# Barwon Water

## Basic Conceptual Geochemical Modelling for Big Swamp

December 2019

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# 1. Introduction

## 1.1 Project objective

Groundwater extraction from the Barwon Downs Borefield, screened in the deep Lower Tertiary Aquifer (LTA) system, has impacted on groundwater baseflows to the Boundary Creek catchment and Big Swamp.

Barwon Water established the Boundary Creek remediation working group in May 2018 to design a remediation plan to address the key environmental issues at Big Swamp and Boundary Creek. Subsequently, a Section 78 notice was issued by the Minister for Water in September 2018 that required Barwon Water to develop and implement a remediation plan for Boundary Creek and Big Swamp. The Section 78 notice directed Barwon Water to:

- Discontinue groundwater extraction from the Barwon Downs Borefield while assessments were completed and remediation work under the remediation plan were completed.
- Prepare and implement a remediation and environment protection plan for Boundary Creek, Big Swamp and the surrounding area.

Barwon Water is in the process of developing options to remediate Boundary Creek and Big Swamp, and are undertaking numerous studies, workshops and stakeholder engagement to identify the most suitable remediation option. To inform the effectiveness of the remediation options assessment, development of a Basic Hydrogeochemical Model (BHM) was requested. The objective of the BHM was:

1. To develop a conceptual hydrogeochemical model for Big Swamp informed by the available hydrogeological data. This included the development of a 3D model of acidity distribution throughout the swamp.
2. Based on the conceptual hydrogeological model, develop suitable geochemical analytical models (i.e. MINTEQ) to inform the assessment of different remediation options, and their ability to achieve the remediation objectives.

## 1.2 Scope of works

GHD Pty Ltd (GHD) was engaged by Barwon Water to complete the basic conceptual geochemical modelling for Big Swamp remediation options and contribute to associated workshops. The scope of works is documented in GHD's proposal dated 20 September 2019.

To meet the project objective and develop a BHM, the following key tasks were undertaken and are documented in this report:

- Compile existing hydrogeological information (i.e. soil and groundwater quality results, swamp geometry, etc.).
- Utilising the existing information, develop a Conceptual Geochemical Model (CGM) for Big Swamp, explaining the acid source and distribution, acidification process and acid fate and transport. The CGM was used as the basis for the development of the geochemical modelling, in association with a 3D model of the interpreted distribution of existing and potential acidity in the swamp.
- Attend technical workshops to discuss remediation options.

- Develop geochemical models, to incorporate the understanding of the primary acid source minerals, the primary acidification process, the speciation of the inorganics in solution and the secondary acidification processes results from the preliminary stages and include the potential effects of the management and mitigation measures under consideration to inform the assessment of effectiveness and risks of each option.

## 1.3 Project specific assumptions and limitations

This report is subject to the following assumptions and limitations.

### 1.3.1 Data assumptions and limitations

The following assumptions and limitations apply to the data utilised in the development of and conduct of the model simulation:

- The topographic, geological, geochemical, hydrological, hydrogeological, hydrogeochemical and environmental data utilised was provided by others and as such GHD does not warrant the quality of the data nor is liable for any errors, omissions and reliability of the data and any consequent errors, omission, results and outcomes of this project.
- The geological, geochemical, hydrological, hydrogeological, hydrogeochemical and environmental data is limited with respect to both spatial and temporal extent and is therefore unlikely to have captured the full range of variance and dynamics that affect these aspects. As such the project outcomes are limited with respect to capturing and simulating the full range of the variability that may occur in Big Swamp and Reach 3 of Boundary Creek.
- No data on the kinetic reaction rates for the acid formation through reduction and degradation through oxidation of the primary acid formation minerals present in Big Swamp was available. Therefore, assessment of the acid formation and attenuation realistically and at representative rates is not feasible. As such all rates and timeframes associated with this project are qualitative and subject to considerable uncertainty.
- No data on the significance of sorption processes and the kinetics for sorption of dissolved phase cations and anions was available. Therefore, assessment of the significance and rate of sorption is not possible, which limits the ability of the basic hydrogeochemical model to fully simulate all hydrogeochemical processes that may occur in Big Swamp and Reach 3 of Boundary Creek.

### 1.3.2 Conceptual geochemical model assumptions and limitations

The literature cited in this report formed the basis on which the opinions related to hydrogeological and hydrogeochemical properties and processes expressed in this report relied. Other literature may also be available, which could result in alteration of the opinions presented in this report.

The following assumptions and limitations apply to the Conceptual Geochemical Model (CGM) utilised in the development of and conduct of the numerical model simulation:

- That the data available is sufficient to identify and characterise, on a qualitative and semi-quantitative basis.
- That the CGM is representative of the primary geochemical processes active in Big Swamp and Reach 3 of Boundary Creek.
- That the CGM provides a sufficient basis to inform the geochemical modelling scenarios.

### 1.3.3 Geochemical modelling assumptions and limitations

Unless otherwise specified geochemical modelling works are subject to the limitations of the software and/or the mathematical formula adopted to conduct the modelling as well as the limitations provided herein. No assessment of variability, confidence and /or uncertainty is typically conducted as part of a geochemical modelling project. No comment on these matters is provided and the reader must make their own judgment on these issues unless it is part of the scope of work to be conducted.

Numerical modelling is based on the CGM developed from the data available at the time of the model development. Therefore, new or additional data could alter the CGM and therefore affect the validity of the numerical model.

The reader needs to be aware that more than one approach is generally possible for numerical modelling simulations, with all approaches potentially producing equally valid results.

The following assumptions and limitations apply to the Geochemical Modelling utilised in the development of and conduct of the model simulation:

- That the equilibrium assumption is sufficiently representative of the geochemical processes that occur in Big Swamp and Reach 3 of Boundary Creek.
- That the omission of sorption from the model due to a lack of representative and reliable data does not significantly adversely affect the representativeness of the model in simulating the actual geochemical processes that occur in Big Swamp and Reach 3 of Boundary Creek.
- That the thermodynamic data in the model database is representative of the thermodynamic energies of the geochemical reactions occurring in the swamp.

# 2. Remediation options workshop

A key objective of the BHM is to support the development of an effective remediation strategy to improve the environmental values of Big Swamp and Reach 3 of Boundary Creek using reasonable and practical remediation methods. The BHM was developed in parallel with the Remediation Options Assessment (ROA) and GHD's project team participated in a series of workshops that formed part of the remediation option evaluation.

During the project a series of workshops were held to evaluate potential management and remediation options that could be applied to Big Swamp and Reach 3 of Boundary Creek. Initially 18 options were considered, which following preliminary evaluation resulted in the adoption of 9 options for more detailed consideration. The remediation options considered are listed in Table 1, with the option not considered beyond the preliminary evaluation stage shown in the grey table fields.

**Table 1 Summary of management or remediation options considered**

| ID | Technology | Description |
|---|---|---|
| O1 | True 'do nothing' | This is a slightly modified version of the original 'do nothing' option presented in the Yeodene Swamp Study (Jacobs. 2008).<br>During the first technical workshop, it was agreed that a true 'do nothing' approach should reflect historical conditions and management practices at the site, which include the following:<br>• Supplementary flow not passed entirely through McDonalds Dam<br>• Continued presence of existing drainage channels across Big Swamp<br>• Water users along Reach 3 of Boundary Creek unable to access water allocation during periods of 'no flow'<br>Unlikely recovery of groundwater levels in the LTA aquifer to pre-pumping conditions in the short term (i.e. 5 years) |
| O2 | Implementation of contingency measures | This is a slightly modified version of the original 'do nothing' option presented in the Yeodene Swamp Study (Jacobs. 2008).<br>During the first technical workshop, it was recognised that a range of contingency measures have been identified to ameliorate some of the issues associated with historical conditions at the site. These contingency measures include:<br>• Minimum supplementary flow of 2 ML/d passed entirely at McDonalds Dam (already implemented)<br>• Infilling of existing drainage channels across Big Swamp (potentially applicable)<br>• Construction of a water pipeline to provide water to users along Reach 3 of Boundary Creek (to be implemented)<br>No interim pumping from the LTA until a new licence from SRW is obtained |
| O3 | Direct treatment of soils with neutralising agents (watershed liming) | This option was included in the Yeodene Swamp Study (Jacobs, 2008) and envisages spreading of agricultural lime (or other suitable neutralising agent) over all or a part of Big Swamp to neutralise acidity of the upper soil profile as wells as increasing pH and alkalinity of the water leaving Big Swamp and discharging into Boundary Creek.<br>Once the areas requiring treatment and the treatment rate (expressed as mass of neutralising agent per unit area) have been evaluated, a variety of implementation methods are possible, including terrestrial applications and aerial methods. |

| ID | Technology | Description |
|---|---|---|
| O4 | Oxic (aerobic) limestone drain (OLD) | This option was included in the Yeodene Swamp Study (Jacobs, 2008) and envisages construction of an open drain channel filled with limestone (or other suitable material) downstream of Big Swamp to improve quality of Boundary Creek water (i.e. increase pH/alkalinity and decrease dissolved metals concentration).<br>Key design parameters of OLDs are mass and size of the limestone aggregate, slope of the drain and water residence time (in the range of several hours).<br>The slope of the drain is inversely proportional to residence time, however higher slopes increase OLDs' efficiencies by limiting the potential for metal precipitation on the surface of the aggregate (armouring). Armouring reduces limestone pore space and surface area, decreasing the limestone dissolution rate and acid neutralising capacity. |
| O5 | Dilution of acidic discharge | This option was included in the Yeodene Swamp Study (Jacobs, 2008) and envisages provision of additional water volumes (i.e. in addition to the supplementary flow of 2 ML/d released upstream of McDonalds Dam as part of the contingency measures) to improve water quality in Boundary Creek.<br>Implementation of this option will require construction of a dedicated water infrastructure and identification of a sustainable source to supply water in the long term (this option does not address generation of acidity in Big Swamp, which will continue).<br>The Yeodene Swamp Study (Jacobs, 2008) seems to indicate that the additional water volumes will be delivered through McDonalds Dam. However, to increase effectiveness and minimise potential side effects to natural environments downstream of the release point, the additional water volumes could also be delivered downstream of Big Swamp (i.e. in the upper reaches of Reach 3 of Boundary Creek).<br>While not mentioned in the Yeodene Swamp Study (Jacobs, 2008), the additional water may also be amended with neutralising agent to increase pH/alkalinity and therefore volumetric requirements. |
| O6 | Water flow diversion and Big Swamp isolation | This option was included in the Yeodene Swamp Study (Jacobs, 2008) and envisages isolation of Big Swamp (source of acidity) and diversion of Boundary Creek flow so that the swamp is by-passed and transport of acid drainage to Reach 3 of Boundary Creek is minimised.<br>Implementation of this option would require building a channel so that water flowing into Boundary Creek does not disperse into Big Swamp, as well as construction of a series of impermeable structures to prevent groundwater within the alluvial swamp sediment to discharge into Reach 3 of Boundary Creek.<br>Additional water retention structures may be also required to minimise risks of acid flushes from Big Swamp into Reach 3 of Boundary Creek. |

| ID | Technology | Description |
|---|---|---|
| O7 | Flooding of Big Swamp (natural anaerobic wetland) | This option was included in the Yeodene Swamp Study (Jacobs, 2008) and envisages flooding of Big Swamp to create permanently waterlogged areas where microbially mediated iron reducing and sulfate reducing reactions have the potential to increase alkalinity, raise pH and remove dissolved metals by precipitation.<br>For sulfate reduction reactions to occur, the following conditions must be realised in the re-flooded portions of Big Swamp:<br>• A permanent water coverage having enough depth to maintain generally anaerobic conditions within the water column<br>• Presence of a bioavailable organic carbon source (electron donor)<br>• pH between 5 and 8<br>• Presence of sulfate and low concentration of competing electron acceptors such as nitrate ($NO_3^-$), manganese ($Mn^{4+}$) and ferric iron ($Fe^{3+}$).<br>Implementation of this option envisages the following steps:<br>• construction of water retention structures (likely to be located at the downstream side of Big Swamp) to realise a permanent water coverage across a significant portion of Big Swamp<br>• infilling of existing drainage channels across Big Swamp to assist with water retention<br>• supply of additional water volumes to achieve the required permanent water coverage<br>• supply of additional organic carbon source (and potentially sulfate) in case of deficiencies of these elements in the natural environment.<br>In addition to promoting favourable geochemical conditions, this option has the additional benefit of maintaining the sulfidic sediments in Big Swamp below water, preventing further oxidation associated release of acidification products in the environment. |
| O8 | Managed groundwater levels within Big Swamp | This is a slightly modified version of the original 'Inundating Yeodene Swamp' option presented in the Yeodene Swamp Study (Jacobs, 2008) developed during the RWG workshop, which accounts for the potential risks associated with re-flooding of the acidified swamp.<br>This option, named 'managed groundwater levels' envisages the following steps:<br>• construction of water retention structures (likely to be located at the downstream side of Big Swamp) to maintain minimum groundwater levels in the Big Swamp alluvium aquifer above the layer of the unoxidised sediments (PASS).<br>• infilling of existing drainage channels across Big Swamp.<br>• supply of additional water volumes to achieve the required minimum groundwater levels.<br>The benefit of this option is to prevent further oxidation of potential ASS within the swamp and associated increase of acidification products released in the environment. |
| O9 | Soil excavation/treatment and rehabilitation | This option involves excavation and removal of the oxidised ASS sediments within Big Swamp which are treated (or disposed) according to EPA Victoria ASS management guidelines.<br>Construction of access tracks and significant removal of vegetation will be required to implement this option. The excavation is likely to be progressed as separate cells to minimise potential exposure of non-oxidised sediments to oxygen.<br>Following removal of the oxidised sediments, lime would be added at the base of the excavations to neutralise potential future acidity generation and then the excavation would be backfilled with suitable imported fill material.<br>After remediation and backfilling, the site would be landscaped and revegetated to resemble the original character of Big Swamp. |

| ID | Technology | Description |
|---|---|---|
| O10 | Deep soil mixing | This option involves the use of a large diameter (one to three metres) hollow-flight auger fitted with special mixing 'paddles' to achieve mixing of a neutralising agent with the oxidised sediments in Big Swamp.<br>Construction of access tracks and significant removal of vegetation will be required to implement this option.<br>Following treatment of the oxidised sediments, the disturbed sections of Big Swamp will require to be rehabilitated through landscaping and planting of vegetation. |
| O11 | Alkaline slurry injection | This option involves injection of a slurry composed of alkaline and impermeable materials to minimise oxygen infiltration and neutralise acidity. Depth of application would be typically to the top of the unoxidised ASS in Big Swamp.<br>Construction of access tracks and significant removal of vegetation will be required to implement this option.<br>Following treatment of the oxidised sediments, the disturbed sections of Big Swamp will require to be rehabilitated through landscaping and planting of vegetation. |
| O12 | In-stream limestone sand | This option involves placement of limestone sand (or other suitable neutralising agent) directly in the streambed of Boundary Creek.<br>The sand is carried into the stream during high flow periods where it dissolves releasing alkalinity and increasing pH. |
| O13 | In-stream active treatment system | This option involves installation of an active treatment system to treat water quality in Reach 3 of Boundary Creek.<br>The system would be installed at the downstream end of Big Swamp and will comprise a range of equipment (i.e. tanks, mixers, pumps) to dose dry or liquid chemicals in the Boundary Creek water to increase alkalinity/pH and remove metals (by precipitation and settling).<br>Depending on system configuration and design parameters, precipitation of metals could be achieved in a settling pond or above ground clarifiers. |
| O14 | Limestone diversion wells | This option envisages that a portion of the flow in Boundary Creek downstream of Big Swamp is diverted into a series of limestone-filled wells to increase alkalinity/pH and precipitate metals.<br>Following treatment, the flow is diverted back into Boundary Creek. |
| O15 | Anoxic limestone drains (ALD) and settling pond | This option envisages construction of a buried drain lined with impermeable material, filled with limestone (or other suitable neutralising agent) and covered by impermeable materials.<br>The water seeping downstream of Big Swamp is diverted into the limestone (to maintain saturated conditions and anoxic conditions) where dissolution of the limestone increases alkalinity and pH.<br>Low oxygen conditions in the ALD would prevent precipitation of metals and armouring issues.<br>The water leaving the ALD is then directed into an aerobic settling stage where metals are precipitated and removed from the water. Removal of metal precipitates (sludges) is required at periodic intervals. |
| O16 | Constructed aerobic wetland | Construction of an aerobic wetland to remove metals by oxidation and hydrolysis. |
| O17 | Constructed vertical flow anaerobic wetland (organic layer, limestone layer and drainage system) | Construction of an anaerobic wetland to increase alkalinity, raise pH and remove metals by precipitation of insoluble hydroxides, carbonates and sulfides.<br>The anaerobic wetland comprises an organic rich substrate at the top, a layer of limestone at the bottom and a drainage system. The wetland is constructed within a watertight basin and water flowing from the top across the organic layer and the limestone layer is collected by the drainage system and released into an aerobic settling pond.<br>Alkalinity is generated by microbial process in the organic layer (if sulfate is available) and through dissolution of the limestone.<br>An aeration and settling stage may be required prior to discharge to increase oxygen and promote precipitation of residual dissolved metals. |

| ID | Technology | Description |
|---|---|---|
| O18 | Permeable reactive barrier | Construction of permeable reactive barriers in Big Swamp (perpendicular to groundwater flow direction) to intercept and treat acidic groundwater. |

# 3. Hydrogeological characterisation

It is noted that the hydrogeological characterisation of the Barwon Downs bore field and the Boundary Creek catchment has been described in detail by Jacobs, 2018, and other reports used to support the groundwater licence application, and therefore a summary has been provided in this document.

## 3.1 Regional hydrogeological setting and the Barwon Downs Borefield

In most years, Barwon Water's water supply is sourced exclusively from surface water resources. However during the Millennium Drought and historically since the 1980's, groundwater was sourced from the Barwon Downs Borefield to supplement the Geelong region water supply. Barwon Downs was relied upon to provide more than 70% of Geelong's daily water requirements during the peak of the Millennium drought period.

The Barwon Downs Borefield is located approximately 70 km south-west of Geelong in the foothills of the Otway Ranges. The borefield extracts from the Lower Tertiary Aquifer (LTA) through six production bores at depths of 600 m. At the borefield location the LTA is a confined aquifer system, overlain by the low permeability marls. However, the LTA outcrops at the surface predominately in an area known as Barongarook High, where the aquifer has its main recharge zone and interacts with the surface water hydrological system (refer Figure 1 and Figure 2)

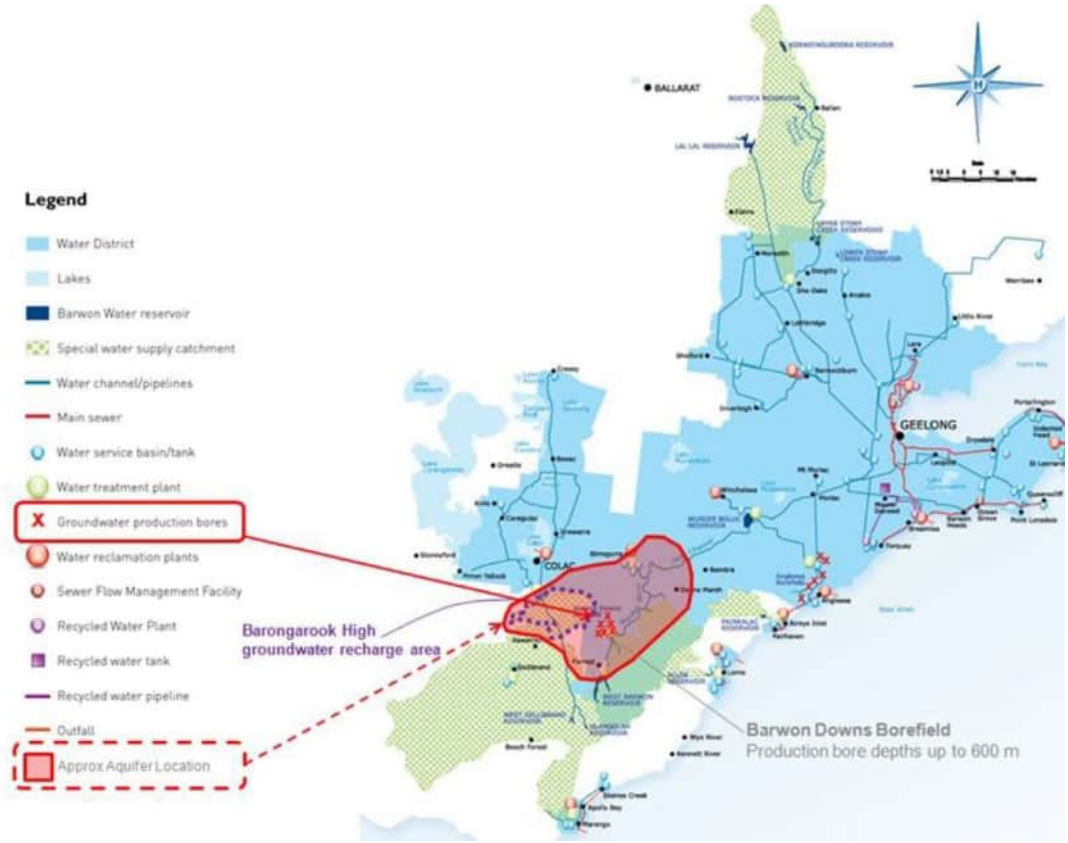



**Figure 1 Borefield location, aquifer extent and recharge area (Jacobs, 2018)**

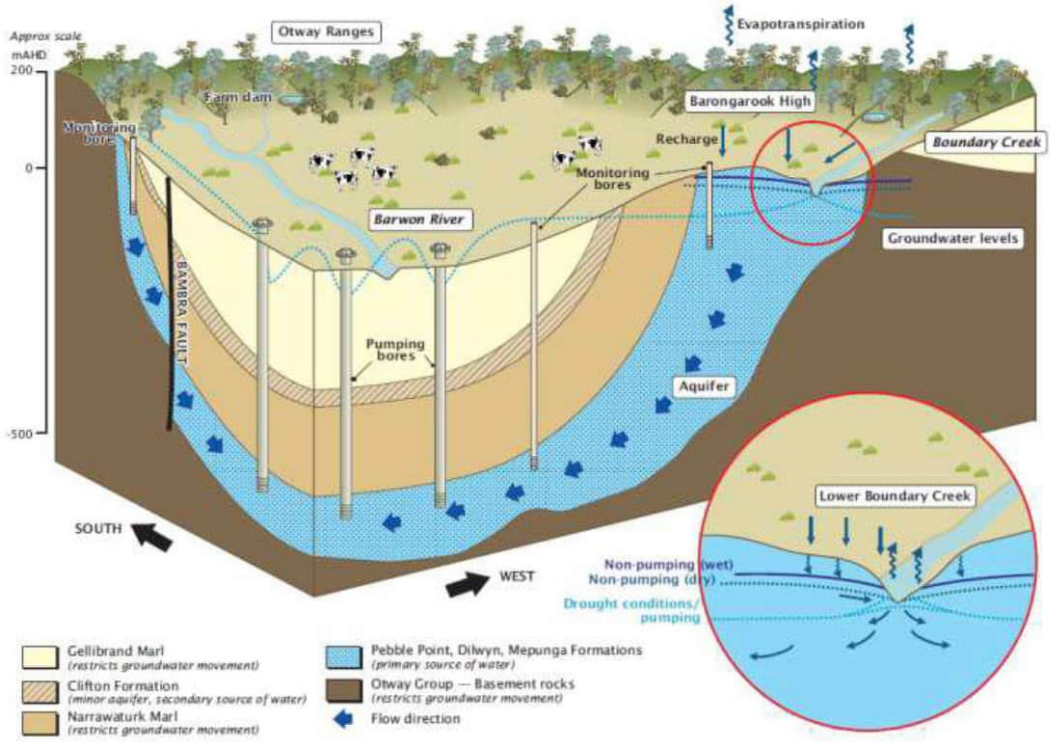



**Figure 2 Schematic of LTA Aquifer, borefield and outcrop area (Jacobs, 2018)**

## 3.2 Impacts of groundwater extraction

Extraction from the deep confined borefield causes the development of a drawdown in the aquifer system, and this drawdown can extend to the outcrop area at the Barongarook High. It is in this recharge zone area, where the LTA is outcropping or subcropping, that the induced groundwater drawdown has the potential to impacts on the groundwater level in the shallow watertable aquifer system, and subsequently the potential to reduce groundwater baseflows, impact on surface water flows/levels or groundwater dependent ecosystems , such as swamplands.

Extensive studies have been completed by Barwon Water to investigate the hydrogeological setting of the Boundary Creek Catchment which flows east across the Barongarook High aquifer recharge area, and joins the Barwon River a couple of kilometres downstream around Yeodene. These extensive investigations have indicated that Boundary Creek flows through 3 distinct hydrogeological settings, classified as Reach 1, 2 and 3 (Jacobs 2017) and are shown in Figure 3 below:

- Reach 1: This is the upper reach of Boundary Creek which predominately flows over outcropping bedrock which is characterised by Palaeozoic sandstone, siltstone and mudstone.
- Reach 2: The central reach of the creek flows over the outcropping regional aquifer (the LTA), which is characterised by permeable sands of the Mepunga, Dillwyn and Pebble point formations. The Yeodene (Big) Swamp is located at the downstream end of Reach 2 on boundary between the regional aquifer and the aquitard. McDonalds Dam, a privately owned dam and is subject to licensing conditions which includes passing flows, is located at the upstream end of Reach 2.

- Reach 3: The lower reach of Boundary Creek flows over an aquitard (the Mid-Tertiary Aquitard or MTD) and is characterised by silty clays of the Gellibrand Marl.

It is noted that shallow Quaternary alluvium occurs locally along the flow path and overlies most of these regional formations. This includes swamp deposits and acid sulfate soils that occur throughout the Yeodene Swamp (Jacobs, 2018).

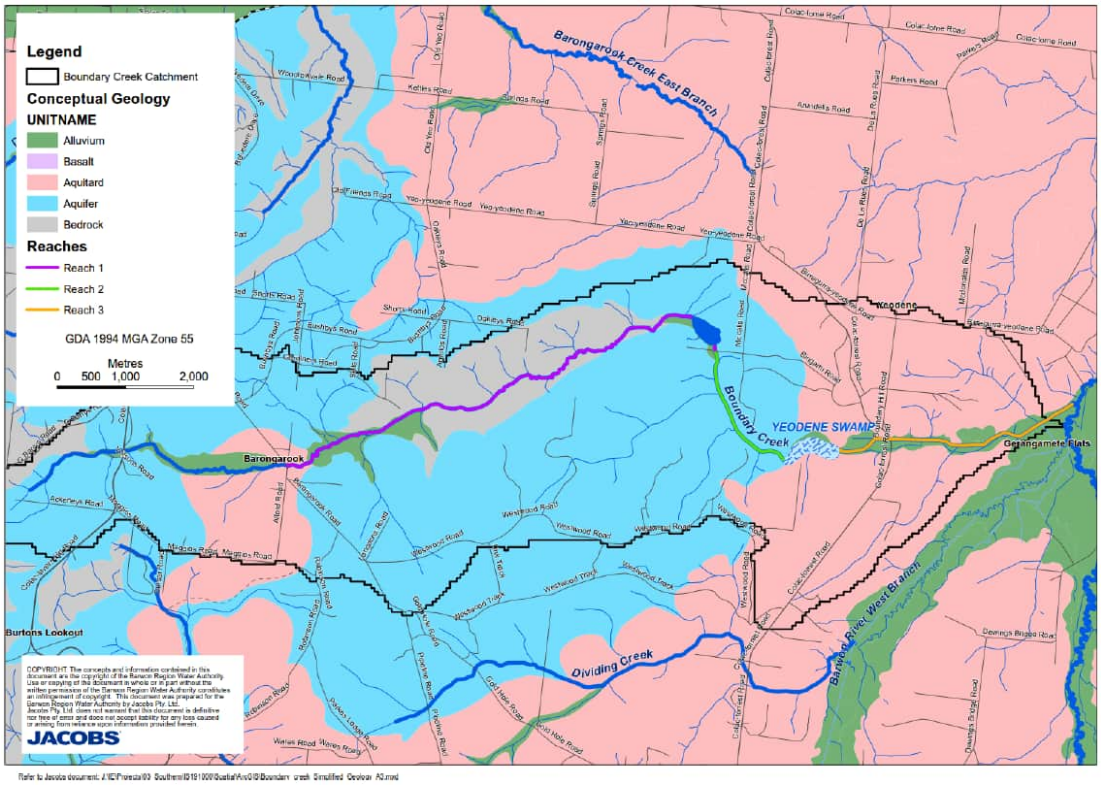



**Figure 3 Simplified geology of the Boundary Creek Catchment (Jacobs, 2018)**

The current conceptual understanding of groundwater- surface water interaction along these Reaches is shown in Figure 4 (Jacobs, 2018). With groundwater seepage occurring from the surface water system to the perched water table aquifer in the shallow alluvials, and subsequently there is a downward hydraulic gradient for groundwater flows from the perched water table aquifer towards the regional LTA system. This downward hydraulic gradient has developed due to the drawdown in the LTA associated with Barwon Water extraction. The groundwater levels are shown in Figure 5 (Jacobs, 2018) , which indicate that prior to 1997 there was a general upward hydraulic gradient from the regional aquifer to Boundary Creek, and the surface water system would have been gaining groundwater baseflow. However, due to the borefield extraction, the hydraulic gradient has been reversed, and Boundary Creek in Reach 2 has generally become a losing feature, the water losses being dependent on numerous factors, such as the stream bed hydraulic conductivity, the hydraulic gradient and the time of the year (i.e. depending on surface water levels, re-wetting of the aquifer etc.).

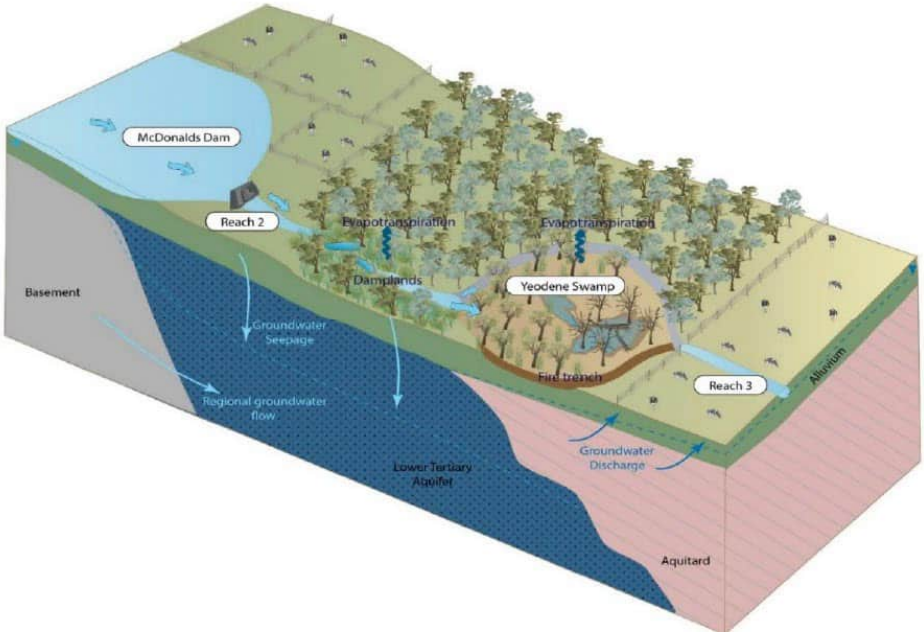



**Figure 4 Conceptual groundwater-surface water interaction along the Boundary Creek (Jacobs, 2018)**

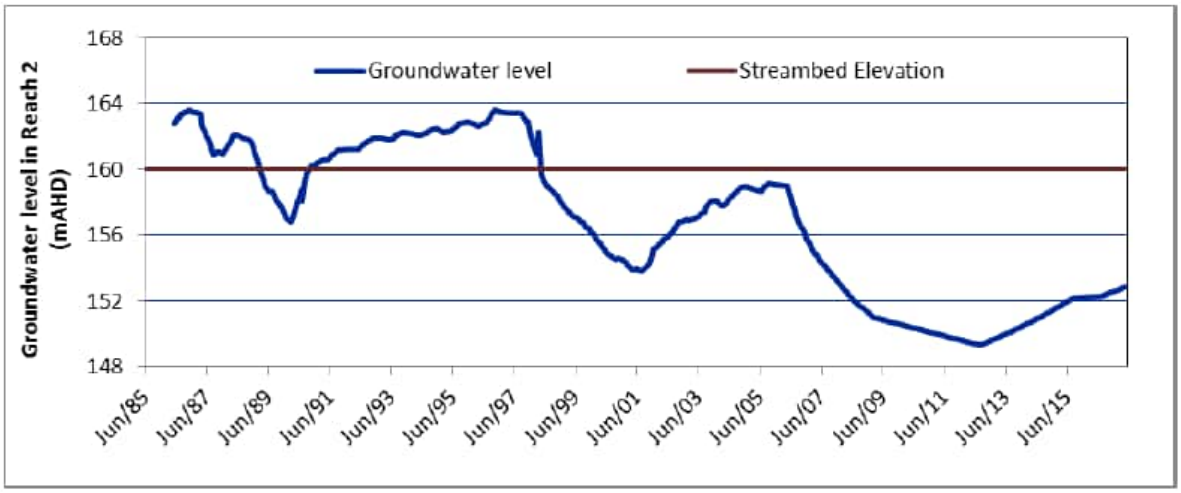



**Figure 5 Historical monitoring of regional aquifer in Reach 2 (Jacobs, 2018)**

Jacobs, 2018 estimated that streamflow declined approximately 3 ML/day through the Damplands and Yeodene Swamp, as a result of evapotranspiration and recharge to the shallow groundwater (i.e. baseflow losses). Barwon Water currently provided 2 ML/day additional flow to Boundary Creek to assist in making up for these baseflow losses.

The impact of the loss of baseflow to Boundary Creek in Reach 2, associated with the borefield extraction and dry climatic conditions, are:

- Reduced stream flow in Boundary Creek.

  As shown in Figure 6 (Yeodene gauge), surface water flows were generally higher prior to 1999, with the creek rarely ceasing to flow, however post 1999 surface water flows are significantly lower and more cease to flow days occurred (also refer Figure 7 and Graph 23).

- Reduced Stream flows into Big (Yeodene) Swamp.

  This swampland is supported by a perched water table aquifer in alluvial sediments, which are expected to overlie both the LTA aquifer at the upper end and the MTD aquifer at the lower end.

The reduction in surface water flows into the swamp have resulted in:

- Lower groundwater levels in the alluvial watertable aquifer, and more storage in the aquifer system in drier months.
- Lower groundwater levels have exposed potential acid sulfate soils, causing oxidisation of the naturally occurring acid sulphate soils in the swamp and the release of acidic water (i.e. pH <4) and high concentrations of metals downstream, when flows do occur during wet period (refer Figure 7).
- The additional storage capacity in the alluvial aquifer system means that when surface flows upstream occur, it takes longer/higher volumes of water to saturate the alluvial aquifer system before surface water flows out of the swamp. This further contributes to the increase in no flow days at the Yeodene Swamp gauge (Figure 7).

The lower groundwater levels and drier conditions in Big Swamp impact on the terrestrial ecology of the swampland (i.e. flora and fauna), and will result a higher risk of peat fires (which have occurred in the past).

The reduced surface water flows and quality downstream of Big Swamp have subsequent impacts on the following key receptors:

- Downstream stock water users.
- Aquatic ecology, fish kills have occurred downstream and in the Barwon River associated with low pH surface water flush events.

The potential impacts associated with the groundwater extraction from the Barwon Downs borefield on the Boundary Creek catchment, are conceptualised in Figure 8 (Barwon Water, 2019).

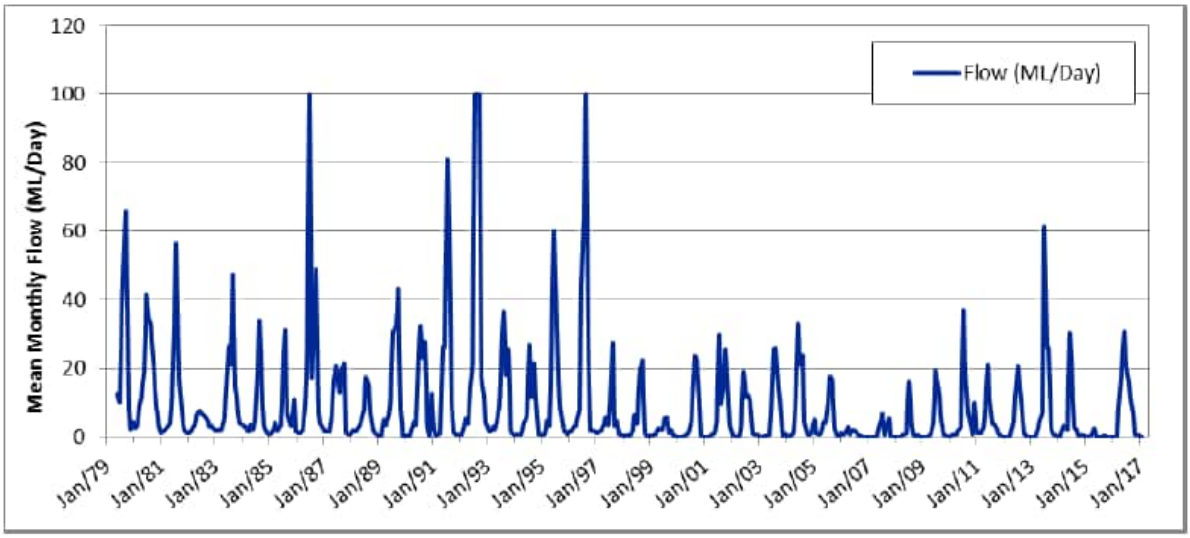



**Figure 6 Average monthly flow in Boundary Creek at Yeodene (Jacobs, 2018)**

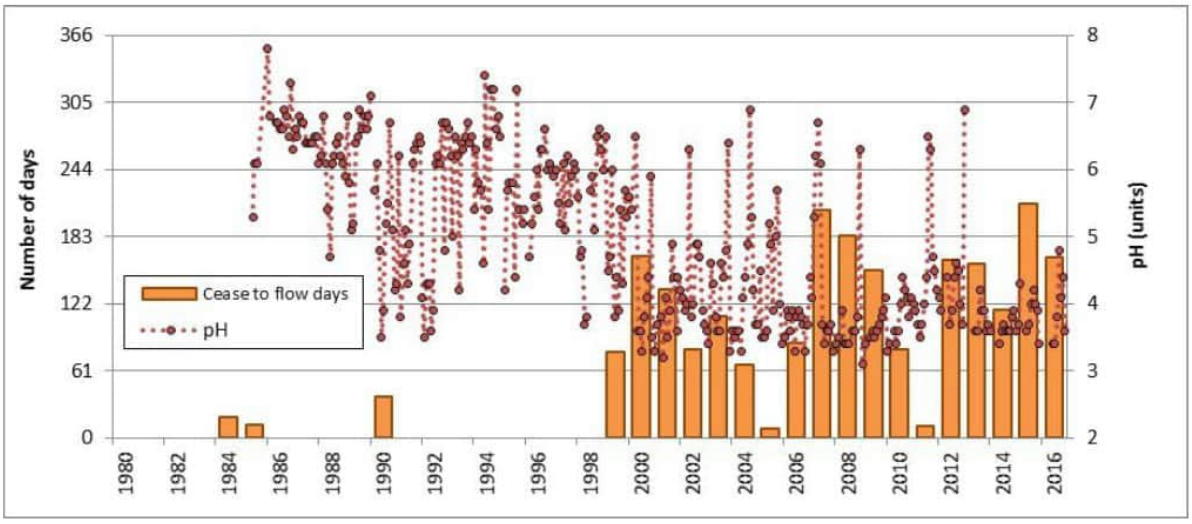



**Figure 7 Number of cease to flow days in Boundary Creek at Yeodene Vs monthly pH at Yeodene.**

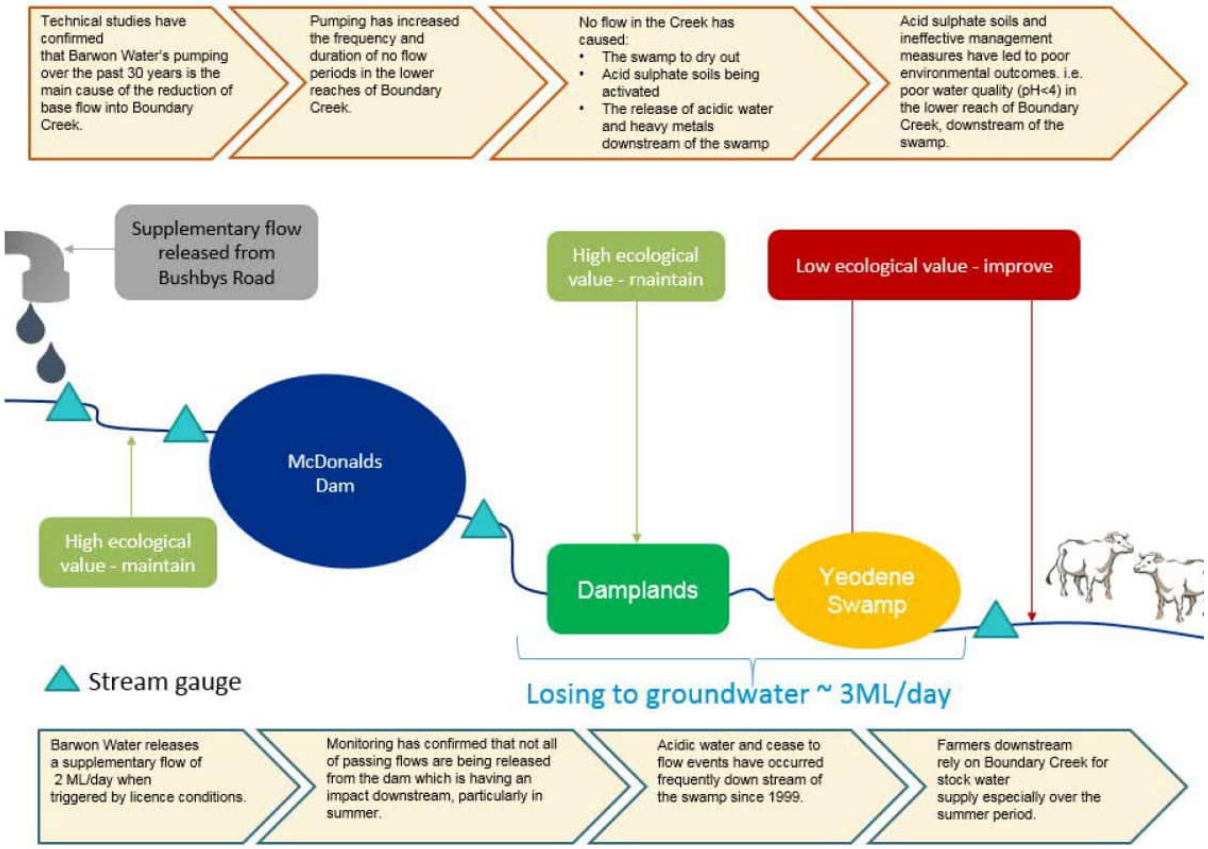



**Figure 8 Boundary Creek Catchment conceptualisation**

# 4. Conceptual geochemical model

This section sets out the Conceptual Geochemical Model (CGM) developed for the acid source, acidification process, acid flux and acid fate and transport for Big Swamp and Reach 3 of Boundary Creek as they are relevant to the project objectives.

This section includes a discussion to the general processes as they apply to Inland Acid Sulphate Soils and then assessment of the available data to evaluate the relevance and significance of these processes with respect to Big Swamp and Reach 3 of Boundary Creek.

Following data evaluation a CGM was developed. The CGM was used as the basis for the development of the geochemical modelling and its primary purpose was to support the remediation solution design and inform the BHM.

## 4.1 Primary acid source assessment for Big Swamp

The primary acid source in Big Swamp is associated with the organic carbon rich sediments that have accumulated in the saturated part of the swamp, where over time primary acid forming minerals generally comprising sulfide minerals have accumulated over recent geological time.

Based on the limited geological and acid formation testing data available, a three dimensional model was developed that mapped the mass of net acid present in Big Swamp. This model is associated with an appreciable amount of uncertainty as a result of the limited lateral and vertical extent of the geological investigation locations completed to date and the consequently limited amount of net acid data available. As such, the results of the three dimensional model should be utilised with an appropriate amount of caution and should be regarded as semi-quantitative. The bore locations from which the geochemical data was used for the 3D model is shown in Figure 9.

### 4.1.1 Three dimensional geological model

The existing topographical and acidification data was used to develop the three dimensional model of the distribution of retained, actual and potential acidity under current hydrological and hydrogeological conditions and those predicted under future flow conditions and water table elevations. For the purpose of this assessment the three dimensional model considered two flow scenarios:

1. Maintenance of an additional 2 ML of flow, with the following conditions considered:
   i) No barrier to restrict flow at the down-stream end of the swamp.
   ii) Installation of a barrier to restrict flow at the down-stream end of the swamp.
2. Maintenance of an additional 20 ML of flow, with the following conditions considered:
   i) No barrier to restrict flow at the down-stream end of the swamp.
   ii) Installation of a barrier to restrict flow at the down-stream end of the swamp.

The three dimensional model was used to provide volumes of swamp sediments that would remain unsaturated and therefore able to generate acid into the future (refer Section 5.5).

Figure 10 and Figure 11 shows the 3D model with the net acidity interpreted between each bore location. The spatial relationship of the net acidity between bore locations was checked using a variogram prior to constructing the 3D contour.

Figure 12 and Figure 13 shows the actual groundwater level in dark blue (July 2019), 20 ML/day modelled groundwater levels (without the head barrier) in red and the 2 ML/day modelled groundwater levels (without the head barrier) in light grey.

Based on the results of the three dimensional model analysis, there appear to be around 600,000 to 700,000 cubic metres of sediments that contain potential primary acid producing minerals based on the available net acidity data.

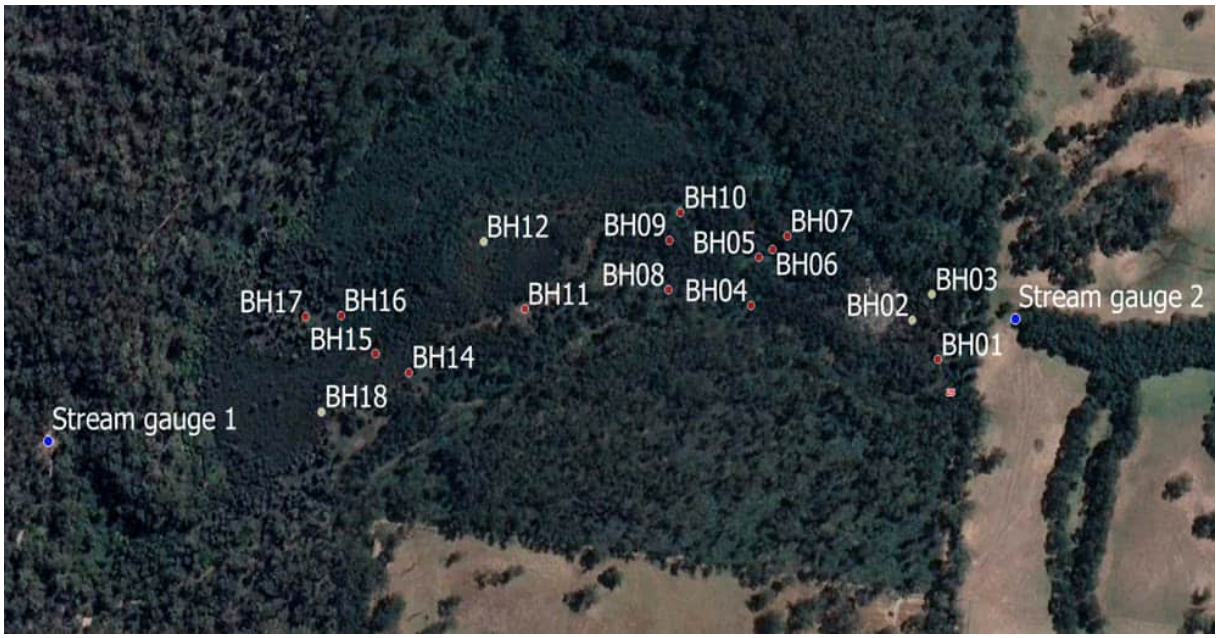



**Figure 9 Bore locations (Jacobs, 2018)**

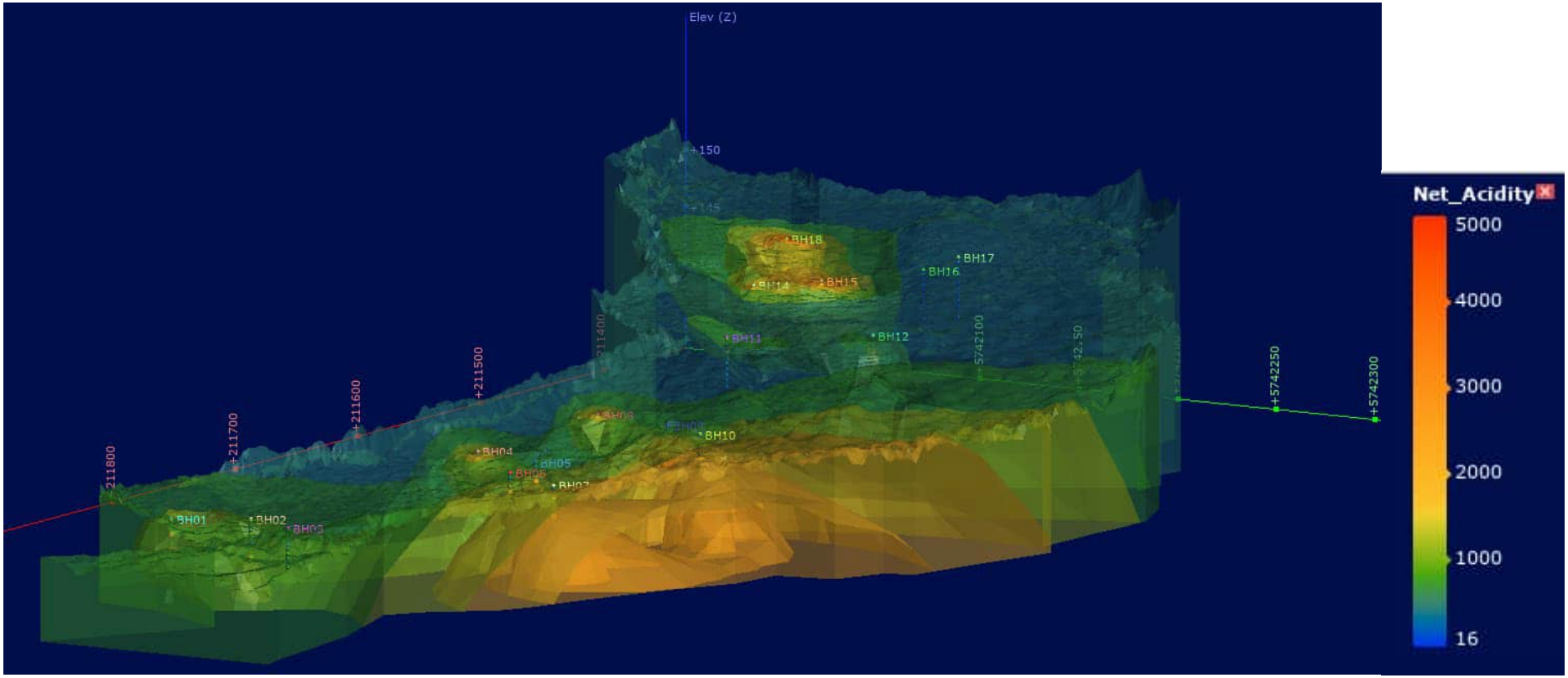



**Figure 10 3D model - net acidity**

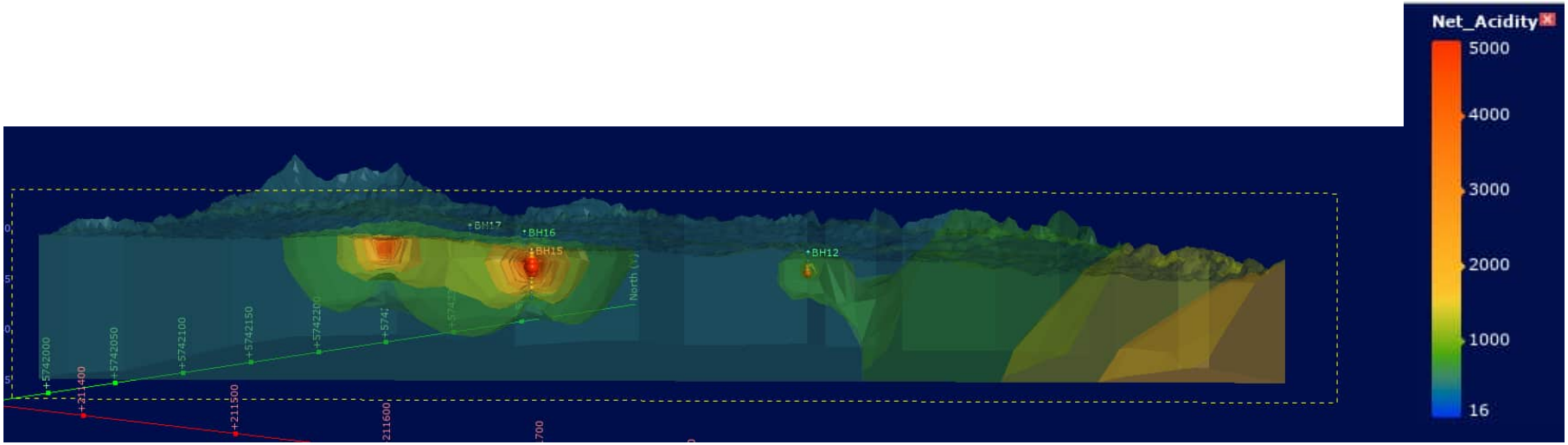



**Figure 11 3D model - net acidity - cross section (Upper swamp South-west to North-east)**

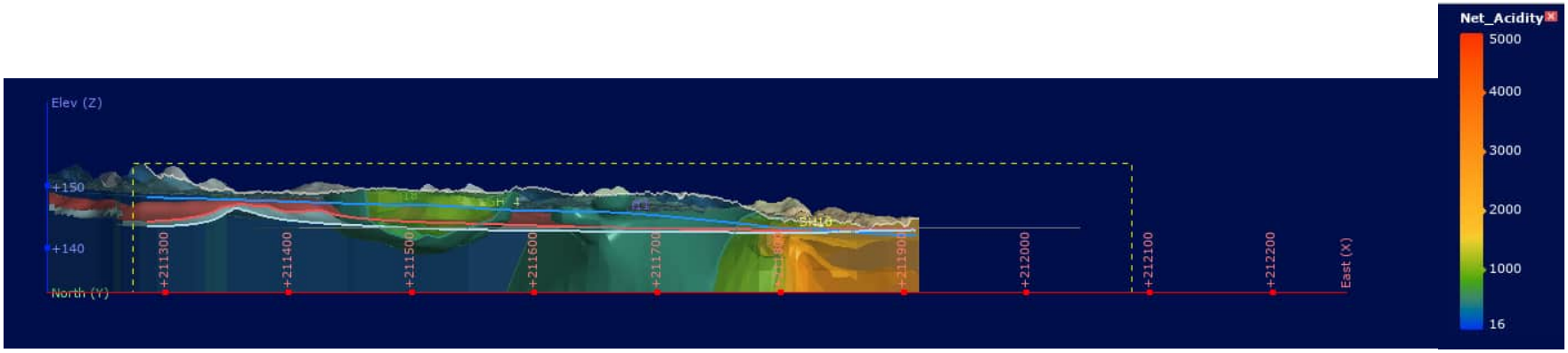



**Figure 12 W-E long section with groundwater levels: actual (blue), 20 ML/day no barrier (red) and 2 ML/day no barrier (grey)**

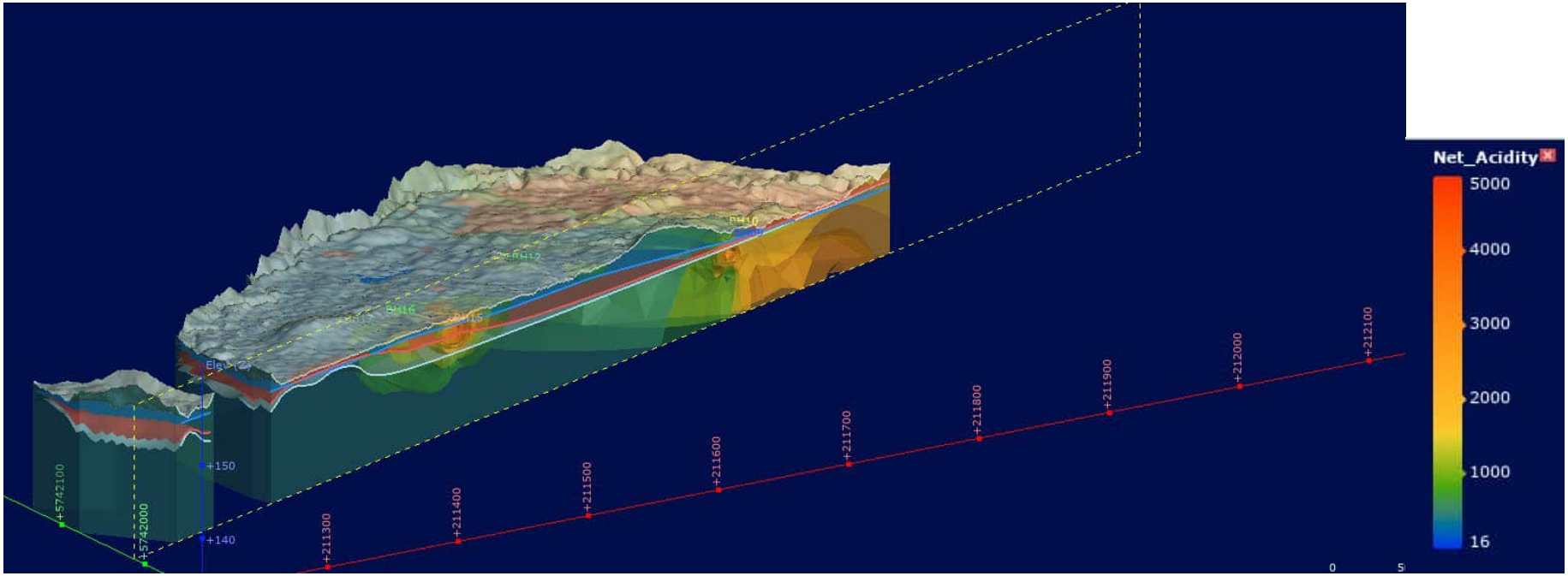
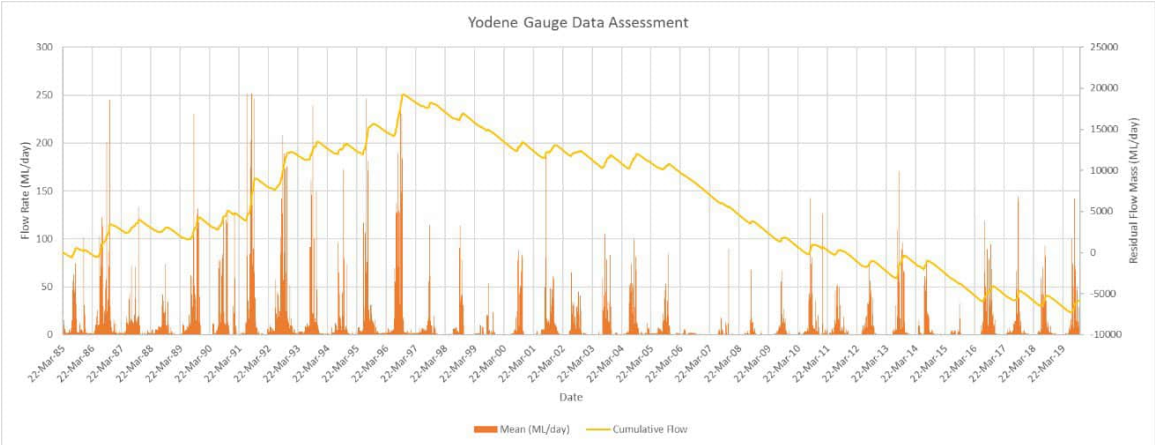



**Figure 13 3D model with groundwater levels: actual (blue), 20 ML/day no barrier (red) and 2 ML/day no barrier (grey)**

## 4.2 Flow and acid flux assessment for Reach 3 of Boundary Creek

The existing flow and pH monitoring data collected for the Yeodene Gauge was used to assess the flow and acid flux from Big Swamp into Reach 3 of Boundary Creek. The stream flow data was assessed through a simple flow and residual mass flow analysis that evaluated stream flow in Reach 3 of Boundary Creek between the mid 1980's to present. The result of the flow analysis are presented on Graph 1 and suggest the following:

- The frequency, duration and quantum of winter flows has declined after the late 1990's.
- The frequency, duration and quantum of winter flows was lowest during the millennial drought.
- Some recovery in frequency duration and quantum of winter flow is observed after 2010 but that recovery is not to the levels of flow observed in the late 1980's and most of the 1990's.
- Flow volumes have been in decline since the 1990's, with the rate of decline only slowing in recent years.




**Graph 1 Summary of streamflow data for Yeodene Gauge**

A statistical analysis of the flow data is summarised in Table 2 and suggests:

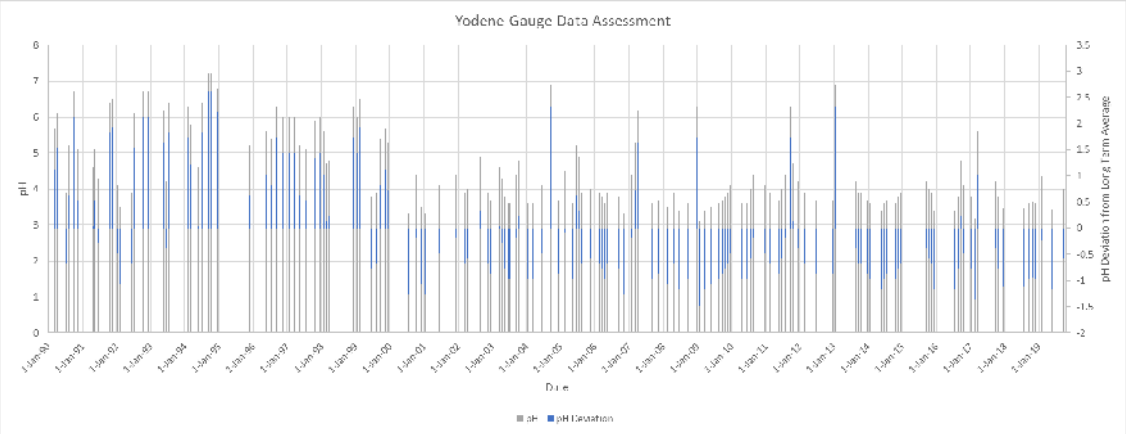
- A decline in flow between the 1990's and 2000's, with the lowest flow occurring in the first decade of the new millennium, coinciding with the millennial drought.
- Some recovery of flow during the 2010's but flow remains notably below that occurring in the 1980's and 1990's.
- Variance in flow volumes declined in the 2000's and 2010's compared to the 1980's and 1990's.

**Table 2 Summary statistics of Yeodene Gauge flow data**

| Flow (ML/day) | All Data | 1980's | 1990's | 2000's | 2010's |
|---|---|---|---|---|---|
| Minimum | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 |
| Median | 1.6 | 3.4 | 2.4 | 0.7 | 1.2 |
| Mean | 8.0 | 10.3 | 11.3 | 4.9 | 6.7 |
| Maximum | 251.8 | 245.0 | 251.8 | 185.2 | 170.4 |
| Standard Deviation | 18.4 | 19.2 | 25.0 | 11.1 | 14.9 |

The pH data for the Yeodene Gauge was assessed over time through a time series plot of the measured pH and the deviation of pH from the long term average, with the result of that assessment summarised on Graph 2. The results suggest:

- pH values in the 1990's were generally above 4.5 for the majority of the time, with pH frequently above 6.
- pH values less than the long term average over the monitoring period were infrequent in the 1990's.
- Since early 2000 pH has frequently been below 4 and an overall decrease in pH is readily discernible.
- The frequency of pH values below the long term average increased noticeable after early 2000.
- No notable change in pH measurements is observed after 2010, despite an increase in flow as shown on Graph 1.




**Graph 2 Summary of pH data for Yeodene Gauge**

A statistical analysis of the pH data is summarised in Table 3 and suggests:

- A decline in pH between the 1990's and 2000's, with lower pH persisting since the first decade of the new millennium, coinciding with the millennial drought.
- No notable recovery in median and mean pH is observed in the 2000's and 2010's and pH remain notably lower in the first two decades of the new millennium than persisted in the 1990's.
- Variance in pH declined in the 2000's and 2010's compared to the 1990's.

**Table 3 Summary statistics of Yeodene Gauge flow data**

| pH (Units) | All Data | 1980's | 1990's | 2000's | 2010's |
|---|---|---|---|---|---|
| Minimum | 3.1 | No Data | 3.5 | 3.1 | 3.2 |
| Median | 4.1 | No Data | 5.8 | 3.8 | 3.8 |
| Mean | 4.6 | No Data | 5.6 | 4.1 | 3.9 |
| Maximum | 7.4 | No Data | 7.4 | 6.9 | 6.9 |
| Standard Deviation | 1.1 | No Data | 1.0 | 0.9 | 0.7 |

## 4.3 General geochemical processes in inland Acid Sulphate Soils

Big Swamp is considered an inland acid sulfate soil (ASS) site, rather than the more common and widespread coastal ASS that occur in low-lying areas adjoining the coastal fringe and primarily formed during a period of higher sea level in the Holocene.

Inland ASS form under a wide range of environmental conditions generally involving a wet swampy setting. Water chemistry in the system can range from freshwater to saline inland environmental settings at various topographic elevations. Inland ASS formation and activation mechanisms involve a wide range of soil and water conditions across a range of climate settings.

The extent of Inland ASS occurrence in Australia has only recently become apparent, primarily as a result of drying of inland wetland and river systems in the millennial drought. Consequently the study of the formation and activation mechanisms of Inland ASS systems is not as advanced as those for Coastal ASS systems.

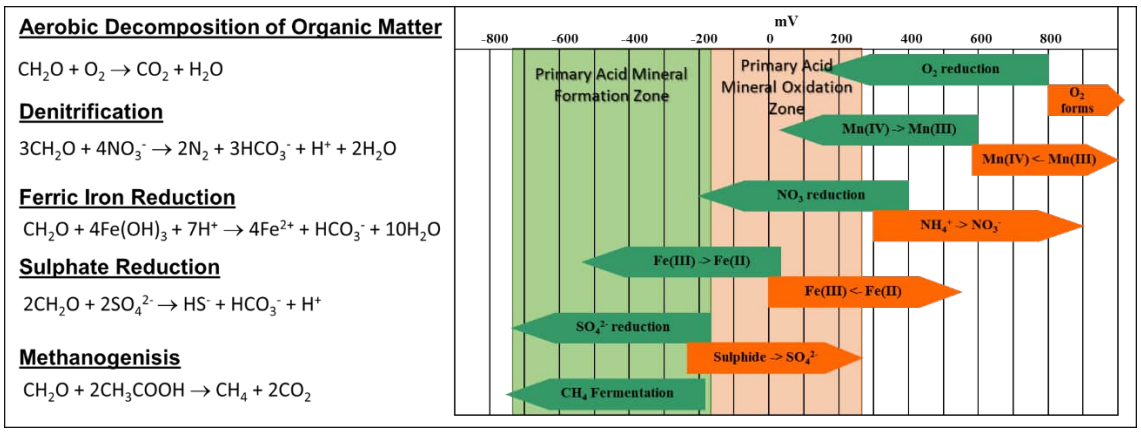
Inland ASS can generally be defined as those ASS, which occur inland of modern-day low lying coastal zones. Inland ASS, provide a range of management challenges in terms of the range and extent of formation mechanisms.

Considering all of these complexities though, there are some common aspects that universally apply to the Inland ASS sites, such as:

- They occur in wet swampy setting that are fed by either or both surface and groundwater.
- They are associated with reducing conditions that are generally created by the degradation of organic matter.
- They are associated with attenuation of dissolved phase sulfate that is fed into the Inland ASS system by either or both the surface and groundwater that enters the system.
- They are associated with acidification that results from the oxidation of the sulfide minerals that are stored in the Inland ASS system, therefore becoming the primary source of the acidification that occurs.

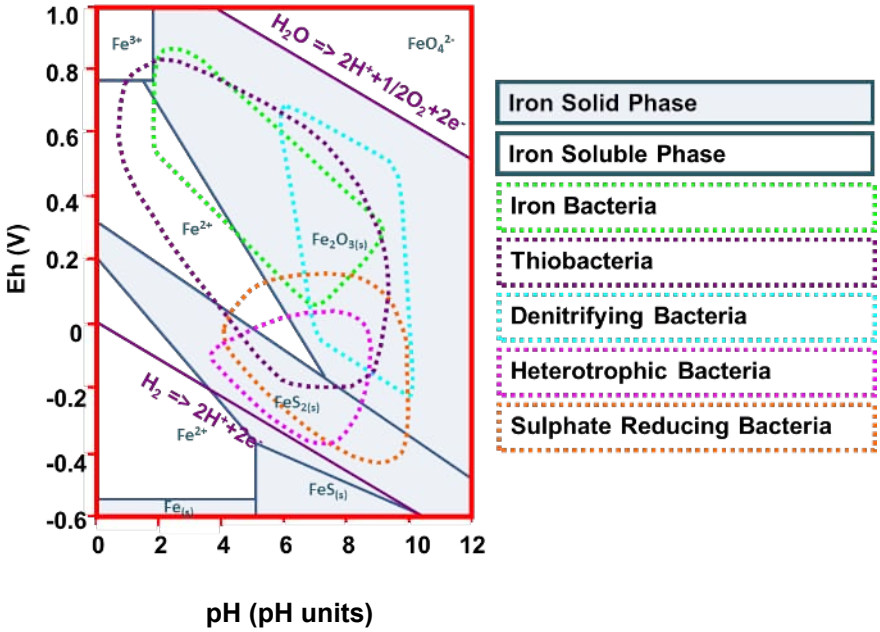
### 4.3.1 Primary acid source mineral formation

In order to inform the CGM, the primary mechanisms that lead to the formation of the acid source in Inland ASS systems needs to be understood. As noted, Inland ASS systems occur in wet, swampy systems where organic matter decomposition results in reducing conditions. Organic matter decomposition is a series of bacteriologically facilitated oxidation / reduction reactions that occur in a specific sequence form thermodynamically most to least favourable. The sequence of oxidation / reduction reactions that lead to the formation of primary acid forming minerals is shown on Graph 3. As shown on Graph 3, the primary acid source mineral formation occurs over the zone when reduction of sulfate occurs, while the primary acid formation processes coincides with the oxidation of sulfide.




## Graph 3 Organic matter degradation reaction sequence

The decomposition of organic matter in Inland ASS environments is facilitated by microbes that liberate the energy released by the oxidation / reduction reaction to fuel their metabolism. Given the complexity and range of pH and Eh conditions over which oxidation / reduction reactions occur, bacterial species have evolved to liberate the energy released by the oxidation / reduction reaction under different environmental conditions. Graph 4 present the activity fields of the common bacteria species that are associated with organic matter degradation superimposed on the iron stability diagram. As is evident, on Graph 4, the primary bacteria species associated with the reduction of sulfate (Heterotrophic and Sulfate Reducing Bacteria) generally occur under slightly acidic, neutral and alkaline conditions. However, these key bacteria species are inactive under highly acidic conditions, which are associated with pH below 4. Thiobacteria are active under highly acidic conditions but only have a limited capacity with respect to sulfate reduction. Therefore, the accumulation of primary acid forming minerals becomes ineffective once oxidation of these minerals occurs and the sediment, pore water, groundwater and surface water pH become acidic.

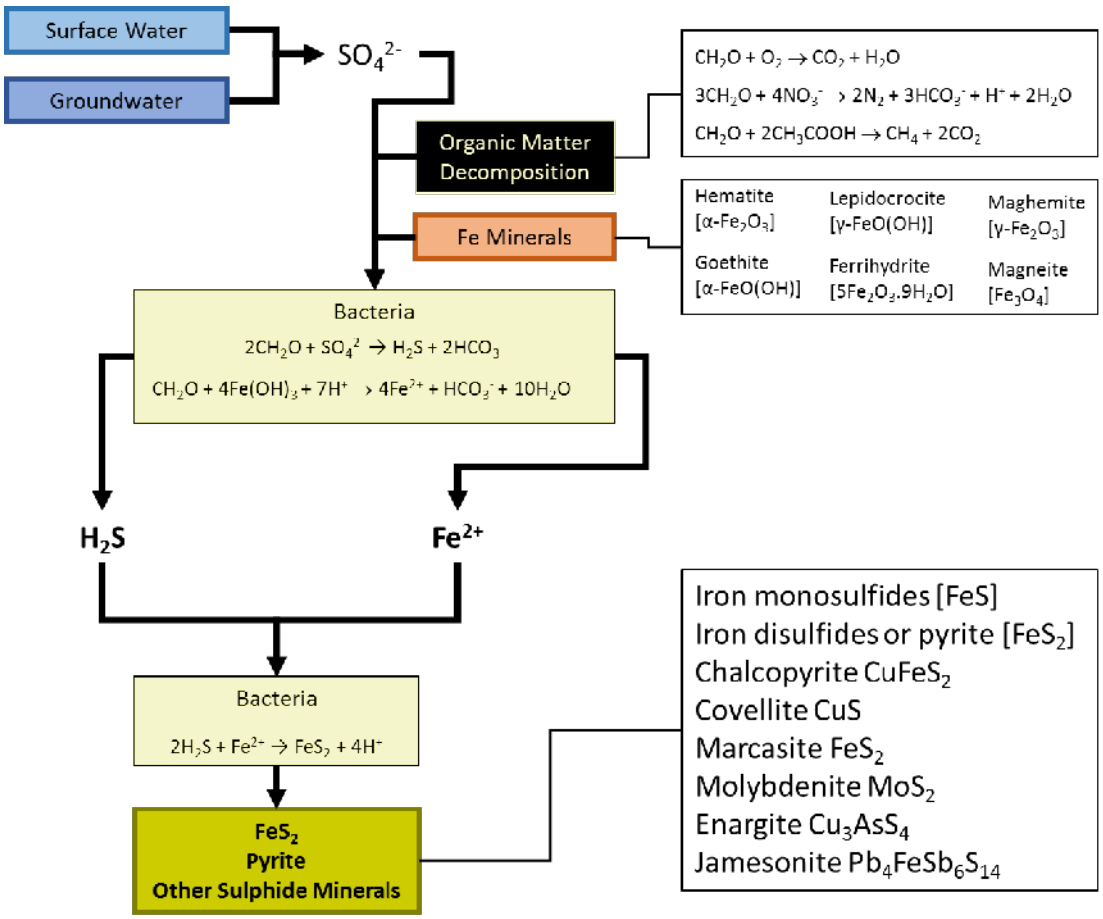



## Graph 4 Environmental conditions and bacterial species activity

The primary acid mineral source formation mechanism and associated reactions that are associated with Inland ASS sites are shown on Graph 5. Iron sulfide minerals are one of the end products that form as part of the process of dissolved sulfate reduction in the Inland ASS system. Dissolved sulfate is utilised as an electron acceptor and is reduced to sulfide, while organic matter is oxidised and donate the electrons for the reduction of sulfate. Sulfate reduction generally occurs in the absence of oxygen as shown on Graph 3.

Sulfate reduction is a natural process that occurs as part of the metabolic process of bacteria and occurs in virtually all lakes, rivers, wetlands and oceans, by various bacteria species as shown on Graph 4. However, the quantities of sulfide minerals that will accumulate in a given environment are a function of several factors, with the following being those most significantly associated with sulfide accumulation:

- Continual addition of dissolved sulfate into the Inland ASS system.
- Saturation of soils and sediments for periods long enough to favour moderately to strongly reducing conditions.
- Availability of labile carbon to fuel the metabolic activity of bacteria.
- Availability of either or both dissolved Fe or Fe containing minerals, such as those listed in Graph 5.




**Graph 5 Primary Acid Source Formation Process active in Big Swamp**

In addition to the accumulated sulfides acting as a potential source of acid when oxidised, an additional source of acid in Inland ASS systems are Monosulfidic black ooze (MBO) which is a subaqueous or waterlogged organic-rich material that contains appreciable concentrations of monosulfides. MBO's are characterised by their gel-like consistence and generally have a field pH of 4 or more when present in saturated undisturbed form. Depending on environmental conditions and composition, MBO can have neutral to slightly alkaline (>pH 7-8).

However, when disturbed and / or drained MBO can become extremely acidic (pH <4). The nutrient rich environment of MBO together with the activity of algae and micro-organisms results in the generation of strongly reducing conditions that result in the formation of iron monosulfides, as shown on Graph 5. As a result MBO form black soils that emit strong sulfidic odours when disturbed.

When subaqueous materials rich in monosulfides are resuspended, for example during the flushing of drains by high runoff events, they rapidly oxidise, which can result in the depletion of dissolved oxygen in the water column, resulting in adverse impact on aquatic flora and fauna, such as fish kills. The risk posed to aqueous flora and fauna is generally highest in enclosed water bodies, such as aquaculture ponds or in estuaries.

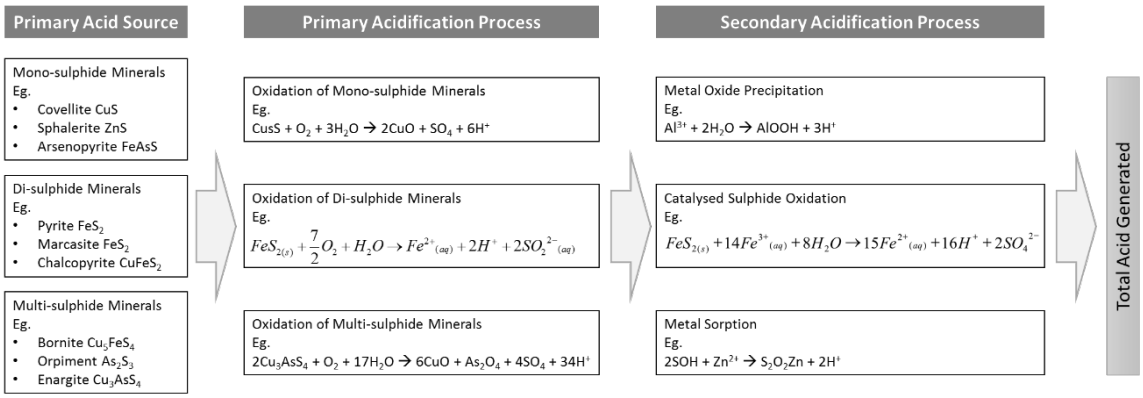
### 4.3.2 General acid generation processes

Acid soils are distinguished by an acidic reaction and a lack of easily soluble minerals that provide buffering capacity. The low readily soluble mineral content results in low ionic strengths in the solutions. In acid soils the pH dependent exchange sites becomes increasingly occupied with hydrogen (nonexchangeable) and the cation exchange capacity decreases. At the permanent sites Ca, Mg, Na, and K are reduced as the solution concentration of these ions increases and the concentration of Al increases. Despite the fact that extractable $H^+$ and $Al^{3+}$ can be high, there is very little exchangeable $H^+$ on exchange sites in acid soils.

ASS generate sulfuric acid through chemical oxidation of sulfide minerals, which result in the release of soluble sulfate. This dissolved sulfate can leach into surface water drainage systems, leading to acidification and the mobilisation of aluminium, heavy metals and arsenic from minerals present in the soils and corrodes steel and concrete infrastructure.

While aluminium is abundant in the minerals present in the soil and rock, dissolved concentrations are low under naturally occurring pH in soil pore-water, groundwater and surface water. Dissolved aluminium is toxic to aquatic and terrestrial flora and fauna. Dissolved aluminium mobilised by acidification processes has been associated with fish kills and death of vegetation. In sub-lethal doses dissolved aluminium stunts growth and breaks down immunity against disease. High concentrations of dissolved heavy metals are also toxic, and heavy deposits of ochre can choke vegetation and block drains.

There are several steps in acid generation which occur in a sequence of reactions that can be divided into primary and secondary acidification processes. The most common source of acid associated with Inland ASS are sulfides, with pyrite generally being the most abundant. Oxidation of mono, di and multi sulfide minerals is generally the primary acidification process. For example, oxidation of pyrite to $Fe^{2+}$ and sulfate is generally the first step in the reaction sequence. This can then be followed by secondary acidification processes, such as oxidation of some $Fe^{2+}$ to $Fe^{3+}$, which significantly increases acid generation through oxidation of pyrite by $Fe^{3+}$ and, finally, oxidation of the remaining $Fe^{2+}$ to Ochre. The overall acid source and primary and secondary acidification processes are summarise on Graph 6.




**Graph 6 Acid sources and primary and secondary acidification processes**

Oxidation of pyrite by oxygen (equation 1) is associated with a slow kinetic rate. Oxidation of $Fe^{2+}$ to $Fe^{3+}$ is a more effective oxidant (equation 2) and oxidation of pyrite by $Fe^{3+}$ (equation 3) proceeds much faster than the reaction of pyrite with oxygen but, also, much faster than the oxidation of $Fe^{2+}$ to $Fe^{3+}$ (equation 2). So the $Fe^{2+}$ to $Fe^{3+}$ transformation is, potentially, the rate-limiting step. However, generation of $Fe^{3+}$ is mediated by iron-oxidising bacteria, particularly Thiobacillus ferooxidans. Equation 3 depends on the pH being low enough for $Fe^{3+}$ to remain soluble (pH < 4), otherwise it is precipitated as ochre (equation 4), so rapid oxidation of pyrite, facilitated by $Fe^{3+}$ generally only takes place at very low pH.

$$\underset{\text{pyrite}}{FeS_{2(s)}} + \underset{\text{dissolved oxygen}}{\tfrac{7}{2}O_2} + H_2O \Rightarrow \underset{\text{dissolved iron II}}{Fe^{2+}_{(aq)}} + \underset{\text{sulphuric acid}}{2H^+_{(aq)} + 2SO_4^{2-}{}_{(aq)}} \quad \ldots.(1)$$

$$Fe^{2+}_{(aq)} + \tfrac{1}{4}O_{2(aq)} + H^+_{(aq)} \Rightarrow \underset{\text{dissolved iron III}}{Fe^{3+}_{(aq)}} + \tfrac{1}{2}H_2O \quad \ldots.(2)$$

$$FeS_{2(s)} + 14Fe^{3+}_{(aq)} + 8H_2O \Rightarrow 15Fe^{2+}_{(aq)} + 16H^+_{(aq)} + 2SO_4^{2-} \quad \ldots.(3)$$

$$Fe^{2+}_{(aq)} + \tfrac{1}{4}O_{2(aq)} + \tfrac{3}{2}H_2O \Rightarrow \underset{\text{ochre}}{FeO.OH_{(s)}} + 2H^+_{(aq)} \quad \ldots.(4)$$

The different stages of oxidation do not necessarily occur at exactly the same point in space and / or time. Field and micromorphological examination of ASS shows a distinct separation of pyrite and its oxidation products ochre, jarosite and gypsum. Under a climate with pronounced wet and dry seasons, oxidation of pyrite may continue after flooding using the oxidising capacity stored as $Fe^{3+}$ oxide during the dry season.

The final step of oxidation of $Fe^{2+}$ ions to ochre (equation 4) requires strongly oxidising conditions, which may be found at some distance from the pyrite source, either within the soil or in drainage or floodwaters. Under conditions of poor drainage, especially in soils rich in organic matter, the $Fe^{2+}$ ions may migrate for several km in acid solution before precipitation as ochre in a more oxidising environment, causing further acid generation through this secondary acidification process.

In soils, a conspicuous intermediate product of sulfide oxidation is the yellow mineral jarosite, which is deposited as coatings around pores and fissures under strongly oxidising conditions, severely acid conditions (Eh greater than +400 mv, pH less than 3.7). Jarosite may occur in a range of solid solutions with natrojarosite and hydrodiumjarosite but the potassium form predominates. Its formation from pyrite may be represented as:

$$FeS_{2(s)} + \tfrac{15}{4}O_{2(aq)} + \tfrac{5}{2}H_2O_{(l)} + \tfrac{1}{3}K^+_{(aq)} \Rightarrow \underset{\text{jarosite}}{\tfrac{1}{3}KFe_3(SO_4)_2(OH)_{6(s)}} + \underset{\text{sulphuric acid}}{\tfrac{4}{3}SO_4^{2-}{}_{(aq)} + 3H^+_{(aq)}}$$

At higher pH values, jarosite is ultimately hydrolysed to goethite.

$$KFe_3(SO_4)_2(OH)_{6(s)} \Rightarrow \underset{\text{goethite}}{3FeO.OH_{(s)}} + 3H^+_{(aq)} + 2SO_4^{2-}{}_{(aq)}$$

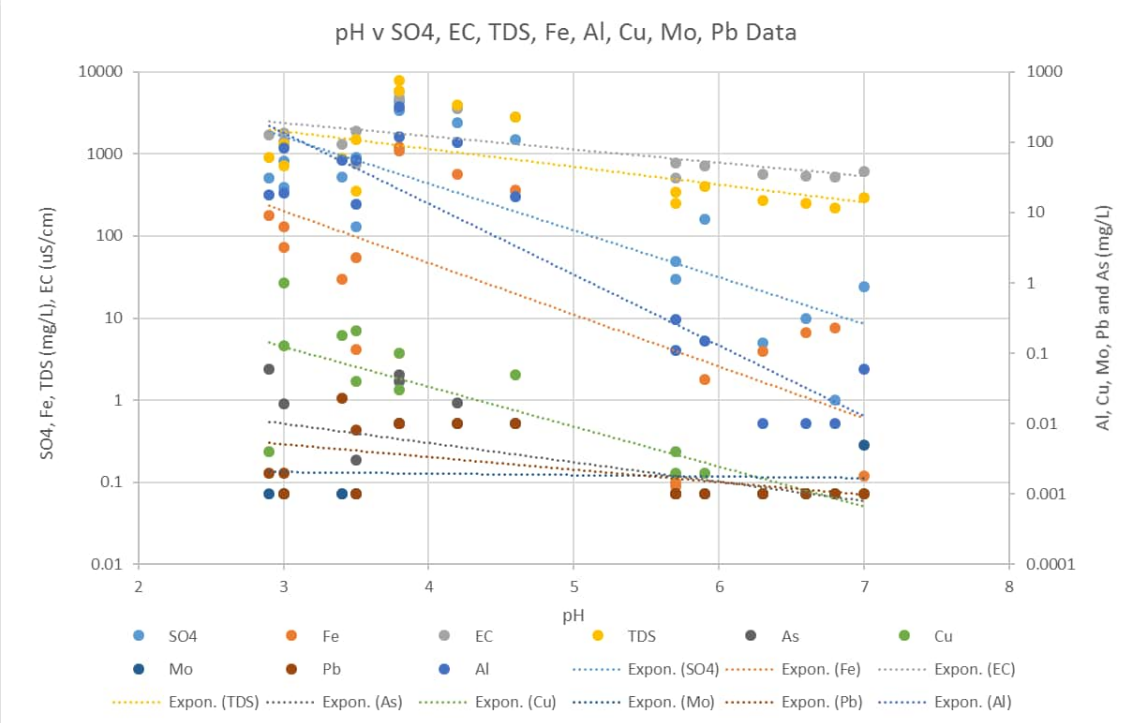
## 4.4 Geochemical processes in Big Swamp and Reach 3 of Boundary Creek

This section provides an assessment of the primary acid source minerals and primary and secondary acidification processes identifiable in Big Swamp and Reach 3 of Boundary Creek.

### 4.4.1 Primary acid source assessment for Big Swamp

Based on the understanding of the general acidification and neutralisation processes set out in the previous sections, the existing water sample analysis data for Big Swamp from May 2017 (Jacobs, 2017a), August 2017 (Jacobs, 2017b) and August 2019 (ALS, 2019) was utilised to assess the potential sulfidic source minerals for acid generation. As noted iron sulfides are generally the most common primary source minerals, as illustrated in Graph 5, with arsenic, copper and lead sulfides providing other potential acid source minerals in Big Swamp based on their presence in dissolved phase.

The dissolved phase concentration measured in pore water and groundwater samples collected from Big Swamp in August 2019 (ALS 2019) was used to assess the relationship between the concentration of these dissolved phase inorganics and pH to evaluate whether oxidation and dissolution of primary acid source minerals was apparent as a primary line of evidence. The results of this assessment are summarised on Graph 7.




**Graph 7 Summary of primary acid source assessment for Big Swamp**

The results of the primary acid source assessment of the data available for Big Swamp as summarised on Graph 7 suggests:

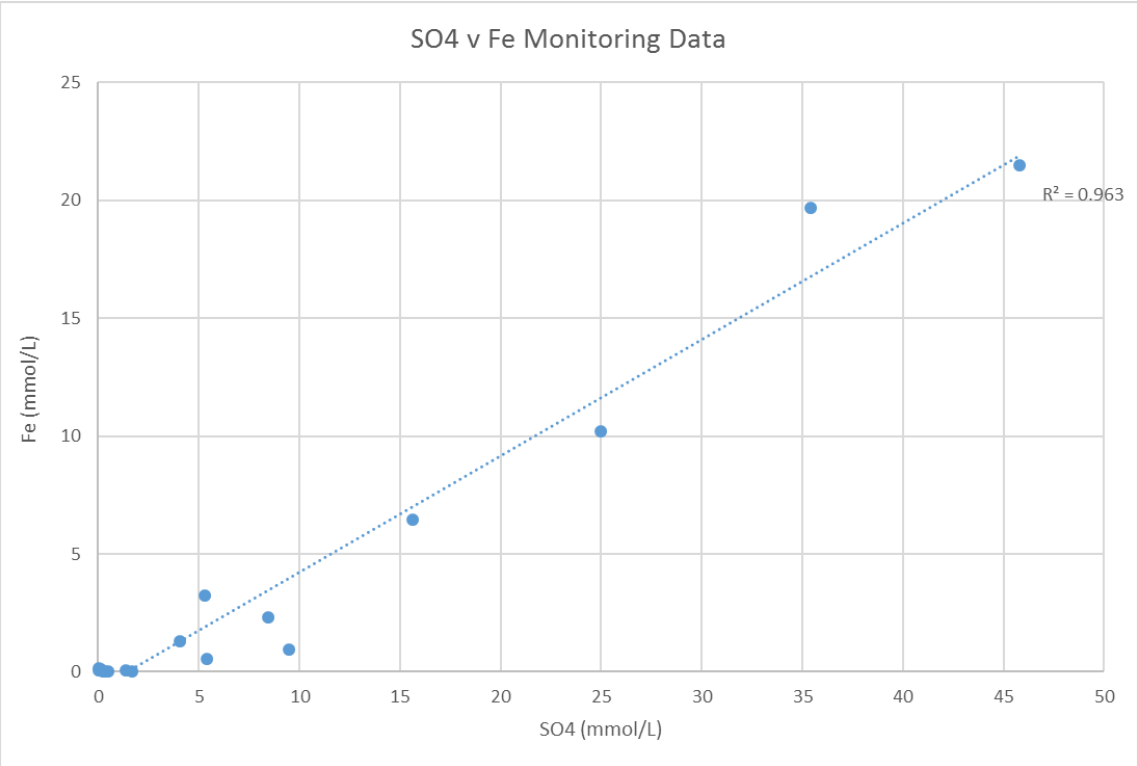
- There is a strong relationship between pH, sulfate and iron when plotted on a log scale, suggesting that iron sulfide minerals such as Iron monosulfides (FeS), Iron disulfides (pyrite) ($FeS_2$) and possibly Marcasite $FeS_2$ are the primary acid source.
- There is a relationship between pH, sulfate and salinity (EC and TDS), suggesting that oxidation and dissolution of sulfide minerals is a source of dissolved solids that increase the ionic strength of the solution.
- Arsenic, copper and lead also show relationships with pH and sulfate. However concentrations of these inorganics are significantly lower than iron concentrations, suggesting that copper sulfide minerals such as Chalcopyrite $CuFeS_2$, Covellite CuS, Enargite $Cu_3AsS_4$ and possibly Jamesonite $Pb_4FeSb_6S_{14}$ if present within the swamp sediments may form a minor acid source. Another potential source of these metals is release of sorbed phase into solution in response to decreasing pH. At present there is insufficient geochemical and mineralogical data to assess which geochemical processes is active with respect to these metals.
- Molybdenum shows no relationship with pH and sulfate, suggesting that molybdenum sulfides are not a detectable acid source in Big Swamp.
- Aluminium, shows a relationship with pH and sulfate, suggesting that mineral weathering and dissolution of aluminium hydroxides and oxides is occurring as a result of the decrease in pH. However, aluminium concentrations are lower than sulfate and iron concentrations, suggesting only limited weathering is occurring, which suggests that buffering capacity in Big Swamp may be limited. This aspect is further discussed in Section 4.6.

Overall there is considered to be sufficient evidence to conclude that iron sulfide minerals form the primary acid source in the Big Swamp sediments, with minor acid contributions from other sulfide minerals if present.

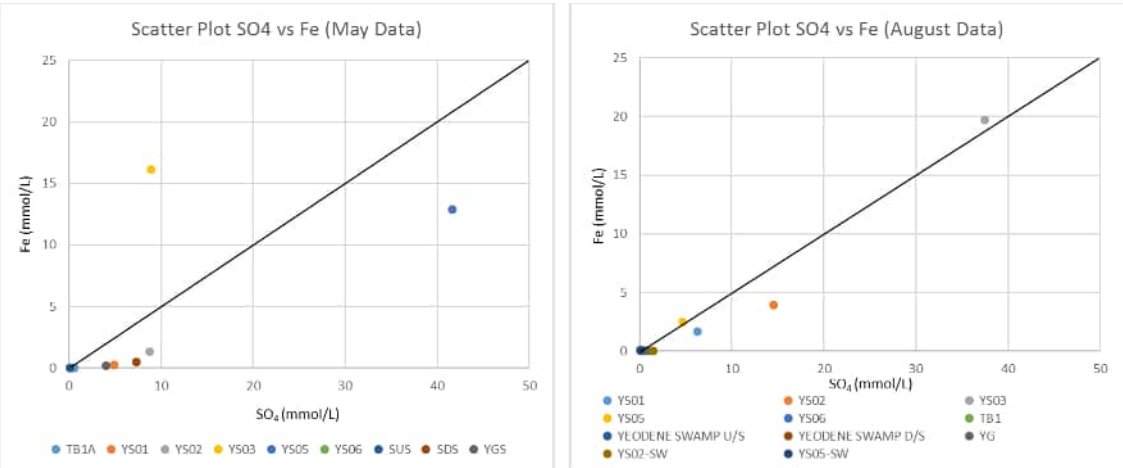
### 4.4.2 Primary acidification processes assessment for Big Swamp

The existing water sample analysis data for Big Swamp was utilised to assess the primary acidification processes associated with the oxidation of sulfidic source minerals. As shown on Graph 7, there is a relationship between pH, iron and sulfate that suggests that iron sulfide mineral are the primary acid source minerals. Oxidation of iron sulfides, such as Iron monosulfides (FeS), Iron disulfides (pyrite) ($FeS_2$) and possibly Marcasite $FeS_2$, are considered to be the primary acidification process responsible of the observed decreases in pH observed in Big Swamp and Reach 3 of Boundary Creek. This assessment finding is supported by the strong positive relationship between sulfate and iron shown in the scatter plots for the recent monitoring data shown on Graph 8 (August 2019). As shown on Graph 8, there is a strong correlation between sulfate and iron at an approximate 2 to 1 ratio, which would be consistent with the oxidation of pyrite (a di-sulfide mineral) as shown in the equation below:

$$2FeS_2 + 7O_2 + 2H_2O \rightarrow 2Fe^{2+} + 4SO_4^{2-} + 4H^+$$




**Graph 8 Sulfate and iron scatter plot – monitoring data for Big Swamp**




**Graph 9 Sulfate and iron scatter plot – Jacobs pore and groundwater data for Big Swamp, with black line showing 2 to 1 relationship**

The relationship between sulfate and iron mole ratio for the Jacobs (2017a, 2017b) monitoring bore data also supports pyrite oxidation as the primary acidification process for the August 2017 data, but not May 2017 as shown on Graph 9. The May data shows a significant deficit in iron compared to sulfate for this monitoring round, indicating that other acidification processed may have been active in Big Swamp in this period as discussed in more detail in Section 4.4.3.

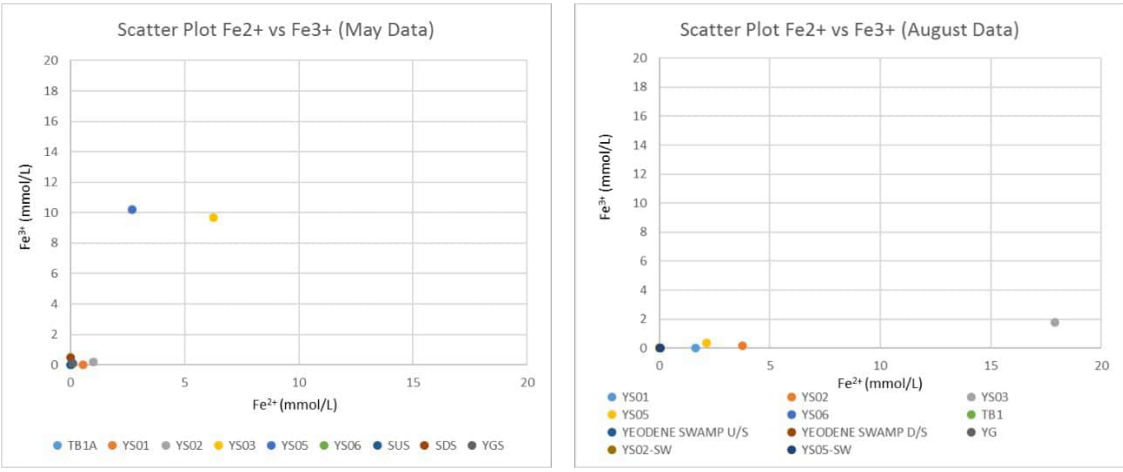
Overall there is considered to be sufficient evidence to conclude that the dominant primary acidification process is oxidation of iron sulfide minerals, with pyrite being the dominant acid source mineral apparent in Big Swamp. If oxidation of iron mono-sulfide was the dominant process, which is commonly associated with MBO, the sulfate to iron ratio's would have plotted near to a 1:1 ratio.

### 4.4.3 Secondary acidification processes in Big Swamp and Reach 3 of Boundary Creek

Secondary acidification processes can occur in the surface water within Big Swamp and the Boundary Creek in Reach 3 down-stream of Big Swamp. Assessment of the available data was undertaken for each of these areas to evaluate the contributions that secondary acidification processes may make to the acid impacts in these two environments.

#### *Big Swamp pore and groundwater quality*

As is evident in the August monitoring event data (Jacobs 2017b) shown on Graph 9 there is an excess of sulfate over iron on the solution, suggesting that some secondary acidification processes are potentially active. The existing water quality monitoring data was assessed to evaluate which secondary acidification processes may be active in Big Swamp. Graph 10 presents the results of the assessment of the iron speciation data provided in the Jacobs (2018) report, which shows differences between the May and August monitoring rounds.

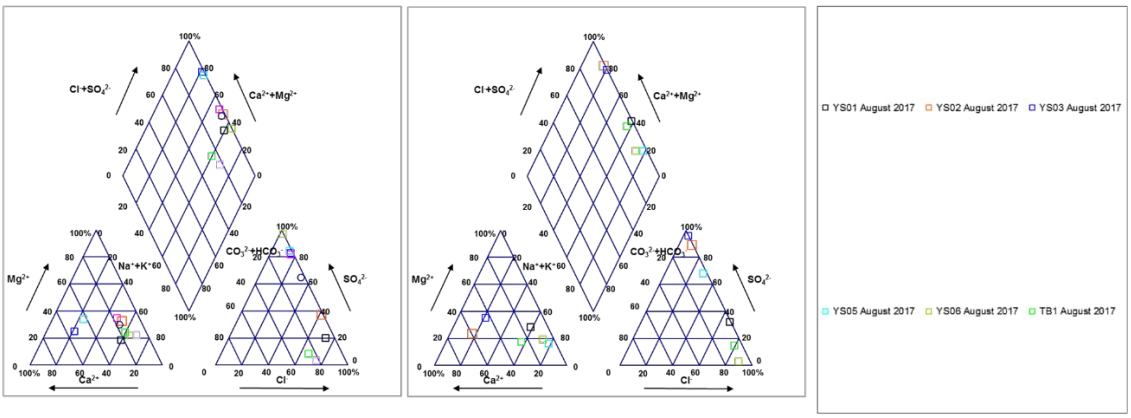



**Graph 10 Ferrous and ferric iron scatter plots for surface water data**

The May 2017 monitoring data for Big Swamp showed two locations (YS03 and YS05) with elevated ferric iron concentration, which suggests that at least in localised areas appreciable amounts of ferric iron may be periodically available to facilitate enhanced pyrite oxidisation as described in equation 3 shown above, suggesting that this secondary acidification process could be active periodically in Big Swamp. However, there currently is insufficient temporal data to confirm this is the case.

Further, as shown on Graph 9, there are periods of excess sulphate over iron, suggesting that dissolved phase minerals may be precipitated as jarosite, which may then be converted to goethite as pH increases resulting in the release of hydrogen and sulfate into solution, while removing iron by precipitation and conversion of jarosite to goethite. The data suggests that these secondary acidification processes may be at least periodically occurring in Big Swamp. However, there currently is insufficient temporal data to confirm this is the case nor can the duration and magnitude of secondary acidification processes as a contributor to the overall acid impact be assessed.

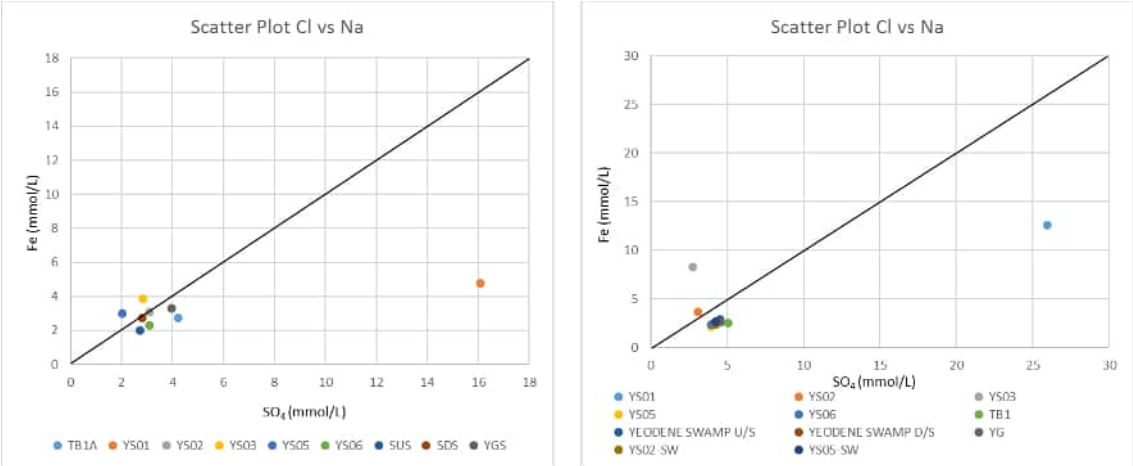
Assessment of the pore water and groundwater monitoring data shows that geochemical conditions in Big Swamp are variable both spatially and temporally suggesting the system is dynamic, as indicated in the piper plots for the May 2017 (Jacobs 2017a) and August 2017 (Jacobs 2017b) data presented on Graph 11. These dynamics will affect the severity and duration of any acid generation events and will affect the impacts on the environment as well as the ability of the environment to recover from acid impacts.




**Graph 11 Piper plot of pore water and groundwater data (May left) (August right)**

### *Reach 3 of Boundary Creek*

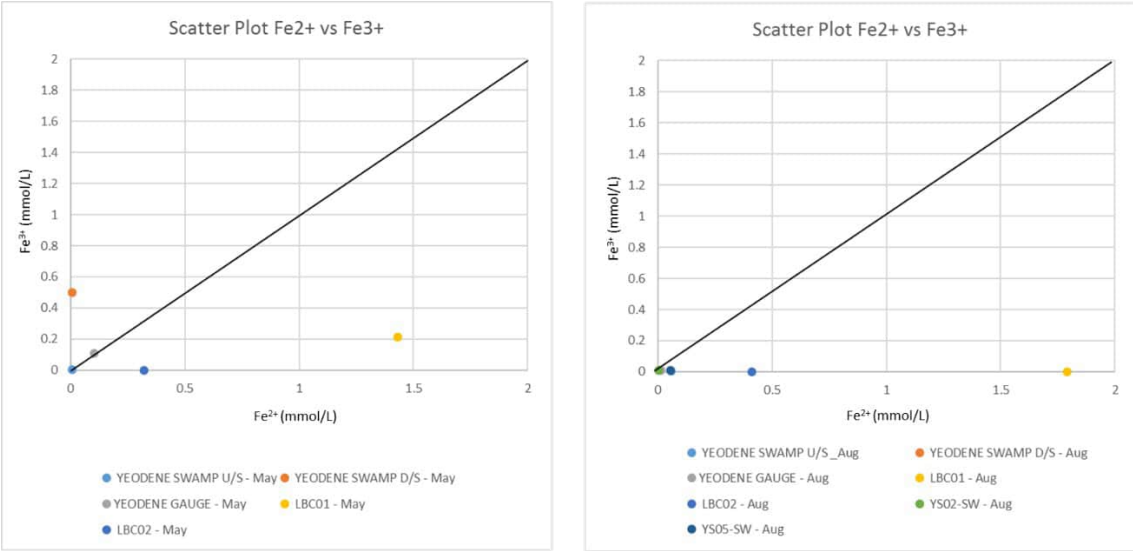
There is limited evidence to suggest that any primary acid source minerals are present in Reach 3 of Boundary Creek as there is no apparent relationship between sulfate and iron as shown on Graph 12 (Jacobs 2017a and 2017b).




**Graph 12 Sulfate and iron scatter plot for surface water data**

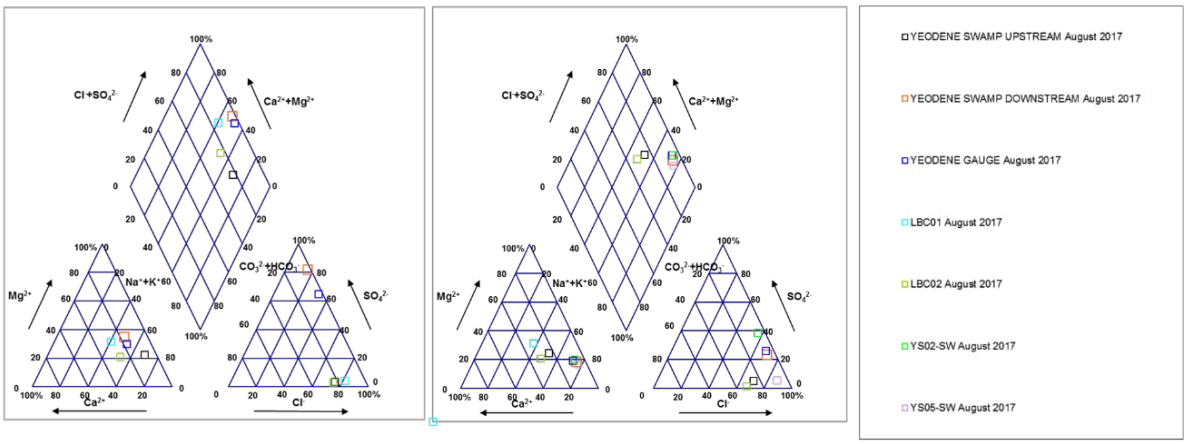
The existing surface water quality monitoring data for Reach 3 of Boundary Creek was assessed to evaluate whether secondary acidification processes may be active in Reach 3. Graph 13 presents the results of the assessment of the iron speciation data provided in the Jacobs (2018) report, which shows differences between the May 2017 and August 2017 monitoring rounds.

The May monitoring data shows that the surface water leaving Big Swamp and entering Reach 3 of Boundary Creek (Yeodene Swamp D/S) has elevated ferric iron concentration, which suggests that at least for some periods appreciable amounts of ferric iron are present in solution. The presence of both ferric and ferrous iron in solution results in an export of acidity from Big Swamp into Reach 3 of Boundary Creek that can lead to secondary acidification though oxidation of ferrous iron to ferric iron and then precipitation of ferric hydroxides.




**Graph 13 Ferrous and ferric iron scatter plots for surface water data**

Assessment of the surface water monitoring data shows that geochemical conditions in Boundary Creek are variable both spatially and temporally suggesting the system is dynamic, as indicated in the piper plots for the May 2017 and August 2017 data presented on Graph 14. These dynamics will affect the severity and duration of any acid generation events and will affect the impacts on the environment as well as the ability of the environment to recover from acid impacts of Reach 3 of Boundary Creek.



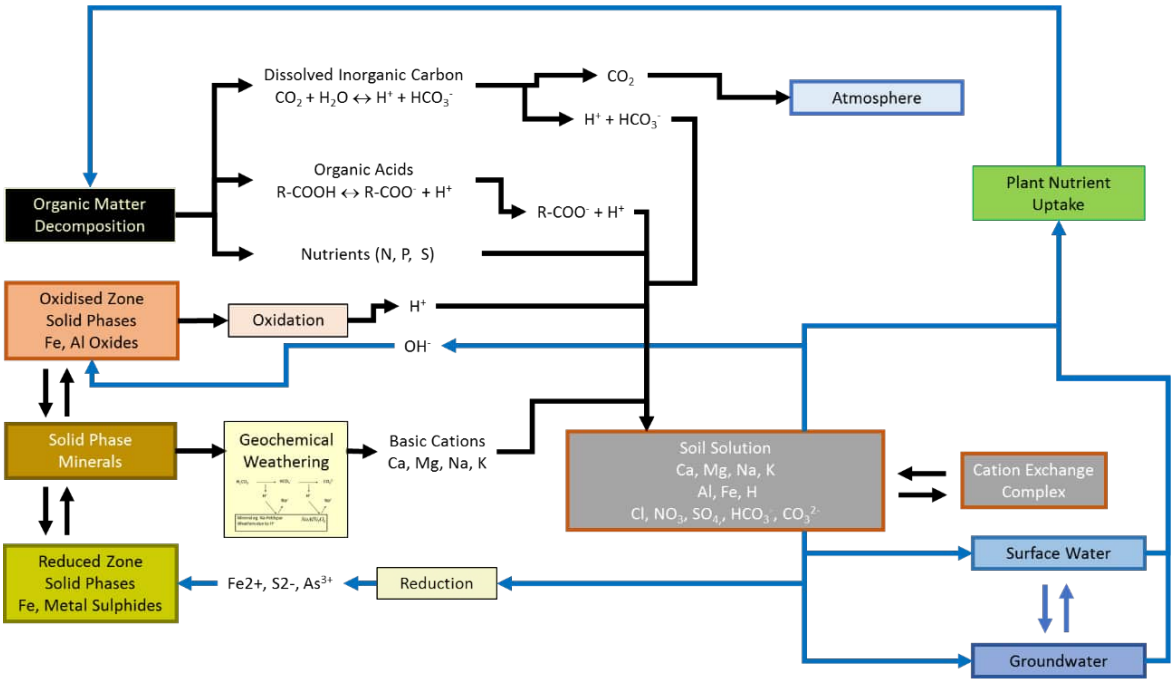

**Graph 14 Piper plot of surface water data (May left) (August right)**

## 4.5 General acid neutralisation processes

The acid neutralisation capacity of soils is controlled by a number of factors, including parent material, climate, vegetation and management. These factors control whether a soil has a neutral, acidic or alkaline reaction. These factors also control the buffering capacity of soils, which provides the capacity to neutralise acids produced by the primary and secondary acidification processes associated with the oxidation of acid source minerals.

There are a number of processes in soils and sediments, which generate or consume protons (acid) and therefore affect pH. These processes interact with the local climate, parent material, and organisms over time to establish the soil pH. Water flow through the system is an important variable as it removes weathering products and supplies protons for exchange reactions. Some of the important processes that either generate or consume protons are provided on Graph 15.

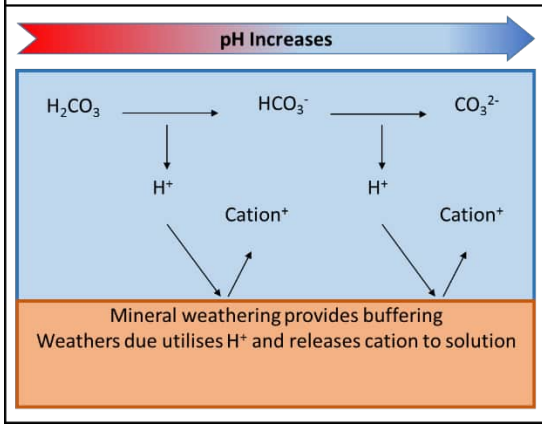
Protons that are generated by these processes interact with the soil exchange complex and the solid phase. Thus, primary minerals, clay and organic matter content and percolation are important aspects of soil pH regulation.




**Graph 15 Conceptual representation of soil processes and factors affecting soil pH**

The release of hydrogen ions into solution as a result of oxidation of sulfide minerals provides protons for mineral weathering and buffering capacity against decrease in pH. The general process involved in buffering is illustrated on Graph 16. The amount of buffering available in soils is dependent in their mineral composition and resistance of these minerals to weathering. Inland ASS soils are characterised by high organic matter content, high sulfide mineral content and low or absence of readily weathered minerals to provide buffering, resulting in significant decreases in pH in response to sulfide mineral oxidation.

**Common Weathering (Buffering) Reactions**




$2NaAlSi_3O_{8(s)} + 9H_2O + 2H^+ \rightarrow Al_2Si_2O_5(OH)_{4(s)} + 2Na^+ + 4H_4SiO_4$
Sodium Feldspar — Kaolinite

$CaAl_2Si_2O_{8(s)} + H_2O + 2H^+ \rightarrow Al_2Si_2O_5(OH)_{4(s)} + Ca^+ + 4H_4SiO_4$
Calcium Feldspar — Kaolinite

$3KAlSi_3O_{8(s)} + 12H_2O + 2H^+ \rightarrow KAl_3Si_3O_{10}(OH)_{2(s)} + 2K^+ + 6H_4SiO_4$
K-Feldspar — Muscovite

$2KAl_3Si_3O_{10}(OH)_{2(s)} + 3H_2O + 2H^+ \rightarrow 3Al_2Si_2O_5(OH)_{4(s)} + 2K^+$
Muscovite — Kaolinite

$Al_2Si_2O_5(OH)_{4(s)} + 5H_2O + 2H^+ \rightarrow 2Al(OH)_{3(s)} + 2H_4SiO_4$
Kaolinite — Gibsite

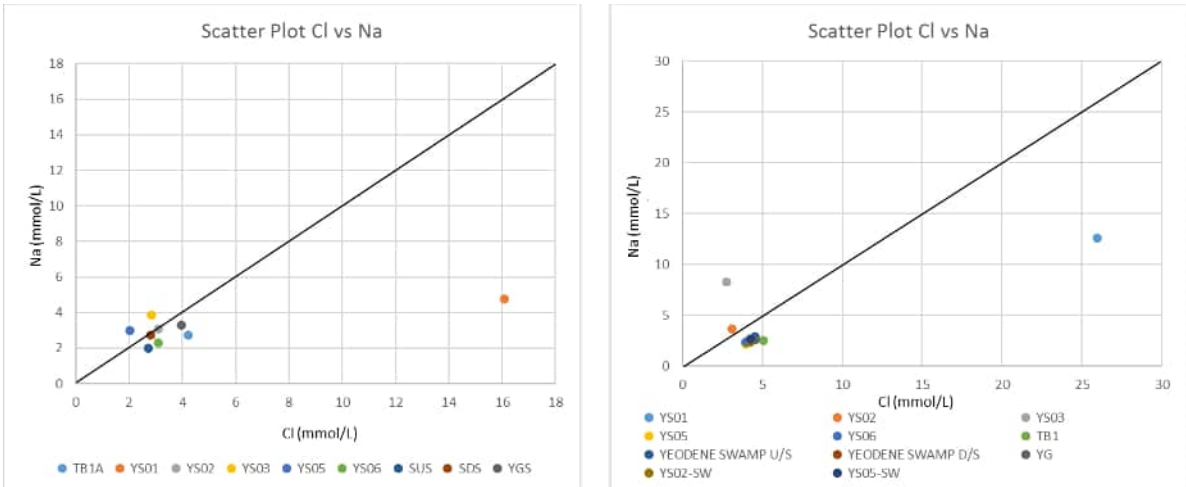
**Graph 16 Common reactions that provide buffering capacity in soils**

## 4.6 Neutralisation capacity assessment for Big Swamp and Reach 3 of Boundary Creek

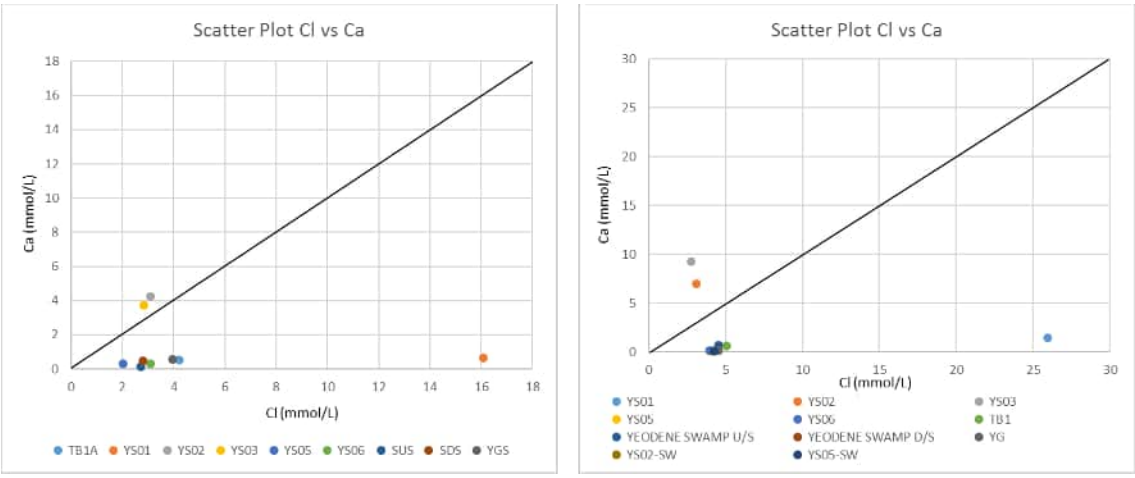
The available water quality monitoring data and results of the Monash University study (2019) was used to assess the neutralising (buffering) capacity of the sediments present in Big Swamp.

The results of the neutralisation capacity assessment indicated that the sediments in Big Swamp had limited neutralisation capacity, based on the following lines of evidence:

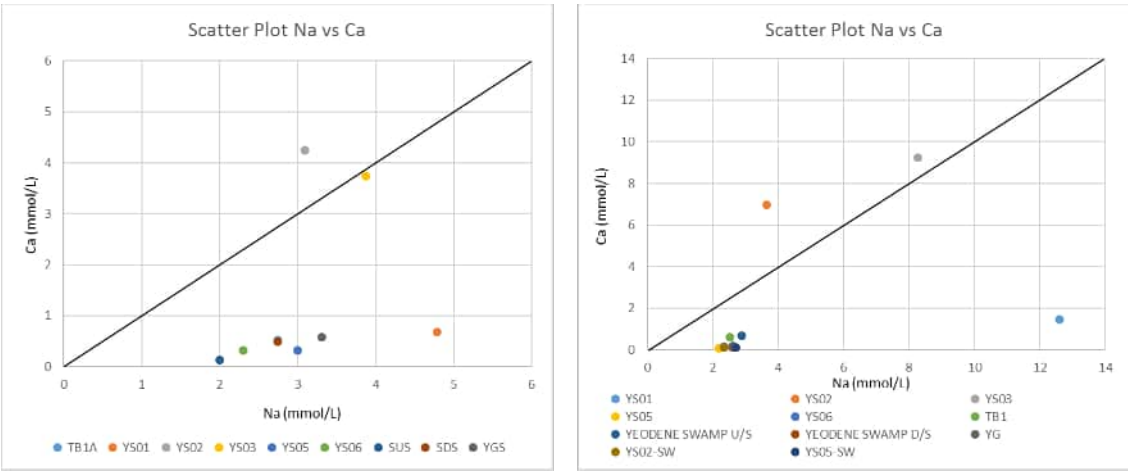
- The salinity range and chloride sodium relationship (Graph 17) shows relatively limited variability suggesting limited dissolution of readily soluble salts or sodium source minerals such as Na-feldspar, in response to decreases in pH.
- The chloride calcium relationship (refer to Graph 18) suggests limited dissolution of calcium source minerals, such as Ca-feldspar, in response to decreases in pH.
- The sodium calcium relationship shows some correlation in terms of concentration and shows some evidence of ion exchange in response to changes in pH. Under changes in pH conditions ion exchange sites can switch preference from di-valent to mono-valent ions, which results in release of di-valent ions such as calcium and removal of mono-valent ions, such as sodium from solution. Ion exchange can provide only limited buffering capacity, and given the results of the scatter plots presented on Graph 19, ion evidence of ion exchange occurring is limited to localised locations within Big Swamp.
- The calcium and bi-carbonate relationship suggests that limited buffering capacity would be provided by calcium carbonate minerals (refer to Graph 20). Graph 20 also supports the evidence on Graph 19 that ion exchange is the primary source of calcium in the water samples analysed.
- The chloride sulfate relationship (refer to Graph 21) suggests that there is limited correlation between the chloride concentration and sulfate concentration, which suggests that salinity (using chloride as an analogy for TDS) is not related to the neutralisation of acid generated by oxidation of sulfide acid source minerals.
- The sulfate sodium (refer to Graph 22) and sulfate calcium (refer to Graph 23) scatter plots show that there is a minor increase in these cations in response to increasing sulfate concentration that results from oxidation of sulfide acid source minerals. This suggests that there may be some limited buffering capacity through weathering of sodium and calcium source minerals or ion exchange, which supports the assessment of the relationship suggested on Graph 17 and Graph 18.



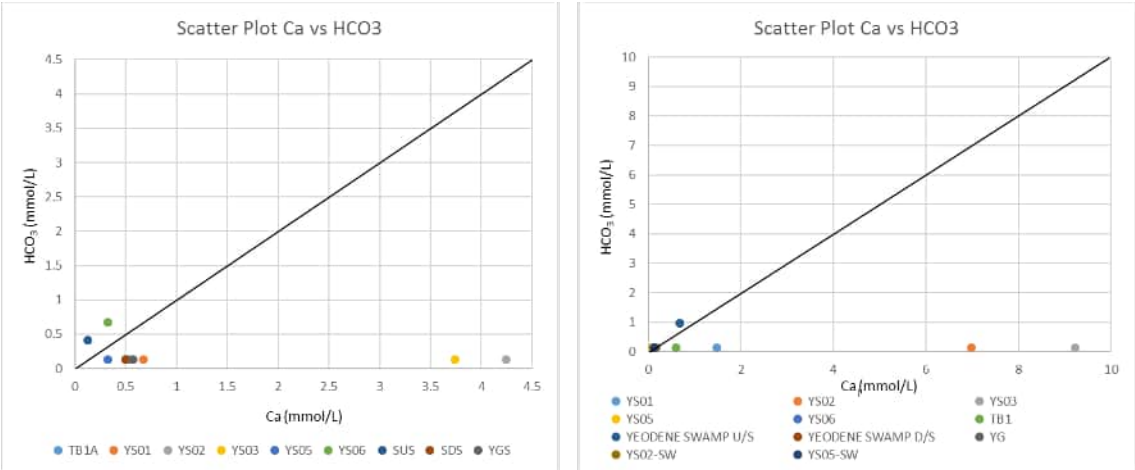

**Graph 17 Chloride, sodium scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio**



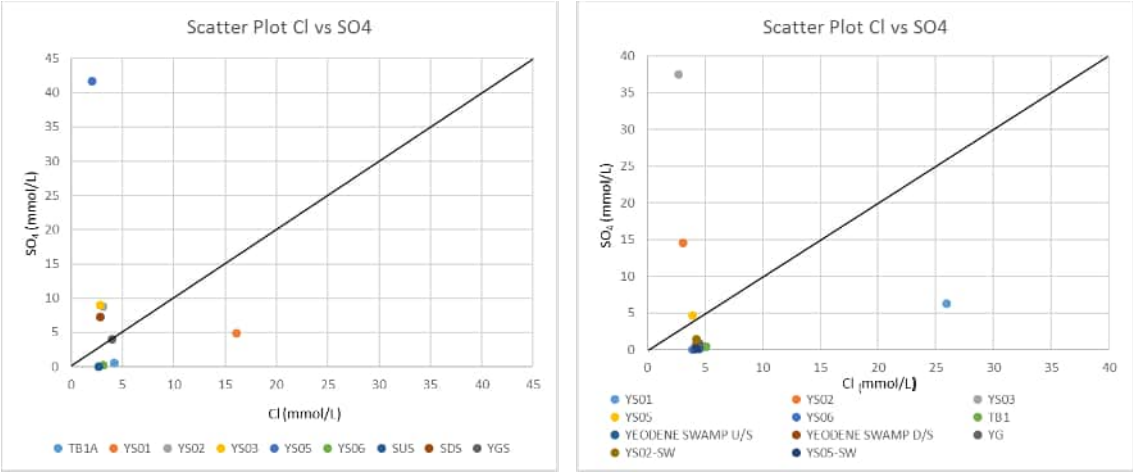

**Graph 18 Chloride, calcium scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio.**



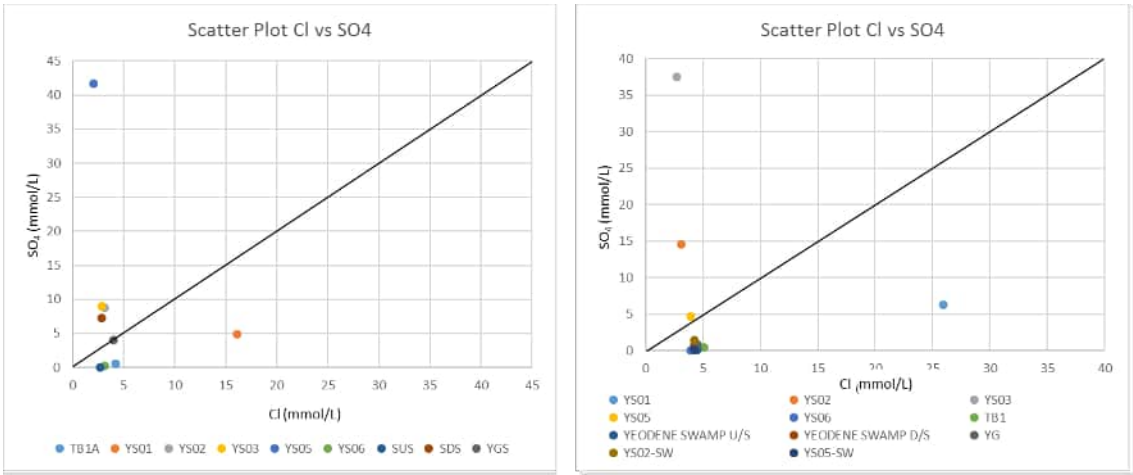

**Graph 19 Sodium, calcium scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio.**



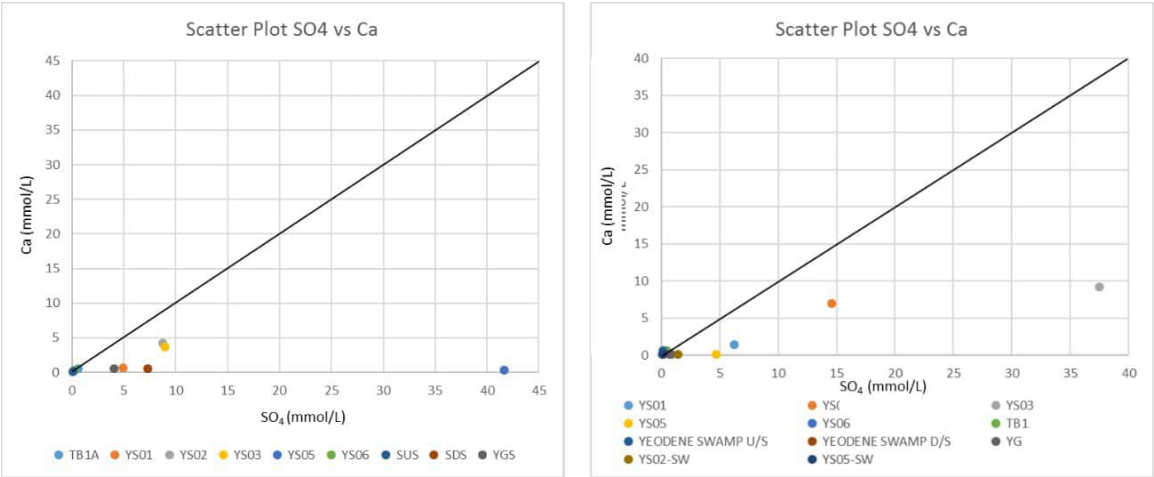

**Graph 20 Calcium, bicarbonate scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio.**




**Graph 21 Chloride, sulfate scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio.**




**Graph 22 Sulfate, sodium scatter plot for May 2017 and August 2017 surface water monitoring data. Black line shows 1 to 1 ratio.**




**Graph 23 Sulfate, calcium scatter plot for May 2017 and August 2017 Surface Water Monitoring Data. Black line shows 1 to 1 relationship.**

The Monash University (2019) incubation studies, documented in a separate progress reports (May/June, July/August and September 2019 reports), focused on 5 soils that were made up of blending soils from samples obtained from Big Swamp. These 5 soils fell into two broad categories, one group (Soil 1 and 2) was comprised of soils that had already oxidised (Acid Soils), while the second group was comprised of soils that had not yet oxidised (Soil 3,4 and 5) and therefore represented potential ASS. The second group of soils was generally distinguished by organic matter content, with Soil 3 and 5 having lower organic carbon content than Soil 4. The preliminary result of the incubation tests suggest that Soil 4 may have sufficient neutralisation capacity in the form of reduction capacity to re-attenuate sulfate by reduction to sulfide and precipitation as sulfide minerals, such as MOB or pyrite. However, Soils 3 and 5, which have lower organic matter content were considered to have insufficient neutralisation capacity in the form of reduction capacity with respect to the amount of acid generated by these soils. Further the Monash study found that while the high organic matter content soils theoretically had sufficient neutralisation capacity for the acid generated by them, the preliminary results suggest that the reaction kinetics for the attenuation of sulfate by reduction to sulfide and precipitation of sulfide mineral appear slow and may not proceed to completion.

Therefore, based on the available information, there is limited evidence that suggests the sediments in Big Swamp have a readily available and efficient buffering capacity. The buffering capacity appears limited by insignificant amounts of soluble minerals and slow kinetic reactions for the reduction of dissolved sulfate to sulfide and precipitation as of sulfide minerals.

## 4.7 Conceptual geochemical model summary

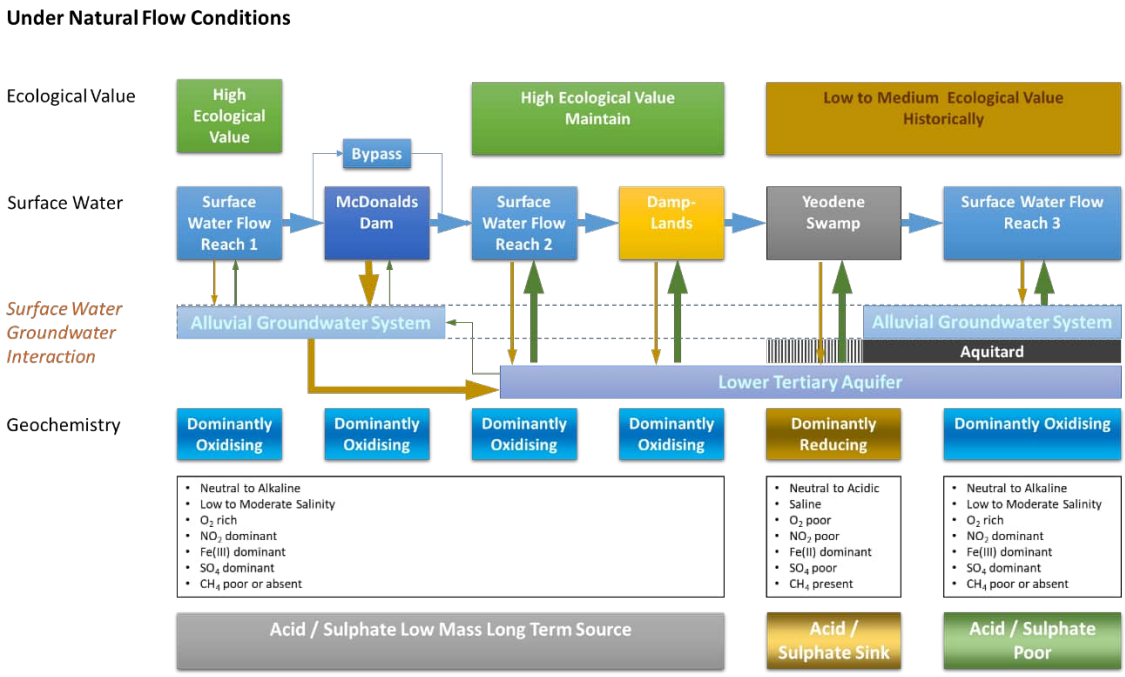
This section presents a summary of the key hydrological, hydrogeological and hydrogeochemical processes associated with Big Swamp and Reach 3 of Boundary Creek that formed the basis of the Conceptual Geochemical Model (CGM).

### 4.7.1 Key processes under natural flow conditions

To inform the baseline assessment and to assist in the development of realistic and practicable remediation and rehabilitation objectives, a baseline CGM was developed on the basis of the primary considerations summarised in Graph 24. The key elements of the conceptual linkages between surface water flow, groundwater surface water interaction and geochemical processes as summarised in Graph 24 are:

- The surface water flow in the catchment has been modified through the landform modification, including the installation of a dam (McDonalds) on Boundary Creek.
- The Boundary Creek catchment has been divided into the following parts, which had different ecological values:
  - Reach 1, up-stream of McDonalds Dam, which is considered to have high ecological values.
  - McDonalds Dam, which retains and stores streamflow and is subject to a theoretical bypass flow of the 2ML/day to maintain environmental flows in Boundary Creek downstream of the dam. The dam represents a highly modified ecosystem and would have low ecological value with respect to the ecological conditions prior to modification.
  - Reach 2, down-stream of McDonalds Dam and up-stream of the Damp-lands, which is considered to have high ecological values.
  - Damp-lands, down-stream of Reach 2 and up-stream of Yeodene Swamp (Big Swamp), which are considered to have high ecological values.
  - Big Swamp, which is located down-stream of the Damplands and up-stream of Reach 3 of Boundary Creek, the swamp was considered to have had high ecological value prior to the occurrence of acidification, vegetation changes and impacts of peat fire.

  - Reach 3 of Boundary Creek, which is located down-stream of Big Swamp and was subject to considerable modification following clearing of the land and use for agriculture, including chanelisation, which resulted in a degraded environmental value prior to pumping by Barwon Water commencing. Therefore, historically Reach 3 of Boundary Creek would have been considered to have had low to medium ecological value prior to the acidification occurring in Big Swamp and consequent acid discharge in to Reach 3.
- Groundwater discharge from the Lower Tertiary Aquifer (LTA) into Reach 2, Damp-lands and possibly Big Swamp was considered to have made a significant baseflow contribution to Boundary Creek prior to drawdown of the potentiometric head in the aquifer associated with groundwater extraction from the Barwon Downs borefield.
- Groundwater discharge into Reach 3 of Boundary Creek and potentially into part or all of Big Swamp was limited by the presence of an aquitard that overlies the LTA.
- Surface water flows in Reach 3 of Boundary Creek under natural flow conditions prior to pumping from the LTA aquifer ranged from lows of 0.1 ML/day to highs of 252 ML/day, with average flows of between 10 and 11 ML/day and Median flow volumes of 2.4 to 3.4 ML/day.
- Geochemical processes relevant to this study that occur in each part of the Boundary Creek catchment can be summarised as follows:
  - Oxidising conditions dominated historically in Reach 1 and 2 of Boundary Creek and the Damp-lands up-stream of Big Swamp, as well as Reach 3 of Boundary Creek, resulting in dissolved sulfate remaining in solution and not subject to accumulation in sediment through reduction. Under these oxidising conditions iron remained predominantly in the ferric iron form leading to low dissolved phase iron concentrations.
  - Reducing conditions dominated in Big Swamp due to the presence of organic matter and persistent wet conditions, which lead to the accumulation of sulfate through reduction to sulphide and precipitation of sulfide minerals from solution. This led to the accumulation of primary acid source minerals in Big Swamp through the formation of pyrite as the dominant sulfide mineral. Based on the available data the Big Swamp is anticipated to contain 600,000 to 700,000 cubic metres of sediments that contain potential primary acid producing minerals.
- Surface water pH in Reach 3 of Boundary Creek under natural flow conditions prior to pumping from the LTA aquifer ranged from lows of 3.5 to highs of 7.4, with an average of 5.6 and Median pH of 5.8.




**Graph 24 Conceptual linkages for system under natural flow conditions**

### 4.7.2 Key processes under anthropogenic flow conditions

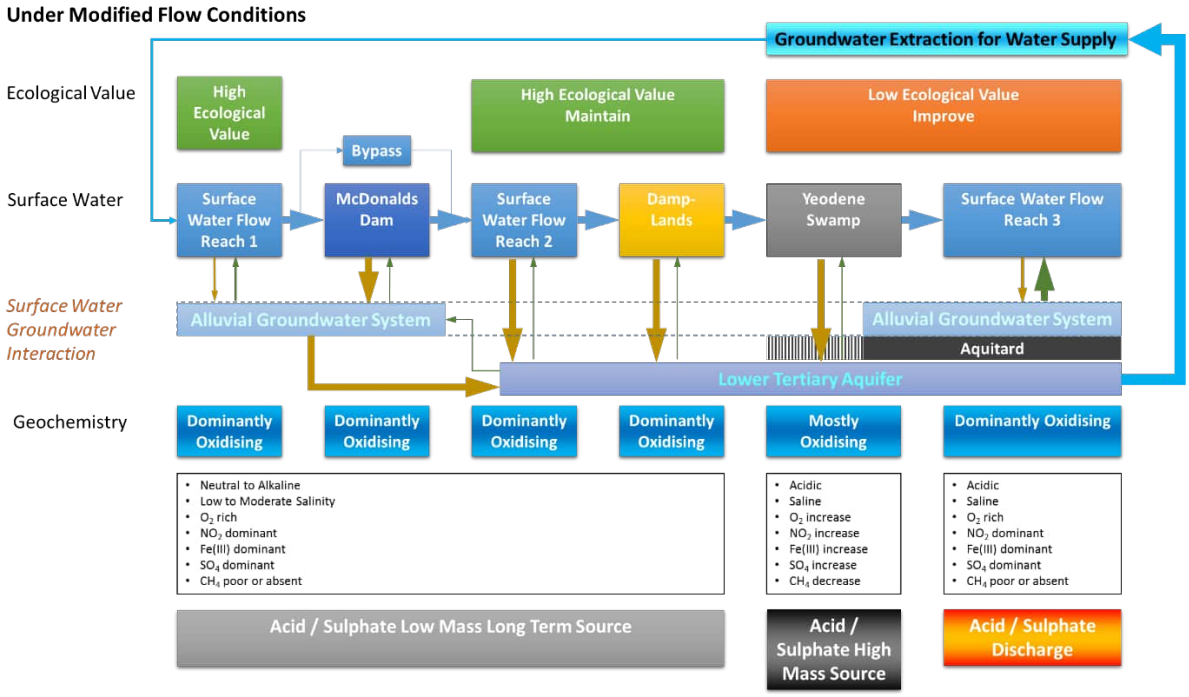
To inform the assessment the geochemical processes occurring under modified flow conditions that resulted from both climate variation and pumping from the LTA aquifer, as well as to assist in the development of realistic and practicable remediation and rehabilitation objectives, a CGM for the conceptual linkages under anthropogenic influences was developed on the basis of the primary considerations summarised in Graph 25. The key elements of the conceptual linkages under modified flow conditions between surface water flow, groundwater surface water interaction and geochemical processes as summarised on Graph 25 are:

- The surface water flow in the catchment has been modified through the landform modification, including the installation of a dam (McDonalds) on Boundary Creek and the pumping from the LTA, which has affected the conceptual linkage and CGM.
- The effects of the modified flow conditions in the Boundary Creek catchment as a result of changes in rainfall and pumping from the LTA has been assessed in the context of the key parts of the catchment, with results indicating:
  - Reach 1, received an anthropogenic input of 2ML/day of additional flow from the total volume extracted from the LTA (or other sources) to compensate to the loss of baseflow contribution from groundwater in Reach 2 and the Damp-lands as a result of pumping from the LTA. Reach 1 is considered to have retained the high ecological values under the modified flow conditions.
  - McDonalds Dam, which retains and stored streamflow and is subject to a theoretical bypass flow of the 2ML/day to maintain environmental flows in Boundary Creek downstream of the dam. The dam represents a highly modified ecosystem and would have low ecological value with respect to the ecological conditions prior to modification. The changed flow regime was considered unlikely to have resulted in any significant changes to the ecological values of the Dam.
  - Reach 2, theoretically received an anthropogenic baseflow contribution of 2ML/day to compensate for baseflow loss as a result of pumping from the LTA. Reach 2 is considered to have retained the high ecological values under the modified flow conditions.

  - Damp-lands, theoretically received an anthropogenic baseflow contribution of 2ML/day to compensate for baseflow loss as a result of pumping from the LTA. The Damp-lands are considered to have retained the high ecological values under the modified flow conditions.
  - Big Swamp, theoretically received an anthropogenic baseflow contribution of 2ML/day to compensate for baseflow loss as a result of pumping from the LTA. However, dewatering of the swamp sediments occurred as a result of loss of groundwater baseflow contributions due to pumping and dry climatic conditions resulting in the formation of acid as a result of conditions becoming predominantly oxidising causing oxidation of the accumulated sulfide minerals resulting in acidification of the sediments, pore water, shallow groundwater and surface water present in Big Swamp. This acidification coupled with vegetation changes and impacts of fire have resulted in the degradation of the ecological values of the swamp from high to low.
  - Reach 3 of Boundary Creek, which is located down-stream of Big Swamp has been adversely impacted by acid discharge from Big Swamp, which has degraded the historically low to medium ecological value prior to the acidification to low under the modified flow regime.
- Groundwater discharge from the Lower Tertiary Aquifer (LTA) into Reach 2, Damp-lands and possibly Big Swamp appears to have ceased, or significantly reduced as a consequence of pumping induced drawdown in the LTA. This is considered to have resulted in a decrease of the water table elevations in the sediments within Big Swamp leading to oxidising conditions that resulted in acidification through oxidation of sulfide mineral and export of acidity from Big Swamp into Reach 3 of Boundary Creek.
- Surface water flows in Reach 3 of Boundary Creek under the modified flow conditions as a result of pumping from the LTA aquifer and climatic conditions ranged from no flow to highs of up to 185 ML/day, which was somewhat similar to the overall range observed prior to modification of the flow regime.

  However, the most significant changes in flow conditions as a result of pumping and climate influences was a decrease in average flows from between 10 and 11 ML/day under natural flow conditions to 5 to 7 ML/day under modified flow conditions (decrease of 4 to 6 ML/day) and a decrease in median flow volumes from 2.4 to 3.4 ML/day under natural flow conditions to 0.7 to 1.2 ML/day under modified flow conditions (decrease of around 2ML/day). In addition the number of no flow days has increased significantly since 1999 (refer Figure 7).
- Changes in geochemical processes that result from the modified flow regime and relevant to this study as they occur in each part of the Boundary Creek catchment can be summarised as follows:
  - Oxidising conditions remain dominant in Reach 1 and 2 of Boundary Creek and the Damp-lands up-stream of Big Swamp, as well as Reach 3 of Boundary Creek. As such no direct changes in geochemical processes as a result of the modified flow conditions are anticipated. However, the oxidising conditions in Reach 3 of Boundary Creek are likely to contribute to acidification as a result of secondary acidification processes.
  - Reducing conditions no longer dominate in Big Swamp due to the decreases in water table elevations and drying of the organic matter rich sediments in the swamp. This led to oxidation of the accumulated sulfate minerals in the sediments that became exposed to oxygen. This oxidation of primary acid source minerals (primarily pyrite) in Big Swamp led to the formation of 600,000 to 700,000 cubic metres of sediments that potentially form acid and contain significant net acidity.

- Surface water pH in Reach 3 of Boundary Creek under modified flow conditions as a result of reduced rainfall and baseflow as a result of pumping from the LTA resulted in changes to pH in those parts of the Boundary Creek catchment, with pH ranging from lows of 3.1 to highs of 6.9, which is similar to the range recorded prior to the modification of the flow regime. However, the most significant changes in pH as a resulted of the modified flow regime were for the average pH which decreased from 5.6 prior to the modification of the flow regime to 4 after modification of the flow regime (difference to 1.6 pH Units) and a decrease in Median pH from 5.8 prior to the modification of the flow regime to 3.8 after modification of the flow regime (difference to 2 pH Units).



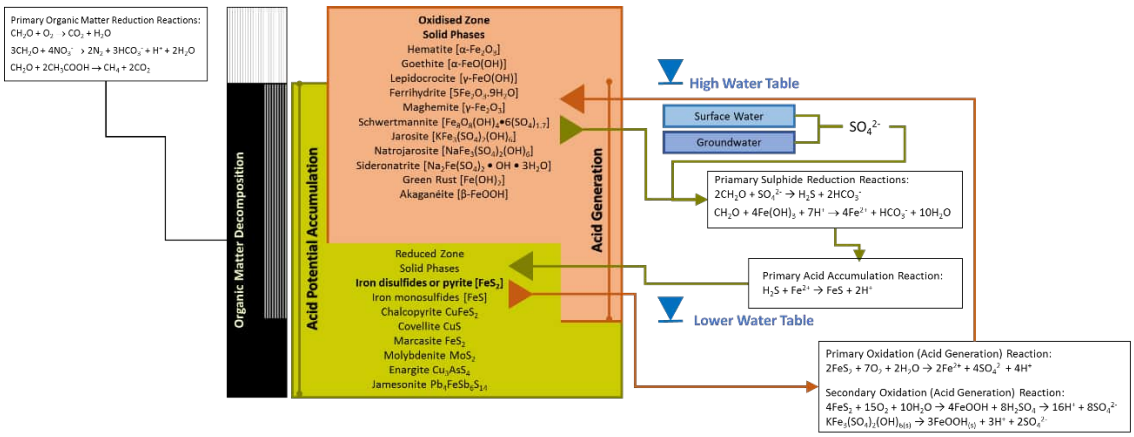

**Graph 25 Conceptual linkages for system under anthropogenic influence**

### 4.7.3 Summary of key geochemical processes occurring in Big Swamp and Reach 3 of Boundary Creek

Following completion of the data assessment a conceptual geochemical model (CGM) was development, which is summarised on Graph 26. In summary the key aspects of the CGM relevant to the project objectives are:

- Acid discharge occurred occasionally from Big Swamp under natural flow conditions and in the absence or limited pumping from the LTA.
- The decrease in baseflow contribution of groundwater from the LTA to Reach 2, Damp-land and possibly Big Swamp as a result of groundwater extraction from the Barwon Downs Borefield in combination with dry climatic conditions has resulted in a decrease in water table elevation within some 600,000 to 700,000 cubic metres of organic rich sediments that are present in Big Swamp and contain primary acid source minerals.
- The decrease in baseflow form groundwater contribution from the LTA and climatic conditions has resulted in a decrease in average and median flow on Reach 3 of Boundary Creek of between 2 to 6 ML/day.

- The decrease in water table elevation in the sediments in Big Swamp has resulted in the oxidation of primary source minerals and has increased the frequency and duration of acid impacts in Reach 3 of Boundary Creek as a result of acid discharge from Big Swamp. Since pumping from the LTA commenced the average and median pH in Reach 3 of Boundary Creek have decreased by between 1.6 to 2 pH Units.
- The acid impacts identified in Big Swamp appear to be the result of acid generated by oxidation of sulfide acid source minerals, particularly pyrite with some minor contributions by other di-sulfidic minerals if present.
- The sediments present in Big Swamp are primarily comprised of decomposing organic matter with limited other mineral content and those minerals present are generally resistant to weathering. Therefore, there is limited buffering capacity in Big Swamp for any acids generated by oxidation of sulfidic minerals.
- The primary sulfate attenuation process that could occurs in Big Swamp is related to reformation of the reducing conditions that results from organic matter decomposition in saturated environments. Based on the available data, this process appears to result in reduction of ferric iron to the ferrous species but there is limited information to suggest that sulfate reduction to sulfide is occurring. Therefore, the attenuation of acid in Big Swamp appears to be limited by insufficient sulfate being present to effectively from sulfide minerals that would attenuate to the net acidity remaining in the system.
- Secondary acidification processes are active in Big Swamp and Reach 3 of Boundary Creek, which further limits the ability of the swamp to limit the attenuation the sulfate.




**Graph 26 Summarised conceptual geochemical model**

The key geochemical processes and their influence on the key Solutes of Concern (SoC) associated with the acidification of sediments in Big Swamp and their fate and transport in solution within Big Swamp and Reach 3 of Boundary Creek are summarised in Table 4.

### Table 4 Summary of geochemical processes and their effect of Solutes of Concern

| Geochemical Process / Solute of Concern / Driver | Change in pH | Change in Oxidation / Reduction Potential | Sorption | Change in Ionic Strength |
|---|---|---|---|---|
| Alkalinity | Primarily driven by dissolved bicarbonate and carbonate. Change in pH affects dominance of these species and provides buffering capacity at more alkaline pH. Bicarbonate forms carbonic acid under low pH (<4.3), which also results in providing buffering capacity with respect to increase of pH. | Not directly affected by changes in redox conditions. | Generally does not participate directly in sorption reactions. | May increases overall alkalinity due to increased concentration of non-carbonate solutes. |
| Aluminium | Solubility primarily affected by pH, with highest solubility under acidic and alkaline conditions and lowest over a pH range 6.5 to 8. | Not directly affected by changes in redox conditions. | Generally not subject to sorption when pH is low (<4.5) but forms sorption sites as pH increases due to precipitation of Al-hydroxide and oxides. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competition for sorption sites. |
| Arsenic | Solubility is affected by pH, with highest solubility under acidic conditions and lower under neutral conditions. | As occurs in two primary oxidation states (3+ and 5+) in solution within surface and groundwater and is therefore sensitive to changes in redox conditions. | Sorbs strongly onto ferric iron hydroxide surfaces but is soluble when ferrous iron is stable in solution and subject to limited sorption under such conditions. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competition for sorption sites. |
| Copper | Solubility is affected by pH, with highest solubility under acidic conditions and lower under neutral conditions. | Cu occurs in two primary oxidation sates (1+ and 2+) in solution within surface and groundwater and is therefore sensitive to changes in redox conditions as the solubility of the redox species differs. | Readily sorbed onto clay minerals but shows limited sorption onto iron hydroxide and some organic matter and as such shows different sorption behaviour to other cations. | Effectiveness of sorption mechanisms is less affected by increasing salinity due to preference for specific sorption sites and ready preference sorption onto such sites when present. |
| Ferric Iron | Solubility is strongly affected by pH with solubility higher under strongly acidic conditions but decreasing rapidly as pH increases above 5. | Sensitive to changes in redox conditions, dominating the total iron concentration under oxidising conditions. | Generally not subject to sorption when pH is low (<3.5) but forms sorption sites as pH increases due to precipitation of Fe-hydroxide and oxides. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competion for sorption sites. |

| Geochemical Process / Solute of Concern / Driver | Change in pH | Change in Oxidation / Reduction Potential | Sorption | Change in Ionic Strength |
|---|---|---|---|---|
| Ferrous Iron | Solubility is strongly affected by pH with solubility higher under acidic conditions but decreasing rapidly as pH increases above 5. | Sensitive to changes in redox conditions, dominating the total iron concentration under moderate reducing conditions. Co-precipitates with sulfide as iron sulfide minerals form under strongly reducing conditions, forming primary acid source minerals. | Can sorb but significance is generally low when pH is low (<3.5) but even when sorbed can lead to subsequent acid formation when oxidised, forming retained acidity or co-precipitate with sulfide under strongly reducing conditions forming primary acid source minerals. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competition for sorption sites. |
| Lead | Solubility primarily affected by pH, with highest solubility under acidic and alkaline conditions and lowest under neutral pH. | Not directly affected by changes in redox conditions. | Generally not subject to sorption when pH is low (<4.5) but readily sorbs to cation sorption sites as pH increases. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competition for sorption sites. |
| Molybdenum | Solubility primarily affected by pH, with highest solubility under acidic and alkaline conditions and lowest under neutral pH. | Not directly affected by changes in redox conditions. | Generally not subject to sorption when pH is low (<4.5) but readily sorbs to cation sorption sites as pH increases. | Effectiveness of sorption mechanisms decreases with increasing salinity due to increased competition for sorption sites. |
| Sulfur | Not sensitive to changes in in pH but can be removed from solution by co-precipitation under more neutral pH. | Sensitive to changes in redox conditions due to the occurrence of multiple oxidation states in solution. The most common form is sulfate under oxidising conditions, with this species generally remaining soluble. Under strongly reducing conditions sulfide is the dominant species and is readily removed from solution by co-precipitation with inorganic cation, most commonly iron or emission as gaseous phase ($HS^-$ and $H_2S$). | Generally not subject to sorption. | Generally not sensitive to salinity. |

| Geochemical Process / Solute of Concern / Driver | Change in pH | Change in Oxidation / Reduction Potential | Sorption | Change in Ionic Strength |
|---|---|---|---|---|
| Bacteriological Activity | Sensitive to pH, with metabolic rate decreasing with decreasing pH and insignificant at pH<4. Also sensitive to fluctuations in pH due to lag time in increasing metabolic rate in response to the occurrences of more favourable conditions. Metabolic activity most effective and efficient under stable and favourable pH conditions. | Sensitive to redox, with metabolic rate decreasing with changes in redox potential due to lag time in increasing metabolic rate in response to the occurrences of more favourable conditions. Metabolic activity most effective and efficient under stable redox conditions. | Metabolic activity not directly affected by sorption, but can decline when co-precipitation of sorbed phases occurs as a result of covering of the biofilms on mineral surfaces subject to mineral precipitate formation. | Some sensitivity to changes in salinity, with metabolic rate most effective and efficient under stable conditions. |
| Notes: | 1. This summary is general in nature and no specific studies of the Big Swamp and Reach 3 of Boundary Creek environment have been undertaken to specifically study the site specific geochemical process affecting the fate and transport of the solutes of concern. | | | |

# 5. Geochemical modelling

This section of the report describes the modelling package used (VISUAL MINTEQ) and outlines the input data and modelling methodology.

## 5.1 Modelling methodology

This section provides a general outline of the approach and methodology adopted for the development of the modelling for this project.

### 5.1.1 General considerations

Modelling a geochemical system requires a clear understanding of the objectives and purpose of the model with respect to the environmental problem to be addressed. This allows the modelling to focus on key issues and begin identifying those processes that are likely to be controlling the behaviour of a geochemical system. Clearly understanding the objectives and purpose also allows for selection of an appropriate approach. In general the objectives and purpose of geochemical modelling can be divided into four broad categories of increasing sophistication, with the level of sophistication adopted generally dependent on the limitations of the available data. The four categories of geochemical modelling can be summarised as follows:

| Modelling Category | Typical questions to be answered |
|---|---|
| 1 Scenario Analysis | • Will reactive process be constrained by kinetic or transport considerations?<br>• What is the maximum rate at which reactive buffering capacity can be depleted?<br>• What are the bounding cases for the system in question? |
| 2 Data Interpretation (laboratory/field) | • Are downstream concentrations the result of chemical attenuation or dilution?<br>• What is the overall rate of a reactive process in the system?<br>• Is local thermodynamic equilibrium a reasonable assumption?<br>• Which reactive processes dominate fate and transport of solutes (solubility, complexation, sorption, colloid transport, etc.)? |
| 3 Procedural Design | • Can the geochemical processes be reliability simulated to support development of a solution to the environmental problem?<br>• Can the geochemical processes be quantitatively simulated to support the design of the remediation system or rehabilitation method that solves the environmental problem? |
| 4 Performance Assessment / Risk Analysis | • At what rate and over what time will an environmental problem occur and persist?<br>• Will the environmental problem pose an unacceptable risk to the beneficial uses of the environment and over what period will this risk to beneficial uses persist at an unacceptable rate?<br>• Can the effectiveness of the remediation or rehabilitation solution developed be reliably and defensibly simulated by the model? |

The majority of environments in which geochemical processes occur are very complex and the features that characterise the hydrological, hydrogeochemist and chemical properties of such systems are also subject to a great deal of spatial and temporal variance.

While geochemical models and theoretically simulate large and complex systems doing so requires a large data set of spatial and temporal data supported by extensive laboratory and flied experimental information. Therefore, the vast majority of geochemical modelling that is conducted required a number of simplifying assumptions and incorporate less details as this will provide results that are more transparent and thereby more easily understood than a complex model.

In general any geochemical model is only truly useful as a predictive tool if the results produced by the model can be verified by data collected form the environment being simulated. In reality, this objective is difficult to achieve for simple models and almost impossible for complex models due to the complexity of natural systems, the inadequacy of field data, and uncertainty relating to how the system will change over time. As a result, any geochemical model can be considered as being constrained by definition and represents a simplification of reality. Therefore, any results produced by the model must be considered as a heuristic tool rather than a source of absolute quantitative fact.

Notwithstanding these limitations of geochemical models, the results produced can provide a degree of predictive success when applied as sub-units within a larger stochastic framework where we can estimate the probability that a forecast may be judged to be true or false. The stochastic approach sits at the core of risk assessment and as such proves a useful means of supporting decision making in the context of uncertainty and lack of specific knowledge of the environment being studied.

In situations where the level of detail required is uncertain from the outset, or situations where there is insufficient data to support the development of a fully representative geochemical model, the most rational and defensible approach is to simplify the system to some specific scenarios for which there is sufficient data to allow for a defensible simulation to be made. The first step in the development of the modelling approach is to assess the CGM in the context of the specific environmental process that requires simulation.

The objective of the CGM is to allow identification of those geochemical processes that are of primary importance and neglect those that are of only minor importance and then develop a geochemical model that considers the primary processes. All geochemical models are based upon principles of mass conservation (mass balance accounting). Mass is neither created nor destroyed in the system, but transferred between solid, aqueous, and gaseous phases.

Geochemical models fall into two distinct categories:

1. Models that do not consider transport processes are referred to as geochemical reaction models.
2. Models that consider both transport processes and geochemical reactions are referred to as coupled transport and reaction models.

### 5.1.2 Conceptual and mathematical formulation of modelling approach

The starting point of any geochemical model development is the CGM, such that one described in Section 4. Geochemical Reaction Models (GRM) are mathematically distinct from Coupled Transport and Reaction Models (CTRM). However, GRMs are not conceptually decoupled from transport considerations and extensively used to evaluate the chemistry of surface and groundwater systems where transport play an important role in the fate and transport of solutes of concern.

GRMs can be used to study geochemical changes and processes that explain the observed changes in solute of concern concentration along flow path. In such uses the GRM is used as an inverse model that attempts to establish reaction mechanisms that explain measured chemical changes that occur as water composition evolves along a flow path. Inverse application of a GRM allows for verification of the model simulation results against the field data collected, which allows for a direct assessment of the robustness and defensibility of the models ability to simulate the geochemical processes of interest occurring in the environment being studied.

GRM's can also be used predict future solute composition in a surface or groundwater as a result of geochemical process considered to be active or to occur at some future point in time. This application of GRMs is considered forward modelling. Forward modelling is generally used to support design studies for the development of remediation or rehabilitation solutions to environmental problems.

The third GRM type is the reaction path model or mass transfer model. Reaction path models can simulate dynamic systems through simulation of changes in dissolved and solid phase mineral composition changes over time with respect to incremental dissolution of target minerals. Reaction path models calculate the dissolved phase mineral composition and secondary mineral precipitation in response to dissolution of a specified target mineral to maintain equilibrium conditions. These model types are used to evaluate the chemical weathering processes that occur in natural systems (diagenetic processes) or to assess the geochemical processes with rehabilitation of environmental problems that involve the use of inorganic treatment minerals. As reaction path models simulate changes through dissolution of primary minerals in a stepwise manner, the variable of time is not included implicitly in the calculations. However, where kinetic reaction rate data is available his can be utilised to relate reaction progress to time and allow calculation of dissolved phase mineral composition as a function of time in a kinetic geochemical reaction model.

All geochemical models require that the reactions included in the simulation must be defined in terms of a set of basis components, which constitute the minimum set of fundamental species that are required to describe all the free and derived species (complexes) present in the aqueous solution.

Most GRM's are based upon an approach in which the conservation of total component concentrations is combined with a description of chemical equilibrium. Chemical equilibrium may be computed in terms of Gibbs' free energy minimisation or in terms of mass action equations involving equilibrium constants. The method of Gibbs' free energy minimisation is generally regarded as being more mathematically robust than the method using equilibrium constants. However, due to a lack of reliable and internally consistent Gibbs' free energy data geochemists have tended to favour the equilibrium constant method and the overwhelming majority of programs available today are therefore based upon this approach.

### 5.1.3 Numerical solution procedures

Geochemical model whether GRMs or CTRMs utilise mathematical formulation (involving equilibrium constants) that create a system of non-linear algebraic equations that are solved using a numerical methods. Most GRMs and CTRMs use a modified Newton-Raphson technique to solve the equations as this represents a fast and reliable procedure in most situation that are simulated. Given that the numerical solution utilises an iterative method, convergence problems may arise if the initial values of unknown variables are not sufficiently close to the equilibrium values. Most current programs incorporate heuristic methods to overcome convergence problems.

Other issues that can arise in numerical simulations can occur in situations where the modelling involved systems that contain multiple phases of the same constituents (i.e. containing gases or minerals as well as water) and where the number of phases exceeds that allowed by the Gibbs' Phase Rule, which can lead to development of a singular matrix in the mathematical formulation of the model and results in failure to find a solution. The best means to avoid the formation of a singular matrix is the development of a robust and defensible CGM and carefully selected input parameters.

### 5.1.4 Uniqueness of geochemical model predictions

An important consideration when using geochemical modelling results to support decision making is uniqueness of the solution provided by the numerical simulation. In general, numerical solutions to the general multicomponent equilibrium problem are unique under conditions of ideality (i.e. dilute concentrations) when the problem is posed in terms of mass balance constraints only. Therefore, this only corresponds to problems where the equilibrium speciation is to be calculated for a solution of known bulk composition.

However, in many situations the simulations mass balance constraints (constraints on fluid bulk composition) are combined with mass action constraints. Mass action constraints include fixed pH, pe, and individual species activity, as well as assumptions of gas and mineral equilibrium. Therefore, in simulations that involve mixed mass balance and mass action constraints the consequent solutions are not always unique even in thermodynamically ideal systems.

This can result in multiple solutions that meet to the objectives of the study and satisfy the problem under study equally well in a mathematical sense. However, some non-unique solutions may not be physically realistic. The mathematical solutions that are not physically realistic are often referred to as metastable equilibria.

Therefore, care is required in interpretation of results derived by model simulations that have non-unique solutions and reference back to the CGM is required in such situations. Under conditions of non-ideality, the uniqueness proofs are also found to be invalid as even an unrealistic and / or non-representative solution can be validated by field data.

### 5.1.5 Processes simulated

Most numerical simulation packages allow for precipitation and dissolution of mineral, dissolution of gases, as well as the possibility of fixing the activity of specified. Reaction types that can be simulated by the numerical models include complexation, ion-exchange, redox reaction, precipitation/dissolution, surface complexation, and other kinds of adsorption.

However, the ability of the numerical model to simulate all processes that the model is capable of considering is usually limited by the quality and quantity of the thermodynamic data available for carrying out reaction calculations. Geochemical simulation models contain databases of relevant aqueous, gaseous, and mineral phase reactions, select mineral or gaseous phases that are likely to precipitate and include them in the calculations. Some geochemical models can simulate titrations, evaporative processes, mixing of different solutions, or perform isotope mass balances. Mass balances based upon radiogenic isotopes are used primarily for estimating the age of groundwater. Geochemical models that simulate mass balances that consider stable isotopes are used to understand the source of a water, or processes that may have influenced the chemical properties of the water over time.

In general application models calculate the activities of aqueous species using the following equations:

- Davies equation
- Debye-Hückel equation
- The extended Debye-Hückel equation

These equations limit the applicability of geochemical model simulations to solutions that have an ionic strengths less than or equal to that of seawater. For simulation of highly saline solutions, such as brines, the Pitzer method for activity calculation can be used. However, simulation of highly saline solutions is limited by a lack of reliable data, particularly for redox sensitive species.

Some geochemical models include numerical routines to simulate kinetically mediated geochemical processes. However, in order to simulate kinetic processes in a robust and defensible manner site specific kinetic data is required and in some instances the kinetic reaction equations themselves need to be entered into the model. Therefore, the applicability of kinetic reaction simulations is generally limited by a lack of relevant representative data. Kinetic reactions models use different numerical methods to those applied to equilibrium systems.

### 5.1.6 Summary of modelling approach adopted

For this project the geochemical modelling was completed using the following approach:

- Qualitative assessment of geochemical processes to be considered in the model based on the conceptual geochemical model.
- Adoption of an equilibrium numerical simulation approach in the absence of sufficient data to inform a kinetic numerical simulation approach.
- Adoption of the Debye-Hückel equation for the numerical equilibrium simulation due to the greater stability of the numerical equation solution for the solutes present in the surface water, pore water and groundwater samples collected and analysed.
- Adoption of an iterative simulation approach for the study of the geochemical processes associated with the potential remediation and rehabilitation options under consideration.
- Developing a model for Big Swamp based on the geochemical processes relevant for the management and remediation options under consideration for rehabilitation.
- Developing a model for Reach 3 of Boundary Creek based on the geochemical processes relevant for the management and remediation options under consideration for improvement of the environmental condition for Boundary Creek downstream of Big Swamp.

A range of hydrogeological and hydrogeochemical conditions as anticipated at the site, or published in the scientific literature, were used to create the models. The models used the maximum measured solute concentrations and utilised a thermodynamic equilibrium model (MINTEQ).

## 5.2 Modelling package

The purpose of the VISUAL MINTEQ modelling package is to provide a tool to assist in the assessment of inorganic compounds and heavy metals in groundwater environments. The model assists in establishing which geochemical processes may be occurring in a geological system and provide insight into the fate of dissolved inorganic solutes present in surface and groundwater environments. The model allows for the most significant chemical reaction and attenuation processes, including:

- Precipitation and dissolution of minerals: Precipitation is the process by which dissolved ions combine via chemical process to form solids. This removes dissolved ions from solution. Dissolution is the process by which solids dissolve, adding dissolved ions to solution.
- Sorption of dissolved ions: Electrically charged surfaces occur on solids in virtually all groundwater systems. In addition, charged dissolved ions occur in the groundwater. Depending on the groundwater environment, the charged surfaces attract positively or negatively charged, dissolved ions. This process removes the charged dissolved ion from solution on a permanent or temporary basis. Sorption processes are reversible, should the environmental condition of groundwater vary. This reversibility can lead to retardation of many dissolved ions, by temporarily removing them from solution.
- Oxidation reduction processes: A number of dissolved ions can occur in more than one oxidation state. For some of these their solubility and / or charge can depend on the oxidation state and therefore control the mobility of that ion.

The data required to predict the equilibrium composition consists of a chemical analysis of the geochemical system to be modelled. This provides total dissolved concentrations for the solutes of interest and the associated geochemical processes that govern their behaviour in the aquatic environment, possibly (but not necessarily) including pH, Eh, or the partial pressures of one or more gases as well.

MINTEQ has an extensive thermodynamic database that is adequate for solving a broad range of problems without need for additional user-supplied equilibrium constants.

The application of a geochemical equilibrium model to an environmental problem involves four steps:

1. Formulate one or more precise and relevant chemical questions that can be answered if one knows the equilibrium composition of the system.
2. Pose the chemical questions to the model in terms of those symbols and formats that it is programmed to understand and from which it may interpret a mathematical problem.
3. Use the geochemical equilibrium model software (in this case, MINTEQ) to solve the mathematical problem.
4. Interpret the output from the model in terms of the original environmental problem.

The first step is almost always the most difficult; the ability to do this well is not obtained from reading a user manual, but by understanding the hydrogeochemical processes active in the groundwater system being studied. Therefore the development of a sound and defensible conceptual geochemical model is a prerequisite to for the development of representative numerical simulation models.

## 5.3 Input data

The model was used to assess the geochemical processes that are likely to be associated with the proposed management and remedial options under consideration for Big Swamp and Reach 3 of Boundary Creek. As surface and groundwater sampling to date is limited, statistical analysis of the data to develop a defensible range of input parameter for the models could not be undertaken. As such, a conservative approach using maximum values was adopted to develop the model input parameters. MINTEQ uses the environmental parameters including pH and oxidation reduction potential as well a major cation / anion and trace element information to establish solute solubility, oxidation reduction reactions and adsorption effects. Geochemical processes for Big Swamp and Reach 3 of Boundary Creek were assessed separately using the available groundwater data for Big Swamp and surface water data for Reach 3 of Boundary Creek included in the Jacobs (2018) report.

The following approach was used for the modelling:

1. Develop model input data list, refer to Table 5 and Table 6
2. Assess validity of equilibrium assumption by running the model.
3. Assess metal mobility in the various environmental conditions identified in the area around the site.

### Model input data

The model input data for the Big Swamp and Reach 3 of Boundary Creek Models is summarised in Table 5 and Table 6.

**Table 5 Summary of MINTEQ input data for Big Swamp Model**

| Parameter | Value / range | Comments |
|---|---|---|
| **Environmental** | | |
| Temperature | 15°C | Based on data from Jacobs (2018) report. Cooler temperatures would result in higher solubility of carbonate minerals and lower solubility for non-carbonate minerals. |
| Activity Co-efficient Estimation | Debye–Hückel Equation | The most applicable equation for calculated TDS |
| pH | Calculated | This parameter was not fixed and was calculated by the model based on the solute concentration and redox conditions. |
| Eh | 900 mV | Based on the value feasible with all solutes remaining in solution. This input parameters was established by adjustment until all solutes remained in solution. |
| **Dissolved ions** | | |
| Ammonia | 0.41 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Chloride | 25.9 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |

| Parameter | Value / range | Comments |
|---|---|---|
| Ferric Iron | 10.2 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Ferrous Iron | 17.9 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Fluoride | 0.01 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrate | 0.001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrite | 0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrogen | 0.05 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Phosphate | 0.002 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Sulfate | 41.6 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Dissolved Organic Matter | 1.40 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Calcium | 9.23 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Magnesium | 7.40 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Potassium | 0.33 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Sodium | 12.61 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Carbonate | 0.96 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Aluminium | 4.81 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Arsenic | 0.005 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Cadmium | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Chromium | 0.0004 mmol/L | Measured in MW7 (May 2011) |

| Parameter | Value / range | Comments |
|---|---|---|
| Copper | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Lead | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Manganese | 0.0455 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Mercury | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nickel | 0.0147 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Zinc | 0.0229 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Adsorption Reaction Models | - | Due to a lack of data, adsorption processes were not included in the model. The relative importance of sorption processes can be assessed by a process of elimination using the other processes including solubility and oxidation reduction reactions.<br>Overall, sorption was not considered to a significant geochemical process with respect to the modelling objectives |
| Gasses at Fixed Partial Pressures | - | Due to a lack of relevant data processes involving gasses with fixed partial pressures, these were not considered. Given that the focus of the model is the assessment of acid generation and attenuation processes, this omission is not considered to have a significant impact on model results. |
| Oxidation Reduction Reactions | $Fe^{2+}/Fe^{3+}$<br>$NO_2^-/NO_3^-$<br>$NH_4^+/NO_3^-$<br>$HS^-/SO_4^{2-}$<br>$H_3AsO_3/AsO_4$ | These were considered to be the most relevant and significant oxidation and reduction processes that could affect the acid generation and attenuation processes. |

Notes:

1. Bicarbonate entered as equivalent amount of carbonate ion.
2. Chromium entered as equivalent amount of $CrO_4^{2-}$ ion.

### Table 6 Summary of MINTEQ input data for Reach 3 of Boundary Creek

| Parameter | Value / range | Comments |
|---|---|---|
| **Environmental** | | |
| Temperature | 15°C | Based on data from Jacobs report. Cooler temperatures would result in higher solubility of carbonate minerals and lower solubility for non-carbonate minerals. |
| Activity Co-efficient Estimation | Debye–Hückel Equation | The most applicable equation for calculated TDS |
| pH | Calculated | This parameter was not fixed and was calculated by the model based on the solute concentration and redox conditions. |
| Eh | 300 mV | Based on the value feasible with all solutes remaining in solution. This input parameters was established by adjustment until all solutes remained in solution. |
| **Dissolved ions** | | |
| Ammonia | 0.72 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Chloride | 21.4 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Ferric Iron | 0.5 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Ferrous Iron | 1.79 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Fluoride | 0.01 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrate | 0.0002 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrite | 0.001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nitrogen | 0.028 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Phosphate | 0.002 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Sulfate | 7.29 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Dissolved Organic Matter | 0.33 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |

| Parameter | Value / range | Comments |
|---|---|---|
| Calcium | 2.99 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Magnesium | 3.00 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Potassium | 0.15 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Sodium | 6.96 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Carbonate | 2.55 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Aluminium | 2.78 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Arsenic | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Cadmium | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Chromium | <0.0001 mmol/L | Measured in MW7 (May 2011) |
| Copper | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Lead | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Manganese | 0.0051 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Mercury | <0.0001 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Nickel | 0.0037 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Zinc | 0.0229 mmol/L | Maximum value measured in the two groundwater sampling rounds conducted. |
| Adsorption Reaction Models | - | Due to a lack of data, adsorption processes were not included in the model. The relative importance of sorption processes can be assessed by a process of elimination using the other processes including solubility and oxidation reduction reactions.<br>Overall, sorption was not considered to a significant geochemical process with respect to the modelling objectives |

| Parameter | Value / range | Comments |
|---|---|---|
| Gasses at Fixed Partial Pressures | - | Due to a lack of relevant data processes involving gasses with fixed partial pressures, these were not considered. Given that the focus of the model is the assessment of acid generation and attenuation processes, this omission is not considered to have a significant impact on model results. |
| Oxidation Reduction Reactions | $Fe^{2+}/Fe^{3+}$<br>$NO_2^-/NO_3^-$<br>$NH_4^+/NO_3^-$<br>$HS^-/SO_4^{2-}$<br>$H_3AsO_3/AsO_4$ | These were considered to be the most relevant and significant oxidation and reduction processes that could affect the acid generation and attenuation processes. |

Notes:
3. Bicarbonate entered as equivalent amount of carbonate ion.
4. Chromium entered as equivalent amount of $CrO_4^{2-}$ ion.

Limited environmental parameter (pH, Eh) data was available for some monitoring rounds and both showed variability over the monitoring period. Major ion data was only available for the May and August monitoring events reported by Jacobs (2018). Therefore, in interpreting the model results it must be acknowledged that:

- The data set does not reflect all temporal changes in environmental parameters such as pH, Eh and temperature.
- That the data set does not show all parameters at 'one moment in time' for sequential monitoring rounds conducted over several years.

Both of these factors can increase the uncertainty around the model results generated and have to be factored into the data interpretation and conclusions drawn.

### 5.3.1 Validity of equilibrium assumption

An initial run of the Big Swamp and Reach 3 Boundary Creek data indicates that most soluble mineral phases would remain in solution, with some aluminium and iron hydroxides predicted to precipitate. Mass distribution output show 100% of sulfate remains in solution and with the majority as the dissolved iron remaining in solution present in ferrous oxidation state. However, the model suggests that some aluminium and the majority of ferric iron would precipitate. This indicates that the acid is being exported from Big Swamp as the precipitation of these minerals would lead to secondary acidification processes occurring in Reach 3 of Boundary Creek.

## 5.4 Modelling scenario for management and remediation option assessment

This section outlines the modelling methodology adopted to assess the management and remediation options proposed for Big Swamp and Reach 3 of Boundary Creek. The modelling results are discussed in the subsequent Section 5.5

### 5.4.1 Lime dosing of soils in Big Swamp

This model utilised the Big Swamp Thermodynamic model to assess the geochemical processes that would result from addition of a neutralising agent into the soils of Big Swamp. The addition of a neutralising agent and its effect on pore water and groundwater geochemistry was simulated through the addition of lime as a finite solid and progressively increasing the amount of available lime until further addition did not produce further predicted changes in geochemistry.

The results of this model are presented in Appendix A.

### 5.4.2 Return of reducing conditions in Big Swamp

This model utilised the Big Swamp Thermodynamic model to assess the geochemical processes that would result from re-saturation of the swamp sediments. Re-saturation was simulated by using this model to calculate the pH and Eh at which all solutes remain in solution and then progressively decreasing the Eh to simulate the re-formation of reducing conditions and assessing the geochemical processes that may be activated. The modelling steps adopted for this assessment were as follows:

- Eh 900 mV, base model with all solutes in solution
- Eh 800 mV, reduction step 1
- Eh 700 mV, reduction step 2
- Eh 600 mV, reduction step 3
- Eh 500 mV, reduction step 4
- Eh 400 mV, reduction step 5
- Eh 300 mV, reduction step 6
- Eh 200 mV, reduction step 8
- Eh 100 mV, reduction step 9

The results of this model are presented in Appendix B.

### 5.4.3 Lime dosing of water discharge from Big Swamp into Reach 3 of Boundary Creek

This model utilised the Reach 3 of Boundary Creek Thermodynamic model to assess the geochemical processes that would result from addition of a neutralising agent into the surface water discharge from Big Swamp. The addition of a neutralising agent was simulated through the addition of lime as a finite solid and progressively increasing the amount of available lime until further addition did not produce further predicted changes in geochemistry.

The results of this model are presented in Appendix C.

### 5.4.4 Anaerobic treatment system for water discharge from Big Swamp into Reach 3 of Boundary Creek

This model utilised the Reach 3 of Boundary Creek Thermodynamic model to assess the geochemical processes that would result from passing the surface water discharging from Big Swamp through a reducing zone in a vertical flow treatment bed. Treatment was simulated by using this model to calculate the pH and Eh at which all solutes remain in solution and then progressively decreasing the Eh to simulate the re-formation of reducing conditions and assessing the geochemical processes that may be activated. The modelling steps adopted for this assessment were as follows:

1. Eh 300 mV, base model with all solutes in solution
2. Eh 250 mV, reduction step 1
3. Eh 200 mV, reduction step 2
4. Eh 150 mV, reduction step 3

The results of this model are presented in Appendix D.

### 5.4.5 Summary of modelling approach for key geochemical processes for remediation and rehabilitation

The modelling of the key geochemical processes associated with the remediation and rehabilitation options under consideration for Big Swamp and Reach 3 of Boundary Creek are summarised in Table 7.

**Table 7 Summary of key geochemical processes being modelled**

| Element \ Simulation | Lime Dosing of Soil | Return of Reducing Conditions | Lime Dosing of Water Discharge | Anaerobic Treatment System |
|---|---|---|---|---|
| Model Type | GRM | GRM | GEM | GEM |
| Model Application | Fw | Fw | Fw | Fw |
| Solute Activity Simulation Equation | DH | DH | DH | DH |
| Ionic Strength | C | C | C | C |
| Charge Balance Error | C | C | C | C |
| pH | C | F | C | F |
| Eh | F | C | F | C |
| Sorption | NI | NI | NI | NI |
| Speciation | C | C | C | C |
| Redox Couples | C | C | C | C |
| Precipitation | C | C | C | C |
| Gaseous Phases | NI | NI | NI | NI |
| Finite Solids | C | NI | C | NI |

Notes:
1. C: Calculated
2. DH: Debye–Hückel Equation
3. Eq: Equilibrium
4. F: Fixed
5. Fw: Forward
6. GRM: Geochemical Reaction Model
7. Iv: Inverse
8. Kn: Kinetic
9. NI: Not Included

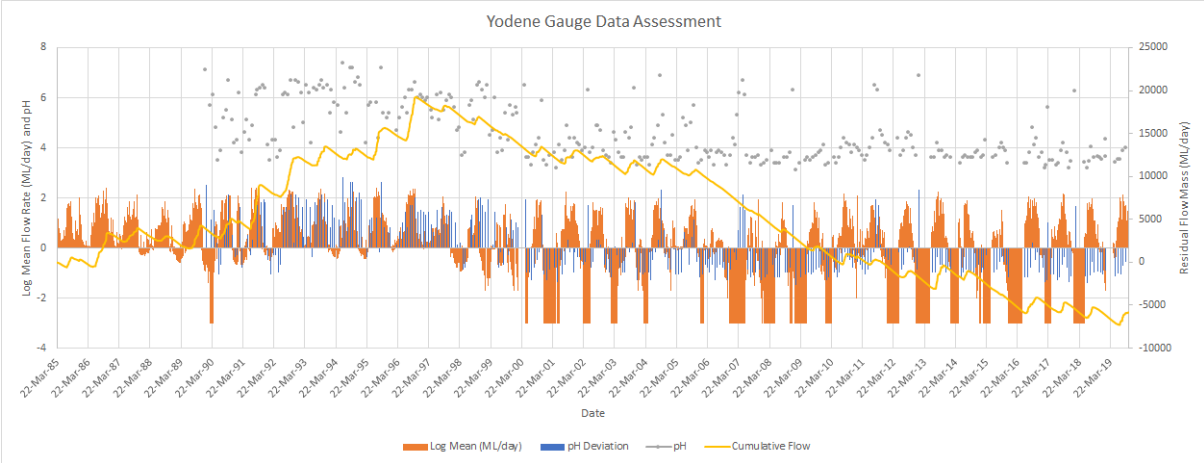
## 5.5 Modelling results and discussion

As set out in Sections 1.1 the primary objective of the geochemical modelling was to assist in evaluation of potential management and remediation options that would improve the environmental values of Big Swamp and Reach 3 of Boundary Creek. This section of the report discusses the modelling results in the context of the available data and the management and remediation options selected for further evaluation.

### 5.5.1 Option O1: True 'do nothing'

Under this option no measures would be taken to meet the project objectives and would rely solely on natural conditions to manage the acidification processes. As Big Swamp and Reach 3 of Boundary Creek currently receive an artificially introduced additional flow of 2ML per day, the historical information on flow and pH, gathered at the Yeodene Gauge was used to assess this option.

For this option the Net Acidity remaining in Big Swamp would continue to leach into the surface water within Big Swamp and discharge into Reach 3 of Boundary Creek. Therefore, use of the historical information available for the Yeodene Gauge was considered to provide relevant data for the evaluation of this option.




**Graph 27 Summary of Yeodene Gauge flow and pH data**

Assessment of the Yeodene Gauge data showed that frequency of occurrences of pH below the long term average of 4.6 increased from early 2000 (refer to Graph 27). The graphical representation of the flow and pH data shows that the frequency of occurrence of pH below the long term average increases after early 2000. This change in frequency appears to coincide with a decline in flow. However, flow decline does not appear to be the only controlling factor for the occurrence of low pH. There are a number of instances where low flow did not coincide with low pH and vice versa.

A statistical assessment of the frequency of pH below the long term average, <3.5 and 4 was undertaken and the results are summarised in Table 8.

**Table 8 Summary of long term pH data trend**

| Period | % pH < long term average (4.6) | % pH < 3.5 | % pH < 4 |
|---|---|---|---|
| 1985 to 2000 | 19% | 0% | 9% |
| 2000 to Jul 2016 | 84% | 10% | 60% |
| Post Jul 2016 | 97% | 31% | 78% |

The results of the three dimensional net acidity model were utilised to assess the total acidity (retained, actual and potential) that remains in Big Swamp (refer to Section 4.1.1) and could be mobilised and enter Reach 3 of Boundary Creek. Based on the Three-Dimensional Model results, the average net acidity present in the swamp sediments that could remain unsaturated was evaluated. However, given the limited data available and the uncertainty in the sediment density, the estimated acid volume is subject to considerable uncertainty. Considering these limitation the sediments that host the net acid mass considered to potentially remain in the unsaturated part of Big Swamp is around 650,000 $m^3$ ± 50% based on the soil volumes, net acidity and the predicted water table elevations.

The time series pH data was used to evaluate the potential amount of acid leaving Big Swamp and migrating into Reach 3 of Boundary Creek down-stream of the swamp. Given the limited data available and the variance in the measured pH the following acid mass flux into Reach 3 of Boundary Creek are subject to considerable uncertainty:

- Acid Flux Leaving Swamp: long term average ~7.2 t/day ± 50% based on pH data recorded Yeodene gauge from 1990 to date.
- Acid Flux Leaving Swamp: Pre 2000 average ~6 t/day ± 50% based on pH data recorded Yeodene gauge from 1990 to 2000.
- Acid Flux Leaving Swamp: Post 2000 average ~7.5 t/day ± 50% based on pH data recorded Yeodene gauge from 2000 to date.

Based on the net acid mass that potentially remains in the unsaturated zone of Big Swamp, the potential mass flux rate into Reach 3 of Big Swamp and the occurrence of asymptotic conditions as a result of the relatively slower oxidation rate of primary acid source minerals, acid flux from the swamp could occur for more than 300 years.

As a final step in the assessment of this remediation option, the variance in pH data in the temporal monitoring data and the relationship to measured acidity was used to evaluate the range in mass flux rate from Big Swamp into Reach 3 of Boundary Creek. Based on the limited data available and the limited temporal frequency the following mass flux rates are subject to considerable uncertainty:

- Low range Acid Flux: 0 t/day
- Median Acid Flux: 1 t/day
- Average Acid Flux: 7.3 t/day
- High range Maximum Acid Flux: 421 t/day

Option 1 was utilised as the baseline scenario as this option represented a passive approach that relied only on natural attenuation processes to deal with the acid generated and solutes of concern mobilised. The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15 (which includes a comparison of the effectiveness of all options).

### 5.5.2 Option O2: Implementation of contingency measures

This option would involve increasing the flow volume into Boundary Creek up-stream of Big Swamp in order to increase the water table elevation in the sediment in Big Swamp. This primary aim of this option is to reduce acid discharge from Big Swamp into Reach 3 of Boundary Creek by increasing the moisture content in the sediments in the swamp that contain primary acid source minerals and reduce acid generation through primary acidification processes. This option is currently being partially implemented through the addition of 2ML/day in surface water flow up-stream of Big Swamp in Reach 1 of Boundary Creek.

Therefore, the effectiveness of this option for the 2ML/day additional flow can be evaluated using the existing recent monitoring data available for the Yeodene Gauge.

Under this option (and to address Options O7 and O8) Jacobs developed two surface water volume addition scenarios and two different surface water flow configurations for each flow scenario were considered, as set out in Section 4.1.1.

For the evaluation of this option as well as Options O7 and O8, the results of the three dimensional net acidity model were utilised to assess the total acidity (retained, actual and potential) that remains in the sediments of Big Swamp and could be mobilised through primary acidification processes and enter Reach 3 of Boundary Creek under the scenarios set out in Section 4.1.1. Based on the model results, the average net acidity present in the swamp sediments that could remain unsaturated was evaluated. However, given the limited data available and the uncertainty in the sediment density, the estimated acid volume is subject to considerable uncertainty. Considering these limitation the sediments that host the net acid mass considered to potentially remain in the unsaturated part of Big Swamp under the scenarios considered are:

- 2ML Day and no Barrier: 650,000 $m^3$ ± 50% depending on density assumption.
- 2ML Day with Barrier: 645,000 $m^3$ ± 50% depending on density assumption.
- 20ML Day with Barrier: 465,000 $m^3$ ± 50% depending on density assumption.

The results for the geochemical modelling scenario for the return of reducing conditions in Big Swamp described in Section 5.4.2 were not used for evaluation of this option due to the availability of field data from the Yeodene Gauge, which was considered preferable to using the projections of a forward GRM.

The time series pH data for the Yeodene Gauge was used to evaluate the potential amount of acid leaving Big Swamp and migrating into Reach 3 of Boundary Creek down-stream of the swamp under various real and simulated flow conditions.

Given the limited data available, the variance in the measured pH and the limited number of modelling scenarios, the following acid mass flux from Big Swamp into Reach 3 of Boundary Creek though surface water flow for this option are subject to considerable uncertainty:

- Acid Flux Leaving Swamp: Post Jul 2006 average ~7.2 t/day ± 50%

Based on the net acid mass that potentially remains in the unsaturated zone of Big Swamp under the two flow scenarios as set out in Section 4.1.1, the potential mass flux rate into Reach 3 of Big Swamp after July 2006 and the potential for asymptotic conditions to occur due to limitations in oxidation rates for potential acid generating primary source minerals, acid flux from the swamp could occur for:

- 2ML Day and no Barrier: 100 years ± 50% depending on density assumption and mass flux variance.
- 2ML Day with Barrier: 80 years ± 50% depending on density assumption and mass flux variance.
- 20ML Day with Barrier: 50 years ± 50% depending on density assumption and mass flux variance.

A key limiting factor in the assessment of this option is the limited amount of temporal data from relevant monitoring points that is available, which results in any source mass, mass flux and timeframes evaluated being subject to considerable uncertainty.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.3 Option O3: Direct treatment of soils with neutralising agents

This option would involve placement of a neutralising agent, such as granular lime, onto the surface of the swamp sediments to provide neutralising capacity to Big Swamp. This options would represent the lowest cost means of adding neutralisation capacity to the sediments in Big Swamp and target primarily dissolved phase acidity in the Surface Water system of Big Swamp.

The addition of lime would result in dissolution of CaO and / or $Ca(OH)_2$ , the common mineral constituents of lime. Dissolution of lime is described by the following reactions:

$$CaO_{(s)} + H2O_{(l)} \rightleftharpoons Ca(OH)_2$$

$$Ca(OH)_2 \rightarrow Ca^{2+} + 2OH^-$$

The release of hydroxide into solution would result in an increase in pH and the addition of solid lime to the sediment surface would increase the pH of the shallow sediments in the swamp.

Initially the rate of pH increase will be limited as the rapid solubilisation of Retained Acid and Actual Acid will occur at a similar or higher rate than the lime dissolution rate. Consequently, while the lime dissolution occurs there are likely to be acid flush events, although at a lower magnitude than if lime was not added.

Once the majority of the retained and actual acid is flushed, pH of the surface soils is likely to increase significantly and remain high until the potential acid generating primary acid forming materials that remain are flushed. This is due to the oxidation rate of disulfide minerals being slower than the lime dissolution rate.

However, as the pH increases ferric ion solubility decreases and precipitation of iron chloride hydroxide occurs, which removes hydroxide from solution, as defined by the following equation.

$$Cl^- + Fe^{3+} + 2OH- \rightleftharpoons ClFe(OH)_{2(s)} \text{ (or straight precipitation of } Fe(OH)_3\text{)}$$

To evaluate this option the Lime Dosing GRM described in Section 5.4.1 was utilised. This iterative dissolution model provided predictions of pH and solute of concern changes in response to the stepwise addition of lime as a finite solid. The effectiveness of the lime dosing was assessed by review of the predicted pH and dissolved phase calcium concentration to identify an effective dosing rate to deal with acid present in the surface waters within Big Swamp.

Based on the predicted calcium concentration in solution after lime dissolution (0.01 mol/L) being similar to the measured ferric iron concentration in the swamp (0.001 to 0.011 mol/L), much of the pH increase gained by lime dissolution is removed by precipitation of ferric iron hydroxides and chlorides, which consume the buffering capacity added, without necessarily also buffering the acid generated by the primary acidification processes, as illustrated in the equations included above. The thermodynamic modelling results indicated that pH increase in solution is largely off-set by precipitation of ferric iron minerals.

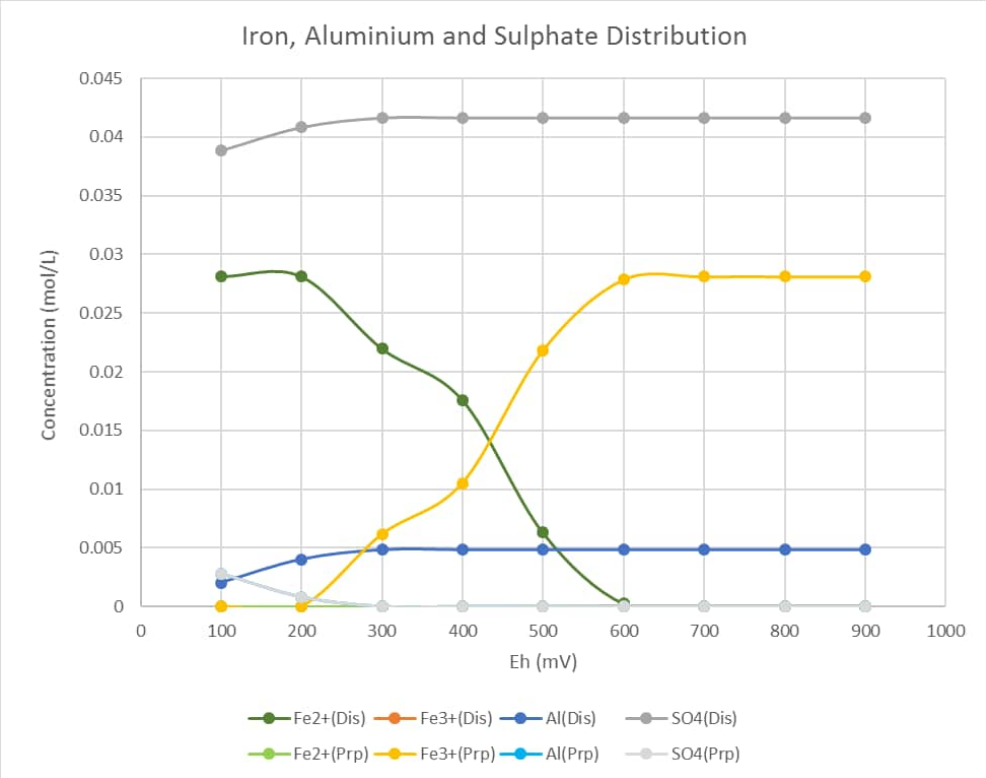
### 5.5.4 Option O7: Flooding of Big Swamp

Under this option a barrier would be built at the down-stream end of Big Swamp to re-flood the swamp (i.e. permanently return to a wetland). The primary aim of this option is to limit further oxidation of potential acid forming primary source minerals through reformation of dominantly reducing conditions in the swamp sediments by increasing moisture content through raising the water table elevation. The primary geochemical processes targeted by this option is the reduction of ferric iron and sulfate, which intends to attenuate acid through precipitation of dominantly iron sulfide minerals and return the swamp to an acid sink.

To evaluate this option the Return of Reducing Conditions GRM for Big Swamp described in Section 5.4.2 was utilised. This iterative reduction model provided predictions of solute of concern changes in response to the stepwise decreases in Eh. The effectiveness of the re-saturation was assessed by review of the predicted inorganic solute phase concentration to identify effectiveness of the option in attenuating solutes of concern and increase pH in the surface water, pore water and groundwater of Big Swamp.

Based on the GRM forward simulation, re-saturation of the sediments in Big Swamp is anticipated to trigger the following geochemical processes:

- The swamp sediments contain high amounts of organic carbon so there should be sufficient carbon source to form and maintain reducing conditions upon re-saturation for the foreseeable future.
- The results of the thermodynamic model based on the staged decrease of Eh support the preliminary results of the Monash study. The model predicted that once reducing conditions dominate the ferric iron present is reduced to ferrous iron and enters solution, while sulfate reduction does not appear to occur to any level of significance. The only removal of sulfate from solution as suggested in the model is precipitation of Aluminium Sulfate. Assessment of the model results showed that solid phase ferric iron would dominate the under the highest oxidising potentials but as reducing conditions form ferric iron is reduced to the ferrous form, which then enters solution. Aluminium would also remain in solution under oxidising and mildly reducing conditions, but as reduction proceeds aluminium solubility decreases, with around 60% of the dissolved aluminium and 7% of dissolved sulfate removed from solution respectively. The solubility of iron, aluminium and sulfate over the modelled Eh range is summarised on Graph 28.




**Graph 28 Summary of iron, aluminium and sulfate concentrations**

The model results suggest that the single most significant limitation to re-formation of acid forming processes through precipitation of iron sulfide minerals is the limited amount of dissolved sulfate in the swamp and the limitation imposed by a lack of effective flushing of the carbonate produced by the reduction of sulfate. This lack of sufficient sulfate for reduction to sulfide to facilitate precipitation of iron sulfides will limit the attenuation of acid through sulfide mineral precipitation. The Monash incubation work and geochemical assessment suggest that the reduction will proceed to the iron reduction stage, leading to ferrous iron in solution and transport out of the swamp, resulting in the export of acidity. These preliminary studies support the model findings, providing an independent line of evidence in regard to the thermodynamic model findings.

One key limitation with respect to understanding of the geochemical processes active in Big Swamp is the lack of kinetic data for the complete oxidation / reduction cycle so reliability of predictions of geochemical processes is limited at this stage.

Based on the geochemical and thermodynamic model the most significant benefit of the re-flooding remediation option would be an increase in water table in the swamp leading to limitation of any potential acidity that remains in the sediments above the historic water table low oxidising and cause further acidification.

The re-saturation of the soils will attempt to move the system behaviour back towards the pre 2000 conditions, however the likelihood of success is limited by the significantly lower sulfate concentrations in the surface water used for the re-flooding than the sulfate concentrations present in the groundwater that migrated through the swamp sediments under the historical flow conditions.

Another aspect considered as part of the re-flooding option is the risk of increased acid flushing events. The re-flooding is likely to lead to an increased risk of acid flushes, which will then abate once the retained and actual acidity is flushed from the system. The interpretation of the historic stream flow and pH data supports this contention.

This interpretation found that the pH in Reach 3 Boundary Creek at the Yeodene Gauge was below the long term average pH (i.e. 4.6):

- Prior to Jan 2000: 19% of measurements
- Post Jan 2000: 86% of measurements, however when splitting this period into the pre 2ML flow addition and post 2ML flow addition the following was observed:
  - Pre 2ML flow addition: 84%
  - Post 2ML flow addition: 97%

  This assessment support the contention that introduction of additional flow is likely to lead to additional acid flushing in the short to medium term, but would reduce the overall acid flux in the long term.
- In the context of acid flushes in response to storm events, this would be situation dependent. The historic record suggests that in the majority of storm events pH was higher during high flow, but there are occasional events where this is not the case. By increasing the saturated volume and inundated area of the swamp there is likely to be an increase in the risk of acid flush events as the retained and actual acidity enters solution leading to acidic conditions in standing water bodies in the swamp. This acid water could then exist the swamp in a first flush event in response to a localised storm event.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.5 Option O8: Managed groundwater levels within Big Swamp

Under this option water levels within the swamp would a managed by use of a series of levees and embankments. To this end the aim of this option is similar to that of Option O3 and O7, in that the aim of this option is to re-saturate the sediments in the swamp to limit the potential for acid generation through the primary acidification processes. As a consequence the GRM used was the same as that used to evaluate Option O7. The geochemical processes associated with this option would also be the same as those already described for Option O7 and are therefore not repeated in this section. The primary difference between this option and Option O7 would be the physical arrangement of the levies used to optimise the increase the water table elevations and re-saturate the sediments across the Big Swamp.

Numerical modelling completed by Jacobs provide groundwater level predictions under a 2 ML/day and 20 ML/day surface flow scenario (with a hydraulic barrier at the lower end of the swamp only). Therefore, the specific effects of a different arrangement of the physical barriers on re-saturation of the sediments on Big Swamp could not be assessed.

The unsaturated sediments and acid flux from the swamp were estimated based on the predicted groundwater levels (refer Option 2 : Section 5.5.2) It is noted that management of the groundwater levels may be done more efficiently at these flows by building small embankments and diversions at different locations along the swamp rather than just at the downstream end. Further numerical groundwater modelling would be required to assess the impacts on groundwater levels (and the reduction of unsaturated swamp area) under a refined embankment system. Therefore, the sediment volumes that contain net acidity with the potential to generate acid is assumed to be the same as for Option O3 and O8.

To evaluate this option the Return of Reducing Conditions GRM for Big Swamp described in Section 5.4.2 was utilised. This iterative dissolution model provided predictions of solute of concern changes in response to the stepwise decreases in Eh.

The effectiveness of the re-saturation was assessed by review of the predicted inorganic solute phase concentration to identify effectiveness of the option in attenuating solutes of concern and increase pH in the surface water, pore water and groundwater of Big Swamp.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.6 Option O9: Soil excavation/treatment and rehabilitation

This option would entail digging up of acid generating sediments in Big Swamp and treating these soils through addition of a neutralising agent to provide buffering capacity for the net acidity (retained, actual and potential) present in the unsaturated sediments. For the purpose of this assessment the neutralising agent applied was assumed to be lime. The chemistry of lime dissolution and the GRM utilised are already discussed under Option O3 in Section 5.5.3 and are therefore not repeated here.

Two scenarios for treatment were considered in the geochemical assessment:

1. Total Treatment of all Net Acidity
2. Treatment of Acid ‘Hot Spots’

Under the total treatment option the three dimensional model of the swamp sediment distribution was used to estimate the total sediment volume present and then using the average net acidity data from the Monash University study to provide a range of values for the lime dosing requirements.

For the 'Hot Spot' treatment option the three dimensional model of the swamp net acidity was used to calculate the lime dosing requirements for a range of progressively increasing net acidity 'Hot Spots'.

The assessment results of the sediment volumes that contain primary acid forming minerals for each of the re-flooding scenarios set out for Option O1 in Section 5.4.1 with results summarised in Table 9. These lime dosing values are subject to considerable uncertainty due the limited data available and the lack of a reliable long term prediction of the water table position in the sediments of Big Swamp.

**Table 9 Summary of lime dosing for net acidity present**

| Volume Scenario | Sediment Volume ($m^3$) | | | Lime Requirement (tonnes) | | |
|---|---|---|---|---|---|---|
| | 2ML/Day No Barrier | 2ML/Day With Barrier | 20ML/Day With Barrier | 2ML/Day No Barrier | 2ML/Day With Barrier | 20ML/Day With Barrier |
| Total Treatment | 610,000 | 600,000 | 435,000 | 135,000 | 133,000 | 96,000 |
| Treatment above 500 mg CaCO3 / kg acidity | 550,000 | 535,000 | 390,000 | 36,000 | 35,000 | 26,000 |
| Treatment above 1500 mg CaCO3 / kg acidity | 65,000 | 62,000 | 45,000 | 13,500 | 13,000 | 9,000 |
| Treatment above 2500 mg CaCO3 / kg acidity | 2800 | 2700 | 1800 | 900 | 870 | 560 |
| Treatment above 3500 mg CaCO3 / kg acidity | 380 | 370 | 250 | 180 | 170 | 105 |
| Treatment above 4500 mg CaCO3 / kg acidity | 100 | 90 | 60 | 55 | 50 | 35 |
| Treatment above 6000 mg CaCO3 / kg acidity | 50 | 50 | 20 | 45 | 40 | 15 |

The volumes and lime dosing rates provided in Table 9 are based on limited geological and geochemical data and are therefore subject to considerable uncertainty. Therefore application of these values in the preliminary remediation design need to be treated with an appropriate amount of caution and conservatism.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.7 Option O10: Deep soil mixing

This option is essentially similar to Option O9 in that a neutralising agent is added to the swamp sediments. However, rather than excavating the sediments and then treating them ex-situ, the sediments are treated in-situ by mixing the neutralising agent into the sediments using a mechanical mixing device.

From a geochemical perspective this option is essentially the same as Option O9 and given the limited data available and the uncertainties associated with the geological and geochemical information currently available this option cannot be distinguished from Option O9 from a geochemical perspective.

The only geochemical differentiator that can be anticipated based on the limited information available is that in-situ mixing is generally less effective than ex-situ methods and therefore some residual acid generation is more likely under this remediation option.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.8 Option O13: In-stream active treatment system

Under this option the surface discharge from Big Swamp into Reach 3 of Boundary Creek would be treated with a neutralising agent to raise pH to acceptable levels and allowing discharge of the treated water after removal of precipitates in an aeration and settlement pond.

Assessment of the geochemical aspects of this option was conducted using the predicted stream flow volumes considered in the hydrogeological model, the treatment volume capacity (up to 4ML/day) and the result of the staged thermodynamic model.

Based on the available stream flow information the following observations were made:

- Stream flows in excess of 4ML/day occur around 34% over the total monitoring period.
- Stream flows in excess of 4ML/day occur around 43% over the monitoring period prior to Jan 2000.
- Stream flows in excess of 4ML/day occur around 27% over the monitoring period post to Jan 2000.

Streamflow's in excess of 4ML/day are likely to occur more frequently than 27% of the time under some of the remediation options considered for Big Swamp, such as re-flooding or increase to flow inputs. Further work and hydrological modelling would be required to establish a more precise estimate of the predicted flow volumes under the various management and remediation options under consideration for Big Swamp.

Based on the observed pH data obtained at the Yeodene Gauge and the relationship between pH and measured acidity in samples collected, the observations made in relation to acid concentrations in the discharge water from Big Swamp entering Reach 3 of Boundary Creek are summarised as follows:

- All data (refer to Table 10)
- Pre 2000 Data (refer to Table 11
- 2000 to Jul 2006 Data (refer to Table 12)
- Jul 2006 to date Data (refer to Table 13)

**Table 10 Summary of acidity in surface water flow – all data**

| Acidity as $CaCO_3$ | Number of Exceedances | Percent of Exceedances |
|---|---|---|
| Acidity >50mg/L | 10343 | 80% |
| Acidity >100mg/L | 10199 | 79% |
| Acidity >300mg/L | 9551 | 74% |
| Acidity >500mg/L | 8746 | 67% |
| Acidity >1000mg/L | 6445 | 50% |

| Acidity as $CaCO_3$ | Number of Exceedances | Percent of Exceedances |
|---|---|---|
| Acidity >1500mg/L | 4165 | 32% |
| Acidity >2000mg/L | 2232 | 17% |
| Acidity >3000mg/L | 173 | 1% |

### Table 11 Summary of acidity in surface water flow – pre 2000 data

| Acidity as $CaCO_3$ | Number of Exceedances | Percent of Exceedances |
|---|---|---|
| Acidity >50mg/L | 3656 | 66% |
| Acidity >100mg/L | 3543 | 64% |
| Acidity >300mg/L | 3103 | 56% |
| Acidity >500mg/L | 2703 | 49% |
| Acidity >1000mg/L | 1626 | 29% |
| Acidity >1500mg/L | 678 | 12% |
| Acidity >2000mg/L | 135 | 2% |
| Acidity >3000mg/L | 0 | 0% |

### Table 12 Summary of acidity in surface water flow – post 2000 data

| Acidity as $CaCO_3$ | Number of Exceedances | Percent of Exceedances |
|---|---|---|
| Acidity >50mg/L | 3656 | 66% |
| Acidity >100mg/L | 3543 | 64% |
| Acidity >300mg/L | 3103 | 56% |
| Acidity >500mg/L | 2703 | 49% |
| Acidity >1000mg/L | 1626 | 29% |
| Acidity >1500mg/L | 678 | 12% |
| Acidity >2000mg/L | 135 | 2% |
| Acidity >3000mg/L | 0 | 0% |

### Table 13 Summary of acidity in surface water flow – post Jul 2006 data

| Acidity as $CaCO_3$ | Number of Exceedances | Percent of Exceedances |
|---|---|---|
| Acidity >50mg/L | 4540 | 91% |
| Acidity >100mg/L | 4512 | 90% |
| Acidity >300mg/L | 4337 | 87% |
| Acidity >500mg/L | 4104 | 82% |
| Acidity >1000mg/L | 3263 | 65% |
| Acidity >1500mg/L | 2383 | 48% |
| Acidity >2000mg/L | 1458 | 29% |
| Acidity >3000mg/L | 109 | 2% |

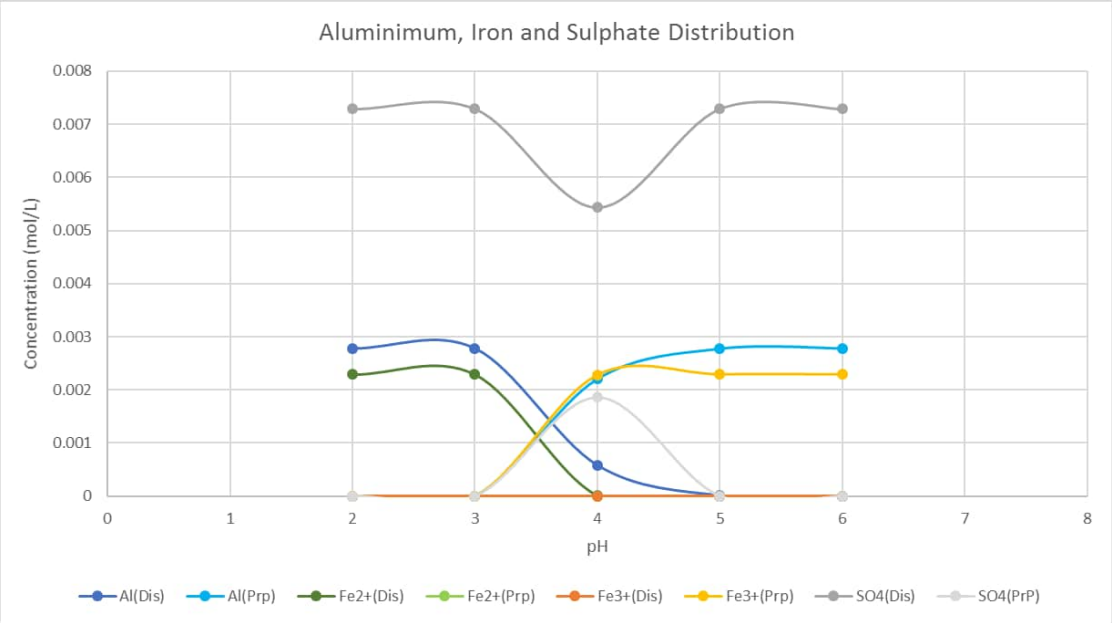
Assessment of the time series data summarised on Table 10 to Table 13 shows that the frequency and intensity of acid flux from Big Swamp into Reach 3 of Boundary Creek increased form early 2000 and intensified further after July 2006, as shown in Graph 27.

To evaluate this option the Lime Dosing GRM for Reach 3 of Boundary Creek described in Section 5.4.3 was utilised. This iterative dissolution model provided predictions of pH and solute of concern changes in response to the stepwise addition of lime to the surface water discharge from Big Swamp into Reach 3 of Boundary Creek as a finite solid. The effectiveness of the lime dosing was assessed by review of the predicted pH and dissolved phase calcium concentration to identify an effective dosing rate to deal with acid present in the surface waters discharge from Big Swamp into Reach 3 of Boundary Creek.

The iterative forward GRM identified a number of geochemical processes that potentially occur in response to addition of lime as neutralising agent to the surface water discharge from Big Swamp. Addition of lime would result in an increase in pH that would lead to precipitation of some minerals. The potential precipitate minerals identified by the GRM are:

- $ClFe(OH)_{2(s)}$ (Predicted by Model) and / or $Fe(OH)_3$ (As observed in Field Studies)
- $AlOHSO_{4(s)}$
- Diaspore (α-AlO(OH)) (Predicted by Model) and / or $Al(OH)_3$ (As observed in Field Studies)
- Nsutite ($Mn_4$+1−x$Mn_2$+x$O_2$-2x$(OH)_{2x}$)
- $FCO_3$-Apatite ($Ca_5(PO_4F_3)$)

The changes in concentration of key solutes of concern (Aluminium, Iron and Sulfate) in solution in response to an increase in pH as a consequence of lime addition are shown on Graph 29. The model suggests that while iron and aluminium are removed from solution, sulfate largely remains soluble, with any removal limited to a specific pH range and to a minor amount.




**Graph 29 Summary of iron, aluminium and sulfate concentrations**

Based on the range of concentrations measured in the stream samples (low, mid and high), the range of flow volumes (low, mid and high) and pH achieved through lime dosing, the following precipitate volumes should be anticipated in the design of the dosing and setting pond:

- pH 2: Minor
- pH 3: Minor
- pH 4: Low 0.3 g/L, mid 0.6 g/L, high 3 g/L
- pH 5: Low 0.8 g/L, mid 1.6 g/L, high 8 g/L

- pH 6: Low 1.6 g/L, mid 3.2 g/L, high 16 g/L

The reagent requirements for specified pH increases, based on the iterative lime addition forward GRM are predicted to result in an increase in TDS, which may result in impacts to the beneficial uses that the water would otherwise be suitable for. Therefore, caution is required in dosing the water discharging from Big Swamp to manage final water quality entering Reach 3 of Boundary Creek to protect beneficial uses of the surface water resource.

The model indicated that once pH reaches 5, minor amounts of calcium that are added as an ion included in the lime minerals is removed from solution by precipitation of FCO3-Apatite, with mineral precipitates removing carbonate from the system. This is likely to reduce the effectiveness of lime dosing in increasing pH and could result in additional precipitate formation, which increases management requirements, for limited additional increase in pH.

Based on the thermodynamic modelling, dosing rates of lime that achieve an increase of pH in would depend on flow rate, with result of the assessment summarised in Table 14.

**Table 14 Summary of lime dosing requirements**

| Flow Rate | 1 pH unit increase (kg) | 2 pH units increase (kg) | 3 pH units increase (kg) |
|---|---|---|---|
| 0.5ML Day | 30 | 40 | 45 |
| 1ML Day | 65 | 75 | 85 |
| 2ML Day | 125 | 150 | 170 |
| 3ML Day | 190 | 225 | 250 |
| 4ML Day | 250 | 300 | 340 |

However, the rates shown in Table 14 are based on very limited data and need to be verified by laboratory and field trials as part of the next stage of works to inform a more detailed design of the treatment system required for implementation of this option.

The effectiveness of this option in achieving management or remediation of the relevant geochemical process aspects for this option are summarised in Table 15.

### 5.5.9 Option O17: Constructed vertical flow anaerobic wetland

The final remediation option considered in the geochemical modelling was the use of a vertical flow anaerobic wetland that comprised an upper layer of organic matter to create reducing conditions followed by a limestone or similar treatment zone designed to provide buffering capacity and neutralise acid.

To evaluate this option the Return of Reducing Conditions GRM for Reach 3 of Boundary Creek described in Section 5.4.4 was utilised. This iterative reduction model provided predictions of solute of concern changes in response to the stepwise decreases in Eh. The effectiveness of the re-saturation was assessed by review of the predicted inorganic solute phase concentration to identify effectiveness of the option in attenuating solutes of concern and increase pH in the surface water of Reach 3 of Boundary Creek.

The interactive forward GRM results suggests that on development of reducing conditions there is limited change to pH within the anaerobic treatment section of the system. The reduction of iron in the anaerobic treatment zone also appears limited and no attenuation of acid was suggested in the model predictions. The only mineral precipitates that form as reducing conditions develop in the anaerobic treatment zone are Metacinnabar and Covellite which result in the removal of mercury and copper from solution. As these ions were only present in trace or

very low concentrations, precipitate clogging of the anaerobic treatment zone of the vertical flow system is not anticipated to be significant. However, the lack of removal of Aluminium and Iron through precipitation in the organic layer allows these solutes to enter the secondary treatment zone, where dissolution of limestone is intended to raise pH.

To evaluate this option the Lime Dosing GRM for Reach 3 of Boundary Creek described in Section 5.4.3 was utilised. This iterative dissolution model provided predictions of pH and solute of concern changes in response to the stepwise addition of lime to the surface water flowing through the limestone treatment zone after treatment in the anaerobic treatment zone as a finite solid. The effectiveness of the treatment by flow the limestone treatment zone was assessed by review of the predicted pH and dissolved phase calcium concentration to evaluate treatment and attenuation of the solutes of concern prior to discharge into Reach 3 of Boundary Creek.

Given the limited removal of acid, aluminium and iron as suggested by the model, the performance of the limestone layer is anticipated to be similar to that of the in stream active treatment system with respect to geochemical processes. The key difference between the two remediation methods is that the organic layer intends to convert ferric iron to the ferrous iron form allowing the ion to migrate into the limestone treatment zone in the more soluble iron from, which should limit the occurrence of iron precipitation in the limestone treatment zone which causes clogging and armouring and reduces the effectiveness of the limestone treatment zone.

However, the formation of aluminium precipitates in response to the increase in pH as predicted in the model for Option O13 would occur within the limestone treatment layer causing clogging and armouring of the limestone reducing the effectiveness of this treatment layer and decreasing the efficiency and effectiveness of the treatment system.

Given the uncertainties that resulted from the limited data available and the overall modelling limitations and given the thermodynamic modelling results, the aeration and settling pond requirements for this remediation option would be similar to those of Option O13.

Additional information based on further monitoring and pilot trials, followed by geochemical modelling would be required to support the more detailed design phase should this remediation option be considered further.

## 5.6 Effectiveness of management and remediation option considered

The results of the GRMs were utilised to assess the potential effectiveness of the management and remediation options under consideration with respect to the key geochemical processes and the fate and transport of solutes of concern, with results summarised in Table 15 based on the assessment and discussion set out in the previous section.

**Table 15 Summary of effectiveness of geochemical processes**

| Remediation Option / Geochemical Process Targeted | Option 1: Do Nothing | Option O2: Implementation of contingency measures | Option O3: Direct treatment of soils with neutralising agents | Option O7: Flooding of Big Swamp | Option O8: Managed groundwater levels within Big Swamp | Option O9: Soil excavation/ treatment and rehabilitation | | Option O10: Deep soil mixing | Option O13: In-stream active treatment system | Option O17: Constructed vertical flow anaerobic wetland |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | All | Hot Spot | | | |
| Remove Primary Acid Source Minerals from Sediments in Big Swamp | 🔴 | 🔴 | 🔴 | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Prevent Further Oxidation of Primary Acid Source Minerals in Sediments of Big Swamp | 🔴 | 🟡 | 🔴 | 🟡 | 🟡 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Neutralise Acidity Generated by Primary Acidification Process in Surface Water of Big Swamp | 🔴 | 🔴 | 🟢 | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Neutralise Acidity Generated by Primary Acidification Process in Pore-Water and Groundwater of Big Swamp | 🔴 | 🔴 | 🟡 | 🟠 | 🟠 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Neutralise Acidity Generated by Secondary Acidification Process in Surface Water of Big Swamp | 🔴 | 🔴 | 🟠 | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Neutralise Acidity Generated by Secondary Acidification Process in Pore-Water and Groundwater of Big Swamp | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟡 | 🟡 | 🔴 | 🔴 |
| Neutralise Acid Discharged from Big Swamp into Reach 3 of Boundary Creek | 🔴 | 🔴 | 🟡 | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🟢 | 🟡 |
| Neutralise Acidity Generated by Secondary Acidification Process in Surface Water of Reach 3 of Boundary Creek | 🔴 | 🔴 | 🔴 | 🔴 | 🔴 | 🟡 | 🟡 | 🟡 | 🟡 | 🟡 |
| Attenuate Aluminium through Precipitation of Mineral Species | 🔴 | 🔴 | 🟡 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟡 | 🟢 |
| Attenuate Aluminium through Sorption | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Arsenic through Precipitation of Mineral Species | 🔴 | 🔴 | 🟡 | 🟡 | 🟡 | 🟢 | 🟢 | 🟢 | 🟡 | 🔴 |
| Attenuate Arsenic through Sorption | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Copper through Precipitation of Mineral Species | 🔴 | 🔴 | 🟠 | 🟡 | 🟡 | 🟢 | 🟢 | 🟢 | 🟡 | 🟠 |
| Attenuate Copper through Sorption | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Ferric Iron through Precipitation of Mineral Species | 🔴 | 🔴 | 🟢 | 🔴 | 🔴 | 🟢 | 🟢 | 🟢 | 🟡 | 🟠 |
| Attenuate Ferris Iron through Sorption | 🔴 | 🔴 | 🟡 | 🔴 | 🔴 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Ferrous Iron through Precipitation of Mineral Species | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟡 | 🟠 |
| Attenuate Ferrous Iron through Sorption | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Lead through Precipitation of Mineral Species | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🟢 | 🟢 | 🟢 | 🟡 | 🟠 |
| Attenuate Lead through Sorption | 🔴 | 🔴 | 🟢 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Molybdenum through Precipitation of Mineral Species | 🔴 | 🔴 | 🟢 | 🟡 | 🟡 | 🟢 | 🟢 | 🟢 | 🟡 | 🟠 |
| Attenuate Molybdenum through Sorption | 🔴 | 🔴 | 🟢 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Sulfur through Precipitation of Mineral Species | 🔴 | 🔴 | 🟠 | 🟠 | 🟠 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |
| Attenuate Sulfur through Sorption | 🔴 | 🔴 | 🟠 | 🔴 | 🔴 | 🟢 | 🟢 | 🟢 | 🟠 | 🟠 |

Notes:
1. 🟢 = Likely to be effective
2. 🟡 = Possibly effective
3. 🟠 = May be effective
4. 🔴 = Unlikely to be effective

# 6. Conclusions

Based on the data review and geochemical modelling the following conclusions can be drawn from the Basic Hydrogeochemical Model:

## 6.1 Formation mechanism

- Big Swamp is an inland ASS system that appears to have formed as a result of long term groundwater seepage, possibly related to the interface zone where the regional LTA aquifer becomes confined by an overlying aquitard.
- The combination of swampy conditions in which organic matter accumulated creating strongly reducing conditions into which the groundwater seepage fed sulfate resulting in reduction of the sulfate to sulfide that led to precipitation of sulfide minerals, forming the primary acid source minerals.
- Over time this system led to accumulation of a stock of primary acid source mineral in the swamp sediments.

## 6.2 Geochemical process under natural flow conditions

- Under natural flow conditions, the swamp sediments were saturated the majority of the time, which maintained reducing conditions which kept the primary source minerals stable and limiting the generation of acid discharge form Big Swamp.
- Under natural dry conditions when surface flow and groundwater seepage rates slow, the water table in the swamp declined and some sediments became unsaturated, leading to oxidation of primary acid source minerals and acid discharge from Big Swamp.
- The historical flow and pH monitoring data for the Yeodene Gauge found that:
  - The cumulative flow analysis data suggests an increasing flow trend in the early and mid 1990's, suggesting relatively wetter conditions prevailed in Big Swamp and Reach 3 of Boundary Creek.
  - Prior to 2000, pH measurements below the long term average (i.e. occurred for around 19% of measurements. Therefore, acid discharge from Big Swamp occurred under natural flow conditions at least periodically.

## 6.3 Anthropogenic effects on acid generation process

- Extraction of groundwater from the LTA during the millennial drought, in combination with the dry climatic conditions, resulted in a lowering of the water table in the sediments of Big Swamp leading to oxidation of primary acid source minerals and an increased occurrence of acid discharge from Big Swamp.
- The historical flow and pH monitoring data for the Yeodene Gauge showed that:
  - The cumulative flow analysis data suggests a decreasing flow trend since the late 1990's, suggesting relatively drier conditions in Big Swamp and Reach 3 of Boundary Creek, leading to drying of the sediments in the swamp.
  - Post 2000, pH measurements below the long term average occurred in around 86% of measurements. This notable change in acid discharge from Big Swamp appears to be a consequence of the oxidation of primary acid source minerals as a result of lowering the water table in the swamp sediments.

## 6.4 Basic hydrogeochemical model

- The available data was used to develop a conceptual geochemical model that informed the development of a thermodynamic model.
- The MINTEQ-2A software package was used to conduct the thermodynamic modelling.
- The Geochemical Reaction Model results assisted in understanding the geochemical processes associated with the potential management and remediation options under consideration for Big Swamp and Reach 3 of Boundary Creek.

## 6.5 Remediation option geochemical processes

The geochemical processes associated with nine remediation options were assessed. The potential effectiveness of the management and remediation options under consideration, with respect to the key geochemical processes and the fate and transport of solutes of concern, are summarised in Table 15, with key conclusions below.

### 6.5.1 Management and remediation of Big Swamp

- The geochemical processes potentially associated with Option O1 (do nothing) were considered to primarily relate to the leaching of the retained and actual acidity in the short to medium term and the long term ongoing acid generation from oxidation of primary acid source minerals that remain in the unsaturated sediments in the swamp. Based on the estimated net acid mass remaining in the unsaturated zone of the swamp, acid flux could occur for more than 300 years.
- Geochemical processes associated with Option O2 implementing contingency measures) would entail re-saturating the sediments in Big Swamp using supplementary surface water flows, in an attempt to re-create reducing conditions to attenuate acid present in the system. Based on the estimated net acid mass remaining in the unsaturated zone of the swamp, acid flux could occur for 50-100 years (±50 years) depending on the surface water flow and barrier scenario. However, the Monash University (2019) study and thermodynamic model suggest that the effectiveness of re-saturation may be limited as there is insufficient sulfate in the system. The study suggested that iron would reduce to the ferrous form, which would increase solubility of iron and allow the ion to migrate in solution, exporting acid that forms down-stream when ferrous iron oxidises to the ferric form and precipitates as ferric hydroxides leading to a decrease in pH. This process also applies to the other re-saturation options, including Options O7 and O8.
- Geochemical processes associated with Option O3 would entail adding a neutralising agent such as lime to the sediment to provide buffering capacity and reduce the potential for acid discharge from Big Swamp into Reach 3 of Boundary Creek. The dissolution of lime adds calcium and hydroxide ions to the solution, which increases pH. These processes also apply to Options O9 and O10, which also add buffering capacity to the sediments in Big Swamp. The addition of buffering capacity and resultant increase in pH leads to precipitation of a range of iron and aluminium hydroxide mineral precipitation as well as some limited removal of sulfate by precipitation of aluminium sulfate over a narrow range of pH. One limiting factor of mineral precipitation as pH increases is armouring of the neutralising agent added resulting in a coating of the surface of the treatment agent granules, which limits or stops dissolution of the neutralising agent reducing its effectiveness.

### 6.5.2 Management and remediation of Reach 3 of Boundary Creek

- The geochemical processes associated with Option O13 would entail adding a neutralising agent by mechanical mixing into the surface water discharging from Big Swamp and then allowing the treated water to discharge into Reach 3 of Boundary Creek after passing through an aeration and settlement pond. The addition of the neutralising agent introduces buffering capacity and rises pH of acidic waters discharging from Big Swamp. The addition of buffering capacity would result in precipitation of aluminium, iron, manganese and calcium minerals. The majority of the mineral precipitates that formed are iron hydroxides, which remove buffering capacity and decrease pH. Some sulfate is also removed from solution by precipitation of aluminium sulfate over a relatively narrow pH range. Also dissolved calcium is removed from solution by precipitation of phosphate minerals, which leads to removal of some buffering capacity.
- The geochemical processes associated with Option O17 would entail adding a neutralising agent under anaerobic conditions in a passive treatment system into the surface water discharging from Big Swamp and then allowing the treated water to discharge into Reach 3 of Boundary Creek after passing through an aeration and settlement pond. The treatment of the acid water in the reduction later of the system (comprising and organic matter layer) would result in the reduction of ferric ion to the more soluble ferrous form which would limit the potential for clogging and armouring of the limestone treatment layer by precipitation of iron hydroxide minerals. However, clogging and armouring of the limestone layer by aluminium sulfate and hydroxide minerals is likely as the pH of the acidic water increases.

## 6.6 General

- The available soil, surface water and groundwater data is currently limited and further spatial and temporal data would be required to support more detailed and representative thermodynamic modelling of the geochemical processes associated with the management and remediation options under consideration.
- The availability of a limited data set for surface and groundwater prevented the undertaking of a statistical analysis of input parameter variance. As a result a conservative approach using the maximum values for the input parameters was adopted.
- Given the data limitation the results of the geochemical assessment are subject to considerable uncertainty and should be used with an appropriate amount of caution in the design of the management and remediation options considered for Big Swamp and Reach 3 of Boundary Creek.
- The geochemical processes associated with each management and remediation option under consideration suggest that no single management and remediation option under consideration is capable of mitigating acid generating processes associated with the primary acid source minerals, primary acidification reactions and secondary acidification reactions. Therefore, a combination of management and remediation processes is likely to be required.

# 7. Recommendations

Based on the data available, the results of the geochemical assessment and modelling and conclusions reached the following recommendations should be implemented with respect to further geochemical data requirements, assessment and modelling:

- Collection of further spatial and temporal geochemical data as follows:
  - Soil samples to further characterise the spatial geochemical characteristics of the sediments in Big Swamp. This should include lateral and vertical extent of sediments within Big Swamp to obtain a more accurate understanding of the sediment volume.
  - Chemical analysis of soil samples to characterise their mineralogical composition, retained acid, actual acidity and potential acidity to provide a more detailed characterisation of the net acidity laterally and vertically.
  - Kinetic reaction rate analysis of soil samples to characterise the rate of acid leaching and oxidation rate of primary acid source minerals through use of simple drying and cyclic drying and wetting simulations (noting some work is currently in progress).
  - Regular collection of surface water sampled on at least a quarterly basis at 10 locations distributed across the swamp to further characterise the spatial and temporal variance in geochemical character of the surface water system.
  - Regular collection of groundwater sampled on at least a quarterly basis at the existing monitoring well locations installed in Big Swamp to further characterise the spatial and temporal variance in geochemical character of the groundwater system.
- Undertake a statistical analysis of the soil, surface water and groundwater data set to assess variance and support the development of an improved conceptual geochemical model and support more robust and reliable decision making in regard to management and remediation options.
- Undertake further thermodynamic modelling using both equilibrium and kinetic approaches to provide improved estimates of the geochemical processes associated with the management and remediation option considered suitable for Big Swamp and Reach 3 of Boundary Creek.

# 8. References


Barwon Water 2019, Request for Proposal – Basic Conceptual Geochemical Modelling for Big Swamp

ALS 2019, August 2019 water quality results

Jacobs, 2018, Yeodene Swamp Study: 2016-2017 Technical Works Program. Report for Barwon Water

Jacobs, 2017, Bore completion Report: Installation of Additional Monitoring Assets Report for Barwon Water

Jacobs 2017a, May 2017 water quality results. Data for Barwon Water

Jacobs 2017b, August 2017 water quality results. Data for Barwon Water

Monash University 2019, Soil test results. Data for Barwon Water

Monash University 2019a, Progress report for Barwon Water on Big Swamp Static testing, May and June 2019.

Monash University 2019b, Progress report for Barwon Water on Big Swamp static testing and process rates, July and August 2019.

Monash University 2019c, September Progress report for Barwon Water on Big Swamp static testing and process rates, September 2019.

# 9. Limitations

*This report: has been prepared by GHD for Barwon Water* and *may only be used and relied on by Barwon Water for the purpose agreed between GHD and the Barwon Water as set out in section 1.2 of this report.*

*GHD otherwise disclaims responsibility to any person other than Barwon Water arising in connection with this report. GHD also excludes implied warranties and conditions, to the extent legally permissible.*

*The services undertaken by GHD in connection with preparing this report were limited to those specifically detailed in the report and are subject to the scope limitations set out in the report.*

*The opinions, conclusions and any recommendations in this report are based on conditions encountered and information reviewed at the date of preparation of the report. GHD has no responsibility or obligation to update this report to account for events or changes occurring subsequent to the date that the report was prepared.*

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# Appendices

# **Appendix A** - Lime dosing of soils in Big Swamp

# A1: Aqueous species in solution

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 9.39E-06 | 9.29E-06 | -5.032 |
| Al(OH)2+ | 2.88E-11 | 2.26E-11 | -10.647 |
| Al(OH)3 (aq) | 8.02E-16 | 8.23E-16 | -15.085 |
| Al(OH)4- | 9.2E-20 | 7.1E-20 | -19.149 |
| Al(SO4)2- | 0.000989 | 0.000763 | -3.117 |
| Al+3 | 0.000381 | 6.61E-05 | -4.18 |
| Al2(OH)2+4 | 6.41E-11 | 1.16E-12 | -11.935 |
| Al2(OH)2CO3+2 | 4.85E-15 | 1.78E-15 | -14.75 |
| Al2PO4+3 | 1.54E-10 | 1.61E-11 | -10.793 |
| Al3(OH)4+5 | 3.86E-16 | 7.31E-19 | -18.136 |
| AlCl+2 | 1.22E-06 | 4.46E-07 | -6.35 |
| AlF+2 | 1.31E-05 | 4.96E-06 | -5.305 |
| AlF2+ | 1.96E-08 | 1.53E-08 | -7.814 |
| AlF3 (aq) | 1.37E-12 | 1.4E-12 | -11.853 |
| AlF4- | 7.12E-18 | 5.49E-18 | -17.26 |
| AlHPO4+ | 1.72E-08 | 1.34E-08 | -7.872 |
| AlOH+2 | 1.74E-07 | 6.59E-08 | -7.181 |
| AlSO4+ | 0.003424 | 0.002644 | -2.578 |
| As3S4(HS)- | 4.9E-224 | 3.8E-224 | -223.418 |
| AsO4-3 | 1.63E-20 | 1.71E-21 | -20.768 |
| AsS(OH)HS- | 1.24E-79 | 9.62E-80 | -79.017 |
| Ca DOM1 | 2.16E-06 | 1.84E-06 | -5.735 |
| Ca(NH3)2+2 | 5.61E-24 | 2.06E-24 | -23.687 |
| Ca(NO3)2 | 6.7E-105 | 6.9E-105 | -104.162 |
| Ca+2 | 0.006371 | 0.002615 | -2.583 |
| CaCl+ | 0.000132 | 0.000103 | -3.988 |
| CaCO3 (aq) | 1.94E-15 | 1.99E-15 | -14.7 |
| CaCrO4 (aq) | 3.12E-11 | 3.2E-11 | -10.495 |
| CaF+ | 2.98E-10 | 2.32E-10 | -9.635 |
| CaH2PO4+ | 3.09E-08 | 2.43E-08 | -7.615 |
| CaHCO3+ | 2.56E-09 | 2.03E-09 | -8.693 |
| CaHPO4 (aq) | 5.71E-12 | 5.86E-12 | -11.232 |
| CaNH3+2 | 3.6E-13 | 1.32E-13 | -12.88 |
| CaNO3+ | 3.31E-51 | 2.57E-51 | -50.59 |
| CaOH+ | 5.22E-14 | 4.14E-14 | -13.383 |
| CaPO4- | 3.09E-18 | 2.43E-18 | -17.615 |
| CaSO4 (aq) | 0.003627 | 0.003721 | -2.429 |
| Cd DOM1 | 1.68E-12 | 1.43E-12 | -11.844 |
| Cd(CO3)2-2 | 1.07E-32 | 3.92E-33 | -32.407 |
| Cd(HS)2 (aq) | 6.42E-84 | 6.58E-84 | -83.182 |
| Cd(HS)3- | 1.1E-126 | 8.3E-127 | -126.081 |
| Cd(HS)4-2 | 7.1E-169 | 2.6E-169 | -168.581 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd(NH3)2+2 | 2.7E-26 | 9.9E-27 | -26.004 |
| Cd(NH3)3+2 | 1.06E-35 | 3.88E-36 | -35.411 |
| Cd(NH3)4+2 | 1.22E-45 | 4.49E-46 | -45.348 |
| Cd(NO2)2 (aq) | 4.91E-81 | 5.03E-81 | -80.298 |
| Cd(NO3)2 (aq) | 1E-106 | 1.1E-106 | -105.972 |
| Cd(OH)2 (aq) | 1.49E-25 | 1.53E-25 | -24.814 |
| Cd(OH)3- | 3.75E-36 | 2.92E-36 | -35.534 |
| Cd(OH)4-2 | 1.58E-47 | 5.8E-48 | -47.236 |
| Cd(SO4)2-2 | 3.28E-10 | 1.2E-10 | -9.919 |
| Cd+2 | 2.21E-09 | 8.09E-10 | -9.092 |
| Cd2OH+3 | 2.55E-25 | 2.67E-26 | -25.574 |
| CdCl+ | 1.6E-09 | 1.24E-09 | -8.905 |
| CdCl2 (aq) | 8.08E-11 | 8.29E-11 | -10.082 |
| CdCO3 (aq) | 9.87E-21 | 1.01E-20 | -19.994 |
| CdF+ | 1.2E-16 | 9.35E-17 | -16.029 |
| CdHCO3+ | 1.93E-15 | 1.5E-15 | -14.824 |
| CdHPO4 (aq) | 1.88E-17 | 1.93E-17 | -16.715 |
| CdHS+ | 2.12E-46 | 1.65E-46 | -45.782 |
| CdNH3+2 | 1.42E-17 | 5.22E-18 | -17.282 |
| CdNO2+ | 3.94E-45 | 3.06E-45 | -44.514 |
| CdNO3+ | 1.27E-57 | 9.9E-58 | -57.004 |
| CdOH+ | 7.46E-18 | 5.8E-18 | -17.236 |
| CdSO4 (aq) | 1.12E-09 | 1.15E-09 | -8.939 |
| Cl-1 | 0.022072 | 0.016569 | -1.781 |
| CO3-2 | 1.41E-15 | 5.34E-16 | -15.272 |
| Cr2O7-2 | 1.4E-11 | 5.13E-12 | -11.29 |
| CrO3Cl- | 2.39E-10 | 1.86E-10 | -9.73 |
| CrO3H2PO4- | 1.67E-12 | 1.3E-12 | -11.887 |
| CrO3HPO4-2 | 1.43E-12 | 5.25E-13 | -12.28 |
| CrO3SO4-2 | 1.02E-08 | 3.73E-09 | -8.428 |
| CrO4-2 | 6.08E-11 | 2.08E-11 | -10.683 |
| Cu DOM1 | 1.61E-09 | 1.38E-09 | -8.862 |
| Cu(CO3)2-2 | 2.41E-28 | 8.83E-29 | -28.054 |
| Cu(N3)2 (aq) | 2.41E-17 | 2.47E-17 | -16.607 |
| Cu(N3)3- | 3.07E-22 | 2.39E-22 | -21.621 |
| Cu(N3)4-2 | 3.31E-28 | 1.22E-28 | -27.915 |
| Cu(NH3)2+2 | 5.58E-22 | 2.05E-22 | -21.689 |
| Cu(NH3)3+2 | 7.17E-30 | 2.63E-30 | -29.58 |
| Cu(NH3)4+2 | 1.91E-38 | 6.99E-39 | -38.156 |
| Cu(NO2)2 (aq) | 2.89E-80 | 2.96E-80 | -79.529 |
| Cu(NO3)2 (aq) | 6.3E-106 | 6.5E-106 | -105.189 |
| Cu(OH)2 (aq) | 1.14E-20 | 1.17E-20 | -19.934 |
| Cu(OH)3- | 4.14E-28 | 3.22E-28 | -27.492 |
| Cu(OH)4-2 | 1.13E-39 | 4.16E-40 | -39.381 |
| Cu+2 | 4.96E-08 | 1.95E-08 | -7.709 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu2(OH)2+2 | 4.45E-22 | 1.63E-22 | -21.787 |
| Cu2OH+3 | 9.4E-20 | 9.84E-21 | -20.007 |
| Cu2S3-2 | 2.2E-145 | 7.9E-146 | -145.1 |
| Cu3(OH)4+2 | 1.04E-35 | 3.82E-36 | -35.418 |
| CuCl+ | 7.52E-10 | 5.75E-10 | -9.24 |
| CuCl2 (aq) | 1.55E-12 | 1.59E-12 | -11.799 |
| CuCl3- | 2.67E-16 | 2.04E-16 | -15.69 |
| CuCl4-2 1 | 6.51E-20 | 2.4E-20 | -19.62 |
| CuCO3 (aq) | 5.99E-17 | 6.14E-17 | -16.212 |
| CuF+ | 8.2E-15 | 6.38E-15 | -14.195 |
| CuHCO3+ | 9.27E-14 | 7.21E-14 | -13.142 |
| CuHPO4 (aq) | 1.19E-15 | 1.22E-15 | -14.912 |
| CuHSO4+ | 1.93E-10 | 1.51E-10 | -9.822 |
| CuN3+ | 3.51E-12 | 2.73E-12 | -11.563 |
| CuNH3+2 | 1.13E-14 | 4.16E-15 | -14.381 |
| CuNO2+ | 9.88E-44 | 7.69E-44 | -43.114 |
| CuNO3+ | 2.42E-56 | 1.89E-56 | -55.724 |
| CuOH+ | 9.52E-14 | 7.28E-14 | -13.138 |
| CuS(aq) | 1.17E-53 | 1.2E-53 | -52.92 |
| CuSO4 (aq) | 2.65E-08 | 2.72E-08 | -7.566 |
| DOC (Gaussian DOM) | 0.001399 | 0.001435 | -2.843 |
| DOM1 | 3.26E-05 | 4.56E-06 | -5.341 |
| F-1 | 1.03E-08 | 7.82E-09 | -8.107 |
| Fe DOM1 | 9.43E-08 | 9.33E-08 | -7.03 |
| Fe(N3)2+ | 3.82E-14 | 2.97E-14 | -13.527 |
| Fe(N3)3 (aq) | 1.2E-18 | 1.23E-18 | -17.91 |
| Fe(NH3)2+2 | 5.73E-22 | 2.1E-22 | -21.678 |
| Fe(NH3)3+2 | 2.65E-32 | 9.72E-33 | -32.012 |
| Fe(NH3)4+2 | 5.23E-43 | 1.92E-43 | -42.717 |
| Fe(NO2)2+ | 2E-79 | 1.56E-79 | -78.807 |
| Fe(NO2)3 (aq) | 6.6E-115 | 6.7E-115 | -114.172 |
| Fe(OH)2 (aq) | 9.05E-20 | 9.29E-20 | -19.032 |
| Fe(OH)2+ | 1.05E-10 | 8.22E-11 | -10.085 |
| Fe(OH)3- | 6.67E-28 | 5.19E-28 | -27.285 |
| Fe(OH)3 (aq) | 5.14E-18 | 5.27E-18 | -17.278 |
| Fe(OH)4- | 8.52E-24 | 6.68E-24 | -23.175 |
| Fe(SO4)2- | 2.33E-08 | 1.81E-08 | -7.742 |
| Fe+2 | 0.010531 | 0.004144 | -2.383 |
| Fe+3 | 1.21E-08 | 2.1E-09 | -8.678 |
| Fe2(OH)2+4 | 5.27E-15 | 9.53E-17 | -16.021 |
| Fe3(OH)4+5 | 1.41E-21 | 2.67E-24 | -23.574 |
| FeCl+ | 5.57E-05 | 4.33E-05 | -4.363 |
| FeCl+2 | 2.07E-09 | 7.62E-10 | -9.118 |
| FeCrO4+ | 2.06E-12 | 1.6E-12 | -11.796 |
| FeF+ | 6.75E-10 | 5.25E-10 | -9.28 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeF+2 | 4.25E-11 | 1.57E-11 | -10.805 |
| FeF2+ | 5.94E-15 | 4.62E-15 | -14.335 |
| FeF3 (aq) | 3.27E-20 | 3.35E-20 | -19.475 |
| FeH2PO4+ | 1.01E-06 | 7.91E-07 | -6.102 |
| FeH2PO4+2 | 4E-11 | 1.51E-11 | -10.82 |
| FeHCO3+ | 3.86E-09 | 3.05E-09 | -8.515 |
| FeHPO4 (aq) | 7.56E-11 | 7.76E-11 | -10.11 |
| FeHPO4+ | 1.57E-10 | 1.23E-10 | -9.91 |
| FeHS+ | 4.43E-42 | 3.45E-42 | -41.462 |
| FeN3+2 | 1.72E-10 | 6.33E-11 | -10.199 |
| FeNH3+2 | 4.87E-12 | 1.79E-12 | -11.748 |
| FeNO2+2 | 3.41E-43 | 1.25E-43 | -42.902 |
| FeOH+ | 1.89E-10 | 1.47E-10 | -9.833 |
| FeOH+2 | 7.4E-09 | 2.73E-09 | -8.564 |
| FeSO4 (aq) | 0.006081 | 0.006238 | -2.205 |
| FeSO4+ | 2.32E-07 | 1.81E-07 | -6.743 |
| H DOM1 | 7.61E-05 | 3.38E-05 | -4.472 |
| H+1 | 0.006241 | 0.005137 | -2.289 |
| H2AsO3- | 4.87E-13 | 3.79E-13 | -12.421 |
| H2AsO4- | 4.8E-07 | 3.74E-07 | -6.427 |
| H2CO3* (aq) | 0.000967 | 0.000992 | -3.003 |
| H2CrO4 (aq) | 6.32E-10 | 6.48E-10 | -9.188 |
| H2PO4- | 6.25E-07 | 4.9E-07 | -6.31 |
| H2S (aq) | 1.46E-40 | 1.49E-40 | -39.826 |
| H3AsO3 | 4.13E-06 | 4.24E-06 | -5.373 |
| H3AsO4 | 3.34E-07 | 3.43E-07 | -6.465 |
| H3PO4 | 3.11E-07 | 3.19E-07 | -6.497 |
| HAsO3-2 | 1.02E-24 | 3.76E-25 | -24.425 |
| HAsO4-2 | 1.95E-11 | 7.14E-12 | -11.146 |
| HCO3- | 9.38E-08 | 7.36E-08 | -7.133 |
| HCrO4- | 4.31E-07 | 3.36E-07 | -6.474 |
| HF (aq) | 4.92E-08 | 5.05E-08 | -7.297 |
| HF2- | 1.96E-15 | 1.48E-15 | -14.829 |
| Hg(CO3)2-2 | 3.94E-36 | 1.44E-36 | -35.84 |
| Hg(HS)2 (aq) | 1.36E-72 | 1.4E-72 | -71.855 |
| Hg(N3)2 (aq) | 1.85E-14 | 1.9E-14 | -13.721 |
| Hg(NH3)2+2 | 3.9E-24 | 1.43E-24 | -23.844 |
| Hg(NH3)4+2 | 4.28E-44 | 1.57E-44 | -43.805 |
| Hg(NO2)2 (aq) | 1.49E-86 | 1.53E-86 | -85.815 |
| Hg(NO2)3- | 2.6E-122 | 2E-122 | -121.7 |
| Hg(NO2)4-2 | 5.3E-159 | 1.9E-159 | -158.715 |
| Hg(NO3)2 (aq) | 1.8E-119 | 1.8E-119 | -118.735 |
| Hg(OH)2 | 3.35E-23 | 3.44E-23 | -22.464 |
| Hg(SO4)2-2 | 5.16E-22 | 1.89E-22 | -21.723 |
| Hg+2 | 6.39E-21 | 2.34E-21 | -20.63 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg2OH+3 | 4.2E-42 | 4.4E-43 | -42.357 |
| Hg3(OH)3+3 | 6.79E-62 | 7.11E-63 | -62.148 |
| HgCl+ | 1.42E-15 | 1.1E-15 | -14.957 |
| HgCl2 (aq) | 1.37E-10 | 1.4E-10 | -9.853 |
| HgCl3-1 | 2.97E-11 | 2.31E-11 | -10.636 |
| HgCl4-2 | 4.67E-12 | 1.71E-12 | -11.766 |
| HgClOH (aq) | 1.45E-16 | 1.49E-16 | -15.827 |
| HgCO3 (aq) | 9.35E-25 | 9.59E-25 | -24.018 |
| HgF+ | 8.78E-28 | 6.83E-28 | -27.166 |
| HgHCO3+ | 1.05E-22 | 8.18E-23 | -22.087 |
| HgHS2- | 1.13E-76 | 8.79E-77 | -76.056 |
| HgN3+ | 7.82E-11 | 6.09E-11 | -10.215 |
| HgNO2+ | 5.6E-53 | 4.36E-53 | -52.36 |
| HgNO3+ | 1.97E-70 | 1.53E-70 | -69.814 |
| HgOH+ | 1.74E-22 | 1.36E-22 | -21.868 |
| HgOHCO3- | 2.8E-29 | 2.18E-29 | -28.662 |
| HgS2-2 | 9.1E-83 | 3.34E-83 | -82.477 |
| HgSO4 (aq) | 2.63E-21 | 2.7E-21 | -20.569 |
| HN3 (aq) | 4.98E-05 | 5.1E-05 | -4.292 |
| HNO2 (aq) | 2.66E-37 | 2.73E-37 | -36.564 |
| HPO4-2 | 1.57E-11 | 5.8E-12 | -11.237 |
| HS-1 | 2.64E-45 | 2E-45 | -44.7 |
| HSO4- | 0.003395 | 0.002621 | -2.582 |
| K+1 | 0.000318 | 0.000239 | -3.622 |
| K2HPO4 (aq) | 3.48E-18 | 3.57E-18 | -17.447 |
| K2PO4- | 5.15E-27 | 4E-27 | -26.397 |
| KCl (aq) | 2.04E-06 | 2.1E-06 | -5.678 |
| KCr2O7- | 1.36E-14 | 1.06E-14 | -13.975 |
| KCrO4- | 2.37E-14 | 1.84E-14 | -13.735 |
| KF (aq) | 8.32E-13 | 8.53E-13 | -12.069 |
| KH2PO4 (aq) | 1.77E-10 | 1.82E-10 | -9.741 |
| KHPO4- | 1.09E-14 | 8.52E-15 | -14.07 |
| KNO3 (aq) | 5.13E-53 | 5.26E-53 | -52.279 |
| KOH (aq) | 3.6E-16 | 3.7E-16 | -15.432 |
| KPO4-2 | 5.48E-24 | 2.01E-24 | -23.697 |
| KSO4- | 1.23E-05 | 9.68E-06 | -5.014 |
| Mg DOM1 | 1.73E-07 | 1.47E-07 | -6.832 |
| Mg(NH3)2+2 | 2.24E-24 | 8.2E-25 | -24.086 |
| Mg+2 | 0.004895 | 0.002089 | -2.68 |
| Mg2CO3+2 | 2.47E-17 | 9.07E-18 | -17.043 |
| MgCl+ | 0.000167 | 0.00013 | -3.885 |
| MgCO3 (aq) | 7.76E-16 | 7.96E-16 | -15.099 |
| MgF+ | 1.4E-09 | 1.08E-09 | -8.966 |
| MgHCO3+ | 1.95E-09 | 1.49E-09 | -8.826 |
| MgHPO4 (aq) | 6.3E-12 | 6.46E-12 | -11.19 |
| MgOH+ | 7.87E-13 | 6.28E-13 | -12.202 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgPO4- | 3.86E-20 | 3.03E-20 | -19.519 |
| MgSO4 (aq) | 0.002343 | 0.002404 | -2.619 |
| Mn+3 | 4.55E-05 | 7.89E-06 | -5.103 |
| N3-1 | 2.48E-07 | 1.93E-07 | -6.714 |
| Na+1 | 0.012083 | 0.009416 | -2.026 |
| Na2HPO4 (aq) | 3.58E-15 | 3.67E-15 | -14.435 |
| Na2PO4- | 1.71E-23 | 1.33E-23 | -22.876 |
| NaCl (aq) | 8.52E-05 | 8.75E-05 | -4.058 |
| NaCO3- | 1.59E-16 | 1.25E-16 | -15.905 |
| NaCrO4- | 1.25E-12 | 9.71E-13 | -12.013 |
| NaF (aq) | 6.35E-11 | 6.52E-11 | -10.186 |
| NaH2PO4 (aq) | 6.98E-09 | 7.16E-09 | -8.145 |
| NaHCO3 (aq) | 4E-10 | 4.11E-10 | -9.386 |
| NaHPO4- | 6.63E-13 | 5.2E-13 | -12.284 |
| NaNO3 (aq) | 7.46E-52 | 7.66E-52 | -51.116 |
| NaOH (aq) | 9.73E-15 | 9.98E-15 | -14.001 |
| NaPO4-2 | 2.38E-22 | 8.74E-23 | -22.058 |
| NaSO4- | 0.000446 | 0.00035 | -3.456 |
| NH3 (aq) | 1.48E-11 | 1.52E-11 | -10.819 |
| NH4+1 | 0.000385 | 0.000284 | -3.546 |
| NH4Cr2O7- | 1.88E-14 | 1.46E-14 | -13.834 |
| NH4SO4- | 2.68E-05 | 2.09E-05 | -4.68 |
| Ni DOM1 | 7.7E-09 | 6.56E-09 | -8.183 |
| Ni(N3)2 (aq) | 1.33E-17 | 1.37E-17 | -16.864 |
| Ni(NH3)2+2 | 2.69E-22 | 9.88E-23 | -22.005 |
| Ni(NH3)3+2 | 2.37E-31 | 8.69E-32 | -31.061 |
| Ni(NH3)4+2 | 6.18E-41 | 2.27E-41 | -40.645 |
| Ni(NH3)5+2 | 5.2E-51 | 1.91E-51 | -50.72 |
| Ni(NH3)6+2 | 9.33E-62 | 3.42E-62 | -61.466 |
| Ni(NO2)2 (aq) | 3.15E-79 | 3.23E-79 | -78.491 |
| Ni(OH)2 (aq) | 1.37E-20 | 1.4E-20 | -19.853 |
| Ni(OH)3- | 3.5E-29 | 2.73E-29 | -28.564 |
| Ni(SO4)2-2 | 3.14E-09 | 1.15E-09 | -8.939 |
| Ni+2 | 1.01E-05 | 3.71E-06 | -5.431 |
| NiCl+ | 2.85E-08 | 2.22E-08 | -7.654 |
| NiCl2 (aq) | 1.28E-11 | 1.31E-11 | -10.883 |
| NiCO3 (aq) | 7.17E-17 | 7.35E-17 | -16.133 |
| NiF+ | 6.72E-13 | 5.23E-13 | -12.281 |
| NiH2PO4+ | 1.53E-11 | 1.19E-11 | -10.923 |
| NiHCO3+ | 3.44E-11 | 2.67E-11 | -10.573 |
| NiHPO4 (aq) | 1.53E-14 | 1.57E-14 | -13.804 |
| NiHS+ | 2.94E-45 | 2.29E-45 | -44.641 |
| NiN3+ | 1.73E-11 | 1.35E-11 | -10.87 |
| NiNH3+2 | 1.01E-13 | 3.69E-14 | -13.433 |
| NiNO2+ | 4.3E-42 | 3.34E-42 | -41.476 |
| NiNO3+ | 3.45E-54 | 2.69E-54 | -53.571 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NiOH+ | 5.65E-14 | 4.39E-14 | -13.357 |
| NiSO4 (aq) | 4.56E-06 | 4.68E-06 | -5.33 |
| NO2-1 | 4.83E-38 | 3.76E-38 | -37.425 |
| NO3-1 | 3.86E-49 | 2.89E-49 | -48.54 |
| OH- | 1.18E-12 | 8.9E-13 | -12.05 |
| Pb DOM1 | 1.1E-09 | 9.36E-10 | -9.029 |
| Pb(CO3)2-2 | 4.51E-29 | 1.66E-29 | -28.781 |
| Pb(HS)2 (aq) | 4.82E-83 | 4.94E-83 | -82.306 |
| Pb(HS)3- | 2.5E-126 | 2E-126 | -125.706 |
| Pb(NO2)2 (aq) | 1.18E-80 | 1.21E-80 | -79.916 |
| Pb(NO3)2 (aq) | 1.5E-104 | 1.5E-104 | -103.816 |
| Pb(OH)2 (aq) | 1.95E-21 | 2E-21 | -20.699 |
| Pb(OH)3- | 5E-30 | 3.89E-30 | -29.41 |
| Pb(SO4)2-2 | 2.52E-09 | 9.25E-10 | -9.034 |
| Pb+2 | 1.82E-08 | 6.66E-09 | -8.177 |
| Pb2OH+3 | 3.28E-20 | 3.43E-21 | -20.464 |
| Pb3(OH)4+2 | 2.85E-40 | 1.05E-40 | -39.981 |
| Pb4(OH)4+4 | 5.93E-44 | 1.07E-45 | -44.969 |
| PbCl+ | 4.56E-09 | 3.55E-09 | -8.45 |
| PbCl2 (aq) | 1.2E-10 | 1.23E-10 | -9.911 |
| PbCl3- | 2.08E-12 | 1.62E-12 | -11.792 |
| PbCl4-2 | 2.67E-14 | 9.79E-15 | -14.009 |
| PbCO3 (aq) | 1.18E-17 | 1.21E-17 | -16.919 |
| PbF+ | 9.45E-15 | 7.35E-15 | -14.133 |
| PbF2 (aq) | 6.89E-22 | 7.07E-22 | -21.15 |
| PbH2PO4+ | 1.03E-13 | 8.02E-14 | -13.096 |
| PbHCO3+ | 3.99E-13 | 3.1E-13 | -12.508 |
| PbHPO4 (aq) | 3.84E-17 | 3.94E-17 | -16.404 |
| PbNO2+ | 1.04E-43 | 8.1E-44 | -43.091 |
| PbNO3+ | 3.76E-56 | 2.92E-56 | -55.534 |
| PbOH+ | 3E-14 | 2.33E-14 | -13.632 |
| PbSO4 (aq) | 2.18E-08 | 2.24E-08 | -7.65 |
| PO4-3 | 3.65E-21 | 3.86E-22 | -21.413 |
| S-2 | 2.1E-60 | 7.75E-61 | -60.111 |
| SO4-2 | 0.020293 | 0.00686 | -2.164 |
| Zn DOM1 | 1.8E-08 | 1.53E-08 | -7.815 |
| Zn(CO3)2-2 | 8.49E-29 | 3.11E-29 | -28.507 |
| Zn(N3)2 (aq) | 1.9E-17 | 1.95E-17 | -16.711 |
| Zn(N3)3- | 2.77E-23 | 2.15E-23 | -22.667 |
| Zn(NH3)2+2 | 1.5E-22 | 5.51E-23 | -22.259 |
| Zn(NH3)3+2 | 6.71E-31 | 2.46E-31 | -30.609 |
| Zn(NH3)4+2 | 1.47E-39 | 5.39E-40 | -39.269 |
| Zn(NO2)2 (aq) | 1.19E-79 | 1.23E-79 | -78.912 |
| Zn(NO3)2 (aq) | 2.2E-103 | 2.3E-103 | -102.642 |
| Zn(OH)2 (aq) | 2.54E-18 | 2.6E-18 | -17.584 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn(OH)3- | 2.06E-27 | 1.6E-27 | -26.796 |
| Zn(OH)4-2 | 1.35E-37 | 4.94E-38 | -37.307 |
| Zn(SO4)2-2 | 1.34E-06 | 4.9E-07 | -6.31 |
| Zn+2 | 1.39E-05 | 5.47E-06 | -5.262 |
| Zn2OH+3 | 2.27E-17 | 2.38E-18 | -17.624 |
| Zn2S3-2 | 1.1E-137 | 3.9E-138 | -137.406 |
| Zn4S6-4 | 1.4E-272 | 2.6E-274 | -273.582 |
| ZnCl+ | 3.17E-07 | 2.42E-07 | -6.616 |
| ZnCl2 (aq) | 2.5E-09 | 2.57E-09 | -8.59 |
| ZnCl3- | 5.77E-11 | 4.49E-11 | -10.348 |
| ZnCl4-2 | 9.36E-13 | 3.43E-13 | -12.464 |
| ZnCO3 (aq) | 1.64E-16 | 1.68E-16 | -15.775 |
| ZnF+ | 9.39E-13 | 7.31E-13 | -12.136 |
| ZnHCO3+ | 1.3E-11 | 1.01E-11 | -10.995 |
| ZnHPO4 (aq) | 5.17E-14 | 5.31E-14 | -13.275 |
| ZnN3+ | 1.95E-11 | 1.52E-11 | -10.818 |
| ZnNH3+2 | 4.27E-14 | 1.57E-14 | -13.805 |
| ZnNO2+ | 1.59E-42 | 1.24E-42 | -41.907 |
| ZnNO3+ | 5.43E-54 | 4.23E-54 | -53.374 |
| ZnOH+ | 6.26E-13 | 4.87E-13 | -12.313 |
| ZnS (aq) | 7.69E-50 | 7.89E-50 | -49.103 |
| ZnSO4 (aq) | 7.33E-06 | 7.52E-06 | -5.124 |

## A2: Species distribution

| Component | % of total concentration | Species name |
|---|---|---|
| Ni+2 | 68.723 | Ni+2 |
| | 0.052 | Ni DOM1 |
| | 0.194 | NiCl+ |
| | 31.009 | NiSO4 (aq) |
| | 0.021 | Ni(SO4)2-2 |
| NH4+1 | 93.479 | NH4+1 |
| | 6.521 | NH4SO4- |
| Cl-1 | 98.028 | Cl-1 |
| | 0.587 | CaCl+ |
| | 0.247 | FeCl+ |
| | 0.743 | MgCl+ |
| | 0.379 | NaCl (aq) |
| Pb+2 | 37.616 | Pb+2 |
| | 2.276 | Pb DOM1 |
| | 9.442 | PbCl+ |
| | 0.248 | PbCl2 (aq) |
| | 45.188 | PbSO4 (aq) |
| | 5.224 | Pb(SO4)2-2 |
| Zn+2 | 60.671 | Zn+2 |
| | 0.079 | Zn DOM1 |
| | 1.384 | ZnCl+ |
| | 0.011 | ZnCl2 (aq) |
| | 32.019 | ZnSO4 (aq) |
| | 5.836 | Zn(SO4)2-2 |
| F-1 | 0.078 | F-1 |
| | 0.373 | HF (aq) |
| | 99.234 | AlF+2 |
| | 0.296 | AlF2+ |
| | 0.011 | MgF+ |
| SO4-2 | 48.735 | SO4-2 |
| | 8.153 | HSO4- |
| | 8.223 | AlSO4+ |
| | 4.748 | Al(SO4)2- |
| | 0.018 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 14.603 | FeSO4 (aq) |
| | 5.627 | MgSO4 (aq) |
| | 8.709 | CaSO4 (aq) |
| | 1.072 | NaSO4- |
| | 0.03 | KSO4- |
| | 0.064 | NH4SO4- |
| Hg(OH)2 | 54.824 | HgCl2 (aq) |
| | 11.907 | HgCl3-1 |
| | 1.874 | HgCl4-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 31.386 | HgN3+ |
| N3-1 | 0.497 | N3-1 |
| | 99.503 | HN3 (aq) |
| PO4-3 | 31.243 | H2PO4- |
| | 15.535 | H3PO4 |
| | 50.432 | FeH2PO4+ |
| | 1.546 | CaH2PO4+ |
| | 0.862 | AlHPO4+ |
| | 0.349 | NaH2PO4 (aq) |
| AsO4-3 | 41.017 | H3AsO4 |
| | 58.981 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 27.035 | DOM1 |
| | 63.137 | H DOM1 |
| | 7.789 | Al DOM1 |
| | 1.794 | Ca DOM1 |
| | 0.078 | Fe DOM1 |
| | 0.143 | Mg DOM1 |
| | 0.015 | Zn DOM1 |
| Ca+2 | 62.88 | Ca+2 |
| | 0.021 | Ca DOM1 |
| | 1.305 | CaCl+ |
| | 35.793 | CaSO4 (aq) |
| Mg+2 | 66.1 | Mg+2 |
| | 2.26 | MgCl+ |
| | 31.637 | MgSO4 (aq) |
| K+1 | 95.673 | K+1 |
| | 0.615 | KCl (aq) |
| | 3.712 | KSO4- |
| Na+1 | 95.787 | Na+1 |
| | 0.676 | NaCl (aq) |
| | 3.537 | NaSO4- |
| CO3-2 | 99.989 | H2CO3* (aq) |
| Al+3 | 7.915 | Al+3 |
| | 0.195 | Al DOM1 |
| | 0.272 | AlF+2 |
| | 0.025 | AlCl+2 |
| | 71.072 | AlSO4+ |
| | 20.517 | Al(SO4)2- |
| Cu+2 | 63.079 | Cu+2 |
| | 2.052 | Cu DOM1 |
| | 0.956 | CuCl+ |
| | 33.66 | CuSO4 (aq) |
| | 0.246 | CuHSO4+ |

| Component | % of total concentration | Species name |
|---|---|---|
| Cd+2 | 41.315 | Cd+2 |
| | 0.031 | Cd DOM1 |
| | 29.961 | CdCl+ |
| | 1.514 | CdCl2 (aq) |
| | 21.031 | CdSO4 (aq) |
| | 6.148 | Cd(SO4)2-2 |
| CrO4-2 | 0.014 | CrO4-2 |
| | 97.474 | HCrO4- |
| | 0.143 | H2CrO4 (aq) |
| | 0.054 | CrO3Cl- |
| | 2.301 | CrO3SO4-2 |
| Mn+3 | 100 | Mn+3 |
| Fe+2 | 63.179 | Fe+2 |
| | 0.334 | FeCl+ |
| | 36.481 | FeSO4 (aq) |
| NO2-1 | 15.374 | NO2-1 |
| | 84.624 | HNO2 (aq) |
| NO3-1 | 98.945 | NO3-1 |
| | 0.848 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.191 | NaNO3 (aq) |
| HS-1 | 97.041 | H2S (aq) |
| | 2.955 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 3.261 | Fe+3 |
| | 25.383 | Fe DOM1 |
| | 1.993 | FeOH+2 |
| | 0.028 | Fe(OH)2+ |
| | 0.011 | FeF+2 |
| | 0.557 | FeCl+2 |
| | 62.397 | FeSO4+ |
| | 6.269 | Fe(SO4)2- |
| | 0.046 | FeN3+2 |
| | 0.011 | FeH2PO4+2 |
| | 0.042 | FeHPO4+ |

# A3: Saturation indices

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 2.678 | -8.797 |
| Al(OH)3 (Soil) | 2.678 | -6.25 |
| Al2O3(s) | 5.366 | -15.858 |
| Al4(OH)10SO4(s) | 3.977 | -18.723 |
| AlAsO4:2H2O(s) | -24.954 | -9.154 |
| AlOHF2(s) | -18.108 | -18.515 |
| AlOHSO4(s) | -4.057 | -0.827 |
| Alunite | -6.773 | -6.65 |
| Anglesite | -10.34 | -2.477 |
| Anhydrite | -4.746 | -0.43 |
| Antlerite | -16.148 | -24.936 |
| Aragonite | -17.855 | -9.576 |
| Arsenolite | -10.735 | -9.172 |
| Artinite | -16.071 | -26.402 |
| As2O5(s) | -55.261 | -20.552 |
| As2S3(am) | -151.692 | -105.307 |
| Atacamite | -10.342 | -18.301 |
| Azurite | -49.101 | -31.948 |
| Bianchite | -7.446 | -5.685 |
| Birnessite | 11.044 | -7.047 |
| Bixbyite | 3.52 | 3.407 |
| Boehmite | 2.681 | -6.612 |
| Brochantite | -19.285 | -35.741 |
| Brucite | 1.892 | -15.901 |
| Ca3(AsO4)2:4H2O(s) | -49.297 | -30.397 |
| Ca3(PO4)2 (am1) | -50.575 | -25.646 |
| Ca3(PO4)2 (am2) | -50.575 | -22.854 |
| Ca3(PO4)2 (beta) | -50.575 | -21.326 |
| Ca4H(PO4)3:3H2O(s) | -76.87 | -29.559 |
| CaCO3xH2O(s) | -17.858 | -10.771 |
| CaCrO4(s) | -13.265 | -11.163 |
| CaHPO4(s) | -26.285 | -6.822 |
| CaHPO4:2H2O(s) | -26.292 | -7.157 |
| Calcite | -17.855 | -9.425 |
| CaS(s) | -44.993 | -56.173 |
| Cd metal (alpha) | -23.085 | -37.058 |
| Cd metal (gamma) | -23.085 | -37.165 |
| Cd(OH)2(s) | -4.52 | -18.74 |
| Cd3(OH)4SO4(s) | -20.296 | -42.856 |
| Cd3(PO4)2(s) | -70.103 | -37.503 |
| Cd3OH2(SO4)2(s) | -27.032 | -33.742 |
| Cd4(OH)6SO4(s) | -24.817 | -53.217 |
| CdCl2(s) | -12.654 | -12.108 |
| CdCl2:1H2O(s) | -12.657 | -11.009 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CdCl2:2.5H2O(s) | -12.662 | -10.705 |
| CdF2(s) | -25.306 | -24.375 |
| CdOHCl(s) | -8.587 | -12.312 |
| CdSO4(s) | -11.256 | -11.4 |
| CdSO4:1H2O(s) | -11.259 | -9.725 |
| CdSO4:2.67H2O(s) | -11.265 | -9.501 |
| Cerrusite | -23.449 | -10.098 |
| Chalcanthite | -9.89 | -7.213 |
| Chalcopyrite | -94.913 | -58.74 |
| Chloropyromorphite(c) | -106.904 | -22.474 |
| Chloropyromorphite(soil) | -106.904 | -26.504 |
| Cinnabar | -69.446 | -22.623 |
| Claudetite | -10.735 | -9.222 |
| Cotunnite | -11.738 | -6.799 |
| Covellite | -50.12 | -27.31 |
| Cr(VI)-Ettringite | -28.56 | -91.961 |
| Cr(VI)-Jarosite | -37.305 | -18.789 |
| CrO3(s) | -15.258 | -12.079 |
| Cryolite | -58.899 | -24.828 |
| Cu azide | -21.137 | -13.296 |
| Cu(OH)2(s) | -3.137 | -12.75 |
| Cu2(OH)3NO3(s) | -57.101 | -66.793 |
| Cu3(AsO4)2:2H2O(s) | -64.67 | -29.57 |
| Cu3(PO4)2(s) | -65.955 | -29.105 |
| Cu3(PO4)2:3H2O(s) | -65.965 | -30.845 |
| CuCO3(s) | -22.982 | -11.482 |
| CuCrO4(s) | -18.392 | -12.952 |
| CuF2(s) | -23.923 | -25.445 |
| CuF2:2H2O(s) | -23.93 | -19.473 |
| CuOCuSO4(s) | -13.007 | -24.148 |
| Cupric Ferrite | -6.764 | -14.03 |
| CuSO4(s) | -9.873 | -13.257 |
| Diaspore | 2.681 | -4.818 |
| Dolomite (disordered) | -35.807 | -19.549 |
| Dolomite (ordered) | -35.807 | -18.957 |
| Epsomite | -4.867 | -2.671 |
| Ettringite | -3.002 | -62.191 |
| FCO3-Apatite | -166.391 | -50.989 |
| Fe(OH)2 (am) | 2.189 | -11.858 |
| Fe(OH)2 (c) | 2.189 | -10.701 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -23.847 | -21.584 |
| Fe3(OH)8(s) | -1.451 | -21.673 |
| FeAsO4:2H2O(s) | -29.452 | -9.252 |
| Ferrihydrite | -1.82 | -5.63 |
| Ferrihydrite (aged) | -1.82 | -5.12 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| FeS (ppt) | -44.793 | -41.91 |
| Fluorite | -18.796 | -8.223 |
| Galena | -50.587 | -35.181 |
| Gibbsite (C) | 2.678 | -5.7 |
| Goethite | -1.817 | -2.676 |
| Goslarite | -7.45 | -5.352 |
| Greenockite | -51.503 | -37.148 |
| Greigite | -189.38 | -144.345 |
| Gypsum | -4.753 | -0.137 |
| Halite | -3.807 | -5.334 |
| Hematite | -3.63 | -2.996 |
| Hercynite | 7.559 | -17.243 |
| Hg(OH)2(s) | -22.464 | -18.968 |
| Hg3O2CO3(s) | -87.229 | -57.649 |
| HgCl2(s) | -30.597 | -8.68 |
| HgSO4(s) | -29.199 | -19.691 |
| Hinsdalite | -30.577 | -28.077 |
| H-Jarosite | -18.938 | -14.905 |
| Huntite | -71.712 | -42.399 |
| Hydrocerrusite | -50.502 | -31.742 |
| Hydromagnesite | -69.932 | -62.494 |
| Hydroxyapatite | -74.867 | -30.534 |
| Hydroxylpyromorphite | -102.837 | -40.047 |
| Hydrozincite | -43.14 | -53.278 |
| K2Cr2O7(s) | -33.185 | -15.451 |
| K2CrO4(s) | -17.927 | -17.302 |
| K-Alum | -12.17 | -6.816 |
| KCl(s) | -5.403 | -6.303 |
| K-Jarosite | -20.267 | -9.886 |
| Langite | -19.289 | -37.784 |
| Larnakite | -13.942 | -13.64 |
| Laurionite | -7.671 | -8.294 |
| Lepidocrocite | -1.817 | -3.188 |
| Lime | 1.993 | -31.886 |
| Litharge | -3.601 | -16.69 |
| Mackinawite | -44.793 | -41.193 |
| Maghemite | -3.63 | -10.016 |
| Magnesioferrite | -1.735 | -20.29 |
| Magnesite | -17.952 | -10.371 |
| Magnetite | -1.437 | -6.108 |
| Malachite | -26.119 | -20.919 |
| Massicot | -3.601 | -16.898 |
| Matlockite | -18.064 | -8.889 |
| Melanothallite | -11.271 | -17.913 |
| Melanterite | -4.57 | -2.236 |
| Metacinnabar | -69.446 | -23.022 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Mg(OH)2 (active) | 1.892 | -16.902 |
| Mg2(OH)3Cl:4H2O(s) | -0.297 | -26.297 |
| Mg3(PO4)2(s) | -50.868 | -27.588 |
| MgCO3:5H2O(s) | -17.969 | -13.429 |
| MgCrO4(s) | -13.363 | -19.284 |
| MgF2(s) | -18.894 | -10.833 |
| MgHPO4:3H2O(s) | -26.393 | -8.218 |
| MgS(s) | -45.091 | -62.771 |
| Minium | 7.764 | -68.323 |
| Mirabilite | -6.25 | -4.653 |
| Mn2(SO4)3(s) | -16.697 | -11.98 |
| Montroydite | -22.46 | -18.744 |
| Morenosite | -7.618 | -5.4 |
| Na2Cr2O7(s) | -29.993 | -19.963 |
| Na2CrO4(s) | -14.735 | -17.785 |
| NaF(s) | -10.133 | -9.638 |
| Na-Jarosite | -18.671 | -14.177 |
| Natron | -19.358 | -17.647 |
| Nesquehonite | -17.963 | -13.44 |
| Ni(OH)2 (am) | -0.859 | -14.333 |
| Ni(OH)2 (c) | -0.859 | -11.649 |
| Ni3(AsO4)2:8H2O(s) | -57.856 | -32.356 |
| Ni3(PO4)2(s) | -59.12 | -27.82 |
| Ni4(OH)6SO4(s) | -10.173 | -42.173 |
| NiCO3(s) | -20.703 | -9.756 |
| NiS (alpha) | -47.842 | -42.322 |
| NiS (beta) | -47.842 | -36.822 |
| NiS (gamma) | -47.842 | -35.122 |
| Nsutite | 11.044 | -6.46 |
| Orpiment | -151.692 | -103.792 |
| Otavite | -24.364 | -12.313 |
| Pb azide (alpha) | -21.605 | -12.63 |
| Pb metal | -22.169 | -26.41 |
| Pb(OH)2(s) | -3.605 | -12.111 |
| Pb10(OH)6O(CO3)6(s) | -155.109 | -146.349 |
| Pb2(OH)3Cl(s) | -11.276 | -20.069 |
| Pb2O(OH)2(s) | -7.206 | -33.396 |
| Pb2O3(s) | 11.365 | -49.675 |
| Pb2OCO3(s) | -27.05 | -26.741 |
| Pb3(AsO4)2(s) | -66.065 | -30.565 |
| Pb3(PO4)2(s) | -67.357 | -23.827 |
| Pb3O2CO3(s) | -30.652 | -42.344 |
| Pb3O2SO4(s) | -17.543 | -28.711 |
| Pb4(OH)6SO4(s) | -21.154 | -42.254 |
| Pb4O3SO4(s) | -21.144 | -43.851 |
| PbCrO4(s) | -18.859 | -5.991 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| PbF2(s) | -24.39 | -16.829 |
| PbHPO4(s) | -31.879 | -8.074 |
| PbO:0.3H2O(s) | -3.602 | -16.582 |
| Periclase | 1.895 | -20.609 |
| Phosgenite | -35.187 | -15.377 |
| Plattnerite | 14.967 | -36.435 |
| Plumbgummite | -52.116 | -19.326 |
| Portlandite | 1.989 | -21.497 |
| Pyrite | -73.211 | -54.399 |
| Realgar | -61.637 | -40.907 |
| Retgersite | -7.615 | -5.547 |
| Siderite | -17.655 | -7.109 |
| Smithsonite | -20.535 | -9.658 |
| Spharelite | -47.673 | -36.67 |
| Spinel | 7.261 | -31.945 |
| Strengite | -30.098 | -3.755 |
| Struvite | -27.64 | -14.38 |
| Sulfur | -28.418 | -26.372 |
| Tenorite(am) | -3.134 | -12.018 |
| Tenorite(c) | -3.134 | -11.169 |
| Thenardite | -6.216 | -6.593 |
| Thermonatrite | -19.328 | -20.029 |
| Tsumebite | -38.628 | -28.838 |
| Vaterite | -17.855 | -10.018 |
| Vivianite | -50.002 | -12.211 |
| Wurtzite | -47.673 | -38.924 |
| Zincite | -0.687 | -12.462 |
| Zincosite | -7.426 | -11.858 |
| Zn metal | -19.255 | -45.976 |
| Zn(NO3)2:6H2O(s) | -102.362 | -105.528 |
| Zn(OH)2 (am) | -0.69 | -13.685 |
| Zn(OH)2 (beta) | -0.69 | -12.95 |
| Zn(OH)2 (delta) | -0.69 | -12.534 |
| Zn(OH)2 (epsilon) | -0.69 | -12.702 |
| Zn(OH)2 (gamma) | -0.69 | -12.922 |
| Zn2(OH)2SO4(s) | -8.116 | -15.616 |
| Zn2(OH)3Cl(s) | -5.447 | -20.638 |
| Zn3(PO4)2:4H2O(s) | -58.627 | -23.207 |
| Zn3AsO42:2.5H2O(s) | -57.331 | -29.831 |
| Zn3O(SO4)2(s) | -15.539 | -36.022 |
| Zn4(OH)6SO4(s) | -9.497 | -37.897 |
| Zn5(OH)8Cl2(s) | -11.585 | -50.085 |
| Zn-Al LDH(s) | -8.625 | -28.455 |
| ZnCl2(s) | -8.824 | -16.314 |
| ZnCO3(s) | -20.535 | -9.735 |
| ZnCO3:1H2O(s) | -20.538 | -10.278 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| ZnF2(s) | -21.476 | -21.305 |
| ZnSO4:1H2O(s) | -7.429 | -7.059 |

## A4: Mass distribution

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 8.15E-07 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.010132 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.022516 | 86.769 | 0 | 0 | 0.003433 | 13.231 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.016669 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 3.71E-07 | 0.003 | 0 | 0 | 0.011444 | 99.997 |
| H+1 | 0.011703 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.13E-06 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.5E-40 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 3.14E-37 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 3.9E-49 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## A5: Finite solids

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 1.14E-02 |

# **Appendix B** - Return of reducing conditions in Big Swamp

# B1: Aqueous species

## B1.1: Eh 100

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 2.39E-05 | 2.36E-05 | -4.627 |
| Al(OH)2+ | 3.25E-09 | 2.53E-09 | -8.597 |
| Al(OH)3 (aq) | 1.47E-12 | 1.51E-12 | -11.822 |
| Al(OH)4- | 2.77E-15 | 2.13E-15 | -14.673 |
| Al(SO4)2- | 0.000401 | 0.000307 | -3.512 |
| Al+3 | 0.000166 | 2.78E-05 | -4.556 |
| Al2(OH)2+4 | 3.31E-09 | 5.47E-11 | -10.262 |
| Al2(OH)2CO3+2 | 6.18E-11 | 2.21E-11 | -10.655 |
| Al2PO4+3 | 6.01E-09 | 5.98E-10 | -9.223 |
| Al3(OH)4+5 | 2.35E-12 | 3.87E-15 | -14.413 |
| AlCl+2 | 5.97E-07 | 2.14E-07 | -6.669 |
| AlF+2 | 1.31E-05 | 4.83E-06 | -5.316 |
| AlF2+ | 4.44E-08 | 3.46E-08 | -7.461 |
| AlF3 (aq) | 7.11E-12 | 7.31E-12 | -11.136 |
| AlF4- | 8.66E-17 | 6.63E-17 | -16.178 |
| AlHPO4+ | 9.42E-08 | 7.29E-08 | -7.137 |
| AlOH+2 | 1.22E-06 | 4.52E-07 | -6.345 |
| AlSO4+ | 0.001419 | 0.001088 | -2.963 |
| As3S4(HS)- | 1.72E-43 | 1.33E-43 | -42.875 |
| AsO4-3 | 7.5E-25 | 7.46E-26 | -25.127 |
| AsS(OH)HS- | 1.22E-18 | 9.42E-19 | -18.026 |
| Ca DOM1 | 1.19E-05 | 1.01E-05 | -4.997 |
| Ca(NH3)2+2 | 1.35E-21 | 4.83E-22 | -21.316 |
| Ca(NO3)2 | 1.1E-164 | 1.1E-164 | -163.942 |
| Ca+2 | 0.005878 | 0.002366 | -2.626 |
| CaCl+ | 0.000137 | 0.000106 | -3.974 |
| CaCO3 (aq) | 4.63E-13 | 4.76E-13 | -12.322 |
| CaCrO4 (aq) | 4.64E-10 | 4.77E-10 | -9.322 |
| CaF+ | 6.28E-10 | 4.86E-10 | -9.313 |
| CaH2PO4+ | 2.24E-08 | 1.75E-08 | -7.758 |
| CaHCO3+ | 3.79E-08 | 2.98E-08 | -7.525 |
| CaHPO4 (aq) | 6.67E-11 | 6.86E-11 | -10.164 |
| CaNH3+2 | 5.36E-12 | 1.92E-12 | -11.716 |
| CaNO3+ | 4.08E-81 | 3.15E-81 | -80.501 |
| CaOH+ | 7.76E-13 | 6.11E-13 | -12.214 |
| CaPO4- | 5.92E-16 | 4.61E-16 | -15.336 |
| CaSO4 (aq) | 0.003205 | 0.003295 | -2.482 |
| Cd DOM1 | 9.67E-12 | 8.21E-12 | -11.086 |
| Cd(CO3)2-2 | 7.23E-28 | 2.59E-28 | -27.586 |
| Cd(HS)2 (aq) | 8.14E-22 | 8.37E-22 | -21.077 |
| Cd(HS)3- | 1.58E-33 | 1.22E-33 | -32.914 |
| Cd(HS)4-2 | 1.25E-44 | 4.47E-45 | -44.35 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd(NH3)2+2 | 6.8E-24 | 2.44E-24 | -23.613 |
| Cd(NH3)3+2 | 4.3E-32 | 1.54E-32 | -31.812 |
| Cd(NH3)4+2 | 8.01E-41 | 2.87E-41 | -40.542 |
| Cd(NO2)2 (aq) | 1.2E-124 | 1.2E-124 | -123.915 |
| Cd(NO3)2 (aq) | 1.8E-166 | 1.9E-166 | -165.731 |
| Cd(OH)2 (aq) | 3.78E-23 | 3.88E-23 | -22.411 |
| Cd(OH)3- | 1.56E-32 | 1.21E-32 | -31.918 |
| Cd(OH)4-2 | 1.09E-42 | 3.92E-43 | -42.407 |
| Cd(SO4)2-2 | 3.05E-10 | 1.09E-10 | -9.961 |
| Cd+2 | 2.14E-09 | 7.68E-10 | -9.115 |
| Cd2OH+3 | 3.94E-24 | 3.92E-25 | -24.406 |
| CdCl+ | 1.74E-09 | 1.35E-09 | -8.87 |
| CdCl2 (aq) | 9.97E-11 | 1.02E-10 | -9.989 |
| CdCO3 (aq) | 2.47E-18 | 2.54E-18 | -17.596 |
| CdF+ | 2.65E-16 | 2.05E-16 | -15.688 |
| CdHCO3+ | 2.99E-14 | 2.31E-14 | -13.636 |
| CdHPO4 (aq) | 2.3E-16 | 2.37E-16 | -15.626 |
| CdHS+ | 2.35E-15 | 1.81E-15 | -14.741 |
| CdNH3+2 | 2.23E-16 | 7.98E-17 | -16.098 |
| CdNO2+ | 5.99E-67 | 4.64E-67 | -66.334 |
| CdNO3+ | 1.65E-87 | 1.27E-87 | -86.895 |
| CdOH+ | 1.16E-16 | 8.99E-17 | -16.046 |
| CdSO4 (aq) | 1.04E-09 | 1.07E-09 | -8.971 |
| Cl-1 | 0.025415 | 0.018911 | -1.723 |
| CO3-2 | 3.82E-13 | 1.41E-13 | -12.851 |
| Cr2O7-2 | 1.47E-11 | 5.26E-12 | -11.279 |
| CrO3Cl- | 1.71E-11 | 1.32E-11 | -10.879 |
| CrO3H2PO4- | 8.3E-14 | 6.42E-14 | -13.192 |
| CrO3HPO4-2 | 1.18E-12 | 4.22E-13 | -12.375 |
| CrO3SO4-2 | 6.33E-10 | 2.27E-10 | -9.644 |
| CrO4-2 | 1.03E-09 | 3.42E-10 | -9.466 |
| Cu DOM1 | 9.1E-15 | 7.72E-15 | -14.112 |
| Cu(CO3)2-2 | 1.59E-29 | 5.72E-30 | -29.243 |
| Cu(N3)2 (aq) | 5.1E-21 | 5.25E-21 | -20.28 |
| Cu(N3)3- | 9.93E-25 | 7.69E-25 | -24.114 |
| Cu(N3)4-2 | 1.65E-29 | 5.91E-30 | -29.229 |
| Cu(NH3)2+2 | 1.38E-25 | 4.93E-26 | -25.307 |
| Cu(NH3)3+2 | 2.85E-32 | 1.02E-32 | -31.991 |
| Cu(NH3)4+2 | 1.22E-39 | 4.37E-40 | -39.359 |
| Cu(NO2)2 (aq) | 6.8E-130 | 7E-130 | -129.155 |
| Cu(NO3)2 (aq) | 1.1E-171 | 1.1E-171 | -170.957 |
| Cu(OH)2 (aq) | 2.81E-24 | 2.89E-24 | -23.539 |
| Cu(OH)3- | 1.69E-30 | 1.31E-30 | -29.884 |
| Cu(OH)4-2 | 7.67E-41 | 2.75E-41 | -40.561 |
| Cu+2 | 4.72E-14 | 1.81E-14 | -13.741 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu2(OH)2+2 | 1.05E-31 | 3.76E-32 | -31.425 |
| Cu2OH+3 | 1.39E-30 | 1.39E-31 | -30.858 |
| Cu2S3-2 | 1.27E-60 | 4.55E-61 | -60.342 |
| Cu3(OH)4+2 | 6.07E-49 | 2.18E-49 | -48.662 |
| CuCl+ | 8.03E-16 | 6.09E-16 | -15.215 |
| CuCl2 (aq) | 1.87E-18 | 1.92E-18 | -17.717 |
| CuCl3- | 3.72E-22 | 2.82E-22 | -21.55 |
| CuCl4-2 1 | 1.05E-25 | 3.78E-26 | -25.422 |
| CuCO3 (aq) | 1.47E-20 | 1.51E-20 | -19.822 |
| CuF+ | 1.77E-20 | 1.37E-20 | -19.863 |
| CuHCO3+ | 1.41E-18 | 1.09E-18 | -17.963 |
| CuHPO4 (aq) | 1.43E-20 | 1.47E-20 | -19.832 |
| CuHSO4+ | 1.09E-17 | 8.43E-18 | -17.074 |
| CuN3+ | 4.96E-17 | 3.84E-17 | -16.416 |
| CuNH3+2 | 1.74E-19 | 6.22E-20 | -19.206 |
| CuNO2+ | 1.47E-71 | 1.14E-71 | -70.943 |
| CuNO3+ | 3.07E-92 | 2.37E-92 | -91.624 |
| CuOH+ | 1.46E-18 | 1.1E-18 | -17.957 |
| CuS(aq) | 2.04E-27 | 2.1E-27 | -26.678 |
| CuSO4 (aq) | 2.4E-14 | 2.47E-14 | -13.607 |
| DOC (Gaussian DOM) | 0.001399 | 0.001438 | -2.842 |
| DOM1 | 5.47E-05 | 7.33E-06 | -5.135 |
| F-1 | 2.41E-08 | 1.81E-08 | -7.742 |
| Fe DOM1 | 5.4E-12 | 5.35E-12 | -11.272 |
| Fe(N3)2+ | 8.33E-17 | 6.45E-17 | -16.191 |
| Fe(N3)3 (aq) | 3.93E-20 | 4.04E-20 | -19.394 |
| Fe(NH3)2+2 | 2.55E-19 | 9.13E-20 | -19.04 |
| Fe(NH3)3+2 | 1.9E-28 | 6.81E-29 | -28.167 |
| Fe(NH3)4+2 | 6.04E-38 | 2.17E-38 | -37.664 |
| Fe(NO2)2+ | 4.9E-128 | 3.8E-128 | -127.425 |
| Fe(NO2)3 (aq) | 2.5E-185 | 2.6E-185 | -184.587 |
| Fe(OH)2 (aq) | 4.04E-17 | 4.15E-17 | -16.382 |
| Fe(OH)2+ | 2.67E-13 | 2.08E-13 | -12.682 |
| Fe(OH)3- | 4.9E-24 | 3.79E-24 | -23.421 |
| Fe(OH)3 (aq) | 2.12E-19 | 2.18E-19 | -18.662 |
| Fe(OH)4- | 5.78E-24 | 4.51E-24 | -23.346 |
| Fe(SO4)2- | 2.13E-13 | 1.65E-13 | -12.784 |
| Fe+2 | 0.018056 | 0.006941 | -2.159 |
| Fe+3 | 1.19E-13 | 1.99E-14 | -13.701 |
| Fe2(OH)2+4 | 1.38E-22 | 2.28E-24 | -23.641 |
| Fe3(OH)4+5 | 9.83E-32 | 1.62E-34 | -33.792 |
| FeCl+ | 0.000107 | 8.28E-05 | -4.082 |
| FeCl+2 | 2.3E-14 | 8.24E-15 | -14.084 |
| FeCrO4+ | 3.23E-16 | 2.5E-16 | -15.602 |
| FeF+ | 2.63E-09 | 2.04E-09 | -8.691 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeF+2 | 9.57E-16 | 3.43E-16 | -15.464 |
| FeF2+ | 3.04E-19 | 2.35E-19 | -18.629 |
| FeF3 (aq) | 3.83E-24 | 3.94E-24 | -23.404 |
| FeH2PO4+ | 1.35E-06 | 1.06E-06 | -5.977 |
| FeH2PO4+2 | 3.09E-16 | 1.14E-16 | -15.942 |
| FeHCO3+ | 1.06E-07 | 8.31E-08 | -7.08 |
| FeHPO4 (aq) | 1.63E-09 | 1.68E-09 | -8.775 |
| FeHPO4+ | 1.94E-14 | 1.51E-14 | -13.821 |
| FeHS+ | 8.64E-11 | 6.69E-11 | -10.175 |
| FeN3+2 | 2.53E-14 | 9.07E-15 | -14.042 |
| FeNH3+2 | 1.35E-10 | 4.82E-11 | -10.317 |
| FeNO2+2 | 5.28E-70 | 1.89E-70 | -69.723 |
| FeOH+ | 5.19E-09 | 4.02E-09 | -8.396 |
| FeOH+2 | 1.18E-12 | 4.22E-13 | -12.375 |
| FeSO4 (aq) | 0.009949 | 0.010229 | -1.99 |
| FeSO4+ | 2.16E-12 | 1.67E-12 | -11.776 |
| H DOM1 | 2.88E-05 | 1.26E-05 | -4.901 |
| H+1 | 0.000386 | 0.000316 | -3.5 |
| H2AsO3- | 9.55E-12 | 7.39E-12 | -11.131 |
| H2AsO4- | 8E-14 | 6.19E-14 | -13.208 |
| H2CO3* (aq) | 0.000965 | 0.000993 | -3.003 |
| H2CrO4 (aq) | 3.94E-11 | 4.05E-11 | -10.393 |
| H2PO4- | 5.01E-07 | 3.9E-07 | -6.409 |
| H2S (aq) | 1.03E-10 | 1.06E-10 | -9.973 |
| H3AsO3 | 4.95E-06 | 5.09E-06 | -5.293 |
| H3AsO4 | 3.4E-15 | 3.49E-15 | -14.457 |
| H3PO4 | 1.52E-08 | 1.56E-08 | -7.806 |
| HAsO3-2 | 3.32E-22 | 1.19E-22 | -21.925 |
| HAsO4-2 | 5.35E-17 | 1.92E-17 | -16.717 |
| HCO3- | 1.53E-06 | 1.2E-06 | -5.922 |
| HCrO4- | 4.4E-07 | 3.41E-07 | -6.468 |
| HF (aq) | 6.99E-09 | 7.19E-09 | -8.143 |
| HF2- | 6.52E-16 | 4.89E-16 | -15.31 |
| Hg(CO3)2-2 | 1.57E-40 | 5.63E-41 | -40.249 |
| Hg(HS)2 (aq) | 1.02E-19 | 1.05E-19 | -18.981 |
| Hg(N3)2 (aq) | 6.31E-19 | 6.49E-19 | -18.188 |
| Hg(NH3)2+2 | 5.79E-31 | 2.08E-31 | -30.683 |
| Hg(NH3)4+2 | 1.65E-48 | 5.91E-49 | -48.228 |
| Hg(NO2)2 (aq) | 2.1E-139 | 2.2E-139 | -138.662 |
| Hg(NO2)3- | 5.9E-197 | 4.5E-197 | -196.344 |
| Hg(NO2)4-2 | 1.9E-255 | 7E-256 | -255.156 |
| Hg(NO3)2 (aq) | 1.8E-188 | 1.9E-188 | -187.724 |
| Hg(OH)2 | 4.99E-30 | 5.13E-30 | -29.29 |
| Hg(SO4)2-2 | 2.83E-31 | 1.01E-31 | -30.994 |
| Hg+2 | 3.66E-30 | 1.31E-30 | -29.883 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg2OH+3 | 2.26E-59 | 2.25E-60 | -59.648 |
| Hg3(OH)3+3 | 5.45E-86 | 5.42E-87 | -86.266 |
| HgCl+ | 9.1E-25 | 7.04E-25 | -24.152 |
| HgCl2 (aq) | 9.94E-20 | 1.02E-19 | -18.991 |
| HgCl3-1 | 2.48E-20 | 1.92E-20 | -19.716 |
| HgCl4-2 | 4.54E-21 | 1.63E-21 | -20.789 |
| HgClOH (aq) | 1.51E-24 | 1.55E-24 | -23.809 |
| HgCO3 (aq) | 1.38E-31 | 1.42E-31 | -30.849 |
| HgF+ | 1.14E-36 | 8.85E-37 | -36.053 |
| HgHCO3+ | 9.61E-31 | 7.44E-31 | -30.129 |
| HgHS2- | 1.38E-22 | 1.07E-22 | -21.971 |
| HgN3+ | 4.69E-14 | 3.63E-14 | -13.44 |
| HgNO2+ | 5.03E-84 | 3.89E-84 | -83.41 |
| HgNO3+ | 1.5E-109 | 1.2E-109 | -108.935 |
| HgOH+ | 1.6E-30 | 1.24E-30 | -29.907 |
| HgOHCO3- | 6.79E-35 | 5.25E-35 | -34.28 |
| HgS2-2 | 1.84E-27 | 6.6E-28 | -27.181 |
| HgSO4 (aq) | 1.44E-30 | 1.48E-30 | -29.831 |
| HN3 (aq) | 4.62E-05 | 4.75E-05 | -4.323 |
| HNO2 (aq) | 2.61E-60 | 2.68E-60 | -59.572 |
| HPO4-2 | 2.09E-10 | 7.5E-11 | -10.125 |
| HS-1 | 3.08E-14 | 2.31E-14 | -13.636 |
| HSO4- | 0.000206 | 0.000158 | -3.802 |
| K+1 | 0.000318 | 0.000237 | -3.626 |
| K2HPO4 (aq) | 4.42E-17 | 4.54E-17 | -16.343 |
| K2PO4- | 1.07E-24 | 8.27E-25 | -24.083 |
| KCl (aq) | 2.31E-06 | 2.37E-06 | -5.625 |
| KCr2O7- | 1.39E-14 | 1.08E-14 | -13.969 |
| KCrO4- | 3.89E-13 | 3.01E-13 | -12.521 |
| KF (aq) | 1.9E-12 | 1.96E-12 | -11.708 |
| KH2PO4 (aq) | 1.39E-10 | 1.43E-10 | -9.844 |
| KHPO4- | 1.4E-13 | 1.09E-13 | -12.962 |
| KNO3 (aq) | 6.87E-83 | 7.07E-83 | -82.151 |
| KOH (aq) | 5.82E-15 | 5.98E-15 | -14.223 |
| KPO4-2 | 1.17E-21 | 4.19E-22 | -21.378 |
| KSO4- | 1.21E-05 | 9.39E-06 | -5.027 |
| Mg DOM1 | 1.04E-06 | 8.83E-07 | -6.054 |
| Mg(NH3)2+2 | 5.89E-22 | 2.11E-22 | -21.675 |
| Mg+2 | 0.004943 | 0.002073 | -2.684 |
| Mg2CO3+2 | 6.57E-15 | 2.36E-15 | -14.628 |
| MgCl+ | 0.000191 | 0.000148 | -3.831 |
| MgCO3 (aq) | 2.03E-13 | 2.09E-13 | -12.681 |
| MgF+ | 3.24E-09 | 2.48E-09 | -8.605 |
| MgHCO3+ | 3.17E-08 | 2.41E-08 | -7.618 |
| MgHPO4 (aq) | 8.07E-11 | 8.29E-11 | -10.081 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgOH+ | 1.28E-11 | 1.02E-11 | -10.992 |
| MgPO4- | 8.11E-18 | 6.32E-18 | -17.199 |
| MgSO4 (aq) | 0.002271 | 0.002335 | -2.632 |
| Mn+3 | 4.55E-05 | 7.61E-06 | -5.119 |
| N3-1 | 3.78E-06 | 2.92E-06 | -5.534 |
| Na+1 | 0.012081 | 0.009357 | -2.029 |
| Na2HPO4 (aq) | 4.56E-14 | 4.69E-14 | -13.329 |
| Na2PO4- | 3.57E-21 | 2.76E-21 | -20.559 |
| NaCl (aq) | 9.65E-05 | 9.92E-05 | -4.004 |
| NaCO3- | 4.19E-14 | 3.27E-14 | -13.486 |
| NaCrO4- | 2.06E-11 | 1.59E-11 | -10.798 |
| NaF (aq) | 1.46E-10 | 1.5E-10 | -9.824 |
| NaH2PO4 (aq) | 5.51E-09 | 5.66E-09 | -8.247 |
| NaHCO3 (aq) | 6.45E-09 | 6.63E-09 | -8.178 |
| NaHPO4- | 8.58E-12 | 6.68E-12 | -11.175 |
| NaNO3 (aq) | 1E-81 | 1.03E-81 | -80.987 |
| NaOH (aq) | 1.58E-13 | 1.62E-13 | -12.79 |
| NaPO4-2 | 5.09E-20 | 1.83E-20 | -19.739 |
| NaSO4- | 0.000437 | 0.00034 | -3.468 |
| NH3 (aq) | 2.38E-10 | 2.45E-10 | -9.612 |
| NH4+1 | 0.000385 | 0.000282 | -3.55 |
| NH4Cr2O7- | 1.92E-14 | 1.49E-14 | -13.827 |
| NH4SO4- | 2.62E-05 | 2.03E-05 | -4.693 |
| Ni DOM1 | 4.62E-08 | 3.92E-08 | -7.407 |
| Ni(N3)2 (aq) | 3.01E-15 | 3.09E-15 | -14.51 |
| Ni(NH3)2+2 | 7.07E-20 | 2.54E-20 | -19.596 |
| Ni(NH3)3+2 | 1E-27 | 3.59E-28 | -27.445 |
| Ni(NH3)4+2 | 4.21E-36 | 1.51E-36 | -35.821 |
| Ni(NH3)5+2 | 5.71E-45 | 2.05E-45 | -44.689 |
| Ni(NH3)6+2 | 1.65E-54 | 5.91E-55 | -54.228 |
| Ni(NO2)2 (aq) | 7.9E-123 | 8.1E-123 | -122.09 |
| Ni(OH)2 (aq) | 3.6E-18 | 3.7E-18 | -17.432 |
| Ni(OH)3- | 1.52E-25 | 1.17E-25 | -24.93 |
| Ni(SO4)2-2 | 3.04E-09 | 1.09E-09 | -8.962 |
| Ni+2 | 1.02E-05 | 3.66E-06 | -5.436 |
| NiCl+ | 3.23E-08 | 2.5E-08 | -7.602 |
| NiCl2 (aq) | 1.64E-11 | 1.69E-11 | -10.773 |
| NiCO3 (aq) | 1.87E-14 | 1.92E-14 | -13.717 |
| NiF+ | 1.55E-12 | 1.2E-12 | -11.922 |
| NiH2PO4+ | 1.21E-11 | 9.39E-12 | -11.027 |
| NiHCO3+ | 5.55E-10 | 4.3E-10 | -9.367 |
| NiHPO4 (aq) | 1.95E-13 | 2.01E-13 | -12.697 |
| NiHS+ | 3.38E-14 | 2.62E-14 | -13.582 |
| NiN3+ | 2.6E-10 | 2.02E-10 | -9.696 |
| NiNH3+2 | 1.64E-12 | 5.87E-13 | -12.231 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NiNO2+ | 6.81E-64 | 5.27E-64 | -63.278 |
| NiNO3+ | 4.65E-84 | 3.6E-84 | -83.444 |
| NiOH+ | 9.17E-13 | 7.09E-13 | -12.149 |
| NiSO4 (aq) | 4.4E-06 | 4.52E-06 | -5.344 |
| NO2-1 | 7.75E-60 | 6E-60 | -59.222 |
| NO3-1 | 5.28E-79 | 3.91E-79 | -78.408 |
| OH- | 1.94E-11 | 1.45E-11 | -10.837 |
| Pb DOM1 | 5.91E-09 | 5.02E-09 | -8.299 |
| Pb(CO3)2-2 | 2.85E-24 | 1.02E-24 | -23.99 |
| Pb(HS)2 (aq) | 5.71E-21 | 5.87E-21 | -20.231 |
| Pb(HS)3- | 3.5E-33 | 2.71E-33 | -32.567 |
| Pb(NO2)2 (aq) | 2.7E-124 | 2.7E-124 | -123.562 |
| Pb(NO3)2 (aq) | 2.4E-164 | 2.5E-164 | -163.604 |
| Pb(OH)2 (aq) | 4.61E-19 | 4.74E-19 | -18.325 |
| Pb(OH)3- | 1.94E-26 | 1.5E-26 | -25.823 |
| Pb(SO4)2-2 | 2.19E-09 | 7.86E-10 | -9.105 |
| Pb+2 | 1.65E-08 | 5.91E-09 | -8.229 |
| Pb2OH+3 | 4.44E-19 | 4.41E-20 | -19.355 |
| Pb3(OH)4+2 | 1.45E-35 | 5.19E-36 | -35.285 |
| Pb4(OH)4+4 | 2.86E-39 | 4.73E-41 | -40.325 |
| PbCl+ | 4.64E-09 | 3.59E-09 | -8.445 |
| PbCl2 (aq) | 1.38E-10 | 1.42E-10 | -9.848 |
| PbCl3- | 2.75E-12 | 2.13E-12 | -11.671 |
| PbCl4-2 | 4.11E-14 | 1.47E-14 | -13.832 |
| PbCO3 (aq) | 2.75E-15 | 2.82E-15 | -14.549 |
| PbF+ | 1.95E-14 | 1.51E-14 | -13.821 |
| PbF2 (aq) | 3.27E-21 | 3.36E-21 | -20.473 |
| PbH2PO4+ | 7.32E-14 | 5.67E-14 | -13.247 |
| PbHCO3+ | 5.78E-12 | 4.47E-12 | -11.349 |
| PbHPO4 (aq) | 4.4E-16 | 4.52E-16 | -15.345 |
| PbNO2+ | 1.48E-65 | 1.15E-65 | -64.941 |
| PbNO3+ | 4.54E-86 | 3.51E-86 | -85.454 |
| PbOH+ | 4.36E-13 | 3.38E-13 | -12.471 |
| PbSO4 (aq) | 1.89E-08 | 1.94E-08 | -7.712 |
| PO4-3 | 8.14E-19 | 8.11E-20 | -19.091 |
| S-2 | 4.06E-28 | 1.46E-28 | -27.837 |
| SO4-2 | 0.020507 | 0.006715 | -2.173 |
| Zn DOM1 | 1.08E-07 | 9.16E-08 | -7.038 |
| Zn(CO3)2-2 | 5.98E-24 | 2.14E-24 | -23.669 |
| Zn(N3)2 (aq) | 4.28E-15 | 4.4E-15 | -14.356 |
| Zn(N3)3- | 9.51E-20 | 7.36E-20 | -19.133 |
| Zn(NH3)2+2 | 3.94E-20 | 1.41E-20 | -19.85 |
| Zn(NH3)3+2 | 2.84E-27 | 1.02E-27 | -26.992 |
| Zn(NH3)4+2 | 1E-34 | 3.59E-35 | -34.445 |
| Zn(NO2)2 (aq) | 3E-123 | 3.1E-123 | -122.511 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn(NO3)2 (aq) | 4E-163 | 4.1E-163 | -162.383 |
| Zn(OH)2 (aq) | 6.68E-16 | 6.87E-16 | -15.163 |
| Zn(OH)3- | 8.91E-24 | 6.9E-24 | -23.161 |
| Zn(OH)4-2 | 9.69E-33 | 3.47E-33 | -32.459 |
| Zn(SO4)2-2 | 1.29E-06 | 4.64E-07 | -6.333 |
| Zn+2 | 1.41E-05 | 5.4E-06 | -5.267 |
| Zn2OH+3 | 3.82E-16 | 3.8E-17 | -16.421 |
| Zn2S3-2 | 7.11E-41 | 2.55E-41 | -40.594 |
| Zn4S6-4 | 6.68E-79 | 1.1E-80 | -79.957 |
| ZnCl+ | 3.6E-07 | 2.73E-07 | -6.563 |
| ZnCl2 (aq) | 3.22E-09 | 3.31E-09 | -8.48 |
| ZnCl3- | 8.53E-11 | 6.6E-11 | -10.18 |
| ZnCl4-2 | 1.61E-12 | 5.76E-13 | -12.24 |
| ZnCO3 (aq) | 4.27E-14 | 4.39E-14 | -13.358 |
| ZnF+ | 2.16E-12 | 1.67E-12 | -11.777 |
| ZnHCO3+ | 2.1E-10 | 1.63E-10 | -9.789 |
| ZnHPO4 (aq) | 6.6E-13 | 6.79E-13 | -12.168 |
| ZnN3+ | 2.93E-10 | 2.27E-10 | -9.644 |
| ZnNH3+2 | 6.96E-13 | 2.5E-13 | -12.603 |
| ZnNO2+ | 2.52E-64 | 1.95E-64 | -63.709 |
| ZnNO3+ | 7.31E-84 | 5.66E-84 | -83.247 |
| ZnOH+ | 1.02E-11 | 7.86E-12 | -11.105 |
| ZnS (aq) | 1.43E-17 | 1.47E-17 | -16.834 |
| ZnSO4 (aq) | 7.08E-06 | 7.28E-06 | -5.138 |

## B1.2: Eh 200

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 2.93E-05 | 2.9E-05 | -4.538 |
| Al(OH)2+ | 1.66E-09 | 1.29E-09 | -8.89 |
| Al(OH)3 (aq) | 3.74E-13 | 3.85E-13 | -12.415 |
| Al(OH)4- | 3.55E-16 | 2.72E-16 | -15.566 |
| Al(SO4)2- | 0.000789 | 0.000604 | -3.219 |
| Al+3 | 0.000339 | 5.63E-05 | -4.249 |
| Al2(OH)2+4 | 3.48E-09 | 5.65E-11 | -10.248 |
| Al2(OH)2CO3+2 | 1.61E-11 | 5.75E-12 | -11.24 |
| Al2PO4+3 | 6.2E-09 | 6.11E-10 | -9.214 |
| Al3(OH)4+5 | 1.27E-12 | 2.03E-15 | -14.692 |
| AlCl+2 | 1.21E-06 | 4.33E-07 | -6.363 |
| AlF+2 | 1.31E-05 | 4.82E-06 | -5.317 |
| AlF2+ | 2.19E-08 | 1.7E-08 | -7.768 |
| AlF3 (aq) | 1.73E-12 | 1.78E-12 | -11.75 |
| AlF4- | 1.04E-17 | 7.95E-18 | -17.1 |
| AlHPO4+ | 9.48E-08 | 7.33E-08 | -7.135 |
| AlOH+2 | 1.25E-06 | 4.59E-07 | -6.338 |
| AlSO4+ | 0.002836 | 0.00217 | -2.663 |
| As3S4(HS)- | 8.7E-110 | 6.7E-110 | -109.173 |
| AsO4-3 | 7.55E-23 | 7.43E-24 | -23.129 |
| AsS(OH)HS- | 6.12E-41 | 4.73E-41 | -40.325 |
| Ca DOM1 | 7.22E-06 | 6.12E-06 | -5.213 |
| Ca(NH3)2+2 | 3.41E-22 | 1.22E-22 | -21.915 |
| Ca(NO3)2 | 1.1E-142 | 1.1E-142 | -141.955 |
| Ca+2 | 0.005923 | 0.002374 | -2.624 |
| CaCl+ | 0.000138 | 0.000106 | -3.973 |
| CaCO3 (aq) | 1.17E-13 | 1.2E-13 | -12.92 |
| CaCrO4 (aq) | 2.33E-10 | 2.4E-10 | -9.621 |
| CaF+ | 3.11E-10 | 2.4E-10 | -9.619 |
| CaH2PO4+ | 2.23E-08 | 1.73E-08 | -7.761 |
| CaHCO3+ | 1.91E-08 | 1.5E-08 | -7.823 |
| CaHPO4 (aq) | 3.32E-11 | 3.41E-11 | -10.467 |
| CaNH3+2 | 2.71E-12 | 9.67E-13 | -12.015 |
| CaNO3+ | 4.03E-70 | 3.11E-70 | -69.507 |
| CaOH+ | 3.91E-13 | 3.07E-13 | -12.512 |
| CaPO4- | 1.48E-16 | 1.15E-16 | -15.939 |
| CaSO4 (aq) | 0.003164 | 0.003255 | -2.488 |
| Cd DOM1 | 5.89E-12 | 4.99E-12 | -11.302 |
| Cd(CO3)2-2 | 4.61E-29 | 1.65E-29 | -28.783 |
| Cd(HS)2 (aq) | 2.05E-44 | 2.11E-44 | -43.675 |
| Cd(HS)3- | 2E-67 | 1.54E-67 | -66.811 |
| Cd(HS)4-2 | 7.94E-90 | 2.83E-90 | -89.548 |
| Cd(NH3)2+2 | 1.72E-24 | 6.14E-25 | -24.212 |
| Cd(NH3)3+2 | 5.44E-33 | 1.94E-33 | -32.712 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd(NH3)4+2 | 5.08E-42 | 1.81E-42 | -41.742 |
| Cd(NO2)2 (aq) | 1.8E-108 | 1.9E-108 | -107.725 |
| Cd(NO3)2 (aq) | 1.8E-144 | 1.8E-144 | -143.744 |
| Cd(OH)2 (aq) | 9.52E-24 | 9.79E-24 | -23.009 |
| Cd(OH)3- | 1.98E-33 | 1.53E-33 | -32.816 |
| Cd(OH)4-2 | 6.95E-44 | 2.48E-44 | -43.605 |
| Cd(SO4)2-2 | 2.98E-10 | 1.06E-10 | -9.973 |
| Cd+2 | 2.16E-09 | 7.71E-10 | -9.113 |
| Cd2OH+3 | 2.01E-24 | 1.98E-25 | -24.703 |
| CdCl+ | 1.75E-09 | 1.35E-09 | -8.869 |
| CdCl2 (aq) | 9.96E-11 | 1.02E-10 | -9.989 |
| CdCO3 (aq) | 6.23E-19 | 6.41E-19 | -18.193 |
| CdF+ | 1.31E-16 | 1.02E-16 | -15.993 |
| CdHCO3+ | 1.51E-14 | 1.17E-14 | -13.933 |
| CdHPO4 (aq) | 1.14E-16 | 1.18E-16 | -15.929 |
| CdHS+ | 1.18E-26 | 9.14E-27 | -26.039 |
| CdNH3+2 | 1.12E-16 | 4.01E-17 | -16.397 |
| CdNO2+ | 7.48E-59 | 5.78E-59 | -58.238 |
| CdNO3+ | 1.63E-76 | 1.26E-76 | -75.901 |
| CdOH+ | 5.85E-17 | 4.52E-17 | -16.344 |
| CdSO4 (aq) | 1.03E-09 | 1.06E-09 | -8.976 |
| Cl-1 | 0.025414 | 0.018877 | -1.724 |
| CO3-2 | 9.66E-14 | 3.55E-14 | -13.45 |
| Cr2O7-2 | 1.47E-11 | 5.25E-12 | -11.28 |
| CrO3Cl- | 3.4E-11 | 2.63E-11 | -10.581 |
| CrO3H2PO4- | 1.64E-13 | 1.27E-13 | -12.898 |
| CrO3HPO4-2 | 1.17E-12 | 4.17E-13 | -12.38 |
| CrO3SO4-2 | 1.25E-09 | 4.45E-10 | -9.351 |
| CrO4-2 | 5.21E-10 | 1.71E-10 | -9.766 |
| Cu DOM1 | 5.61E-09 | 4.75E-09 | -8.323 |
| Cu(CO3)2-2 | 1.03E-24 | 3.68E-25 | -24.434 |
| Cu(N3)2 (aq) | 1.41E-15 | 1.45E-15 | -14.839 |
| Cu(N3)3- | 1.43E-19 | 1.11E-19 | -18.957 |
| Cu(N3)4-2 | 1.24E-24 | 4.43E-25 | -24.354 |
| Cu(NH3)2+2 | 3.52E-20 | 1.26E-20 | -19.901 |
| Cu(NH3)3+2 | 3.65E-27 | 1.3E-27 | -26.885 |
| Cu(NH3)4+2 | 7.83E-35 | 2.79E-35 | -34.554 |
| Cu(NO2)2 (aq) | 1.1E-107 | 1.1E-107 | -106.96 |
| Cu(NO3)2 (aq) | 1.1E-143 | 1.1E-143 | -142.965 |
| Cu(OH)2 (aq) | 7.17E-19 | 7.37E-19 | -18.132 |
| Cu(OH)3- | 2.16E-25 | 1.67E-25 | -24.777 |
| Cu(OH)4-2 | 4.94E-36 | 1.76E-36 | -35.754 |
| Cu+2 | 4.82E-08 | 1.84E-08 | -7.734 |
| Cu2(OH)2+2 | 2.73E-20 | 9.76E-21 | -20.011 |
| Cu2OH+3 | 7.29E-19 | 7.18E-20 | -19.144 |
| Cu2S3-2 | 2.09E-83 | 7.47E-84 | -83.127 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu3(OH)4+2 | 4.04E-32 | 1.44E-32 | -31.841 |
| CuCl+ | 8.16E-10 | 6.18E-10 | -9.209 |
| CuCl2 (aq) | 1.89E-12 | 1.94E-12 | -11.711 |
| CuCl3- | 3.77E-16 | 2.85E-16 | -15.545 |
| CuCl4-2 1 | 1.07E-19 | 3.81E-20 | -19.419 |
| CuCO3 (aq) | 3.74E-15 | 3.85E-15 | -14.414 |
| CuF+ | 8.89E-15 | 6.87E-15 | -14.163 |
| CuHCO3+ | 7.19E-13 | 5.55E-13 | -12.255 |
| CuHPO4 (aq) | 7.2E-15 | 7.41E-15 | -14.13 |
| CuHSO4+ | 2.18E-11 | 1.68E-11 | -10.774 |
| CuN3+ | 2.63E-11 | 2.03E-11 | -10.692 |
| CuNH3+2 | 8.88E-14 | 3.17E-14 | -13.499 |
| CuNO2+ | 1.86E-57 | 1.44E-57 | -56.842 |
| CuNO3+ | 3.07E-75 | 2.37E-75 | -74.625 |
| CuOH+ | 7.42E-13 | 5.62E-13 | -12.25 |
| CuS(aq) | 5.22E-33 | 5.37E-33 | -32.27 |
| CuSO4 (aq) | 2.4E-08 | 2.47E-08 | -7.607 |
| DOC (Gaussian DOM) | 0.001399 | 0.001439 | -2.842 |
| DOM1 | 4.83E-05 | 6.41E-06 | -5.193 |
| F-1 | 1.19E-08 | 8.92E-09 | -8.049 |
| Fe DOM1 | 1.84E-10 | 1.82E-10 | -9.739 |
| Fe(N3)2+ | 1.27E-15 | 9.85E-16 | -15.007 |
| Fe(N3)3 (aq) | 3.12E-19 | 3.21E-19 | -18.493 |
| Fe(NH3)2+2 | 6.43E-20 | 2.3E-20 | -19.639 |
| Fe(NH3)3+2 | 2.4E-29 | 8.57E-30 | -29.067 |
| Fe(NH3)4+2 | 3.82E-39 | 1.37E-39 | -38.865 |
| Fe(NO2)2+ | 4.2E-110 | 3.3E-110 | -109.486 |
| Fe(NO2)3 (aq) | 2.7E-159 | 2.8E-159 | -158.554 |
| Fe(OH)2 (aq) | 1.02E-17 | 1.05E-17 | -16.981 |
| Fe(OH)2+ | 3.77E-12 | 2.94E-12 | -11.532 |
| Fe(OH)3- | 6.19E-25 | 4.79E-25 | -24.32 |
| Fe(OH)3 (aq) | 1.5E-18 | 1.54E-18 | -17.812 |
| Fe(OH)4- | 2.06E-23 | 1.6E-23 | -22.796 |
| Fe(SO4)2- | 1.16E-11 | 8.97E-12 | -11.047 |
| Fe+2 | 0.018191 | 0.00696 | -2.157 |
| Fe+3 | 6.75E-12 | 1.12E-12 | -11.951 |
| Fe2(OH)2+4 | 1.12E-19 | 1.82E-21 | -20.741 |
| Fe3(OH)4+5 | 1.14E-27 | 1.82E-30 | -29.741 |
| FeCl+ | 0.000107 | 8.29E-05 | -4.081 |
| FeCl+2 | 1.3E-12 | 4.63E-13 | -12.335 |
| FeCrO4+ | 9.12E-15 | 7.05E-15 | -14.152 |
| FeF+ | 1.3E-09 | 1.01E-09 | -8.997 |
| FeF+2 | 2.67E-14 | 9.53E-15 | -14.021 |
| FeF2+ | 4.16E-18 | 3.21E-18 | -17.493 |
| FeF3 (aq) | 2.58E-23 | 2.66E-23 | -22.575 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeH2PO4+ | 1.34E-06 | 1.05E-06 | -5.98 |
| FeH2PO4+2 | 1.73E-14 | 6.36E-15 | -14.197 |
| FeHCO3+ | 5.32E-08 | 4.18E-08 | -7.378 |
| FeHPO4 (aq) | 8.12E-10 | 8.35E-10 | -9.078 |
| FeHPO4+ | 5.41E-13 | 4.21E-13 | -12.376 |
| FeHS+ | 4.35E-22 | 3.36E-22 | -21.473 |
| FeN3+2 | 7.45E-13 | 2.66E-13 | -12.575 |
| FeNH3+2 | 6.79E-11 | 2.42E-11 | -10.616 |
| FeNO2+2 | 3.71E-60 | 1.32E-60 | -59.878 |
| FeOH+ | 2.61E-09 | 2.02E-09 | -8.695 |
| FeOH+2 | 3.34E-11 | 1.19E-11 | -10.924 |
| FeSO4 (aq) | 0.009814 | 0.010095 | -1.996 |
| FeSO4+ | 1.2E-10 | 9.28E-11 | -10.033 |
| H DOM1 | 3.5E-05 | 1.52E-05 | -4.819 |
| H+1 | 0.00077 | 0.000631 | -3.2 |
| H2AsO3- | 4.79E-12 | 3.71E-12 | -11.431 |
| H2AsO4- | 3.18E-11 | 2.45E-11 | -10.61 |
| H2CO3* (aq) | 0.000966 | 0.000994 | -3.003 |
| H2CrO4 (aq) | 7.84E-11 | 8.07E-11 | -10.093 |
| H2PO4- | 4.96E-07 | 3.86E-07 | -6.413 |
| H2S (aq) | 1.03E-21 | 1.06E-21 | -20.973 |
| H3AsO3 | 4.95E-06 | 5.09E-06 | -5.293 |
| H3AsO4 | 2.69E-12 | 2.76E-12 | -11.558 |
| H3PO4 | 3E-08 | 3.08E-08 | -7.511 |
| HAsO3-2 | 8.37E-23 | 2.99E-23 | -22.524 |
| HAsO4-2 | 1.07E-14 | 3.82E-15 | -14.418 |
| HCO3- | 7.71E-07 | 6E-07 | -6.222 |
| HCrO4- | 4.4E-07 | 3.4E-07 | -6.468 |
| HF (aq) | 6.88E-09 | 7.07E-09 | -8.15 |
| HF2- | 3.17E-16 | 2.37E-16 | -15.625 |
| Hg(CO3)2-2 | 1.61E-36 | 5.76E-37 | -36.24 |
| Hg(HS)2 (aq) | 4.13E-37 | 4.25E-37 | -36.372 |
| Hg(N3)2 (aq) | 6.95E-15 | 7.15E-15 | -14.146 |
| Hg(NH3)2+2 | 2.36E-26 | 8.41E-27 | -26.075 |
| Hg(NH3)4+2 | 1.68E-44 | 6E-45 | -44.222 |
| Hg(NO2)2 (aq) | 5.3E-118 | 5.4E-118 | -117.265 |
| Hg(NO2)3- | 1.8E-167 | 1.4E-167 | -166.853 |
| Hg(NO2)4-2 | 7.5E-218 | 2.7E-218 | -217.57 |
| Hg(NO3)2 (aq) | 2.9E-161 | 2.9E-161 | -160.53 |
| Hg(OH)2 | 2.02E-25 | 2.08E-25 | -24.682 |
| Hg(SO4)2-2 | 4.45E-26 | 1.59E-26 | -25.799 |
| Hg+2 | 5.93E-25 | 2.12E-25 | -24.674 |
| Hg2OH+3 | 2.99E-49 | 2.94E-50 | -49.532 |
| Hg3(OH)3+3 | 2.92E-71 | 2.88E-72 | -71.541 |
| HgCl+ | 1.47E-19 | 1.14E-19 | -18.945 |
| HgCl2 (aq) | 1.6E-14 | 1.64E-14 | -13.784 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgCl3-1 | 3.99E-15 | 3.09E-15 | -14.51 |
| HgCl4-2 | 7.31E-16 | 2.61E-16 | -15.583 |
| HgClOH (aq) | 1.22E-19 | 1.26E-19 | -18.901 |
| HgCO3 (aq) | 5.6E-27 | 5.76E-27 | -26.24 |
| HgF+ | 9.12E-32 | 7.05E-32 | -31.152 |
| HgHCO3+ | 7.8E-26 | 6.03E-26 | -25.22 |
| HgHS2- | 2.82E-40 | 2.18E-40 | -39.662 |
| HgN3+ | 2.49E-10 | 1.93E-10 | -9.715 |
| HgNO2+ | 1.01E-70 | 7.81E-71 | -70.107 |
| HgNO3+ | 2.39E-93 | 1.85E-93 | -92.734 |
| HgOH+ | 1.3E-25 | 1E-25 | -24.999 |
| HgOHCO3- | 1.38E-30 | 1.07E-30 | -29.971 |
| HgS2-2 | 1.89E-45 | 6.73E-46 | -45.172 |
| HgSO4 (aq) | 2.28E-25 | 2.35E-25 | -24.629 |
| HN3 (aq) | 4.8E-05 | 4.94E-05 | -4.306 |
| HNO2 (aq) | 6.46E-52 | 6.64E-52 | -51.178 |
| HPO4-2 | 1.04E-10 | 3.72E-11 | -10.43 |
| HS-1 | 1.55E-25 | 1.16E-25 | -24.936 |
| HSO4- | 0.000405 | 0.00031 | -3.508 |
| K+1 | 0.000318 | 0.000236 | -3.626 |
| K2HPO4 (aq) | 2.18E-17 | 2.25E-17 | -16.648 |
| K2PO4- | 2.65E-25 | 2.05E-25 | -24.688 |
| KCl (aq) | 2.3E-06 | 2.37E-06 | -5.626 |
| KCr2O7- | 1.39E-14 | 1.07E-14 | -13.97 |
| KCrO4- | 1.95E-13 | 1.51E-13 | -12.822 |
| KF (aq) | 9.38E-13 | 9.64E-13 | -12.016 |
| KH2PO4 (aq) | 1.38E-10 | 1.42E-10 | -9.849 |
| KHPO4- | 6.94E-14 | 5.41E-14 | -13.267 |
| KNO3 (aq) | 6.75E-72 | 6.94E-72 | -71.159 |
| KOH (aq) | 2.91E-15 | 3E-15 | -14.524 |
| KPO4-2 | 2.91E-22 | 1.04E-22 | -21.983 |
| KSO4- | 1.19E-05 | 9.24E-06 | -5.035 |
| Mg DOM1 | 6.32E-07 | 5.36E-07 | -6.271 |
| Mg(NH3)2+2 | 1.49E-22 | 5.31E-23 | -22.275 |
| Mg+2 | 0.004974 | 0.002078 | -2.682 |
| Mg2CO3+2 | 1.67E-15 | 5.96E-16 | -15.225 |
| MgCl+ | 0.000191 | 0.000148 | -3.831 |
| MgCO3 (aq) | 5.11E-14 | 5.26E-14 | -13.279 |
| MgF+ | 1.6E-09 | 1.23E-09 | -8.911 |
| MgHCO3+ | 1.6E-08 | 1.21E-08 | -7.917 |
| MgHPO4 (aq) | 4.01E-11 | 4.12E-11 | -10.385 |
| MgOH+ | 6.45E-12 | 5.12E-12 | -11.291 |
| MgPO4- | 2.02E-18 | 1.57E-18 | -17.803 |
| MgSO4 (aq) | 0.00224 | 0.002304 | -2.637 |
| Mn+3 | 4.55E-05 | 7.55E-06 | -5.122 |
| N3-1 | 1.97E-06 | 1.52E-06 | -5.817 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Na+1 | 0.012088 | 0.009351 | -2.029 |
| Na2HPO4 (aq) | 2.26E-14 | 2.32E-14 | -13.634 |
| Na2PO4- | 8.87E-22 | 6.85E-22 | -21.164 |
| NaCl (aq) | 9.62E-05 | 9.9E-05 | -4.005 |
| NaCO3- | 1.06E-14 | 8.21E-15 | -14.085 |
| NaCrO4- | 1.03E-11 | 7.96E-12 | -11.099 |
| NaF (aq) | 7.18E-11 | 7.39E-11 | -10.132 |
| NaH2PO4 (aq) | 5.44E-09 | 5.6E-09 | -8.252 |
| NaHCO3 (aq) | 3.23E-09 | 3.33E-09 | -8.478 |
| NaHPO4- | 4.25E-12 | 3.31E-12 | -11.48 |
| NaNO3 (aq) | 9.84E-71 | 1.01E-70 | -69.995 |
| NaOH (aq) | 7.89E-14 | 8.11E-14 | -13.091 |
| NaPO4-2 | 1.27E-20 | 4.53E-21 | -20.344 |
| NaSO4- | 0.00043 | 0.000335 | -3.475 |
| NH3 (aq) | 1.19E-10 | 1.22E-10 | -9.912 |
| NH4+1 | 0.000386 | 0.000282 | -3.55 |
| NH4Cr2O7- | 1.92E-14 | 1.48E-14 | -13.829 |
| NH4SO4- | 2.58E-05 | 1.99E-05 | -4.7 |
| Ni DOM1 | 2.81E-08 | 2.38E-08 | -7.623 |
| Ni(N3)2 (aq) | 8.18E-16 | 8.42E-16 | -15.075 |
| Ni(NH3)2+2 | 1.79E-20 | 6.38E-21 | -20.195 |
| Ni(NH3)3+2 | 1.27E-28 | 4.52E-29 | -28.345 |
| Ni(NH3)4+2 | 2.67E-37 | 9.51E-38 | -37.022 |
| Ni(NH3)5+2 | 1.81E-46 | 6.46E-47 | -46.19 |
| Ni(NH3)6+2 | 2.62E-56 | 9.35E-57 | -56.029 |
| Ni(NO2)2 (aq) | 1.2E-106 | 1.3E-106 | -105.9 |
| Ni(OH)2 (aq) | 9.06E-19 | 9.31E-19 | -18.031 |
| Ni(OH)3- | 1.92E-26 | 1.48E-26 | -25.829 |
| Ni(SO4)2-2 | 2.97E-09 | 1.06E-09 | -8.975 |
| Ni+2 | 1.03E-05 | 3.67E-06 | -5.435 |
| NiCl+ | 3.24E-08 | 2.51E-08 | -7.601 |
| NiCl2 (aq) | 1.64E-11 | 1.69E-11 | -10.773 |
| NiCO3 (aq) | 4.71E-15 | 4.84E-15 | -14.315 |
| NiF+ | 7.66E-13 | 5.92E-13 | -12.227 |
| NiH2PO4+ | 1.21E-11 | 9.32E-12 | -11.031 |
| NiHCO3+ | 2.8E-10 | 2.16E-10 | -9.665 |
| NiHPO4 (aq) | 9.71E-14 | 9.98E-14 | -13.001 |
| NiHS+ | 1.7E-25 | 1.32E-25 | -24.881 |
| NiN3+ | 1.36E-10 | 1.05E-10 | -9.977 |
| NiNH3+2 | 8.27E-13 | 2.95E-13 | -12.53 |
| NiNO2+ | 8.5E-56 | 6.57E-56 | -55.183 |
| NiNO3+ | 4.59E-73 | 3.55E-73 | -72.45 |
| NiOH+ | 4.61E-13 | 3.57E-13 | -12.448 |
| NiSO4 (aq) | 4.34E-06 | 4.47E-06 | -5.35 |
| NO2-1 | 9.64E-52 | 7.45E-52 | -51.128 |
| NO3-1 | 5.19E-68 | 3.84E-68 | -67.415 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| OH- | 9.73E-12 | 7.29E-12 | -11.137 |
| Pb DOM1 | 3.79E-09 | 3.21E-09 | -8.493 |
| Pb(CO3)2-2 | 1.92E-25 | 6.85E-26 | -25.164 |
| Pb(HS)2 (aq) | 1.52E-43 | 1.56E-43 | -42.806 |
| Pb(HS)3- | 4.67E-67 | 3.61E-67 | -66.443 |
| Pb(NO2)2 (aq) | 4.3E-108 | 4.5E-108 | -107.35 |
| Pb(NO3)2 (aq) | 2.5E-142 | 2.5E-142 | -141.595 |
| Pb(OH)2 (aq) | 1.22E-19 | 1.26E-19 | -18.9 |
| Pb(OH)3- | 2.59E-27 | 2E-27 | -26.698 |
| Pb(SO4)2-2 | 2.26E-09 | 8.05E-10 | -9.094 |
| Pb+2 | 1.75E-08 | 6.25E-09 | -8.204 |
| Pb2OH+3 | 2.51E-19 | 2.47E-20 | -19.607 |
| Pb3(OH)4+2 | 1.09E-36 | 3.88E-37 | -36.412 |
| Pb4(OH)4+4 | 2.3E-40 | 3.74E-42 | -41.428 |
| PbCl+ | 4.9E-09 | 3.79E-09 | -8.421 |
| PbCl2 (aq) | 1.45E-10 | 1.49E-10 | -9.825 |
| PbCl3- | 2.9E-12 | 2.24E-12 | -11.65 |
| PbCl4-2 | 4.33E-14 | 1.55E-14 | -13.811 |
| PbCO3 (aq) | 7.3E-16 | 7.51E-16 | -15.124 |
| PbF+ | 1.02E-14 | 7.87E-15 | -14.104 |
| PbF2 (aq) | 8.4E-22 | 8.64E-22 | -21.063 |
| PbH2PO4+ | 7.67E-14 | 5.93E-14 | -13.227 |
| PbHCO3+ | 3.07E-12 | 2.37E-12 | -11.624 |
| PbHPO4 (aq) | 2.3E-16 | 2.37E-16 | -15.625 |
| PbNO2+ | 1.95E-57 | 1.51E-57 | -56.822 |
| PbNO3+ | 4.72E-75 | 3.65E-75 | -74.438 |
| PbOH+ | 2.32E-13 | 1.79E-13 | -12.747 |
| PbSO4 (aq) | 1.97E-08 | 2.02E-08 | -7.694 |
| PO4-3 | 2.05E-19 | 2.01E-20 | -19.696 |
| S-2 | 1.03E-39 | 3.66E-40 | -39.436 |
| SO4-2 | 0.020314 | 0.006609 | -2.18 |
| Zn DOM1 | 6.58E-08 | 5.58E-08 | -7.253 |
| Zn(CO3)2-2 | 3.82E-25 | 1.36E-25 | -24.865 |
| Zn(N3)2 (aq) | 1.17E-15 | 1.2E-15 | -14.92 |
| Zn(N3)3- | 1.35E-20 | 1.05E-20 | -19.98 |
| Zn(NH3)2+2 | 9.99E-21 | 3.56E-21 | -20.448 |
| Zn(NH3)3+2 | 3.6E-28 | 1.28E-28 | -27.891 |
| Zn(NH3)4+2 | 6.35E-36 | 2.27E-36 | -35.645 |
| Zn(NO2)2 (aq) | 4.7E-107 | 4.8E-107 | -106.32 |
| Zn(NO3)2 (aq) | 3.9E-141 | 4E-141 | -140.396 |
| Zn(OH)2 (aq) | 1.69E-16 | 1.73E-16 | -15.761 |
| Zn(OH)3- | 1.13E-24 | 8.73E-25 | -24.059 |
| Zn(OH)4-2 | 6.17E-34 | 2.2E-34 | -33.657 |
| Zn(SO4)2-2 | 1.27E-06 | 4.52E-07 | -6.345 |
| Zn+2 | 1.42E-05 | 5.43E-06 | -5.265 |
| Zn2OH+3 | 1.95E-16 | 1.92E-17 | -16.716 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn2S3-2 | 1.15E-75 | 4.09E-76 | -75.388 |
| Zn4S6-4 | 1.8E-148 | 2.8E-150 | -149.546 |
| ZnCl+ | 3.62E-07 | 2.74E-07 | -6.562 |
| ZnCl2 (aq) | 3.22E-09 | 3.31E-09 | -8.48 |
| ZnCl3- | 8.54E-11 | 6.6E-11 | -10.18 |
| ZnCl4-2 | 1.61E-12 | 5.75E-13 | -12.24 |
| ZnCO3 (aq) | 1.08E-14 | 1.11E-14 | -13.955 |
| ZnF+ | 1.07E-12 | 8.29E-13 | -12.081 |
| ZnHCO3+ | 1.06E-10 | 8.2E-11 | -10.086 |
| ZnHPO4 (aq) | 3.29E-13 | 3.38E-13 | -12.471 |
| ZnN3+ | 1.54E-10 | 1.19E-10 | -9.925 |
| ZnNH3+2 | 3.52E-13 | 1.26E-13 | -12.901 |
| ZnNO2+ | 3.16E-56 | 2.44E-56 | -55.613 |
| ZnNO3+ | 7.24E-73 | 5.59E-73 | -72.252 |
| ZnOH+ | 5.12E-12 | 3.96E-12 | -11.402 |
| ZnS (aq) | 3.6E-29 | 3.71E-29 | -28.431 |
| ZnSO4 (aq) | 7E-06 | 7.2E-06 | -5.143 |

## B1.3: Eh 300

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 2.31E-05 | 2.28E-05 | -4.641 |
| Al(OH)2+ | 4.47E-10 | 3.5E-10 | -9.456 |
| Al(OH)3 (aq) | 4.97E-14 | 5.11E-14 | -13.292 |
| Al(OH)4- | 2.29E-17 | 1.77E-17 | -16.753 |
| Al(SO4)2- | 0.001005 | 0.000774 | -3.111 |
| Al+3 | 0.000374 | 6.39E-05 | -4.194 |
| Al2(OH)2+4 | 1E-09 | 1.74E-11 | -10.759 |
| Al2(OH)2CO3+2 | 1.18E-12 | 4.28E-13 | -12.369 |
| Al2PO4+3 | 2.22E-09 | 2.27E-10 | -9.643 |
| Al3(OH)4+5 | 9.54E-14 | 1.7E-16 | -15.77 |
| AlCl+2 | 1.27E-06 | 4.6E-07 | -6.337 |
| AlF+2 | 1.31E-05 | 4.92E-06 | -5.308 |
| AlF2+ | 2E-08 | 1.56E-08 | -7.806 |
| AlF3 (aq) | 1.43E-12 | 1.46E-12 | -11.834 |
| AlF4- | 7.65E-18 | 5.89E-18 | -17.23 |
| AlHPO4+ | 6.3E-08 | 4.89E-08 | -7.311 |
| AlOH+2 | 6.81E-07 | 2.55E-07 | -6.594 |
| AlSO4+ | 0.0034 | 0.002617 | -2.582 |
| As3S4(HS)- | 2.5E-175 | 1.9E-175 | -174.72 |
| AsO4-3 | 6.52E-21 | 6.67E-22 | -21.176 |
| AsS(OH)HS- | 5.34E-63 | 4.15E-63 | -62.382 |
| Ca DOM1 | 4.94E-06 | 4.2E-06 | -5.376 |
| Ca(NH3)2+2 | 8.07E-23 | 2.93E-23 | -22.533 |
| Ca(NO3)2 | 6.9E-121 | 7.1E-121 | -120.148 |
| Ca+2 | 0.005769 | 0.002348 | -2.629 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCl+ | 0.000127 | 9.86E-05 | -4.006 |
| CaCO3 (aq) | 2.8E-14 | 2.87E-14 | -13.542 |
| CaCrO4 (aq) | 1.14E-10 | 1.17E-10 | -9.933 |
| CaF+ | 2.75E-10 | 2.14E-10 | -9.67 |
| CaH2PO4+ | 2.62E-08 | 2.05E-08 | -7.688 |
| CaHCO3+ | 9.24E-09 | 7.3E-09 | -8.136 |
| CaHPO4 (aq) | 1.93E-11 | 1.99E-11 | -10.702 |
| CaNH3+2 | 1.3E-12 | 4.72E-13 | -12.326 |
| CaNO3+ | 3.19E-59 | 2.48E-59 | -58.606 |
| CaOH+ | 1.88E-13 | 1.49E-13 | -12.828 |
| CaPO4- | 4.21E-17 | 3.29E-17 | -16.482 |
| CaSO4 (aq) | 0.003331 | 0.003421 | -2.466 |
| Cd DOM1 | 4.13E-12 | 3.51E-12 | -11.454 |
| Cd(CO3)2-2 | 2.68E-30 | 9.75E-31 | -30.011 |
| Cd(HS)2 (aq) | 8.94E-67 | 9.18E-67 | -66.037 |
| Cd(HS)3- | 5.7E-101 | 4.4E-101 | -100.357 |
| Cd(HS)4-2 | 1.5E-134 | 5.3E-135 | -134.277 |
| Cd(NH3)2+2 | 4.17E-25 | 1.52E-25 | -24.819 |
| Cd(NH3)3+2 | 6.52E-34 | 2.37E-34 | -33.626 |
| Cd(NH3)4+2 | 3E-43 | 1.09E-43 | -42.962 |
| Cd(NO2)2 (aq) | 2.1E-92 | 2.16E-92 | -91.666 |
| Cd(NO3)2 (aq) | 1.2E-122 | 1.2E-122 | -121.926 |
| Cd(OH)2 (aq) | 2.31E-24 | 2.37E-24 | -23.624 |
| Cd(OH)3- | 2.33E-34 | 1.81E-34 | -33.742 |
| Cd(OH)4-2 | 3.97E-45 | 1.44E-45 | -44.841 |
| Cd(SO4)2-2 | 3.36E-10 | 1.22E-10 | -9.914 |
| Cd+2 | 2.15E-09 | 7.81E-10 | -9.107 |
| Cd2OH+3 | 9.72E-25 | 9.96E-26 | -25.002 |
| CdCl+ | 1.65E-09 | 1.28E-09 | -8.892 |
| CdCl2 (aq) | 8.87E-11 | 9.11E-11 | -10.041 |
| CdCO3 (aq) | 1.53E-19 | 1.57E-19 | -18.804 |
| CdF+ | 1.19E-16 | 9.26E-17 | -16.034 |
| CdHCO3+ | 7.48E-15 | 5.81E-15 | -14.236 |
| CdHPO4 (aq) | 6.84E-17 | 7.02E-17 | -16.154 |
| CdHS+ | 7.81E-38 | 6.06E-38 | -37.217 |
| CdNH3+2 | 5.52E-17 | 2.01E-17 | -16.698 |
| CdNO2+ | 8.02E-51 | 6.23E-51 | -50.206 |
| CdNO3+ | 1.32E-65 | 1.03E-65 | -64.989 |
| CdOH+ | 2.89E-17 | 2.24E-17 | -16.649 |
| CdSO4 (aq) | 1.11E-09 | 1.14E-09 | -8.944 |
| Cl-1 | 0.023635 | 0.017675 | -1.753 |
| CO3-2 | 2.29E-14 | 8.57E-15 | -14.067 |
| Cr2O7-2 | 1.46E-11 | 5.3E-12 | -11.276 |
| CrO3Cl- | 6.49E-11 | 5.04E-11 | -10.298 |
| CrO3H2PO4- | 4E-13 | 3.1E-13 | -12.508 |
| CrO3HPO4-2 | 1.38E-12 | 5.02E-13 | -12.299 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CrO3SO4-2 | 2.67E-09 | 9.69E-10 | -9.013 |
| CrO4-2 | 2.51E-10 | 8.45E-11 | -10.073 |
| Cu DOM1 | 3.94E-09 | 3.35E-09 | -8.475 |
| Cu(CO3)2-2 | 6E-26 | 2.18E-26 | -25.662 |
| Cu(N3)2 (aq) | 3.59E-16 | 3.69E-16 | -15.433 |
| Cu(N3)3- | 1.82E-20 | 1.41E-20 | -19.851 |
| Cu(N3)4-2 | 7.79E-26 | 2.83E-26 | -25.548 |
| Cu(NH3)2+2 | 8.55E-21 | 3.1E-21 | -20.508 |
| Cu(NH3)3+2 | 4.38E-28 | 1.59E-28 | -27.799 |
| Cu(NH3)4+2 | 4.63E-36 | 1.68E-36 | -35.774 |
| Cu(NO2)2 (aq) | 1.22E-91 | 1.26E-91 | -90.901 |
| Cu(NO3)2 (aq) | 6.9E-122 | 7.1E-122 | -121.147 |
| Cu(OH)2 (aq) | 1.74E-19 | 1.79E-19 | -18.747 |
| Cu(OH)3- | 2.55E-26 | 1.98E-26 | -25.703 |
| Cu(OH)4-2 | 2.82E-37 | 1.02E-37 | -36.99 |
| Cu+2 | 4.8E-08 | 1.87E-08 | -7.728 |
| Cu2(OH)2+2 | 6.61E-21 | 2.4E-21 | -20.62 |
| Cu2OH+3 | 3.53E-19 | 3.61E-20 | -19.442 |
| Cu2S3-2 | 7.1E-118 | 2.6E-118 | -117.591 |
| Cu3(OH)4+2 | 2.37E-33 | 8.61E-34 | -33.065 |
| CuCl+ | 7.7E-10 | 5.87E-10 | -9.231 |
| CuCl2 (aq) | 1.68E-12 | 1.73E-12 | -11.762 |
| CuCl3- | 3.12E-16 | 2.37E-16 | -15.625 |
| CuCl4-2 1 | 8.16E-20 | 2.97E-20 | -19.527 |
| CuCO3 (aq) | 9.19E-16 | 9.44E-16 | -15.025 |
| CuF+ | 8.07E-15 | 6.26E-15 | -14.203 |
| CuHCO3+ | 3.56E-13 | 2.77E-13 | -12.558 |
| CuHPO4 (aq) | 4.31E-15 | 4.42E-15 | -14.354 |
| CuHSO4+ | 4.75E-11 | 3.68E-11 | -10.434 |
| CuN3+ | 1.33E-11 | 1.03E-11 | -10.986 |
| CuNH3+2 | 4.37E-14 | 1.59E-14 | -13.8 |
| CuNO2+ | 2E-49 | 1.55E-49 | -48.809 |
| CuNO3+ | 2.5E-64 | 1.94E-64 | -63.713 |
| CuOH+ | 3.66E-13 | 2.79E-13 | -12.555 |
| CuS(aq) | 1.71E-44 | 1.75E-44 | -43.756 |
| CuSO4 (aq) | 2.59E-08 | 2.66E-08 | -7.575 |
| DOC (Gaussian DOM) | 0.001399 | 0.001436 | -2.843 |
| DOM1 | 4.33E-05 | 5.94E-06 | -5.226 |
| F-1 | 1.06E-08 | 8.02E-09 | -8.096 |
| Fe DOM1 | 5.55E-09 | 5.49E-09 | -8.26 |
| Fe(N3)2+ | 1.38E-14 | 1.07E-14 | -13.969 |
| Fe(N3)3 (aq) | 1.71E-18 | 1.76E-18 | -17.756 |
| Fe(NH3)2+2 | 1.19E-20 | 4.33E-21 | -20.364 |
| Fe(NH3)3+2 | 2.2E-30 | 7.97E-31 | -30.098 |
| Fe(NH3)4+2 | 1.73E-40 | 6.27E-41 | -40.203 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe(NO2)2+ | 2.06E-92 | 1.6E-92 | -91.795 |
| Fe(NO2)3 (aq) | 1.4E-133 | 1.5E-133 | -132.836 |
| Fe(OH)2 (aq) | 1.89E-18 | 1.94E-18 | -17.713 |
| Fe(OH)2+ | 3.9E-11 | 3.05E-11 | -10.515 |
| Fe(OH)3- | 5.58E-26 | 4.33E-26 | -25.363 |
| Fe(OH)3 (aq) | 7.64E-18 | 7.84E-18 | -17.105 |
| Fe(OH)4- | 5.09E-23 | 3.98E-23 | -22.4 |
| Fe(SO4)2- | 5.67E-10 | 4.4E-10 | -9.357 |
| Fe+2 | 0.013821 | 0.005384 | -2.269 |
| Fe+3 | 2.85E-10 | 4.86E-11 | -10.313 |
| Fe2(OH)2+4 | 4.71E-17 | 8.2E-19 | -18.086 |
| Fe3(OH)4+5 | 4.78E-24 | 8.51E-27 | -26.07 |
| FeCl+ | 7.73E-05 | 6E-05 | -4.222 |
| FeCl+2 | 5.16E-11 | 1.88E-11 | -10.726 |
| FeCrO4+ | 1.94E-13 | 1.51E-13 | -12.822 |
| FeF+ | 9.02E-10 | 7E-10 | -9.155 |
| FeF+2 | 1.02E-12 | 3.72E-13 | -12.43 |
| FeF2+ | 1.45E-16 | 1.13E-16 | -15.948 |
| FeF3 (aq) | 8.16E-22 | 8.38E-22 | -21.077 |
| FeH2PO4+ | 1.24E-06 | 9.68E-07 | -6.014 |
| FeH2PO4+2 | 8.82E-13 | 3.3E-13 | -12.481 |
| FeHCO3+ | 2.01E-08 | 1.59E-08 | -7.799 |
| FeHPO4 (aq) | 3.7E-10 | 3.8E-10 | -9.42 |
| FeHPO4+ | 1.37E-11 | 1.08E-11 | -10.969 |
| FeHS+ | 2.19E-33 | 1.7E-33 | -32.769 |
| FeN3+2 | 1.59E-11 | 5.79E-12 | -11.238 |
| FeNH3+2 | 2.55E-11 | 9.25E-12 | -11.034 |
| FeNO2+2 | 1.68E-50 | 6.11E-51 | -50.214 |
| FeOH+ | 9.84E-10 | 7.64E-10 | -9.117 |
| FeOH+2 | 6.94E-10 | 2.53E-10 | -9.597 |
| FeSO4 (aq) | 0.008083 | 0.0083 | -2.081 |
| FeSO4+ | 5.51E-09 | 4.28E-09 | -8.369 |
| H DOM1 | 4.87E-05 | 2.14E-05 | -4.669 |
| H+1 | 0.001561 | 0.001283 | -2.892 |
| H2AsO3- | 2.34E-12 | 1.81E-12 | -11.741 |
| H2AsO4- | 1.17E-08 | 9.11E-09 | -8.04 |
| H2CO3* (aq) | 0.000967 | 0.000993 | -3.003 |
| H2CrO4 (aq) | 1.6E-10 | 1.64E-10 | -9.784 |
| H2PO4- | 5.9E-07 | 4.62E-07 | -6.336 |
| H2S (aq) | 1.38E-32 | 1.42E-32 | -31.849 |
| H3AsO3 | 4.93E-06 | 5.07E-06 | -5.295 |
| H3AsO4 | 2.03E-09 | 2.09E-09 | -8.681 |
| H3PO4 | 7.3E-08 | 7.5E-08 | -7.125 |
| HAsO3-2 | 1.98E-23 | 7.2E-24 | -23.143 |
| HAsO4-2 | 1.92E-12 | 6.97E-13 | -12.157 |
| HCO3- | 3.77E-07 | 2.95E-07 | -6.53 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HCrO4- | 4.39E-07 | 3.41E-07 | -6.467 |
| HF (aq) | 1.26E-08 | 1.29E-08 | -7.888 |
| HF2- | 5.17E-16 | 3.9E-16 | -15.409 |
| Hg(CO3)2-2 | 3.2E-36 | 1.16E-36 | -35.935 |
| Hg(HS)2 (aq) | 6.13E-58 | 6.29E-58 | -57.201 |
| Hg(N3)2 (aq) | 1.44E-14 | 1.48E-14 | -13.829 |
| Hg(NH3)2+2 | 1.95E-25 | 7.08E-26 | -25.15 |
| Hg(NH3)4+2 | 3.39E-44 | 1.23E-44 | -43.91 |
| Hg(NO2)2 (aq) | 2.1E-100 | 2.1E-100 | -99.674 |
| Hg(NO2)3- | 7.5E-142 | 5.8E-142 | -141.235 |
| Hg(NO2)4-2 | 3.3E-184 | 1.2E-184 | -183.926 |
| Hg(NO3)2 (aq) | 6.4E-138 | 6.6E-138 | -137.18 |
| Hg(OH)2 | 1.67E-24 | 1.72E-24 | -23.765 |
| Hg(SO4)2-2 | 1.7E-24 | 6.19E-25 | -24.208 |
| Hg+2 | 2.01E-23 | 7.31E-24 | -23.136 |
| Hg2OH+3 | 1.67E-46 | 1.71E-47 | -46.766 |
| Hg3(OH)3+3 | 1.35E-67 | 1.39E-68 | -67.858 |
| HgCl+ | 4.73E-18 | 3.67E-18 | -17.435 |
| HgCl2 (aq) | 4.85E-13 | 4.98E-13 | -12.303 |
| HgCl3-1 | 1.13E-13 | 8.75E-14 | -13.058 |
| HgCl4-2 | 1.91E-14 | 6.93E-15 | -14.16 |
| HgClOH (aq) | 1.93E-18 | 1.99E-18 | -17.702 |
| HgCO3 (aq) | 4.68E-26 | 4.8E-26 | -25.318 |
| HgF+ | 2.82E-30 | 2.19E-30 | -29.66 |
| HgHCO3+ | 1.32E-24 | 1.02E-24 | -23.99 |
| HgHS2- | 2.04E-61 | 1.59E-61 | -60.799 |
| HgN3+ | 2.49E-10 | 1.93E-10 | -9.714 |
| HgNO2+ | 3.69E-61 | 2.87E-61 | -60.543 |
| HgNO3+ | 6.61E-81 | 5.13E-81 | -80.289 |
| HgOH+ | 2.18E-24 | 1.69E-24 | -23.771 |
| HgOHCO3- | 5.63E-30 | 4.37E-30 | -29.36 |
| HgS2-2 | 6.64E-67 | 2.41E-67 | -66.618 |
| HgSO4 (aq) | 8.39E-24 | 8.61E-24 | -23.065 |
| HN3 (aq) | 4.9E-05 | 5.03E-05 | -4.298 |
| HNO2 (aq) | 1.4E-43 | 1.44E-43 | -42.843 |
| HPO4-2 | 6.01E-11 | 2.19E-11 | -10.66 |
| HS-1 | 1.01E-36 | 7.59E-37 | -36.12 |
| HSO4- | 0.000871 | 0.00067 | -3.174 |
| K+1 | 0.000318 | 0.000238 | -3.624 |
| K2HPO4 (aq) | 1.3E-17 | 1.34E-17 | -16.874 |
| K2PO4- | 7.72E-26 | 5.99E-26 | -25.223 |
| KCl (aq) | 2.17E-06 | 2.23E-06 | -5.652 |
| KCr2O7- | 1.4E-14 | 1.09E-14 | -13.964 |
| KCrO4- | 9.6E-14 | 7.45E-14 | -13.128 |
| KF (aq) | 8.48E-13 | 8.71E-13 | -12.06 |
| KH2PO4 (aq) | 1.66E-10 | 1.7E-10 | -9.769 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| KHPO4- | 4.09E-14 | 3.2E-14 | -13.495 |
| KNO3 (aq) | 5.47E-61 | 5.62E-61 | -60.25 |
| KOH (aq) | 1.43E-15 | 1.47E-15 | -14.832 |
| KPO4-2 | 8.32E-23 | 3.02E-23 | -22.52 |
| KSO4- | 1.26E-05 | 9.87E-06 | -5.006 |
| Mg DOM1 | 4.34E-07 | 3.69E-07 | -6.433 |
| Mg(NH3)2+2 | 3.53E-23 | 1.28E-23 | -22.892 |
| Mg+2 | 0.004865 | 0.00206 | -2.686 |
| Mg2CO3+2 | 3.9E-16 | 1.42E-16 | -15.849 |
| MgCl+ | 0.000177 | 0.000137 | -3.863 |
| MgCO3 (aq) | 1.23E-14 | 1.26E-14 | -13.9 |
| MgF+ | 1.42E-09 | 1.09E-09 | -8.961 |
| MgHCO3+ | 7.74E-09 | 5.9E-09 | -8.229 |
| MgHPO4 (aq) | 2.34E-11 | 2.4E-11 | -10.619 |
| MgOH+ | 3.12E-12 | 2.48E-12 | -11.605 |
| MgPO4- | 5.77E-19 | 4.52E-19 | -18.345 |
| MgSO4 (aq) | 0.002364 | 0.002428 | -2.615 |
| Mn+3 | 4.55E-05 | 7.77E-06 | -5.11 |
| N3-1 | 9.83E-07 | 7.63E-07 | -6.117 |
| Na+1 | 0.012067 | 0.009379 | -2.028 |
| Na2HPO4 (aq) | 1.34E-14 | 1.37E-14 | -13.862 |
| Na2PO4- | 2.57E-22 | 2E-22 | -21.7 |
| NaCl (aq) | 9.05E-05 | 9.29E-05 | -4.032 |
| NaCO3- | 2.54E-15 | 1.99E-15 | -14.701 |
| NaCrO4- | 5.07E-12 | 3.94E-12 | -11.405 |
| NaF (aq) | 6.49E-11 | 6.66E-11 | -10.177 |
| NaH2PO4 (aq) | 6.54E-09 | 6.72E-09 | -8.173 |
| NaHCO3 (aq) | 1.6E-09 | 1.64E-09 | -8.785 |
| NaHPO4- | 2.5E-12 | 1.95E-12 | -11.709 |
| NaNO3 (aq) | 7.97E-60 | 8.18E-60 | -59.087 |
| NaOH (aq) | 3.88E-14 | 3.98E-14 | -13.4 |
| NaPO4-2 | 3.62E-21 | 1.32E-21 | -20.881 |
| NaSO4- | 0.000456 | 0.000357 | -3.447 |
| NH3 (aq) | 5.89E-11 | 6.04E-11 | -10.219 |
| NH4+1 | 0.000384 | 0.000283 | -3.549 |
| NH4Cr2O7- | 1.94E-14 | 1.5E-14 | -13.823 |
| NH4SO4- | 2.74E-05 | 2.13E-05 | -4.672 |
| Ni DOM1 | 1.93E-08 | 1.64E-08 | -7.784 |
| Ni(N3)2 (aq) | 2.05E-16 | 2.1E-16 | -15.678 |
| Ni(NH3)2+2 | 4.25E-21 | 1.54E-21 | -20.811 |
| Ni(NH3)3+2 | 1.49E-29 | 5.41E-30 | -29.267 |
| Ni(NH3)4+2 | 1.55E-38 | 5.61E-39 | -38.251 |
| Ni(NH3)5+2 | 5.18E-48 | 1.88E-48 | -47.725 |
| Ni(NH3)6+2 | 3.7E-58 | 1.34E-58 | -57.871 |
| Ni(NO2)2 (aq) | 1.38E-90 | 1.41E-90 | -89.85 |
| Ni(OH)2 (aq) | 2.16E-19 | 2.22E-19 | -18.655 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(OH)3- | 2.22E-27 | 1.73E-27 | -26.763 |
| Ni(SO4)2-2 | 3.28E-09 | 1.19E-09 | -8.924 |
| Ni+2 | 1.01E-05 | 3.65E-06 | -5.438 |
| NiCl+ | 3E-08 | 2.33E-08 | -7.632 |
| NiCl2 (aq) | 1.43E-11 | 1.47E-11 | -10.833 |
| NiCO3 (aq) | 1.13E-15 | 1.16E-15 | -14.934 |
| NiF+ | 6.82E-13 | 5.29E-13 | -12.276 |
| NiH2PO4+ | 1.43E-11 | 1.11E-11 | -10.956 |
| NiHCO3+ | 1.36E-10 | 1.06E-10 | -9.976 |
| NiHPO4 (aq) | 5.69E-14 | 5.84E-14 | -13.234 |
| NiHS+ | 1.1E-36 | 8.56E-37 | -36.068 |
| NiN3+ | 6.76E-11 | 5.25E-11 | -10.28 |
| NiNH3+2 | 3.98E-13 | 1.45E-13 | -12.839 |
| NiNO2+ | 8.94E-48 | 6.94E-48 | -47.159 |
| NiNO3+ | 3.66E-62 | 2.84E-62 | -61.547 |
| NiOH+ | 2.23E-13 | 1.73E-13 | -12.761 |
| NiSO4 (aq) | 4.59E-06 | 4.72E-06 | -5.326 |
| NO2-1 | 1.02E-43 | 7.92E-44 | -43.101 |
| NO3-1 | 4.16E-57 | 3.1E-57 | -56.509 |
| OH- | 4.73E-12 | 3.57E-12 | -11.448 |
| Pb DOM1 | 2.64E-09 | 2.25E-09 | -8.649 |
| Pb(CO3)2-2 | 1.11E-26 | 4.02E-27 | -26.395 |
| Pb(HS)2 (aq) | 6.56E-66 | 6.74E-66 | -65.171 |
| Pb(HS)3- | 1.3E-100 | 1E-100 | -99.991 |
| Pb(NO2)2 (aq) | 4.95E-92 | 5.08E-92 | -91.294 |
| Pb(NO3)2 (aq) | 1.6E-120 | 1.7E-120 | -119.78 |
| Pb(OH)2 (aq) | 2.95E-20 | 3.03E-20 | -19.519 |
| Pb(OH)3- | 3.04E-28 | 2.36E-28 | -27.627 |
| Pb(SO4)2-2 | 2.52E-09 | 9.15E-10 | -9.038 |
| Pb+2 | 1.73E-08 | 6.29E-09 | -8.202 |
| Pb2OH+3 | 1.2E-19 | 1.23E-20 | -19.912 |
| Pb3(OH)4+2 | 6.23E-38 | 2.26E-38 | -37.646 |
| Pb4(OH)4+4 | 1.26E-41 | 2.19E-43 | -42.659 |
| PbCl+ | 4.6E-09 | 3.57E-09 | -8.447 |
| PbCl2 (aq) | 1.28E-10 | 1.32E-10 | -9.88 |
| PbCl3- | 2.38E-12 | 1.85E-12 | -11.733 |
| PbCl4-2 | 3.29E-14 | 1.2E-14 | -13.922 |
| PbCO3 (aq) | 1.78E-16 | 1.83E-16 | -15.738 |
| PbF+ | 9.17E-15 | 7.12E-15 | -14.147 |
| PbF2 (aq) | 6.85E-22 | 7.03E-22 | -21.153 |
| PbH2PO4+ | 9.19E-14 | 7.13E-14 | -13.147 |
| PbHCO3+ | 1.51E-12 | 1.17E-12 | -11.93 |
| PbHPO4 (aq) | 1.37E-16 | 1.4E-16 | -15.853 |
| PbNO2+ | 2.08E-49 | 1.61E-49 | -48.793 |
| PbNO3+ | 3.81E-64 | 2.96E-64 | -63.529 |
| PbOH+ | 1.14E-13 | 8.81E-14 | -13.055 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| PbSO4 (aq) | 2.11E-08 | 2.16E-08 | -7.665 |
| PO4-3 | 5.66E-20 | 5.83E-21 | -20.234 |
| S-2 | 3.24E-51 | 1.18E-51 | -50.928 |
| SO4-2 | 0.021069 | 0.007025 | -2.153 |
| Zn DOM1 | 4.5E-08 | 3.82E-08 | -7.417 |
| Zn(CO3)2-2 | 2.17E-26 | 7.87E-27 | -26.104 |
| Zn(N3)2 (aq) | 2.9E-16 | 2.98E-16 | -15.526 |
| Zn(N3)3- | 1.68E-21 | 1.3E-21 | -20.886 |
| Zn(NH3)2+2 | 2.36E-21 | 8.57E-22 | -21.067 |
| Zn(NH3)3+2 | 4.2E-29 | 1.53E-29 | -28.817 |
| Zn(NH3)4+2 | 3.66E-37 | 1.33E-37 | -36.876 |
| Zn(NO2)2 (aq) | 5.2E-91 | 5.34E-91 | -90.273 |
| Zn(NO3)2 (aq) | 2.5E-119 | 2.6E-119 | -118.589 |
| Zn(OH)2 (aq) | 3.99E-17 | 4.1E-17 | -16.388 |
| Zn(OH)3- | 1.3E-25 | 1.01E-25 | -24.996 |
| Zn(OH)4-2 | 3.43E-35 | 1.25E-35 | -34.904 |
| Zn(SO4)2-2 | 1.39E-06 | 5.04E-07 | -6.297 |
| Zn+2 | 1.38E-05 | 5.36E-06 | -5.271 |
| Zn2OH+3 | 8.96E-17 | 9.17E-18 | -17.037 |
| Zn2S3-2 | 3.7E-110 | 1.3E-110 | -109.875 |
| Zn4S6-4 | 1.7E-217 | 3E-219 | -218.52 |
| ZnCl+ | 3.33E-07 | 2.54E-07 | -6.596 |
| ZnCl2 (aq) | 2.79E-09 | 2.87E-09 | -8.542 |
| ZnCl3- | 6.89E-11 | 5.35E-11 | -10.272 |
| ZnCl4-2 | 1.2E-12 | 4.36E-13 | -12.36 |
| ZnCO3 (aq) | 2.58E-15 | 2.65E-15 | -14.577 |
| ZnF+ | 9.48E-13 | 7.36E-13 | -12.133 |
| ZnHCO3+ | 5.13E-11 | 3.98E-11 | -10.4 |
| ZnHPO4 (aq) | 1.91E-13 | 1.97E-13 | -12.707 |
| ZnN3+ | 7.58E-11 | 5.89E-11 | -10.23 |
| ZnNH3+2 | 1.69E-13 | 6.13E-14 | -13.213 |
| ZnNO2+ | 3.3E-48 | 2.56E-48 | -47.592 |
| ZnNO3+ | 5.73E-62 | 4.45E-62 | -61.352 |
| ZnOH+ | 2.46E-12 | 1.91E-12 | -11.718 |
| ZnS (aq) | 1.15E-40 | 1.18E-40 | -39.929 |
| ZnSO4 (aq) | 7.36E-06 | 7.56E-06 | -5.122 |

## B1.4: Eh 400

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 9.27E-06 | 9.18E-06 | -5.037 |
| Al(OH)2+ | 2.76E-11 | 2.17E-11 | -10.664 |
| Al(OH)3 (aq) | 7.53E-16 | 7.73E-16 | -15.112 |
| Al(OH)4- | 8.46E-20 | 6.53E-20 | -19.185 |
| Al(SO4)2- | 0.000986 | 0.000761 | -3.119 |
| Al+3 | 0.000383 | 6.63E-05 | -4.178 |
| Al2(OH)2+4 | 6.2E-11 | 1.12E-12 | -11.951 |
| Al2(OH)2CO3+2 | 4.48E-15 | 1.64E-15 | -14.785 |
| Al2PO4+3 | 1.44E-10 | 1.51E-11 | -10.822 |
| Al3(OH)4+5 | 3.58E-16 | 6.77E-19 | -18.17 |
| AlCl+2 | 1.24E-06 | 4.53E-07 | -6.343 |
| AlF+2 | 1.31E-05 | 4.96E-06 | -5.305 |
| AlF2+ | 1.95E-08 | 1.53E-08 | -7.816 |
| AlF3 (aq) | 1.35E-12 | 1.39E-12 | -11.857 |
| AlF4- | 7.02E-18 | 5.42E-18 | -17.266 |
| AlHPO4+ | 1.64E-08 | 1.28E-08 | -7.894 |
| AlOH+2 | 1.71E-07 | 6.46E-08 | -7.189 |
| AlSO4+ | 0.003426 | 0.002644 | -2.578 |
| As3S4(HS)- | 1.8E-223 | 1.4E-223 | -222.852 |
| AsO4-3 | 1.48E-20 | 1.54E-21 | -20.811 |
| AsS(OH)HS- | 1.88E-79 | 1.46E-79 | -78.834 |
| Ca DOM1 | 1.94E-06 | 1.65E-06 | -5.782 |
| Ca(NH3)2+2 | 4.9E-24 | 1.8E-24 | -23.746 |
| Ca(NO3)2 | 3.9E-105 | 4E-105 | -104.393 |
| Ca+2 | 0.005812 | 0.002384 | -2.623 |
| CaCl+ | 0.000122 | 9.5E-05 | -4.022 |
| CaCO3 (aq) | 1.7E-15 | 1.74E-15 | -14.759 |
| CaCrO4 (aq) | 2.78E-11 | 2.85E-11 | -10.545 |
| CaF+ | 2.7E-10 | 2.11E-10 | -9.676 |
| CaH2PO4+ | 2.74E-08 | 2.15E-08 | -7.668 |
| CaHCO3+ | 2.29E-09 | 1.81E-09 | -8.742 |
| CaHPO4 (aq) | 4.94E-12 | 5.07E-12 | -11.295 |
| CaNH3+2 | 3.21E-13 | 1.18E-13 | -12.929 |
| CaNO3+ | 2.42E-51 | 1.88E-51 | -50.725 |
| CaOH+ | 4.66E-14 | 3.69E-14 | -13.433 |
| CaPO4- | 2.62E-18 | 2.05E-18 | -17.687 |
| CaSO4 (aq) | 0.003296 | 0.003381 | -2.471 |
| Cd DOM1 | 1.65E-12 | 1.4E-12 | -11.853 |
| Cd(CO3)2-2 | 9.76E-33 | 3.58E-33 | -32.446 |
| Cd(HS)2 (aq) | 9.43E-84 | 9.67E-84 | -83.014 |
| Cd(HS)3- | 1.9E-126 | 1.5E-126 | -125.83 |
| Cd(HS)4-2 | 1.6E-168 | 5.7E-169 | -168.245 |
| Cd(NH3)2+2 | 2.58E-26 | 9.44E-27 | -26.025 |
| Cd(NH3)3+2 | 9.89E-36 | 3.62E-36 | -35.441 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd(NH3)4+2 | 1.12E-45 | 4.1E-46 | -45.387 |
| Cd(NO2)2 (aq) | 3.44E-81 | 3.53E-81 | -80.452 |
| Cd(NO3)2 (aq) | 6.7E-107 | 6.9E-107 | -106.164 |
| Cd(OH)2 (aq) | 1.43E-25 | 1.46E-25 | -24.835 |
| Cd(OH)3- | 3.5E-36 | 2.73E-36 | -35.564 |
| Cd(OH)4-2 | 1.44E-47 | 5.3E-48 | -47.276 |
| Cd(SO4)2-2 | 3.25E-10 | 1.19E-10 | -9.924 |
| Cd+2 | 2.2E-09 | 8.06E-10 | -9.094 |
| Cd2OH+3 | 2.48E-25 | 2.59E-26 | -25.586 |
| CdCl+ | 1.61E-09 | 1.26E-09 | -8.901 |
| CdCl2 (aq) | 8.26E-11 | 8.47E-11 | -10.072 |
| CdCO3 (aq) | 9.42E-21 | 9.66E-21 | -20.015 |
| CdF+ | 1.19E-16 | 9.27E-17 | -16.033 |
| CdHCO3+ | 1.88E-15 | 1.46E-15 | -14.835 |
| CdHPO4 (aq) | 1.78E-17 | 1.82E-17 | -16.739 |
| CdHS+ | 2.57E-46 | 2E-46 | -45.699 |
| CdNH3+2 | 1.39E-17 | 5.09E-18 | -17.293 |
| CdNO2+ | 3.29E-45 | 2.56E-45 | -44.592 |
| CdNO3+ | 1.02E-57 | 7.92E-58 | -57.101 |
| CdOH+ | 7.27E-18 | 5.66E-18 | -17.247 |
| CdSO4 (aq) | 1.12E-09 | 1.14E-09 | -8.942 |
| Cl-1 | 0.022357 | 0.016778 | -1.775 |
| CO3-2 | 1.35E-15 | 5.11E-16 | -15.291 |
| Cr2O7-2 | 1.4E-11 | 5.13E-12 | -11.29 |
| CrO3Cl- | 2.47E-10 | 1.93E-10 | -9.715 |
| CrO3H2PO4- | 1.65E-12 | 1.29E-12 | -11.891 |
| CrO3HPO4-2 | 1.39E-12 | 5.09E-13 | -12.294 |
| CrO3SO4-2 | 1.04E-08 | 3.8E-09 | -8.42 |
| CrO4-2 | 5.95E-11 | 2.03E-11 | -10.693 |
| Cu DOM1 | 1.59E-09 | 1.35E-09 | -8.868 |
| Cu(CO3)2-2 | 2.21E-28 | 8.1E-29 | -28.092 |
| Cu(N3)2 (aq) | 2.31E-17 | 2.37E-17 | -16.626 |
| Cu(N3)3- | 2.88E-22 | 2.24E-22 | -21.649 |
| Cu(N3)4-2 | 3.04E-28 | 1.12E-28 | -27.953 |
| Cu(NH3)2+2 | 5.35E-22 | 1.96E-22 | -21.708 |
| Cu(NH3)3+2 | 6.72E-30 | 2.46E-30 | -29.608 |
| Cu(NH3)4+2 | 1.75E-38 | 6.41E-39 | -38.193 |
| Cu(NO2)2 (aq) | 2.03E-80 | 2.08E-80 | -79.681 |
| Cu(NO3)2 (aq) | 4.1E-106 | 4.2E-106 | -105.379 |
| Cu(OH)2 (aq) | 1.09E-20 | 1.12E-20 | -19.952 |
| Cu(OH)3- | 3.88E-28 | 3.02E-28 | -27.52 |
| Cu(OH)4-2 | 1.04E-39 | 3.81E-40 | -39.419 |
| Cu+2 | 4.97E-08 | 1.95E-08 | -7.709 |
| Cu2(OH)2+2 | 4.27E-22 | 1.57E-22 | -21.805 |
| Cu2OH+3 | 9.23E-20 | 9.65E-21 | -20.016 |
| Cu2S3-2 | 3.6E-145 | 1.3E-145 | -144.875 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu3(OH)4+2 | 9.56E-36 | 3.51E-36 | -35.455 |
| CuCl+ | 7.62E-10 | 5.83E-10 | -9.235 |
| CuCl2 (aq) | 1.59E-12 | 1.63E-12 | -11.788 |
| CuCl3- | 2.78E-16 | 2.12E-16 | -15.673 |
| CuCl4-2 1 | 6.86E-20 | 2.52E-20 | -19.598 |
| CuCO3 (aq) | 5.74E-17 | 5.88E-17 | -16.23 |
| CuF+ | 8.17E-15 | 6.36E-15 | -14.197 |
| CuHCO3+ | 9.08E-14 | 7.06E-14 | -13.151 |
| CuHPO4 (aq) | 1.13E-15 | 1.16E-15 | -14.934 |
| CuHSO4+ | 1.97E-10 | 1.54E-10 | -9.814 |
| CuN3+ | 3.44E-12 | 2.68E-12 | -11.572 |
| CuNH3+2 | 1.11E-14 | 4.07E-15 | -14.39 |
| CuNO2+ | 8.3E-44 | 6.46E-44 | -43.19 |
| CuNO3+ | 1.95E-56 | 1.52E-56 | -55.819 |
| CuOH+ | 9.32E-14 | 7.12E-14 | -13.147 |
| CuS(aq) | 1.39E-53 | 1.43E-53 | -52.845 |
| CuSO4 (aq) | 2.64E-08 | 2.71E-08 | -7.567 |
| DOC (Gaussian DOM) | 0.001399 | 0.001435 | -2.843 |
| DOM1 | 3.24E-05 | 4.54E-06 | -5.343 |
| F-1 | 1.03E-08 | 7.79E-09 | -8.109 |
| Fe DOM1 | 9.81E-08 | 9.71E-08 | -7.013 |
| Fe(N3)2+ | 3.87E-14 | 3.01E-14 | -13.522 |
| Fe(N3)3 (aq) | 1.19E-18 | 1.22E-18 | -17.914 |
| Fe(NH3)2+2 | 5.8E-22 | 2.12E-22 | -21.673 |
| Fe(NH3)3+2 | 2.62E-32 | 9.62E-33 | -32.017 |
| Fe(NH3)4+2 | 5.07E-43 | 1.86E-43 | -42.731 |
| Fe(NO2)2+ | 1.49E-79 | 1.16E-79 | -78.936 |
| Fe(NO2)3 (aq) | 4.1E-115 | 4.2E-115 | -114.377 |
| Fe(OH)2 (aq) | 9.16E-20 | 9.4E-20 | -19.027 |
| Fe(OH)2+ | 1.06E-10 | 8.32E-11 | -10.08 |
| Fe(OH)3- | 6.6E-28 | 5.14E-28 | -27.289 |
| Fe(OH)3 (aq) | 5.09E-18 | 5.22E-18 | -17.282 |
| Fe(OH)4- | 8.25E-24 | 6.47E-24 | -23.189 |
| Fe(SO4)2- | 2.45E-08 | 1.9E-08 | -7.721 |
| Fe+2 | 0.01114 | 0.00438 | -2.359 |
| Fe+3 | 1.28E-08 | 2.22E-09 | -8.654 |
| Fe2(OH)2+4 | 5.65E-15 | 1.02E-16 | -15.992 |
| Fe3(OH)4+5 | 1.53E-21 | 2.88E-24 | -23.54 |
| FeCl+ | 5.96E-05 | 4.64E-05 | -4.334 |
| FeCl+2 | 2.21E-09 | 8.15E-10 | -9.089 |
| FeCrO4+ | 2.13E-12 | 1.65E-12 | -11.781 |
| FeF+ | 7.11E-10 | 5.53E-10 | -9.257 |
| FeF+2 | 4.48E-11 | 1.65E-11 | -10.783 |
| FeF2+ | 6.22E-15 | 4.85E-15 | -14.314 |
| FeF3 (aq) | 3.41E-20 | 3.5E-20 | -19.456 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeH2PO4+ | 1.03E-06 | 8.11E-07 | -6.091 |
| FeH2PO4+2 | 4.1E-11 | 1.55E-11 | -10.809 |
| FeHCO3+ | 3.99E-09 | 3.16E-09 | -8.501 |
| FeHPO4 (aq) | 7.58E-11 | 7.78E-11 | -10.109 |
| FeHPO4+ | 1.57E-10 | 1.23E-10 | -9.908 |
| FeHS+ | 5.69E-42 | 4.43E-42 | -41.354 |
| FeN3+2 | 1.79E-10 | 6.54E-11 | -10.184 |
| FeNH3+2 | 5.04E-12 | 1.85E-12 | -11.733 |
| FeNO2+2 | 3.03E-43 | 1.11E-43 | -42.955 |
| FeOH+ | 1.95E-10 | 1.52E-10 | -9.818 |
| FeOH+2 | 7.66E-09 | 2.82E-09 | -8.55 |
| FeSO4 (aq) | 0.006407 | 0.006573 | -2.182 |
| FeSO4+ | 2.44E-07 | 1.9E-07 | -6.721 |
| H DOM1 | 7.66E-05 | 3.4E-05 | -4.469 |
| H+1 | 0.00638 | 0.005251 | -2.28 |
| H2AsO3- | 4.81E-13 | 3.74E-13 | -12.427 |
| H2AsO4- | 4.54E-07 | 3.53E-07 | -6.452 |
| H2CO3* (aq) | 0.000967 | 0.000992 | -3.003 |
| H2CrO4 (aq) | 6.45E-10 | 6.62E-10 | -9.179 |
| H2PO4- | 6.06E-07 | 4.75E-07 | -6.323 |
| H2S (aq) | 1.81E-40 | 1.85E-40 | -39.732 |
| H3AsO3 | 4.17E-06 | 4.28E-06 | -5.369 |
| H3AsO4 | 3.23E-07 | 3.31E-07 | -6.48 |
| H3PO4 | 3.08E-07 | 3.16E-07 | -6.5 |
| HAsO3-2 | 9.9E-25 | 3.63E-25 | -24.44 |
| HAsO4-2 | 1.8E-11 | 6.6E-12 | -11.18 |
| HCO3- | 9.18E-08 | 7.2E-08 | -7.143 |
| HCrO4- | 4.31E-07 | 3.35E-07 | -6.475 |
| HF (aq) | 5.01E-08 | 5.14E-08 | -7.289 |
| HF2- | 1.99E-15 | 1.5E-15 | -14.823 |
| Hg(CO3)2-2 | 3.66E-36 | 1.34E-36 | -35.873 |
| Hg(HS)2 (aq) | 2.03E-72 | 2.09E-72 | -71.681 |
| Hg(N3)2 (aq) | 1.72E-14 | 1.76E-14 | -13.754 |
| Hg(NH3)2+2 | 3.78E-24 | 1.39E-24 | -23.858 |
| Hg(NH3)4+2 | 3.97E-44 | 1.46E-44 | -43.837 |
| Hg(NO2)2 (aq) | 1.06E-86 | 1.09E-86 | -85.962 |
| Hg(NO2)3- | 1.5E-122 | 1.2E-122 | -121.923 |
| Hg(NO2)4-2 | 2.6E-159 | 9.7E-160 | -159.014 |
| Hg(NO3)2 (aq) | 1.2E-119 | 1.2E-119 | -118.92 |
| Hg(OH)2 | 3.25E-23 | 3.33E-23 | -22.477 |
| Hg(SO4)2-2 | 5.2E-22 | 1.9E-22 | -21.72 |
| Hg+2 | 6.48E-21 | 2.37E-21 | -20.625 |
| Hg2OH+3 | 4.22E-42 | 4.42E-43 | -42.355 |
| Hg3(OH)3+3 | 6.62E-62 | 6.92E-63 | -62.16 |
| HgCl+ | 1.45E-15 | 1.13E-15 | -14.946 |
| HgCl2 (aq) | 1.42E-10 | 1.46E-10 | -9.837 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgCl3-1 | 3.12E-11 | 2.43E-11 | -10.614 |
| HgCl4-2 | 4.98E-12 | 1.83E-12 | -11.739 |
| HgClOH (aq) | 1.46E-16 | 1.5E-16 | -15.825 |
| HgCO3 (aq) | 9.07E-25 | 9.3E-25 | -24.031 |
| HgF+ | 8.86E-28 | 6.89E-28 | -27.162 |
| HgHCO3+ | 1.04E-22 | 8.11E-23 | -22.091 |
| HgHS2- | 1.65E-76 | 1.29E-76 | -75.891 |
| HgN3+ | 7.11E-11 | 5.53E-11 | -10.257 |
| HgNO2+ | 4.76E-53 | 3.71E-53 | -52.431 |
| HgNO3+ | 1.6E-70 | 1.25E-70 | -69.904 |
| HgOH+ | 1.73E-22 | 1.34E-22 | -21.872 |
| HgOHCO3- | 2.65E-29 | 2.07E-29 | -28.685 |
| HgS2-2 | 1.3E-82 | 4.77E-83 | -82.321 |
| HgSO4 (aq) | 2.65E-21 | 2.72E-21 | -20.565 |
| HN3 (aq) | 4.98E-05 | 5.1E-05 | -4.292 |
| HNO2 (aq) | 2.28E-37 | 2.34E-37 | -36.631 |
| HPO4-2 | 1.5E-11 | 5.5E-12 | -11.259 |
| HS-1 | 3.21E-45 | 2.42E-45 | -44.615 |
| HSO4- | 0.00346 | 0.002671 | -2.573 |
| K+1 | 0.000318 | 0.000239 | -3.622 |
| K2HPO4 (aq) | 3.31E-18 | 3.39E-18 | -17.47 |
| K2PO4- | 4.78E-27 | 3.72E-27 | -26.43 |
| KCl (aq) | 2.07E-06 | 2.12E-06 | -5.673 |
| KCr2O7- | 1.36E-14 | 1.06E-14 | -13.976 |
| KCrO4- | 2.31E-14 | 1.8E-14 | -13.745 |
| KF (aq) | 8.28E-13 | 8.5E-13 | -12.071 |
| KH2PO4 (aq) | 1.72E-10 | 1.76E-10 | -9.754 |
| KHPO4- | 1.03E-14 | 8.08E-15 | -14.093 |
| KNO3 (aq) | 4.12E-53 | 4.22E-53 | -52.374 |
| KOH (aq) | 3.52E-16 | 3.61E-16 | -15.442 |
| KPO4-2 | 5.09E-24 | 1.87E-24 | -23.729 |
| KSO4- | 1.23E-05 | 9.65E-06 | -5.016 |
| Mg DOM1 | 1.7E-07 | 1.45E-07 | -6.839 |
| Mg(NH3)2+2 | 2.14E-24 | 7.85E-25 | -24.105 |
| Mg+2 | 0.0049 | 0.002089 | -2.68 |
| Mg2CO3+2 | 2.37E-17 | 8.68E-18 | -17.061 |
| MgCl+ | 0.00017 | 0.000132 | -3.88 |
| MgCO3 (aq) | 7.43E-16 | 7.62E-16 | -15.118 |
| MgF+ | 1.4E-09 | 1.08E-09 | -8.968 |
| MgHCO3+ | 1.91E-09 | 1.46E-09 | -8.835 |
| MgHPO4 (aq) | 5.98E-12 | 6.13E-12 | -11.212 |
| MgOH+ | 7.7E-13 | 6.15E-13 | -12.211 |
| MgPO4- | 3.59E-20 | 2.81E-20 | -19.551 |
| MgSO4 (aq) | 0.002336 | 0.002397 | -2.62 |
| Mn+3 | 4.55E-05 | 7.88E-06 | -5.103 |
| N3-1 | 2.43E-07 | 1.89E-07 | -6.723 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Na+1 | 0.012083 | 0.009414 | -2.026 |
| Na2HPO4 (aq) | 3.4E-15 | 3.48E-15 | -14.458 |
| Na2PO4- | 1.59E-23 | 1.24E-23 | -22.908 |
| NaCl (aq) | 8.63E-05 | 8.85E-05 | -4.053 |
| NaCO3- | 1.52E-16 | 1.19E-16 | -15.924 |
| NaCrO4- | 1.22E-12 | 9.49E-13 | -12.023 |
| NaF (aq) | 6.32E-11 | 6.49E-11 | -10.188 |
| NaH2PO4 (aq) | 6.77E-09 | 6.94E-09 | -8.159 |
| NaHCO3 (aq) | 3.92E-10 | 4.02E-10 | -9.396 |
| NaHPO4- | 6.29E-13 | 4.93E-13 | -12.307 |
| NaNO3 (aq) | 5.99E-52 | 6.15E-52 | -51.211 |
| NaOH (aq) | 9.52E-15 | 9.76E-15 | -14.01 |
| NaPO4-2 | 2.21E-22 | 8.12E-23 | -22.091 |
| NaSO4- | 0.000445 | 0.000349 | -3.457 |
| NH3 (aq) | 1.45E-11 | 1.48E-11 | -10.828 |
| NH4+1 | 0.000385 | 0.000284 | -3.546 |
| NH4Cr2O7- | 1.88E-14 | 1.46E-14 | -13.835 |
| NH4SO4- | 2.68E-05 | 2.08E-05 | -4.681 |
| Ni DOM1 | 7.58E-09 | 6.46E-09 | -8.19 |
| Ni(N3)2 (aq) | 1.28E-17 | 1.31E-17 | -16.883 |
| Ni(NH3)2+2 | 2.58E-22 | 9.46E-23 | -22.024 |
| Ni(NH3)3+2 | 2.22E-31 | 8.14E-32 | -31.089 |
| Ni(NH3)4+2 | 5.66E-41 | 2.08E-41 | -40.683 |
| Ni(NH3)5+2 | 4.66E-51 | 1.71E-51 | -50.767 |
| Ni(NH3)6+2 | 8.18E-62 | 3E-62 | -61.523 |
| Ni(NO2)2 (aq) | 2.22E-79 | 2.28E-79 | -78.643 |
| Ni(OH)2 (aq) | 1.31E-20 | 1.34E-20 | -19.872 |
| Ni(OH)3- | 3.28E-29 | 2.55E-29 | -28.593 |
| Ni(SO4)2-2 | 3.12E-09 | 1.15E-09 | -8.941 |
| Ni+2 | 1.01E-05 | 3.71E-06 | -5.431 |
| NiCl+ | 2.89E-08 | 2.25E-08 | -7.648 |
| NiCl2 (aq) | 1.31E-11 | 1.34E-11 | -10.871 |
| NiCO3 (aq) | 6.87E-17 | 7.04E-17 | -16.152 |
| NiF+ | 6.7E-13 | 5.21E-13 | -12.283 |
| NiH2PO4+ | 1.49E-11 | 1.16E-11 | -10.936 |
| NiHCO3+ | 3.36E-11 | 2.62E-11 | -10.582 |
| NiHPO4 (aq) | 1.45E-14 | 1.49E-14 | -13.826 |
| NiHS+ | 3.57E-45 | 2.78E-45 | -44.556 |
| NiN3+ | 1.7E-11 | 1.32E-11 | -10.879 |
| NiNH3+2 | 9.85E-14 | 3.61E-14 | -13.442 |
| NiNO2+ | 3.61E-42 | 2.81E-42 | -41.552 |
| NiNO3+ | 2.77E-54 | 2.16E-54 | -53.666 |
| NiOH+ | 5.53E-14 | 4.3E-14 | -13.367 |
| NiSO4 (aq) | 4.55E-06 | 4.66E-06 | -5.331 |
| NO2-1 | 4.05E-38 | 3.16E-38 | -37.501 |
| NO3-1 | 3.1E-49 | 2.32E-49 | -48.635 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| OH- | 1.15E-12 | 8.71E-13 | -12.06 |
| Pb DOM1 | 1.08E-09 | 9.21E-10 | -9.036 |
| Pb(CO3)2-2 | 4.14E-29 | 1.52E-29 | -28.819 |
| Pb(HS)2 (aq) | 7.11E-83 | 7.29E-83 | -82.137 |
| Pb(HS)3- | 4.5E-126 | 3.5E-126 | -125.453 |
| Pb(NO2)2 (aq) | 8.33E-81 | 8.55E-81 | -80.068 |
| Pb(NO3)2 (aq) | 9.6E-105 | 9.9E-105 | -104.006 |
| Pb(OH)2 (aq) | 1.87E-21 | 1.92E-21 | -20.718 |
| Pb(OH)3- | 4.69E-30 | 3.65E-30 | -29.438 |
| Pb(SO4)2-2 | 2.51E-09 | 9.19E-10 | -9.036 |
| Pb+2 | 1.82E-08 | 6.66E-09 | -8.176 |
| Pb2OH+3 | 3.22E-20 | 3.36E-21 | -20.473 |
| Pb3(OH)4+2 | 2.62E-40 | 9.59E-41 | -40.018 |
| Pb4(OH)4+4 | 5.46E-44 | 9.86E-46 | -45.006 |
| PbCl+ | 4.62E-09 | 3.59E-09 | -8.444 |
| PbCl2 (aq) | 1.23E-10 | 1.26E-10 | -9.9 |
| PbCl3- | 2.16E-12 | 1.68E-12 | -11.775 |
| PbCl4-2 | 2.81E-14 | 1.03E-14 | -13.987 |
| PbCO3 (aq) | 1.13E-17 | 1.15E-17 | -16.938 |
| PbF+ | 9.42E-15 | 7.33E-15 | -14.135 |
| PbF2 (aq) | 6.84E-22 | 7.02E-22 | -21.154 |
| PbH2PO4+ | 1E-13 | 7.79E-14 | -13.109 |
| PbHCO3+ | 3.9E-13 | 3.04E-13 | -12.517 |
| PbHPO4 (aq) | 3.65E-17 | 3.74E-17 | -16.427 |
| PbNO2+ | 8.74E-44 | 6.8E-44 | -43.167 |
| PbNO3+ | 3.02E-56 | 2.35E-56 | -55.629 |
| PbOH+ | 2.93E-14 | 2.28E-14 | -13.642 |
| PbSO4 (aq) | 2.18E-08 | 2.23E-08 | -7.651 |
| PO4-3 | 3.39E-21 | 3.58E-22 | -21.446 |
| S-2 | 2.5E-60 | 9.21E-61 | -60.036 |
| SO4-2 | 0.020246 | 0.006838 | -2.165 |
| Zn DOM1 | 1.77E-08 | 1.51E-08 | -7.821 |
| Zn(CO3)2-2 | 7.79E-29 | 2.85E-29 | -28.545 |
| Zn(N3)2 (aq) | 1.82E-17 | 1.87E-17 | -16.729 |
| Zn(N3)3- | 2.59E-23 | 2.02E-23 | -22.695 |
| Zn(NH3)2+2 | 1.44E-22 | 5.28E-23 | -22.278 |
| Zn(NH3)3+2 | 6.29E-31 | 2.31E-31 | -30.637 |
| Zn(NH3)4+2 | 1.35E-39 | 4.94E-40 | -39.307 |
| Zn(NO2)2 (aq) | 8.41E-80 | 8.63E-80 | -79.064 |
| Zn(NO3)2 (aq) | 1.4E-103 | 1.5E-103 | -102.832 |
| Zn(OH)2 (aq) | 2.43E-18 | 2.49E-18 | -17.603 |
| Zn(OH)3- | 1.93E-27 | 1.5E-27 | -26.824 |
| Zn(OH)4-2 | 1.23E-37 | 4.53E-38 | -37.344 |
| Zn(SO4)2-2 | 1.33E-06 | 4.87E-07 | -6.312 |
| Zn+2 | 1.39E-05 | 5.47E-06 | -5.262 |
| Zn2OH+3 | 2.23E-17 | 2.33E-18 | -17.632 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn2S3-2 | 1.8E-137 | 6.6E-138 | -137.181 |
| Zn4S6-4 | 4.1E-272 | 7.4E-274 | -273.131 |
| ZnCl+ | 3.21E-07 | 2.45E-07 | -6.61 |
| ZnCl2 (aq) | 2.57E-09 | 2.64E-09 | -8.579 |
| ZnCl3- | 6E-11 | 4.67E-11 | -10.331 |
| ZnCl4-2 | 9.86E-13 | 3.61E-13 | -12.442 |
| ZnCO3 (aq) | 1.57E-16 | 1.61E-16 | -15.793 |
| ZnF+ | 9.36E-13 | 7.29E-13 | -12.138 |
| ZnHCO3+ | 1.27E-11 | 9.91E-12 | -11.004 |
| ZnHPO4 (aq) | 4.91E-14 | 5.04E-14 | -13.297 |
| ZnN3+ | 1.91E-11 | 1.49E-11 | -10.828 |
| ZnNH3+2 | 4.19E-14 | 1.54E-14 | -13.814 |
| ZnNO2+ | 1.34E-42 | 1.04E-42 | -41.983 |
| ZnNO3+ | 4.36E-54 | 3.4E-54 | -53.469 |
| ZnOH+ | 6.13E-13 | 4.77E-13 | -12.322 |
| ZnS (aq) | 9.15E-50 | 9.39E-50 | -49.028 |
| ZnSO4 (aq) | 7.31E-06 | 7.5E-06 | -5.125 |

## B1.5: Eh 500

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 4.05E-06 | 4.01E-06 | -5.397 |
| Al(OH)2+ | 3.24E-12 | 2.56E-12 | -11.591 |
| Al(OH)3 (aq) | 2.94E-17 | 3.01E-17 | -16.521 |
| Al(OH)4- | 1.08E-21 | 8.4E-22 | -21.076 |
| Al(SO4)2- | 0.000935 | 0.000727 | -3.138 |
| Al+3 | 0.0004 | 7.21E-05 | -4.142 |
| Al2(OH)2+4 | 7.19E-12 | 1.44E-13 | -12.842 |
| Al2(OH)2CO3+2 | 6.09E-17 | 2.29E-17 | -16.64 |
| Al2PO4+3 | 1.78E-11 | 1.97E-12 | -11.705 |
| Al3(OH)4+5 | 4.65E-18 | 1.03E-20 | -19.988 |
| AlCl+2 | 1.13E-06 | 4.24E-07 | -6.372 |
| AlF+2 | 1.3E-05 | 5.06E-06 | -5.296 |
| AlF2+ | 1.85E-08 | 1.46E-08 | -7.834 |
| AlF3 (aq) | 1.22E-12 | 1.25E-12 | -11.903 |
| AlF4- | 5.89E-18 | 4.58E-18 | -17.339 |
| AlHPO4+ | 5.96E-09 | 4.66E-09 | -8.331 |
| AlOH+2 | 5.96E-08 | 2.32E-08 | -7.635 |
| AlSO4+ | 0.003465 | 0.002695 | -2.569 |
| As3S4(HS)- | 9.4E-284 | 7.4E-284 | -283.131 |
| AsO4-3 | 5.11E-21 | 5.66E-22 | -21.247 |
| AsS(OH)HS- | 7.2E-100 | 5.6E-100 | -99.249 |
| Ca DOM1 | 8.06E-07 | 6.89E-07 | -6.162 |
| Ca(NH3)2+2 | 5.55E-25 | 2.09E-25 | -24.68 |
| Ca(NO3)2 | 9.48E-87 | 9.71E-87 | -86.013 |
| Ca+2 | 0.005906 | 0.002476 | -2.606 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCl+ | 0.000108 | 8.49E-05 | -4.071 |
| CaCO3 (aq) | 1.92E-16 | 1.96E-16 | -15.707 |
| CaCrO4 (aq) | 9.18E-12 | 9.39E-12 | -11.027 |
| CaF+ | 2.62E-10 | 2.05E-10 | -9.687 |
| CaH2PO4+ | 2.87E-08 | 2.27E-08 | -7.644 |
| CaHCO3+ | 7.77E-10 | 6.19E-10 | -9.208 |
| CaHPO4 (aq) | 1.73E-12 | 1.77E-12 | -11.752 |
| CaNH3+2 | 1.09E-13 | 4.09E-14 | -13.388 |
| CaNO3+ | 3.8E-42 | 2.97E-42 | -41.527 |
| CaOH+ | 1.59E-14 | 1.26E-14 | -13.898 |
| CaPO4- | 2.99E-19 | 2.36E-19 | -18.626 |
| CaSO4 (aq) | 0.003217 | 0.003293 | -2.482 |
| Cd DOM1 | 7.16E-13 | 6.13E-13 | -12.213 |
| Cd(CO3)2-2 | 1.22E-34 | 4.58E-35 | -34.339 |
| Cd(HS)2 (aq) | 4.4E-103 | 4.5E-103 | -102.349 |
| Cd(HS)3- | 1.8E-155 | 1.4E-155 | -154.849 |
| Cd(HS)4-2 | 3E-207 | 1.1E-207 | -206.95 |
| Cd(NH3)2+2 | 3.06E-27 | 1.15E-27 | -26.94 |
| Cd(NH3)3+2 | 3.92E-37 | 1.48E-37 | -36.831 |
| Cd(NH3)4+2 | 1.49E-47 | 5.59E-48 | -47.253 |
| Cd(NO2)2 (aq) | 7.38E-68 | 7.55E-68 | -67.122 |
| Cd(NO3)2 (aq) | 1.68E-88 | 1.72E-88 | -87.764 |
| Cd(OH)2 (aq) | 1.69E-26 | 1.73E-26 | -25.762 |
| Cd(OH)3- | 1.36E-37 | 1.06E-37 | -36.974 |
| Cd(OH)4-2 | 1.81E-49 | 6.81E-50 | -49.167 |
| Cd(SO4)2-2 | 3.03E-10 | 1.14E-10 | -9.944 |
| Cd+2 | 2.33E-09 | 8.76E-10 | -9.058 |
| Cd2OH+3 | 9.12E-26 | 1.01E-26 | -25.996 |
| CdCl+ | 1.5E-09 | 1.17E-09 | -8.93 |
| CdCl2 (aq) | 6.66E-11 | 6.81E-11 | -10.167 |
| CdCO3 (aq) | 1.11E-21 | 1.14E-21 | -20.943 |
| CdF+ | 1.21E-16 | 9.46E-17 | -16.024 |
| CdHCO3+ | 6.68E-16 | 5.23E-16 | -15.281 |
| CdHPO4 (aq) | 6.5E-18 | 6.65E-18 | -17.177 |
| CdHS+ | 5.73E-56 | 4.49E-56 | -55.348 |
| CdNH3+2 | 4.92E-18 | 1.85E-18 | -17.733 |
| CdNO2+ | 1.58E-38 | 1.23E-38 | -37.909 |
| CdNO3+ | 1.67E-48 | 1.31E-48 | -47.883 |
| CdOH+ | 2.59E-18 | 2.03E-18 | -17.693 |
| CdSO4 (aq) | 1.14E-09 | 1.17E-09 | -8.933 |
| Cl-1 | 0.019054 | 0.014436 | -1.841 |
| CO3-2 | 1.43E-16 | 5.55E-17 | -16.256 |
| Cr2O7-2 | 1.26E-11 | 4.75E-12 | -11.323 |
| CrO3Cl- | 6.17E-10 | 4.83E-10 | -9.316 |
| CrO3H2PO4- | 4.88E-12 | 3.82E-12 | -11.418 |
| CrO3HPO4-2 | 1.33E-12 | 4.98E-13 | -12.302 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CrO3SO4-2 | 2.77E-08 | 1.04E-08 | -7.983 |
| CrO4-2 | 1.83E-11 | 6.44E-12 | -11.191 |
| Cu DOM1 | 6.66E-10 | 5.7E-10 | -9.244 |
| Cu(CO3)2-2 | 2.66E-30 | 9.99E-31 | -30 |
| Cu(N3)2 (aq) | 2.64E-18 | 2.7E-18 | -17.568 |
| Cu(N3)3- | 1.08E-23 | 8.45E-24 | -23.073 |
| Cu(N3)4-2 | 3.69E-30 | 1.39E-30 | -29.858 |
| Cu(NH3)2+2 | 6.11E-23 | 2.3E-23 | -22.639 |
| Cu(NH3)3+2 | 2.57E-31 | 9.67E-32 | -31.015 |
| Cu(NH3)4+2 | 2.24E-40 | 8.41E-41 | -40.075 |
| Cu(NO2)2 (aq) | 4.2E-67 | 4.3E-67 | -66.367 |
| Cu(NO3)2 (aq) | 9.87E-88 | 1.01E-87 | -86.996 |
| Cu(OH)2 (aq) | 1.24E-21 | 1.27E-21 | -20.896 |
| Cu(OH)3- | 1.45E-29 | 1.14E-29 | -28.945 |
| Cu(OH)4-2 | 1.26E-41 | 4.73E-42 | -41.326 |
| Cu+2 | 5.07E-08 | 2.05E-08 | -7.689 |
| Cu2(OH)2+2 | 4.97E-23 | 1.87E-23 | -22.729 |
| Cu2OH+3 | 3.15E-20 | 3.49E-21 | -20.457 |
| Cu2S3-2 | 1.2E-175 | 4.6E-176 | -175.336 |
| Cu3(OH)4+2 | 1.27E-37 | 4.76E-38 | -37.322 |
| CuCl+ | 6.81E-10 | 5.25E-10 | -9.28 |
| CuCl2 (aq) | 1.23E-12 | 1.26E-12 | -11.899 |
| CuCl3- | 1.84E-16 | 1.42E-16 | -15.849 |
| CuCl4-2 1 | 3.82E-20 | 1.45E-20 | -19.839 |
| CuCO3 (aq) | 6.53E-18 | 6.69E-18 | -17.175 |
| CuF+ | 7.98E-15 | 6.25E-15 | -14.204 |
| CuHCO3+ | 3.11E-14 | 2.43E-14 | -13.614 |
| CuHPO4 (aq) | 4E-16 | 4.09E-16 | -15.388 |
| CuHSO4+ | 5.84E-10 | 4.57E-10 | -9.34 |
| CuN3+ | 1.18E-12 | 9.26E-13 | -12.034 |
| CuNH3+2 | 3.8E-15 | 1.43E-15 | -14.845 |
| CuNO2+ | 3.83E-37 | 3E-37 | -36.523 |
| CuNO3+ | 3.08E-47 | 2.41E-47 | -46.617 |
| CuOH+ | 3.19E-14 | 2.46E-14 | -13.609 |
| CuS(aq) | 9.96E-64 | 1.02E-63 | -62.991 |
| CuSO4 (aq) | 2.6E-08 | 2.66E-08 | -7.575 |
| DOC (Gaussian DOM) | 0.001399 | 0.001432 | -2.844 |
| DOM1 | 2.34E-05 | 3.44E-06 | -5.463 |
| F-1 | 9.58E-09 | 7.31E-09 | -8.136 |
| Fe DOM1 | 8.23E-07 | 8.15E-07 | -6.089 |
| Fe(N3)2+ | 8.76E-14 | 6.86E-14 | -13.164 |
| Fe(N3)3 (aq) | 8.96E-19 | 9.17E-19 | -18.038 |
| Fe(NH3)2+2 | 2.36E-23 | 8.86E-24 | -23.053 |
| Fe(NH3)3+2 | 3.57E-34 | 1.34E-34 | -33.872 |
| Fe(NH3)4+2 | 2.31E-45 | 8.68E-46 | -45.062 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe(NO2)2+ | 6.09E-65 | 4.77E-65 | -64.321 |
| Fe(NO2)3 (aq) | 7.49E-94 | 7.67E-94 | -93.115 |
| Fe(OH)2 (aq) | 3.72E-21 | 3.81E-21 | -20.419 |
| Fe(OH)2+ | 2.39E-10 | 1.89E-10 | -9.723 |
| Fe(OH)3- | 8.76E-30 | 6.87E-30 | -29.163 |
| Fe(OH)3 (aq) | 3.82E-18 | 3.92E-18 | -17.407 |
| Fe(OH)4- | 2.03E-24 | 1.6E-24 | -23.796 |
| Fe(SO4)2- | 4.47E-07 | 3.5E-07 | -6.456 |
| Fe+2 | 0.004045 | 0.001632 | -2.787 |
| Fe+3 | 2.57E-07 | 4.64E-08 | -7.333 |
| Fe2(OH)2+4 | 2.42E-13 | 4.85E-15 | -14.314 |
| Fe3(OH)4+5 | 1.41E-19 | 3.12E-22 | -21.506 |
| FeCl+ | 1.9E-05 | 1.49E-05 | -4.828 |
| FeCl+2 | 3.87E-08 | 1.47E-08 | -7.834 |
| FeCrO4+ | 1.4E-11 | 1.1E-11 | -10.959 |
| FeF+ | 2.47E-10 | 1.93E-10 | -9.713 |
| FeF+2 | 8.53E-10 | 3.23E-10 | -9.49 |
| FeF2+ | 1.14E-13 | 8.94E-14 | -13.049 |
| FeF3 (aq) | 5.91E-19 | 6.06E-19 | -18.218 |
| FeH2PO4+ | 3.9E-07 | 3.08E-07 | -6.512 |
| FeH2PO4+2 | 8.5E-10 | 3.31E-10 | -9.481 |
| FeHCO3+ | 4.86E-10 | 3.87E-10 | -9.412 |
| FeHPO4 (aq) | 9.51E-12 | 9.73E-12 | -11.012 |
| FeHPO4+ | 1.1E-09 | 8.67E-10 | -9.062 |
| FeHS+ | 4.35E-52 | 3.4E-52 | -51.468 |
| FeN3+2 | 1.2E-09 | 4.52E-10 | -9.345 |
| FeNH3+2 | 6.13E-13 | 2.3E-13 | -12.637 |
| FeNO2+2 | 2.74E-35 | 1.03E-35 | -34.987 |
| FeOH+ | 2.38E-11 | 1.87E-11 | -10.729 |
| FeOH+2 | 5.13E-08 | 1.94E-08 | -7.711 |
| FeSO4 (aq) | 0.002243 | 0.002296 | -2.639 |
| FeSO4+ | 4.75E-06 | 3.73E-06 | -5.428 |
| H DOM1 | 9.13E-05 | 4.14E-05 | -4.383 |
| H+1 | 0.019259 | 0.015921 | -1.798 |
| H2AsO3- | 4.7E-15 | 3.68E-15 | -14.434 |
| H2AsO4- | 1.52E-06 | 1.19E-06 | -5.924 |
| H2CO3* (aq) | 0.000967 | 0.00099 | -3.004 |
| H2CrO4 (aq) | 1.89E-09 | 1.93E-09 | -8.714 |
| H2PO4- | 6.13E-07 | 4.84E-07 | -6.315 |
| H2S (aq) | 1.13E-49 | 1.16E-49 | -48.936 |
| H3AsO3 | 1.25E-07 | 1.28E-07 | -6.894 |
| H3AsO4 | 3.3E-06 | 3.38E-06 | -5.471 |
| H3PO4 | 9.53E-07 | 9.76E-07 | -6.011 |
| HAsO3-2 | 3.13E-27 | 1.18E-27 | -26.929 |
| HAsO4-2 | 1.95E-11 | 7.33E-12 | -11.135 |
| HCO3- | 3E-08 | 2.37E-08 | -7.625 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HCrO4- | 4.12E-07 | 3.23E-07 | -6.491 |
| HF (aq) | 1.43E-07 | 1.46E-07 | -6.835 |
| HF2- | 5.27E-15 | 4.02E-15 | -14.396 |
| Hg(CO3)2-2 | 8.18E-38 | 3.07E-38 | -37.512 |
| Hg(HS)2 (aq) | 1.69E-91 | 1.73E-91 | -90.762 |
| Hg(N3)2 (aq) | 3.98E-16 | 4.07E-16 | -15.39 |
| Hg(NH3)2+2 | 8.04E-25 | 3.02E-25 | -24.52 |
| Hg(NH3)4+2 | 9.44E-46 | 3.55E-46 | -45.45 |
| Hg(NO2)2 (aq) | 4.09E-73 | 4.18E-73 | -72.379 |
| Hg(NO2)3- | 2.6E-102 | 2E-102 | -101.693 |
| Hg(NO2)4-2 | 1.9E-132 | 7.3E-133 | -132.136 |
| Hg(NO3)2 (aq) | 5.3E-101 | 5.4E-101 | -100.267 |
| Hg(OH)2 | 6.89E-24 | 7.06E-24 | -23.151 |
| Hg(SO4)2-2 | 8.67E-22 | 3.26E-22 | -21.487 |
| Hg+2 | 1.23E-20 | 4.62E-21 | -20.335 |
| Hg2OH+3 | 4.98E-42 | 5.52E-43 | -42.258 |
| Hg3(OH)3+3 | 1.65E-62 | 1.83E-63 | -62.737 |
| HgCl+ | 2.42E-15 | 1.9E-15 | -14.722 |
| HgCl2 (aq) | 2.05E-10 | 2.1E-10 | -9.678 |
| HgCl3-1 | 3.85E-11 | 3.01E-11 | -10.521 |
| HgCl4-2 | 5.18E-12 | 1.95E-12 | -11.71 |
| HgClOH (aq) | 8.07E-17 | 8.26E-17 | -16.083 |
| HgCO3 (aq) | 1.92E-25 | 1.97E-25 | -24.706 |
| HgF+ | 1.61E-27 | 1.26E-27 | -26.9 |
| HgHCO3+ | 6.63E-23 | 5.19E-23 | -22.284 |
| HgHS2- | 4.49E-96 | 3.52E-96 | -95.454 |
| HgN3+ | 5.37E-13 | 4.2E-13 | -12.376 |
| HgNO2+ | 4.09E-46 | 3.2E-46 | -45.495 |
| HgNO3+ | 4.71E-61 | 3.69E-61 | -60.433 |
| HgOH+ | 1.1E-22 | 8.63E-23 | -22.064 |
| HgOHCO3- | 1.84E-30 | 1.44E-30 | -29.842 |
| HgS2-2 | 1.1E-102 | 4.3E-103 | -102.366 |
| HgSO4 (aq) | 4.85E-21 | 4.97E-21 | -20.304 |
| HN3 (aq) | 4.99E-05 | 5.11E-05 | -4.292 |
| HNO2 (aq) | 3.08E-30 | 3.15E-30 | -29.502 |
| HPO4-2 | 4.88E-12 | 1.85E-12 | -11.733 |
| HS-1 | 6.56E-55 | 5E-55 | -54.301 |
| HSO4- | 0.009759 | 0.007592 | -2.12 |
| K+1 | 0.000319 | 0.000242 | -3.617 |
| K2HPO4 (aq) | 1.14E-18 | 1.17E-18 | -17.933 |
| K2PO4- | 5.39E-28 | 4.22E-28 | -27.375 |
| KCl (aq) | 1.81E-06 | 1.85E-06 | -5.733 |
| KCr2O7- | 1.27E-14 | 9.91E-15 | -14.004 |
| KCrO4- | 7.39E-15 | 5.79E-15 | -14.238 |
| KF (aq) | 7.89E-13 | 8.08E-13 | -12.093 |
| KH2PO4 (aq) | 1.77E-10 | 1.82E-10 | -9.741 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| KHPO4- | 3.48E-15 | 2.75E-15 | -14.561 |
| KNO3 (aq) | 6.35E-44 | 6.5E-44 | -43.187 |
| KOH (aq) | 1.18E-16 | 1.21E-16 | -15.918 |
| KPO4-2 | 5.57E-25 | 2.09E-25 | -24.679 |
| KSO4- | 1.16E-05 | 9.16E-06 | -5.038 |
| Mg DOM1 | 7.05E-08 | 6.03E-08 | -7.22 |
| Mg(NH3)2+2 | 2.42E-25 | 9.11E-26 | -25.04 |
| Mg+2 | 0.00498 | 0.002165 | -2.664 |
| Mg2CO3+2 | 2.69E-18 | 1.01E-18 | -17.995 |
| MgCl+ | 0.00015 | 0.000118 | -3.929 |
| MgCO3 (aq) | 8.37E-17 | 8.57E-17 | -16.067 |
| MgF+ | 1.35E-09 | 1.05E-09 | -8.98 |
| MgHCO3+ | 6.47E-10 | 4.98E-10 | -9.302 |
| MgHPO4 (aq) | 2.09E-12 | 2.13E-12 | -11.671 |
| MgOH+ | 2.62E-13 | 2.1E-13 | -12.678 |
| MgPO4- | 4.09E-21 | 3.23E-21 | -20.491 |
| MgSO4 (aq) | 0.002275 | 0.002329 | -2.633 |
| Mn+3 | 4.55E-05 | 8.2E-06 | -5.086 |
| N3-1 | 7.97E-08 | 6.24E-08 | -7.205 |
| Na+1 | 0.012121 | 0.009508 | -2.022 |
| Na2HPO4 (aq) | 1.17E-15 | 1.19E-15 | -14.923 |
| Na2PO4- | 1.78E-24 | 1.4E-24 | -23.855 |
| NaCl (aq) | 7.52E-05 | 7.69E-05 | -4.114 |
| NaCO3- | 1.65E-17 | 1.31E-17 | -16.884 |
| NaCrO4- | 3.89E-13 | 3.04E-13 | -12.517 |
| NaF (aq) | 6.01E-11 | 6.15E-11 | -10.211 |
| NaH2PO4 (aq) | 6.97E-09 | 7.14E-09 | -8.146 |
| NaHCO3 (aq) | 1.3E-10 | 1.34E-10 | -9.874 |
| NaHPO4- | 2.12E-13 | 1.67E-13 | -12.776 |
| NaNO3 (aq) | 9.22E-43 | 9.43E-43 | -42.025 |
| NaOH (aq) | 3.18E-15 | 3.25E-15 | -14.488 |
| NaPO4-2 | 2.41E-23 | 9.08E-24 | -23.042 |
| NaSO4- | 0.000418 | 0.00033 | -3.481 |
| NH3 (aq) | 4.85E-12 | 4.97E-12 | -11.304 |
| NH4+1 | 0.000386 | 0.000288 | -3.54 |
| NH4Cr2O7- | 1.76E-14 | 1.37E-14 | -13.862 |
| NH4SO4- | 2.53E-05 | 1.98E-05 | -4.703 |
| Ni DOM1 | 3.15E-09 | 2.69E-09 | -8.57 |
| Ni(N3)2 (aq) | 1.45E-18 | 1.48E-18 | -17.829 |
| Ni(NH3)2+2 | 2.92E-23 | 1.1E-23 | -22.959 |
| Ni(NH3)3+2 | 8.42E-33 | 3.17E-33 | -32.5 |
| Ni(NH3)4+2 | 7.18E-43 | 2.7E-43 | -42.568 |
| Ni(NH3)5+2 | 1.98E-53 | 7.45E-54 | -53.128 |
| Ni(NH3)6+2 | 1.16E-64 | 4.37E-65 | -64.359 |
| Ni(NO2)2 (aq) | 4.54E-66 | 4.65E-66 | -65.333 |
| Ni(OH)2 (aq) | 1.48E-21 | 1.52E-21 | -20.819 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(OH)3- | 1.21E-30 | 9.51E-31 | -30.022 |
| Ni(SO4)2-2 | 2.78E-09 | 1.05E-09 | -8.981 |
| Ni+2 | 1.02E-05 | 3.85E-06 | -5.415 |
| NiCl+ | 2.56E-08 | 2.01E-08 | -7.697 |
| NiCl2 (aq) | 1.01E-11 | 1.03E-11 | -10.986 |
| NiCO3 (aq) | 7.75E-18 | 7.94E-18 | -17.1 |
| NiF+ | 6.49E-13 | 5.08E-13 | -12.294 |
| NiH2PO4+ | 1.56E-11 | 1.22E-11 | -10.912 |
| NiHCO3+ | 1.14E-11 | 8.94E-12 | -11.048 |
| NiHPO4 (aq) | 5.08E-15 | 5.2E-15 | -14.284 |
| NiHS+ | 7.6E-55 | 5.95E-55 | -54.225 |
| NiN3+ | 5.78E-12 | 4.52E-12 | -11.345 |
| NiNH3+2 | 3.33E-14 | 1.25E-14 | -13.902 |
| NiNO2+ | 1.65E-35 | 1.29E-35 | -34.889 |
| NiNO3+ | 4.35E-45 | 3.4E-45 | -44.468 |
| NiOH+ | 1.88E-14 | 1.47E-14 | -13.832 |
| NiSO4 (aq) | 4.43E-06 | 4.54E-06 | -5.343 |
| NO2-1 | 1.79E-31 | 1.4E-31 | -30.854 |
| NO3-1 | 4.66E-40 | 3.52E-40 | -39.453 |
| OH- | 3.76E-13 | 2.87E-13 | -12.542 |
| Pb DOM1 | 4.66E-10 | 3.99E-10 | -9.399 |
| Pb(CO3)2-2 | 5.12E-31 | 1.93E-31 | -30.715 |
| Pb(HS)2 (aq) | 3.3E-102 | 3.3E-102 | -101.475 |
| Pb(HS)3- | 4.3E-155 | 3.3E-155 | -154.476 |
| Pb(NO2)2 (aq) | 1.77E-67 | 1.81E-67 | -66.742 |
| Pb(NO3)2 (aq) | 2.4E-86 | 2.45E-86 | -85.61 |
| Pb(OH)2 (aq) | 2.19E-22 | 2.25E-22 | -21.648 |
| Pb(OH)3- | 1.8E-31 | 1.41E-31 | -30.851 |
| Pb(SO4)2-2 | 2.32E-09 | 8.71E-10 | -9.06 |
| Pb+2 | 1.91E-08 | 7.18E-09 | -8.144 |
| Pb2OH+3 | 1.16E-20 | 1.29E-21 | -20.89 |
| Pb3(OH)4+2 | 3.78E-42 | 1.42E-42 | -41.848 |
| Pb4(OH)4+4 | 7.87E-46 | 1.57E-47 | -46.803 |
| PbCl+ | 4.26E-09 | 3.33E-09 | -8.477 |
| PbCl2 (aq) | 9.82E-11 | 1E-10 | -9.998 |
| PbCl3- | 1.47E-12 | 1.15E-12 | -11.938 |
| PbCl4-2 | 1.62E-14 | 6.08E-15 | -14.216 |
| PbCO3 (aq) | 1.32E-18 | 1.35E-18 | -17.87 |
| PbF+ | 9.47E-15 | 7.42E-15 | -14.13 |
| PbF2 (aq) | 6.52E-22 | 6.67E-22 | -21.176 |
| PbH2PO4+ | 1.09E-13 | 8.55E-14 | -13.068 |
| PbHCO3+ | 1.38E-13 | 1.08E-13 | -12.968 |
| PbHPO4 (aq) | 1.32E-17 | 1.35E-17 | -16.868 |
| PbNO2+ | 4.15E-37 | 3.25E-37 | -36.488 |
| PbNO3+ | 4.91E-47 | 3.85E-47 | -46.415 |
| PbOH+ | 1.04E-14 | 8.11E-15 | -14.091 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| PbSO4 (aq) | 2.2E-08 | 2.26E-08 | -7.647 |
| PO4-3 | 3.52E-22 | 3.97E-23 | -22.401 |
| S-2 | 1.65E-70 | 6.27E-71 | -70.203 |
| SO4-2 | 0.018337 | 0.006411 | -2.193 |
| Zn DOM1 | 7.43E-09 | 6.35E-09 | -8.197 |
| Zn(CO3)2-2 | 9.37E-31 | 3.52E-31 | -30.453 |
| Zn(N3)2 (aq) | 2.08E-18 | 2.13E-18 | -17.672 |
| Zn(N3)3- | 9.71E-25 | 7.61E-25 | -24.119 |
| Zn(NH3)2+2 | 1.65E-23 | 6.19E-24 | -23.208 |
| Zn(NH3)3+2 | 2.41E-32 | 9.06E-33 | -32.043 |
| Zn(NH3)4+2 | 1.72E-41 | 6.48E-42 | -41.188 |
| Zn(NO2)2 (aq) | 1.74E-66 | 1.78E-66 | -65.75 |
| Zn(NO3)2 (aq) | 3.48E-85 | 3.56E-85 | -84.448 |
| Zn(OH)2 (aq) | 2.78E-19 | 2.84E-19 | -18.546 |
| Zn(OH)3- | 7.2E-29 | 5.64E-29 | -28.249 |
| Zn(OH)4-2 | 1.49E-39 | 5.61E-40 | -39.251 |
| Zn(SO4)2-2 | 1.19E-06 | 4.49E-07 | -6.348 |
| Zn+2 | 1.42E-05 | 5.73E-06 | -5.242 |
| Zn2OH+3 | 7.62E-18 | 8.44E-19 | -18.074 |
| Zn2S3-2 | 6.1E-168 | 2.3E-168 | -167.641 |
| ZnCl+ | 2.87E-07 | 2.21E-07 | -6.655 |
| ZnCl2 (aq) | 2E-09 | 2.05E-09 | -8.689 |
| ZnCl3- | 3.98E-11 | 3.11E-11 | -10.507 |
| ZnCl4-2 | 5.52E-13 | 2.07E-13 | -12.683 |
| ZnCO3 (aq) | 1.79E-17 | 1.83E-17 | -16.737 |
| ZnF+ | 9.15E-13 | 7.17E-13 | -12.145 |
| ZnHCO3+ | 4.36E-12 | 3.42E-12 | -11.466 |
| ZnHPO4 (aq) | 1.73E-14 | 1.77E-14 | -13.751 |
| ZnN3+ | 6.57E-12 | 5.15E-12 | -11.289 |
| ZnNH3+2 | 1.43E-14 | 5.38E-15 | -14.269 |
| ZnNO2+ | 6.17E-36 | 4.83E-36 | -35.316 |
| ZnNO3+ | 6.9E-45 | 5.41E-45 | -44.267 |
| ZnOH+ | 2.1E-13 | 1.65E-13 | -12.783 |
| ZnS (aq) | 6.54E-60 | 6.69E-60 | -59.174 |
| ZnSO4 (aq) | 7.2E-06 | 7.37E-06 | -5.132 |

## B1.6: Eh 600

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.21E-06 | 3.17E-06 | -5.498 |
| Al(OH)2+ | 1.79E-12 | 1.42E-12 | -11.848 |
| Al(OH)3 (aq) | 1.19E-17 | 1.22E-17 | -16.915 |
| Al(OH)4- | 3.16E-22 | 2.47E-22 | -21.607 |
| Al(SO4)2- | 0.000911 | 0.000712 | -3.148 |
| Al+3 | 0.000407 | 7.52E-05 | -4.124 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al2(OH)2+4 | 3.91E-12 | 8.3E-14 | -13.081 |
| Al2(OH)2CO3+2 | 1.84E-17 | 7.01E-18 | -17.154 |
| Al2PO4+3 | 1E-11 | 1.15E-12 | -11.94 |
| Al3(OH)4+5 | 1.35E-18 | 3.29E-21 | -20.483 |
| AlCl+2 | 1.06E-06 | 4.03E-07 | -6.395 |
| AlF+2 | 1.3E-05 | 5.12E-06 | -5.291 |
| AlF2+ | 1.82E-08 | 1.44E-08 | -7.842 |
| AlF3 (aq) | 1.17E-12 | 1.19E-12 | -11.923 |
| AlF4- | 5.44E-18 | 4.25E-18 | -17.372 |
| AlHPO4+ | 4.55E-09 | 3.58E-09 | -8.447 |
| AlOH+2 | 4.46E-08 | 1.76E-08 | -7.754 |
| AlSO4+ | 0.003483 | 0.002721 | -2.565 |
| AsO4-3 | 2.15E-21 | 2.46E-22 | -21.609 |
| AsS(OH)HS- | 1.9E-128 | 1.5E-128 | -127.828 |
| Ca DOM1 | 6.24E-07 | 5.35E-07 | -6.272 |
| Ca(NH3)2+2 | 3.01E-25 | 1.15E-25 | -24.94 |
| Ca(NO3)2 | 1.71E-61 | 1.75E-61 | -60.757 |
| Ca+2 | 0.005948 | 0.002525 | -2.598 |
| CaCl+ | 0.0001 | 7.9E-05 | -4.103 |
| CaCO3 (aq) | 1.04E-16 | 1.06E-16 | -15.974 |
| CaCrO4 (aq) | 6.71E-12 | 6.86E-12 | -11.164 |
| CaF+ | 2.58E-10 | 2.03E-10 | -9.691 |
| CaH2PO4+ | 2.95E-08 | 2.34E-08 | -7.632 |
| CaHCO3+ | 5.75E-10 | 4.6E-10 | -9.338 |
| CaHPO4 (aq) | 1.3E-12 | 1.33E-12 | -11.877 |
| CaNH3+2 | 8.03E-14 | 3.06E-14 | -13.514 |
| CaNO3+ | 1.62E-29 | 1.28E-29 | -28.894 |
| CaOH+ | 1.17E-14 | 9.4E-15 | -14.027 |
| CaPO4- | 1.63E-19 | 1.29E-19 | -18.888 |
| CaSO4 (aq) | 0.003183 | 0.003254 | -2.488 |
| Cd DOM1 | 5.69E-13 | 4.88E-13 | -12.312 |
| Cd(CO3)2-2 | 3.54E-35 | 1.35E-35 | -34.869 |
| Cd(HS)2 (aq) | 1.3E-128 | 1.3E-128 | -127.872 |
| Cd(HS)3- | 9.1E-194 | 7.2E-194 | -193.144 |
| Cd(HS)4-2 | 2.5E-258 | 9.6E-259 | -258.016 |
| Cd(NH3)2+2 | 1.7E-27 | 6.49E-28 | -27.188 |
| Cd(NH3)3+2 | 1.61E-37 | 6.13E-38 | -37.213 |
| Cd(NH3)4+2 | 4.46E-48 | 1.7E-48 | -47.769 |
| Cd(NO2)2 (aq) | 4.88E-49 | 4.99E-49 | -48.302 |
| Cd(NO3)2 (aq) | 3.12E-63 | 3.19E-63 | -62.496 |
| Cd(OH)2 (aq) | 9.41E-27 | 9.62E-27 | -26.017 |
| Cd(OH)3- | 5.49E-38 | 4.31E-38 | -37.365 |
| Cd(OH)4-2 | 5.28E-50 | 2.01E-50 | -49.696 |
| Cd(SO4)2-2 | 2.93E-10 | 1.12E-10 | -9.951 |
| Cd+2 | 2.4E-09 | 9.17E-10 | -9.038 |
| Cd2OH+3 | 7.04E-26 | 8.07E-27 | -26.093 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl+ | 1.43E-09 | 1.12E-09 | -8.95 |
| CdCl2 (aq) | 5.8E-11 | 5.94E-11 | -10.227 |
| CdCO3 (aq) | 6.19E-22 | 6.33E-22 | -21.198 |
| CdF+ | 1.22E-16 | 9.62E-17 | -16.017 |
| CdHCO3+ | 5.07E-16 | 3.99E-16 | -15.399 |
| CdHPO4 (aq) | 5.01E-18 | 5.13E-18 | -17.29 |
| CdHS+ | 1.01E-68 | 7.95E-69 | -68.1 |
| CdNH3+2 | 3.73E-18 | 1.42E-18 | -17.847 |
| CdNO2+ | 4.13E-29 | 3.25E-29 | -28.489 |
| CdNO3+ | 7.33E-36 | 5.76E-36 | -35.239 |
| CdOH+ | 1.97E-18 | 1.55E-18 | -17.81 |
| CdSO4 (aq) | 1.16E-09 | 1.18E-09 | -8.927 |
| Cl-1 | 0.017287 | 0.013168 | -1.88 |
| CO3-2 | 7.46E-17 | 2.95E-17 | -16.531 |
| Cr2O7-2 | 1.2E-11 | 4.58E-12 | -11.339 |
| CrO3Cl- | 7.56E-10 | 5.94E-10 | -9.226 |
| CrO3H2PO4- | 6.61E-12 | 5.2E-12 | -11.284 |
| CrO3HPO4-2 | 1.29E-12 | 4.94E-13 | -12.306 |
| CrO3SO4-2 | 3.56E-08 | 1.36E-08 | -7.867 |
| CrO4-2 | 1.28E-11 | 4.61E-12 | -11.336 |
| Cu DOM1 | 5.16E-10 | 4.42E-10 | -9.355 |
| Cu(CO3)2-2 | 7.53E-31 | 2.87E-31 | -30.542 |
| Cu(N3)2 (aq) | 1.43E-18 | 1.46E-18 | -17.835 |
| Cu(N3)3- | 4.24E-24 | 3.33E-24 | -23.477 |
| Cu(N3)4-2 | 1.04E-30 | 3.98E-31 | -30.4 |
| Cu(NH3)2+2 | 3.32E-23 | 1.27E-23 | -22.898 |
| Cu(NH3)3+2 | 1.02E-31 | 3.91E-32 | -31.408 |
| Cu(NH3)4+2 | 6.55E-41 | 2.5E-41 | -40.602 |
| Cu(NO2)2 (aq) | 2.71E-48 | 2.77E-48 | -47.558 |
| Cu(NO3)2 (aq) | 1.78E-62 | 1.82E-62 | -61.739 |
| Cu(OH)2 (aq) | 6.74E-22 | 6.89E-22 | -21.162 |
| Cu(OH)3- | 5.71E-30 | 4.49E-30 | -29.348 |
| Cu(OH)4-2 | 3.57E-42 | 1.36E-42 | -41.866 |
| Cu+2 | 5.1E-08 | 2.09E-08 | -7.68 |
| Cu2(OH)2+2 | 2.71E-23 | 1.03E-23 | -22.986 |
| Cu2OH+3 | 2.31E-20 | 2.65E-21 | -20.577 |
| Cu2S3-2 | 2.4E-214 | 9E-215 | -214.044 |
| Cu3(OH)4+2 | 3.74E-38 | 1.43E-38 | -37.845 |
| CuCl+ | 6.31E-10 | 4.88E-10 | -9.311 |
| CuCl2 (aq) | 1.05E-12 | 1.07E-12 | -11.97 |
| CuCl3- | 1.42E-16 | 1.1E-16 | -15.96 |
| CuCl4-2 1 | 2.65E-20 | 1.02E-20 | -19.99 |
| CuCO3 (aq) | 3.54E-18 | 3.62E-18 | -17.441 |
| CuF+ | 7.88E-15 | 6.19E-15 | -14.208 |
| CuHCO3+ | 2.3E-14 | 1.81E-14 | -13.743 |
| CuHPO4 (aq) | 3E-16 | 3.07E-16 | -15.513 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CuHSO4+ | 7.88E-10 | 6.2E-10 | -9.208 |
| CuN3+ | 8.75E-13 | 6.88E-13 | -12.163 |
| CuNH3+2 | 2.8E-15 | 1.07E-15 | -14.971 |
| CuNO2+ | 9.78E-28 | 7.69E-28 | -27.114 |
| CuNO3+ | 1.32E-34 | 1.04E-34 | -33.985 |
| CuOH+ | 2.36E-14 | 1.83E-14 | -13.738 |
| CuS(aq) | 1.26E-76 | 1.28E-76 | -75.892 |
| CuSO4 (aq) | 2.57E-08 | 2.63E-08 | -7.58 |
| DOC (Gaussian DOM) | 0.001399 | 0.00143 | -2.845 |
| DOM1 | 2.1E-05 | 3.17E-06 | -5.498 |
| F-1 | 9.26E-09 | 7.1E-09 | -8.149 |
| Fe DOM1 | 1.51E-06 | 1.5E-06 | -5.825 |
| Fe(N3)2+ | 1.12E-13 | 8.78E-14 | -13.056 |
| Fe(N3)3 (aq) | 8.37E-19 | 8.55E-19 | -18.068 |
| Fe(NH3)2+2 | 5.39E-25 | 2.06E-25 | -24.687 |
| Fe(NH3)3+2 | 6E-36 | 2.29E-36 | -35.64 |
| Fe(NH3)4+2 | 2.85E-47 | 1.09E-47 | -46.964 |
| Fe(NO2)2+ | 9.25E-46 | 7.27E-46 | -45.138 |
| Fe(NO2)3 (aq) | 2.87E-65 | 2.94E-65 | -64.532 |
| Fe(OH)2 (aq) | 8.51E-23 | 8.7E-23 | -22.06 |
| Fe(OH)2+ | 3.06E-10 | 2.43E-10 | -9.615 |
| Fe(OH)3- | 1.45E-31 | 1.14E-31 | -30.941 |
| Fe(OH)3 (aq) | 3.58E-18 | 3.66E-18 | -17.436 |
| Fe(OH)4- | 1.38E-24 | 1.09E-24 | -23.962 |
| Fe(SO4)2- | 1.01E-06 | 7.92E-07 | -6.101 |
| Fe+2 | 0.000171 | 7.02E-05 | -4.154 |
| Fe+3 | 6.07E-07 | 1.12E-07 | -6.951 |
| Fe2(OH)2+4 | 7.07E-13 | 1.5E-14 | -13.824 |
| Fe3(OH)4+5 | 5.09E-19 | 1.24E-21 | -20.908 |
| FeCl+ | 7.42E-07 | 5.83E-07 | -6.234 |
| FeCl+2 | 8.37E-08 | 3.23E-08 | -7.491 |
| FeCrO4+ | 2.41E-11 | 1.9E-11 | -10.722 |
| FeF+ | 1.03E-11 | 8.08E-12 | -11.093 |
| FeF+2 | 1.97E-09 | 7.58E-10 | -9.12 |
| FeF2+ | 2.58E-13 | 2.03E-13 | -12.692 |
| FeF3 (aq) | 1.31E-18 | 1.34E-18 | -17.873 |
| FeH2PO4+ | 1.68E-08 | 1.34E-08 | -7.874 |
| FeH2PO4+2 | 2.04E-09 | 8.05E-10 | -9.094 |
| FeHCO3+ | 1.52E-11 | 1.21E-11 | -10.916 |
| FeHPO4 (aq) | 3.01E-13 | 3.08E-13 | -12.512 |
| FeHPO4+ | 1.94E-09 | 1.54E-09 | -8.813 |
| FeHS+ | 3.15E-66 | 2.48E-66 | -65.606 |
| FeN3+2 | 2.08E-09 | 7.94E-10 | -9.1 |
| FeNH3+2 | 1.91E-14 | 7.28E-15 | -14.138 |
| FeNO2+2 | 1.64E-25 | 6.24E-26 | -25.205 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeOH+ | 7.43E-13 | 5.85E-13 | -12.233 |
| FeOH+2 | 8.87E-08 | 3.42E-08 | -7.466 |
| FeSO4 (aq) | 9.36E-05 | 9.57E-05 | -4.019 |
| FeSO4+ | 1.11E-05 | 8.72E-06 | -5.06 |
| H DOM1 | 9.41E-05 | 4.31E-05 | -4.365 |
| H+1 | 0.026349 | 0.021837 | -1.661 |
| H2AsO3- | 2.29E-18 | 1.8E-18 | -17.745 |
| H2AsO4- | 1.24E-06 | 9.73E-07 | -6.012 |
| H2CO3* (aq) | 0.000967 | 0.000989 | -3.005 |
| H2CrO4 (aq) | 2.55E-09 | 2.6E-09 | -8.585 |
| H2PO4- | 6.16E-07 | 4.89E-07 | -6.311 |
| H2S (aq) | 2.63E-62 | 2.69E-62 | -61.57 |
| H3AsO3 | 8.36E-11 | 8.55E-11 | -10.068 |
| H3AsO4 | 3.71E-06 | 3.79E-06 | -5.421 |
| H3PO4 | 1.32E-06 | 1.35E-06 | -5.869 |
| HAsO3-2 | 1.1E-30 | 4.19E-31 | -30.378 |
| HAsO4-2 | 1.15E-11 | 4.37E-12 | -11.359 |
| HCO3- | 2.18E-08 | 1.73E-08 | -7.763 |
| HCrO4- | 4.03E-07 | 3.17E-07 | -6.499 |
| HF (aq) | 1.91E-07 | 1.95E-07 | -6.71 |
| HF2- | 6.78E-15 | 5.2E-15 | -14.284 |
| Hg(CO3)2-2 | 2.78E-38 | 1.06E-38 | -37.974 |
| Hg(HS)2 (aq) | 5.9E-117 | 6.1E-117 | -116.217 |
| Hg(N3)2 (aq) | 1.38E-16 | 1.41E-16 | -15.852 |
| Hg(NH3)2+2 | 5.24E-25 | 2E-25 | -24.699 |
| Hg(NH3)4+2 | 3.32E-46 | 1.27E-46 | -45.897 |
| Hg(NO2)2 (aq) | 3.16E-54 | 3.23E-54 | -53.49 |
| Hg(NO2)3- | 5.02E-74 | 3.94E-74 | -73.404 |
| Hg(NO2)4-2 | 9.34E-95 | 3.57E-95 | -94.448 |
| Hg(NO3)2 (aq) | 1.14E-75 | 1.17E-75 | -74.932 |
| Hg(OH)2 | 4.49E-24 | 4.59E-24 | -23.338 |
| Hg(SO4)2-2 | 9.82E-22 | 3.75E-22 | -21.426 |
| Hg+2 | 1.48E-20 | 5.66E-21 | -20.247 |
| Hg2OH+3 | 5.27E-42 | 6.03E-43 | -42.22 |
| Hg3(OH)3+3 | 1.14E-62 | 1.3E-63 | -62.885 |
| HgCl+ | 2.69E-15 | 2.12E-15 | -14.674 |
| HgCl2 (aq) | 2.09E-10 | 2.14E-10 | -9.67 |
| HgCl3-1 | 3.56E-11 | 2.8E-11 | -10.553 |
| HgCl4-2 | 4.33E-12 | 1.65E-12 | -11.782 |
| HgClOH (aq) | 6.58E-17 | 6.73E-17 | -16.172 |
| HgCO3 (aq) | 1.25E-25 | 1.28E-25 | -24.894 |
| HgF+ | 1.91E-27 | 1.5E-27 | -26.824 |
| HgHCO3+ | 5.89E-23 | 4.63E-23 | -22.334 |
| HgHS2- | 1.1E-121 | 9E-122 | -121.046 |
| HgN3+ | 1.35E-13 | 1.06E-13 | -12.975 |
| HgNO2+ | 1.25E-36 | 9.85E-37 | -36.007 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgNO3+ | 2.42E-48 | 1.9E-48 | -47.721 |
| HgOH+ | 9.8E-23 | 7.7E-23 | -22.114 |
| HgOHCO3- | 8.68E-31 | 6.82E-31 | -30.166 |
| HgS2-2 | 2.1E-128 | 8E-129 | -128.095 |
| HgSO4 (aq) | 5.77E-21 | 5.9E-21 | -20.229 |
| HN3 (aq) | 4.99E-05 | 5.11E-05 | -4.292 |
| HNO2 (aq) | 1.06E-20 | 1.09E-20 | -19.965 |
| HPO4-2 | 3.53E-12 | 1.36E-12 | -11.866 |
| HS-1 | 1.1E-67 | 8.47E-68 | -67.072 |
| HSO4- | 0.012915 | 0.010091 | -1.996 |
| K+1 | 0.00032 | 0.000243 | -3.614 |
| K2HPO4 (aq) | 8.52E-19 | 8.71E-19 | -18.06 |
| K2PO4- | 2.92E-28 | 2.3E-28 | -27.639 |
| KCl (aq) | 1.66E-06 | 1.7E-06 | -5.77 |
| KCr2O7- | 1.23E-14 | 9.63E-15 | -14.016 |
| KCrO4- | 5.31E-15 | 4.17E-15 | -14.38 |
| KF (aq) | 7.73E-13 | 7.9E-13 | -12.102 |
| KH2PO4 (aq) | 1.8E-10 | 1.84E-10 | -9.734 |
| KHPO4- | 2.57E-15 | 2.04E-15 | -14.691 |
| KNO3 (aq) | 2.69E-31 | 2.75E-31 | -30.56 |
| KOH (aq) | 8.67E-17 | 8.86E-17 | -16.053 |
| KPO4-2 | 2.96E-25 | 1.13E-25 | -24.947 |
| KSO4- | 1.13E-05 | 8.94E-06 | -5.049 |
| Mg DOM1 | 5.45E-08 | 4.67E-08 | -7.331 |
| Mg(NH3)2+2 | 1.31E-25 | 5.01E-26 | -25.3 |
| Mg+2 | 0.005018 | 0.002206 | -2.656 |
| Mg2CO3+2 | 1.46E-18 | 5.58E-19 | -18.253 |
| MgCl+ | 0.000139 | 0.000109 | -3.961 |
| MgCO3 (aq) | 4.53E-17 | 4.64E-17 | -16.334 |
| MgF+ | 1.33E-09 | 1.04E-09 | -8.984 |
| MgHCO3+ | 4.77E-10 | 3.7E-10 | -9.432 |
| MgHPO4 (aq) | 1.57E-12 | 1.6E-12 | -11.796 |
| MgOH+ | 1.94E-13 | 1.56E-13 | -12.807 |
| MgPO4- | 2.23E-21 | 1.77E-21 | -20.753 |
| MgSO4 (aq) | 0.002249 | 0.0023 | -2.638 |
| Mn+3 | 4.55E-05 | 8.39E-06 | -5.076 |
| N3-1 | 5.78E-08 | 4.55E-08 | -7.342 |
| Na+1 | 0.012139 | 0.009559 | -2.02 |
| Na2HPO4 (aq) | 8.68E-16 | 8.88E-16 | -15.052 |
| Na2PO4- | 9.63E-25 | 7.57E-25 | -24.121 |
| NaCl (aq) | 6.9E-05 | 7.06E-05 | -4.151 |
| NaCO3- | 8.79E-18 | 6.97E-18 | -17.157 |
| NaCrO4- | 2.79E-13 | 2.19E-13 | -12.659 |
| NaF (aq) | 5.88E-11 | 6.01E-11 | -10.221 |
| NaH2PO4 (aq) | 7.09E-09 | 7.24E-09 | -8.14 |
| NaHCO3 (aq) | 9.56E-11 | 9.78E-11 | -10.01 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NaHPO4- | 1.56E-13 | 1.24E-13 | -12.907 |
| NaNO3 (aq) | 3.9E-30 | 3.99E-30 | -29.399 |
| NaOH (aq) | 2.33E-15 | 2.38E-15 | -14.623 |
| NaPO4-2 | 1.28E-23 | 4.9E-24 | -23.31 |
| NaSO4- | 0.000406 | 0.000322 | -3.492 |
| NH3 (aq) | 3.57E-12 | 3.65E-12 | -11.438 |
| NH4+1 | 0.000387 | 0.000291 | -3.537 |
| NH4Cr2O7- | 1.7E-14 | 1.34E-14 | -13.874 |
| NH4SO4- | 2.46E-05 | 1.93E-05 | -4.713 |
| Ni DOM1 | 2.43E-09 | 2.09E-09 | -8.68 |
| Ni(N3)2 (aq) | 7.84E-19 | 8.02E-19 | -18.096 |
| Ni(NH3)2+2 | 1.59E-23 | 6.05E-24 | -23.218 |
| Ni(NH3)3+2 | 3.35E-33 | 1.28E-33 | -32.893 |
| Ni(NH3)4+2 | 2.1E-43 | 8.03E-44 | -43.095 |
| Ni(NH3)5+2 | 4.26E-54 | 1.63E-54 | -53.789 |
| Ni(NH3)6+2 | 1.84E-65 | 7.02E-66 | -65.154 |
| Ni(NO2)2 (aq) | 2.93E-47 | 2.99E-47 | -46.524 |
| Ni(OH)2 (aq) | 8.04E-22 | 8.22E-22 | -21.085 |
| Ni(OH)3- | 4.78E-31 | 3.76E-31 | -30.425 |
| Ni(SO4)2-2 | 2.62E-09 | 1E-09 | -9 |
| Ni+2 | 1.03E-05 | 3.92E-06 | -5.406 |
| NiCl+ | 2.38E-08 | 1.87E-08 | -7.729 |
| NiCl2 (aq) | 8.57E-12 | 8.77E-12 | -11.057 |
| NiCO3 (aq) | 4.2E-18 | 4.3E-18 | -17.367 |
| NiF+ | 6.41E-13 | 5.04E-13 | -12.298 |
| NiH2PO4+ | 1.6E-11 | 1.26E-11 | -10.9 |
| NiHCO3+ | 8.45E-12 | 6.64E-12 | -11.178 |
| NiHPO4 (aq) | 3.82E-15 | 3.9E-15 | -14.409 |
| NiHS+ | 1.31E-67 | 1.03E-67 | -66.988 |
| NiN3+ | 4.28E-12 | 3.36E-12 | -11.474 |
| NiNH3+2 | 2.46E-14 | 9.4E-15 | -14.027 |
| NiNO2+ | 4.21E-26 | 3.31E-26 | -25.48 |
| NiNO3+ | 1.86E-32 | 1.46E-32 | -31.836 |
| NiOH+ | 1.39E-14 | 1.09E-14 | -13.961 |
| NiSO4 (aq) | 4.39E-06 | 4.49E-06 | -5.348 |
| NO2-1 | 4.48E-22 | 3.52E-22 | -21.454 |
| NO3-1 | 1.95E-27 | 1.48E-27 | -26.829 |
| OH- | 2.73E-13 | 2.09E-13 | -12.679 |
| Pb DOM1 | 3.66E-10 | 3.14E-10 | -9.503 |
| Pb(CO3)2-2 | 1.47E-31 | 5.62E-32 | -31.25 |
| Pb(HS)2 (aq) | 9.7E-128 | 9.9E-128 | -127.003 |
| Pb(HS)3- | 2.1E-193 | 1.7E-193 | -192.775 |
| Pb(NO2)2 (aq) | 1.16E-48 | 1.18E-48 | -47.926 |
| Pb(NO3)2 (aq) | 4.39E-61 | 4.49E-61 | -60.348 |
| Pb(OH)2 (aq) | 1.21E-22 | 1.24E-22 | -21.908 |
| Pb(OH)3- | 7.19E-32 | 5.65E-32 | -31.248 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(SO4)2-2 | 2.22E-09 | 8.47E-10 | -9.072 |
| Pb+2 | 1.95E-08 | 7.43E-09 | -8.129 |
| Pb2OH+3 | 8.79E-21 | 1.01E-21 | -20.997 |
| Pb3(OH)4+2 | 1.17E-42 | 4.45E-43 | -42.352 |
| Pb4(OH)4+4 | 2.4E-46 | 5.1E-48 | -47.292 |
| PbCl+ | 4E-09 | 3.15E-09 | -8.502 |
| PbCl2 (aq) | 8.46E-11 | 8.65E-11 | -10.063 |
| PbCl3- | 1.15E-12 | 9.05E-13 | -12.043 |
| PbCl4-2 | 1.14E-14 | 4.36E-15 | -14.361 |
| PbCO3 (aq) | 7.26E-19 | 7.42E-19 | -18.13 |
| PbF+ | 9.48E-15 | 7.45E-15 | -14.128 |
| PbF2 (aq) | 6.37E-22 | 6.51E-22 | -21.186 |
| PbH2PO4+ | 1.14E-13 | 8.93E-14 | -13.049 |
| PbHCO3+ | 1.03E-13 | 8.12E-14 | -13.09 |
| PbHPO4 (aq) | 1.01E-17 | 1.03E-17 | -16.987 |
| PbNO2+ | 1.08E-27 | 8.46E-28 | -27.073 |
| PbNO3+ | 2.13E-34 | 1.67E-34 | -33.776 |
| PbOH+ | 7.79E-15 | 6.12E-15 | -14.213 |
| PbSO4 (aq) | 2.21E-08 | 2.26E-08 | -7.646 |
| PO4-3 | 1.82E-22 | 2.13E-23 | -22.672 |
| S-2 | 2.01E-83 | 7.73E-84 | -83.112 |
| SO4-2 | 0.017427 | 0.006213 | -2.207 |
| Zn DOM1 | 5.77E-09 | 4.95E-09 | -8.306 |
| Zn(CO3)2-2 | 2.66E-31 | 1.02E-31 | -30.993 |
| Zn(N3)2 (aq) | 1.13E-18 | 1.16E-18 | -17.936 |
| Zn(N3)3- | 3.83E-25 | 3.01E-25 | -24.521 |
| Zn(NH3)2+2 | 8.97E-24 | 3.42E-24 | -23.466 |
| Zn(NH3)3+2 | 9.64E-33 | 3.68E-33 | -32.434 |
| Zn(NH3)4+2 | 5.07E-42 | 1.94E-42 | -41.713 |
| Zn(NO2)2 (aq) | 1.13E-47 | 1.15E-47 | -46.939 |
| Zn(NO3)2 (aq) | 6.31E-60 | 6.45E-60 | -59.19 |
| Zn(OH)2 (aq) | 1.51E-19 | 1.55E-19 | -18.811 |
| Zn(OH)3- | 2.85E-29 | 2.24E-29 | -28.65 |
| Zn(OH)4-2 | 4.25E-40 | 1.62E-40 | -39.79 |
| Zn(SO4)2-2 | 1.13E-06 | 4.32E-07 | -6.365 |
| Zn+2 | 1.43E-05 | 5.87E-06 | -5.231 |
| Zn2OH+3 | 5.63E-18 | 6.45E-19 | -18.19 |
| Zn2S3-2 | 1.2E-206 | 4.5E-207 | -206.347 |
| ZnCl+ | 2.67E-07 | 2.07E-07 | -6.685 |
| ZnCl2 (aq) | 1.7E-09 | 1.74E-09 | -8.759 |
| ZnCl3- | 3.08E-11 | 2.42E-11 | -10.616 |
| ZnCl4-2 | 3.85E-13 | 1.47E-13 | -12.832 |
| ZnCO3 (aq) | 9.73E-18 | 9.95E-18 | -17.002 |
| ZnF+ | 9.07E-13 | 7.13E-13 | -12.147 |
| ZnHCO3+ | 3.24E-12 | 2.55E-12 | -11.594 |
| ZnHPO4 (aq) | 1.31E-14 | 1.34E-14 | -13.874 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnN3+ | 4.88E-12 | 3.84E-12 | -11.416 |
| ZnNH3+2 | 1.06E-14 | 4.05E-15 | -14.393 |
| ZnNO2+ | 1.58E-26 | 1.24E-26 | -25.905 |
| ZnNO3+ | 2.96E-32 | 2.33E-32 | -31.633 |
| ZnOH+ | 1.56E-13 | 1.23E-13 | -12.91 |
| ZnS (aq) | 8.27E-73 | 8.46E-73 | -72.073 |
| ZnSO4 (aq) | 7.15E-06 | 7.31E-06 | -5.136 |

## B1.7: Eh 700

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.18E-06 | 3.15E-06 | -5.502 |
| Al(OH)2+ | 1.75E-12 | 1.39E-12 | -11.857 |
| Al(OH)3 (aq) | 1.15E-17 | 1.18E-17 | -16.929 |
| Al(OH)4- | 3.02E-22 | 2.36E-22 | -21.627 |
| Al(SO4)2- | 0.00091 | 0.000711 | -3.148 |
| Al+3 | 0.000408 | 7.53E-05 | -4.123 |
| Al2(OH)2+4 | 3.82E-12 | 8.13E-14 | -13.09 |
| Al2(OH)2CO3+2 | 1.76E-17 | 6.71E-18 | -17.173 |
| Al2PO4+3 | 9.82E-12 | 1.13E-12 | -11.948 |
| Al3(OH)4+5 | 1.29E-18 | 3.15E-21 | -20.501 |
| AlCl+2 | 1.05E-06 | 4.02E-07 | -6.396 |
| AlF+2 | 1.3E-05 | 5.12E-06 | -5.29 |
| AlF2+ | 1.81E-08 | 1.44E-08 | -7.842 |
| AlF3 (aq) | 1.17E-12 | 1.19E-12 | -11.924 |
| AlF4- | 5.42E-18 | 4.24E-18 | -17.373 |
| AlHPO4+ | 4.51E-09 | 3.54E-09 | -8.451 |
| AlOH+2 | 4.41E-08 | 1.74E-08 | -7.759 |
| AlSO4+ | 0.003484 | 0.002723 | -2.565 |
| AsO4-3 | 2.08E-21 | 2.38E-22 | -21.623 |
| AsS(OH)HS- | 7.9E-160 | 6.2E-160 | -159.205 |
| Ca DOM1 | 6.18E-07 | 5.3E-07 | -6.276 |
| Ca(NH3)2+2 | 2.94E-25 | 1.12E-25 | -24.949 |
| Ca(NO3)2 | 1.31E-33 | 1.34E-33 | -32.872 |
| Ca+2 | 0.00595 | 0.002527 | -2.597 |
| CaCl+ | 0.0001 | 7.87E-05 | -4.104 |
| CaCO3 (aq) | 1.02E-16 | 1.04E-16 | -15.984 |
| CaCrO4 (aq) | 6.63E-12 | 6.78E-12 | -11.169 |
| CaF+ | 2.58E-10 | 2.03E-10 | -9.692 |
| CaH2PO4+ | 2.95E-08 | 2.34E-08 | -7.631 |
| CaHCO3+ | 5.68E-10 | 4.55E-10 | -9.342 |
| CaHPO4 (aq) | 1.28E-12 | 1.31E-12 | -11.882 |
| CaNH3+2 | 7.94E-14 | 3.03E-14 | -13.518 |
| CaNO3+ | 1.42E-15 | 1.12E-15 | -14.952 |
| CaOH+ | 1.16E-14 | 9.29E-15 | -14.032 |
| CaPO4- | 1.59E-19 | 1.26E-19 | -18.898 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaSO4 (aq) | 0.003181 | 0.003253 | -2.488 |
| Cd DOM1 | 5.64E-13 | 4.84E-13 | -12.316 |
| Cd(CO3)2-2 | 3.38E-35 | 1.29E-35 | -34.889 |
| Cd(HS)2 (aq) | 1.7E-156 | 1.7E-156 | -155.766 |
| Cd(HS)3- | 1.3E-235 | 1E-235 | -234.985 |
| Cd(NH3)2+2 | 1.66E-27 | 6.36E-28 | -27.197 |
| Cd(NH3)3+2 | 1.55E-37 | 5.93E-38 | -37.227 |
| Cd(NH3)4+2 | 4.27E-48 | 1.63E-48 | -47.788 |
| Cd(NO2)2 (aq) | 3.96E-28 | 4.04E-28 | -27.393 |
| Cd(NO3)2 (aq) | 2.39E-35 | 2.44E-35 | -34.612 |
| Cd(OH)2 (aq) | 9.21E-27 | 9.42E-27 | -26.026 |
| Cd(OH)3- | 5.3E-38 | 4.17E-38 | -37.38 |
| Cd(OH)4-2 | 5.04E-50 | 1.93E-50 | -49.716 |
| Cd(SO4)2-2 | 2.93E-10 | 1.12E-10 | -9.951 |
| Cd+2 | 2.41E-09 | 9.19E-10 | -9.037 |
| Cd2OH+3 | 6.98E-26 | 8E-27 | -26.097 |
| CdCl+ | 1.42E-09 | 1.12E-09 | -8.951 |
| CdCl2 (aq) | 5.77E-11 | 5.9E-11 | -10.229 |
| CdCO3 (aq) | 6.06E-22 | 6.2E-22 | -21.208 |
| CdF+ | 1.23E-16 | 9.63E-17 | -16.016 |
| CdHCO3+ | 5.02E-16 | 3.95E-16 | -15.403 |
| CdHPO4 (aq) | 4.97E-18 | 5.08E-18 | -17.294 |
| CdHS+ | 1.14E-82 | 8.99E-83 | -82.046 |
| CdNH3+2 | 3.69E-18 | 1.41E-18 | -17.851 |
| CdNO2+ | 1.18E-18 | 9.25E-19 | -18.034 |
| CdNO3+ | 6.43E-22 | 5.05E-22 | -21.297 |
| CdOH+ | 1.95E-18 | 1.53E-18 | -17.815 |
| CdSO4 (aq) | 1.16E-09 | 1.18E-09 | -8.927 |
| Cl-1 | 0.017211 | 0.013113 | -1.882 |
| CO3-2 | 7.28E-17 | 2.88E-17 | -16.541 |
| Cr2O7-2 | 1.2E-11 | 4.58E-12 | -11.339 |
| CrO3Cl- | 7.61E-10 | 5.98E-10 | -9.223 |
| CrO3H2PO4- | 6.69E-12 | 5.26E-12 | -11.279 |
| CrO3HPO4-2 | 1.29E-12 | 4.94E-13 | -12.306 |
| CrO3SO4-2 | 3.59E-08 | 1.37E-08 | -7.863 |
| CrO4-2 | 1.27E-11 | 4.56E-12 | -11.341 |
| Cu DOM1 | 5.11E-10 | 4.38E-10 | -9.359 |
| Cu(CO3)2-2 | 7.18E-31 | 2.74E-31 | -30.562 |
| Cu(N3)2 (aq) | 1.4E-18 | 1.43E-18 | -17.845 |
| Cu(N3)3- | 4.09E-24 | 3.22E-24 | -23.492 |
| Cu(N3)4-2 | 9.96E-31 | 3.8E-31 | -30.42 |
| Cu(NH3)2+2 | 3.24E-23 | 1.24E-23 | -22.907 |
| Cu(NH3)3+2 | 9.9E-32 | 3.78E-32 | -31.422 |
| Cu(NH3)4+2 | 6.26E-41 | 2.39E-41 | -40.622 |
| Cu(NO2)2 (aq) | 2.19E-27 | 2.24E-27 | -26.65 |
| Cu(NO3)2 (aq) | 1.37E-34 | 1.4E-34 | -33.855 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(OH)2 (aq) | 6.59E-22 | 6.74E-22 | -21.171 |
| Cu(OH)3- | 5.51E-30 | 4.33E-30 | -29.363 |
| Cu(OH)4-2 | 3.4E-42 | 1.3E-42 | -41.886 |
| Cu+2 | 5.1E-08 | 2.09E-08 | -7.68 |
| Cu2(OH)2+2 | 2.65E-23 | 1.01E-23 | -22.995 |
| Cu2OH+3 | 2.28E-20 | 2.62E-21 | -20.582 |
| Cu2S3-2 | 3.3E-256 | 1.3E-256 | -255.901 |
| Cu3(OH)4+2 | 3.58E-38 | 1.37E-38 | -37.865 |
| CuCl+ | 6.28E-10 | 4.87E-10 | -9.313 |
| CuCl2 (aq) | 1.04E-12 | 1.06E-12 | -11.973 |
| CuCl3- | 1.4E-16 | 1.08E-16 | -15.965 |
| CuCl4-2 1 | 2.61E-20 | 1.01E-20 | -19.997 |
| CuCO3 (aq) | 3.46E-18 | 3.54E-18 | -17.451 |
| CuF+ | 7.88E-15 | 6.19E-15 | -14.208 |
| CuHCO3+ | 2.27E-14 | 1.79E-14 | -13.748 |
| CuHPO4 (aq) | 2.97E-16 | 3.04E-16 | -15.517 |
| CuHSO4+ | 7.97E-10 | 6.27E-10 | -9.203 |
| CuN3+ | 8.65E-13 | 6.8E-13 | -12.167 |
| CuNH3+2 | 2.77E-15 | 1.06E-15 | -14.975 |
| CuNO2+ | 2.78E-17 | 2.19E-17 | -16.66 |
| CuNO3+ | 1.15E-20 | 9.07E-21 | -20.043 |
| CuOH+ | 2.34E-14 | 1.81E-14 | -13.742 |
| CuS(aq) | 1.4E-90 | 1.43E-90 | -89.844 |
| CuSO4 (aq) | 2.57E-08 | 2.63E-08 | -7.58 |
| DOC (Gaussian DOM) | 0.001399 | 0.00143 | -2.845 |
| DOM1 | 2.09E-05 | 3.16E-06 | -5.5 |
| F-1 | 9.24E-09 | 7.09E-09 | -8.149 |
| Fe DOM1 | 1.54E-06 | 1.53E-06 | -5.815 |
| Fe(N3)2+ | 1.13E-13 | 8.86E-14 | -13.052 |
| Fe(N3)3 (aq) | 8.35E-19 | 8.53E-19 | -18.069 |
| Fe(NH3)2+2 | 9.69E-27 | 3.7E-27 | -26.432 |
| Fe(NH3)3+2 | 1.07E-37 | 4.07E-38 | -37.39 |
| Fe(NH3)4+2 | 5.01E-49 | 1.91E-49 | -48.718 |
| Fe(NO2)2+ | 7.73E-25 | 6.08E-25 | -24.216 |
| Fe(NO2)3 (aq) | 6.83E-34 | 6.98E-34 | -33.156 |
| Fe(OH)2 (aq) | 1.53E-24 | 1.57E-24 | -23.805 |
| Fe(OH)2+ | 3.09E-10 | 2.45E-10 | -9.611 |
| Fe(OH)3- | 2.58E-33 | 2.03E-33 | -32.691 |
| Fe(OH)3 (aq) | 3.57E-18 | 3.65E-18 | -17.437 |
| Fe(OH)4- | 1.36E-24 | 1.08E-24 | -23.968 |
| Fe(SO4)2- | 1.04E-06 | 8.17E-07 | -6.088 |
| Fe+2 | 3.16E-06 | 1.29E-06 | -5.889 |
| Fe+3 | 6.27E-07 | 1.16E-07 | -6.937 |
| Fe2(OH)2+4 | 7.36E-13 | 1.57E-14 | -13.805 |
| Fe3(OH)4+5 | 5.34E-19 | 1.3E-21 | -20.885 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeCl+ | 1.36E-08 | 1.07E-08 | -7.971 |
| FeCl+2 | 8.61E-08 | 3.32E-08 | -7.479 |
| FeCrO4+ | 2.46E-11 | 1.94E-11 | -10.713 |
| FeF+ | 1.89E-13 | 1.49E-13 | -12.828 |
| FeF+2 | 2.03E-09 | 7.83E-10 | -9.106 |
| FeF2+ | 2.66E-13 | 2.1E-13 | -12.678 |
| FeF3 (aq) | 1.35E-18 | 1.38E-18 | -17.86 |
| FeH2PO4+ | 3.1E-10 | 2.46E-10 | -9.609 |
| FeH2PO4+2 | 2.11E-09 | 8.32E-10 | -9.08 |
| FeHCO3+ | 2.76E-13 | 2.21E-13 | -12.656 |
| FeHPO4 (aq) | 5.48E-15 | 5.61E-15 | -14.251 |
| FeHPO4+ | 1.98E-09 | 1.57E-09 | -8.803 |
| FeHS+ | 6.55E-82 | 5.15E-82 | -81.288 |
| FeN3+2 | 2.12E-09 | 8.11E-10 | -9.091 |
| FeNH3+2 | 3.47E-16 | 1.33E-16 | -15.878 |
| FeNO2+2 | 4.8E-15 | 1.84E-15 | -14.736 |
| FeOH+ | 1.35E-14 | 1.06E-14 | -13.973 |
| FeOH+2 | 9.06E-08 | 3.49E-08 | -7.457 |
| FeSO4 (aq) | 1.72E-06 | 1.76E-06 | -5.755 |
| FeSO4+ | 1.14E-05 | 9E-06 | -5.046 |
| H DOM1 | 9.42E-05 | 4.32E-05 | -4.364 |
| H+1 | 0.026658 | 0.022096 | -1.656 |
| H2AsO3- | 7.37E-22 | 5.8E-22 | -21.237 |
| H2AsO4- | 1.23E-06 | 9.65E-07 | -6.016 |
| H2CO3* (aq) | 0.000967 | 0.000989 | -3.005 |
| H2CrO4 (aq) | 2.57E-09 | 2.63E-09 | -8.58 |
| H2PO4- | 6.17E-07 | 4.89E-07 | -6.311 |
| H2S (aq) | 3.01E-76 | 3.08E-76 | -75.512 |
| H3AsO3 | 2.73E-14 | 2.79E-14 | -13.555 |
| H3AsO4 | 3.72E-06 | 3.8E-06 | -5.42 |
| H3PO4 | 1.34E-06 | 1.37E-06 | -5.864 |
| HAsO3-2 | 3.5E-34 | 1.34E-34 | -33.874 |
| HAsO4-2 | 1.12E-11 | 4.28E-12 | -11.368 |
| HCO3- | 2.15E-08 | 1.71E-08 | -7.768 |
| HCrO4- | 4.03E-07 | 3.17E-07 | -6.499 |
| HF (aq) | 1.93E-07 | 1.97E-07 | -6.706 |
| HF2- | 6.84E-15 | 5.25E-15 | -14.28 |
| Hg(CO3)2-2 | 2.67E-38 | 1.02E-38 | -37.991 |
| Hg(HS)2 (aq) | 7.6E-145 | 7.8E-145 | -144.108 |
| Hg(N3)2 (aq) | 1.32E-16 | 1.35E-16 | -15.869 |
| Hg(NH3)2+2 | 5.16E-25 | 1.97E-25 | -24.705 |
| Hg(NH3)4+2 | 3.2E-46 | 1.22E-46 | -45.913 |
| Hg(NO2)2 (aq) | 2.58E-33 | 2.64E-33 | -32.578 |
| Hg(NO2)3- | 1.16E-42 | 9.15E-43 | -42.038 |
| Hg(NO2)4-2 | 6.16E-53 | 2.35E-53 | -52.628 |
| Hg(NO3)2 (aq) | 8.84E-48 | 9.04E-48 | -47.044 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(OH)2 | 4.43E-24 | 4.53E-24 | -23.344 |
| Hg(SO4)2-2 | 9.88E-22 | 3.77E-22 | -21.423 |
| Hg+2 | 1.5E-20 | 5.71E-21 | -20.243 |
| Hg2OH+3 | 5.29E-42 | 6.07E-43 | -42.217 |
| Hg3(OH)3+3 | 1.13E-62 | 1.29E-63 | -62.888 |
| HgCl+ | 2.71E-15 | 2.13E-15 | -14.672 |
| HgCl2 (aq) | 2.09E-10 | 2.14E-10 | -9.67 |
| HgCl3-1 | 3.55E-11 | 2.79E-11 | -10.554 |
| HgCl4-2 | 4.29E-12 | 1.64E-12 | -11.786 |
| HgClOH (aq) | 6.54E-17 | 6.68E-17 | -16.175 |
| HgCO3 (aq) | 1.23E-25 | 1.26E-25 | -24.9 |
| HgF+ | 1.92E-27 | 1.51E-27 | -26.821 |
| HgHCO3+ | 5.88E-23 | 4.62E-23 | -22.335 |
| HgHS2- | 1.5E-149 | 1.1E-149 | -148.942 |
| HgN3+ | 1.28E-13 | 1.01E-13 | -12.997 |
| HgNO2+ | 3.6E-26 | 2.83E-26 | -25.549 |
| HgNO3+ | 2.14E-34 | 1.68E-34 | -33.775 |
| HgOH+ | 9.77E-23 | 7.68E-23 | -22.115 |
| HgOHCO3- | 8.45E-31 | 6.65E-31 | -30.177 |
| HgS2-2 | 2.6E-156 | 1E-156 | -155.996 |
| HgSO4 (aq) | 5.81E-21 | 5.94E-21 | -20.226 |
| HN3 (aq) | 4.99E-05 | 5.11E-05 | -4.292 |
| HNO2 (aq) | 3.05E-10 | 3.12E-10 | -9.506 |
| HPO4-2 | 3.49E-12 | 1.34E-12 | -11.871 |
| HS-1 | 1.25E-81 | 9.56E-82 | -81.02 |
| HSO4- | 0.013048 | 0.010197 | -1.992 |
| K+1 | 0.00032 | 0.000243 | -3.614 |
| K2HPO4 (aq) | 8.43E-19 | 8.62E-19 | -18.065 |
| K2PO4- | 2.86E-28 | 2.24E-28 | -27.649 |
| KCl (aq) | 1.66E-06 | 1.69E-06 | -5.772 |
| KCr2O7- | 1.22E-14 | 9.62E-15 | -14.017 |
| KCrO4- | 5.24E-15 | 4.12E-15 | -14.385 |
| KF (aq) | 7.72E-13 | 7.89E-13 | -12.103 |
| KH2PO4 (aq) | 1.81E-10 | 1.85E-10 | -9.734 |
| KHPO4- | 2.54E-15 | 2.01E-15 | -14.696 |
| KNO3 (aq) | 2.36E-17 | 2.41E-17 | -16.618 |
| KOH (aq) | 8.57E-17 | 8.76E-17 | -16.058 |
| KPO4-2 | 2.89E-25 | 1.11E-25 | -24.957 |
| KSO4- | 1.13E-05 | 8.93E-06 | -5.049 |
| Mg DOM1 | 5.4E-08 | 4.63E-08 | -7.335 |
| Mg(NH3)2+2 | 1.28E-25 | 4.9E-26 | -25.31 |
| Mg+2 | 0.005019 | 0.002208 | -2.656 |
| Mg2CO3+2 | 1.43E-18 | 5.46E-19 | -18.263 |
| MgCl+ | 0.000139 | 0.000109 | -3.963 |
| MgCO3 (aq) | 4.43E-17 | 4.53E-17 | -16.344 |
| MgF+ | 1.33E-09 | 1.04E-09 | -8.984 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHCO3+ | 4.72E-10 | 3.66E-10 | -9.437 |
| MgHPO4 (aq) | 1.55E-12 | 1.58E-12 | -11.8 |
| MgOH+ | 1.92E-13 | 1.54E-13 | -12.812 |
| MgPO4- | 2.18E-21 | 1.73E-21 | -20.763 |
| MgSO4 (aq) | 0.002248 | 0.002299 | -2.639 |
| Mn+3 | 4.55E-05 | 8.4E-06 | -5.076 |
| N3-1 | 5.72E-08 | 4.49E-08 | -7.347 |
| Na+1 | 0.01214 | 0.009561 | -2.019 |
| Na2HPO4 (aq) | 8.59E-16 | 8.78E-16 | -15.056 |
| Na2PO4- | 9.41E-25 | 7.4E-25 | -24.131 |
| NaCl (aq) | 6.87E-05 | 7.03E-05 | -4.153 |
| NaCO3- | 8.59E-18 | 6.81E-18 | -17.167 |
| NaCrO4- | 2.75E-13 | 2.17E-13 | -12.665 |
| NaF (aq) | 5.87E-11 | 6E-11 | -10.222 |
| NaH2PO4 (aq) | 7.09E-09 | 7.25E-09 | -8.14 |
| NaHCO3 (aq) | 9.45E-11 | 9.66E-11 | -10.015 |
| NaHPO4- | 1.54E-13 | 1.22E-13 | -12.912 |
| NaNO3 (aq) | 3.41E-16 | 3.49E-16 | -15.457 |
| NaOH (aq) | 2.3E-15 | 2.36E-15 | -14.628 |
| NaPO4-2 | 1.25E-23 | 4.79E-24 | -23.32 |
| NaSO4- | 0.000405 | 0.000321 | -3.493 |
| NH3 (aq) | 3.53E-12 | 3.61E-12 | -11.443 |
| NH4+1 | 0.000387 | 0.000291 | -3.537 |
| NH4Cr2O7- | 1.7E-14 | 1.34E-14 | -13.874 |
| NH4SO4- | 2.46E-05 | 1.93E-05 | -4.714 |
| Ni DOM1 | 2.41E-09 | 2.07E-09 | -8.685 |
| Ni(N3)2 (aq) | 7.67E-19 | 7.84E-19 | -18.106 |
| Ni(NH3)2+2 | 1.55E-23 | 5.92E-24 | -23.227 |
| Ni(NH3)3+2 | 3.24E-33 | 1.24E-33 | -32.907 |
| Ni(NH3)4+2 | 2.01E-43 | 7.68E-44 | -43.115 |
| Ni(NH3)5+2 | 4.02E-54 | 1.54E-54 | -53.813 |
| Ni(NH3)6+2 | 1.72E-65 | 6.56E-66 | -65.183 |
| Ni(NO2)2 (aq) | 2.37E-26 | 2.42E-26 | -25.616 |
| Ni(OH)2 (aq) | 7.86E-22 | 8.03E-22 | -21.095 |
| Ni(OH)3- | 4.62E-31 | 3.63E-31 | -30.44 |
| Ni(SO4)2-2 | 2.62E-09 | 9.99E-10 | -9 |
| Ni+2 | 1.03E-05 | 3.93E-06 | -5.406 |
| NiCl+ | 2.37E-08 | 1.86E-08 | -7.73 |
| NiCl2 (aq) | 8.51E-12 | 8.7E-12 | -11.06 |
| NiCO3 (aq) | 4.11E-18 | 4.2E-18 | -17.377 |
| NiF+ | 6.4E-13 | 5.03E-13 | -12.298 |
| NiH2PO4+ | 1.61E-11 | 1.26E-11 | -10.899 |
| NiHCO3+ | 8.36E-12 | 6.57E-12 | -11.182 |
| NiHPO4 (aq) | 3.78E-15 | 3.86E-15 | -14.413 |
| NiHS+ | 1.48E-81 | 1.16E-81 | -80.935 |
| NiN3+ | 4.23E-12 | 3.32E-12 | -11.478 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NiNH3+2 | 2.43E-14 | 9.3E-15 | -14.032 |
| NiNO2+ | 1.2E-15 | 9.43E-16 | -15.026 |
| NiNO3+ | 1.63E-18 | 1.28E-18 | -17.893 |
| NiOH+ | 1.38E-14 | 1.08E-14 | -13.966 |
| NiSO4 (aq) | 4.39E-06 | 4.48E-06 | -5.348 |
| NO2-1 | 1.27E-11 | 1E-11 | -11 |
| NO3-1 | 1.71E-13 | 1.3E-13 | -12.888 |
| OH- | 2.7E-13 | 2.07E-13 | -12.684 |
| Pb DOM1 | 3.63E-10 | 3.11E-10 | -9.507 |
| Pb(CO3)2-2 | 1.41E-31 | 5.37E-32 | -31.27 |
| Pb(HS)2 (aq) | 1.2E-155 | 1.3E-155 | -154.897 |
| Pb(HS)3- | 3.1E-235 | 2.4E-235 | -234.617 |
| Pb(NO2)2 (aq) | 9.38E-28 | 9.59E-28 | -27.018 |
| Pb(NO3)2 (aq) | 3.37E-33 | 3.44E-33 | -32.463 |
| Pb(OH)2 (aq) | 1.18E-22 | 1.21E-22 | -21.918 |
| Pb(OH)3- | 6.95E-32 | 5.47E-32 | -31.262 |
| Pb(SO4)2-2 | 2.21E-09 | 8.46E-10 | -9.073 |
| Pb+2 | 1.95E-08 | 7.44E-09 | -8.128 |
| Pb2OH+3 | 8.7E-21 | 9.97E-22 | -21.001 |
| Pb3(OH)4+2 | 1.12E-42 | 4.26E-43 | -42.37 |
| Pb4(OH)4+4 | 2.3E-46 | 4.9E-48 | -47.31 |
| PbCl+ | 3.99E-09 | 3.14E-09 | -8.503 |
| PbCl2 (aq) | 8.4E-11 | 8.59E-11 | -10.066 |
| PbCl3- | 1.14E-12 | 8.95E-13 | -12.048 |
| PbCl4-2 | 1.12E-14 | 4.29E-15 | -14.367 |
| PbCO3 (aq) | 7.1E-19 | 7.26E-19 | -18.139 |
| PbF+ | 9.49E-15 | 7.46E-15 | -14.127 |
| PbF2 (aq) | 6.36E-22 | 6.51E-22 | -21.187 |
| PbH2PO4+ | 1.14E-13 | 8.94E-14 | -13.048 |
| PbHCO3+ | 1.02E-13 | 8.04E-14 | -13.095 |
| PbHPO4 (aq) | 9.99E-18 | 1.02E-17 | -16.991 |
| PbNO2+ | 3.06E-17 | 2.41E-17 | -16.618 |
| PbNO3+ | 1.87E-20 | 1.47E-20 | -19.834 |
| PbOH+ | 7.7E-15 | 6.06E-15 | -14.218 |
| PbSO4 (aq) | 2.21E-08 | 2.26E-08 | -7.646 |
| PO4-3 | 1.78E-22 | 2.08E-23 | -22.682 |
| S-2 | 2.24E-97 | 8.63E-98 | -97.064 |
| SO4-2 | 0.017389 | 0.006205 | -2.207 |
| Zn DOM1 | 5.72E-09 | 4.9E-09 | -8.31 |
| Zn(CO3)2-2 | 2.54E-31 | 9.71E-32 | -31.013 |
| Zn(N3)2 (aq) | 1.11E-18 | 1.13E-18 | -17.946 |
| Zn(N3)3- | 3.7E-25 | 2.91E-25 | -24.536 |
| Zn(NH3)2+2 | 8.77E-24 | 3.35E-24 | -23.475 |
| Zn(NH3)3+2 | 9.31E-33 | 3.56E-33 | -32.449 |
| Zn(NH3)4+2 | 4.85E-42 | 1.85E-42 | -41.733 |
| Zn(NO2)2 (aq) | 9.11E-27 | 9.32E-27 | -26.031 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn(NO3)2 (aq) | 4.83E-32 | 4.94E-32 | -31.306 |
| Zn(OH)2 (aq) | 1.48E-19 | 1.51E-19 | -18.82 |
| Zn(OH)3- | 2.75E-29 | 2.16E-29 | -28.665 |
| Zn(OH)4-2 | 4.06E-40 | 1.55E-40 | -39.81 |
| Zn(SO4)2-2 | 1.13E-06 | 4.31E-07 | -6.366 |
| Zn+2 | 1.43E-05 | 5.88E-06 | -5.231 |
| Zn2OH+3 | 5.57E-18 | 6.39E-19 | -18.195 |
| Zn2S3-2 | 1.6E-248 | 6.3E-249 | -248.203 |
| ZnCl+ | 2.66E-07 | 2.06E-07 | -6.686 |
| ZnCl2 (aq) | 1.69E-09 | 1.73E-09 | -8.762 |
| ZnCl3- | 3.04E-11 | 2.39E-11 | -10.621 |
| ZnCl4-2 | 3.79E-13 | 1.45E-13 | -12.839 |
| ZnCO3 (aq) | 9.52E-18 | 9.73E-18 | -17.012 |
| ZnF+ | 9.07E-13 | 7.13E-13 | -12.147 |
| ZnHCO3+ | 3.21E-12 | 2.52E-12 | -11.599 |
| ZnHPO4 (aq) | 1.29E-14 | 1.32E-14 | -13.879 |
| ZnN3+ | 4.83E-12 | 3.8E-12 | -11.421 |
| ZnNH3+2 | 1.05E-14 | 4.01E-15 | -14.397 |
| ZnNO2+ | 4.5E-16 | 3.54E-16 | -15.451 |
| ZnNO3+ | 2.59E-18 | 2.04E-18 | -17.691 |
| ZnOH+ | 1.55E-13 | 1.22E-13 | -12.915 |
| ZnS (aq) | 9.24E-87 | 9.44E-87 | -86.025 |
| ZnSO4 (aq) | 7.15E-06 | 7.31E-06 | -5.136 |

## B1.8: Eh 800

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.14E-06 | 3.11E-06 | -5.507 |
| Al(OH)2+ | 1.7E-12 | 1.35E-12 | -11.871 |
| Al(OH)3 (aq) | 1.09E-17 | 1.12E-17 | -16.951 |
| Al(OH)4- | 2.82E-22 | 2.2E-22 | -21.657 |
| Al(SO4)2- | 0.000904 | 0.000707 | -3.151 |
| Al+3 | 0.000411 | 7.58E-05 | -4.12 |
| Al2(OH)2+4 | 3.74E-12 | 7.94E-14 | -13.1 |
| Al2(OH)2CO3+2 | 1.65E-17 | 6.31E-18 | -17.2 |
| Al2PO4+3 | 9.47E-12 | 1.09E-12 | -11.964 |
| Al3(OH)4+5 | 1.23E-18 | 2.98E-21 | -20.525 |
| AlCl+2 | 1.06E-06 | 4.05E-07 | -6.393 |
| AlF+2 | 1.3E-05 | 5.12E-06 | -5.291 |
| AlF2+ | 1.8E-08 | 1.43E-08 | -7.846 |
| AlF3 (aq) | 1.15E-12 | 1.17E-12 | -11.93 |
| AlF4- | 5.3E-18 | 4.14E-18 | -17.383 |
| AlHPO4+ | 4.4E-09 | 3.46E-09 | -8.462 |
| AlOH+2 | 4.36E-08 | 1.72E-08 | -7.764 |
| AlSO4+ | 0.003486 | 0.002724 | -2.565 |
| AsO4-3 | 1.97E-21 | 2.26E-22 | -21.646 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| AsS(OH)HS- | 3.9E-191 | 3E-191 | -190.519 |
| Ca DOM1 | 6.08E-07 | 5.21E-07 | -6.283 |
| Ca(NH3)2+2 | 9.33E-35 | 3.56E-35 | -34.449 |
| Ca(NO3)2 | 2.86E-15 | 2.92E-15 | -14.535 |
| Ca+2 | 0.005962 | 0.002532 | -2.597 |
| CaCl+ | 0.0001 | 7.88E-05 | -4.103 |
| CaCO3 (aq) | 9.79E-17 | 1E-16 | -15.999 |
| CaCrO4 (aq) | 6.51E-12 | 6.66E-12 | -11.177 |
| CaF+ | 2.57E-10 | 2.02E-10 | -9.694 |
| CaH2PO4+ | 2.92E-08 | 2.31E-08 | -7.636 |
| CaHCO3+ | 5.59E-10 | 4.47E-10 | -9.35 |
| CaHPO4 (aq) | 1.25E-12 | 1.27E-12 | -11.895 |
| CaNH3+2 | 1.41E-18 | 5.4E-19 | -18.268 |
| CaNO3+ | 2.1E-06 | 1.65E-06 | -5.783 |
| CaOH+ | 1.14E-14 | 9.14E-15 | -14.039 |
| CaPO4- | 1.52E-19 | 1.2E-19 | -18.919 |
| CaSO4 (aq) | 0.003167 | 0.003238 | -2.49 |
| Cd DOM1 | 5.55E-13 | 4.76E-13 | -12.323 |
| Cd(CO3)2-2 | 3.14E-35 | 1.2E-35 | -34.921 |
| Cd(HS)2 (aq) | 2.4E-184 | 2.5E-184 | -183.608 |
| Cd(HS)3- | 2.3E-277 | 1.8E-277 | -276.749 |
| Cd(NH3)2+2 | 5.27E-37 | 2.01E-37 | -36.696 |
| Cd(NH3)3+2 | 8.75E-52 | 3.34E-52 | -51.476 |
| Cd(NH3)4+2 | 4.27E-67 | 1.63E-67 | -66.787 |
| Cd(NO2)2 (aq) | 9.37E-17 | 9.58E-17 | -16.019 |
| Cd(NO3)2 (aq) | 5.2E-17 | 5.32E-17 | -16.274 |
| Cd(OH)2 (aq) | 8.88E-27 | 9.08E-27 | -26.042 |
| Cd(OH)3- | 5.02E-38 | 3.95E-38 | -37.404 |
| Cd(OH)4-2 | 4.68E-50 | 1.79E-50 | -49.748 |
| Cd(SO4)2-2 | 2.9E-10 | 1.11E-10 | -9.956 |
| Cd+2 | 2.41E-09 | 9.2E-10 | -9.036 |
| Cd2OH+3 | 6.88E-26 | 7.88E-27 | -26.104 |
| CdCl+ | 1.43E-09 | 1.12E-09 | -8.951 |
| CdCl2 (aq) | 5.78E-11 | 5.9E-11 | -10.229 |
| CdCO3 (aq) | 5.85E-22 | 5.98E-22 | -21.223 |
| CdF+ | 1.22E-16 | 9.58E-17 | -16.019 |
| CdHCO3+ | 4.94E-16 | 3.88E-16 | -15.411 |
| CdHPO4 (aq) | 4.82E-18 | 4.93E-18 | -17.307 |
| CdHS+ | 1.37E-96 | 1.08E-96 | -95.967 |
| CdNH3+2 | 6.58E-23 | 2.51E-23 | -22.6 |
| CdNO2+ | 5.73E-13 | 4.51E-13 | -12.346 |
| CdNO3+ | 9.49E-13 | 7.46E-13 | -12.127 |
| CdOH+ | 1.92E-18 | 1.51E-18 | -17.822 |
| CdSO4 (aq) | 1.15E-09 | 1.18E-09 | -8.929 |
| Cl-1 | 0.017209 | 0.01311 | -1.882 |
| CO3-2 | 7.01E-17 | 2.77E-17 | -16.557 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cr2O7-2 | 1.2E-11 | 4.57E-12 | -11.341 |
| CrO3Cl- | 7.75E-10 | 6.09E-10 | -9.215 |
| CrO3H2PO4- | 6.72E-12 | 5.29E-12 | -11.277 |
| CrO3HPO4-2 | 1.28E-12 | 4.87E-13 | -12.312 |
| CrO3SO4-2 | 3.63E-08 | 1.39E-08 | -7.858 |
| CrO4-2 | 1.24E-11 | 4.47E-12 | -11.35 |
| Cu DOM1 | 5.02E-10 | 4.31E-10 | -9.366 |
| Cu(CO3)2-2 | 6.67E-31 | 2.55E-31 | -30.594 |
| Cu(N3)2 (aq) | 1.35E-18 | 1.38E-18 | -17.861 |
| Cu(N3)3- | 3.88E-24 | 3.05E-24 | -23.516 |
| Cu(N3)4-2 | 9.25E-31 | 3.53E-31 | -30.452 |
| Cu(NH3)2+2 | 1.03E-32 | 3.92E-33 | -32.407 |
| Cu(NH3)3+2 | 5.58E-46 | 2.13E-46 | -45.672 |
| Cu(NH3)4+2 | 6.26E-60 | 2.39E-60 | -59.621 |
| Cu(NO2)2 (aq) | 5.19E-16 | 5.3E-16 | -15.275 |
| Cu(NO3)2 (aq) | 2.97E-16 | 3.04E-16 | -15.517 |
| Cu(OH)2 (aq) | 6.36E-22 | 6.5E-22 | -21.187 |
| Cu(OH)3- | 5.22E-30 | 4.1E-30 | -29.387 |
| Cu(OH)4-2 | 3.16E-42 | 1.21E-42 | -41.918 |
| Cu+2 | 5.11E-08 | 2.09E-08 | -7.679 |
| Cu2(OH)2+2 | 2.56E-23 | 9.76E-24 | -23.011 |
| Cu2OH+3 | 2.25E-20 | 2.58E-21 | -20.589 |
| Cu2S3-2 | 5.4E-298 | 2E-298 | -297.689 |
| Cu3(OH)4+2 | 3.33E-38 | 1.27E-38 | -37.896 |
| CuCl+ | 6.29E-10 | 4.87E-10 | -9.312 |
| CuCl2 (aq) | 1.04E-12 | 1.06E-12 | -11.973 |
| CuCl3- | 1.4E-16 | 1.08E-16 | -15.965 |
| CuCl4-2 1 | 2.61E-20 | 1.01E-20 | -19.997 |
| CuCO3 (aq) | 3.34E-18 | 3.41E-18 | -17.467 |
| CuF+ | 7.83E-15 | 6.16E-15 | -14.211 |
| CuHCO3+ | 2.24E-14 | 1.76E-14 | -13.755 |
| CuHPO4 (aq) | 2.88E-16 | 2.95E-16 | -15.531 |
| CuHSO4+ | 8.09E-10 | 6.36E-10 | -9.197 |
| CuN3+ | 8.5E-13 | 6.68E-13 | -12.175 |
| CuNH3+2 | 4.94E-20 | 1.88E-20 | -19.725 |
| CuNO2+ | 1.36E-11 | 1.07E-11 | -10.972 |
| CuNO3+ | 1.7E-11 | 1.34E-11 | -10.873 |
| CuOH+ | 2.3E-14 | 1.78E-14 | -13.75 |
| CuS(aq) | 1.7E-104 | 1.7E-104 | -103.773 |
| CuSO4 (aq) | 2.56E-08 | 2.62E-08 | -7.582 |
| DOC (Gaussian DOM) | 0.001399 | 0.00143 | -2.845 |
| DOM1 | 2.07E-05 | 3.14E-06 | -5.503 |
| F-1 | 9.18E-09 | 7.04E-09 | -8.152 |
| Fe DOM1 | 1.6E-06 | 1.58E-06 | -5.801 |
| Fe(N3)2+ | 1.14E-13 | 8.98E-14 | -13.047 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe(N3)3 (aq) | 8.3E-19 | 8.49E-19 | -18.071 |
| Fe(NH3)2+2 | 5.75E-38 | 2.19E-38 | -37.659 |
| Fe(NH3)3+2 | 1.12E-53 | 4.29E-54 | -53.367 |
| Fe(NH3)4+2 | 9.39E-70 | 3.58E-70 | -69.446 |
| Fe(NO2)2+ | 1.92E-13 | 1.51E-13 | -12.82 |
| Fe(NO2)3 (aq) | 8.26E-17 | 8.45E-17 | -16.073 |
| Fe(OH)2 (aq) | 2.77E-26 | 2.83E-26 | -25.549 |
| Fe(OH)2+ | 3.13E-10 | 2.48E-10 | -9.605 |
| Fe(OH)3- | 4.58E-35 | 3.61E-35 | -34.443 |
| Fe(OH)3 (aq) | 3.55E-18 | 3.63E-18 | -17.44 |
| Fe(OH)4- | 1.32E-24 | 1.05E-24 | -23.979 |
| Fe(SO4)2- | 1.08E-06 | 8.49E-07 | -6.071 |
| Fe+2 | 5.92E-08 | 2.42E-08 | -7.615 |
| Fe+3 | 6.6E-07 | 1.22E-07 | -6.914 |
| Fe2(OH)2+4 | 7.86E-13 | 1.67E-14 | -13.777 |
| Fe3(OH)4+5 | 5.79E-19 | 1.41E-21 | -20.851 |
| FeCl+ | 2.55E-10 | 2.01E-10 | -9.698 |
| FeCl+2 | 9.07E-08 | 3.5E-08 | -7.456 |
| FeCrO4+ | 2.54E-11 | 2E-11 | -10.699 |
| FeF+ | 3.52E-15 | 2.77E-15 | -14.558 |
| FeF+2 | 2.12E-09 | 8.18E-10 | -9.087 |
| FeF2+ | 2.76E-13 | 2.18E-13 | -12.662 |
| FeF3 (aq) | 1.39E-18 | 1.42E-18 | -17.848 |
| FeH2PO4+ | 5.75E-12 | 4.56E-12 | -11.341 |
| FeH2PO4+2 | 2.19E-09 | 8.65E-10 | -9.063 |
| FeHCO3+ | 5.08E-15 | 4.06E-15 | -14.391 |
| FeHPO4 (aq) | 9.97E-17 | 1.02E-16 | -15.992 |
| FeHPO4+ | 2.02E-09 | 1.6E-09 | -8.795 |
| FeHS+ | 1.47E-97 | 1.16E-97 | -96.936 |
| FeN3+2 | 2.19E-09 | 8.38E-10 | -9.077 |
| FeNH3+2 | 1.16E-22 | 4.42E-23 | -22.355 |
| FeNO2+2 | 2.46E-09 | 9.39E-10 | -9.027 |
| FeOH+ | 2.49E-16 | 1.96E-16 | -15.708 |
| FeOH+2 | 9.36E-08 | 3.61E-08 | -7.443 |
| FeSO4 (aq) | 3.21E-08 | 3.28E-08 | -7.484 |
| FeSO4+ | 1.19E-05 | 9.41E-06 | -5.026 |
| H DOM1 | 9.44E-05 | 4.33E-05 | -4.364 |
| H+1 | 0.02717 | 0.02252 | -1.647 |
| H2AsO3- | 2.4E-25 | 1.88E-25 | -24.725 |
| H2AsO4- | 1.21E-06 | 9.51E-07 | -6.022 |
| H2CO3* (aq) | 0.000967 | 0.000989 | -3.005 |
| H2CrO4 (aq) | 2.62E-09 | 2.68E-09 | -8.572 |
| H2PO4- | 6.09E-07 | 4.83E-07 | -6.316 |
| H2S (aq) | 3.67E-90 | 3.76E-90 | -89.425 |
| H3AsO3 | 9.04E-18 | 9.24E-18 | -17.034 |
| H3AsO4 | 3.74E-06 | 3.82E-06 | -5.418 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| H3PO4 | 1.35E-06 | 1.38E-06 | -5.861 |
| HAsO3-2 | 1.12E-37 | 4.26E-38 | -37.371 |
| HAsO4-2 | 1.09E-11 | 4.14E-12 | -11.383 |
| HCO3- | 2.11E-08 | 1.67E-08 | -7.776 |
| HCrO4- | 4.03E-07 | 3.16E-07 | -6.5 |
| HF (aq) | 1.95E-07 | 1.99E-07 | -6.701 |
| HF2- | 6.87E-15 | 5.27E-15 | -14.278 |
| Hg(CO3)2-2 | 2.48E-38 | 9.47E-39 | -38.023 |
| Hg(HS)2 (aq) | 1.1E-172 | 1.1E-172 | -171.95 |
| Hg(N3)2 (aq) | 1.23E-16 | 1.26E-16 | -15.901 |
| Hg(NH3)2+2 | 1.63E-34 | 6.23E-35 | -34.205 |
| Hg(NH3)4+2 | 3.2E-65 | 1.22E-65 | -64.913 |
| Hg(NO2)2 (aq) | 6.11E-22 | 6.24E-22 | -21.205 |
| Hg(NO2)3- | 1.34E-25 | 1.05E-25 | -24.978 |
| Hg(NO2)4-2 | 3.45E-30 | 1.32E-30 | -29.881 |
| Hg(NO3)2 (aq) | 1.92E-29 | 1.97E-29 | -28.707 |
| Hg(OH)2 | 4.26E-24 | 4.36E-24 | -23.36 |
| Hg(SO4)2-2 | 9.76E-22 | 3.73E-22 | -21.429 |
| Hg+2 | 1.5E-20 | 5.71E-21 | -20.243 |
| Hg2OH+3 | 5.2E-42 | 5.96E-43 | -42.225 |
| Hg3(OH)3+3 | 1.07E-62 | 1.22E-63 | -62.913 |
| HgCl+ | 2.71E-15 | 2.13E-15 | -14.672 |
| HgCl2 (aq) | 2.09E-10 | 2.14E-10 | -9.669 |
| HgCl3-1 | 3.55E-11 | 2.79E-11 | -10.554 |
| HgCl4-2 | 4.29E-12 | 1.64E-12 | -11.786 |
| HgClOH (aq) | 6.41E-17 | 6.56E-17 | -16.183 |
| HgCO3 (aq) | 1.19E-25 | 1.21E-25 | -24.916 |
| HgF+ | 1.91E-27 | 1.5E-27 | -26.824 |
| HgHCO3+ | 5.77E-23 | 4.53E-23 | -22.343 |
| HgHS2- | 2E-177 | 1.6E-177 | -176.793 |
| HgN3+ | 1.17E-13 | 9.17E-14 | -13.037 |
| HgNO2+ | 1.75E-20 | 1.38E-20 | -19.862 |
| HgNO3+ | 3.15E-25 | 2.48E-25 | -24.606 |
| HgOH+ | 9.59E-23 | 7.54E-23 | -22.123 |
| HgOHCO3- | 7.99E-31 | 6.28E-31 | -30.202 |
| HgS2-2 | 3.7E-184 | 1.4E-184 | -183.856 |
| HgSO4 (aq) | 5.78E-21 | 5.91E-21 | -20.229 |
| HN3 (aq) | 4.99E-05 | 5.11E-05 | -4.292 |
| HNO2 (aq) | 0.000151 | 0.000155 | -3.81 |
| HPO4-2 | 3.38E-12 | 1.3E-12 | -11.885 |
| HS-1 | 1.49E-95 | 1.15E-95 | -94.941 |
| HSO4- | 0.013215 | 0.010326 | -1.986 |
| K+1 | 0.00032 | 0.000243 | -3.614 |
| K2HPO4 (aq) | 8.17E-19 | 8.35E-19 | -18.078 |
| K2PO4- | 2.71E-28 | 2.13E-28 | -27.671 |
| KCl (aq) | 1.65E-06 | 1.69E-06 | -5.772 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| KCr2O7- | 1.22E-14 | 9.6E-15 | -14.018 |
| KCrO4- | 5.14E-15 | 4.04E-15 | -14.394 |
| KF (aq) | 7.66E-13 | 7.84E-13 | -12.106 |
| KH2PO4 (aq) | 1.78E-10 | 1.82E-10 | -9.739 |
| KHPO4- | 2.46E-15 | 1.95E-15 | -14.71 |
| KNO3 (aq) | 3.47E-08 | 3.55E-08 | -7.45 |
| KOH (aq) | 8.41E-17 | 8.59E-17 | -16.066 |
| KPO4-2 | 2.75E-25 | 1.05E-25 | -24.979 |
| KSO4- | 1.12E-05 | 8.87E-06 | -5.052 |
| Mg DOM1 | 5.31E-08 | 4.55E-08 | -7.342 |
| Mg(NH3)2+2 | 4.07E-35 | 1.55E-35 | -34.809 |
| Mg+2 | 0.005029 | 0.002212 | -2.655 |
| Mg2CO3+2 | 1.38E-18 | 5.27E-19 | -18.278 |
| MgCl+ | 0.000139 | 0.000109 | -3.962 |
| MgCO3 (aq) | 4.28E-17 | 4.37E-17 | -16.359 |
| MgF+ | 1.32E-09 | 1.03E-09 | -8.987 |
| MgHCO3+ | 4.64E-10 | 3.59E-10 | -9.444 |
| MgHPO4 (aq) | 1.5E-12 | 1.54E-12 | -11.813 |
| MgOH+ | 1.88E-13 | 1.52E-13 | -12.819 |
| MgPO4- | 2.07E-21 | 1.64E-21 | -20.784 |
| MgSO4 (aq) | 0.002238 | 0.002288 | -2.641 |
| Mn+3 | 4.55E-05 | 8.4E-06 | -5.076 |
| N3-1 | 5.61E-08 | 4.41E-08 | -7.356 |
| Na+1 | 0.012142 | 0.009562 | -2.019 |
| Na2HPO4 (aq) | 8.32E-16 | 8.51E-16 | -15.07 |
| Na2PO4- | 8.95E-25 | 7.04E-25 | -24.153 |
| NaCl (aq) | 6.87E-05 | 7.03E-05 | -4.153 |
| NaCO3- | 8.27E-18 | 6.56E-18 | -17.183 |
| NaCrO4- | 2.7E-13 | 2.12E-13 | -12.673 |
| NaF (aq) | 5.83E-11 | 5.96E-11 | -10.225 |
| NaH2PO4 (aq) | 7E-09 | 7.16E-09 | -8.145 |
| NaHCO3 (aq) | 9.27E-11 | 9.48E-11 | -10.023 |
| NaHPO4- | 1.5E-13 | 1.19E-13 | -12.926 |
| NaNO3 (aq) | 5.03E-07 | 5.15E-07 | -6.288 |
| NaOH (aq) | 2.26E-15 | 2.31E-15 | -14.636 |
| NaPO4-2 | 1.19E-23 | 4.55E-24 | -23.342 |
| NaSO4- | 0.000403 | 0.000319 | -3.496 |
| NH3 (aq) | 6.27E-17 | 6.42E-17 | -16.193 |
| NH4+1 | 7.02E-09 | 5.27E-09 | -8.278 |
| NH4Cr2O7- | 3.07E-19 | 2.41E-19 | -18.617 |
| NH4SO4- | 4.43E-10 | 3.48E-10 | -9.458 |
| Ni DOM1 | 2.37E-09 | 2.03E-09 | -8.692 |
| Ni(N3)2 (aq) | 7.39E-19 | 7.56E-19 | -18.122 |
| Ni(NH3)2+2 | 4.91E-33 | 1.87E-33 | -32.727 |
| Ni(NH3)3+2 | 1.83E-47 | 6.97E-48 | -47.157 |
| Ni(NH3)4+2 | 2.01E-62 | 7.68E-63 | -62.115 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)5+2 | 7.16E-78 | 2.73E-78 | -77.563 |
| Ni(NH3)6+2 | 5.43E-94 | 2.07E-94 | -93.683 |
| Ni(NO2)2 (aq) | 5.61E-15 | 5.74E-15 | -14.241 |
| Ni(OH)2 (aq) | 7.57E-22 | 7.74E-22 | -21.111 |
| Ni(OH)3- | 4.37E-31 | 3.44E-31 | -30.464 |
| Ni(SO4)2-2 | 2.59E-09 | 9.88E-10 | -9.005 |
| Ni+2 | 1.03E-05 | 3.93E-06 | -5.405 |
| NiCl+ | 2.37E-08 | 1.86E-08 | -7.73 |
| NiCl2 (aq) | 8.52E-12 | 8.71E-12 | -11.06 |
| NiCO3 (aq) | 3.96E-18 | 4.05E-18 | -17.393 |
| NiF+ | 6.37E-13 | 5E-13 | -12.301 |
| NiH2PO4+ | 1.59E-11 | 1.25E-11 | -10.904 |
| NiHCO3+ | 8.21E-12 | 6.46E-12 | -11.19 |
| NiHPO4 (aq) | 3.66E-15 | 3.75E-15 | -14.426 |
| NiHS+ | 1.77E-95 | 1.39E-95 | -94.856 |
| NiN3+ | 4.16E-12 | 3.27E-12 | -11.486 |
| NiNH3+2 | 4.34E-19 | 1.66E-19 | -18.781 |
| NiNO2+ | 5.84E-10 | 4.59E-10 | -9.338 |
| NiNO3+ | 2.4E-09 | 1.89E-09 | -8.724 |
| NiOH+ | 1.35E-14 | 1.06E-14 | -13.973 |
| NiSO4 (aq) | 4.36E-06 | 4.46E-06 | -5.35 |
| NO2-1 | 6.19E-06 | 4.86E-06 | -5.313 |
| NO3-1 | 0.000252 | 0.000191 | -3.719 |
| OH- | 2.65E-13 | 2.03E-13 | -12.692 |
| Pb DOM1 | 3.57E-10 | 3.06E-10 | -9.514 |
| Pb(CO3)2-2 | 1.31E-31 | 4.99E-32 | -31.302 |
| Pb(HS)2 (aq) | 1.8E-183 | 1.8E-183 | -182.739 |
| Pb(HS)3- | 5.3E-277 | 4.2E-277 | -276.38 |
| Pb(NO2)2 (aq) | 2.22E-16 | 2.27E-16 | -15.643 |
| Pb(NO3)2 (aq) | 7.33E-15 | 7.5E-15 | -14.125 |
| Pb(OH)2 (aq) | 1.14E-22 | 1.17E-22 | -21.933 |
| Pb(OH)3- | 6.59E-32 | 5.18E-32 | -31.286 |
| Pb(SO4)2-2 | 2.19E-09 | 8.37E-10 | -9.077 |
| Pb+2 | 1.95E-08 | 7.46E-09 | -8.127 |
| Pb2OH+3 | 8.58E-21 | 9.84E-22 | -21.007 |
| Pb3(OH)4+2 | 1.04E-42 | 3.98E-43 | -42.4 |
| Pb4(OH)4+4 | 2.16E-46 | 4.59E-48 | -47.339 |
| PbCl+ | 4E-09 | 3.14E-09 | -8.502 |
| PbCl2 (aq) | 8.42E-11 | 8.61E-11 | -10.065 |
| PbCl3- | 1.14E-12 | 8.97E-13 | -12.047 |
| PbCl4-2 | 1.13E-14 | 4.3E-15 | -14.367 |
| PbCO3 (aq) | 6.85E-19 | 7.01E-19 | -18.155 |
| PbF+ | 9.44E-15 | 7.42E-15 | -14.13 |
| PbF2 (aq) | 6.29E-22 | 6.43E-22 | -21.192 |
| PbH2PO4+ | 1.13E-13 | 8.86E-14 | -13.053 |
| PbHCO3+ | 1.01E-13 | 7.91E-14 | -13.102 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| PbHPO4 (aq) | 9.7E-18 | 9.92E-18 | -17.003 |
| PbNO2+ | 1.49E-11 | 1.17E-11 | -10.93 |
| PbNO3+ | 2.76E-11 | 2.17E-11 | -10.664 |
| PbOH+ | 7.58E-15 | 5.96E-15 | -14.225 |
| PbSO4 (aq) | 2.2E-08 | 2.25E-08 | -7.647 |
| PO4-3 | 1.69E-22 | 1.98E-23 | -22.704 |
| S-2 | 2.6E-111 | 1E-111 | -110.994 |
| SO4-2 | 0.017285 | 0.006165 | -2.21 |
| Zn DOM1 | 5.63E-09 | 4.82E-09 | -8.317 |
| Zn(CO3)2-2 | 2.36E-31 | 9.02E-32 | -31.045 |
| Zn(N3)2 (aq) | 1.07E-18 | 1.09E-18 | -17.962 |
| Zn(N3)3- | 3.5E-25 | 2.75E-25 | -24.56 |
| Zn(NH3)2+2 | 2.78E-33 | 1.06E-33 | -32.974 |
| Zn(NH3)3+2 | 5.25E-47 | 2E-47 | -46.698 |
| Zn(NH3)4+2 | 4.85E-61 | 1.85E-61 | -60.732 |
| Zn(NO2)2 (aq) | 2.16E-15 | 2.21E-15 | -14.656 |
| Zn(NO3)2 (aq) | 1.05E-13 | 1.08E-13 | -12.968 |
| Zn(OH)2 (aq) | 1.43E-19 | 1.46E-19 | -18.836 |
| Zn(OH)3- | 2.6E-29 | 2.05E-29 | -28.689 |
| Zn(OH)4-2 | 3.77E-40 | 1.44E-40 | -39.842 |
| Zn(SO4)2-2 | 1.12E-06 | 4.26E-07 | -6.37 |
| Zn+2 | 1.44E-05 | 5.89E-06 | -5.23 |
| Zn2OH+3 | 5.5E-18 | 6.3E-19 | -18.201 |
| Zn2S3-2 | 2.7E-290 | 1E-290 | -289.991 |
| ZnCl+ | 2.67E-07 | 2.06E-07 | -6.685 |
| ZnCl2 (aq) | 1.69E-09 | 1.73E-09 | -8.761 |
| ZnCl3- | 3.05E-11 | 2.4E-11 | -10.62 |
| ZnCl4-2 | 3.8E-13 | 1.45E-13 | -12.839 |
| ZnCO3 (aq) | 9.18E-18 | 9.39E-18 | -17.027 |
| ZnF+ | 9.02E-13 | 7.09E-13 | -12.149 |
| ZnHCO3+ | 3.15E-12 | 2.48E-12 | -11.606 |
| ZnHPO4 (aq) | 1.26E-14 | 1.28E-14 | -13.891 |
| ZnN3+ | 4.75E-12 | 3.73E-12 | -11.428 |
| ZnNH3+2 | 1.87E-19 | 7.14E-20 | -19.146 |
| ZnNO2+ | 2.2E-10 | 1.73E-10 | -9.763 |
| ZnNO3+ | 3.83E-09 | 3.01E-09 | -8.521 |
| ZnOH+ | 1.52E-13 | 1.2E-13 | -12.922 |
| ZnS (aq) | 1.1E-100 | 1.1E-100 | -99.954 |
| ZnSO4 (aq) | 7.12E-06 | 7.28E-06 | -5.138 |

## B1.9: Eh 900

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.14E-06 | 3.11E-06 | -5.508 |
| Al(OH)2+ | 1.69E-12 | 1.34E-12 | -11.874 |
| Al(OH)3 (aq) | 1.08E-17 | 1.11E-17 | -16.956 |
| Al(OH)4- | 2.78E-22 | 2.17E-22 | -21.663 |
| Al(SO4)2- | 0.000903 | 0.000705 | -3.152 |
| Al+3 | 0.000412 | 7.59E-05 | -4.119 |
| Al2(OH)2+4 | 3.73E-12 | 7.9E-14 | -13.102 |
| Al2(OH)2CO3+2 | 1.63E-17 | 6.23E-18 | -17.206 |
| Al2PO4+3 | 9.41E-12 | 1.08E-12 | -11.968 |
| Al3(OH)4+5 | 1.21E-18 | 2.95E-21 | -20.53 |
| AlCl+2 | 1.06E-06 | 4.06E-07 | -6.392 |
| AlF+2 | 1.3E-05 | 5.12E-06 | -5.291 |
| AlF2+ | 1.8E-08 | 1.42E-08 | -7.847 |
| AlF3 (aq) | 1.14E-12 | 1.17E-12 | -11.933 |
| AlF4- | 5.26E-18 | 4.11E-18 | -17.386 |
| AlHPO4+ | 4.37E-09 | 3.44E-09 | -8.464 |
| AlOH+2 | 4.35E-08 | 1.72E-08 | -7.765 |
| AlSO4+ | 0.003486 | 0.002724 | -2.565 |
| AsO4-3 | 1.95E-21 | 2.23E-22 | -21.651 |
| AsS(OH)HS- | 1.4E-222 | 1.1E-222 | -221.965 |
| Ca DOM1 | 6.06E-07 | 5.19E-07 | -6.285 |
| Ca(NH3)2+2 | 2.73E-62 | 1.04E-62 | -61.982 |
| Ca(NO3)2 | 7.49E-15 | 7.66E-15 | -14.116 |
| Ca+2 | 0.005966 | 0.002533 | -2.596 |
| CaCl+ | 0.0001 | 7.89E-05 | -4.103 |
| CaCO3 (aq) | 9.71E-17 | 9.93E-17 | -16.003 |
| CaCrO4 (aq) | 6.48E-12 | 6.63E-12 | -11.179 |
| CaF+ | 2.56E-10 | 2.02E-10 | -9.695 |
| CaH2PO4+ | 2.91E-08 | 2.31E-08 | -7.637 |
| CaHCO3+ | 5.57E-10 | 4.45E-10 | -9.351 |
| CaHPO4 (aq) | 1.24E-12 | 1.27E-12 | -11.898 |
| CaNH3+2 | 2.42E-32 | 9.24E-33 | -32.034 |
| CaNO3+ | 3.4E-06 | 2.67E-06 | -5.573 |
| CaOH+ | 1.14E-14 | 9.1E-15 | -14.041 |
| CaPO4- | 1.5E-19 | 1.19E-19 | -18.924 |
| CaSO4 (aq) | 0.003162 | 0.003233 | -2.49 |
| Cd DOM1 | 5.53E-13 | 4.74E-13 | -12.324 |
| Cd(CO3)2-2 | 3.09E-35 | 1.18E-35 | -34.928 |
| Cd(HS)2 (aq) | 2.7E-212 | 2.7E-212 | -211.562 |
| Cd(NH3)2+2 | 1.54E-64 | 5.89E-65 | -64.23 |
| Cd(NH3)3+2 | 4.38E-93 | 1.67E-93 | -92.777 |
| Cd(NH3)4+2 | 3.7E-122 | 1.4E-122 | -121.855 |
| Cd(NO2)2 (aq) | 2.52E-23 | 2.58E-23 | -22.589 |
| Cd(NO3)2 (aq) | 1.37E-16 | 1.4E-16 | -15.855 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd(OH)2 (aq) | 8.81E-27 | 9.01E-27 | -26.045 |
| Cd(OH)3- | 4.96E-38 | 3.9E-38 | -37.409 |
| Cd(OH)4-2 | 4.61E-50 | 1.76E-50 | -49.755 |
| Cd(SO4)2-2 | 2.89E-10 | 1.1E-10 | -9.958 |
| Cd+2 | 2.41E-09 | 9.21E-10 | -9.036 |
| Cd2OH+3 | 6.86E-26 | 7.85E-27 | -26.105 |
| CdCl+ | 1.43E-09 | 1.12E-09 | -8.95 |
| CdCl2 (aq) | 5.78E-11 | 5.91E-11 | -10.229 |
| CdCO3 (aq) | 5.8E-22 | 5.93E-22 | -21.227 |
| CdF+ | 1.22E-16 | 9.56E-17 | -16.02 |
| CdHCO3+ | 4.92E-16 | 3.87E-16 | -15.413 |
| CdHPO4 (aq) | 4.79E-18 | 4.9E-18 | -17.31 |
| CdHS+ | 1.4E-110 | 1.1E-110 | -109.944 |
| CdNH3+2 | 1.13E-36 | 4.29E-37 | -36.367 |
| CdNO2+ | 2.97E-16 | 2.34E-16 | -15.631 |
| CdNO3+ | 1.54E-12 | 1.21E-12 | -11.918 |
| CdOH+ | 1.91E-18 | 1.5E-18 | -17.824 |
| CdSO4 (aq) | 1.15E-09 | 1.18E-09 | -8.93 |
| Cl-1 | 0.017209 | 0.013108 | -1.882 |
| CO3-2 | 6.95E-17 | 2.75E-17 | -16.561 |
| Cr2O7-2 | 1.2E-11 | 4.56E-12 | -11.341 |
| CrO3Cl- | 7.78E-10 | 6.11E-10 | -9.214 |
| CrO3H2PO4- | 6.73E-12 | 5.29E-12 | -11.276 |
| CrO3HPO4-2 | 1.27E-12 | 4.86E-13 | -12.314 |
| CrO3SO4-2 | 3.64E-08 | 1.39E-08 | -7.857 |
| CrO4-2 | 1.24E-11 | 4.45E-12 | -11.352 |
| Cu DOM1 | 5.01E-10 | 4.29E-10 | -9.368 |
| Cu(CO3)2-2 | 6.56E-31 | 2.5E-31 | -30.601 |
| Cu(N3)2 (aq) | 1.34E-18 | 1.37E-18 | -17.864 |
| Cu(N3)3- | 3.83E-24 | 3.01E-24 | -23.522 |
| Cu(N3)4-2 | 9.1E-31 | 3.47E-31 | -30.459 |
| Cu(NH3)2+2 | 3E-60 | 1.15E-60 | -59.941 |
| Cu(NH3)3+2 | 2.79E-87 | 1.06E-87 | -86.973 |
| Cu(NH3)4+2 | 5.4E-115 | 2E-115 | -114.689 |
| Cu(NO2)2 (aq) | 1.4E-22 | 1.43E-22 | -21.846 |
| Cu(NO3)2 (aq) | 7.8E-16 | 7.97E-16 | -15.098 |
| Cu(OH)2 (aq) | 6.3E-22 | 6.45E-22 | -21.191 |
| Cu(OH)3- | 5.15E-30 | 4.05E-30 | -29.392 |
| Cu(OH)4-2 | 3.11E-42 | 1.19E-42 | -41.926 |
| Cu+2 | 5.12E-08 | 2.09E-08 | -7.679 |
| Cu2(OH)2+2 | 2.54E-23 | 9.68E-24 | -23.014 |
| Cu2OH+3 | 2.24E-20 | 2.57E-21 | -20.59 |
| Cu3(OH)4+2 | 3.28E-38 | 1.25E-38 | -37.902 |
| CuCl+ | 6.29E-10 | 4.87E-10 | -9.312 |
| CuCl2 (aq) | 1.04E-12 | 1.07E-12 | -11.973 |
| CuCl3- | 1.4E-16 | 1.08E-16 | -15.965 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CuCl4-2 1 | 2.61E-20 | 1.01E-20 | -19.997 |
| CuCO3 (aq) | 3.31E-18 | 3.39E-18 | -17.47 |
| CuF+ | 7.82E-15 | 6.14E-15 | -14.212 |
| CuHCO3+ | 2.23E-14 | 1.75E-14 | -13.757 |
| CuHPO4 (aq) | 2.86E-16 | 2.93E-16 | -15.533 |
| CuHSO4+ | 8.11E-10 | 6.37E-10 | -9.196 |
| CuN3+ | 8.47E-13 | 6.66E-13 | -12.177 |
| CuNH3+2 | 8.45E-34 | 3.22E-34 | -33.492 |
| CuNO2+ | 7.03E-15 | 5.53E-15 | -14.257 |
| CuNO3+ | 2.76E-11 | 2.17E-11 | -10.664 |
| CuOH+ | 2.29E-14 | 1.77E-14 | -13.752 |
| CuS(aq) | 1.7E-118 | 1.8E-118 | -117.752 |
| CuSO4 (aq) | 2.56E-08 | 2.61E-08 | -7.583 |
| DOC (Gaussian DOM) | 0.001399 | 0.00143 | -2.845 |
| DOM1 | 2.07E-05 | 3.14E-06 | -5.504 |
| F-1 | 9.16E-09 | 7.02E-09 | -8.153 |
| Fe DOM1 | 1.61E-06 | 1.59E-06 | -5.798 |
| Fe(N3)2+ | 1.15E-13 | 9.01E-14 | -13.045 |
| Fe(N3)3 (aq) | 8.29E-19 | 8.48E-19 | -18.072 |
| Fe(NH3)2+2 | 3.03E-67 | 1.16E-67 | -66.937 |
| Fe(NH3)3+2 | 1.01E-96 | 3.87E-97 | -96.412 |
| Fe(NH3)4+2 | 1.4E-126 | 5.5E-127 | -126.258 |
| Fe(NO2)2+ | 5.23E-20 | 4.11E-20 | -19.386 |
| Fe(NO2)3 (aq) | 1.16E-26 | 1.19E-26 | -25.924 |
| Fe(OH)2 (aq) | 4.94E-28 | 5.05E-28 | -27.296 |
| Fe(OH)2+ | 3.14E-10 | 2.49E-10 | -9.604 |
| Fe(OH)3- | 8.14E-37 | 6.42E-37 | -36.193 |
| Fe(OH)3 (aq) | 3.55E-18 | 3.63E-18 | -17.44 |
| Fe(OH)4- | 1.32E-24 | 1.04E-24 | -23.982 |
| Fe(SO4)2- | 1.09E-06 | 8.56E-07 | -6.068 |
| Fe+2 | 1.07E-09 | 4.37E-10 | -9.36 |
| Fe+3 | 6.68E-07 | 1.23E-07 | -6.909 |
| Fe2(OH)2+4 | 7.99E-13 | 1.69E-14 | -13.771 |
| Fe3(OH)4+5 | 5.9E-19 | 1.43E-21 | -20.844 |
| FeCl+ | 4.6E-12 | 3.61E-12 | -11.442 |
| FeCl+2 | 9.18E-08 | 3.54E-08 | -7.452 |
| FeCrO4+ | 2.56E-11 | 2.01E-11 | -10.696 |
| FeF+ | 6.33E-17 | 4.98E-17 | -16.303 |
| FeF+2 | 2.14E-09 | 8.25E-10 | -9.083 |
| FeF2+ | 2.78E-13 | 2.19E-13 | -12.659 |
| FeF3 (aq) | 1.4E-18 | 1.43E-18 | -17.846 |
| FeH2PO4+ | 1.03E-13 | 8.19E-14 | -13.087 |
| FeH2PO4+2 | 2.21E-09 | 8.73E-10 | -9.059 |
| FeHCO3+ | 9.11E-17 | 7.29E-17 | -16.137 |
| FeHPO4 (aq) | 1.78E-18 | 1.82E-18 | -17.739 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHPO4+ | 2.03E-09 | 1.61E-09 | -8.793 |
| FeHS+ | 2.8E-113 | 2.2E-113 | -112.658 |
| FeN3+2 | 2.21E-09 | 8.44E-10 | -9.074 |
| FeNH3+2 | 3.57E-38 | 1.36E-38 | -37.866 |
| FeNO2+2 | 1.29E-12 | 4.93E-13 | -12.308 |
| FeOH+ | 4.46E-18 | 3.52E-18 | -17.454 |
| FeOH+2 | 9.43E-08 | 3.63E-08 | -7.44 |
| FeSO4 (aq) | 5.77E-10 | 5.9E-10 | -9.229 |
| FeSO4+ | 1.21E-05 | 9.5E-06 | -5.022 |
| H DOM1 | 9.44E-05 | 4.33E-05 | -4.364 |
| H+1 | 0.027288 | 0.022615 | -1.646 |
| H2AsO3- | 7.65E-29 | 6.02E-29 | -28.221 |
| H2AsO4- | 1.21E-06 | 9.48E-07 | -6.023 |
| H2CO3* (aq) | 0.000967 | 0.000989 | -3.005 |
| H2CrO4 (aq) | 2.63E-09 | 2.69E-09 | -8.57 |
| H2PO4- | 6.07E-07 | 4.81E-07 | -6.318 |
| H2S (aq) | 3.9E-104 | 4E-104 | -103.401 |
| H3AsO3 | 2.9E-21 | 2.96E-21 | -20.528 |
| H3AsO4 | 3.74E-06 | 3.83E-06 | -5.417 |
| H3PO4 | 1.35E-06 | 1.38E-06 | -5.861 |
| HAsO3-2 | 3.55E-41 | 1.35E-41 | -40.868 |
| HAsO4-2 | 1.08E-11 | 4.11E-12 | -11.386 |
| HCO3- | 2.1E-08 | 1.67E-08 | -7.778 |
| HCrO4- | 4.02E-07 | 3.16E-07 | -6.5 |
| HF (aq) | 1.95E-07 | 2E-07 | -6.7 |
| HF2- | 6.87E-15 | 5.27E-15 | -14.278 |
| Hg(CO3)2-2 | 2.44E-38 | 9.32E-39 | -38.031 |
| Hg(HS)2 (aq) | 1.2E-200 | 1.2E-200 | -199.905 |
| Hg(N3)2 (aq) | 1.21E-16 | 1.23E-16 | -15.908 |
| Hg(NH3)2+2 | 4.78E-62 | 1.82E-62 | -61.739 |
| Hg(NH3)4+2 | 2.7E-120 | 1E-120 | -119.981 |
| Hg(NO2)2 (aq) | 1.64E-28 | 1.68E-28 | -27.775 |
| Hg(NO2)3- | 1.87E-35 | 1.47E-35 | -34.833 |
| Hg(NO2)4-2 | 2.49E-43 | 9.52E-44 | -43.022 |
| Hg(NO3)2 (aq) | 5.04E-29 | 5.15E-29 | -28.288 |
| Hg(OH)2 | 4.23E-24 | 4.33E-24 | -23.364 |
| Hg(SO4)2-2 | 9.73E-22 | 3.71E-22 | -21.43 |
| Hg+2 | 1.5E-20 | 5.72E-21 | -20.243 |
| Hg2OH+3 | 5.19E-42 | 5.94E-43 | -42.226 |
| Hg3(OH)3+3 | 1.06E-62 | 1.21E-63 | -62.918 |
| HgCl+ | 2.71E-15 | 2.13E-15 | -14.672 |
| HgCl2 (aq) | 2.09E-10 | 2.14E-10 | -9.669 |
| HgCl3-1 | 3.55E-11 | 2.79E-11 | -10.554 |
| HgCl4-2 | 4.29E-12 | 1.64E-12 | -11.786 |
| HgClOH (aq) | 6.39E-17 | 6.53E-17 | -16.185 |
| HgCO3 (aq) | 1.18E-25 | 1.2E-25 | -24.92 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgF+ | 1.9E-27 | 1.5E-27 | -26.825 |
| HgHCO3+ | 5.75E-23 | 4.52E-23 | -22.345 |
| HgHS2- | 2.3E-205 | 1.8E-205 | -204.749 |
| HgN3+ | 1.14E-13 | 8.98E-14 | -13.047 |
| HgNO2+ | 9.08E-24 | 7.13E-24 | -23.147 |
| HgNO3+ | 5.1E-25 | 4.01E-25 | -24.397 |
| HgOH+ | 9.55E-23 | 7.51E-23 | -22.124 |
| HgOHCO3- | 7.89E-31 | 6.2E-31 | -30.207 |
| HgS2-2 | 4E-212 | 1.5E-212 | -211.813 |
| HgSO4 (aq) | 5.77E-21 | 5.9E-21 | -20.229 |
| HN3 (aq) | 4.99E-05 | 5.11E-05 | -4.292 |
| HNO2 (aq) | 7.88E-08 | 8.06E-08 | -7.094 |
| HPO4-2 | 3.36E-12 | 1.29E-12 | -11.888 |
| HS-1 | 1.6E-109 | 1.2E-109 | -108.918 |
| HSO4- | 0.013248 | 0.010352 | -1.985 |
| K+1 | 0.00032 | 0.000243 | -3.614 |
| K2HPO4 (aq) | 8.11E-19 | 8.29E-19 | -18.082 |
| K2PO4- | 2.68E-28 | 2.11E-28 | -27.676 |
| KCl (aq) | 1.65E-06 | 1.69E-06 | -5.772 |
| KCr2O7- | 1.22E-14 | 9.59E-15 | -14.018 |
| KCrO4- | 5.12E-15 | 4.02E-15 | -14.396 |
| KF (aq) | 7.65E-13 | 7.82E-13 | -12.107 |
| KH2PO4 (aq) | 1.78E-10 | 1.82E-10 | -9.741 |
| KHPO4- | 2.44E-15 | 1.94E-15 | -14.713 |
| KNO3 (aq) | 5.62E-08 | 5.75E-08 | -7.24 |
| KOH (aq) | 8.37E-17 | 8.56E-17 | -16.068 |
| KPO4-2 | 2.72E-25 | 1.04E-25 | -24.984 |
| KSO4- | 1.12E-05 | 8.85E-06 | -5.053 |
| Mg DOM1 | 5.29E-08 | 4.53E-08 | -7.343 |
| Mg(NH3)2+2 | 1.19E-62 | 4.54E-63 | -62.343 |
| Mg+2 | 0.005032 | 0.002213 | -2.655 |
| Mg2CO3+2 | 1.37E-18 | 5.23E-19 | -18.281 |
| MgCl+ | 0.000139 | 0.000109 | -3.962 |
| MgCO3 (aq) | 4.24E-17 | 4.34E-17 | -16.363 |
| MgF+ | 1.32E-09 | 1.03E-09 | -8.987 |
| MgHCO3+ | 4.62E-10 | 3.58E-10 | -9.446 |
| MgHPO4 (aq) | 1.49E-12 | 1.53E-12 | -11.816 |
| MgOH+ | 1.88E-13 | 1.51E-13 | -12.821 |
| MgPO4- | 2.05E-21 | 1.63E-21 | -20.789 |
| MgSO4 (aq) | 0.002235 | 0.002285 | -2.641 |
| Mn+3 | 4.55E-05 | 8.39E-06 | -5.076 |
| N3-1 | 5.59E-08 | 4.39E-08 | -7.357 |
| Na+1 | 0.012143 | 0.009562 | -2.019 |
| Na2HPO4 (aq) | 8.26E-16 | 8.45E-16 | -15.073 |
| Na2PO4- | 8.85E-25 | 6.96E-25 | -24.158 |
| NaCl (aq) | 6.87E-05 | 7.03E-05 | -4.153 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NaCO3- | 8.2E-18 | 6.5E-18 | -17.187 |
| NaCrO4- | 2.69E-13 | 2.11E-13 | -12.675 |
| NaF (aq) | 5.81E-11 | 5.95E-11 | -10.226 |
| NaH2PO4 (aq) | 6.98E-09 | 7.14E-09 | -8.146 |
| NaHCO3 (aq) | 9.23E-11 | 9.44E-11 | -10.025 |
| NaHPO4- | 1.49E-13 | 1.18E-13 | -12.929 |
| NaNO3 (aq) | 8.15E-07 | 8.33E-07 | -6.079 |
| NaOH (aq) | 2.25E-15 | 2.3E-15 | -14.638 |
| NaPO4-2 | 1.18E-23 | 4.5E-24 | -23.347 |
| NaSO4- | 0.000402 | 0.000319 | -3.496 |
| NH3 (aq) | 1.07E-30 | 1.1E-30 | -29.96 |
| NH4+1 | 1.2E-22 | 9.04E-23 | -22.044 |
| NH4Cr2O7- | 5.27E-33 | 4.14E-33 | -32.383 |
| NH4SO4- | 7.59E-24 | 5.96E-24 | -23.224 |
| Ni DOM1 | 2.36E-09 | 2.03E-09 | -8.693 |
| Ni(N3)2 (aq) | 7.33E-19 | 7.5E-19 | -18.125 |
| Ni(NH3)2+2 | 1.44E-60 | 5.48E-61 | -60.261 |
| Ni(NH3)3+2 | 9.13E-89 | 3.48E-89 | -88.458 |
| Ni(NH3)4+2 | 1.7E-117 | 6.6E-118 | -117.183 |
| Ni(NH3)5+2 | 1E-146 | 4E-147 | -146.398 |
| Ni(NH3)6+2 | 1.4E-176 | 5.2E-177 | -176.285 |
| Ni(NO2)2 (aq) | 1.51E-21 | 1.54E-21 | -20.812 |
| Ni(OH)2 (aq) | 7.51E-22 | 7.68E-22 | -21.115 |
| Ni(OH)3- | 4.32E-31 | 3.39E-31 | -30.469 |
| Ni(SO4)2-2 | 2.58E-09 | 9.85E-10 | -9.007 |
| Ni+2 | 1.03E-05 | 3.94E-06 | -5.405 |
| NiCl+ | 2.37E-08 | 1.86E-08 | -7.73 |
| NiCl2 (aq) | 8.52E-12 | 8.71E-12 | -11.06 |
| NiCO3 (aq) | 3.93E-18 | 4.02E-18 | -17.396 |
| NiF+ | 6.35E-13 | 4.99E-13 | -12.302 |
| NiH2PO4+ | 1.58E-11 | 1.24E-11 | -10.905 |
| NiHCO3+ | 8.18E-12 | 6.43E-12 | -11.192 |
| NiHPO4 (aq) | 3.64E-15 | 3.72E-15 | -14.429 |
| NiHS+ | 1.9E-109 | 1.5E-109 | -108.833 |
| NiN3+ | 4.14E-12 | 3.25E-12 | -11.488 |
| NiNH3+2 | 7.42E-33 | 2.83E-33 | -32.548 |
| NiNO2+ | 3.03E-13 | 2.38E-13 | -12.623 |
| NiNO3+ | 3.89E-09 | 3.06E-09 | -8.515 |
| NiOH+ | 1.35E-14 | 1.06E-14 | -13.975 |
| NiSO4 (aq) | 4.36E-06 | 4.45E-06 | -5.351 |
| NO2-1 | 3.21E-09 | 2.52E-09 | -8.598 |
| NO3-1 | 0.000407 | 0.000309 | -3.51 |
| OH- | 2.64E-13 | 2.02E-13 | -12.694 |
| Pb DOM1 | 3.56E-10 | 3.05E-10 | -9.515 |
| Pb(CO3)2-2 | 1.29E-31 | 4.91E-32 | -31.309 |
| Pb(HS)2 (aq) | 2E-211 | 2E-211 | -210.693 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(NO2)2 (aq) | 5.98E-23 | 6.12E-23 | -22.213 |
| Pb(NO3)2 (aq) | 1.92E-14 | 1.97E-14 | -13.706 |
| Pb(OH)2 (aq) | 1.13E-22 | 1.16E-22 | -21.936 |
| Pb(OH)3- | 6.51E-32 | 5.12E-32 | -31.291 |
| Pb(SO4)2-2 | 2.19E-09 | 8.35E-10 | -9.078 |
| Pb+2 | 1.96E-08 | 7.47E-09 | -8.127 |
| Pb2OH+3 | 8.57E-21 | 9.81E-22 | -21.008 |
| Pb3(OH)4+2 | 1.03E-42 | 3.92E-43 | -42.406 |
| Pb4(OH)4+4 | 2.13E-46 | 4.52E-48 | -47.344 |
| PbCl+ | 4E-09 | 3.15E-09 | -8.502 |
| PbCl2 (aq) | 8.43E-11 | 8.62E-11 | -10.065 |
| PbCl3- | 1.14E-12 | 8.97E-13 | -12.047 |
| PbCl4-2 | 1.13E-14 | 4.3E-15 | -14.367 |
| PbCO3 (aq) | 6.8E-19 | 6.95E-19 | -18.158 |
| PbF+ | 9.43E-15 | 7.41E-15 | -14.13 |
| PbF2 (aq) | 6.26E-22 | 6.4E-22 | -21.194 |
| PbH2PO4+ | 1.12E-13 | 8.84E-14 | -13.054 |
| PbHCO3+ | 1E-13 | 7.88E-14 | -13.103 |
| PbHPO4 (aq) | 9.64E-18 | 9.86E-18 | -17.006 |
| PbNO2+ | 7.75E-15 | 6.09E-15 | -14.215 |
| PbNO3+ | 4.47E-11 | 3.51E-11 | -10.454 |
| PbOH+ | 7.56E-15 | 5.94E-15 | -14.226 |
| PbSO4 (aq) | 2.2E-08 | 2.25E-08 | -7.648 |
| PO4-3 | 1.67E-22 | 1.96E-23 | -22.709 |
| S-2 | 2.8E-125 | 1.1E-125 | -124.973 |
| SO4-2 | 0.017262 | 0.006154 | -2.211 |
| Zn DOM1 | 5.61E-09 | 4.81E-09 | -8.318 |
| Zn(CO3)2-2 | 2.32E-31 | 8.87E-32 | -31.052 |
| Zn(N3)2 (aq) | 1.06E-18 | 1.08E-18 | -17.965 |
| Zn(N3)3- | 3.46E-25 | 2.72E-25 | -24.565 |
| Zn(NH3)2+2 | 8.13E-61 | 3.1E-61 | -60.508 |
| Zn(NH3)3+2 | 2.63E-88 | 1E-88 | -87.999 |
| Zn(NH3)4+2 | 4.2E-116 | 1.6E-116 | -115.8 |
| Zn(NO2)2 (aq) | 5.81E-22 | 5.94E-22 | -21.226 |
| Zn(NO3)2 (aq) | 2.76E-13 | 2.82E-13 | -12.549 |
| Zn(OH)2 (aq) | 1.42E-19 | 1.45E-19 | -18.839 |
| Zn(OH)3- | 2.57E-29 | 2.02E-29 | -28.694 |
| Zn(OH)4-2 | 3.71E-40 | 1.42E-40 | -39.849 |
| Zn(SO4)2-2 | 1.11E-06 | 4.25E-07 | -6.372 |
| Zn+2 | 1.44E-05 | 5.89E-06 | -5.23 |
| Zn2OH+3 | 5.48E-18 | 6.27E-19 | -18.202 |
| ZnCl+ | 2.67E-07 | 2.06E-07 | -6.685 |
| ZnCl2 (aq) | 1.7E-09 | 1.73E-09 | -8.761 |
| ZnCl3- | 3.05E-11 | 2.4E-11 | -10.62 |
| ZnCl4-2 | 3.8E-13 | 1.45E-13 | -12.839 |
| ZnCO3 (aq) | 9.11E-18 | 9.31E-18 | -17.031 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnF+ | 9.01E-13 | 7.08E-13 | -12.15 |
| ZnHCO3+ | 3.14E-12 | 2.47E-12 | -11.608 |
| ZnHPO4 (aq) | 1.25E-14 | 1.28E-14 | -13.894 |
| ZnN3+ | 4.73E-12 | 3.72E-12 | -11.429 |
| ZnNH3+2 | 3.2E-33 | 1.22E-33 | -32.913 |
| ZnNO2+ | 1.14E-13 | 8.95E-14 | -13.048 |
| ZnNO3+ | 6.21E-09 | 4.88E-09 | -8.312 |
| ZnOH+ | 1.52E-13 | 1.19E-13 | -12.924 |
| ZnS (aq) | 1.1E-114 | 1.2E-114 | -113.932 |
| ZnSO4 (aq) | 7.11E-06 | 7.27E-06 | -5.138 |

# B2: Species distribution

## B2.1: Eh 100

| Component | % of total concentration | Species name |
|---|---|---|
| CrO4-2 | 0.234 | CrO4-2 |
| | 99.494 | HCrO4- |
| | 0.105 | CaCrO4 (aq) |
| | 0.143 | CrO3SO4-2 |
| NH4+1 | 93.633 | NH4+1 |
| | 6.367 | NH4SO4- |
| Cl-1 | 97.939 | Cl-1 |
| | 0.529 | CaCl+ |
| | 0.412 | FeCl+ |
| | 0.735 | MgCl+ |
| | 0.372 | NaCl (aq) |
| Fe+2 | 64.226 | Fe+2 |
| | 0.381 | FeCl+ |
| | 35.388 | FeSO4 (aq) |
| Zn+2 | 61.376 | Zn+2 |
| | 0.471 | Zn DOM1 |
| | 1.573 | ZnCl+ |
| | 0.014 | ZnCl2 (aq) |
| | 30.909 | ZnSO4 (aq) |
| | 5.654 | Zn(SO4)2-2 |
| F-1 | 0.183 | F-1 |
| | 0.053 | HF (aq) |
| | 99.041 | AlF+2 |
| | 0.672 | AlF2+ |
| | 0.025 | MgF+ |
| | 0.02 | FeF+ |
| Pb+2 | 34.136 | Pb+2 |
| | 12.253 | Pb DOM1 |
| | 9.615 | PbCl+ |
| | 0.286 | PbCl2 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 39.149 | PbSO4 (aq) |
| | 4.542 | Pb(SO4)2-2 |
| | 0.012 | PbHCO3+ |
| Ni+2 | 69.501 | Ni+2 |
| | 0.314 | Ni DOM1 |
| | 0.22 | NiCl+ |
| | 29.939 | NiSO4 (aq) |
| | 0.021 | Ni(SO4)2-2 |
| N3-1 | 7.553 | N3-1 |
| | 92.446 | HN3 (aq) |
| PO4-3 | 0.01 | HPO4-2 |
| | 25.034 | H2PO4- |
| | 0.76 | H3PO4 |
| | 67.69 | FeH2PO4+ |
| | 0.082 | FeHPO4 (aq) |
| | 1.121 | CaH2PO4+ |
| | 4.712 | AlHPO4+ |
| | 0.301 | Al2PO4+3 |
| | 0.275 | NaH2PO4 (aq) |
| AsO4-3 | 4.072 | H3AsO4 |
| | 0.064 | HAsO4-2 |
| | 95.864 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 45.417 | DOM1 |
| | 23.937 | H DOM1 |
| | 19.799 | Al DOM1 |
| | 9.851 | Ca DOM1 |
| | 0.863 | Mg DOM1 |
| | 0.038 | Ni DOM1 |
| | 0.09 | Zn DOM1 |
| Ca+2 | 63.672 | Ca+2 |
| | 0.129 | Ca DOM1 |
| | 1.487 | CaCl+ |
| | 34.711 | CaSO4 (aq) |
| Mg+2 | 66.747 | Mg+2 |
| | 0.014 | Mg DOM1 |
| | 2.574 | MgCl+ |
| | 30.664 | MgSO4 (aq) |
| K+1 | 95.681 | K+1 |
| | 0.694 | KCl (aq) |
| | 3.625 | KSO4- |
| Na+1 | 95.772 | Na+1 |
| | 0.765 | NaCl (aq) |
| | 3.463 | NaSO4- |
| CO3-2 | 0.159 | HCO3- |

| Component | % of total concentration | Species name |
|---|---|---|
| | 99.822 | H2CO3* (aq) |
| | 0.011 | FeHCO3+ |
| SO4-2 | 52.788 | SO4-2 |
| | 0.53 | HSO4- |
| | 3.653 | AlSO4+ |
| | 2.065 | Al(SO4)2- |
| | 0.018 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 25.61 | FeSO4 (aq) |
| | 5.846 | MgSO4 (aq) |
| | 8.249 | CaSO4 (aq) |
| | 1.124 | NaSO4- |
| | 0.031 | KSO4- |
| | 0.067 | NH4SO4- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 40.107 | Cd+2 |
| | 0.181 | Cd DOM1 |
| | 32.635 | CdCl+ |
| | 1.867 | CdCl2 (aq) |
| | 19.491 | CdSO4 (aq) |
| | 5.719 | Cd(SO4)2-2 |
| Fe+3 | 1.265 | Fe+3 |
| | 57.409 | Fe DOM1 |
| | 12.501 | FeOH+2 |
| | 2.833 | Fe(OH)2+ |
| | 0.01 | FeF+2 |
| | 0.244 | FeCl+2 |
| | 22.995 | FeSO4+ |
| | 2.259 | Fe(SO4)2- |
| | 0.269 | FeN3+2 |
| | 0.206 | FeHPO4+ |
| NO2-1 | 74.833 | NO2-1 |
| | 25.158 | HNO2 (aq) |
| NO3-1 | 99.031 | NO3-1 |
| | 0.765 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.188 | NaNO3 (aq) |
| HS-1 | 0.016 | HS-1 |
| | 54.469 | H2S (aq) |
| | 0.018 | NiHS+ |
| | 45.495 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Hg(OH)2 | 99.998 | HgN3+ |
| Cu+2 | 58.122 | Cu+2 |
| | 11.212 | Cu DOM1 |
| | 0.99 | CuCl+ |

| Component | % of total concentration | Species name |
|---|---|---|
| | 29.596 | CuSO4 (aq) |
| | 0.013 | CuHSO4+ |
| | 0.061 | CuN3+ |
| Al+3 | 8.208 | Al+3 |
| | 1.178 | Al DOM1 |
| | 0.06 | AlOH+2 |
| | 0.646 | AlF+2 |
| | 0.029 | AlCl+2 |
| | 70.07 | AlSO4+ |
| | 19.8 | Al(SO4)2- |

## B2.2: Eh 200

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 99.989 | HgN3+ |
| NH4+1 | 93.733 | NH4+1 |
| | 6.267 | NH4SO4- |
| Cl-1 | 97.934 | Cl-1 |
| | 0.531 | CaCl+ |
| | 0.413 | FeCl+ |
| | 0.736 | MgCl+ |
| | 0.371 | NaCl (aq) |
| Fe+2 | 64.706 | Fe+2 |
| | 0.382 | FeCl+ |
| | 34.908 | FeSO4 (aq) |
| Zn+2 | 62.008 | Zn+2 |
| | 0.287 | Zn DOM1 |
| | 1.581 | ZnCl+ |
| | 0.014 | ZnCl2 (aq) |
| | 30.576 | ZnSO4 (aq) |
| | 5.532 | Zn(SO4)2-2 |
| F-1 | 0.09 | F-1 |
| | 0.052 | HF (aq) |
| | 99.501 | AlF+2 |
| | 0.332 | AlF2+ |
| | 0.012 | MgF+ |
| SO4-2 | 49.75 | SO4-2 |
| | 0.992 | HSO4- |
| | 6.945 | AlSO4+ |
| | 3.863 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 24.035 | FeSO4 (aq) |
| | 5.486 | MgSO4 (aq) |
| | 7.749 | CaSO4 (aq) |
| | 1.053 | NaSO4- |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.029 | KSO4- |
| | 0.063 | NH4SO4- |
| Ni+2 | 70.026 | Ni+2 |
| | 0.191 | Ni DOM1 |
| | 0.221 | NiCl+ |
| | 29.539 | NiSO4 (aq) |
| | 0.02 | Ni(SO4)2-2 |
| N3-1 | 3.94 | N3-1 |
| | 96.059 | HN3 (aq) |
| PO4-3 | 24.791 | H2PO4- |
| | 1.499 | H3PO4 |
| | 67.216 | FeH2PO4+ |
| | 0.041 | FeHPO4 (aq) |
| | 1.114 | CaH2PO4+ |
| | 4.741 | AlHPO4+ |
| | 0.31 | Al2PO4+3 |
| | 0.272 | NaH2PO4 (aq) |
| AsO4-3 | 7.799 | H3AsO4 |
| | 0.031 | HAsO4-2 |
| | 92.17 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 40.054 | DOM1 |
| | 29.032 | H DOM1 |
| | 24.311 | Al DOM1 |
| | 5.992 | Ca DOM1 |
| | 0.524 | Mg DOM1 |
| | 0.023 | Ni DOM1 |
| | 0.055 | Zn DOM1 |
| Ca+2 | 64.158 | Ca+2 |
| | 0.078 | Ca DOM1 |
| | 1.492 | CaCl+ |
| | 34.271 | CaSO4 (aq) |
| Mg+2 | 67.163 | Mg+2 |
| | 2.58 | MgCl+ |
| | 30.248 | MgSO4 (aq) |
| K+1 | 95.74 | K+1 |
| | 0.692 | KCl (aq) |
| | 3.568 | KSO4- |
| Na+1 | 95.827 | Na+1 |
| | 0.763 | NaCl (aq) |
| | 3.41 | NaSO4- |
| CO3-2 | 0.08 | HCO3- |
| | 99.911 | H2CO3* (aq) |
| Pb+2 | 36.266 | Pb+2 |
| | 7.854 | Pb DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 10.161 | PbCl+ |
| | 0.301 | PbCl2 (aq) |
| | 40.73 | PbSO4 (aq) |
| | 4.674 | Pb(SO4)2-2 |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 40.448 | Cd+2 |
| | 0.11 | Cd DOM1 |
| | 32.74 | CdCl+ |
| | 1.867 | CdCl2 (aq) |
| | 19.249 | CdSO4 (aq) |
| | 5.586 | Cd(SO4)2-2 |
| CrO4-2 | 0.118 | CrO4-2 |
| | 99.513 | HCrO4- |
| | 0.018 | H2CrO4 (aq) |
| | 0.053 | CaCrO4 (aq) |
| | 0.282 | CrO3SO4-2 |
| Cu+2 | 61.239 | Cu+2 |
| | 7.126 | Cu DOM1 |
| | 1.037 | CuCl+ |
| | 30.532 | CuSO4 (aq) |
| | 0.028 | CuHSO4+ |
| | 0.033 | CuN3+ |
| Fe+3 | 1.863 | Fe+3 |
| | 50.828 | Fe DOM1 |
| | 9.209 | FeOH+2 |
| | 1.042 | Fe(OH)2+ |
| | 0.358 | FeCl+2 |
| | 33.128 | FeSO4+ |
| | 3.203 | Fe(SO4)2- |
| | 0.206 | FeN3+2 |
| | 0.149 | FeHPO4+ |
| NO2-1 | 59.886 | NO2-1 |
| | 40.106 | HNO2 (aq) |
| NO3-1 | 99.03 | NO3-1 |
| | 0.767 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.188 | NaNO3 (aq) |
| HS-1 | 0.011 | HS-1 |
| | 70.385 | H2S (aq) |
| | 0.012 | NiHS+ |
| | 29.592 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Al+3 | 8.469 | Al+3 |
| | 0.731 | Al DOM1 |
| | 0.031 | AlOH+2 |
| | 0.328 | AlF+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.03 | AlCl+2 |
| | 70.736 | AlSO4+ |
| | 19.672 | Al(SO4)2- |

## B2.3: Eh 300

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 0.194 | HgCl2 (aq) |
| | 0.045 | HgCl3-1 |
| | 99.747 | HgN3+ |
| NH4+1 | 93.344 | NH4+1 |
| | 6.656 | NH4SO4- |
| Cl-1 | 98.029 | Cl-1 |
| | 0.527 | CaCl+ |
| | 0.321 | FeCl+ |
| | 0.732 | MgCl+ |
| | 0.375 | NaCl (aq) |
| Pb+2 | 35.859 | Pb+2 |
| | 5.473 | Pb DOM1 |
| | 9.532 | PbCl+ |
| | 0.266 | PbCl2 (aq) |
| | 43.639 | PbSO4 (aq) |
| | 5.223 | Pb(SO4)2-2 |
| Zn+2 | 60.13 | Zn+2 |
| | 0.196 | Zn DOM1 |
| | 1.453 | ZnCl+ |
| | 0.012 | ZnCl2 (aq) |
| | 32.143 | ZnSO4 (aq) |
| | 6.065 | Zn(SO4)2-2 |
| F-1 | 0.081 | F-1 |
| | 0.095 | HF (aq) |
| | 99.501 | AlF+2 |
| | 0.303 | AlF2+ |
| | 0.011 | MgF+ |
| SO4-2 | 50.597 | SO4-2 |
| | 2.091 | HSO4- |
| | 8.166 | AlSO4+ |
| | 4.828 | Al(SO4)2- |
| | 0.018 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 19.412 | FeSO4 (aq) |
| | 5.678 | MgSO4 (aq) |
| | 8 | CaSO4 (aq) |
| | 1.096 | NaSO4- |
| | 0.03 | KSO4- |
| | 0.066 | NH4SO4- |

| Component | % of total concentration | Species name |
|---|---|---|
| Ni+2 | 68.383 | Ni+2 |
| | 0.131 | Ni DOM1 |
| | 0.204 | NiCl+ |
| | 31.258 | NiSO4 (aq) |
| | 0.022 | Ni(SO4)2-2 |
| N3-1 | 1.966 | N3-1 |
| | 98.033 | HN3 (aq) |
| PO4-3 | 29.515 | H2PO4- |
| | 3.651 | H3PO4 |
| | 61.9 | FeH2PO4+ |
| | 0.019 | FeHPO4 (aq) |
| | 1.311 | CaH2PO4+ |
| | 3.151 | AlHPO4+ |
| | 0.111 | Al2PO4+3 |
| | 0.327 | NaH2PO4 (aq) |
| AsO4-3 | 14.75 | H3AsO4 |
| | 0.014 | HAsO4-2 |
| | 85.236 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 35.914 | DOM1 |
| | 40.413 | H DOM1 |
| | 19.147 | Al DOM1 |
| | 4.103 | Ca DOM1 |
| | 0.36 | Mg DOM1 |
| | 0.016 | Ni DOM1 |
| | 0.037 | Zn DOM1 |
| Ca+2 | 62.487 | Ca+2 |
| | 0.054 | Ca DOM1 |
| | 1.375 | CaCl+ |
| | 36.083 | CaSO4 (aq) |
| Mg+2 | 65.686 | Mg+2 |
| | 2.384 | MgCl+ |
| | 31.924 | MgSO4 (aq) |
| K+1 | 95.555 | K+1 |
| | 0.652 | KCl (aq) |
| | 3.793 | KSO4- |
| Na+1 | 95.664 | Na+1 |
| | 0.717 | NaCl (aq) |
| | 3.618 | NaSO4- |
| CO3-2 | 0.039 | HCO3- |
| | 99.957 | H2CO3* (aq) |
| Al+3 | 7.772 | Al+3 |
| | 0.479 | Al DOM1 |
| | 0.014 | AlOH+2 |
| | 0.273 | AlF+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.026 | AlCl+2 |
| | 70.571 | AlSO4+ |
| | 20.863 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 40.277 | Cd+2 |
| | 0.077 | Cd DOM1 |
| | 30.928 | CdCl+ |
| | 1.661 | CdCl2 (aq) |
| | 20.77 | CdSO4 (aq) |
| | 6.286 | Cd(SO4)2-2 |
| CrO4-2 | 0.057 | CrO4-2 |
| | 99.255 | HCrO4- |
| | 0.036 | H2CrO4 (aq) |
| | 0.026 | CaCrO4 (aq) |
| | 0.015 | CrO3Cl- |
| | 0.603 | CrO3SO4-2 |
| Cu+2 | 60.979 | Cu+2 |
| | 5.003 | Cu DOM1 |
| | 0.979 | CuCl+ |
| | 32.959 | CuSO4 (aq) |
| | 0.06 | CuHSO4+ |
| | 0.017 | CuN3+ |
| Fe+2 | 62.871 | Fe+2 |
| | 0.352 | FeCl+ |
| | 36.771 | FeSO4 (aq) |
| NO2-1 | 42.197 | NO2-1 |
| | 57.798 | HNO2 (aq) |
| NO3-1 | 99.034 | NO3-1 |
| | 0.761 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.19 | NaNO3 (aq) |
| HS-1 | 86.269 | H2S (aq) |
| | 13.717 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 2.238 | Fe+3 |
| | 43.607 | Fe DOM1 |
| | 5.453 | FeOH+2 |
| | 0.307 | Fe(OH)2+ |
| | 0.406 | FeCl+2 |
| | 43.288 | FeSO4+ |
| | 4.452 | Fe(SO4)2- |
| | 0.125 | FeN3+2 |
| | 0.108 | FeHPO4+ |

## B2.4: Eh 400

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 56.958 | HgCl2 (aq) |
| | 12.53 | HgCl3-1 |
| | 1.998 | HgCl4-2 |
| | 28.506 | HgN3+ |
| NH4+1 | 93.5 | NH4+1 |
| | 6.5 | NH4SO4- |
| Cl-1 | 98.065 | Cl-1 |
| | 0.536 | CaCl+ |
| | 0.261 | FeCl+ |
| | 0.744 | MgCl+ |
| | 0.379 | NaCl (aq) |
| Pb+2 | 37.664 | Pb+2 |
| | 2.242 | Pb DOM1 |
| | 9.569 | PbCl+ |
| | 0.254 | PbCl2 (aq) |
| | 45.067 | PbSO4 (aq) |
| | 5.197 | Pb(SO4)2-2 |
| Zn+2 | 60.761 | Zn+2 |
| | 0.077 | Zn DOM1 |
| | 1.402 | ZnCl+ |
| | 0.011 | ZnCl2 (aq) |
| | 31.94 | ZnSO4 (aq) |
| | 5.807 | Zn(SO4)2-2 |
| F-1 | 0.078 | F-1 |
| | 0.379 | HF (aq) |
| | 99.229 | AlF+2 |
| | 0.295 | AlF2+ |
| | 0.011 | MgF+ |
| SO4-2 | 48.621 | SO4-2 |
| | 8.309 | HSO4- |
| | 8.226 | AlSO4+ |
| | 4.734 | Al(SO4)2- |
| | 0.018 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 15.386 | FeSO4 (aq) |
| | 5.611 | MgSO4 (aq) |
| | 7.915 | CaSO4 (aq) |
| | 1.068 | NaSO4- |
| | 0.03 | KSO4- |
| | 0.064 | NH4SO4- |
| Ni+2 | 68.806 | Ni+2 |
| | 0.052 | Ni DOM1 |
| | 0.196 | NiCl+ |
| | 30.924 | NiSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.021 | Ni(SO4)2-2 |
| N3-1 | 0.486 | N3-1 |
| | 99.514 | HN3 (aq) |
| PO4-3 | 30.313 | H2PO4- |
| | 15.403 | H3PO4 |
| | 51.725 | FeH2PO4+ |
| | 1.368 | CaH2PO4+ |
| | 0.821 | AlHPO4+ |
| | 0.338 | NaH2PO4 (aq) |
| AsO4-3 | 41.543 | H3AsO4 |
| | 58.455 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 26.909 | DOM1 |
| | 63.544 | H DOM1 |
| | 7.691 | Al DOM1 |
| | 1.61 | Ca DOM1 |
| | 0.081 | Fe DOM1 |
| | 0.141 | Mg DOM1 |
| | 0.015 | Zn DOM1 |
| Ca+2 | 62.957 | Ca+2 |
| | 0.021 | Ca DOM1 |
| | 1.323 | CaCl+ |
| | 35.699 | CaSO4 (aq) |
| Mg+2 | 66.161 | Mg+2 |
| | 2.29 | MgCl+ |
| | 31.547 | MgSO4 (aq) |
| K+1 | 95.678 | K+1 |
| | 0.622 | KCl (aq) |
| | 3.7 | KSO4- |
| Na+1 | 95.79 | Na+1 |
| | 0.684 | NaCl (aq) |
| | 3.526 | NaSO4- |
| CO3-2 | 99.99 | H2CO3* (aq) |
| Al+3 | 7.95 | Al+3 |
| | 0.192 | Al DOM1 |
| | 0.272 | AlF+2 |
| | 0.026 | AlCl+2 |
| | 71.097 | AlSO4+ |
| | 20.458 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 41.2 | Cd+2 |
| | 0.031 | Cd DOM1 |
| | 30.24 | CdCl+ |
| | 1.547 | CdCl2 (aq) |
| | 20.89 | CdSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 6.092 | Cd(SO4)2-2 |
| CrO4-2 | 0.013 | CrO4-2 |
| | 97.427 | HCrO4- |
| | 0.146 | H2CrO4 (aq) |
| | 0.056 | CrO3Cl- |
| | 2.344 | CrO3SO4-2 |
| Cu+2 | 63.174 | Cu+2 |
| | 2.022 | Cu DOM1 |
| | 0.969 | CuCl+ |
| | 33.578 | CuSO4 (aq) |
| | 0.251 | CuHSO4+ |
| Fe+2 | 63.268 | Fe+2 |
| | 0.338 | FeCl+ |
| | 36.388 | FeSO4 (aq) |
| NO2-1 | 15.094 | NO2-1 |
| | 84.904 | HNO2 (aq) |
| NO3-1 | 99.02 | NO3-1 |
| | 0.774 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.191 | NaNO3 (aq) |
| HS-1 | 96.942 | H2S (aq) |
| | 3.054 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 3.287 | Fe+3 |
| | 25.148 | Fe DOM1 |
| | 1.964 | FeOH+2 |
| | 0.027 | Fe(OH)2+ |
| | 0.011 | FeF+2 |
| | 0.568 | FeCl+2 |
| | 62.626 | FeSO4+ |
| | 6.272 | Fe(SO4)2- |
| | 0.046 | FeN3+2 |
| | 0.011 | FeH2PO4+2 |
| | 0.04 | FeHPO4+ |

## B2.5: Eh 500

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 82.267 | HgCl2 (aq) |
| | 15.438 | HgCl3-1 |
| | 2.078 | HgCl4-2 |
| | 0.215 | HgN3+ |
| NH4+1 | 93.856 | NH4+1 |
| | 6.144 | NH4SO4- |
| Cl-1 | 98.165 | Cl-1 |
| | 0.559 | CaCl+ |
| | 0.098 | FeCl+ |
| | 0.774 | MgCl+ |
| | 0.387 | NaCl (aq) |
| Pb+2 | 39.567 | Pb+2 |
| | 0.966 | Pb DOM1 |
| | 8.817 | PbCl+ |
| | 0.203 | PbCl2 (aq) |
| | 45.642 | PbSO4 (aq) |
| | 4.8 | Pb(SO4)2-2 |
| Zn+2 | 62.05 | Zn+2 |
| | 0.032 | Zn DOM1 |
| | 1.254 | ZnCl+ |
| | 31.443 | ZnSO4 (aq) |
| | 5.213 | Zn(SO4)2-2 |
| F-1 | 0.073 | F-1 |
| | 1.082 | HF (aq) |
| | 98.543 | AlF+2 |
| | 0.281 | AlF2+ |
| | 0.01 | MgF+ |
| SO4-2 | 44.036 | SO4-2 |
| | 23.437 | HSO4- |
| | 8.321 | AlSO4+ |
| | 4.49 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 5.386 | FeSO4 (aq) |
| | 0.011 | FeSO4+ |
| | 5.464 | MgSO4 (aq) |
| | 7.725 | CaSO4 (aq) |
| | 1.004 | NaSO4- |
| | 0.028 | KSO4- |
| | 0.061 | NH4SO4- |
| Ni+2 | 69.62 | Ni+2 |
| | 0.021 | Ni DOM1 |
| | 0.174 | NiCl+ |
| | 30.165 | NiSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.019 | Ni(SO4)2-2 |
| N3-1 | 0.159 | N3-1 |
| | 99.838 | HN3 (aq) |
| PO4-3 | 30.656 | H2PO4- |
| | 47.665 | H3PO4 |
| | 19.487 | FeH2PO4+ |
| | 0.042 | FeH2PO4+2 |
| | 0.055 | FeHPO4+ |
| | 1.437 | CaH2PO4+ |
| | 0.298 | AlHPO4+ |
| | 0.349 | NaH2PO4 (aq) |
| AsO4-3 | 68.489 | H3AsO4 |
| | 31.511 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 19.425 | DOM1 |
| | 75.797 | H DOM1 |
| | 3.358 | Al DOM1 |
| | 0.669 | Ca DOM1 |
| | 0.683 | Fe DOM1 |
| | 0.058 | Mg DOM1 |
| Ca+2 | 63.975 | Ca+2 |
| | 1.174 | CaCl+ |
| | 34.841 | CaSO4 (aq) |
| Mg+2 | 67.247 | Mg+2 |
| | 2.029 | MgCl+ |
| | 30.723 | MgSO4 (aq) |
| K+1 | 95.968 | K+1 |
| | 0.543 | KCl (aq) |
| | 3.489 | KSO4- |
| Na+1 | 96.088 | Na+1 |
| | 0.596 | NaCl (aq) |
| | 3.316 | NaSO4- |
| CO3-2 | 99.997 | H2CO3* (aq) |
| Al+3 | 8.304 | Al+3 |
| | 0.084 | Al DOM1 |
| | 0.27 | AlF+2 |
| | 0.023 | AlCl+2 |
| | 71.915 | AlSO4+ |
| | 19.402 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 43.641 | Cd+2 |
| | 0.013 | Cd DOM1 |
| | 28.095 | CdCl+ |
| | 1.247 | CdCl2 (aq) |
| | 21.332 | CdSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 5.672 | Cd(SO4)2-2 |
| CrO4-2 | 93.166 | HCrO4- |
| | 0.427 | H2CrO4 (aq) |
| | 0.14 | CrO3Cl- |
| | 6.251 | CrO3SO4-2 |
| Cu+2 | 64.496 | Cu+2 |
| | 0.847 | Cu DOM1 |
| | 0.866 | CuCl+ |
| | 33.046 | CuSO4 (aq) |
| | 0.742 | CuHSO4+ |
| Fe+2 | 64.135 | Fe+2 |
| | 0.301 | FeCl+ |
| | 35.558 | FeSO4 (aq) |
| NO2-1 | 5.493 | NO2-1 |
| | 94.505 | HNO2 (aq) |
| NO3-1 | 98.983 | NO3-1 |
| | 0.806 | CaNO3+ |
| | 0.013 | KNO3 (aq) |
| | 0.196 | NaNO3 (aq) |
| HS-1 | 99.616 | H2S (aq) |
| | 0.382 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 4.039 | Fe+3 |
| | 12.916 | Fe DOM1 |
| | 0.805 | FeOH+2 |
| | 0.013 | FeF+2 |
| | 0.607 | FeCl+2 |
| | 74.56 | FeSO4+ |
| | 7.007 | Fe(SO4)2- |
| | 0.019 | FeN3+2 |
| | 0.013 | FeH2PO4+2 |
| | 0.017 | FeHPO4+ |

## B2.6: Eh 600

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 83.915 | HgCl2 (aq) |
| | 14.294 | HgCl3-1 |
| | 1.736 | HgCl4-2 |
| | 0.054 | HgN3+ |
| NH4+1 | 94.022 | NH4+1 |
| | 5.978 | NH4SO4- |
| Cl-1 | 98.225 | Cl-1 |
| | 0.571 | CaCl+ |
| | 0.791 | MgCl+ |
| | 0.392 | NaCl (aq) |
| Pb+2 | 40.347 | Pb+2 |
| | 0.759 | Pb DOM1 |
| | 8.292 | PbCl+ |
| | 0.175 | PbCl2 (aq) |
| | 45.828 | PbSO4 (aq) |
| | 4.596 | Pb(SO4)2-2 |
| Zn+2 | 62.625 | Zn+2 |
| | 0.025 | Zn DOM1 |
| | 1.165 | ZnCl+ |
| | 31.238 | ZnSO4 (aq) |
| | 4.939 | Zn(SO4)2-2 |
| F-1 | 0.07 | F-1 |
| | 1.444 | HF (aq) |
| | 98.184 | AlF+2 |
| | 0.275 | AlF2+ |
| | 0.015 | FeF+2 |
| | 0.01 | MgF+ |
| SO4-2 | 41.852 | SO4-2 |
| | 31.015 | HSO4- |
| | 8.364 | AlSO4+ |
| | 4.374 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 0.225 | FeSO4 (aq) |
| | 0.027 | FeSO4+ |
| | 5.402 | MgSO4 (aq) |
| | 7.643 | CaSO4 (aq) |
| | 0.975 | NaSO4- |
| | 0.027 | KSO4- |
| | 0.059 | NH4SO4- |
| Ni+2 | 69.958 | Ni+2 |
| | 0.017 | Ni DOM1 |
| | 0.162 | NiCl+ |
| | 29.846 | NiSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.018 | Ni(SO4)2-2 |
| N3-1 | 0.116 | N3-1 |
| | 99.88 | HN3 (aq) |
| PO4-3 | 30.823 | H2PO4- |
| | 66.07 | H3PO4 |
| | 0.842 | FeH2PO4+ |
| | 0.102 | FeH2PO4+2 |
| | 0.097 | FeHPO4+ |
| | 1.473 | CaH2PO4+ |
| | 0.227 | AlHPO4+ |
| | 0.354 | NaH2PO4 (aq) |
| AsO4-3 | 74.974 | H3AsO4 |
| | 25.026 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 17.398 | DOM1 |
| | 78.119 | H DOM1 |
| | 2.66 | Al DOM1 |
| | 0.518 | Ca DOM1 |
| | 1.253 | Fe DOM1 |
| | 0.045 | Mg DOM1 |
| Ca+2 | 64.431 | Ca+2 |
| | 1.088 | CaCl+ |
| | 34.474 | CaSO4 (aq) |
| Mg+2 | 67.75 | Mg+2 |
| | 1.879 | MgCl+ |
| | 30.371 | MgSO4 (aq) |
| K+1 | 96.11 | K+1 |
| | 0.5 | KCl (aq) |
| | 3.391 | KSO4- |
| Na+1 | 96.235 | Na+1 |
| | 0.547 | NaCl (aq) |
| | 3.218 | NaSO4- |
| CO3-2 | 99.998 | H2CO3* (aq) |
| Al+3 | 8.455 | Al+3 |
| | 0.067 | Al DOM1 |
| | 0.269 | AlF+2 |
| | 0.022 | AlCl+2 |
| | 72.287 | AlSO4+ |
| | 18.899 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.014 | Cd+2 |
| | 0.011 | Cd DOM1 |
| | 26.727 | CdCl+ |
| | 1.088 | CdCl2 (aq) |
| | 21.666 | CdSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 5.495 | Cd(SO4)2-2 |
| CrO4-2 | 91.193 | HCrO4- |
| | 0.575 | H2CrO4 (aq) |
| | 0.171 | CrO3Cl- |
| | 8.043 | CrO3SO4-2 |
| Cu+2 | 64.837 | Cu+2 |
| | 0.655 | Cu DOM1 |
| | 0.801 | CuCl+ |
| | 32.701 | CuSO4 (aq) |
| | 1.002 | CuHSO4+ |
| Fe+2 | 64.509 | Fe+2 |
| | 0.279 | FeCl+ |
| | 35.206 | FeSO4 (aq) |
| NO2-1 | 4.047 | NO2-1 |
| | 95.951 | HNO2 (aq) |
| NO3-1 | 98.963 | NO3-1 |
| | 0.823 | CaNO3+ |
| | 0.014 | KNO3 (aq) |
| | 0.198 | NaNO3 (aq) |
| HS-1 | 99.987 | H2S (aq) |
| | 0.012 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 4.223 | Fe+3 |
| | 10.508 | Fe DOM1 |
| | 0.617 | FeOH+2 |
| | 0.014 | FeF+2 |
| | 0.583 | FeCl+2 |
| | 76.995 | FeSO4+ |
| | 7.016 | Fe(SO4)2- |
| | 0.014 | FeN3+2 |
| | 0.014 | FeH2PO4+2 |
| | 0.014 | FeHPO4+ |

## B2.7: Eh700

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 83.983 | HgCl2 (aq) |
| | 14.243 | HgCl3-1 |
| | 1.721 | HgCl4-2 |
| | 0.051 | HgN3+ |
| NH4+1 | 94.028 | NH4+1 |
| | 5.972 | NH4SO4- |
| Cl-1 | 98.227 | Cl-1 |
| | 0.571 | CaCl+ |
| | 0.791 | MgCl+ |
| | 0.392 | NaCl (aq) |
| Pb+2 | 40.379 | Pb+2 |
| | 0.752 | Pb DOM1 |
| | 8.268 | PbCl+ |
| | 0.174 | PbCl2 (aq) |
| | 45.836 | PbSO4 (aq) |
| | 4.588 | Pb(SO4)2-2 |
| Zn+2 | 62.648 | Zn+2 |
| | 0.025 | Zn DOM1 |
| | 1.161 | ZnCl+ |
| | 31.23 | ZnSO4 (aq) |
| | 4.928 | Zn(SO4)2-2 |
| F-1 | 0.07 | F-1 |
| | 1.459 | HF (aq) |
| | 98.168 | AlF+2 |
| | 0.275 | AlF2+ |
| | 0.015 | FeF+2 |
| | 0.01 | MgF+ |
| SO4-2 | 41.761 | SO4-2 |
| | 31.336 | HSO4- |
| | 8.366 | AlSO4+ |
| | 4.369 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.011 | NiSO4 (aq) |
| | 0.027 | FeSO4+ |
| | 5.399 | MgSO4 (aq) |
| | 7.64 | CaSO4 (aq) |
| | 0.974 | NaSO4- |
| | 0.027 | KSO4- |
| | 0.059 | NH4SO4- |
| Ni+2 | 69.971 | Ni+2 |
| | 0.016 | Ni DOM1 |
| | 0.161 | NiCl+ |
| | 29.834 | NiSO4 (aq) |
| | 0.018 | Ni(SO4)2-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| N3-1 | 0.114 | N3-1 |
| | 99.881 | HN3 (aq) |
| PO4-3 | 30.83 | H2PO4- |
| | 66.884 | H3PO4 |
| | 0.016 | FeH2PO4+ |
| | 0.105 | FeH2PO4+2 |
| | 0.099 | FeHPO4+ |
| | 1.475 | CaH2PO4+ |
| | 0.225 | AlHPO4+ |
| | 0.355 | NaH2PO4 (aq) |
| AsO4-3 | 75.198 | H3AsO4 |
| | 24.802 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 17.323 | DOM1 |
| | 78.193 | H DOM1 |
| | 2.637 | Al DOM1 |
| | 0.513 | Ca DOM1 |
| | 1.282 | Fe DOM1 |
| | 0.045 | Mg DOM1 |
| Ca+2 | 64.449 | Ca+2 |
| | 1.085 | CaCl+ |
| | 34.459 | CaSO4 (aq) |
| Mg+2 | 67.771 | Mg+2 |
| | 1.872 | MgCl+ |
| | 30.357 | MgSO4 (aq) |
| K+1 | 96.116 | K+1 |
| | 0.498 | KCl (aq) |
| | 3.386 | KSO4- |
| Na+1 | 96.241 | Na+1 |
| | 0.545 | NaCl (aq) |
| | 3.214 | NaSO4- |
| CO3-2 | 99.998 | H2CO3* (aq) |
| Al+3 | 8.461 | Al+3 |
| | 0.066 | Al DOM1 |
| | 0.269 | AlF+2 |
| | 0.022 | AlCl+2 |
| | 72.302 | AlSO4+ |
| | 18.879 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.075 | Cd+2 |
| | 0.011 | Cd DOM1 |
| | 26.665 | CdCl+ |
| | 1.081 | CdCl2 (aq) |
| | 21.682 | CdSO4 (aq) |
| | 5.488 | Cd(SO4)2-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| CrO4-2 | 91.112 | HCrO4- |
| | 0.582 | H2CrO4 (aq) |
| | 0.172 | CrO3Cl- |
| | 8.117 | CrO3SO4-2 |
| Cu+2 | 64.849 | Cu+2 |
| | 0.649 | Cu DOM1 |
| | 0.799 | CuCl+ |
| | 32.687 | CuSO4 (aq) |
| | 1.013 | CuHSO4+ |
| Fe+2 | 64.523 | Fe+2 |
| | 0.278 | FeCl+ |
| | 35.192 | FeSO4 (aq) |
| NO2-1 | 4 | NO2-1 |
| | 95.998 | HNO2 (aq) |
| NO3-1 | 98.962 | NO3-1 |
| | 0.824 | CaNO3+ |
| | 0.014 | KNO3 (aq) |
| | 0.198 | NaNO3 (aq) |
| HS-1 | 99.999 | H2S (aq) |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 4.23 | Fe+3 |
| | 10.427 | Fe DOM1 |
| | 0.611 | FeOH+2 |
| | 0.014 | FeF+2 |
| | 0.581 | FeCl+2 |
| | 77.079 | FeSO4+ |
| | 7.014 | Fe(SO4)2- |
| | 0.014 | FeN3+2 |
| | 0.014 | FeH2PO4+2 |
| | 0.013 | FeHPO4+ |

## B2.8: Eh 800

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 83.989 | HgCl2 (aq) |
| | 14.242 | HgCl3-1 |
| | 1.721 | HgCl4-2 |
| | 0.047 | HgN3+ |
| NH4+1 | 94.065 | NH4+1 |
| | 5.935 | NH4SO4- |
| Cl-1 | 98.225 | Cl-1 |
| | 0.572 | CaCl+ |
| | 0.793 | MgCl+ |
| | 0.392 | NaCl (aq) |
| Pb+2 | 40.499 | Pb+2 |
| | 0.741 | Pb DOM1 |
| | 8.289 | PbCl+ |
| | 0.175 | PbCl2 (aq) |
| | 45.663 | PbSO4 (aq) |
| | 4.543 | Pb(SO4)2-2 |
| | 0.031 | PbNO2+ |
| | 0.057 | PbNO3+ |
| Zn+2 | 62.809 | Zn+2 |
| | 0.025 | Zn DOM1 |
| | 1.164 | ZnCl+ |
| | 31.1 | ZnSO4 (aq) |
| | 4.878 | Zn(SO4)2-2 |
| | 0.017 | ZnNO3+ |
| F-1 | 0.07 | F-1 |
| | 1.476 | HF (aq) |
| | 98.153 | AlF+2 |
| | 0.273 | AlF2+ |
| | 0.016 | FeF+2 |
| SO4-2 | 41.51 | SO4-2 |
| | 31.735 | HSO4- |
| | 8.371 | AlSO4+ |
| | 4.344 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.01 | NiSO4 (aq) |
| | 0.029 | FeSO4+ |
| | 5.374 | MgSO4 (aq) |
| | 7.605 | CaSO4 (aq) |
| | 0.968 | NaSO4- |
| | 0.027 | KSO4- |
| Ni+2 | 70.098 | Ni+2 |
| | 0.016 | Ni DOM1 |
| | 0.161 | NiCl+ |
| | 29.687 | NiSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.018 | Ni(SO4)2-2 |
| | 0.016 | NiNO3+ |
| N3-1 | 0.112 | N3-1 |
| | 99.883 | HN3 (aq) |
| PO4-3 | 30.444 | H2PO4- |
| | 67.305 | H3PO4 |
| | 0.109 | FeH2PO4+2 |
| | 0.101 | FeHPO4+ |
| | 1.459 | CaH2PO4+ |
| | 0.22 | AlHPO4+ |
| | 0.35 | NaH2PO4 (aq) |
| AsO4-3 | 75.549 | H3AsO4 |
| | 24.451 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 17.213 | DOM1 |
| | 78.297 | H DOM1 |
| | 2.608 | Al DOM1 |
| | 0.504 | Ca DOM1 |
| | 1.326 | Fe DOM1 |
| | 0.044 | Mg DOM1 |
| Ca+2 | 64.584 | Ca+2 |
| | 1.086 | CaCl+ |
| | 34.3 | CaSO4 (aq) |
| | 0.023 | CaNO3+ |
| Mg+2 | 67.908 | Mg+2 |
| | 1.875 | MgCl+ |
| | 30.216 | MgSO4 (aq) |
| K+1 | 96.127 | K+1 |
| | 0.498 | KCl (aq) |
| | 3.365 | KSO4- |
| | 0.01 | KNO3 (aq) |
| Na+1 | 96.257 | Na+1 |
| | 0.545 | NaCl (aq) |
| | 3.194 | NaSO4- |
| CO3-2 | 99.998 | H2CO3* (aq) |
| Al+3 | 8.524 | Al+3 |
| | 0.065 | Al DOM1 |
| | 0.269 | AlF+2 |
| | 0.022 | AlCl+2 |
| | 72.349 | AlSO4+ |
| | 18.77 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.165 | Cd+2 |
| | 0.01 | Cd DOM1 |
| | 26.706 | CdCl+ |

| Component | % of total concentration | Species name |
|---|---|---|
| | 1.082 | CdCl2 (aq) |
| | 21.579 | CdSO4 (aq) |
| | 5.428 | Cd(SO4)2-2 |
| | 0.011 | CdNO2+ |
| | 0.018 | CdNO3+ |
| CrO4-2 | 91.004 | HCrO4- |
| | 0.592 | H2CrO4 (aq) |
| | 0.175 | CrO3Cl- |
| | 8.212 | CrO3SO4-2 |
| Cu+2 | 64.967 | Cu+2 |
| | 0.639 | Cu DOM1 |
| | 0.8 | CuCl+ |
| | 32.526 | CuSO4 (aq) |
| | 1.028 | CuHSO4+ |
| | 0.017 | CuNO2+ |
| | 0.022 | CuNO3+ |
| Fe+2 | 64.677 | Fe+2 |
| | 0.279 | FeCl+ |
| | 35.038 | FeSO4 (aq) |
| NO2-1 | 3.928 | NO2-1 |
| | 96.07 | HNO2 (aq) |
| NO3-1 | 98.96 | NO3-1 |
| | 0.825 | CaNO3+ |
| | 0.014 | KNO3 (aq) |
| | 0.198 | NaNO3 (aq) |
| HS-1 | 99.999 | H2S (aq) |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 4.264 | Fe+3 |
| | 10.32 | Fe DOM1 |
| | 0.605 | FeOH+2 |
| | 0.014 | FeF+2 |
| | 0.586 | FeCl+2 |
| | 77.175 | FeSO4+ |
| | 6.978 | Fe(SO4)2- |
| | 0.016 | FeNO2+2 |
| | 0.014 | FeN3+2 |
| | 0.014 | FeH2PO4+2 |
| | 0.013 | FeHPO4+ |

## B2.9: Eh 900

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 83.989 | HgCl2 (aq) |
| | 14.242 | HgCl3-1 |
| | 1.722 | HgCl4-2 |
| | 0.046 | HgN3+ |
| NH4+1 | 94.075 | NH4+1 |
| | 5.925 | NH4SO4- |
| Cl-1 | 98.225 | Cl-1 |
| | 0.573 | CaCl+ |
| | 0.793 | MgCl+ |
| | 0.392 | NaCl (aq) |
| Pb+2 | 40.547 | Pb+2 |
| | 0.738 | Pb DOM1 |
| | 8.296 | PbCl+ |
| | 0.175 | PbCl2 (aq) |
| | 45.617 | PbSO4 (aq) |
| | 4.532 | Pb(SO4)2-2 |
| | 0.093 | PbNO3+ |
| Zn+2 | 62.856 | Zn+2 |
| | 0.024 | Zn DOM1 |
| | 1.164 | ZnCl+ |
| | 31.056 | ZnSO4 (aq) |
| | 4.864 | Zn(SO4)2-2 |
| | 0.027 | ZnNO3+ |
| F-1 | 0.069 | F-1 |
| | 1.479 | HF (aq) |
| | 98.151 | AlF+2 |
| | 0.272 | AlF2+ |
| | 0.016 | FeF+2 |
| SO4-2 | 41.456 | SO4-2 |
| | 31.816 | HSO4- |
| | 8.372 | AlSO4+ |
| | 4.336 | Al(SO4)2- |
| | 0.017 | ZnSO4 (aq) |
| | 0.01 | NiSO4 (aq) |
| | 0.029 | FeSO4+ |
| | 5.366 | MgSO4 (aq) |
| | 7.593 | CaSO4 (aq) |
| | 0.966 | NaSO4- |
| | 0.027 | KSO4- |
| Ni+2 | 70.139 | Ni+2 |
| | 0.016 | Ni DOM1 |
| | 0.161 | NiCl+ |
| | 29.64 | NiSO4 (aq) |
| | 0.018 | Ni(SO4)2-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.026 | NiNO3+ |
| N3-1 | 0.112 | N3-1 |
| | 99.884 | HN3 (aq) |
| PO4-3 | 30.359 | H2PO4- |
| | 67.395 | H3PO4 |
| | 0.11 | FeH2PO4+2 |
| | 0.102 | FeHPO4+ |
| | 1.455 | CaH2PO4+ |
| | 0.219 | AlHPO4+ |
| | 0.349 | NaH2PO4 (aq) |
| AsO4-3 | 75.625 | H3AsO4 |
| | 24.375 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 17.191 | DOM1 |
| | 78.318 | H DOM1 |
| | 2.602 | Al DOM1 |
| | 0.502 | Ca DOM1 |
| | 1.335 | Fe DOM1 |
| | 0.044 | Mg DOM1 |
| Ca+2 | 64.622 | Ca+2 |
| | 1.087 | CaCl+ |
| | 34.248 | CaSO4 (aq) |
| | 0.037 | CaNO3+ |
| Mg+2 | 67.952 | Mg+2 |
| | 1.876 | MgCl+ |
| | 30.172 | MgSO4 (aq) |
| K+1 | 96.126 | K+1 |
| | 0.498 | KCl (aq) |
| | 3.359 | KSO4- |
| | 0.017 | KNO3 (aq) |
| Na+1 | 96.26 | Na+1 |
| | 0.545 | NaCl (aq) |
| | 3.188 | NaSO4- |
| CO3-2 | 99.998 | H2CO3* (aq) |
| Al+3 | 8.544 | Al+3 |
| | 0.065 | Al DOM1 |
| | 0.269 | AlF+2 |
| | 0.022 | AlCl+2 |
| | 72.359 | AlSO4+ |
| | 18.739 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.2 | Cd+2 |
| | 0.01 | Cd DOM1 |
| | 26.716 | CdCl+ |
| | 1.082 | CdCl2 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 21.549 | CdSO4 (aq) |
| | 5.413 | Cd(SO4)2-2 |
| | 0.029 | CdNO3+ |
| CrO4-2 | 90.98 | HCrO4- |
| | 0.595 | H2CrO4 (aq) |
| | 0.176 | CrO3Cl- |
| | 8.232 | CrO3SO4-2 |
| Cu+2 | 65.016 | Cu+2 |
| | 0.636 | Cu DOM1 |
| | 0.8 | CuCl+ |
| | 32.48 | CuSO4 (aq) |
| | 1.031 | CuHSO4+ |
| | 0.035 | CuNO3+ |
| Fe+2 | 64.726 | Fe+2 |
| | 0.279 | FeCl+ |
| | 34.989 | FeSO4 (aq) |
| NO2-1 | 3.913 | NO2-1 |
| | 96.085 | HNO2 (aq) |
| NO3-1 | 98.96 | NO3-1 |
| | 0.826 | CaNO3+ |
| | 0.014 | KNO3 (aq) |
| | 0.198 | NaNO3 (aq) |
| HS-1 | 99.999 | H2S (aq) |
| H3AsO3 | 100 | H3AsO3 |
| Fe+3 | 4.276 | Fe+3 |
| | 10.298 | Fe DOM1 |
| | 0.604 | FeOH+2 |
| | 0.014 | FeF+2 |
| | 0.587 | FeCl+2 |
| | 77.21 | FeSO4+ |
| | 6.969 | Fe(SO4)2- |
| | 0.014 | FeN3+2 |
| | 0.014 | FeH2PO4+2 |
| | 0.013 | FeHPO4+ |

# B3 Saturation indicies

## B3.1: Eh 100

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 5.941 | -5.534 |
| Al(OH)3 (Soil) | 5.941 | -2.987 |
| Al2O3(s) | 11.885 | -9.34 |
| Al4(OH)10SO4(s) | 14.593 | -8.107 |
| AlAsO4:2H2O(s) | -29.685 | -13.885 |
| AlOHF2(s) | -16.542 | -16.949 |
| AlOHSO4(s) | -3.23 | 0 |
| Alunite | -0.646 | -0.523 |
| Anglesite | -10.402 | -2.539 |
| Anhydrite | -4.799 | -0.483 |
| Antlerite | -29.401 | -38.189 |
| Aragonite | -15.477 | -7.198 |
| Arsenolite | -10.584 | -9.021 |
| Artinite | -11.223 | -21.554 |
| As2O5(s) | -71.252 | -36.543 |
| As2S3(am) | -61.99 | -15.605 |
| Atacamite | -18.709 | -26.668 |
| Azurite | -59.928 | -42.774 |
| Bianchite | -7.446 | -5.685 |
| Birnessite | 10.628 | -7.463 |
| Bixbyite | 10.76 | 10.647 |
| Boehmite | 5.942 | -3.352 |
| Brochantite | -36.145 | -52.6 |
| Brucite | 4.315 | -13.479 |
| Ca3(AsO4)2:4H2O(s) | -58.137 | -39.237 |
| Ca3(PO4)2 (am1) | -46.06 | -21.132 |
| Ca3(PO4)2 (am2) | -46.06 | -18.339 |
| Ca3(PO4)2 (beta) | -46.06 | -16.812 |
| Ca4H(PO4)3:3H2O(s) | -71.28 | -23.969 |
| CaCO3xH2O(s) | -15.478 | -8.391 |
| CaCrO4(s) | -12.092 | -9.99 |
| CaHPO4(s) | -25.217 | -5.754 |
| CaHPO4:2H2O(s) | -25.219 | -6.084 |
| Calcite | -15.477 | -7.046 |
| CaS(s) | -12.762 | -23.942 |
| Cd metal (alpha) | -12.613 | -26.586 |
| Cd metal (gamma) | -12.613 | -26.693 |
| Cd(OH)2(s) | -2.117 | -16.336 |
| Cd3(OH)4SO4(s) | -15.522 | -38.082 |
| Cd3(PO4)2(s) | -65.527 | -32.927 |
| Cd3OH2(SO4)2(s) | -24.693 | -31.403 |
| Cd4(OH)6SO4(s) | -17.639 | -46.039 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CdCl2(s) | -12.561 | -12.016 |
| CdCl2:1H2O(s) | -12.562 | -10.915 |
| CdCl2:2.5H2O(s) | -12.564 | -10.607 |
| CdF2(s) | -24.6 | -23.668 |
| CdOHCl(s) | -7.339 | -11.065 |
| CdSO4(s) | -11.288 | -11.432 |
| CdSO4:1H2O(s) | -11.289 | -9.755 |
| CdSO4:2.67H2O(s) | -11.291 | -9.527 |
| Cerrusite | -21.079 | -7.729 |
| Chalcanthite | -15.919 | -13.243 |
| Chalcopyrite | -36.173 | 0 |
| Chloropyromorphite(c) | -100.14 | -15.71 |
| Chloropyromorphite(soil) | -100.14 | -19.74 |
| Cinnabar | -46.424 | 0.399 |
| Claudetite | -10.584 | -9.071 |
| Cotunnite | -11.675 | -6.736 |
| Covellite | -23.878 | -1.068 |
| Cr(VI)-Ettringite | -11.303 | -74.704 |
| Cr(VI)-Jarosite | -42.666 | -24.15 |
| CrO3(s) | -16.465 | -13.286 |
| Cryolite | -57.097 | -23.026 |
| Cu azide | -24.81 | -16.969 |
| Cu(OH)2(s) | -6.743 | -16.356 |
| Cu2(OH)3NO3(s) | -95.394 | -105.086 |
| Cu3(AsO4)2:2H2O(s) | -91.481 | -56.381 |
| Cu3(PO4)2(s) | -79.406 | -42.556 |
| Cu3(PO4)2:3H2O(s) | -79.409 | -44.289 |
| CuCO3(s) | -26.592 | -15.092 |
| CuCrO4(s) | -23.207 | -17.767 |
| CuF2(s) | -29.226 | -30.748 |
| CuF2:2H2O(s) | -29.228 | -24.771 |
| CuOCuSO4(s) | -22.657 | -33.798 |
| Cupric Ferrite | -13.148 | -20.414 |
| CuSO4(s) | -15.914 | -19.298 |
| Diaspore | 5.942 | -1.558 |
| Dolomite (disordered) | -31.011 | -14.753 |
| Dolomite (ordered) | -31.011 | -14.161 |
| Epsomite | -4.863 | -2.667 |
| Ettringite | 10.575 | -48.613 |
| FCO3-Apatite | -151.84 | -36.438 |
| Fe(OH)2 (am) | 4.839 | -9.208 |
| Fe(OH)2 (c) | 4.839 | -8.051 |
| Fe(OH)2.7Cl.3(s) | -4.771 | -1.731 |
| Fe2(SO4)3(s) | -33.921 | -31.658 |
| Fe3(OH)8(s) | -1.569 | -21.791 |
| FeAsO4:2H2O(s) | -38.83 | -18.63 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ferrihydrite | -3.204 | -7.014 |
| Ferrihydrite (aged) | -3.204 | -6.504 |
| FeS (ppt) | -12.295 | -9.412 |
| Fluorite | -18.111 | -7.538 |
| Galena | -18.365 | -2.959 |
| Gibbsite (C) | 5.941 | -2.437 |
| Goethite | -3.203 | -4.062 |
| Goslarite | -7.447 | -5.35 |
| Greenockite | -19.251 | -4.897 |
| Greigite | -70.106 | -25.071 |
| Gypsum | -4.801 | -0.185 |
| Halite | -3.752 | -5.28 |
| Hematite | -6.405 | -5.771 |
| Hercynite | 16.725 | -8.076 |
| Hg(OH)2(s) | -29.29 | -25.794 |
| Hg3O2CO3(s) | -107.717 | -78.137 |
| HgCl2(s) | -39.735 | -17.817 |
| HgSO4(s) | -38.461 | -28.953 |
| Hinsdalite | -22.167 | -19.667 |
| H-Jarosite | -27.956 | -23.923 |
| Huntite | -62.079 | -32.766 |
| Hydrocerrusite | -43.389 | -24.629 |
| Hydromagnesite | -57.826 | -50.388 |
| Hydroxyapatite | -66.904 | -22.571 |
| Hydroxylpyromorphite | -94.917 | -32.127 |
| Hydrozincite | -31.044 | -41.182 |
| K2Cr2O7(s) | -33.182 | -15.448 |
| K2CrO4(s) | -16.717 | -16.093 |
| K-Alum | -12.54 | -7.186 |
| KCl(s) | -5.349 | -6.249 |
| K-Jarosite | -28.081 | -17.7 |
| Langite | -36.146 | -54.641 |
| Larnakite | -11.631 | -11.33 |
| Laurionite | -6.453 | -7.076 |
| Lepidocrocite | -3.203 | -4.574 |
| Lime | 4.373 | -29.505 |
| Litharge | -1.23 | -14.318 |
| Mackinawite | -12.295 | -8.695 |
| Maghemite | -6.405 | -12.791 |
| Magnesioferrite | -2.09 | -20.645 |
| Magnesite | -15.534 | -7.953 |
| Magnetite | -1.565 | -6.235 |
| Malachite | -33.335 | -28.135 |
| Massicot | -1.23 | -14.526 |
| Matlockite | -17.694 | -8.519 |
| Melanothallite | -17.188 | -23.831 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Melanterite | -4.338 | -2.005 |
| Metacinnabar | -46.424 | 0 |
| Mg(OH)2 (active) | 4.315 | -14.479 |
| Mg2(OH)3Cl:4H2O(s) | 3.403 | -22.597 |
| Mg3(PO4)2(s) | -46.233 | -22.953 |
| MgCO3:5H2O(s) | -15.539 | -10.999 |
| MgCrO4(s) | -12.149 | -18.07 |
| MgF2(s) | -18.168 | -10.107 |
| MgHPO4:3H2O(s) | -25.278 | -7.103 |
| MgS(s) | -12.82 | -30.5 |
| Minium | 6.808 | -69.278 |
| Mirabilite | -6.241 | -4.644 |
| Mn2(SO4)3(s) | -16.756 | -12.039 |
| Montroydite | -29.289 | -25.572 |
| Morenosite | -7.616 | -5.397 |
| Na2Cr2O7(s) | -29.988 | -19.958 |
| Na2CrO4(s) | -13.523 | -16.573 |
| NaF(s) | -9.771 | -9.276 |
| Na-Jarosite | -26.484 | -21.989 |
| Natron | -16.918 | -15.207 |
| Nesquehonite | -15.537 | -11.014 |
| Ni(OH)2 (am) | 1.562 | -11.912 |
| Ni(OH)2 (c) | 1.562 | -9.228 |
| Ni3(AsO4)2:8H2O(s) | -66.571 | -41.071 |
| Ni3(PO4)2(s) | -54.491 | -23.191 |
| Ni4(OH)6SO4(s) | -2.924 | -34.924 |
| NiCO3(s) | -18.287 | -7.34 |
| NiS (alpha) | -15.572 | -10.052 |
| NiS (beta) | -15.572 | -4.552 |
| NiS (gamma) | -15.572 | -2.852 |
| Nsutite | 10.628 | -6.876 |
| Orpiment | -61.99 | -14.09 |
| Otavite | -21.966 | -9.914 |
| Pb azide (alpha) | -19.297 | -10.323 |
| Pb metal | -11.727 | -15.967 |
| Pb(OH)2(s) | -1.231 | -9.737 |
| Pb10(OH)6O(CO3)6(s) | -131.397 | -122.637 |
| Pb2(OH)3Cl(s) | -7.684 | -16.477 |
| Pb2O(OH)2(s) | -2.46 | -28.65 |
| Pb2O3(s) | 8.038 | -53.002 |
| Pb2OCO3(s) | -22.309 | -21.999 |
| Pb3(AsO4)2(s) | -74.941 | -39.441 |
| Pb3(PO4)2(s) | -62.868 | -19.338 |
| Pb3O2CO3(s) | -23.539 | -35.231 |
| Pb3O2SO4(s) | -12.861 | -24.028 |
| Pb4(OH)6SO4(s) | -14.093 | -35.193 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb4O3SO4(s) | -14.091 | -36.797 |
| PbCrO4(s) | -17.694 | -4.826 |
| PbF2(s) | -23.713 | -16.152 |
| PbHPO4(s) | -30.82 | -7.015 |
| PbO:0.3H2O(s) | -1.23 | -14.21 |
| Periclase | 4.316 | -18.188 |
| Phosgenite | -32.755 | -12.945 |
| Plattnerite | 9.268 | -42.134 |
| Plumbgummite | -42.585 | -9.795 |
| Portlandite | 4.372 | -19.114 |
| Pyrite | -18.933 | -0.122 |
| Realgar | -27.676 | -6.946 |
| Retgersite | -7.615 | -5.547 |
| Siderite | -15.009 | -4.464 |
| Smithsonite | -18.118 | -7.241 |
| Spharelite | -15.404 | -4.401 |
| Spinel | 16.2 | -23.006 |
| Strengite | -32.794 | -6.451 |
| Struvite | -25.324 | -12.064 |
| Sulfur | -6.638 | -4.592 |
| Tenorite(am) | -6.742 | -15.627 |
| Tenorite(c) | -6.742 | -14.777 |
| Thenardite | -6.231 | -6.608 |
| Thermonatrite | -16.909 | -17.61 |
| Tsumebite | -38.796 | -29.006 |
| Vaterite | -15.477 | -7.64 |
| Vivianite | -44.666 | -6.875 |
| Wurtzite | -15.404 | -6.655 |
| Zincite | 1.732 | -10.043 |
| Zincosite | -7.44 | -11.872 |
| Zn metal | -8.766 | -35.487 |
| Zn(NO3)2:6H2O(s) | -162.089 | -165.255 |
| Zn(OH)2 (am) | 1.731 | -11.264 |
| Zn(OH)2 (beta) | 1.731 | -10.529 |
| Zn(OH)2 (delta) | 1.731 | -10.113 |
| Zn(OH)2 (epsilon) | 1.731 | -10.281 |
| Zn(OH)2 (gamma) | 1.731 | -10.501 |
| Zn2(OH)2SO4(s) | -5.71 | -13.21 |
| Zn2(OH)3Cl(s) | -1.761 | -16.952 |
| Zn3(PO4)2:4H2O(s) | -53.988 | -18.568 |
| Zn3AsO42:2.5H2O(s) | -66.059 | -38.559 |
| Zn3O(SO4)2(s) | -13.149 | -33.632 |
| Zn4(OH)6SO4(s) | -2.248 | -30.648 |
| Zn5(OH)8Cl2(s) | -1.791 | -40.291 |
| Zn-Al LDH(s) | -0.522 | -20.352 |
| ZnCl2(s) | -8.714 | -16.205 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| ZnCO3(s) | -18.118 | -7.318 |
| ZnCO3:1H2O(s) | -18.119 | -7.859 |
| ZnF2(s) | -20.752 | -20.581 |
| ZnSO4:1H2O(s) | -7.441 | -7.071 |

## B3.2: Eh 200

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 5.348 | -6.127 |
| Al(OH)3 (Soil) | 5.348 | -3.58 |
| Al2O3(s) | 10.699 | -10.526 |
| Al4(OH)10SO4(s) | 12.814 | -9.886 |
| AlAsO4:2H2O(s) | -27.38 | -11.58 |
| AlOHF2(s) | -17.149 | -17.556 |
| AlOHSO4(s) | -3.23 | 0 |
| Alunite | -1.539 | -1.416 |
| Anglesite | -10.384 | -2.521 |
| Anhydrite | -4.804 | -0.488 |
| Antlerite | -12.587 | -21.375 |
| Aragonite | -16.075 | -7.796 |
| Arsenolite | -10.584 | -9.021 |
| Artinite | -12.42 | -22.751 |
| As2O5(s) | -65.455 | -30.746 |
| As2S3(am) | -94.989 | -48.604 |
| Atacamite | -7.596 | -15.555 |
| Azurite | -43.705 | -26.552 |
| Bianchite | -7.451 | -5.69 |
| Birnessite | 11.174 | -6.917 |
| Bixbyite | 8.953 | 8.841 |
| Boehmite | 5.349 | -3.945 |
| Brochantite | -13.923 | -30.378 |
| Brucite | 3.716 | -14.077 |
| Ca3(AsO4)2:4H2O(s) | -54.135 | -35.235 |
| Ca3(PO4)2 (am1) | -47.265 | -22.337 |
| Ca3(PO4)2 (am2) | -47.265 | -19.544 |
| Ca3(PO4)2 (beta) | -47.265 | -18.017 |
| Ca4H(PO4)3:3H2O(s) | -72.788 | -25.477 |
| CaCO3xH2O(s) | -16.076 | -8.989 |
| CaCrO4(s) | -12.391 | -10.289 |
| CaHPO4(s) | -25.52 | -6.057 |
| CaHPO4:2H2O(s) | -25.522 | -6.387 |
| Calcite | -16.075 | -7.644 |
| CaS(s) | -24.361 | -35.541 |
| Cd metal (alpha) | -16.11 | -30.082 |
| Cd metal (gamma) | -16.11 | -30.189 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cd(OH)2(s) | -2.715 | -16.934 |
| Cd3(OH)4SO4(s) | -16.723 | -39.283 |
| Cd3(PO4)2(s) | -66.731 | -34.131 |
| Cd3OH2(SO4)2(s) | -25.301 | -32.011 |
| Cd4(OH)6SO4(s) | -19.439 | -47.839 |
| CdCl2(s) | -12.561 | -12.016 |
| CdCl2:1H2O(s) | -12.562 | -10.915 |
| CdCl2:2.5H2O(s) | -12.564 | -10.607 |
| CdF2(s) | -25.212 | -24.281 |
| CdOHCl(s) | -7.638 | -11.364 |
| CdSO4(s) | -11.293 | -11.437 |
| CdSO4:1H2O(s) | -11.294 | -9.76 |
| CdSO4:2.67H2O(s) | -11.296 | -9.532 |
| Cerrusite | -21.654 | -8.304 |
| Chalcanthite | -9.919 | -7.243 |
| Chalcopyrite | -53.364 | -17.191 |
| Chloropyromorphite(c) | -101.833 | -17.403 |
| Chloropyromorphite(soil) | -101.833 | -21.433 |
| Cinnabar | -52.816 | -5.993 |
| Claudetite | -10.584 | -9.071 |
| Cotunnite | -11.652 | -6.713 |
| Covellite | -29.47 | -6.661 |
| Cr(VI)-Ettringite | -15.181 | -78.582 |
| Cr(VI)-Jarosite | -39.817 | -21.3 |
| CrO3(s) | -16.165 | -12.986 |
| Cryolite | -58.633 | -24.562 |
| Cu azide | -19.369 | -11.528 |
| Cu(OH)2(s) | -1.336 | -10.949 |
| Cu2(OH)3NO3(s) | -73.287 | -82.979 |
| Cu3(AsO4)2:2H2O(s) | -69.463 | -34.363 |
| Cu3(PO4)2(s) | -62.595 | -25.745 |
| Cu3(PO4)2:3H2O(s) | -62.598 | -27.478 |
| CuCO3(s) | -21.184 | -9.684 |
| CuCrO4(s) | -17.5 | -12.06 |
| CuF2(s) | -23.833 | -25.355 |
| CuF2:2H2O(s) | -23.835 | -19.378 |
| CuOCuSO4(s) | -11.25 | -22.39 |
| Cupric Ferrite | -6.04 | -13.306 |
| CuSO4(s) | -9.914 | -13.298 |
| Diaspore | 5.349 | -2.151 |
| Dolomite (disordered) | -32.207 | -15.949 |
| Dolomite (ordered) | -32.207 | -15.357 |
| Epsomite | -4.869 | -2.672 |
| Ettringite | 7.578 | -51.611 |
| FCO3-Apatite | -156.209 | -40.807 |
| Fe(OH)2 (am) | 4.241 | -9.806 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe(OH)2 (c) | 4.241 | -8.649 |
| Fe(OH)2.7Cl.3(s) | -3.831 | -0.791 |
| Fe2(SO4)3(s) | -30.441 | -28.178 |
| Fe3(OH)8(s) | -0.467 | -20.689 |
| FeAsO4:2H2O(s) | -35.082 | -14.882 |
| Ferrihydrite | -2.354 | -6.164 |
| Ferrihydrite (aged) | -2.354 | -5.654 |
| FeS (ppt) | -23.893 | -21.01 |
| Fluorite | -18.723 | -8.15 |
| Galena | -29.94 | -14.534 |
| Gibbsite (C) | 5.348 | -3.03 |
| Goethite | -2.353 | -3.212 |
| Goslarite | -7.452 | -5.354 |
| Greenockite | -30.849 | -16.495 |
| Greigite | -113.003 | -67.968 |
| Gypsum | -4.806 | -0.19 |
| Halite | -3.753 | -5.281 |
| Hematite | -4.704 | -4.071 |
| Hercynite | 14.94 | -9.861 |
| Hg(OH)2(s) | -24.682 | -21.185 |
| Hg3O2CO3(s) | -93.891 | -64.311 |
| HgCl2(s) | -34.528 | -12.61 |
| HgSO4(s) | -33.259 | -23.751 |
| Hinsdalite | -23.633 | -21.133 |
| H-Jarosite | -24.219 | -20.186 |
| Huntite | -64.472 | -35.159 |
| Hydrocerrusite | -45.115 | -26.355 |
| Hydromagnesite | -60.818 | -53.38 |
| Hydroxyapatite | -69.011 | -24.678 |
| Hydroxylpyromorphite | -96.91 | -34.12 |
| Hydrozincite | -34.031 | -44.169 |
| K2Cr2O7(s) | -33.184 | -15.45 |
| K2CrO4(s) | -17.019 | -16.394 |
| K-Alum | -12.247 | -6.893 |
| KCl(s) | -5.35 | -6.25 |
| K-Jarosite | -24.644 | -14.263 |
| Langite | -13.924 | -32.419 |
| Larnakite | -12.19 | -11.888 |
| Laurionite | -6.729 | -7.352 |
| Lepidocrocite | -2.353 | -3.724 |
| Lime | 3.775 | -30.104 |
| Litharge | -1.805 | -14.894 |
| Mackinawite | -23.893 | -20.293 |
| Maghemite | -4.704 | -11.09 |
| Magnesioferrite | -0.988 | -19.543 |
| Magnesite | -16.132 | -8.551 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Magnetite | -0.463 | -5.133 |
| Malachite | -22.521 | -17.32 |
| Massicot | -1.805 | -15.102 |
| Matlockite | -17.978 | -8.803 |
| Melanothallite | -11.182 | -17.825 |
| Melanterite | -4.344 | -2.011 |
| Metacinnabar | -52.816 | -6.391 |
| Mg(OH)2 (active) | 3.716 | -15.078 |
| Mg2(OH)3Cl:4H2O(s) | 2.504 | -23.496 |
| Mg3(PO4)2(s) | -47.439 | -24.159 |
| MgCO3:5H2O(s) | -16.137 | -11.597 |
| MgCrO4(s) | -12.448 | -18.369 |
| MgF2(s) | -18.781 | -10.72 |
| MgHPO4:3H2O(s) | -25.581 | -7.406 |
| MgS(s) | -24.418 | -42.098 |
| Minium | 7.979 | -68.107 |
| Mirabilite | -6.248 | -4.651 |
| Mn2(SO4)3(s) | -16.784 | -12.066 |
| Montroydite | -24.681 | -20.964 |
| Morenosite | -7.622 | -5.403 |
| Na2Cr2O7(s) | -29.989 | -19.959 |
| Na2CrO4(s) | -13.824 | -16.874 |
| NaF(s) | -10.079 | -9.584 |
| Na-Jarosite | -23.047 | -18.552 |
| Natron | -17.518 | -15.807 |
| Nesquehonite | -16.135 | -11.613 |
| Ni(OH)2 (am) | 0.963 | -12.51 |
| Ni(OH)2 (c) | 0.963 | -9.827 |
| Ni3(AsO4)2:8H2O(s) | -62.571 | -37.071 |
| Ni3(PO4)2(s) | -55.696 | -24.396 |
| Ni4(OH)6SO4(s) | -4.725 | -36.725 |
| NiCO3(s) | -18.885 | -7.938 |
| NiS (alpha) | -27.171 | -21.651 |
| NiS (beta) | -27.171 | -16.151 |
| NiS (gamma) | -27.171 | -14.451 |
| Nsutite | 11.174 | -6.33 |
| Orpiment | -94.989 | -47.089 |
| Otavite | -22.563 | -10.512 |
| Pb azide (alpha) | -19.839 | -10.865 |
| Pb metal | -15.201 | -19.441 |
| Pb(OH)2(s) | -1.806 | -10.312 |
| Pb10(OH)6O(CO3)6(s) | -137.151 | -128.391 |
| Pb2(OH)3Cl(s) | -8.536 | -17.329 |
| Pb2O(OH)2(s) | -3.612 | -29.802 |
| Pb2O3(s) | 9.785 | -51.255 |
| Pb2OCO3(s) | -23.46 | -23.15 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb3(AsO4)2(s) | -70.871 | -35.371 |
| Pb3(PO4)2(s) | -64.005 | -20.475 |
| Pb3O2CO3(s) | -25.265 | -36.957 |
| Pb3O2SO4(s) | -13.995 | -25.162 |
| Pb4(OH)6SO4(s) | -15.803 | -36.903 |
| Pb4O3SO4(s) | -15.8 | -38.507 |
| PbCrO4(s) | -17.97 | -5.102 |
| PbF2(s) | -24.303 | -16.742 |
| PbHPO4(s) | -31.1 | -7.295 |
| PbO:0.3H2O(s) | -1.806 | -14.786 |
| Periclase | 3.717 | -18.787 |
| Phosgenite | -33.307 | -13.497 |
| Plattnerite | 11.59 | -39.811 |
| Plumbgummite | -44.349 | -11.559 |
| Portlandite | 3.774 | -19.712 |
| Pyrite | -38.633 | -19.822 |
| Realgar | -40.125 | -19.395 |
| Retgersite | -7.621 | -5.553 |
| Siderite | -15.607 | -5.062 |
| Smithsonite | -18.715 | -7.838 |
| Spharelite | -27.001 | -15.999 |
| Spinel | 14.415 | -24.791 |
| Strengite | -31.649 | -5.306 |
| Struvite | -25.929 | -12.669 |
| Sulfur | -14.74 | -12.694 |
| Tenorite(am) | -1.335 | -10.22 |
| Tenorite(c) | -1.335 | -9.37 |
| Thenardite | -6.238 | -6.615 |
| Thermonatrite | -17.509 | -18.21 |
| Tsumebite | -34.245 | -24.455 |
| Vaterite | -16.075 | -8.238 |
| Vivianite | -45.872 | -8.081 |
| Wurtzite | -27.001 | -18.252 |
| Zincite | 1.134 | -10.641 |
| Zincosite | -7.445 | -11.877 |
| Zn metal | -12.261 | -38.983 |
| Zn(NO3)2:6H2O(s) | -140.102 | -143.268 |
| Zn(OH)2 (am) | 1.133 | -11.861 |
| Zn(OH)2 (beta) | 1.133 | -11.126 |
| Zn(OH)2 (delta) | 1.133 | -10.711 |
| Zn(OH)2 (epsilon) | 1.133 | -10.879 |
| Zn(OH)2 (gamma) | 1.133 | -11.098 |
| Zn2(OH)2SO4(s) | -6.312 | -13.812 |
| Zn2(OH)3Cl(s) | -2.657 | -17.848 |
| Zn3(PO4)2:4H2O(s) | -55.191 | -19.771 |
| Zn3AsO42:2.5H2O(s) | -62.055 | -34.555 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn3O(SO4)2(s) | -13.756 | -34.238 |
| Zn4(OH)6SO4(s) | -4.046 | -32.446 |
| Zn5(OH)8Cl2(s) | -4.181 | -42.681 |
| Zn-Al LDH(s) | -2.31 | -22.14 |
| ZnCl2(s) | -8.713 | -16.204 |
| ZnCO3(s) | -18.715 | -7.915 |
| ZnCO3:1H2O(s) | -18.716 | -8.456 |
| ZnF2(s) | -21.364 | -21.192 |
| ZnSO4:1H2O(s) | -7.446 | -7.076 |

## B3.3: Eh 300

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 4.471 | -7.004 |
| Al(OH)3 (Soil) | 4.471 | -4.457 |
| Al2O3(s) | 8.952 | -12.272 |
| Al4(OH)10SO4(s) | 9.954 | -12.746 |
| AlAsO4:2H2O(s) | -25.377 | -9.577 |
| AlOHF2(s) | -17.497 | -17.904 |
| AlOHSO4(s) | -3.459 | -0.229 |
| Alunite | -3.183 | -3.06 |
| Anglesite | -10.355 | -2.492 |
| Anhydrite | -4.783 | -0.466 |
| Antlerite | -13.784 | -22.572 |
| Aragonite | -16.696 | -8.417 |
| Arsenolite | -10.58 | -9.018 |
| Artinite | -13.672 | -24.003 |
| As2O5(s) | -59.693 | -24.983 |
| As2S3(am) | -127.606 | -81.221 |
| Atacamite | -8.544 | -16.503 |
| Azurite | -45.542 | -28.389 |
| Bianchite | -7.444 | -5.683 |
| Birnessite | 11.698 | -6.393 |
| Bixbyite | 7.122 | 7.009 |
| Boehmite | 4.475 | -4.819 |
| Brochantite | -15.736 | -32.191 |
| Brucite | 3.091 | -14.702 |
| Ca3(AsO4)2:4H2O(s) | -50.253 | -31.353 |
| Ca3(PO4)2 (am1) | -48.357 | -23.428 |
| Ca3(PO4)2 (am2) | -48.357 | -20.635 |
| Ca3(PO4)2 (beta) | -48.357 | -19.108 |
| Ca4H(PO4)3:3H2O(s) | -74.122 | -26.811 |
| CaCO3xH2O(s) | -16.7 | -9.613 |
| CaCrO4(s) | -12.703 | -10.601 |
| CaHPO4(s) | -25.755 | -6.292 |
| CaHPO4:2H2O(s) | -25.762 | -6.627 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Calcite | -16.696 | -8.266 |
| CaS(s) | -35.857 | -47.037 |
| Cd metal (alpha) | -19.602 | -33.575 |
| Cd metal (gamma) | -19.602 | -33.682 |
| Cd(OH)2(s) | -3.33 | -17.55 |
| Cd3(OH)4SO4(s) | -17.922 | -40.482 |
| Cd3(PO4)2(s) | -67.791 | -35.191 |
| Cd3OH2(SO4)2(s) | -25.852 | -32.562 |
| Cd4(OH)6SO4(s) | -21.252 | -49.652 |
| CdCl2(s) | -12.613 | -12.067 |
| CdCl2:1H2O(s) | -12.616 | -10.968 |
| CdCl2:2.5H2O(s) | -12.621 | -10.664 |
| CdF2(s) | -25.299 | -24.368 |
| CdOHCl(s) | -7.972 | -11.697 |
| CdSO4(s) | -11.261 | -11.405 |
| CdSO4:1H2O(s) | -11.264 | -9.73 |
| CdSO4:2.67H2O(s) | -11.27 | -9.506 |
| Cerrusite | -22.268 | -8.918 |
| Chalcanthite | -9.899 | -7.222 |
| Chalcopyrite | -76.453 | -40.281 |
| Chloropyromorphite(c) | -103.464 | -19.034 |
| Chloropyromorphite(soil) | -103.464 | -23.064 |
| Cinnabar | -62.77 | -15.947 |
| Claudetite | -10.58 | -9.067 |
| Cotunnite | -11.707 | -6.768 |
| Covellite | -40.956 | -18.147 |
| Cr(VI)-Ettringite | -19.811 | -83.212 |
| Cr(VI)-Jarosite | -37.379 | -18.863 |
| CrO3(s) | -15.854 | -12.675 |
| Cryolite | -58.852 | -24.781 |
| Cu azide | -19.963 | -12.122 |
| Cu(OH)2(s) | -1.951 | -11.564 |
| Cu2(OH)3NO3(s) | -63.3 | -72.993 |
| Cu3(AsO4)2:2H2O(s) | -65.543 | -30.443 |
| Cu3(PO4)2(s) | -63.654 | -26.804 |
| Cu3(PO4)2:3H2O(s) | -63.664 | -28.544 |
| CuCO3(s) | -21.795 | -10.295 |
| CuCrO4(s) | -17.802 | -12.362 |
| CuF2(s) | -23.92 | -25.442 |
| CuF2:2H2O(s) | -23.927 | -19.469 |
| CuOCuSO4(s) | -11.83 | -22.971 |
| Cupric Ferrite | -5.233 | -12.499 |
| CuSO4(s) | -9.882 | -13.265 |
| Diaspore | 4.475 | -3.025 |
| Dolomite (disordered) | -33.449 | -17.191 |
| Dolomite (ordered) | -33.449 | -16.599 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Epsomite | -4.863 | -2.666 |
| Ettringite | 3.949 | -55.239 |
| FCO3-Apatite | -159.694 | -44.292 |
| Fe(OH)2 (am) | 3.508 | -10.539 |
| Fe(OH)2 (c) | 3.508 | -9.382 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -27.086 | -24.824 |
| Fe3(OH)8(s) | 0.213 | -20.009 |
| FeAsO4:2H2O(s) | -31.496 | -11.296 |
| Ferrihydrite | -1.648 | -5.458 |
| Ferrihydrite (aged) | -1.648 | -4.948 |
| FeS (ppt) | -35.497 | -32.614 |
| Fluorite | -18.821 | -8.248 |
| Galena | -41.43 | -26.023 |
| Gibbsite (C) | 4.471 | -3.907 |
| Goethite | -1.644 | -2.504 |
| Goslarite | -7.448 | -5.35 |
| Greenockite | -42.335 | -27.981 |
| Greigite | -155.807 | -110.772 |
| Gypsum | -4.789 | -0.173 |
| Halite | -3.78 | -5.308 |
| Hematite | -3.285 | -2.651 |
| Hercynite | 12.464 | -12.338 |
| Hg(OH)2(s) | -23.765 | -20.268 |
| Hg3O2CO3(s) | -91.131 | -61.551 |
| HgCl2(s) | -33.047 | -11.129 |
| HgSO4(s) | -31.695 | -22.187 |
| Hinsdalite | -25.841 | -23.341 |
| H-Jarosite | -20.81 | -16.778 |
| Huntite | -66.955 | -37.643 |
| Hydrocerrusite | -46.962 | -28.202 |
| Hydromagnesite | -63.935 | -56.497 |
| Hydroxyapatite | -70.961 | -26.628 |
| Hydroxylpyromorphite | -98.822 | -36.032 |
| Hydrozincite | -37.155 | -47.293 |
| K2Cr2O7(s) | -33.176 | -15.442 |
| K2CrO4(s) | -17.322 | -16.697 |
| K-Alum | -12.166 | -6.812 |
| KCl(s) | -5.377 | -6.277 |
| K-Jarosite | -21.539 | -11.158 |
| Langite | -15.739 | -34.234 |
| Larnakite | -12.776 | -12.475 |
| Laurionite | -7.066 | -7.689 |
| Lepidocrocite | -1.644 | -3.015 |
| Lime | 3.151 | -30.727 |
| Litharge | -2.421 | -15.509 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Mackinawite | -35.497 | -31.897 |
| Maghemite | -3.285 | -9.671 |
| Magnesioferrite | -0.191 | -18.746 |
| Magnesite | -16.753 | -9.171 |
| Magnetite | 0.226 | -4.444 |
| Malachite | -23.747 | -18.546 |
| Massicot | -2.421 | -15.718 |
| Matlockite | -18.05 | -8.875 |
| Melanothallite | -11.234 | -17.876 |
| Melanterite | -4.446 | -2.112 |
| Metacinnabar | -62.77 | -16.345 |
| Mg(OH)2 (active) | 3.091 | -15.703 |
| Mg2(OH)3Cl:4H2O(s) | 1.527 | -24.473 |
| Mg3(PO4)2(s) | -48.527 | -25.247 |
| MgCO3:5H2O(s) | -16.77 | -12.23 |
| MgCrO4(s) | -12.76 | -18.681 |
| MgF2(s) | -18.878 | -10.816 |
| MgHPO4:3H2O(s) | -25.822 | -7.647 |
| MgS(s) | -35.914 | -53.594 |
| Minium | 9.011 | -67.076 |
| Mirabilite | -6.243 | -4.646 |
| Mn2(SO4)3(s) | -16.68 | -11.962 |
| Montroydite | -23.761 | -20.044 |
| Morenosite | -7.615 | -5.396 |
| Na2Cr2O7(s) | -29.983 | -19.953 |
| Na2CrO4(s) | -14.129 | -17.179 |
| NaF(s) | -10.124 | -9.629 |
| Na-Jarosite | -19.943 | -15.448 |
| Natron | -18.156 | -16.445 |
| Nesquehonite | -16.763 | -12.24 |
| Ni(OH)2 (am) | 0.339 | -13.134 |
| Ni(OH)2 (c) | 0.339 | -10.451 |
| Ni3(AsO4)2:8H2O(s) | -58.691 | -33.191 |
| Ni3(PO4)2(s) | -56.781 | -25.481 |
| Ni4(OH)6SO4(s) | -6.573 | -38.573 |
| NiCO3(s) | -19.504 | -8.557 |
| NiS (alpha) | -38.666 | -33.146 |
| NiS (beta) | -38.666 | -27.646 |
| NiS (gamma) | -38.666 | -25.946 |
| Nsutite | 11.698 | -5.806 |
| Orpiment | -127.606 | -79.706 |
| Otavite | -23.174 | -11.123 |
| Pb azide (alpha) | -20.437 | -11.462 |
| Pb metal | -18.696 | -22.937 |
| Pb(OH)2(s) | -2.425 | -10.931 |
| Pb10(OH)6O(CO3)6(s) | -143.306 | -134.546 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2(OH)3Cl(s) | -9.49 | -18.283 |
| Pb2O(OH)2(s) | -4.846 | -31.036 |
| Pb2O3(s) | 11.433 | -49.607 |
| Pb2OCO3(s) | -24.69 | -24.38 |
| Pb3(AsO4)2(s) | -66.956 | -31.456 |
| Pb3(PO4)2(s) | -65.073 | -21.543 |
| Pb3O2CO3(s) | -27.111 | -38.803 |
| Pb3O2SO4(s) | -15.198 | -26.365 |
| Pb4(OH)6SO4(s) | -17.629 | -38.729 |
| Pb4O3SO4(s) | -17.619 | -40.326 |
| PbCrO4(s) | -18.275 | -5.406 |
| PbF2(s) | -24.393 | -16.831 |
| PbHPO4(s) | -31.328 | -7.523 |
| PbO:0.3H2O(s) | -2.422 | -15.402 |
| Periclase | 3.094 | -19.409 |
| Phosgenite | -33.975 | -14.165 |
| Plattnerite | 13.854 | -37.548 |
| Plumbgummite | -46.814 | -14.024 |
| Portlandite | 3.148 | -20.338 |
| Pyrite | -58.23 | -39.419 |
| Realgar | -52.436 | -31.706 |
| Retgersite | -7.611 | -5.543 |
| Siderite | -16.336 | -5.79 |
| Smithsonite | -19.337 | -8.46 |
| Spharelite | -38.499 | -27.496 |
| Spinel | 12.047 | -27.16 |
| Strengite | -30.554 | -4.211 |
| Struvite | -26.469 | -13.209 |
| Sulfur | -22.733 | -20.688 |
| Tenorite(am) | -1.948 | -10.832 |
| Tenorite(c) | -1.948 | -9.983 |
| Thenardite | -6.209 | -6.586 |
| Thermonatrite | -18.126 | -18.827 |
| Tsumebite | -35.711 | -25.921 |
| Vaterite | -16.696 | -8.86 |
| Vivianite | -47.302 | -9.511 |
| Wurtzite | -38.499 | -29.75 |
| Zincite | 0.51 | -11.265 |
| Zincosite | -7.424 | -11.856 |
| Zn metal | -15.765 | -42.486 |
| Zn(NO3)2:6H2O(s) | -118.309 | -121.475 |
| Zn(OH)2 (am) | 0.506 | -12.488 |
| Zn(OH)2 (beta) | 0.506 | -11.753 |
| Zn(OH)2 (delta) | 0.506 | -11.338 |
| Zn(OH)2 (epsilon) | 0.506 | -11.506 |
| Zn(OH)2 (gamma) | 0.506 | -11.725 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn2(OH)2SO4(s) | -6.917 | -14.417 |
| Zn2(OH)3Cl(s) | -3.628 | -18.819 |
| Zn3(PO4)2:4H2O(s) | -56.294 | -20.874 |
| Zn3AsO42:2.5H2O(s) | -58.171 | -30.671 |
| Zn3O(SO4)2(s) | -14.338 | -34.82 |
| Zn4(OH)6SO4(s) | -5.904 | -34.304 |
| Zn5(OH)8Cl2(s) | -6.75 | -45.25 |
| Zn-Al LDH(s) | -4.438 | -24.268 |
| ZnCl2(s) | -8.776 | -16.267 |
| ZnCO3(s) | -19.337 | -8.537 |
| ZnCO3:1H2O(s) | -19.341 | -9.081 |
| ZnF2(s) | -21.462 | -21.291 |
| ZnSO4:1H2O(s) | -7.427 | -7.057 |

## B3.4: Eh 400

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 2.651 | -8.824 |
| Al(OH)3 (Soil) | 2.651 | -6.277 |
| Al2O3(s) | 5.312 | -15.912 |
| Al4(OH)10SO4(s) | 3.886 | -18.814 |
| AlAsO4:2H2O(s) | -24.996 | -9.196 |
| AlOHF2(s) | -18.119 | -18.526 |
| AlOHSO4(s) | -4.067 | -0.837 |
| Alunite | -6.828 | -6.705 |
| Anglesite | -10.341 | -2.478 |
| Anhydrite | -4.788 | -0.472 |
| Antlerite | -16.186 | -24.974 |
| Aragonite | -17.914 | -9.635 |
| Arsenolite | -10.727 | -9.164 |
| Artinite | -16.109 | -26.44 |
| As2O5(s) | -55.291 | -20.582 |
| As2S3(am) | -151.402 | -105.018 |
| Atacamite | -10.364 | -18.323 |
| Azurite | -49.157 | -32.004 |
| Bianchite | -7.447 | -5.686 |
| Birnessite | 11.005 | -7.086 |
| Bixbyite | 3.462 | 3.349 |
| Boehmite | 2.654 | -6.639 |
| Brochantite | -19.343 | -35.798 |
| Brucite | 1.873 | -15.92 |
| Ca3(AsO4)2:4H2O(s) | -49.504 | -30.604 |
| Ca3(PO4)2 (am1) | -50.76 | -25.831 |
| Ca3(PO4)2 (am2) | -50.76 | -23.038 |
| Ca3(PO4)2 (beta) | -50.76 | -21.511 |
| Ca4H(PO4)3:3H2O(s) | -77.118 | -29.806 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CaCO3xH2O(s) | -17.917 | -10.83 |
| CaCrO4(s) | -13.315 | -11.213 |
| CaHPO4(s) | -26.348 | -6.885 |
| CaHPO4:2H2O(s) | -26.355 | -7.22 |
| Calcite | -17.914 | -9.484 |
| CaS(s) | -44.958 | -56.138 |
| Cd metal (alpha) | -23.087 | -37.059 |
| Cd metal (gamma) | -23.087 | -37.166 |
| Cd(OH)2(s) | -4.541 | -18.76 |
| Cd3(OH)4SO4(s) | -20.34 | -42.9 |
| Cd3(PO4)2(s) | -70.172 | -37.572 |
| Cd3OH2(SO4)2(s) | -27.058 | -33.768 |
| Cd4(OH)6SO4(s) | -24.881 | -53.281 |
| CdCl2(s) | -12.644 | -12.098 |
| CdCl2:1H2O(s) | -12.648 | -11 |
| CdCl2:2.5H2O(s) | -12.653 | -10.695 |
| CdF2(s) | -25.311 | -24.38 |
| CdOHCl(s) | -8.592 | -12.318 |
| CdSO4(s) | -11.259 | -11.403 |
| CdSO4:1H2O(s) | -11.262 | -9.728 |
| CdSO4:2.67H2O(s) | -11.268 | -9.504 |
| Cerrusite | -23.468 | -10.117 |
| Chalcanthite | -9.891 | -7.214 |
| Chalcopyrite | -94.739 | -58.566 |
| Chloropyromorphite(c) | -106.994 | -22.564 |
| Chloropyromorphite(soil) | -106.994 | -26.594 |
| Cinnabar | -69.366 | -22.543 |
| Claudetite | -10.727 | -9.214 |
| Cotunnite | -11.727 | -6.788 |
| Covellite | -50.045 | -27.235 |
| Cr(VI)-Ettringite | -28.942 | -92.343 |
| Cr(VI)-Jarosite | -37.31 | -18.794 |
| CrO3(s) | -15.249 | -12.07 |
| Cryolite | -58.909 | -24.838 |
| Cu azide | -21.156 | -13.315 |
| Cu(OH)2(s) | -3.156 | -12.769 |
| Cu2(OH)3NO3(s) | -57.224 | -66.916 |
| Cu3(AsO4)2:2H2O(s) | -64.756 | -29.656 |
| Cu3(PO4)2(s) | -66.018 | -29.168 |
| Cu3(PO4)2:3H2O(s) | -66.029 | -30.909 |
| CuCO3(s) | -23 | -11.5 |
| CuCrO4(s) | -18.402 | -12.962 |
| CuF2(s) | -23.926 | -25.448 |
| CuF2:2H2O(s) | -23.933 | -19.476 |
| CuOCuSO4(s) | -13.027 | -24.168 |
| Cupric Ferrite | -6.792 | -14.058 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CuSO4(s) | -9.874 | -13.258 |
| Diaspore | 2.654 | -4.845 |
| Dolomite (disordered) | -35.885 | -19.627 |
| Dolomite (ordered) | -35.885 | -19.035 |
| Epsomite | -4.869 | -2.672 |
| Ettringite | -3.359 | -62.547 |
| FCO3-Apatite | -166.947 | -51.545 |
| Fe(OH)2 (am) | 2.194 | -11.853 |
| Fe(OH)2 (c) | 2.194 | -10.696 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -23.803 | -21.54 |
| Fe3(OH)8(s) | -1.455 | -21.677 |
| FeAsO4:2H2O(s) | -29.472 | -9.272 |
| Ferrihydrite | -1.825 | -5.635 |
| Ferrihydrite (aged) | -1.825 | -5.125 |
| FeS (ppt) | -44.694 | -41.811 |
| Fluorite | -18.84 | -8.267 |
| Galena | -50.512 | -35.106 |
| Gibbsite (C) | 2.651 | -5.727 |
| Goethite | -1.821 | -2.68 |
| Goslarite | -7.451 | -5.353 |
| Greenockite | -51.429 | -37.075 |
| Greigite | -189.008 | -143.973 |
| Gypsum | -4.795 | -0.178 |
| Halite | -3.801 | -5.329 |
| Hematite | -3.639 | -3.005 |
| Hercynite | 7.51 | -17.292 |
| Hg(OH)2(s) | -22.477 | -18.981 |
| Hg3O2CO3(s) | -87.269 | -57.689 |
| HgCl2(s) | -30.581 | -8.663 |
| HgSO4(s) | -29.195 | -19.687 |
| Hinsdalite | -30.663 | -28.163 |
| H-Jarosite | -18.916 | -14.883 |
| Huntite | -71.828 | -42.515 |
| Hydrocerrusite | -50.559 | -31.799 |
| Hydromagnesite | -70.026 | -62.588 |
| Hydroxyapatite | -75.174 | -30.841 |
| Hydroxylpyromorphite | -102.942 | -40.152 |
| Hydrozincite | -43.234 | -53.372 |
| K2Cr2O7(s) | -33.185 | -15.452 |
| K2CrO4(s) | -17.937 | -17.312 |
| K-Alum | -12.171 | -6.817 |
| KCl(s) | -5.397 | -6.297 |
| K-Jarosite | -20.255 | -9.874 |
| Langite | -19.346 | -37.841 |
| Larnakite | -13.962 | -13.66 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Laurionite | -7.675 | -8.298 |
| Lepidocrocite | -1.821 | -3.192 |
| Lime | 1.933 | -31.945 |
| Litharge | -3.62 | -16.708 |
| Mackinawite | -44.694 | -41.094 |
| Maghemite | -3.639 | -10.025 |
| Magnesioferrite | -1.763 | -20.318 |
| Magnesite | -17.971 | -10.39 |
| Magnetite | -1.441 | -6.112 |
| Malachite | -26.156 | -20.956 |
| Massicot | -3.62 | -16.917 |
| Matlockite | -18.06 | -8.885 |
| Melanothallite | -11.259 | -17.902 |
| Melanterite | -4.547 | -2.214 |
| Metacinnabar | -69.366 | -22.941 |
| Mg(OH)2 (active) | 1.873 | -16.921 |
| Mg2(OH)3Cl:4H2O(s) | -0.32 | -26.32 |
| Mg3(PO4)2(s) | -50.931 | -27.651 |
| MgCO3:5H2O(s) | -17.988 | -13.448 |
| MgCrO4(s) | -13.373 | -19.294 |
| MgF2(s) | -18.897 | -10.836 |
| MgHPO4:3H2O(s) | -26.416 | -8.241 |
| MgS(s) | -45.016 | -62.696 |
| Minium | 7.689 | -68.398 |
| Mirabilite | -6.251 | -4.654 |
| Mn2(SO4)3(s) | -16.702 | -11.985 |
| Montroydite | -22.474 | -18.757 |
| Morenosite | -7.62 | -5.401 |
| Na2Cr2O7(s) | -29.994 | -19.964 |
| Na2CrO4(s) | -14.745 | -17.795 |
| NaF(s) | -10.135 | -9.64 |
| Na-Jarosite | -18.659 | -14.164 |
| Natron | -19.378 | -17.666 |
| Nesquehonite | -17.981 | -13.459 |
| Ni(OH)2 (am) | -0.878 | -14.352 |
| Ni(OH)2 (c) | -0.878 | -11.668 |
| Ni3(AsO4)2:8H2O(s) | -57.943 | -32.443 |
| Ni3(PO4)2(s) | -59.184 | -27.884 |
| Ni4(OH)6SO4(s) | -10.23 | -42.23 |
| NiCO3(s) | -20.722 | -9.775 |
| NiS (alpha) | -47.767 | -42.247 |
| NiS (beta) | -47.767 | -36.747 |
| NiS (gamma) | -47.767 | -35.047 |
| Nsutite | 11.005 | -6.499 |
| Orpiment | -151.402 | -103.503 |
| Otavite | -24.385 | -12.334 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb azide (alpha) | -21.623 | -12.649 |
| Pb metal | -22.169 | -26.41 |
| Pb(OH)2(s) | -3.624 | -12.129 |
| Pb10(OH)6O(CO3)6(s) | -155.296 | -146.536 |
| Pb2(OH)3Cl(s) | -11.299 | -20.092 |
| Pb2O(OH)2(s) | -7.244 | -33.434 |
| Pb2O3(s) | 11.309 | -49.731 |
| Pb2OCO3(s) | -27.088 | -26.778 |
| Pb3(AsO4)2(s) | -66.152 | -30.652 |
| Pb3(PO4)2(s) | -67.42 | -23.89 |
| Pb3O2CO3(s) | -30.708 | -42.4 |
| Pb3O2SO4(s) | -17.582 | -28.749 |
| Pb4(OH)6SO4(s) | -21.212 | -42.312 |
| Pb4O3SO4(s) | -21.202 | -43.909 |
| PbCrO4(s) | -18.869 | -6 |
| PbF2(s) | -24.394 | -16.832 |
| PbHPO4(s) | -31.902 | -8.097 |
| PbO:0.3H2O(s) | -3.621 | -16.601 |
| Periclase | 1.876 | -20.627 |
| Phosgenite | -35.194 | -15.384 |
| Plattnerite | 14.929 | -36.472 |
| Plumbgummite | -52.224 | -19.434 |
| Portlandite | 1.93 | -21.556 |
| Pyrite | -73.037 | -54.226 |
| Realgar | -61.53 | -40.8 |
| Retgersite | -7.616 | -5.548 |
| Siderite | -17.65 | -7.104 |
| Smithsonite | -20.553 | -9.676 |
| Spharelite | -47.598 | -36.595 |
| Spinel | 7.188 | -32.018 |
| Strengite | -30.106 | -3.763 |
| Struvite | -27.672 | -14.412 |
| Sulfur | -28.343 | -26.297 |
| Tenorite(am) | -3.153 | -12.037 |
| Tenorite(c) | -3.153 | -11.187 |
| Thenardite | -6.218 | -6.595 |
| Thermonatrite | -19.347 | -20.048 |
| Tsumebite | -38.688 | -28.898 |
| Vaterite | -17.914 | -10.078 |
| Vivianite | -49.994 | -12.203 |
| Wurtzite | -47.598 | -38.849 |
| Zincite | -0.706 | -12.481 |
| Zincosite | -7.427 | -11.859 |
| Zn metal | -19.255 | -45.976 |
| Zn(NO3)2:6H2O(s) | -102.553 | -105.718 |
| Zn(OH)2 (am) | -0.709 | -13.704 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn(OH)2 (beta) | -0.709 | -12.969 |
| Zn(OH)2 (delta) | -0.709 | -12.553 |
| Zn(OH)2 (epsilon) | -0.709 | -12.721 |
| Zn(OH)2 (gamma) | -0.709 | -12.94 |
| Zn2(OH)2SO4(s) | -8.136 | -15.636 |
| Zn2(OH)3Cl(s) | -5.47 | -20.661 |
| Zn3(PO4)2:4H2O(s) | -58.691 | -23.271 |
| Zn3AsO42:2.5H2O(s) | -57.417 | -29.917 |
| Zn3O(SO4)2(s) | -15.56 | -36.042 |
| Zn4(OH)6SO4(s) | -9.554 | -37.954 |
| Zn5(OH)8Cl2(s) | -11.649 | -50.149 |
| Zn-Al LDH(s) | -8.689 | -28.519 |
| ZnCl2(s) | -8.812 | -16.303 |
| ZnCO3(s) | -20.553 | -9.753 |
| ZnCO3:1H2O(s) | -20.557 | -10.297 |
| ZnF2(s) | -21.479 | -21.308 |
| ZnSO4:1H2O(s) | -7.43 | -7.06 |

## B3.5: Eh 500

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 1.242 | -10.233 |
| Al(OH)3 (Soil) | 1.242 | -7.686 |
| Al2O3(s) | 2.494 | -18.73 |
| Al4(OH)10SO4(s) | -0.814 | -23.514 |
| AlAsO4:2H2O(s) | -25.396 | -9.596 |
| AlOHF2(s) | -18.619 | -19.026 |
| AlOHSO4(s) | -4.54 | -1.31 |
| Alunite | -9.66 | -9.537 |
| Anglesite | -10.337 | -2.474 |
| Anhydrite | -4.799 | -0.483 |
| Antlerite | -18.081 | -26.869 |
| Aragonite | -18.862 | -10.583 |
| Arsenolite | -13.778 | -12.215 |
| Artinite | -18.006 | -28.337 |
| As2O5(s) | -53.273 | -18.563 |
| As2S3(am) | -182.064 | -135.679 |
| Atacamite | -11.834 | -19.793 |
| Azurite | -51.989 | -34.836 |
| Bianchite | -7.455 | -5.694 |
| Birnessite | 10.845 | -7.246 |
| Bixbyite | 0.606 | 0.494 |
| Boehmite | 1.245 | -8.048 |
| Brochantite | -22.181 | -38.636 |
| Brucite | 0.925 | -16.868 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(AsO4)2:4H2O(s) | -50.327 | -31.427 |
| Ca3(PO4)2 (am1) | -52.621 | -27.693 |
| Ca3(PO4)2 (am2) | -52.621 | -24.9 |
| Ca3(PO4)2 (beta) | -52.621 | -23.373 |
| Ca4H(PO4)3:3H2O(s) | -79.437 | -32.126 |
| CaCO3xH2O(s) | -18.865 | -11.778 |
| CaCrO4(s) | -13.797 | -11.695 |
| CaHPO4(s) | -26.806 | -7.342 |
| CaHPO4:2H2O(s) | -26.812 | -7.678 |
| Calcite | -18.862 | -10.432 |
| CaS(s) | -55.109 | -66.289 |
| Cd metal (alpha) | -26.549 | -40.521 |
| Cd metal (gamma) | -26.549 | -40.628 |
| Cd(OH)2(s) | -5.468 | -19.687 |
| Cd3(OH)4SO4(s) | -22.187 | -44.747 |
| Cd3(PO4)2(s) | -71.975 | -39.375 |
| Cd3OH2(SO4)2(s) | -27.969 | -34.679 |
| Cd4(OH)6SO4(s) | -27.655 | -56.055 |
| CdCl2(s) | -12.739 | -12.193 |
| CdCl2:1H2O(s) | -12.742 | -11.094 |
| CdCl2:2.5H2O(s) | -12.747 | -10.79 |
| CdF2(s) | -25.33 | -24.398 |
| CdOHCl(s) | -9.103 | -12.829 |
| CdSO4(s) | -11.251 | -11.394 |
| CdSO4:1H2O(s) | -11.254 | -9.72 |
| CdSO4:2.67H2O(s) | -11.26 | -9.496 |
| Cerrusite | -24.4 | -11.049 |
| Chalcanthite | -9.899 | -7.222 |
| Chalcopyrite | -115.481 | -79.309 |
| Chloropyromorphite(c) | -109.764 | -25.334 |
| Chloropyromorphite(soil) | -109.764 | -29.364 |
| Cinnabar | -79.243 | -32.42 |
| Claudetite | -13.778 | -12.265 |
| Cotunnite | -11.825 | -6.886 |
| Covellite | -60.191 | -37.382 |
| Cr(VI)-Ettringite | -36.046 | -99.447 |
| Cr(VI)-Jarosite | -37.231 | -18.715 |
| CrO3(s) | -14.784 | -11.605 |
| Cryolite | -59.024 | -24.953 |
| Cu azide | -22.098 | -14.257 |
| Cu(OH)2(s) | -4.1 | -13.713 |
| Cu2(OH)3NO3(s) | -49.447 | -59.14 |
| Cu3(AsO4)2:2H2O(s) | -65.568 | -30.468 |
| Cu3(PO4)2(s) | -67.869 | -31.019 |
| Cu3(PO4)2:3H2O(s) | -67.88 | -32.76 |
| CuCO3(s) | -23.945 | -12.445 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CuCrO4(s) | -18.88 | -13.44 |
| CuF2(s) | -23.961 | -25.483 |
| CuF2:2H2O(s) | -23.968 | -19.511 |
| CuOCuSO4(s) | -13.978 | -25.119 |
| Cupric Ferrite | -7.985 | -15.251 |
| CuSO4(s) | -9.882 | -13.266 |
| Diaspore | 1.245 | -6.254 |
| Dolomite (disordered) | -37.782 | -21.524 |
| Dolomite (ordered) | -37.782 | -20.932 |
| Epsomite | -4.881 | -2.684 |
| Ettringite | -9.052 | -68.241 |
| FCO3-Apatite | -172.602 | -57.2 |
| Fe(OH)2 (am) | 0.802 | -13.245 |
| Fe(OH)2 (c) | 0.802 | -12.088 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -21.246 | -18.983 |
| Fe3(OH)8(s) | -3.097 | -23.319 |
| FeAsO4:2H2O(s) | -28.587 | -8.387 |
| Ferrihydrite | -1.949 | -5.76 |
| Ferrihydrite (aged) | -1.949 | -5.25 |
| FeS (ppt) | -55.29 | -52.407 |
| Fluorite | -18.878 | -8.305 |
| Galena | -60.646 | -45.24 |
| Gibbsite (C) | 1.242 | -7.136 |
| Goethite | -1.946 | -2.805 |
| Goslarite | -7.458 | -5.361 |
| Greenockite | -61.56 | -47.206 |
| Greigite | -227.464 | -182.429 |
| Gypsum | -4.806 | -0.19 |
| Halite | -3.862 | -5.39 |
| Hematite | -3.889 | -3.255 |
| Hercynite | 3.3 | -21.502 |
| Hg(OH)2(s) | -23.151 | -19.655 |
| Hg3O2CO3(s) | -89.293 | -59.713 |
| HgCl2(s) | -30.422 | -8.504 |
| HgSO4(s) | -28.934 | -19.426 |
| Hinsdalite | -34.396 | -31.896 |
| H-Jarosite | -17.42 | -13.387 |
| Huntite | -75.623 | -46.31 |
| Hydrocerrusite | -53.354 | -34.594 |
| Hydromagnesite | -74.769 | -67.332 |
| Hydroxyapatite | -78.441 | -34.108 |
| Hydroxylpyromorphite | -106.128 | -43.338 |
| Hydrozincite | -47.952 | -58.09 |
| K2Cr2O7(s) | -33.208 | -15.475 |
| K2CrO4(s) | -18.424 | -17.8 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K-Alum | -12.185 | -6.832 |
| KCl(s) | -5.457 | -6.357 |
| K-Jarosite | -19.235 | -8.854 |
| Langite | -22.184 | -40.679 |
| Larnakite | -14.888 | -14.586 |
| Laurionite | -8.19 | -8.813 |
| Lepidocrocite | -1.946 | -3.317 |
| Lime | 0.986 | -32.892 |
| Litharge | -4.551 | -17.639 |
| Mackinawite | -55.29 | -51.69 |
| Maghemite | -3.889 | -10.275 |
| Magnesioferrite | -2.961 | -21.516 |
| Magnesite | -18.92 | -11.339 |
| Magnetite | -3.083 | -7.754 |
| Malachite | -28.044 | -22.844 |
| Massicot | -4.551 | -17.848 |
| Matlockite | -18.12 | -8.945 |
| Melanothallite | -11.37 | -18.013 |
| Melanterite | -5.004 | -2.67 |
| Metacinnabar | -79.243 | -32.819 |
| Mg(OH)2 (active) | 0.925 | -17.869 |
| Mg2(OH)3Cl:4H2O(s) | -1.799 | -27.799 |
| Mg3(PO4)2(s) | -52.796 | -29.516 |
| MgCO3:5H2O(s) | -18.937 | -14.397 |
| MgCrO4(s) | -13.855 | -19.776 |
| MgF2(s) | -18.937 | -10.875 |
| MgHPO4:3H2O(s) | -26.874 | -8.699 |
| MgS(s) | -55.167 | -72.847 |
| Minium | 7.43 | -68.656 |
| Mirabilite | -6.271 | -4.674 |
| Mn2(SO4)3(s) | -16.751 | -12.034 |
| Montroydite | -23.148 | -19.431 |
| Morenosite | -7.631 | -5.412 |
| Na2Cr2O7(s) | -30.018 | -19.988 |
| Na2CrO4(s) | -15.235 | -18.284 |
| NaF(s) | -10.158 | -9.663 |
| Na-Jarosite | -17.64 | -13.146 |
| Natron | -20.333 | -18.622 |
| Nesquehonite | -18.93 | -14.408 |
| Ni(OH)2 (am) | -1.825 | -15.299 |
| Ni(OH)2 (c) | -1.825 | -12.615 |
| Ni3(AsO4)2:8H2O(s) | -58.766 | -33.266 |
| Ni3(PO4)2(s) | -61.047 | -29.747 |
| Ni4(OH)6SO4(s) | -13.084 | -45.084 |
| NiCO3(s) | -21.67 | -10.723 |
| NiS (alpha) | -57.917 | -52.397 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| NiS (beta) | -57.917 | -46.897 |
| NiS (gamma) | -57.917 | -45.197 |
| Nsutite | 10.845 | -6.659 |
| Orpiment | -182.064 | -134.164 |
| Otavite | -25.313 | -13.262 |
| Pb azide (alpha) | -22.553 | -13.579 |
| Pb metal | -25.635 | -29.876 |
| Pb(OH)2(s) | -4.554 | -13.06 |
| Pb10(OH)6O(CO3)6(s) | -164.612 | -155.852 |
| Pb2(OH)3Cl(s) | -12.744 | -21.537 |
| Pb2O(OH)2(s) | -9.106 | -35.296 |
| Pb2O3(s) | 11.982 | -49.058 |
| Pb2OCO3(s) | -28.951 | -28.641 |
| Pb3(AsO4)2(s) | -66.926 | -31.426 |
| Pb3(PO4)2(s) | -69.234 | -25.704 |
| Pb3O2CO3(s) | -33.502 | -45.194 |
| Pb3O2SO4(s) | -19.439 | -30.607 |
| Pb4(OH)6SO4(s) | -24 | -45.1 |
| Pb4O3SO4(s) | -23.99 | -46.697 |
| PbCrO4(s) | -19.335 | -6.466 |
| PbF2(s) | -24.416 | -16.854 |
| PbHPO4(s) | -32.343 | -8.538 |
| PbO:0.3H2O(s) | -4.552 | -17.532 |
| Periclase | 0.928 | -21.575 |
| Phosgenite | -36.224 | -16.414 |
| Plattnerite | 16.533 | -34.869 |
| Plumbgummite | -56.402 | -23.612 |
| Portlandite | 0.983 | -22.503 |
| Pyrite | -90.301 | -71.49 |
| Realgar | -73.526 | -52.796 |
| Retgersite | -7.628 | -5.56 |
| Siderite | -19.043 | -8.497 |
| Smithsonite | -21.497 | -10.621 |
| Spharelite | -57.744 | -46.742 |
| Spinel | 3.423 | -35.784 |
| Strengite | -29.742 | -3.398 |
| Struvite | -28.606 | -15.346 |
| Sulfur | -35.011 | -32.966 |
| Tenorite(am) | -4.096 | -12.981 |
| Tenorite(c) | -4.096 | -12.131 |
| Thenardite | -6.237 | -6.614 |
| Thermonatrite | -20.303 | -21.004 |
| Tsumebite | -41.004 | -31.214 |
| Vaterite | -18.862 | -11.026 |
| Vivianite | -53.192 | -15.401 |
| Wurtzite | -57.744 | -48.996 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zincite | -1.649 | -13.424 |
| Zincosite | -7.435 | -11.867 |
| Zn metal | -22.733 | -49.454 |
| Zn(NO3)2:6H2O(s) | -84.169 | -87.335 |
| Zn(OH)2 (am) | -1.652 | -14.647 |
| Zn(OH)2 (beta) | -1.652 | -13.912 |
| Zn(OH)2 (delta) | -1.652 | -13.496 |
| Zn(OH)2 (epsilon) | -1.652 | -13.664 |
| Zn(OH)2 (gamma) | -1.652 | -13.884 |
| Zn2(OH)2SO4(s) | -9.087 | -16.587 |
| Zn2(OH)3Cl(s) | -6.94 | -22.131 |
| Zn3(PO4)2:4H2O(s) | -60.541 | -25.121 |
| Zn3AsO42:2.5H2O(s) | -58.228 | -30.728 |
| Zn3O(SO4)2(s) | -16.519 | -37.001 |
| Zn4(OH)6SO4(s) | -12.392 | -40.792 |
| Zn5(OH)8Cl2(s) | -15.533 | -54.033 |
| Zn-Al LDH(s) | -11.985 | -31.815 |
| ZnCl2(s) | -8.923 | -16.414 |
| ZnCO3(s) | -21.497 | -10.697 |
| ZnCO3:1H2O(s) | -21.501 | -11.241 |
| ZnF2(s) | -21.514 | -21.342 |
| ZnSO4:1H2O(s) | -7.438 | -7.068 |

## B3.6: Eh 600

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 0.848 | -10.627 |
| Al(OH)3 (Soil) | 0.848 | -8.08 |
| Al2O3(s) | 1.707 | -19.518 |
| Al4(OH)10SO4(s) | -2.129 | -24.829 |
| AlAsO4:2H2O(s) | -25.74 | -9.94 |
| AlOHF2(s) | -18.764 | -19.171 |
| AlOHSO4(s) | -4.673 | -1.443 |
| Alunite | -10.455 | -10.331 |
| Anglesite | -10.336 | -2.473 |
| Anhydrite | -4.804 | -0.488 |
| Antlerite | -18.618 | -27.406 |
| Aragonite | -19.128 | -10.849 |
| Arsenolite | -20.126 | -18.563 |
| Artinite | -18.539 | -28.87 |
| As2O5(s) | -53.173 | -18.464 |
| As2S3(am) | -226.314 | -179.929 |
| Atacamite | -12.269 | -20.228 |
| Azurite | -52.788 | -35.634 |
| Bianchite | -7.458 | -5.698 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Birnessite | 12.055 | -6.036 |
| Bixbyite | -0.197 | -0.31 |
| Boehmite | 0.852 | -8.442 |
| Brochantite | -22.983 | -39.439 |
| Brucite | 0.658 | -17.135 |
| Ca3(AsO4)2:4H2O(s) | -51.025 | -32.125 |
| Ca3(PO4)2 (am1) | -53.137 | -28.208 |
| Ca3(PO4)2 (am2) | -53.137 | -25.416 |
| Ca3(PO4)2 (beta) | -53.137 | -23.888 |
| Ca4H(PO4)3:3H2O(s) | -80.077 | -32.766 |
| CaCO3xH2O(s) | -19.132 | -12.045 |
| CaCrO4(s) | -13.934 | -11.832 |
| CaHPO4(s) | -26.93 | -7.467 |
| CaHPO4:2H2O(s) | -26.937 | -7.802 |
| Calcite | -19.128 | -10.698 |
| CaS(s) | -68.009 | -79.189 |
| Cd metal (alpha) | -30.027 | -44 |
| Cd metal (gamma) | -30.027 | -44.107 |
| Cd(OH)2(s) | -5.723 | -19.942 |
| Cd3(OH)4SO4(s) | -22.69 | -45.25 |
| Cd3(PO4)2(s) | -72.457 | -39.857 |
| Cd3OH2(SO4)2(s) | -28.211 | -34.921 |
| Cd4(OH)6SO4(s) | -28.413 | -56.813 |
| CdCl2(s) | -12.799 | -12.253 |
| CdCl2:1H2O(s) | -12.802 | -11.154 |
| CdCl2:2.5H2O(s) | -12.807 | -10.85 |
| CdF2(s) | -25.335 | -24.404 |
| CdOHCl(s) | -9.261 | -12.986 |
| CdSO4(s) | -11.244 | -11.388 |
| CdSO4:1H2O(s) | -11.248 | -9.713 |
| CdSO4:2.67H2O(s) | -11.253 | -9.49 |
| Cerrusite | -24.66 | -11.309 |
| Chalcanthite | -9.904 | -7.227 |
| Chalcopyrite | -142.657 | -106.484 |
| Chloropyromorphite(c) | -110.54 | -26.11 |
| Chloropyromorphite(soil) | -110.54 | -30.14 |
| Cinnabar | -92.064 | -45.241 |
| Claudetite | -20.126 | -18.613 |
| Cotunnite | -11.89 | -6.951 |
| Covellite | -73.092 | -50.282 |
| Cr(VI)-Ettringite | -38.041 | -101.442 |
| Cr(VI)-Jarosite | -37.194 | -18.678 |
| CrO3(s) | -14.654 | -11.475 |
| Cryolite | -59.075 | -25.004 |
| Cu azide | -22.365 | -14.524 |
| Cu(OH)2(s) | -4.365 | -13.978 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cu2(OH)3NO3(s) | -37.218 | -46.91 |
| Cu3(AsO4)2:2H2O(s) | -66.266 | -31.166 |
| Cu3(PO4)2(s) | -68.385 | -31.535 |
| Cu3(PO4)2:3H2O(s) | -68.395 | -33.275 |
| CuCO3(s) | -24.211 | -12.711 |
| CuCrO4(s) | -19.016 | -13.576 |
| CuF2(s) | -23.978 | -25.499 |
| CuF2:2H2O(s) | -23.984 | -19.527 |
| CuOCuSO4(s) | -14.249 | -25.39 |
| Cupric Ferrite | -8.309 | -15.575 |
| CuSO4(s) | -9.887 | -13.271 |
| Diaspore | 0.852 | -6.648 |
| Dolomite (disordered) | -38.316 | -22.058 |
| Dolomite (ordered) | -38.316 | -21.466 |
| Epsomite | -4.887 | -2.69 |
| Ettringite | -10.653 | -69.842 |
| FCO3-Apatite | -174.18 | -58.778 |
| Fe(OH)2 (am) | -0.839 | -14.886 |
| Fe(OH)2 (c) | -0.839 | -13.729 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -20.522 | -18.259 |
| Fe3(OH)8(s) | -4.796 | -25.018 |
| FeAsO4:2H2O(s) | -28.567 | -8.367 |
| Ferrihydrite | -1.979 | -5.789 |
| Ferrihydrite (aged) | -1.979 | -5.279 |
| FeS (ppt) | -69.565 | -66.682 |
| Fluorite | -18.895 | -8.322 |
| Galena | -73.54 | -58.134 |
| Gibbsite (C) | 0.848 | -7.53 |
| Goethite | -1.975 | -2.835 |
| Goslarite | -7.462 | -5.364 |
| Greenockite | -74.449 | -60.095 |
| Greigite | -279.701 | -234.666 |
| Gypsum | -4.811 | -0.195 |
| Halite | -3.9 | -5.428 |
| Hematite | -3.947 | -3.313 |
| Hercynite | 0.871 | -23.931 |
| Hg(OH)2(s) | -23.338 | -19.842 |
| Hg3O2CO3(s) | -89.853 | -60.273 |
| HgCl2(s) | -30.414 | -8.496 |
| HgSO4(s) | -28.859 | -19.351 |
| Hinsdalite | -35.435 | -32.935 |
| H-Jarosite | -16.986 | -12.953 |
| Huntite | -76.69 | -47.377 |
| Hydrocerrusite | -54.133 | -35.373 |
| Hydromagnesite | -76.103 | -68.666 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Hydroxyapatite | -79.346 | -35.013 |
| Hydroxylpyromorphite | -107.003 | -44.213 |
| Hydrozincite | -49.274 | -59.412 |
| K2Cr2O7(s) | -33.217 | -15.484 |
| K2CrO4(s) | -18.563 | -17.939 |
| K-Alum | -12.192 | -6.838 |
| KCl(s) | -5.494 | -6.394 |
| K-Jarosite | -18.935 | -8.554 |
| Langite | -22.987 | -41.482 |
| Larnakite | -15.146 | -14.845 |
| Laurionite | -8.352 | -8.975 |
| Lepidocrocite | -1.975 | -3.346 |
| Lime | 0.721 | -33.158 |
| Litharge | -4.811 | -17.899 |
| Mackinawite | -69.565 | -65.965 |
| Maghemite | -3.947 | -10.333 |
| Magnesioferrite | -3.285 | -21.841 |
| Magnesite | -19.187 | -11.605 |
| Magnetite | -4.783 | -9.453 |
| Malachite | -28.577 | -23.376 |
| Massicot | -4.811 | -18.107 |
| Matlockite | -18.158 | -8.983 |
| Melanothallite | -11.441 | -18.084 |
| Melanterite | -6.384 | -4.051 |
| Metacinnabar | -92.064 | -45.64 |
| Mg(OH)2 (active) | 0.658 | -18.136 |
| Mg2(OH)3Cl:4H2O(s) | -2.234 | -28.234 |
| Mg3(PO4)2(s) | -53.313 | -30.033 |
| MgCO3:5H2O(s) | -19.204 | -14.664 |
| MgCrO4(s) | -13.992 | -19.913 |
| MgF2(s) | -18.954 | -10.892 |
| MgHPO4:3H2O(s) | -26.999 | -8.824 |
| MgS(s) | -68.068 | -85.748 |
| Minium | 9.875 | -66.211 |
| Mirabilite | -6.28 | -4.683 |
| Mn2(SO4)3(s) | -16.772 | -12.055 |
| Montroydite | -23.335 | -19.618 |
| Morenosite | -7.637 | -5.418 |
| Na2Cr2O7(s) | -30.029 | -19.999 |
| Na2CrO4(s) | -15.375 | -18.425 |
| NaF(s) | -10.168 | -9.673 |
| Na-Jarosite | -17.341 | -12.846 |
| Natron | -20.604 | -18.892 |
| Nesquehonite | -19.197 | -14.675 |
| Ni(OH)2 (am) | -2.091 | -15.565 |
| Ni(OH)2 (c) | -2.091 | -12.881 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ni3(AsO4)2:8H2O(s) | -59.464 | -33.964 |
| Ni3(PO4)2(s) | -61.562 | -30.262 |
| Ni4(OH)6SO4(s) | -13.887 | -45.887 |
| NiCO3(s) | -21.937 | -10.99 |
| NiS (alpha) | -70.817 | -65.297 |
| NiS (beta) | -70.817 | -59.797 |
| NiS (gamma) | -70.817 | -58.097 |
| Nsutite | 12.055 | -5.449 |
| Orpiment | -226.314 | -178.415 |
| Otavite | -25.568 | -13.517 |
| Pb azide (alpha) | -22.814 | -13.839 |
| Pb metal | -29.118 | -33.359 |
| Pb(OH)2(s) | -4.814 | -13.32 |
| Pb10(OH)6O(CO3)6(s) | -167.211 | -158.451 |
| Pb2(OH)3Cl(s) | -13.166 | -21.959 |
| Pb2O(OH)2(s) | -9.625 | -35.815 |
| Pb2O3(s) | 14.686 | -46.354 |
| Pb2OCO3(s) | -29.47 | -29.161 |
| Pb3(AsO4)2(s) | -67.605 | -32.105 |
| Pb3(PO4)2(s) | -69.73 | -26.2 |
| Pb3O2CO3(s) | -34.281 | -45.973 |
| Pb3O2SO4(s) | -19.957 | -31.125 |
| Pb4(OH)6SO4(s) | -24.778 | -45.878 |
| Pb4O3SO4(s) | -24.768 | -47.474 |
| PbCrO4(s) | -19.465 | -6.596 |
| PbF2(s) | -24.426 | -16.865 |
| PbHPO4(s) | -32.462 | -8.657 |
| PbO:0.3H2O(s) | -4.812 | -17.792 |
| Periclase | 0.662 | -21.842 |
| Phosgenite | -36.55 | -16.74 |
| Plattnerite | 19.497 | -31.905 |
| Plumbgummite | -57.561 | -24.771 |
| Portlandite | 0.717 | -22.769 |
| Pyrite | -113.987 | -95.176 |
| Realgar | -90.946 | -70.216 |
| Retgersite | -7.633 | -5.565 |
| Siderite | -20.685 | -10.139 |
| Smithsonite | -21.762 | -10.885 |
| Spharelite | -70.643 | -59.64 |
| Spinel | 2.368 | -36.838 |
| Strengite | -29.629 | -3.286 |
| Struvite | -28.865 | -15.605 |
| Sulfur | -44.422 | -42.376 |
| Tenorite(am) | -4.362 | -13.246 |
| Tenorite(c) | -4.362 | -12.397 |
| Thenardite | -6.246 | -6.623 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Thermonatrite | -20.573 | -21.274 |
| Tsumebite | -41.648 | -31.858 |
| Vaterite | -19.128 | -11.292 |
| Vivianite | -57.832 | -20.042 |
| Wurtzite | -70.643 | -61.894 |
| Zincite | -1.913 | -13.688 |
| Zincosite | -7.438 | -11.87 |
| Zn metal | -26.221 | -52.942 |
| Zn(NO3)2:6H2O(s) | -58.911 | -62.077 |
| Zn(OH)2 (am) | -1.917 | -14.911 |
| Zn(OH)2 (beta) | -1.917 | -14.176 |
| Zn(OH)2 (delta) | -1.917 | -13.761 |
| Zn(OH)2 (epsilon) | -1.917 | -13.929 |
| Zn(OH)2 (gamma) | -1.917 | -14.148 |
| Zn2(OH)2SO4(s) | -9.355 | -16.855 |
| Zn2(OH)3Cl(s) | -7.371 | -22.562 |
| Zn3(PO4)2:4H2O(s) | -61.051 | -25.631 |
| Zn3AsO42:2.5H2O(s) | -58.921 | -31.421 |
| Zn3O(SO4)2(s) | -16.789 | -37.272 |
| Zn4(OH)6SO4(s) | -13.188 | -41.588 |
| Zn5(OH)8Cl2(s) | -16.659 | -55.159 |
| Zn-Al LDH(s) | -12.908 | -32.738 |
| ZnCl2(s) | -8.992 | -16.483 |
| ZnCO3(s) | -21.762 | -10.962 |
| ZnCO3:1H2O(s) | -21.766 | -11.506 |
| ZnF2(s) | -21.529 | -21.357 |
| ZnSO4:1H2O(s) | -7.442 | -7.071 |

## B3.7: Eh 700

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 0.834 | -10.641 |
| Al(OH)3 (Soil) | 0.834 | -8.095 |
| Al2O3(s) | 1.677 | -19.547 |
| Al4(OH)10SO4(s) | -2.177 | -24.877 |
| AlAsO4:2H2O(s) | -25.753 | -9.953 |
| AlOHF2(s) | -18.769 | -19.176 |
| AlOHSO4(s) | -4.678 | -1.448 |
| Alunite | -10.484 | -10.361 |
| Anglesite | -10.336 | -2.473 |
| Anhydrite | -4.805 | -0.488 |
| Antlerite | -18.638 | -27.426 |
| Aragonite | -19.138 | -10.859 |
| Arsenolite | -27.099 | -25.536 |
| Artinite | -18.559 | -28.89 |
| As2O5(s) | -53.17 | -18.461 |
| As2S3(am) | -275.115 | -228.73 |
| Atacamite | -12.285 | -20.244 |
| Azurite | -52.817 | -35.664 |
| Bianchite | -7.459 | -5.698 |
| Birnessite | 13.784 | -4.307 |
| Bixbyite | -0.227 | -0.34 |
| Boehmite | 0.837 | -8.457 |
| Brochantite | -23.013 | -39.469 |
| Brucite | 0.649 | -17.145 |
| Ca3(AsO4)2:4H2O(s) | -51.052 | -32.152 |
| Ca3(PO4)2 (am1) | -53.156 | -28.227 |
| Ca3(PO4)2 (am2) | -53.156 | -25.435 |
| Ca3(PO4)2 (beta) | -53.156 | -23.907 |
| Ca4H(PO4)3:3H2O(s) | -80.101 | -32.789 |
| CaCO3xH2O(s) | -19.142 | -12.055 |
| CaCrO4(s) | -13.939 | -11.837 |
| CaHPO4(s) | -26.935 | -7.471 |
| CaHPO4:2H2O(s) | -26.942 | -7.807 |
| Calcite | -19.138 | -10.708 |
| CaS(s) | -81.961 | -93.141 |
| Cd metal (alpha) | -33.524 | -47.497 |
| Cd metal (gamma) | -33.524 | -47.604 |
| Cd(OH)2(s) | -5.732 | -19.951 |
| Cd3(OH)4SO4(s) | -22.708 | -45.268 |
| Cd3(PO4)2(s) | -72.474 | -39.874 |
| Cd3OH2(SO4)2(s) | -28.22 | -34.93 |
| Cd4(OH)6SO4(s) | -28.441 | -56.841 |
| CdCl2(s) | -12.801 | -12.256 |
| CdCl2:1H2O(s) | -12.805 | -11.157 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| CdCl2:2.5H2O(s) | -12.81 | -10.853 |
| CdF2(s) | -25.335 | -24.404 |
| CdOHCl(s) | -9.267 | -12.992 |
| CdSO4(s) | -11.244 | -11.388 |
| CdSO4:1H2O(s) | -11.247 | -9.713 |
| CdSO4:2.67H2O(s) | -11.253 | -9.489 |
| Cerrusite | -24.669 | -11.319 |
| Chalcanthite | -9.904 | -7.228 |
| Chalcopyrite | -172.296 | -136.124 |
| Chloropyromorphite(c) | -110.569 | -26.139 |
| Chloropyromorphite(soil) | -110.569 | -30.169 |
| Cinnabar | -106.013 | -59.19 |
| Claudetite | -27.099 | -25.586 |
| Cotunnite | -11.893 | -6.954 |
| Covellite | -87.044 | -64.234 |
| Cr(VI)-Ettringite | -38.115 | -101.516 |
| Cr(VI)-Jarosite | -37.192 | -18.676 |
| CrO3(s) | -14.649 | -11.471 |
| Cryolite | -59.077 | -25.006 |
| Cu azide | -22.375 | -14.534 |
| Cu(OH)2(s) | -4.375 | -13.988 |
| Cu2(OH)3NO3(s) | -23.291 | -32.983 |
| Cu3(AsO4)2:2H2O(s) | -66.293 | -31.193 |
| Cu3(PO4)2(s) | -68.403 | -31.553 |
| Cu3(PO4)2:3H2O(s) | -68.414 | -33.294 |
| CuCO3(s) | -24.221 | -12.721 |
| CuCrO4(s) | -19.021 | -13.581 |
| CuF2(s) | -23.978 | -25.5 |
| CuF2:2H2O(s) | -23.985 | -19.528 |
| CuOCuSO4(s) | -14.259 | -25.4 |
| Cupric Ferrite | -8.321 | -15.587 |
| CuSO4(s) | -9.887 | -13.271 |
| Diaspore | 0.837 | -6.663 |
| Dolomite (disordered) | -38.335 | -22.077 |
| Dolomite (ordered) | -38.335 | -21.485 |
| Epsomite | -4.887 | -2.69 |
| Ettringite | -10.713 | -69.901 |
| FCO3-Apatite | -174.238 | -58.836 |
| Fe(OH)2 (am) | -2.584 | -16.631 |
| Fe(OH)2 (c) | -2.584 | -15.474 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -20.495 | -18.232 |
| Fe3(OH)8(s) | -6.543 | -26.765 |
| FeAsO4:2H2O(s) | -28.567 | -8.367 |
| Ferrihydrite | -1.98 | -5.79 |
| Ferrihydrite (aged) | -1.98 | -5.28 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| FeS (ppt) | -85.253 | -82.369 |
| Fluorite | -18.896 | -8.323 |
| Galena | -87.492 | -72.086 |
| Gibbsite (C) | 0.834 | -7.545 |
| Goethite | -1.976 | -2.836 |
| Goslarite | -7.462 | -5.364 |
| Greenockite | -88.401 | -74.046 |
| Greigite | -337.217 | -292.182 |
| Gypsum | -4.811 | -0.195 |
| Halite | -3.902 | -5.429 |
| Hematite | -3.949 | -3.315 |
| Hercynite | -0.903 | -25.705 |
| Hg(OH)2(s) | -23.344 | -19.848 |
| Hg3O2CO3(s) | -89.871 | -60.291 |
| HgCl2(s) | -30.413 | -8.496 |
| HgSO4(s) | -28.856 | -19.348 |
| Hinsdalite | -35.473 | -32.973 |
| H-Jarosite | -16.969 | -12.937 |
| Huntite | -76.729 | -47.417 |
| Hydrocerrusite | -54.162 | -35.402 |
| Hydromagnesite | -76.153 | -68.715 |
| Hydroxyapatite | -79.38 | -35.047 |
| Hydroxylpyromorphite | -107.035 | -44.245 |
| Hydrozincite | -49.323 | -59.461 |
| K2Cr2O7(s) | -33.218 | -15.484 |
| K2CrO4(s) | -18.568 | -17.944 |
| K-Alum | -12.192 | -6.838 |
| KCl(s) | -5.496 | -6.396 |
| K-Jarosite | -18.924 | -8.543 |
| Langite | -23.017 | -41.512 |
| Larnakite | -15.156 | -14.854 |
| Laurionite | -8.358 | -8.981 |
| Lepidocrocite | -1.976 | -3.347 |
| Lime | 0.711 | -33.168 |
| Litharge | -4.82 | -17.909 |
| Mackinawite | -85.253 | -81.653 |
| Maghemite | -3.949 | -10.335 |
| Magnesioferrite | -3.297 | -21.853 |
| Magnesite | -19.197 | -11.615 |
| Magnetite | -6.53 | -11.2 |
| Malachite | -28.596 | -23.396 |
| Massicot | -4.82 | -18.117 |
| Matlockite | -18.16 | -8.985 |
| Melanothallite | -11.445 | -18.087 |
| Melanterite | -8.12 | -5.786 |
| Metacinnabar | -106.013 | -59.588 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Mg(OH)2 (active) | 0.649 | -18.145 |
| Mg2(OH)3Cl:4H2O(s) | -2.251 | -28.251 |
| Mg3(PO4)2(s) | -53.332 | -30.052 |
| MgCO3:5H2O(s) | -19.214 | -14.674 |
| MgCrO4(s) | -13.997 | -19.918 |
| MgF2(s) | -18.954 | -10.893 |
| MgHPO4:3H2O(s) | -27.004 | -8.829 |
| MgS(s) | -82.02 | -99.7 |
| Minium | 13.335 | -62.752 |
| Mirabilite | -6.28 | -4.683 |
| Mn2(SO4)3(s) | -16.773 | -12.056 |
| Montroydite | -23.341 | -19.624 |
| Morenosite | -7.637 | -5.418 |
| Na2Cr2O7(s) | -30.03 | -19.999 |
| Na2CrO4(s) | -15.38 | -18.43 |
| NaF(s) | -10.169 | -9.674 |
| Na-Jarosite | -17.33 | -12.835 |
| Natron | -20.614 | -18.902 |
| Nesquehonite | -19.207 | -14.684 |
| Ni(OH)2 (am) | -2.101 | -15.575 |
| Ni(OH)2 (c) | -2.101 | -12.891 |
| Ni3(AsO4)2:8H2O(s) | -59.491 | -33.991 |
| Ni3(PO4)2(s) | -61.581 | -30.281 |
| Ni4(OH)6SO4(s) | -13.917 | -45.917 |
| NiCO3(s) | -21.947 | -11 |
| NiS (alpha) | -84.77 | -79.25 |
| NiS (beta) | -84.77 | -73.75 |
| NiS (gamma) | -84.77 | -72.05 |
| Nsutite | 13.784 | -3.72 |
| Orpiment | -275.115 | -227.215 |
| Otavite | -25.578 | -13.526 |
| Pb azide (alpha) | -22.823 | -13.849 |
| Pb metal | -32.616 | -36.856 |
| Pb(OH)2(s) | -4.824 | -13.33 |
| Pb10(OH)6O(CO3)6(s) | -167.307 | -158.547 |
| Pb2(OH)3Cl(s) | -13.182 | -21.975 |
| Pb2O(OH)2(s) | -9.644 | -35.834 |
| Pb2O3(s) | 18.155 | -42.885 |
| Pb2OCO3(s) | -29.49 | -29.18 |
| Pb3(AsO4)2(s) | -67.631 | -32.131 |
| Pb3(PO4)2(s) | -69.749 | -26.219 |
| Pb3O2CO3(s) | -34.31 | -46.002 |
| Pb3O2SO4(s) | -19.976 | -31.144 |
| Pb4(OH)6SO4(s) | -24.807 | -45.907 |
| Pb4O3SO4(s) | -24.796 | -47.503 |
| PbCrO4(s) | -19.47 | -6.601 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| PbF2(s) | -24.427 | -16.865 |
| PbHPO4(s) | -32.466 | -8.661 |
| PbO:0.3H2O(s) | -4.821 | -17.801 |
| Periclase | 0.652 | -21.852 |
| Phosgenite | -36.562 | -16.752 |
| Plattnerite | 22.975 | -28.426 |
| Plumbgummite | -57.604 | -24.814 |
| Portlandite | 0.707 | -22.779 |
| Pyrite | -140.129 | -121.318 |
| Realgar | -110.119 | -89.389 |
| Retgersite | -7.633 | -5.565 |
| Siderite | -22.43 | -11.884 |
| Smithsonite | -21.772 | -10.895 |
| Spharelite | -84.595 | -73.592 |
| Spinel | 2.329 | -36.877 |
| Strengite | -29.625 | -3.282 |
| Struvite | -28.874 | -15.614 |
| Sulfur | -54.876 | -52.83 |
| Tenorite(am) | -4.372 | -13.256 |
| Tenorite(c) | -4.372 | -12.407 |
| Thenardite | -6.246 | -6.623 |
| Thermonatrite | -20.583 | -21.284 |
| Tsumebite | -41.672 | -31.882 |
| Vaterite | -19.138 | -11.302 |
| Vivianite | -63.057 | -25.266 |
| Wurtzite | -84.595 | -75.846 |
| Zincite | -1.923 | -13.698 |
| Zincosite | -7.438 | -11.87 |
| Zn metal | -29.719 | -56.44 |
| Zn(NO3)2:6H2O(s) | -31.026 | -34.192 |
| Zn(OH)2 (am) | -1.926 | -14.921 |
| Zn(OH)2 (beta) | -1.926 | -14.186 |
| Zn(OH)2 (delta) | -1.926 | -13.77 |
| Zn(OH)2 (epsilon) | -1.926 | -13.938 |
| Zn(OH)2 (gamma) | -1.926 | -14.158 |
| Zn2(OH)2SO4(s) | -9.365 | -16.865 |
| Zn2(OH)3Cl(s) | -7.387 | -22.578 |
| Zn3(PO4)2:4H2O(s) | -61.07 | -25.65 |
| Zn3AsO42:2.5H2O(s) | -58.948 | -31.448 |
| Zn3O(SO4)2(s) | -16.8 | -37.282 |
| Zn4(OH)6SO4(s) | -13.217 | -41.617 |
| Zn5(OH)8Cl2(s) | -16.701 | -55.201 |
| Zn-Al LDH(s) | -12.942 | -32.772 |
| ZnCl2(s) | -8.996 | -16.486 |
| ZnCO3(s) | -21.772 | -10.972 |
| ZnCO3:1H2O(s) | -21.775 | -11.515 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| ZnF2(s) | -21.529 | -21.358 |
| ZnSO4:1H2O(s) | -7.442 | -7.072 |

## B3.8: Eh 800

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 0.812 | -10.663 |
| Al(OH)3 (Soil) | 0.812 | -8.117 |
| Al2O3(s) | 1.634 | -19.591 |
| Al4(OH)10SO4(s) | -2.251 | -24.951 |
| AlAsO4:2H2O(s) | -25.773 | -9.973 |
| AlOHF2(s) | -18.781 | -19.188 |
| AlOHSO4(s) | -4.686 | -1.456 |
| Alunite | -10.53 | -10.407 |
| Anglesite | -10.337 | -2.474 |
| Anhydrite | -4.807 | -0.49 |
| Antlerite | -18.672 | -27.46 |
| Aragonite | -19.154 | -10.875 |
| Arsenolite | -34.058 | -32.496 |
| Artinite | -18.59 | -28.921 |
| As2O5(s) | -53.166 | -18.457 |
| As2S3(am) | -323.813 | -277.429 |
| Atacamite | -12.309 | -20.268 |
| Azurite | -52.865 | -35.711 |
| Bianchite | -7.46 | -5.699 |
| Birnessite | 15.5 | -2.591 |
| Bixbyite | -0.277 | -0.389 |
| Boehmite | 0.815 | -8.478 |
| Brochantite | -23.063 | -39.518 |
| Brucite | 0.633 | -17.16 |
| Ca3(AsO4)2:4H2O(s) | -51.095 | -32.195 |
| Ca3(PO4)2 (am1) | -53.197 | -28.269 |
| Ca3(PO4)2 (am2) | -53.197 | -25.476 |
| Ca3(PO4)2 (beta) | -53.197 | -23.949 |
| Ca4H(PO4)3:3H2O(s) | -80.155 | -32.844 |
| CaCO3xH2O(s) | -19.157 | -12.07 |
| CaCrO4(s) | -13.947 | -11.845 |
| CaHPO4(s) | -26.948 | -7.484 |
| CaHPO4:2H2O(s) | -26.955 | -7.82 |
| Calcite | -19.154 | -10.724 |
| CaS(s) | -95.89 | -107.07 |
| Cd metal (alpha) | -37.022 | -50.995 |
| Cd metal (gamma) | -37.022 | -51.101 |
| Cd(OH)2(s) | -5.748 | -19.967 |
| Cd3(OH)4SO4(s) | -22.742 | -45.302 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cd3(PO4)2(s) | -72.516 | -39.916 |
| Cd3OH2(SO4)2(s) | -28.24 | -34.95 |
| Cd4(OH)6SO4(s) | -28.49 | -56.89 |
| CdCl2(s) | -12.801 | -12.255 |
| CdCl2:1H2O(s) | -12.804 | -11.156 |
| CdCl2:2.5H2O(s) | -12.809 | -10.852 |
| CdF2(s) | -25.341 | -24.409 |
| CdOHCl(s) | -9.274 | -13 |
| CdSO4(s) | -11.246 | -11.39 |
| CdSO4:1H2O(s) | -11.249 | -9.715 |
| CdSO4:2.67H2O(s) | -11.255 | -9.492 |
| Cerrusite | -24.685 | -11.334 |
| Chalcanthite | -9.906 | -7.23 |
| Chalcopyrite | -201.882 | -165.709 |
| Chloropyromorphite(c) | -110.629 | -26.199 |
| Chloropyromorphite(soil) | -110.629 | -30.229 |
| Cinnabar | -119.942 | -73.119 |
| Claudetite | -34.058 | -32.546 |
| Cotunnite | -11.892 | -6.953 |
| Covellite | -100.973 | -78.163 |
| Cr(VI)-Ettringite | -38.23 | -101.631 |
| Cr(VI)-Jarosite | -37.192 | -18.676 |
| CrO3(s) | -14.642 | -11.463 |
| Cryolite | -59.093 | -25.022 |
| Cu azide | -22.391 | -14.549 |
| Cu(OH)2(s) | -4.391 | -14.004 |
| Cu2(OH)3NO3(s) | -14.145 | -23.838 |
| Cu3(AsO4)2:2H2O(s) | -66.336 | -31.236 |
| Cu3(PO4)2(s) | -68.446 | -31.596 |
| Cu3(PO4)2:3H2O(s) | -68.456 | -33.336 |
| CuCO3(s) | -24.237 | -12.737 |
| CuCrO4(s) | -19.029 | -13.589 |
| CuF2(s) | -23.984 | -25.506 |
| CuF2:2H2O(s) | -23.991 | -19.534 |
| CuOCuSO4(s) | -14.277 | -25.418 |
| Cupric Ferrite | -8.342 | -15.608 |
| CuSO4(s) | -9.889 | -13.273 |
| Diaspore | 0.815 | -6.684 |
| Dolomite (disordered) | -38.367 | -22.109 |
| Dolomite (ordered) | -38.367 | -21.517 |
| Epsomite | -4.889 | -2.692 |
| Ettringite | -10.809 | -69.998 |
| FCO3-Apatite | -174.364 | -58.962 |
| Fe(OH)2 (am) | -4.327 | -18.374 |
| Fe(OH)2 (c) | -4.327 | -17.217 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe2(SO4)3(s) | -20.459 | -18.196 |
| Fe3(OH)8(s) | -8.292 | -28.514 |
| FeAsO4:2H2O(s) | -28.567 | -8.367 |
| Ferrihydrite | -1.982 | -5.792 |
| Ferrihydrite (aged) | -1.982 | -5.282 |
| FeS (ppt) | -100.909 | -98.026 |
| Fluorite | -18.901 | -8.328 |
| Galena | -101.421 | -86.014 |
| Gibbsite (C) | 0.812 | -7.567 |
| Goethite | -1.979 | -2.838 |
| Goslarite | -7.464 | -5.366 |
| Greenockite | -102.33 | -87.975 |
| Greigite | -394.618 | -349.583 |
| Gypsum | -4.813 | -0.197 |
| Halite | -3.902 | -5.429 |
| Hematite | -3.954 | -3.32 |
| Hercynite | -2.69 | -27.492 |
| Hg(OH)2(s) | -23.36 | -19.864 |
| Hg3O2CO3(s) | -89.92 | -60.34 |
| HgCl2(s) | -30.413 | -8.496 |
| HgSO4(s) | -28.859 | -19.35 |
| Hinsdalite | -35.538 | -33.038 |
| H-Jarosite | -16.949 | -12.917 |
| Huntite | -76.792 | -47.479 |
| Hydrocerrusite | -54.208 | -35.448 |
| Hydromagnesite | -76.231 | -68.793 |
| Hydroxyapatite | -79.45 | -35.117 |
| Hydroxylpyromorphite | -107.103 | -44.313 |
| Hydrozincite | -49.401 | -59.538 |
| K2Cr2O7(s) | -33.219 | -15.485 |
| K2CrO4(s) | -18.577 | -17.953 |
| K-Alum | -12.195 | -6.841 |
| KCl(s) | -5.496 | -6.396 |
| K-Jarosite | -18.912 | -8.531 |
| Langite | -23.066 | -41.561 |
| Larnakite | -15.173 | -14.871 |
| Laurionite | -8.365 | -8.988 |
| Lepidocrocite | -1.979 | -3.35 |
| Lime | 0.695 | -33.183 |
| Litharge | -4.836 | -17.924 |
| Mackinawite | -100.909 | -97.309 |
| Maghemite | -3.954 | -10.34 |
| Magnesioferrite | -3.318 | -21.873 |
| Magnesite | -19.213 | -11.631 |
| Magnetite | -8.278 | -12.949 |
| Malachite | -28.628 | -23.428 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Massicot | -4.836 | -18.132 |
| Matlockite | -18.162 | -8.987 |
| Melanothallite | -11.444 | -18.087 |
| Melanterite | -9.849 | -7.516 |
| Metacinnabar | -119.942 | -73.518 |
| Mg(OH)2 (active) | 0.633 | -18.161 |
| Mg2(OH)3Cl:4H2O(s) | -2.274 | -28.274 |
| Mg3(PO4)2(s) | -53.373 | -30.093 |
| MgCO3:5H2O(s) | -19.23 | -14.69 |
| MgCrO4(s) | -14.005 | -19.926 |
| MgF2(s) | -18.96 | -10.899 |
| MgHPO4:3H2O(s) | -27.017 | -8.842 |
| MgS(s) | -95.949 | -113.629 |
| Minium | 16.77 | -59.316 |
| Mirabilite | -6.283 | -4.686 |
| Mn2(SO4)3(s) | -16.782 | -12.064 |
| Montroydite | -23.357 | -19.64 |
| Morenosite | -7.639 | -5.42 |
| Na2Cr2O7(s) | -30.031 | -20 |
| Na2CrO4(s) | -15.389 | -18.439 |
| NaF(s) | -10.172 | -9.677 |
| Na-Jarosite | -17.318 | -12.823 |
| Natron | -20.63 | -18.919 |
| Nesquehonite | -19.223 | -14.7 |
| Ni(OH)2 (am) | -2.117 | -15.59 |
| Ni(OH)2 (c) | -2.117 | -12.907 |
| Ni3(AsO4)2:8H2O(s) | -59.534 | -34.034 |
| Ni3(PO4)2(s) | -61.623 | -30.323 |
| Ni4(OH)6SO4(s) | -13.966 | -45.966 |
| NiCO3(s) | -21.963 | -11.015 |
| NiS (alpha) | -98.699 | -93.179 |
| NiS (beta) | -98.699 | -87.679 |
| NiS (gamma) | -98.699 | -85.979 |
| Nsutite | 15.5 | -2.004 |
| Orpiment | -323.813 | -275.914 |
| Otavite | -25.593 | -13.542 |
| Pb azide (alpha) | -22.838 | -13.864 |
| Pb metal | -36.113 | -40.354 |
| Pb(OH)2(s) | -4.839 | -13.345 |
| Pb10(OH)6O(CO3)6(s) | -167.46 | -158.7 |
| Pb2(OH)3Cl(s) | -13.204 | -21.997 |
| Pb2O(OH)2(s) | -9.675 | -35.865 |
| Pb2O3(s) | 21.606 | -39.434 |
| Pb2OCO3(s) | -29.52 | -29.211 |
| Pb3(AsO4)2(s) | -67.673 | -32.173 |
| Pb3(PO4)2(s) | -69.789 | -26.259 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb3O2CO3(s) | -34.356 | -46.048 |
| Pb3O2SO4(s) | -20.008 | -31.176 |
| Pb4(OH)6SO4(s) | -24.854 | -45.954 |
| Pb4O3SO4(s) | -24.844 | -47.551 |
| PbCrO4(s) | -19.477 | -6.609 |
| PbF2(s) | -24.432 | -16.87 |
| PbHPO4(s) | -32.478 | -8.673 |
| PbO:0.3H2O(s) | -4.837 | -17.817 |
| Periclase | 0.636 | -21.867 |
| Phosgenite | -36.576 | -16.766 |
| Plattnerite | 26.442 | -24.96 |
| Plumbgummite | -57.679 | -24.889 |
| Portlandite | 0.692 | -22.794 |
| Pyrite | -166.217 | -147.405 |
| Realgar | -129.253 | -108.523 |
| Retgersite | -7.636 | -5.568 |
| Siderite | -24.173 | -13.627 |
| Smithsonite | -21.787 | -10.911 |
| Spharelite | -98.524 | -87.521 |
| Spinel | 2.27 | -36.936 |
| Strengite | -29.625 | -3.282 |
| Struvite | -33.637 | -20.377 |
| Sulfur | -65.308 | -63.262 |
| Tenorite(am) | -4.388 | -13.272 |
| Tenorite(c) | -4.388 | -12.422 |
| Thenardite | -6.249 | -6.626 |
| Thermonatrite | -20.6 | -21.3 |
| Tsumebite | -41.715 | -31.925 |
| Vaterite | -19.154 | -11.318 |
| Vivianite | -68.281 | -30.49 |
| Wurtzite | -98.524 | -89.775 |
| Zincite | -1.939 | -13.713 |
| Zincosite | -7.44 | -11.872 |
| Zn metal | -33.216 | -59.937 |
| Zn(NO3)2:6H2O(s) | -12.688 | -15.854 |
| Zn(OH)2 (am) | -1.942 | -14.936 |
| Zn(OH)2 (beta) | -1.942 | -14.201 |
| Zn(OH)2 (delta) | -1.942 | -13.786 |
| Zn(OH)2 (epsilon) | -1.942 | -13.954 |
| Zn(OH)2 (gamma) | -1.942 | -14.173 |
| Zn2(OH)2SO4(s) | -9.382 | -16.882 |
| Zn2(OH)3Cl(s) | -7.41 | -22.601 |
| Zn3(PO4)2:4H2O(s) | -61.111 | -25.691 |
| Zn3AsO42:2.5H2O(s) | -58.99 | -31.49 |
| Zn3O(SO4)2(s) | -16.819 | -37.301 |
| Zn4(OH)6SO4(s) | -13.266 | -41.666 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn5(OH)8Cl2(s) | -16.762 | -55.262 |
| Zn-Al LDH(s) | -12.995 | -32.825 |
| ZnCl2(s) | -8.995 | -16.486 |
| ZnCO3(s) | -21.787 | -10.987 |
| ZnCO3:1H2O(s) | -21.791 | -11.531 |
| ZnF2(s) | -21.535 | -21.363 |
| ZnSO4:1H2O(s) | -7.443 | -7.073 |

## B3.9: Eh 900

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 0.807 | -10.668 |
| Al(OH)3 (Soil) | 0.807 | -8.121 |
| Al2O3(s) | 1.624 | -19.6 |
| Al4(OH)10SO4(s) | -2.267 | -24.967 |
| AlAsO4:2H2O(s) | -25.777 | -9.977 |
| AlOHF2(s) | -18.784 | -19.191 |
| AlOHSO4(s) | -4.688 | -1.458 |
| Alunite | -10.54 | -10.417 |
| Anglesite | -10.338 | -2.475 |
| Anhydrite | -4.807 | -0.491 |
| Antlerite | -18.679 | -27.467 |
| Aragonite | -19.158 | -10.879 |
| Arsenolite | -41.047 | -39.484 |
| Artinite | -18.597 | -28.928 |
| As2O5(s) | -53.165 | -18.456 |
| As2S3(am) | -372.727 | -326.343 |
| Atacamite | -12.314 | -20.273 |
| Azurite | -52.875 | -35.722 |
| Bianchite | -7.461 | -5.7 |
| Birnessite | 17.242 | -0.849 |
| Bixbyite | -0.289 | -0.401 |
| Boehmite | 0.811 | -8.483 |
| Brochantite | -23.074 | -39.529 |
| Brucite | 0.629 | -17.164 |
| Ca3(AsO4)2:4H2O(s) | -51.105 | -32.205 |
| Ca3(PO4)2 (am1) | -53.207 | -28.278 |
| Ca3(PO4)2 (am2) | -53.207 | -25.486 |
| Ca3(PO4)2 (beta) | -53.207 | -23.958 |
| Ca4H(PO4)3:3H2O(s) | -80.168 | -32.856 |
| CaCO3xH2O(s) | -19.161 | -12.074 |
| CaCrO4(s) | -13.949 | -11.847 |
| CaHPO4(s) | -26.951 | -7.487 |
| CaHPO4:2H2O(s) | -26.958 | -7.823 |
| Calcite | -19.158 | -10.727 |
| CaS(s) | -109.869 | -121.049 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cd metal (alpha) | -40.52 | -54.493 |
| Cd metal (gamma) | -40.52 | -54.599 |
| Cd(OH)2(s) | -5.751 | -19.971 |
| Cd3(OH)4SO4(s) | -22.75 | -45.31 |
| Cd3(PO4)2(s) | -72.525 | -39.925 |
| Cd3OH2(SO4)2(s) | -28.245 | -34.955 |
| Cd4(OH)6SO4(s) | -28.501 | -56.901 |
| CdCl2(s) | -12.801 | -12.255 |
| CdCl2:1H2O(s) | -12.804 | -11.156 |
| CdCl2:2.5H2O(s) | -12.809 | -10.852 |
| CdF2(s) | -25.343 | -24.411 |
| CdOHCl(s) | -9.276 | -13.001 |
| CdSO4(s) | -11.247 | -11.391 |
| CdSO4:1H2O(s) | -11.25 | -9.716 |
| CdSO4:2.67H2O(s) | -11.256 | -9.492 |
| Cerrusite | -24.688 | -11.337 |
| Chalcanthite | -9.907 | -7.23 |
| Chalcopyrite | -231.584 | -195.411 |
| Chloropyromorphite(c) | -110.643 | -26.213 |
| Chloropyromorphite(soil) | -110.643 | -30.243 |
| Cinnabar | -133.921 | -87.098 |
| Claudetite | -41.047 | -39.534 |
| Cotunnite | -11.892 | -6.953 |
| Covellite | -114.952 | -92.142 |
| Cr(VI)-Ettringite | -38.255 | -101.656 |
| Cr(VI)-Jarosite | -37.192 | -18.676 |
| CrO3(s) | -14.64 | -11.461 |
| Cryolite | -59.098 | -25.027 |
| Cu azide | -22.394 | -14.553 |
| Cu(OH)2(s) | -4.395 | -14.008 |
| Cu2(OH)3NO3(s) | -13.941 | -23.634 |
| Cu3(AsO4)2:2H2O(s) | -66.346 | -31.246 |
| Cu3(PO4)2(s) | -68.455 | -31.605 |
| Cu3(PO4)2:3H2O(s) | -68.465 | -33.345 |
| CuCO3(s) | -24.24 | -12.74 |
| CuCrO4(s) | -19.031 | -13.591 |
| CuF2(s) | -23.986 | -25.508 |
| CuF2:2H2O(s) | -23.993 | -19.535 |
| CuOCuSO4(s) | -14.281 | -25.422 |
| Cupric Ferrite | -8.346 | -15.613 |
| CuSO4(s) | -9.89 | -13.274 |
| Diaspore | 0.811 | -6.689 |
| Dolomite (disordered) | -38.374 | -22.116 |
| Dolomite (ordered) | -38.374 | -21.524 |
| Epsomite | -4.89 | -2.693 |
| Ettringite | -10.831 | -70.02 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| FCO3-Apatite | -174.393 | -58.991 |
| Fe(OH)2 (am) | -6.075 | -20.122 |
| Fe(OH)2 (c) | -6.075 | -18.965 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -20.451 | -18.188 |
| Fe3(OH)8(s) | -10.04 | -30.262 |
| FeAsO4:2H2O(s) | -28.567 | -8.367 |
| Ferrihydrite | -1.983 | -5.793 |
| Ferrihydrite (aged) | -1.983 | -5.283 |
| FeS (ppt) | -116.632 | -113.749 |
| Fluorite | -18.903 | -8.33 |
| Galena | -115.399 | -99.993 |
| Gibbsite (C) | 0.807 | -7.571 |
| Goethite | -1.979 | -2.839 |
| Goslarite | -7.464 | -5.367 |
| Greenockite | -116.308 | -101.954 |
| Greigite | -452.268 | -407.233 |
| Gypsum | -4.814 | -0.198 |
| Halite | -3.902 | -5.429 |
| Hematite | -3.955 | -3.321 |
| Hercynite | -4.447 | -29.249 |
| Hg(OH)2(s) | -23.364 | -19.868 |
| Hg3O2CO3(s) | -89.931 | -60.351 |
| HgCl2(s) | -30.413 | -8.496 |
| HgSO4(s) | -28.859 | -19.351 |
| Hinsdalite | -35.552 | -33.052 |
| H-Jarosite | -16.945 | -12.912 |
| Huntite | -76.806 | -47.493 |
| Hydrocerrusite | -54.218 | -35.458 |
| Hydromagnesite | -76.249 | -68.811 |
| Hydroxyapatite | -79.466 | -35.133 |
| Hydroxylpyromorphite | -107.118 | -44.328 |
| Hydrozincite | -49.418 | -59.556 |
| K2Cr2O7(s) | -33.219 | -15.486 |
| K2CrO4(s) | -18.579 | -17.955 |
| K-Alum | -12.195 | -6.842 |
| KCl(s) | -5.496 | -6.396 |
| K-Jarosite | -18.91 | -8.529 |
| Langite | -23.077 | -41.573 |
| Larnakite | -15.177 | -14.875 |
| Laurionite | -8.367 | -8.99 |
| Lepidocrocite | -1.979 | -3.35 |
| Lime | 0.691 | -33.187 |
| Litharge | -4.839 | -17.927 |
| Mackinawite | -116.632 | -113.032 |
| Maghemite | -3.955 | -10.341 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Magnesioferrite | -3.322 | -21.878 |
| Magnesite | -19.216 | -11.635 |
| Magnetite | -10.027 | -14.697 |
| Malachite | -28.635 | -23.435 |
| Massicot | -4.839 | -18.135 |
| Matlockite | -18.163 | -8.988 |
| Melanothallite | -11.444 | -18.087 |
| Melanterite | -11.594 | -9.261 |
| Metacinnabar | -133.921 | -87.497 |
| Mg(OH)2 (active) | 0.629 | -18.165 |
| Mg2(OH)3Cl:4H2O(s) | -2.279 | -28.279 |
| Mg3(PO4)2(s) | -53.383 | -30.103 |
| MgCO3:5H2O(s) | -19.233 | -14.693 |
| MgCrO4(s) | -14.007 | -19.928 |
| MgF2(s) | -18.962 | -10.9 |
| MgHPO4:3H2O(s) | -27.02 | -8.845 |
| MgS(s) | -109.928 | -127.608 |
| Minium | 20.255 | -55.832 |
| Mirabilite | -6.284 | -4.687 |
| Mn2(SO4)3(s) | -16.785 | -12.067 |
| Montroydite | -23.361 | -19.644 |
| Morenosite | -7.64 | -5.421 |
| Na2Cr2O7(s) | -30.031 | -20.001 |
| Na2CrO4(s) | -15.391 | -18.441 |
| NaF(s) | -10.173 | -9.678 |
| Na-Jarosite | -17.316 | -12.821 |
| Natron | -20.634 | -18.922 |
| Nesquehonite | -19.226 | -14.704 |
| Ni(OH)2 (am) | -2.121 | -15.594 |
| Ni(OH)2 (c) | -2.121 | -12.911 |
| Ni3(AsO4)2:8H2O(s) | -59.544 | -34.044 |
| Ni3(PO4)2(s) | -61.633 | -30.333 |
| Ni4(OH)6SO4(s) | -13.978 | -45.978 |
| NiCO3(s) | -21.966 | -11.019 |
| NiS (alpha) | -112.678 | -107.158 |
| NiS (beta) | -112.678 | -101.658 |
| NiS (gamma) | -112.678 | -99.958 |
| Nsutite | 17.242 | -0.262 |
| Orpiment | -372.727 | -324.828 |
| Otavite | -25.597 | -13.546 |
| Pb azide (alpha) | -22.842 | -13.867 |
| Pb metal | -39.611 | -43.851 |
| Pb(OH)2(s) | -4.842 | -13.348 |
| Pb10(OH)6O(CO3)6(s) | -167.493 | -158.733 |
| Pb2(OH)3Cl(s) | -13.209 | -22.002 |
| Pb2O(OH)2(s) | -9.681 | -35.871 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O3(s) | 25.094 | -35.946 |
| Pb2OCO3(s) | -29.527 | -29.217 |
| Pb3(AsO4)2(s) | -67.682 | -32.182 |
| Pb3(PO4)2(s) | -69.798 | -26.268 |
| Pb3O2CO3(s) | -34.366 | -46.058 |
| Pb3O2SO4(s) | -20.016 | -31.183 |
| Pb4(OH)6SO4(s) | -24.865 | -45.965 |
| Pb4O3SO4(s) | -24.855 | -47.561 |
| PbCrO4(s) | -19.479 | -6.61 |
| PbF2(s) | -24.434 | -16.872 |
| PbHPO4(s) | -32.481 | -8.676 |
| PbO:0.3H2O(s) | -4.84 | -17.82 |
| Periclase | 0.633 | -21.871 |
| Phosgenite | -36.58 | -16.77 |
| Plattnerite | 29.933 | -21.469 |
| Plumbgummite | -57.695 | -24.905 |
| Portlandite | 0.688 | -22.798 |
| Pyrite | -192.421 | -173.609 |
| Realgar | -148.469 | -127.74 |
| Retgersite | -7.636 | -5.568 |
| Siderite | -25.921 | -15.375 |
| Smithsonite | -21.791 | -10.914 |
| Spharelite | -112.502 | -101.5 |
| Spinel | 2.257 | -36.949 |
| Strengite | -29.625 | -3.282 |
| Struvite | -47.407 | -34.147 |
| Sulfur | -75.788 | -73.743 |
| Tenorite(am) | -4.391 | -13.276 |
| Tenorite(c) | -4.391 | -12.426 |
| Thenardite | -6.25 | -6.627 |
| Thermonatrite | -20.603 | -21.304 |
| Tsumebite | -41.725 | -31.935 |
| Vaterite | -19.158 | -11.321 |
| Vivianite | -73.523 | -35.733 |
| Wurtzite | -112.502 | -103.754 |
| Zincite | -1.942 | -13.717 |
| Zincosite | -7.441 | -11.872 |
| Zn metal | -36.714 | -63.435 |
| Zn(NO3)2:6H2O(s) | -12.269 | -15.435 |
| Zn(OH)2 (am) | -1.945 | -14.94 |
| Zn(OH)2 (beta) | -1.945 | -14.205 |
| Zn(OH)2 (delta) | -1.945 | -13.789 |
| Zn(OH)2 (epsilon) | -1.945 | -13.957 |
| Zn(OH)2 (gamma) | -1.945 | -14.177 |
| Zn2(OH)2SO4(s) | -9.386 | -16.886 |
| Zn2(OH)3Cl(s) | -7.415 | -22.606 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn3(PO4)2:4H2O(s) | -61.121 | -25.701 |
| Zn3AsO42:2.5H2O(s) | -59 | -31.5 |
| Zn3O(SO4)2(s) | -16.823 | -37.306 |
| Zn4(OH)6SO4(s) | -13.277 | -41.677 |
| Zn5(OH)8Cl2(s) | -16.776 | -55.276 |
| Zn-Al LDH(s) | -13.006 | -32.836 |
| ZnCl2(s) | -8.995 | -16.486 |
| ZnCO3(s) | -21.791 | -10.991 |
| ZnCO3:1H2O(s) | -21.794 | -11.534 |
| ZnF2(s) | -21.537 | -21.365 |
| ZnSO4:1H2O(s) | -7.444 | -7.074 |

# B4 Mass distribution

## B4.1: Eh 100

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.002025 | 42.035 | 0 | 0 | 0.002793 | 57.965 |
| AsO4-3 | 8.34E-14 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.02595 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 8.12E-14 | 0 | 0 | 0 | 7.87E-08 | 100 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.028113 | 100 | 0 | 0 | 7.87E-08 | 0 |
| Fe+3 | 9.41E-12 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.002603 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.69E-14 | 0.019 | 0 | 0 | 2.49E-10 | 99.981 |
| HS-1 | 1.9E-10 | 0.12 | 0 | 0 | 1.58E-07 | 99.88 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.04E-59 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 5.33E-79 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| SO4-2 | 0.038848 | 93.293 | 0 | 0 | 0.002793 | 6.707 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B3.2: Eh 200

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004009 | 83.203 | 0 | 0 | 0.000809 | 16.797 |
| AsO4-3 | 3.45E-11 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.02595 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.028114 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 3.62E-10 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.003195 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.47E-21 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.61E-51 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 5.25E-68 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.040831 | 98.057 | 0 | 0 | 0.000809 | 1.943 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.3: Eh 300

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 1.38E-08 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.024111 | 92.913 | 0 | 0 | 0.001839 | 7.087 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.021983 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.27E-08 | 0 | 0 | 0 | 0.006131 | 100 |
| H+1 | 0.004467 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.93E-06 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.6E-32 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 2.42E-43 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 4.2E-57 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.4: Eh 400

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 7.77E-07 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.022798 | 87.854 | 0 | 0 | 0.003152 | 12.146 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.017607 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 3.9E-07 | 0.004 | 0 | 0 | 0.010506 | 99.996 |
| H+1 | 0.011907 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.17E-06 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.86E-40 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 2.69E-37 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 3.13E-49 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.5: Eh 500

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 4.82E-06 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.01941 | 74.798 | 0 | 0 | 0.00654 | 25.202 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.006308 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 6.37E-06 | 0.029 | 0 | 0 | 0.021799 | 99.971 |
| H+1 | 0.031112 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 1.25E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.14E-49 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 3.25E-30 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 4.71E-40 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.6: Eh 600

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.0176 | 67.822 | 0 | 0 | 0.00835 | 32.178 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.000266 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.44E-05 | 0.052 | 0 | 0 | 0.027833 | 99.948 |
| H+1 | 0.041361 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 8.36E-11 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 2.63E-62 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 5E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.11E-20 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.97E-27 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 2E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.04164 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.7: Eh 700

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.017522 | 67.521 | 0 | 0 | 0.008428 | 32.479 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 4.89E-06 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.48E-05 | 0.053 | 0 | 0 | 0.028094 | 99.947 |
| H+1 | 0.041804 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 2.73E-14 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 3.01E-76 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 5E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 3.18E-10 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.72E-13 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 2E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.04164 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.8: Eh 800

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.01752 | 67.517 | 0 | 0 | 0.008429 | 32.483 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 9.15E-08 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.55E-05 | 0.055 | 0 | 0 | 0.028098 | 99.945 |
| H+1 | 0.042635 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 9.04E-18 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 3.67E-90 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 7.46E-09 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 0.000158 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 0.000254 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## B4.9: Eh 900

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.004818 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 4.95E-06 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.009232 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 5.34E-09 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.01752 | 67.517 | 0 | 0 | 0.008429 | 32.483 |
| CO3-2 | 0.000967 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 4.42E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 7.87E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.001399 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 0.000121 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 1.65E-09 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.56E-05 | 0.056 | 0 | 0 | 0.028098 | 99.944 |
| H+1 | 0.042634 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 2.9E-21 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 2.49E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 3.9E-104 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.007406 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 4.55E-05 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 0.00005 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.012614 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 1.28E-22 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 1.47E-05 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 8.2E-08 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 0.000412 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 4.83E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 0.000002 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.041641 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

# B5 Finite solids

## B5.1: Eh 100

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Metacinnabar | 2.49E-10 |
| Chalcopyrite | 7.87E-08 |
| AlOHSO4(s) | 2.79E-03 |

## B5.2: Eh 200

| Solid | Equilibrium amount (mol/l) |
|---|---|
| AlOHSO4(s) | 8.09E-04 |

## B5.3: Eh 300

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 6.13E-03 |

## B5.4: Eh 400

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 1.05E-02 |

## B5.5: Eh 500

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.18E-02 |

## B5.6: Eh 600

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.78E-02 |

## B5.7: Eh 700

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.81E-02 |

## B5.8: Eh 800

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.81E-02 |

## B5.9: Eh 900

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.81E-02 |

# **Appendix C** - Lime dosing of water discharge from Big Swamp into Reach 3 of Boundary Creek

# C1: Aqueous species

## C1.1 pH 2

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 4.28E-06 | 4.24E-06 | -5.372 |
| Al(OH)2+ | 2.19E-11 | 1.83E-11 | -10.739 |
| Al(OH)3 (aq) | 3.41E-16 | 3.45E-16 | -15.463 |
| Al(OH)4- | 1.87E-20 | 1.54E-20 | -19.812 |
| Al(SO4)2- | 0.000103 | 8.5E-05 | -4.07 |
| Al+3 | 0.000799 | 0.0002 | -3.7 |
| Al2(OH)2+4 | 6.05E-11 | 2.84E-12 | -11.547 |
| Al2(OH)2CO3+2 | 6.41E-15 | 2.98E-15 | -14.525 |
| Al2PO4+3 | 3.17E-10 | 5.67E-11 | -10.246 |
| Al3(OH)4+5 | 1.72E-16 | 1.45E-18 | -17.84 |
| AlCl+2 | 3.01E-06 | 1.4E-06 | -5.854 |
| AlF+2 | 1.31E-05 | 6.3E-06 | -5.2 |
| AlF2+ | 9.86E-09 | 8.21E-09 | -8.086 |
| AlF3 (aq) | 3.12E-13 | 3.16E-13 | -12.501 |
| AlF4- | 6.31E-19 | 5.21E-19 | -18.283 |
| AlHPO4+ | 3.69E-08 | 3.05E-08 | -7.516 |
| AlOH+2 | 2.14E-07 | 1.03E-07 | -6.988 |
| AlSO4+ | 0.001857 | 0.001533 | -2.814 |
| As3S4(HS)- | 3.1E-130 | 2.5E-130 | -129.598 |
| AsO4-3 | 1.28E-26 | 2.29E-27 | -26.641 |
| AsS(OH)HS- | 1.41E-48 | 1.17E-48 | -47.933 |
| Ca DOM1 | 2.18E-07 | 1.93E-07 | -6.714 |
| Ca(NH3)2+2 | 3.34E-24 | 1.55E-24 | -23.809 |
| Ca(NO3)2 | 3.5E-138 | 3.5E-138 | -137.457 |
| Ca+2 | 0.003614 | 0.001812 | -2.742 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCl+ | 8.97E-05 | 7.41E-05 | -4.13 |
| CaCO3 (aq) | 9.38E-16 | 9.48E-16 | -15.023 |
| CaCrO4 (aq) | 1E-11 | 1.01E-11 | -10.995 |
| CaF+ | 8.15E-11 | 6.77E-11 | -10.17 |
| CaH2PO4+ | 2.95E-08 | 2.46E-08 | -7.609 |
| CaHCO3+ | 2.24E-09 | 1.88E-09 | -8.726 |
| CaHPO4 (aq) | 3.02E-12 | 3.05E-12 | -11.515 |
| CaNH3+2 | 2.05E-13 | 9.54E-14 | -13.02 |
| CaNO3+ | 5.84E-68 | 4.82E-68 | -67.317 |
| CaOH+ | 1.77E-14 | 1.48E-14 | -13.829 |
| CaPO4- | 7.8E-19 | 6.5E-19 | -18.187 |
| CaSO4 (aq) | 0.00049 | 0.000495 | -3.305 |
| Cd DOM1 | 7.82E-13 | 6.92E-13 | -12.16 |
| Cd(CO3)2-2 | 1.27E-32 | 5.9E-33 | -32.229 |
| Cd(HS)2 (aq) | 1.13E-51 | 1.14E-51 | -50.944 |
| Cd(HS)3- | 1.28E-78 | 1.05E-78 | -77.977 |
| Cd(HS)4-2 | 5.3E-105 | 2.5E-105 | -104.61 |
| Cd(NH3)2+2 | 7.4E-26 | 3.45E-26 | -25.463 |
| Cd(NH3)3+2 | 3.03E-35 | 1.41E-35 | -34.85 |
| Cd(NH3)4+2 | 3.66E-45 | 1.7E-45 | -44.769 |
| Cd(NO2)2 (aq) | 1.6E-105 | 1.6E-105 | -104.783 |
| Cd(NO3)2 (aq) | 2.5E-139 | 2.5E-139 | -138.603 |
| Cd(OH)2 (aq) | 1.3E-25 | 1.31E-25 | -24.882 |
| Cd(OH)3- | 1.57E-36 | 1.29E-36 | -35.888 |
| Cd(OH)4-2 | 2.86E-48 | 1.33E-48 | -47.876 |
| Cd(SO4)2-2 | 3.05E-11 | 1.42E-11 | -10.848 |
| Cd+2 | 5.55E-09 | 2.58E-09 | -8.588 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cd2OH+3 | 7.88E-25 | 1.41E-25 | -24.851 |
| CdCl+ | 5E-09 | 4.13E-09 | -8.384 |
| CdCl2 (aq) | 2.83E-10 | 2.86E-10 | -9.544 |
| CdCO3 (aq) | 2.2E-20 | 2.22E-20 | -19.654 |
| CdF+ | 1.52E-16 | 1.26E-16 | -15.901 |
| CdHCO3+ | 7.75E-15 | 6.4E-15 | -14.194 |
| CdHPO4 (aq) | 4.58E-17 | 4.63E-17 | -16.334 |
| CdHS+ | 4.7E-30 | 3.88E-30 | -29.411 |
| CdNH3+2 | 3.74E-17 | 1.74E-17 | -16.759 |
| CdNO2+ | 3.79E-57 | 3.13E-57 | -56.504 |
| CdNO3+ | 1.04E-73 | 8.56E-74 | -73.068 |
| CdOH+ | 1.16E-17 | 9.59E-18 | -17.018 |
| CdSO4 (aq) | 6.99E-10 | 7.07E-10 | -9.151 |
| Cl-1 | 0.02117 | 0.017213 | -1.764 |
| CO3-2 | 7.62E-16 | 3.67E-16 | -15.436 |
| Cr2O7-2 | 8.65E-12 | 4.03E-12 | -11.395 |
| CrO3Cl- | 4.02E-10 | 3.32E-10 | -9.479 |
| CrO3H2PO4- | 3.95E-12 | 3.26E-12 | -11.486 |
| CrO3HPO4-2 | 1.46E-12 | 6.78E-13 | -12.169 |
| CrO3SO4-2 | 2.65E-09 | 1.23E-09 | -8.91 |
| CrO4-2 | 2.08E-11 | 9.48E-12 | -11.023 |
| Cu DOM1 | 3.23E-10 | 2.86E-10 | -9.544 |
| Cu(CO3)2-2 | 1.23E-28 | 5.71E-29 | -28.243 |
| Cu(N3)2 (aq) | 2.82E-18 | 2.85E-18 | -17.545 |
| Cu(N3)3- | 9.68E-24 | 8E-24 | -23.097 |
| Cu(N3)4-2 | 2.53E-30 | 1.18E-30 | -29.929 |
| Cu(NH3)2+2 | 6.57E-22 | 3.06E-22 | -21.515 |
| Cu(NH3)3+2 | 8.82E-30 | 4.1E-30 | -29.387 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NH3)4+2 | 2.45E-38 | 1.14E-38 | -37.944 |
| Cu(NO2)2 (aq) | 4.1E-105 | 4.2E-105 | -104.38 |
| Cu(NO3)2 (aq) | 6.4E-139 | 6.5E-139 | -138.187 |
| Cu(OH)2 (aq) | 4.24E-21 | 4.29E-21 | -20.368 |
| Cu(OH)3- | 7.43E-29 | 6.14E-29 | -28.212 |
| Cu(OH)4-2 | 8.81E-41 | 4.1E-41 | -40.387 |
| Cu+2 | 5.44E-08 | 2.68E-08 | -7.572 |
| Cu2(OH)2+2 | 1.77E-22 | 8.24E-23 | -22.084 |
| Cu2OH+3 | 5.36E-20 | 9.59E-21 | -20.018 |
| Cu2S3-2 | 1.73E-98 | 8.1E-99 | -98.093 |
| Cu3(OH)4+2 | 1.52E-36 | 7.08E-37 | -36.15 |
| CuCl+ | 9.98E-10 | 8.19E-10 | -9.087 |
| CuCl2 (aq) | 2.32E-12 | 2.35E-12 | -11.629 |
| CuCl3- | 3.83E-16 | 3.14E-16 | -15.503 |
| CuCl4-2 1 | 8.09E-20 | 3.83E-20 | -19.416 |
| CuCO3 (aq) | 5.72E-17 | 5.78E-17 | -16.238 |
| CuF+ | 4.46E-15 | 3.68E-15 | -14.434 |
| CuHCO3+ | 1.6E-13 | 1.32E-13 | -12.879 |
| CuHPO4 (aq) | 1.25E-15 | 1.26E-15 | -14.898 |
| CuHSO4+ | 9.35E-11 | 7.73E-11 | -10.112 |
| CuN3+ | 1.32E-12 | 1.09E-12 | -11.964 |
| CuNH3+2 | 1.28E-14 | 5.96E-15 | -14.225 |
| CuNO2+ | 4.09E-56 | 3.38E-56 | -55.471 |
| CuNO3+ | 8.48E-73 | 7E-73 | -72.155 |
| CuOH+ | 6.29E-14 | 5.17E-14 | -13.287 |
| CuS(aq) | 6.17E-38 | 6.24E-38 | -37.205 |
| CuSO4 (aq) | 7.08E-09 | 7.16E-09 | -8.145 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| DOC (Gaussian DOM) | 0.000333 | 0.000337 | -3.473 |
| DOM1 | 5.69E-06 | 1.27E-06 | -5.896 |
| F-1 | 4.03E-09 | 3.29E-09 | -8.483 |
| Fe DOM1 | 6.02E-11 | 5.97E-11 | -10.224 |
| Fe(N3)2+ | 1.28E-17 | 1.06E-17 | -16.976 |
| Fe(N3)3 (aq) | 1.25E-22 | 1.27E-22 | -21.897 |
| Fe(NH3)2+2 | 1.17E-22 | 5.43E-23 | -22.265 |
| Fe(NH3)3+2 | 5.64E-33 | 2.62E-33 | -32.581 |
| Fe(NH3)4+2 | 1.16E-43 | 5.4E-44 | -43.267 |
| Fe(NO2)2+ | 8.2E-107 | 6.8E-107 | -106.17 |
| Fe(NO2)3 (aq) | 9.3E-155 | 9.4E-155 | -154.029 |
| Fe(OH)2 (aq) | 5.84E-21 | 5.91E-21 | -20.229 |
| Fe(OH)2+ | 1.12E-13 | 9.31E-14 | -13.031 |
| Fe(OH)3- | 2.06E-29 | 1.71E-29 | -28.767 |
| Fe(OH)3 (aq) | 3.06E-21 | 3.09E-21 | -20.51 |
| Fe(OH)4- | 2.44E-27 | 2.03E-27 | -26.693 |
| Fe(SO4)2- | 3.42E-12 | 2.83E-12 | -11.549 |
| Fe+2 | 0.001998 | 0.000983 | -3.007 |
| Fe+3 | 3.55E-11 | 8.88E-12 | -11.052 |
| Fe2(OH)2+4 | 9.74E-21 | 4.57E-22 | -21.34 |
| Fe3(OH)4+5 | 1.72E-30 | 1.45E-32 | -31.84 |
| FeCl+ | 1.29E-05 | 1.07E-05 | -4.972 |
| FeCl+2 | 7.05E-12 | 3.34E-12 | -11.476 |
| FeCrO4+ | 3.74E-15 | 3.09E-15 | -14.51 |
| FeF+ | 6.35E-11 | 5.25E-11 | -10.28 |
| FeF+2 | 5.88E-14 | 2.79E-14 | -13.555 |
| FeF2+ | 4.18E-18 | 3.47E-18 | -17.46 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeF3 (aq) | 1.05E-23 | 1.06E-23 | -22.976 |
| FeH2PO4+ | 3.3E-07 | 2.75E-07 | -6.561 |
| FeH2PO4+2 | 1.95E-13 | 9.37E-14 | -13.028 |
| FeHCO3+ | 1.16E-09 | 9.68E-10 | -9.014 |
| FeHPO4 (aq) | 1.37E-11 | 1.38E-11 | -10.859 |
| FeHPO4+ | 4.7E-13 | 3.91E-13 | -12.407 |
| FeHS+ | 7.29E-27 | 6.02E-27 | -26.221 |
| FeN3+2 | 1.67E-13 | 7.75E-14 | -13.11 |
| FeNH3+2 | 9.51E-13 | 4.43E-13 | -12.354 |
| FeNO2+2 | 3.64E-58 | 1.7E-58 | -57.771 |
| FeOH+ | 2.17E-11 | 1.8E-11 | -10.744 |
| FeOH+2 | 1.26E-11 | 5.97E-12 | -11.224 |
| FeSO4 (aq) | 0.000281 | 0.000284 | -3.546 |
| FeSO4+ | 1.77E-10 | 1.47E-10 | -9.834 |
| H DOM1 | 1.85E-05 | 9.95E-06 | -5.002 |
| H+1 | 0.011666 | 0.01 | -2 |
| H2AsO3- | 2.76E-14 | 2.28E-14 | -13.642 |
| H2AsO4- | 2.3E-12 | 1.9E-12 | -11.722 |
| H2CO3* (aq) | 0.002552 | 0.002581 | -2.588 |
| H2CrO4 (aq) | 1.11E-09 | 1.12E-09 | -8.95 |
| H2PO4- | 8.62E-07 | 7.18E-07 | -6.144 |
| H2S (aq) | 2.11E-24 | 2.14E-24 | -23.67 |
| H3AsO3 | 4.91E-07 | 4.96E-07 | -6.305 |
| H3AsO4 | 3.35E-12 | 3.38E-12 | -11.471 |
| H3PO4 | 8.99E-07 | 9.09E-07 | -6.042 |
| HAsO3-2 | 2.49E-26 | 1.16E-26 | -25.936 |
| HAsO4-2 | 4E-17 | 1.86E-17 | -16.73 |
| HCO3- | 1.18E-07 | 9.84E-08 | -7.007 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HCrO4- | 3.61E-07 | 2.98E-07 | -6.525 |
| HF (aq) | 4.09E-08 | 4.14E-08 | -7.383 |
| HF2- | 6.27E-16 | 5.12E-16 | -15.291 |
| Hg(CO3)2-2 | 3.9E-36 | 1.82E-36 | -35.741 |
| Hg(HS)2 (aq) | 1.99E-40 | 2.02E-40 | -39.696 |
| Hg(N3)2 (aq) | 1.13E-15 | 1.14E-15 | -14.942 |
| Hg(NH3)2+2 | 8.94E-24 | 4.16E-24 | -23.381 |
| Hg(NH3)4+2 | 1.07E-43 | 4.97E-44 | -43.304 |
| Hg(NO2)2 (aq) | 4.1E-111 | 4.2E-111 | -110.378 |
| Hg(NO2)3- | 2.1E-159 | 1.8E-159 | -158.757 |
| Hg(NO2)4-2 | 1.2E-208 | 5.4E-209 | -208.266 |
| Hg(NO3)2 (aq) | 3.6E-152 | 3.6E-152 | -151.445 |
| Hg(OH)2 | 2.43E-23 | 2.46E-23 | -22.609 |
| Hg(SO4)2-2 | 4.01E-23 | 1.86E-23 | -22.73 |
| Hg+2 | 1.34E-20 | 6.25E-21 | -20.204 |
| Hg2OH+3 | 9.06E-42 | 1.62E-42 | -41.79 |
| Hg3(OH)3+3 | 1.05E-61 | 1.87E-62 | -61.727 |
| HgCl+ | 3.7E-15 | 3.06E-15 | -14.515 |
| HgCl2 (aq) | 3.99E-10 | 4.04E-10 | -9.394 |
| HgCl3-1 | 8.37E-11 | 6.91E-11 | -10.16 |
| HgCl4-2 | 1.14E-11 | 5.33E-12 | -11.273 |
| HgClOH (aq) | 2.12E-16 | 2.14E-16 | -15.67 |
| HgCO3 (aq) | 1.74E-24 | 1.76E-24 | -23.755 |
| HgF+ | 9.29E-28 | 7.67E-28 | -27.115 |
| HgHCO3+ | 3.53E-22 | 2.92E-22 | -21.535 |
| HgHS2- | 7.9E-45 | 6.52E-45 | -44.186 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgN3+ | 4.03E-12 | 3.33E-12 | -11.477 |
| HgNO2+ | 4.51E-65 | 3.73E-65 | -64.429 |
| HgNO3+ | 1.34E-86 | 1.11E-86 | -85.956 |
| HgOH+ | 2.27E-22 | 1.87E-22 | -21.728 |
| HgOHCO3- | 2.5E-29 | 2.06E-29 | -28.685 |
| HgS2-2 | 2.73E-51 | 1.27E-51 | -50.896 |
| HgSO4 (aq) | 1.37E-21 | 1.38E-21 | -20.86 |
| HN3 (aq) | 2.85E-05 | 2.88E-05 | -4.541 |
| HNO2 (aq) | 1.68E-49 | 1.7E-49 | -48.769 |
| HPO4-2 | 9.2E-12 | 4.36E-12 | -11.36 |
| HS-1 | 1.8E-29 | 1.47E-29 | -28.833 |
| HSO4- | 0.001187 | 0.00098 | -3.009 |
| K+1 | 0.000149 | 0.000121 | -3.918 |
| K2HPO4 (aq) | 6.82E-19 | 6.89E-19 | -18.162 |
| K2PO4- | 4.8E-28 | 3.97E-28 | -27.402 |
| KCl (aq) | 1.09E-06 | 1.1E-06 | -5.957 |
| KCr2O7- | 5.09E-15 | 4.2E-15 | -14.376 |
| KCrO4- | 5.16E-15 | 4.26E-15 | -14.371 |
| KF (aq) | 1.8E-13 | 1.82E-13 | -12.74 |
| KH2PO4 (aq) | 1.33E-10 | 1.35E-10 | -9.871 |
| KHPO4- | 3.89E-15 | 3.24E-15 | -14.489 |
| KNO3 (aq) | 7.13E-70 | 7.21E-70 | -69.142 |
| KOH (aq) | 9.58E-17 | 9.68E-17 | -16.014 |
| KPO4-2 | 8.45E-25 | 3.93E-25 | -24.405 |
| KSO4- | 1.13E-06 | 9.42E-07 | -6.026 |
| Mg DOM1 | 1.61E-08 | 1.42E-08 | -7.847 |
| Mg(NH3)2+2 | 1.23E-24 | 5.71E-25 | -24.243 |
| Mg+2 | 0.002607 | 0.001335 | -2.875 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Mg2CO3+2 | 5.46E-18 | 2.54E-18 | -17.595 |
| MgCl+ | 0.000105 | 8.65E-05 | -4.063 |
| MgCO3 (aq) | 3.45E-16 | 3.49E-16 | -15.457 |
| MgF+ | 3.52E-10 | 2.91E-10 | -9.536 |
| MgHCO3+ | 1.55E-09 | 1.27E-09 | -8.895 |
| MgHPO4 (aq) | 3.07E-12 | 3.11E-12 | -11.508 |
| MgOH+ | 2.47E-13 | 2.08E-13 | -12.683 |
| MgPO4- | 8.98E-21 | 7.48E-21 | -20.126 |
| MgSO4 (aq) | 0.000292 | 0.000295 | -3.53 |
| Mn+3 | 5.1E-06 | 1.27E-06 | -5.895 |
| N3-1 | 6.78E-08 | 5.6E-08 | -7.252 |
| Na+1 | 0.006857 | 0.005678 | -2.246 |
| Na2HPO4 (aq) | 9.93E-16 | 1E-15 | -14.998 |
| Na2PO4- | 2.26E-24 | 1.87E-24 | -23.728 |
| NaCl (aq) | 5.42E-05 | 5.48E-05 | -4.261 |
| NaCO3- | 6.19E-17 | 5.15E-17 | -16.288 |
| NaCrO4- | 3.24E-13 | 2.67E-13 | -12.573 |
| NaF (aq) | 1.64E-11 | 1.65E-11 | -10.781 |
| NaH2PO4 (aq) | 6.25E-09 | 6.32E-09 | -8.199 |
| NaHCO3 (aq) | 3.27E-10 | 3.31E-10 | -9.48 |
| NaHPO4- | 2.83E-13 | 2.36E-13 | -12.627 |
| NaNO3 (aq) | 1.24E-68 | 1.25E-68 | -67.903 |
| NaOH (aq) | 3.08E-15 | 3.12E-15 | -14.506 |
| NaPO4-2 | 4.38E-23 | 2.04E-23 | -22.691 |
| NaSO4- | 4.87E-05 | 4.06E-05 | -4.392 |
| NH3 (aq) | 1.57E-11 | 1.58E-11 | -10.8 |
| NH4+1 | 0.000716 | 0.000578 | -3.238 |
| NH4Cr2O7- | 2.83E-14 | 2.33E-14 | -13.632 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NH4SO4- | 9.88E-06 | 8.16E-06 | -5.089 |
| Ni DOM1 | 4.73E-10 | 4.19E-10 | -9.378 |
| Ni(N3)2 (aq) | 4.8E-19 | 4.85E-19 | -18.314 |
| Ni(NH3)2+2 | 9.77E-23 | 4.54E-23 | -22.343 |
| Ni(NH3)3+2 | 8.96E-32 | 4.17E-32 | -31.38 |
| Ni(NH3)4+2 | 2.44E-41 | 1.14E-41 | -40.945 |
| Ni(NH3)5+2 | 2.14E-51 | 9.97E-52 | -51.001 |
| Ni(NH3)6+2 | 4.01E-62 | 1.87E-62 | -61.729 |
| Ni(NO2)2 (aq) | 1.4E-104 | 1.4E-104 | -103.854 |
| Ni(OH)2 (aq) | 1.57E-21 | 1.59E-21 | -20.8 |
| Ni(OH)3- | 1.93E-30 | 1.6E-30 | -29.797 |
| Ni(SO4)2-2 | 3.86E-11 | 1.79E-11 | -10.746 |
| Ni+2 | 3.36E-06 | 1.56E-06 | -5.806 |
| NiCl+ | 1.18E-08 | 9.73E-09 | -8.012 |
| NiCl2 (aq) | 5.9E-12 | 5.97E-12 | -11.224 |
| NiCO3 (aq) | 2.11E-17 | 2.13E-17 | -16.672 |
| NiF+ | 1.13E-13 | 9.3E-14 | -13.032 |
| NiH2PO4+ | 8.93E-12 | 7.37E-12 | -11.132 |
| NiHCO3+ | 1.83E-11 | 1.51E-11 | -10.822 |
| NiHPO4 (aq) | 4.93E-15 | 4.99E-15 | -14.302 |
| NiHS+ | 8.59E-30 | 7.1E-30 | -29.149 |
| NiN3+ | 2E-12 | 1.65E-12 | -11.783 |
| NiNH3+2 | 3.49E-14 | 1.62E-14 | -13.789 |
| NiNO2+ | 5.47E-55 | 4.52E-55 | -54.345 |
| NiNO3+ | 3.71E-71 | 3.07E-71 | -70.513 |
| NiOH+ | 1.16E-14 | 9.6E-15 | -14.018 |
| NiSO4 (aq) | 3.75E-07 | 3.79E-07 | -6.421 |
| NO2-1 | 1.46E-50 | 1.2E-50 | -49.919 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| NO3-1 | 9.62E-66 | 7.8E-66 | -65.108 |
| OH- | 5.65E-13 | 4.61E-13 | -12.336 |
| Pb DOM1 | 3.96E-10 | 3.51E-10 | -9.455 |
| Pb(CO3)2-2 | 4.15E-29 | 1.93E-29 | -28.714 |
| Pb(HS)2 (aq) | 6.55E-51 | 6.62E-51 | -50.179 |
| Pb(HS)3- | 2.35E-78 | 1.94E-78 | -77.712 |
| Pb(NO2)2 (aq) | 3E-105 | 3.1E-105 | -104.511 |
| Pb(NO3)2 (aq) | 2.7E-137 | 2.8E-137 | -136.558 |
| Pb(OH)2 (aq) | 1.31E-21 | 1.33E-21 | -20.877 |
| Pb(OH)3- | 1.62E-30 | 1.34E-30 | -29.874 |
| Pb(SO4)2-2 | 1.82E-10 | 8.45E-11 | -10.073 |
| Pb+2 | 3.54E-08 | 1.65E-08 | -7.783 |
| Pb2OH+3 | 6.09E-20 | 1.09E-20 | -19.963 |
| Pb3(OH)4+2 | 2.45E-40 | 1.14E-40 | -39.943 |
| Pb4(OH)4+4 | 6.18E-44 | 2.9E-45 | -44.538 |
| PbCl+ | 1.1E-08 | 9.12E-09 | -8.04 |
| PbCl2 (aq) | 3.24E-10 | 3.28E-10 | -9.484 |
| PbCl3- | 5.43E-12 | 4.49E-12 | -11.348 |
| PbCl4-2 | 6.07E-14 | 2.82E-14 | -13.549 |
| PbCO3 (aq) | 2.03E-17 | 2.05E-17 | -16.689 |
| PbF+ | 9.28E-15 | 7.67E-15 | -14.115 |
| PbF2 (aq) | 3.07E-22 | 3.1E-22 | -21.508 |
| PbH2PO4+ | 3.52E-13 | 2.91E-13 | -12.536 |
| PbHCO3+ | 1.24E-12 | 1.03E-12 | -11.989 |
| PbHPO4 (aq) | 7.26E-17 | 7.34E-17 | -16.134 |
| PbNO2+ | 7.78E-56 | 6.43E-56 | -55.192 |
| PbNO3+ | 2.37E-72 | 1.96E-72 | -71.708 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| PbOH+ | 3.62E-14 | 2.99E-14 | -13.525 |
| PbSO4 (aq) | 1.05E-08 | 1.06E-08 | -7.973 |
| PO4-3 | 8E-22 | 1.49E-22 | -21.826 |
| S-2 | 6.18E-45 | 2.93E-45 | -44.533 |
| SO4-2 | 0.002911 | 0.001318 | -2.88 |
| Zn DOM1 | 4.67E-09 | 4.13E-09 | -8.384 |
| Zn(CO3)2-2 | 5.61E-29 | 2.61E-29 | -28.583 |
| Zn(N3)2 (aq) | 2.88E-18 | 2.91E-18 | -17.536 |
| Zn(N3)3- | 1.13E-24 | 9.33E-25 | -24.03 |
| Zn(NH3)2+2 | 2.3E-22 | 1.07E-22 | -21.971 |
| Zn(NH3)3+2 | 1.07E-30 | 4.98E-31 | -30.302 |
| Zn(NH3)4+2 | 2.45E-39 | 1.14E-39 | -38.944 |
| Zn(NO2)2 (aq) | 2.2E-104 | 2.2E-104 | -103.65 |
| Zn(NO3)2 (aq) | 2.9E-136 | 3E-136 | -135.527 |
| Zn(OH)2 (aq) | 1.23E-18 | 1.24E-18 | -17.906 |
| Zn(OH)3- | 4.79E-28 | 3.96E-28 | -27.403 |
| Zn(OH)4-2 | 1.36E-38 | 6.31E-39 | -38.2 |
| Zn(SO4)2-2 | 6.92E-08 | 3.22E-08 | -7.492 |
| Zn+2 | 1.98E-05 | 9.73E-06 | -5.012 |
| Zn2OH+3 | 2.18E-17 | 3.9E-18 | -17.409 |
| Zn2S3-2 | 1.44E-90 | 6.71E-91 | -90.173 |
| Zn4S6-4 | 1.6E-178 | 7.7E-180 | -179.116 |
| ZnCl+ | 5.45E-07 | 4.48E-07 | -6.349 |
| ZnCl2 (aq) | 4.88E-09 | 4.94E-09 | -8.307 |
| ZnCl3- | 1.09E-10 | 8.96E-11 | -10.047 |
| ZnCl4-2 | 1.53E-12 | 7.12E-13 | -12.147 |
| ZnCO3 (aq) | 2.03E-16 | 2.05E-16 | -15.688 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnF+ | 6.63E-13 | 5.48E-13 | -12.261 |
| ZnHCO3+ | 2.91E-11 | 2.41E-11 | -10.619 |
| ZnHPO4 (aq) | 7.03E-14 | 7.11E-14 | -13.148 |
| ZnN3+ | 9.49E-12 | 7.84E-12 | -11.106 |
| ZnNH3+2 | 6.26E-14 | 2.91E-14 | -13.536 |
| ZnNO2+ | 8.55E-55 | 7.06E-55 | -54.151 |
| ZnNO3+ | 2.46E-70 | 2.03E-70 | -69.692 |
| ZnOH+ | 5.43E-13 | 4.49E-13 | -12.348 |
| ZnS (aq) | 5.25E-34 | 5.31E-34 | -33.275 |
| ZnSO4 (aq) | 2.54E-06 | 2.57E-06 | -5.59 |

## C1.2 pH 3

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 1.3E-05 | 1.29E-05 | -4.89 |
| Al(OH)2+ | 1.85E-09 | 1.56E-09 | -8.808 |
| Al(OH)3 (aq) | 2.91E-13 | 2.94E-13 | -12.532 |
| Al(OH)4- | 1.57E-16 | 1.31E-16 | -15.882 |
| Al(SO4)2- | 0.000136 | 0.000113 | -3.945 |
| Al+3 | 0.000647 | 0.000171 | -3.768 |
| Al2(OH)2+4 | 3.84E-09 | 2.07E-10 | -9.685 |
| Al2(OH)2CO3+2 | 4.51E-11 | 2.17E-11 | -10.663 |
| Al2PO4+3 | 2.83E-08 | 5.47E-09 | -8.262 |
| Al3(OH)4+5 | 8.64E-13 | 8.99E-15 | -14.046 |
| AlCl+2 | 2.51E-06 | 1.21E-06 | -5.918 |
| AlF+2 | 1.31E-05 | 6.53E-06 | -5.185 |
| AlF2+ | 1.23E-08 | 1.03E-08 | -7.987 |
| AlF3 (aq) | 4.76E-13 | 4.81E-13 | -12.318 |
| AlF4- | 1.15E-18 | 9.62E-19 | -18.017 |
| AlHPO4+ | 4.12E-07 | 3.43E-07 | -6.464 |
| AlOH+2 | 1.77E-06 | 8.79E-07 | -6.056 |
| AlSO4+ | 0.001965 | 0.001637 | -2.786 |
| As3S4(HS)- | 1.2E-188 | 9.7E-189 | -188.014 |
| AsO4-3 | 1.17E-21 | 2.27E-22 | -21.644 |
| AsS(OH)HS- | 2.19E-67 | 1.83E-67 | -66.738 |
| Ca DOM1 | 7.68E-07 | 6.83E-07 | -6.166 |
| Ca(NH3)2+2 | 3.26E-22 | 1.57E-22 | -21.804 |
| Ca(NO3)2 | 3.5E-118 | 3.5E-118 | -117.455 |
| Ca+2 | 0.003494 | 0.001803 | -2.744 |
| CaCl+ | 8.94E-05 | 7.45E-05 | -4.128 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCO3 (aq) | 9.33E-14 | 9.42E-14 | -13.026 |
| CaCrO4 (aq) | 1.01E-10 | 1.02E-10 | -9.989 |
| CaF+ | 9.75E-11 | 8.16E-11 | -10.088 |
| CaH2PO4+ | 3.85E-08 | 3.23E-08 | -7.491 |
| CaHCO3+ | 2.21E-08 | 1.87E-08 | -7.729 |
| CaHPO4 (aq) | 3.97E-11 | 4.01E-11 | -10.397 |
| CaNH3+2 | 1.99E-12 | 9.57E-13 | -12.019 |
| CaNO3+ | 5.79E-58 | 4.82E-58 | -57.317 |
| CaOH+ | 1.75E-13 | 1.47E-13 | -12.831 |
| CaPO4- | 1.02E-16 | 8.53E-17 | -16.069 |
| CaSO4 (aq) | 0.00061 | 0.000616 | -3.211 |
| Cd DOM1 | 2.76E-12 | 2.45E-12 | -11.61 |
| Cd(CO3)2-2 | 1.22E-28 | 5.87E-29 | -28.232 |
| Cd(HS)2 (aq) | 1.77E-69 | 1.79E-69 | -68.748 |
| Cd(HS)3- | 2.5E-105 | 2.1E-105 | -104.683 |
| Cd(HS)4-2 | 1.3E-140 | 6.1E-141 | -140.218 |
| Cd(NH3)2+2 | 7.25E-24 | 3.49E-24 | -23.457 |
| Cd(NH3)3+2 | 2.99E-32 | 1.44E-32 | -31.841 |
| Cd(NH3)4+2 | 3.64E-41 | 1.75E-41 | -40.756 |
| Cd(NO2)2 (aq) | 1.65E-89 | 1.67E-89 | -88.778 |
| Cd(NO3)2 (aq) | 2.5E-119 | 2.5E-119 | -118.599 |
| Cd(OH)2 (aq) | 1.3E-23 | 1.31E-23 | -22.883 |
| Cd(OH)3- | 1.55E-33 | 1.29E-33 | -32.89 |
| Cd(OH)4-2 | 2.75E-44 | 1.32E-44 | -43.878 |
| Cd(SO4)2-2 | 4.59E-11 | 2.21E-11 | -10.655 |
| Cd+2 | 5.35E-09 | 2.58E-09 | -8.589 |
| Cd2OH+3 | 7.26E-24 | 1.4E-24 | -23.853 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl+ | 5E-09 | 4.17E-09 | -8.38 |
| CdCl2 (aq) | 2.88E-10 | 2.91E-10 | -9.536 |
| CdCO3 (aq) | 2.19E-18 | 2.21E-18 | -17.655 |
| CdF+ | 1.83E-16 | 1.52E-16 | -15.818 |
| CdHCO3+ | 7.66E-14 | 6.38E-14 | -13.195 |
| CdHPO4 (aq) | 6.04E-16 | 6.1E-16 | -15.215 |
| CdHS+ | 5.83E-39 | 4.86E-39 | -38.313 |
| CdNH3+2 | 3.63E-16 | 1.75E-16 | -15.757 |
| CdNO2+ | 3.78E-49 | 3.15E-49 | -48.502 |
| CdNO3+ | 1.03E-63 | 8.59E-64 | -63.066 |
| CdOH+ | 1.15E-16 | 9.57E-17 | -16.019 |
| CdSO4 (aq) | 8.73E-10 | 8.82E-10 | -9.055 |
| Cl-1 | 0.02117 | 0.017395 | -1.76 |
| CO3-2 | 7.36E-14 | 3.66E-14 | -13.436 |
| Cr2O7-2 | 8.67E-12 | 4.18E-12 | -11.379 |
| CrO3Cl- | 4.11E-11 | 3.42E-11 | -10.466 |
| CrO3H2PO4- | 5.27E-13 | 4.39E-13 | -12.358 |
| CrO3HPO4-2 | 1.89E-12 | 9.11E-13 | -12.041 |
| CrO3SO4-2 | 3.26E-10 | 1.57E-10 | -9.805 |
| CrO4-2 | 2.04E-10 | 9.65E-11 | -10.015 |
| Cu DOM1 | 1.13E-09 | 1E-09 | -8.999 |
| Cu(CO3)2-2 | 1.17E-24 | 5.61E-25 | -24.251 |
| Cu(N3)2 (aq) | 2.66E-16 | 2.69E-16 | -15.571 |
| Cu(N3)3- | 8.86E-21 | 7.38E-21 | -20.132 |
| Cu(N3)4-2 | 2.21E-26 | 1.06E-26 | -25.973 |
| Cu(NH3)2+2 | 6.36E-20 | 3.07E-20 | -19.514 |
| Cu(NH3)3+2 | 8.6E-27 | 4.14E-27 | -26.382 |
| Cu(NH3)4+2 | 2.41E-34 | 1.16E-34 | -33.936 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO2)2 (aq) | 4.12E-89 | 4.16E-89 | -88.381 |
| Cu(NO3)2 (aq) | 6.4E-119 | 6.5E-119 | -118.189 |
| Cu(OH)2 (aq) | 4.18E-19 | 4.22E-19 | -18.375 |
| Cu(OH)3- | 7.25E-26 | 6.04E-26 | -25.219 |
| Cu(OH)4-2 | 8.37E-37 | 4.03E-37 | -36.395 |
| Cu+2 | 5.21E-08 | 2.64E-08 | -7.578 |
| Cu2(OH)2+2 | 1.66E-20 | 8.01E-21 | -20.097 |
| Cu2OH+3 | 4.82E-19 | 9.33E-20 | -19.03 |
| Cu2S3-2 | 3.2E-122 | 1.5E-122 | -121.81 |
| Cu3(OH)4+2 | 1.41E-32 | 6.78E-33 | -32.169 |
| CuCl+ | 9.85E-10 | 8.17E-10 | -9.088 |
| CuCl2 (aq) | 2.34E-12 | 2.37E-12 | -11.626 |
| CuCl3- | 3.86E-16 | 3.2E-16 | -15.495 |
| CuCl4-2 1 | 8.04E-20 | 3.94E-20 | -19.404 |
| CuCO3 (aq) | 5.64E-15 | 5.7E-15 | -14.244 |
| CuF+ | 5.29E-15 | 4.41E-15 | -14.356 |
| CuHCO3+ | 1.56E-12 | 1.3E-12 | -11.885 |
| CuHPO4 (aq) | 1.63E-14 | 1.64E-14 | -13.784 |
| CuHSO4+ | 1.14E-11 | 9.52E-12 | -11.021 |
| CuN3+ | 1.26E-11 | 1.05E-11 | -10.979 |
| CuNH3+2 | 1.23E-13 | 5.92E-14 | -13.227 |
| CuNO2+ | 4.03E-48 | 3.36E-48 | -47.474 |
| CuNO3+ | 8.34E-63 | 6.95E-63 | -62.158 |
| CuOH+ | 6.14E-13 | 5.09E-13 | -12.293 |
| CuS(aq) | 7.64E-46 | 7.71E-46 | -45.113 |
| CuSO4 (aq) | 8.74E-09 | 8.83E-09 | -8.054 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.473 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| DOM1 | 8.46E-06 | 2.02E-06 | -5.694 |
| F-1 | 4.84E-09 | 3.99E-09 | -8.399 |
| Fe DOM1 | 2.13E-10 | 2.11E-10 | -9.675 |
| Fe(N3)2+ | 1.21E-15 | 1.01E-15 | -14.997 |
| Fe(N3)3 (aq) | 1.17E-19 | 1.18E-19 | -18.928 |
| Fe(NH3)2+2 | 1.14E-20 | 5.49E-21 | -20.26 |
| Fe(NH3)3+2 | 5.55E-30 | 2.67E-30 | -29.573 |
| Fe(NH3)4+2 | 1.15E-39 | 5.56E-40 | -39.255 |
| Fe(NO2)2+ | 8.18E-91 | 6.82E-91 | -90.166 |
| Fe(NO2)3 (aq) | 9.4E-131 | 9.5E-131 | -130.023 |
| Fe(OH)2 (aq) | 5.81E-19 | 5.87E-19 | -18.231 |
| Fe(OH)2+ | 1.1E-11 | 9.26E-12 | -11.033 |
| Fe(OH)3- | 2.03E-26 | 1.7E-26 | -25.77 |
| Fe(OH)3 (aq) | 3.04E-18 | 3.07E-18 | -17.512 |
| Fe(OH)4- | 2.4E-23 | 2.01E-23 | -22.696 |
| Fe(SO4)2- | 5.28E-12 | 4.4E-12 | -11.357 |
| Fe+2 | 0.001928 | 0.000979 | -3.009 |
| Fe+3 | 3.35E-11 | 8.84E-12 | -11.054 |
| Fe2(OH)2+4 | 8.4E-19 | 4.52E-20 | -19.345 |
| Fe3(OH)4+5 | 1.37E-26 | 1.42E-28 | -27.847 |
| FeCl+ | 1.29E-05 | 1.07E-05 | -4.969 |
| FeCl+2 | 6.86E-12 | 3.37E-12 | -11.473 |
| FeCrO4+ | 3.76E-14 | 3.13E-14 | -13.504 |
| FeF+ | 7.6E-11 | 6.34E-11 | -10.198 |
| FeF+2 | 6.85E-14 | 3.36E-14 | -13.473 |
| FeF2+ | 6.06E-18 | 5.07E-18 | -17.295 |
| FeF3 (aq) | 1.86E-23 | 1.88E-23 | -22.727 |
| FeH2PO4+ | 4.3E-07 | 3.61E-07 | -6.442 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeH2PO4+2 | 2.47E-13 | 1.23E-13 | -12.91 |
| FeHCO3+ | 1.14E-08 | 9.62E-09 | -8.017 |
| FeHPO4 (aq) | 1.8E-10 | 1.82E-10 | -9.74 |
| FeHPO4+ | 6.12E-12 | 5.14E-12 | -11.289 |
| FeHS+ | 9.02E-36 | 7.51E-36 | -35.124 |
| FeN3+2 | 1.57E-12 | 7.55E-13 | -12.122 |
| FeNH3+2 | 9.22E-12 | 4.44E-12 | -11.352 |
| FeNO2+2 | 3.53E-50 | 1.7E-50 | -49.77 |
| FeOH+ | 2.14E-10 | 1.8E-10 | -9.746 |
| FeOH+2 | 1.21E-10 | 5.94E-11 | -10.226 |
| FeSO4 (aq) | 0.00035 | 0.000354 | -3.451 |
| FeSO4+ | 2.18E-10 | 1.82E-10 | -9.739 |
| H DOM1 | 6.39E-06 | 3.54E-06 | -5.451 |
| H+1 | 0.00116 | 0.001 | -3 |
| H2AsO3- | 2.72E-13 | 2.26E-13 | -12.645 |
| H2AsO4- | 2.26E-09 | 1.88E-09 | -8.725 |
| H2CO3* (aq) | 0.002551 | 0.002576 | -2.589 |
| H2CrO4 (aq) | 1.13E-10 | 1.14E-10 | -9.942 |
| H2PO4- | 1.13E-06 | 9.47E-07 | -6.024 |
| H2S (aq) | 2.65E-34 | 2.68E-34 | -33.572 |
| H3AsO3 | 4.88E-07 | 4.93E-07 | -6.307 |
| H3AsO4 | 3.33E-10 | 3.36E-10 | -9.474 |
| H3PO4 | 1.19E-07 | 1.2E-07 | -6.921 |
| HAsO3-2 | 2.39E-24 | 1.15E-24 | -23.939 |
| HAsO4-2 | 3.83E-13 | 1.85E-13 | -12.734 |
| HCO3- | 1.17E-06 | 9.82E-07 | -6.008 |
| HCrO4- | 3.65E-07 | 3.04E-07 | -6.517 |
| HF (aq) | 4.97E-09 | 5.01E-09 | -8.3 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HF2- | 9.12E-17 | 7.52E-17 | -16.124 |
| Hg(CO3)2-2 | 4.79E-35 | 2.31E-35 | -34.637 |
| Hg(HS)2 (aq) | 4E-61 | 4.04E-61 | -60.394 |
| Hg(N3)2 (aq) | 1.38E-14 | 1.39E-14 | -13.857 |
| Hg(NH3)2+2 | 1.12E-24 | 5.39E-25 | -24.269 |
| Hg(NH3)4+2 | 1.36E-42 | 6.54E-43 | -42.184 |
| Hg(NO2)2 (aq) | 5.36E-98 | 5.41E-98 | -97.267 |
| Hg(NO2)3- | 2.7E-138 | 2.3E-138 | -137.643 |
| Hg(NO2)4-2 | 1.5E-179 | 7.1E-180 | -179.149 |
| Hg(NO3)2 (aq) | 4.6E-135 | 4.6E-135 | -134.334 |
| Hg(OH)2 | 3.1E-24 | 3.13E-24 | -23.505 |
| Hg(SO4)2-2 | 7.7E-26 | 3.71E-26 | -25.43 |
| Hg+2 | 1.66E-23 | 7.97E-24 | -23.098 |
| Hg2OH+3 | 1.36E-46 | 2.63E-47 | -46.579 |
| Hg3(OH)3+3 | 2.01E-67 | 3.88E-68 | -67.412 |
| HgCl+ | 4.73E-18 | 3.94E-18 | -17.404 |
| HgCl2 (aq) | 5.21E-13 | 5.26E-13 | -12.279 |
| HgCl3-1 | 1.09E-13 | 9.1E-14 | -13.041 |
| HgCl4-2 | 1.47E-14 | 7.08E-15 | -14.15 |
| HgClOH (aq) | 2.73E-18 | 2.75E-18 | -17.56 |
| HgCO3 (aq) | 2.22E-25 | 2.24E-25 | -24.65 |
| HgF+ | 1.42E-30 | 1.19E-30 | -29.926 |
| HgHCO3+ | 4.46E-24 | 3.71E-24 | -23.43 |
| HgHS2- | 1.57E-64 | 1.31E-64 | -63.884 |
| HgN3+ | 4.98E-10 | 4.15E-10 | -9.382 |
| HgNO2+ | 5.74E-60 | 4.78E-60 | -59.32 |
| HgNO3+ | 1.7E-79 | 1.42E-79 | -78.848 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgOH+ | 2.86E-24 | 2.39E-24 | -23.622 |
| HgOHCO3- | 3.15E-29 | 2.63E-29 | -28.581 |
| HgS2-2 | 5.29E-70 | 2.55E-70 | -69.594 |
| HgSO4 (aq) | 2.18E-24 | 2.2E-24 | -23.657 |
| HN3 (aq) | 2.79E-05 | 2.82E-05 | -4.55 |
| HNO2 (aq) | 1.7E-42 | 1.71E-42 | -41.766 |
| HPO4-2 | 1.17E-10 | 5.75E-11 | -10.24 |
| HS-1 | 2.23E-38 | 1.84E-38 | -37.735 |
| HSO4- | 0.000147 | 0.000123 | -3.912 |
| K+1 | 0.000148 | 0.000122 | -3.914 |
| K2HPO4 (aq) | 9.15E-18 | 9.24E-18 | -17.034 |
| K2PO4- | 6.39E-26 | 5.32E-26 | -25.274 |
| KCl (aq) | 1.11E-06 | 1.12E-06 | -5.949 |
| KCr2O7- | 5.28E-15 | 4.4E-15 | -14.357 |
| KCrO4- | 5.25E-14 | 4.37E-14 | -13.359 |
| KF (aq) | 2.2E-13 | 2.22E-13 | -12.653 |
| KH2PO4 (aq) | 1.77E-10 | 1.79E-10 | -9.747 |
| KHPO4- | 5.14E-14 | 4.31E-14 | -13.365 |
| KNO3 (aq) | 7.24E-60 | 7.31E-60 | -59.136 |
| KOH (aq) | 9.66E-16 | 9.76E-16 | -15.011 |
| KPO4-2 | 1.09E-22 | 5.23E-23 | -22.281 |
| KSO4- | 1.41E-06 | 1.19E-06 | -5.926 |
| Mg DOM1 | 5.68E-08 | 5.05E-08 | -7.297 |
| Mg(NH3)2+2 | 1.2E-22 | 5.79E-23 | -22.237 |
| Mg+2 | 0.002534 | 0.001333 | -2.875 |
| Mg2CO3+2 | 5.25E-16 | 2.53E-16 | -15.597 |
| MgCl+ | 0.000105 | 8.73E-05 | -4.059 |
| MgCO3 (aq) | 3.45E-14 | 3.48E-14 | -13.458 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgF+ | 4.23E-10 | 3.52E-10 | -9.453 |
| MgHCO3+ | 1.53E-08 | 1.27E-08 | -7.896 |
| MgHPO4 (aq) | 4.05E-11 | 4.09E-11 | -10.388 |
| MgOH+ | 2.45E-12 | 2.07E-12 | -11.683 |
| MgPO4- | 1.17E-18 | 9.86E-19 | -18.006 |
| MgSO4 (aq) | 0.000365 | 0.000368 | -3.434 |
| Mn+3 | 5.1E-06 | 1.34E-06 | -5.872 |
| N3-1 | 6.58E-07 | 5.48E-07 | -6.261 |
| Na+1 | 0.006844 | 0.005716 | -2.243 |
| Na2HPO4 (aq) | 1.33E-14 | 1.34E-14 | -13.872 |
| Na2PO4- | 3E-22 | 2.5E-22 | -21.602 |
| NaCl (aq) | 5.52E-05 | 5.57E-05 | -4.254 |
| NaCO3- | 6.17E-15 | 5.18E-15 | -14.286 |
| NaCrO4- | 3.29E-12 | 2.74E-12 | -11.562 |
| NaF (aq) | 2E-11 | 2.02E-11 | -10.695 |
| NaH2PO4 (aq) | 8.31E-09 | 8.39E-09 | -8.076 |
| NaHCO3 (aq) | 3.29E-09 | 3.33E-09 | -8.478 |
| NaHPO4- | 3.73E-12 | 3.13E-12 | -11.504 |
| NaNO3 (aq) | 1.25E-58 | 1.26E-58 | -57.898 |
| NaOH (aq) | 3.1E-14 | 3.13E-14 | -13.504 |
| NaPO4-2 | 5.62E-21 | 2.71E-21 | -20.568 |
| NaSO4- | 6.07E-05 | 5.1E-05 | -4.292 |
| NH3 (aq) | 1.58E-10 | 1.6E-10 | -9.797 |
| NH4+1 | 0.000714 | 0.000582 | -3.235 |
| NH4Cr2O7- | 2.93E-14 | 2.44E-14 | -13.612 |
| NH4SO4- | 1.23E-05 | 1.03E-05 | -4.988 |
| Ni DOM1 | 1.68E-09 | 1.5E-09 | -8.825 |
| Ni(N3)2 (aq) | 4.62E-17 | 4.66E-17 | -16.331 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)2+2 | 9.63E-21 | 4.64E-21 | -20.334 |
| Ni(NH3)3+2 | 8.91E-29 | 4.29E-29 | -28.367 |
| Ni(NH3)4+2 | 2.44E-37 | 1.18E-37 | -36.929 |
| Ni(NH3)5+2 | 2.17E-46 | 1.04E-46 | -45.982 |
| Ni(NH3)6+2 | 4.09E-56 | 1.97E-56 | -55.706 |
| Ni(NO2)2 (aq) | 1.41E-88 | 1.42E-88 | -87.846 |
| Ni(OH)2 (aq) | 1.58E-19 | 1.59E-19 | -18.798 |
| Ni(OH)3- | 1.92E-27 | 1.6E-27 | -26.796 |
| Ni(SO4)2-2 | 5.85E-11 | 2.82E-11 | -10.55 |
| Ni+2 | 3.26E-06 | 1.57E-06 | -5.804 |
| NiCl+ | 1.19E-08 | 9.88E-09 | -8.005 |
| NiCl2 (aq) | 6.07E-12 | 6.13E-12 | -11.213 |
| NiCO3 (aq) | 2.12E-15 | 2.14E-15 | -14.67 |
| NiF+ | 1.36E-13 | 1.13E-13 | -12.946 |
| NiH2PO4+ | 1.17E-11 | 9.78E-12 | -11.01 |
| NiHCO3+ | 1.82E-10 | 1.51E-10 | -9.82 |
| NiHPO4 (aq) | 6.55E-14 | 6.61E-14 | -13.18 |
| NiHS+ | 1.07E-38 | 8.94E-39 | -38.049 |
| NiN3+ | 1.95E-11 | 1.62E-11 | -10.79 |
| NiNH3+2 | 3.42E-13 | 1.65E-13 | -12.784 |
| NiNO2+ | 5.49E-47 | 4.57E-47 | -46.34 |
| NiNO3+ | 3.72E-61 | 3.1E-61 | -60.509 |
| NiOH+ | 1.16E-13 | 9.64E-14 | -13.016 |
| NiSO4 (aq) | 4.72E-07 | 4.76E-07 | -6.322 |
| NO2-1 | 1.46E-42 | 1.21E-42 | -41.916 |
| NO3-1 | 9.56E-56 | 7.85E-56 | -55.105 |
| OH- | 5.58E-12 | 4.61E-12 | -11.337 |
| Pb DOM1 | 1.34E-09 | 1.19E-09 | -8.923 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(CO3)2-2 | 3.82E-25 | 1.84E-25 | -24.735 |
| Pb(HS)2 (aq) | 9.87E-69 | 9.97E-69 | -68.001 |
| Pb(HS)3- | 4.4E-105 | 3.7E-105 | -104.436 |
| Pb(NO2)2 (aq) | 2.96E-89 | 2.99E-89 | -88.525 |
| Pb(NO3)2 (aq) | 2.7E-117 | 2.7E-117 | -116.572 |
| Pb(OH)2 (aq) | 1.26E-19 | 1.27E-19 | -18.896 |
| Pb(OH)3- | 1.53E-27 | 1.28E-27 | -26.894 |
| Pb(SO4)2-2 | 2.62E-10 | 1.26E-10 | -9.898 |
| Pb+2 | 3.28E-08 | 1.58E-08 | -7.802 |
| Pb2OH+3 | 5.16E-19 | 9.98E-20 | -19.001 |
| Pb3(OH)4+2 | 2.07E-36 | 9.97E-37 | -36.001 |
| Pb4(OH)4+4 | 4.51E-40 | 2.43E-41 | -40.615 |
| PbCl+ | 1.06E-08 | 8.83E-09 | -8.054 |
| PbCl2 (aq) | 3.18E-10 | 3.21E-10 | -9.494 |
| PbCl3- | 5.32E-12 | 4.43E-12 | -11.353 |
| PbCl4-2 | 5.85E-14 | 2.82E-14 | -13.55 |
| PbCO3 (aq) | 1.94E-15 | 1.96E-15 | -14.708 |
| PbF+ | 1.07E-14 | 8.9E-15 | -14.051 |
| PbF2 (aq) | 4.33E-22 | 4.37E-22 | -21.36 |
| PbH2PO4+ | 4.41E-13 | 3.67E-13 | -12.435 |
| PbHCO3+ | 1.18E-11 | 9.81E-12 | -11.008 |
| PbHPO4 (aq) | 9.18E-16 | 9.27E-16 | -15.033 |
| PbNO2+ | 7.43E-48 | 6.19E-48 | -47.208 |
| PbNO3+ | 2.26E-62 | 1.88E-62 | -61.725 |
| PbOH+ | 3.43E-13 | 2.86E-13 | -12.544 |
| PbSO4 (aq) | 1.26E-08 | 1.27E-08 | -7.895 |
| PO4-3 | 9.76E-20 | 1.97E-20 | -19.706 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| S-2 | 7.48E-53 | 3.67E-53 | -52.435 |
| SO4-2 | 0.003499 | 0.001647 | -2.783 |
| Zn DOM1 | 1.64E-08 | 1.46E-08 | -7.835 |
| Zn(CO3)2-2 | 5.38E-25 | 2.59E-25 | -24.586 |
| Zn(N3)2 (aq) | 2.75E-16 | 2.78E-16 | -15.557 |
| Zn(N3)3- | 1.04E-21 | 8.7E-22 | -21.06 |
| Zn(NH3)2+2 | 2.25E-20 | 1.08E-20 | -19.966 |
| Zn(NH3)3+2 | 1.06E-27 | 5.09E-28 | -27.294 |
| Zn(NH3)4+2 | 2.43E-35 | 1.17E-35 | -34.932 |
| Zn(NO2)2 (aq) | 2.24E-88 | 2.26E-88 | -87.646 |
| Zn(NO3)2 (aq) | 3E-116 | 3E-116 | -115.524 |
| Zn(OH)2 (aq) | 1.22E-16 | 1.24E-16 | -15.908 |
| Zn(OH)3- | 4.72E-25 | 3.93E-25 | -24.405 |
| Zn(OH)4-2 | 1.3E-34 | 6.27E-35 | -34.203 |
| Zn(SO4)2-2 | 1.04E-07 | 5.01E-08 | -7.3 |
| Zn+2 | 1.91E-05 | 9.7E-06 | -5.013 |
| Zn2OH+3 | 2E-16 | 3.87E-17 | -16.412 |
| Zn2S3-2 | 2.7E-114 | 1.3E-114 | -113.881 |
| Zn4S6-4 | 5.4E-226 | 2.9E-227 | -226.533 |
| ZnCl+ | 5.44E-07 | 4.51E-07 | -6.346 |
| ZnCl2 (aq) | 4.98E-09 | 5.02E-09 | -8.299 |
| ZnCl3- | 1.11E-10 | 9.22E-11 | -10.035 |
| ZnCl4-2 | 1.54E-12 | 7.4E-13 | -12.131 |
| ZnCO3 (aq) | 2.02E-14 | 2.04E-14 | -13.69 |
| ZnF+ | 7.94E-13 | 6.62E-13 | -12.179 |
| ZnHCO3+ | 2.87E-10 | 2.39E-10 | -9.621 |
| ZnHPO4 (aq) | 9.25E-13 | 9.34E-13 | -12.03 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnN3+ | 9.17E-11 | 7.64E-11 | -10.117 |
| ZnNH3+2 | 6.07E-13 | 2.93E-13 | -12.534 |
| ZnNO2+ | 8.5E-47 | 7.08E-47 | -46.15 |
| ZnNO3+ | 2.45E-60 | 2.04E-60 | -59.691 |
| ZnOH+ | 5.36E-12 | 4.47E-12 | -11.35 |
| ZnS (aq) | 6.57E-42 | 6.63E-42 | -41.178 |
| ZnSO4 (aq) | 3.17E-06 | 3.2E-06 | -5.494 |

## C1.3 pH 4

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 1.02E-05 | 1.01E-05 | -4.995 |
| Al(OH)2+ | 3.4E-08 | 2.89E-08 | -7.539 |
| Al(OH)3 (aq) | 5.41E-11 | 5.45E-11 | -10.264 |
| Al(OH)4- | 2.88E-13 | 2.43E-13 | -12.614 |
| Al(SO4)2- | 3.19E-05 | 2.69E-05 | -4.57 |
| Al+3 | 0.00011 | 3.16E-05 | -4.5 |
| Al2(OH)2+4 | 1.06E-08 | 7.11E-10 | -9.148 |
| Al2(OH)2CO3+2 | 1.46E-08 | 7.43E-09 | -8.129 |
| Al2PO4+3 | 9.24E-08 | 2.02E-08 | -7.695 |
| Al3(OH)4+5 | 3.93E-11 | 5.74E-13 | -12.241 |
| AlCl+2 | 4.34E-07 | 2.21E-07 | -6.656 |
| AlF+2 | 1.3E-05 | 6.8E-06 | -5.167 |
| AlF2+ | 7.09E-08 | 6.03E-08 | -7.22 |
| AlF3 (aq) | 1.57E-11 | 1.58E-11 | -10.802 |
| AlF4- | 2.1E-16 | 1.77E-16 | -15.751 |
| AlHPO4+ | 8.09E-07 | 6.83E-07 | -6.165 |
| AlOH+2 | 3.11E-06 | 1.63E-06 | -5.788 |
| AlSO4+ | 0.000407 | 0.000343 | -3.464 |
| As3S4(HS)- | 1.4E-249 | 1.1E-249 | -248.942 |
| AsO4-3 | 1.85E-17 | 4.04E-18 | -17.394 |
| AsS(OH)HS- | 4.92E-87 | 4.16E-87 | -86.381 |
| Ca DOM1 | 3.28E-06 | 2.94E-06 | -5.532 |
| Ca(NH3)2+2 | 3.24E-20 | 1.65E-20 | -19.783 |
| Ca(NO3)2 | 3.65E-98 | 3.68E-98 | -97.434 |
| Ca+2 | 0.003399 | 0.001835 | -2.736 |
| CaCl+ | 8.84E-05 | 7.46E-05 | -4.127 |
| CaCO3 (aq) | 9.46E-12 | 9.53E-12 | -11.021 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCrO4 (aq) | 1.04E-09 | 1.05E-09 | -8.978 |
| CaF+ | 5.5E-10 | 4.67E-10 | -9.331 |
| CaH2PO4+ | 4.15E-08 | 3.53E-08 | -7.452 |
| CaHCO3+ | 2.21E-07 | 1.89E-07 | -6.724 |
| CaHPO4 (aq) | 4.34E-10 | 4.38E-10 | -9.359 |
| CaNH3+2 | 1.95E-11 | 9.89E-12 | -11.005 |
| CaNO3+ | 5.9E-48 | 4.99E-48 | -47.302 |
| CaOH+ | 1.76E-12 | 1.5E-12 | -11.823 |
| CaPO4- | 1.09E-14 | 9.31E-15 | -14.031 |
| CaSO4 (aq) | 0.000703 | 0.000709 | -3.149 |
| Cd DOM1 | 1.19E-11 | 1.07E-11 | -10.972 |
| Cd(CO3)2-2 | 1.17E-24 | 5.95E-25 | -24.225 |
| Cd(HS)2 (aq) | 2.33E-87 | 2.34E-87 | -86.63 |
| Cd(HS)3- | 3.6E-132 | 3.1E-132 | -131.512 |
| Cd(HS)4-2 | 2E-176 | 1E-176 | -175.993 |
| Cd(NH3)2+2 | 7.27E-22 | 3.7E-22 | -21.432 |
| Cd(NH3)3+2 | 3.05E-29 | 1.55E-29 | -28.81 |
| Cd(NH3)4+2 | 3.76E-37 | 1.91E-37 | -36.718 |
| Cd(NO2)2 (aq) | 1.75E-73 | 1.76E-73 | -72.754 |
| Cd(NO3)2 (aq) | 2.6E-99 | 2.7E-99 | -98.575 |
| Cd(OH)2 (aq) | 1.33E-21 | 1.34E-21 | -20.872 |
| Cd(OH)3- | 1.57E-30 | 1.32E-30 | -29.878 |
| Cd(OH)4-2 | 2.67E-40 | 1.36E-40 | -39.867 |
| Cd(SO4)2-2 | 5.71E-11 | 2.9E-11 | -10.537 |
| Cd+2 | 5.21E-09 | 2.65E-09 | -8.577 |
| Cd2OH+3 | 6.77E-23 | 1.48E-23 | -22.83 |
| CdCl+ | 4.98E-09 | 4.21E-09 | -8.376 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl2 (aq) | 2.87E-10 | 2.9E-10 | -9.538 |
| CdCO3 (aq) | 2.24E-16 | 2.26E-16 | -15.646 |
| CdF+ | 1.04E-15 | 8.77E-16 | -15.057 |
| CdHCO3+ | 7.71E-13 | 6.51E-13 | -12.186 |
| CdHPO4 (aq) | 6.66E-15 | 6.72E-15 | -14.173 |
| CdHS+ | 6.68E-48 | 5.64E-48 | -47.249 |
| CdNH3+2 | 3.59E-15 | 1.82E-15 | -14.739 |
| CdNO2+ | 3.88E-41 | 3.28E-41 | -40.484 |
| CdNO3+ | 1.06E-53 | 8.95E-54 | -53.048 |
| CdOH+ | 1.16E-15 | 9.82E-16 | -15.008 |
| CdSO4 (aq) | 1.02E-09 | 1.02E-09 | -8.99 |
| Cl-1 | 0.020503 | 0.01712 | -1.766 |
| CO3-2 | 6.94E-12 | 3.64E-12 | -11.439 |
| Cr2O7-2 | 8.34E-12 | 4.24E-12 | -11.373 |
| CrO3Cl- | 4.02E-12 | 3.39E-12 | -11.47 |
| CrO3H2PO4- | 5.61E-14 | 4.74E-14 | -13.324 |
| CrO3HPO4-2 | 1.94E-12 | 9.84E-13 | -12.007 |
| CrO3SO4-2 | 3.51E-11 | 1.79E-11 | -10.748 |
| CrO4-2 | 1.94E-09 | 9.72E-10 | -9.012 |
| Cu DOM1 | 4.55E-09 | 4.08E-09 | -8.389 |
| Cu(CO3)2-2 | 1.05E-20 | 5.35E-21 | -20.272 |
| Cu(N3)2 (aq) | 1.77E-14 | 1.78E-14 | -13.749 |
| Cu(N3)3- | 4.8E-18 | 4.06E-18 | -17.392 |
| Cu(N3)4-2 | 9.53E-23 | 4.85E-23 | -22.315 |
| Cu(NH3)2+2 | 5.99E-18 | 3.04E-18 | -17.517 |
| Cu(NH3)3+2 | 8.22E-24 | 4.18E-24 | -23.379 |
| Cu(NH3)4+2 | 2.33E-30 | 1.19E-30 | -29.926 |
| Cu(NO2)2 (aq) | 4.1E-73 | 4.13E-73 | -72.384 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO3)2 (aq) | 6.4E-99 | 6.4E-99 | -98.191 |
| Cu(OH)2 (aq) | 4.04E-17 | 4.07E-17 | -16.391 |
| Cu(OH)3- | 6.89E-23 | 5.82E-23 | -22.235 |
| Cu(OH)4-2 | 7.64E-33 | 3.89E-33 | -32.411 |
| Cu+2 | 4.78E-08 | 2.55E-08 | -7.594 |
| Cu2(OH)2+2 | 1.46E-18 | 7.44E-19 | -18.129 |
| Cu2OH+3 | 3.97E-18 | 8.67E-19 | -18.062 |
| Cu2S3-2 | 4.1E-146 | 2.1E-146 | -145.682 |
| Cu3(OH)4+2 | 1.19E-28 | 6.07E-29 | -28.217 |
| CuCl+ | 9.21E-10 | 7.75E-10 | -9.111 |
| CuCl2 (aq) | 2.19E-12 | 2.21E-12 | -11.655 |
| CuCl3- | 3.49E-16 | 2.94E-16 | -15.532 |
| CuCl4-2 1 | 6.89E-20 | 3.57E-20 | -19.448 |
| CuCO3 (aq) | 5.42E-13 | 5.46E-13 | -12.263 |
| CuF+ | 2.82E-14 | 2.38E-14 | -13.623 |
| CuHCO3+ | 1.48E-11 | 1.25E-11 | -10.904 |
| CuHPO4 (aq) | 1.69E-13 | 1.7E-13 | -12.77 |
| CuHSO4+ | 1.23E-12 | 1.04E-12 | -11.984 |
| CuN3+ | 9.93E-11 | 8.38E-11 | -10.077 |
| CuNH3+2 | 1.14E-12 | 5.8E-13 | -12.237 |
| CuNO2+ | 3.89E-40 | 3.28E-40 | -39.484 |
| CuNO3+ | 8.05E-53 | 6.8E-53 | -52.168 |
| CuOH+ | 5.84E-12 | 4.91E-12 | -11.309 |
| CuS(aq) | 8.34E-54 | 8.41E-54 | -53.075 |
| CuSO4 (aq) | 9.55E-09 | 9.62E-09 | -8.017 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.474 |
| DOM1 | 1.23E-05 | 3.27E-06 | -5.485 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| F-1 | 2.67E-08 | 2.24E-08 | -7.65 |
| Fe DOM1 | 5E-12 | 4.96E-12 | -11.304 |
| Fe(N3)2+ | 4.55E-16 | 3.84E-16 | -15.415 |
| Fe(N3)3 (aq) | 3.71E-19 | 3.74E-19 | -18.427 |
| Fe(NH3)2+2 | 6.18E-21 | 3.14E-21 | -20.503 |
| Fe(NH3)3+2 | 3.05E-29 | 1.55E-29 | -28.809 |
| Fe(NH3)4+2 | 6.44E-38 | 3.27E-38 | -37.485 |
| Fe(NO2)2+ | 4.62E-77 | 3.9E-77 | -76.409 |
| Fe(NO2)3 (aq) | 5.5E-109 | 5.5E-109 | -108.259 |
| Fe(OH)2 (aq) | 3.23E-19 | 3.26E-19 | -18.487 |
| Fe(OH)2+ | 6.04E-12 | 5.14E-12 | -11.289 |
| Fe(OH)3- | 1.11E-25 | 9.43E-26 | -25.026 |
| Fe(OH)3 (aq) | 1.69E-17 | 1.71E-17 | -16.768 |
| Fe(OH)4- | 1.31E-21 | 1.12E-21 | -20.952 |
| Fe(SO4)2- | 3.7E-14 | 3.12E-14 | -13.506 |
| Fe+2 | 1.02E-05 | 5.44E-06 | -5.265 |
| Fe+3 | 1.71E-13 | 4.91E-14 | -13.309 |
| Fe2(OH)2+4 | 2.08E-21 | 1.39E-22 | -21.856 |
| Fe3(OH)4+5 | 1.67E-29 | 2.44E-31 | -30.613 |
| FeCl+ | 6.95E-08 | 5.87E-08 | -7.231 |
| FeCl+2 | 3.55E-14 | 1.84E-14 | -13.735 |
| FeCrO4+ | 2.08E-15 | 1.75E-15 | -14.756 |
| FeF+ | 2.34E-12 | 1.97E-12 | -11.704 |
| FeF+2 | 2.03E-15 | 1.05E-15 | -14.98 |
| FeF2+ | 1.05E-18 | 8.88E-19 | -18.052 |
| FeF3 (aq) | 1.83E-23 | 1.84E-23 | -22.734 |
| FeH2PO4+ | 2.53E-09 | 2.15E-09 | -8.667 |
| FeH2PO4+2 | 1.4E-15 | 7.33E-16 | -15.135 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHCO3+ | 6.21E-10 | 5.31E-10 | -9.275 |
| FeHPO4 (aq) | 1.07E-11 | 1.08E-11 | -10.965 |
| FeHPO4+ | 3.6E-13 | 3.06E-13 | -12.514 |
| FeHS+ | 5.59E-47 | 4.72E-47 | -46.326 |
| FeN3+2 | 6.84E-14 | 3.48E-14 | -13.459 |
| FeNH3+2 | 4.92E-13 | 2.5E-13 | -12.601 |
| FeNO2+2 | 1.88E-44 | 9.57E-45 | -44.019 |
| FeOH+ | 1.18E-11 | 9.97E-12 | -11.001 |
| FeOH+2 | 6.37E-12 | 3.3E-12 | -11.482 |
| FeSO4 (aq) | 2.2E-06 | 2.22E-06 | -5.653 |
| FeSO4+ | 1.35E-12 | 1.15E-12 | -11.941 |
| H DOM1 | 2.59E-06 | 1.5E-06 | -5.825 |
| H+1 | 0.000115 | 0.0001 | -4 |
| H2AsO3- | 4.77E-13 | 4.03E-13 | -12.395 |
| H2AsO4- | 3.97E-07 | 3.35E-07 | -6.475 |
| H2CO3* (aq) | 0.002541 | 0.002561 | -2.592 |
| H2CrO4 (aq) | 1.14E-11 | 1.15E-11 | -10.939 |
| H2PO4- | 1.19E-06 | 1.02E-06 | -5.993 |
| H2S (aq) | 3.01E-44 | 3.03E-44 | -43.518 |
| H3AsO3 | 8.7E-08 | 8.77E-08 | -7.057 |
| H3AsO4 | 5.93E-09 | 5.98E-09 | -8.223 |
| H3PO4 | 1.28E-08 | 1.29E-08 | -7.891 |
| HAsO3-2 | 4.03E-23 | 2.05E-23 | -22.688 |
| HAsO4-2 | 6.47E-10 | 3.29E-10 | -9.483 |
| HCO3- | 1.15E-05 | 9.76E-06 | -5.011 |
| HCrO4- | 3.62E-07 | 3.06E-07 | -6.514 |
| HF (aq) | 2.79E-09 | 2.82E-09 | -8.551 |
| HF2- | 2.83E-16 | 2.37E-16 | -15.625 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(CO3)2-2 | 5.49E-36 | 2.79E-36 | -35.554 |
| Hg(HS)2 (aq) | 6.27E-84 | 6.32E-84 | -83.199 |
| Hg(N3)2 (aq) | 1.16E-15 | 1.17E-15 | -14.932 |
| Hg(NH3)2+2 | 1.34E-27 | 6.8E-28 | -27.168 |
| Hg(NH3)4+2 | 1.67E-43 | 8.5E-44 | -43.071 |
| Hg(NO2)2 (aq) | 6.77E-87 | 6.83E-87 | -86.166 |
| Hg(NO2)3- | 3.4E-119 | 2.9E-119 | -118.536 |
| Hg(NO2)4-2 | 1.8E-152 | 9.2E-153 | -152.036 |
| Hg(NO3)2 (aq) | 5.8E-120 | 5.8E-120 | -119.234 |
| Hg(OH)2 | 3.8E-27 | 3.83E-27 | -26.417 |
| Hg(SO4)2-2 | 1.14E-30 | 5.81E-31 | -30.236 |
| Hg+2 | 1.92E-28 | 9.76E-29 | -28.011 |
| Hg2OH+3 | 1.81E-55 | 3.95E-56 | -55.404 |
| Hg3(OH)3+3 | 3.25E-79 | 7.11E-80 | -79.148 |
| HgCl+ | 5.62E-23 | 4.75E-23 | -22.324 |
| HgCl2 (aq) | 6.19E-18 | 6.23E-18 | -17.205 |
| HgCl3-1 | 1.26E-18 | 1.06E-18 | -17.974 |
| HgCl4-2 | 1.6E-19 | 8.14E-20 | -19.09 |
| HgClOH (aq) | 3.29E-22 | 3.32E-22 | -21.479 |
| HgCO3 (aq) | 2.7E-28 | 2.72E-28 | -27.565 |
| HgF+ | 9.66E-35 | 8.15E-35 | -34.089 |
| HgHCO3+ | 5.35E-28 | 4.52E-28 | -27.345 |
| HgHS2- | 2.42E-86 | 2.05E-86 | -85.689 |
| HgN3+ | 4.99E-10 | 4.21E-10 | -9.376 |
| HgNO2+ | 7.04E-57 | 5.94E-57 | -56.226 |
| HgNO3+ | 2.09E-74 | 1.76E-74 | -73.754 |
| HgOH+ | 3.46E-28 | 2.92E-28 | -27.535 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgOHCO3- | 3.78E-31 | 3.2E-31 | -30.496 |
| HgS2-2 | 7.85E-91 | 3.99E-91 | -90.399 |
| HgSO4 (aq) | 3.02E-29 | 3.05E-29 | -28.516 |
| HN3 (aq) | 2.32E-05 | 2.34E-05 | -4.632 |
| HNO2 (aq) | 1.72E-35 | 1.74E-35 | -34.76 |
| HPO4-2 | 1.19E-09 | 6.17E-10 | -9.209 |
| HS-1 | 2.49E-47 | 2.08E-47 | -46.681 |
| HSO4- | 1.64E-05 | 1.39E-05 | -4.858 |
| K+1 | 0.000148 | 0.000124 | -3.908 |
| K2HPO4 (aq) | 1.01E-16 | 1.02E-16 | -15.991 |
| K2PO4- | 6.96E-24 | 5.88E-24 | -23.231 |
| KCl (aq) | 1.11E-06 | 1.12E-06 | -5.95 |
| KCr2O7- | 5.36E-15 | 4.53E-15 | -14.344 |
| KCrO4- | 5.29E-13 | 4.47E-13 | -12.35 |
| KF (aq) | 1.26E-12 | 1.27E-12 | -11.897 |
| KH2PO4 (aq) | 1.93E-10 | 1.95E-10 | -9.71 |
| KHPO4- | 5.52E-13 | 4.7E-13 | -12.328 |
| KNO3 (aq) | 7.47E-50 | 7.53E-50 | -49.123 |
| KOH (aq) | 9.83E-15 | 9.9E-15 | -14.004 |
| KPO4-2 | 1.12E-20 | 5.7E-21 | -20.244 |
| KSO4- | 1.6E-06 | 1.36E-06 | -5.866 |
| Mg DOM1 | 2.43E-07 | 2.18E-07 | -6.662 |
| Mg(NH3)2+2 | 1.2E-20 | 6.09E-21 | -20.215 |
| Mg+2 | 0.002478 | 0.00136 | -2.866 |
| Mg2CO3+2 | 5.15E-14 | 2.62E-14 | -13.582 |
| MgCl+ | 0.000104 | 8.77E-05 | -4.057 |
| MgCO3 (aq) | 3.5E-12 | 3.53E-12 | -11.452 |
| MgF+ | 2.39E-09 | 2.02E-09 | -8.695 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHCO3+ | 1.53E-07 | 1.29E-07 | -6.89 |
| MgHPO4 (aq) | 4.44E-10 | 4.48E-10 | -9.349 |
| MgOH+ | 2.47E-11 | 2.12E-11 | -10.675 |
| MgPO4- | 1.27E-16 | 1.08E-16 | -15.967 |
| MgSO4 (aq) | 0.000422 | 0.000425 | -3.372 |
| Mn+3 | 5.1E-06 | 1.46E-06 | -5.835 |
| N3-1 | 5.38E-06 | 4.54E-06 | -5.343 |
| Na+1 | 0.006836 | 0.005786 | -2.238 |
| Na2HPO4 (aq) | 1.46E-13 | 1.48E-13 | -12.831 |
| Na2PO4- | 3.25E-20 | 2.75E-20 | -19.561 |
| NaCl (aq) | 5.51E-05 | 5.55E-05 | -4.255 |
| NaCO3- | 6.13E-13 | 5.21E-13 | -12.283 |
| NaCrO4- | 3.31E-11 | 2.8E-11 | -10.553 |
| NaF (aq) | 1.14E-10 | 1.15E-10 | -9.94 |
| NaH2PO4 (aq) | 9.04E-09 | 9.11E-09 | -8.04 |
| NaHCO3 (aq) | 3.32E-08 | 3.35E-08 | -7.475 |
| NaHPO4- | 4E-11 | 3.4E-11 | -10.468 |
| NaNO3 (aq) | 1.29E-48 | 1.3E-48 | -47.886 |
| NaOH (aq) | 3.15E-13 | 3.17E-13 | -12.499 |
| NaPO4-2 | 5.78E-19 | 2.94E-19 | -18.532 |
| NaSO4- | 6.86E-05 | 5.84E-05 | -4.234 |
| NH3 (aq) | 1.61E-09 | 1.62E-09 | -8.79 |
| NH4+1 | 0.000712 | 0.000591 | -3.228 |
| NH4Cr2O7- | 2.98E-14 | 2.51E-14 | -13.6 |
| NH4SO4- | 1.4E-05 | 1.18E-05 | -4.928 |
| Ni DOM1 | 7.25E-09 | 6.5E-09 | -8.187 |
| Ni(N3)2 (aq) | 3.27E-15 | 3.3E-15 | -14.482 |
| Ni(NH3)2+2 | 9.67E-19 | 4.92E-19 | -18.308 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)3+2 | 9.08E-26 | 4.62E-26 | -25.336 |
| Ni(NH3)4+2 | 2.53E-33 | 1.29E-33 | -32.891 |
| Ni(NH3)5+2 | 2.27E-41 | 1.16E-41 | -40.937 |
| Ni(NH3)6+2 | 4.35E-50 | 2.21E-50 | -49.655 |
| Ni(NO2)2 (aq) | 1.5E-72 | 1.51E-72 | -71.821 |
| Ni(OH)2 (aq) | 1.62E-17 | 1.64E-17 | -16.786 |
| Ni(OH)3- | 1.95E-24 | 1.65E-24 | -23.784 |
| Ni(SO4)2-2 | 7.28E-11 | 3.7E-11 | -10.431 |
| Ni+2 | 3.18E-06 | 1.62E-06 | -5.792 |
| NiCl+ | 1.18E-08 | 9.99E-09 | -8 |
| NiCl2 (aq) | 6.05E-12 | 6.1E-12 | -11.215 |
| NiCO3 (aq) | 2.17E-13 | 2.18E-13 | -12.661 |
| NiF+ | 7.75E-13 | 6.54E-13 | -12.184 |
| NiH2PO4+ | 1.28E-11 | 1.08E-11 | -10.967 |
| NiHCO3+ | 1.83E-09 | 1.55E-09 | -8.811 |
| NiHPO4 (aq) | 7.23E-13 | 7.29E-13 | -12.137 |
| NiHS+ | 1.23E-47 | 1.04E-47 | -46.983 |
| NiN3+ | 1.64E-10 | 1.38E-10 | -9.859 |
| NiNH3+2 | 3.38E-12 | 1.72E-12 | -11.765 |
| NiNO2+ | 5.65E-39 | 4.77E-39 | -38.321 |
| NiNO3+ | 3.83E-51 | 3.23E-51 | -50.49 |
| NiOH+ | 1.17E-12 | 9.91E-13 | -12.004 |
| NiSO4 (aq) | 5.49E-07 | 5.54E-07 | -6.257 |
| NO2-1 | 1.46E-34 | 1.23E-34 | -33.91 |
| NO3-1 | 9.55E-46 | 7.97E-46 | -45.099 |
| OH- | 5.5E-11 | 4.61E-11 | -10.337 |
| Pb DOM1 | 5.25E-09 | 4.71E-09 | -8.327 |
| Pb(CO3)2-2 | 3.34E-21 | 1.7E-21 | -20.769 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(HS)2 (aq) | 1.18E-86 | 1.19E-86 | -85.924 |
| Pb(HS)3- | 5.9E-132 | 4.9E-132 | -131.306 |
| Pb(NO2)2 (aq) | 2.85E-73 | 2.88E-73 | -72.541 |
| Pb(NO3)2 (aq) | 2.56E-97 | 2.58E-97 | -96.589 |
| Pb(OH)2 (aq) | 1.18E-17 | 1.19E-17 | -16.926 |
| Pb(OH)3- | 1.41E-24 | 1.19E-24 | -23.923 |
| Pb(SO4)2-2 | 2.97E-10 | 1.51E-10 | -9.821 |
| Pb+2 | 2.9E-08 | 1.47E-08 | -7.831 |
| Pb2OH+3 | 3.99E-18 | 8.71E-19 | -18.06 |
| Pb3(OH)4+2 | 1.6E-32 | 8.13E-33 | -32.09 |
| Pb4(OH)4+4 | 2.77E-36 | 1.85E-37 | -36.733 |
| PbCl+ | 9.61E-09 | 8.12E-09 | -8.091 |
| PbCl2 (aq) | 2.88E-10 | 2.9E-10 | -9.537 |
| PbCl3- | 4.67E-12 | 3.95E-12 | -11.404 |
| PbCl4-2 | 4.86E-14 | 2.47E-14 | -13.607 |
| PbCO3 (aq) | 1.8E-13 | 1.82E-13 | -12.74 |
| PbF+ | 5.53E-14 | 4.67E-14 | -13.331 |
| PbF2 (aq) | 1.28E-20 | 1.29E-20 | -19.891 |
| PbH2PO4+ | 4.36E-13 | 3.68E-13 | -12.434 |
| PbHCO3+ | 1.08E-10 | 9.11E-11 | -10.04 |
| PbHPO4 (aq) | 9.22E-15 | 9.29E-15 | -14.032 |
| PbNO2+ | 6.95E-40 | 5.87E-40 | -39.231 |
| PbNO3+ | 2.12E-52 | 1.79E-52 | -51.748 |
| PbOH+ | 3.16E-12 | 2.67E-12 | -11.573 |
| PbSO4 (aq) | 1.33E-08 | 1.35E-08 | -7.871 |
| PO4-3 | 9.29E-18 | 2.11E-18 | -17.676 |
| S-2 | 8.02E-61 | 4.15E-61 | -60.382 |
| SO4-2 | 0.003728 | 0.001863 | -2.73 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn DOM1 | 7.02E-08 | 6.3E-08 | -7.201 |
| Zn(CO3)2-2 | 5.13E-21 | 2.61E-21 | -20.583 |
| Zn(N3)2 (aq) | 1.93E-14 | 1.95E-14 | -13.711 |
| Zn(N3)3- | 5.99E-19 | 5.05E-19 | -18.296 |
| Zn(NH3)2+2 | 2.23E-18 | 1.14E-18 | -17.945 |
| Zn(NH3)3+2 | 1.07E-24 | 5.42E-25 | -24.266 |
| Zn(NH3)4+2 | 2.49E-31 | 1.27E-31 | -30.897 |
| Zn(NO2)2 (aq) | 2.35E-72 | 2.37E-72 | -71.625 |
| Zn(NO3)2 (aq) | 3.12E-96 | 3.14E-96 | -95.503 |
| Zn(OH)2 (aq) | 1.25E-14 | 1.26E-14 | -13.9 |
| Zn(OH)3- | 4.74E-22 | 4.01E-22 | -21.397 |
| Zn(OH)4-2 | 1.26E-30 | 6.39E-31 | -30.195 |
| Zn(SO4)2-2 | 1.28E-07 | 6.53E-08 | -7.185 |
| Zn+2 | 1.85E-05 | 9.88E-06 | -5.005 |
| Zn2OH+3 | 1.84E-15 | 4.02E-16 | -15.396 |
| Zn2S3-2 | 3.9E-138 | 2E-138 | -137.705 |
| Zn4S6-4 | 9.9E-274 | 6.6E-275 | -274.18 |
| ZnCl+ | 5.38E-07 | 4.52E-07 | -6.345 |
| ZnCl2 (aq) | 4.92E-09 | 4.96E-09 | -8.305 |
| ZnCl3- | 1.06E-10 | 8.95E-11 | -10.048 |
| ZnCl4-2 | 1.39E-12 | 7.07E-13 | -12.15 |
| ZnCO3 (aq) | 2.05E-12 | 2.07E-12 | -11.684 |
| ZnF+ | 4.48E-12 | 3.79E-12 | -11.422 |
| ZnHCO3+ | 2.87E-09 | 2.42E-09 | -8.615 |
| ZnHPO4 (aq) | 1.01E-11 | 1.02E-11 | -10.991 |
| ZnN3+ | 7.64E-10 | 6.45E-10 | -9.19 |
| ZnNH3+2 | 5.95E-12 | 3.03E-12 | -11.519 |
| ZnNO2+ | 8.68E-39 | 7.33E-39 | -38.135 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnNO3+ | 2.5E-50 | 2.11E-50 | -49.676 |
| ZnOH+ | 5.39E-11 | 4.55E-11 | -10.342 |
| ZnS (aq) | 7.58E-50 | 7.64E-50 | -49.117 |
| ZnSO4 (aq) | 3.66E-06 | 3.69E-06 | -5.433 |

## C1.4 pH 5

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.49E-08 | 3.47E-08 | -7.46 |
| Al(OH)2+ | 3.41E-09 | 2.89E-09 | -8.539 |
| Al(OH)3 (aq) | 5.4E-11 | 5.45E-11 | -10.264 |
| Al(OH)4- | 2.89E-12 | 2.43E-12 | -11.614 |
| Al(SO4)2- | 7.03E-08 | 5.91E-08 | -7.228 |
| Al+3 | 1.13E-07 | 3.16E-08 | -7.5 |
| Al2(OH)2+4 | 1.13E-12 | 7.11E-14 | -13.148 |
| Al2(OH)2CO3+2 | 1.42E-10 | 7.13E-11 | -10.147 |
| Al2PO4+3 | 1.62E-11 | 3.42E-12 | -11.466 |
| Al3(OH)4+5 | 4.34E-16 | 5.74E-18 | -17.241 |
| AlCl+2 | 4.39E-10 | 2.2E-10 | -9.658 |
| AlF+2 | 2.44E-06 | 1.26E-06 | -5.9 |
| AlF2+ | 2.44E-06 | 2.06E-06 | -5.685 |
| AlF3 (aq) | 9.92E-08 | 1E-07 | -7 |
| AlF4- | 2.47E-10 | 2.08E-10 | -9.682 |
| AlHPO4+ | 1.38E-08 | 1.16E-08 | -7.936 |
| AlOH+2 | 3.16E-08 | 1.63E-08 | -7.788 |
| AlSO4+ | 6.05E-07 | 5.09E-07 | -6.293 |
| AsO4-3 | 2.32E-15 | 4.88E-16 | -15.311 |
| AsS(OH)HS- | 1.3E-108 | 1.1E-108 | -107.957 |
| Ca DOM1 | 1.03E-05 | 9.22E-06 | -5.035 |
| Ca(NH3)2+2 | 2.92E-18 | 1.46E-18 | -17.835 |
| Ca(NO3)2 | 3.24E-78 | 3.27E-78 | -77.485 |
| Ca+2 | 0.003149 | 0.001677 | -2.775 |
| CaCl+ | 8.08E-05 | 6.79E-05 | -4.168 |
| CaCO3 (aq) | 8.29E-10 | 8.36E-10 | -9.078 |
| CaCrO4 (aq) | 8.85E-09 | 8.92E-09 | -8.05 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaF+ | 9.34E-08 | 7.89E-08 | -7.103 |
| CaH2PO4+ | 6.45E-08 | 5.47E-08 | -7.262 |
| CaHCO3+ | 1.95E-06 | 1.66E-06 | -5.78 |
| CaHPO4 (aq) | 6.73E-09 | 6.79E-09 | -8.168 |
| CaNH3+2 | 1.78E-10 | 8.91E-11 | -10.05 |
| CaNO3+ | 5.34E-38 | 4.49E-38 | -37.348 |
| CaOH+ | 1.61E-11 | 1.37E-11 | -10.863 |
| CaPO4- | 1.7E-12 | 1.44E-12 | -11.841 |
| CaSO4 (aq) | 0.000952 | 0.00096 | -3.018 |
| Cd DOM1 | 3.86E-11 | 3.45E-11 | -10.462 |
| Cd(CO3)2-2 | 1.04E-20 | 5.18E-21 | -20.285 |
| Cd(HS)2 (aq) | 4.8E-105 | 4.9E-105 | -104.313 |
| Cd(HS)3- | 1.1E-158 | 9.5E-159 | -158.024 |
| Cd(HS)4-2 | 9.3E-212 | 4.6E-212 | -211.334 |
| Cd(NH3)2+2 | 6.78E-20 | 3.39E-20 | -19.469 |
| Cd(NH3)3+2 | 2.8E-26 | 1.4E-26 | -25.853 |
| Cd(NH3)4+2 | 3.41E-33 | 1.71E-33 | -32.768 |
| Cd(NO2)2 (aq) | 1.61E-57 | 1.62E-57 | -56.791 |
| Cd(NO3)2 (aq) | 2.42E-79 | 2.44E-79 | -78.612 |
| Cd(OH)2 (aq) | 1.26E-19 | 1.27E-19 | -18.897 |
| Cd(OH)3- | 1.49E-27 | 1.25E-27 | -26.903 |
| Cd(OH)4-2 | 2.57E-36 | 1.28E-36 | -35.891 |
| Cd(SO4)2-2 | 1.2E-10 | 6.03E-11 | -10.22 |
| Cd+2 | 5E-09 | 2.5E-09 | -8.602 |
| Cd2OH+3 | 6.27E-22 | 1.32E-22 | -21.879 |
| CdCl+ | 4.71E-09 | 3.96E-09 | -8.402 |
| CdCl2 (aq) | 2.69E-10 | 2.71E-10 | -9.566 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCO3 (aq) | 2.03E-14 | 2.05E-14 | -13.689 |
| CdF+ | 1.82E-13 | 1.53E-13 | -12.815 |
| CdHCO3+ | 7.02E-12 | 5.91E-12 | -11.229 |
| CdHPO4 (aq) | 1.07E-13 | 1.08E-13 | -12.968 |
| CdHS+ | 9.39E-57 | 7.9E-57 | -56.102 |
| CdNH3+2 | 3.4E-14 | 1.7E-14 | -13.77 |
| CdNO2+ | 3.63E-33 | 3.06E-33 | -32.515 |
| CdNO3+ | 9.91E-44 | 8.33E-44 | -43.079 |
| CdOH+ | 1.1E-14 | 9.28E-15 | -14.032 |
| CdSO4 (aq) | 1.42E-09 | 1.43E-09 | -8.844 |
| Cl-1 | 0.020517 | 0.01705 | -1.768 |
| CO3-2 | 6.77E-10 | 3.49E-10 | -9.457 |
| Cr2O7-2 | 7.31E-12 | 3.66E-12 | -11.437 |
| CrO3Cl- | 3.73E-13 | 3.14E-13 | -12.504 |
| CrO3H2PO4- | 8.88E-15 | 7.47E-15 | -14.127 |
| CrO3HPO4-2 | 3.1E-12 | 1.55E-12 | -11.81 |
| CrO3SO4-2 | 4.91E-12 | 2.46E-12 | -11.609 |
| CrO4-2 | 1.83E-08 | 9.03E-09 | -8.044 |
| Cu DOM1 | 1.23E-08 | 1.1E-08 | -7.957 |
| Cu(CO3)2-2 | 7.76E-17 | 3.89E-17 | -16.411 |
| Cu(N3)2 (aq) | 1.91E-13 | 1.92E-13 | -12.716 |
| Cu(N3)3- | 1.93E-16 | 1.62E-16 | -15.791 |
| Cu(N3)4-2 | 1.43E-20 | 7.16E-21 | -20.145 |
| Cu(NH3)2+2 | 4.66E-16 | 2.33E-16 | -15.632 |
| Cu(NH3)3+2 | 6.31E-21 | 3.16E-21 | -20.501 |
| Cu(NH3)4+2 | 1.77E-26 | 8.83E-27 | -26.054 |
| Cu(NO2)2 (aq) | 3.14E-57 | 3.17E-57 | -56.499 |
| Cu(NO3)2 (aq) | 4.89E-79 | 4.93E-79 | -78.307 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(OH)2 (aq) | 3.18E-15 | 3.21E-15 | -14.494 |
| Cu(OH)3- | 5.46E-20 | 4.59E-20 | -19.338 |
| Cu(OH)4-2 | 6.12E-29 | 3.06E-29 | -28.514 |
| Cu+2 | 3.82E-08 | 2.01E-08 | -7.697 |
| Cu2(OH)2+2 | 9.24E-17 | 4.62E-17 | -16.335 |
| Cu2OH+3 | 2.56E-17 | 5.39E-18 | -17.269 |
| Cu2S3-2 | 8.4E-170 | 4.2E-170 | -169.376 |
| Cu3(OH)4+2 | 5.94E-25 | 2.97E-25 | -24.527 |
| CuCl+ | 7.26E-10 | 6.08E-10 | -9.216 |
| CuCl2 (aq) | 1.71E-12 | 1.73E-12 | -11.762 |
| CuCl3- | 2.73E-16 | 2.29E-16 | -15.64 |
| CuCl4-2 1 | 5.43E-20 | 2.77E-20 | -19.558 |
| CuCO3 (aq) | 4.1E-11 | 4.13E-11 | -10.384 |
| CuF+ | 4.14E-12 | 3.48E-12 | -11.459 |
| CuHCO3+ | 1.12E-10 | 9.44E-11 | -10.025 |
| CuHPO4 (aq) | 2.25E-12 | 2.27E-12 | -11.643 |
| CuHSO4+ | 1.44E-13 | 1.21E-13 | -12.916 |
| CuN3+ | 2.91E-10 | 2.45E-10 | -9.612 |
| CuNH3+2 | 9E-12 | 4.5E-12 | -11.346 |
| CuNO2+ | 3.03E-32 | 2.55E-32 | -31.593 |
| CuNO3+ | 6.28E-43 | 5.28E-43 | -42.277 |
| CuOH+ | 4.62E-11 | 3.87E-11 | -10.412 |
| CuS(aq) | 9.74E-62 | 9.82E-62 | -61.008 |
| CuSO4 (aq) | 1.12E-08 | 1.12E-08 | -7.949 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.474 |
| DOM1 | 1.64E-05 | 4.23E-06 | -5.374 |
| F-1 | 4.97E-06 | 4.15E-06 | -5.382 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe DOM1 | 3.42E-14 | 3.4E-14 | -13.469 |
| Fe(N3)2+ | 1.25E-17 | 1.05E-17 | -16.979 |
| Fe(N3)3 (aq) | 3.75E-20 | 3.78E-20 | -19.422 |
| Fe(NH3)2+2 | 1.22E-21 | 6.1E-22 | -21.215 |
| Fe(NH3)3+2 | 5.94E-29 | 2.97E-29 | -28.527 |
| Fe(NH3)4+2 | 1.23E-36 | 6.18E-37 | -36.209 |
| Fe(NO2)2+ | 9.01E-64 | 7.57E-64 | -63.121 |
| Fe(NO2)3 (aq) | 1.05E-87 | 1.06E-87 | -86.977 |
| Fe(OH)2 (aq) | 6.46E-20 | 6.51E-20 | -19.186 |
| Fe(OH)2+ | 1.21E-12 | 1.03E-12 | -11.988 |
| Fe(OH)3- | 2.23E-25 | 1.88E-25 | -24.725 |
| Fe(OH)3 (aq) | 3.38E-17 | 3.41E-17 | -16.467 |
| Fe(OH)4- | 2.63E-20 | 2.23E-20 | -19.651 |
| Fe(SO4)2- | 1.63E-16 | 1.37E-16 | -15.863 |
| Fe+2 | 2.07E-08 | 1.09E-08 | -7.964 |
| Fe+3 | 3.51E-16 | 9.81E-17 | -16.009 |
| Fe2(OH)2+4 | 8.87E-25 | 5.56E-26 | -25.255 |
| Fe3(OH)4+5 | 1.47E-33 | 1.94E-35 | -34.712 |
| FeCl+ | 1.39E-10 | 1.17E-10 | -9.933 |
| FeCl+2 | 7.18E-17 | 3.66E-17 | -16.437 |
| FeCrO4+ | 3.87E-17 | 3.25E-17 | -16.488 |
| FeF+ | 8.68E-13 | 7.3E-13 | -12.137 |
| FeF+2 | 7.6E-16 | 3.87E-16 | -15.412 |
| FeF2+ | 7.19E-17 | 6.07E-17 | -16.217 |
| FeF3 (aq) | 2.31E-19 | 2.33E-19 | -18.632 |
| FeH2PO4+ | 8.6E-12 | 7.29E-12 | -11.138 |
| FeH2PO4+2 | 4.81E-18 | 2.48E-18 | -17.605 |
| FeHCO3+ | 1.2E-11 | 1.02E-11 | -10.992 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHPO4 (aq) | 3.64E-13 | 3.67E-13 | -12.436 |
| FeHPO4+ | 1.22E-14 | 1.04E-14 | -13.984 |
| FeHS+ | 1.66E-58 | 1.4E-58 | -57.855 |
| FeN3+2 | 5.14E-16 | 2.57E-16 | -15.59 |
| FeNH3+2 | 9.85E-15 | 4.93E-15 | -14.307 |
| FeNO2+2 | 3.77E-39 | 1.89E-39 | -38.725 |
| FeOH+ | 2.36E-13 | 1.99E-13 | -12.701 |
| FeOH+2 | 1.29E-13 | 6.58E-14 | -13.182 |
| FeSO4 (aq) | 6.52E-09 | 6.58E-09 | -8.182 |
| FeSO4+ | 4.01E-15 | 3.39E-15 | -14.47 |
| H DOM1 | 8.99E-07 | 5.13E-07 | -6.29 |
| H+1 | 1.15E-05 | 0.00001 | -5 |
| H2AsO3- | 5.79E-15 | 4.87E-15 | -14.312 |
| H2AsO4- | 4.82E-07 | 4.05E-07 | -6.392 |
| H2CO3* (aq) | 0.002438 | 0.002459 | -2.609 |
| H2CrO4 (aq) | 1.06E-12 | 1.07E-12 | -11.971 |
| H2PO4- | 2.03E-06 | 1.72E-06 | -5.764 |
| H2S (aq) | 4.45E-54 | 4.49E-54 | -53.348 |
| H3AsO3 | 1.05E-10 | 1.06E-10 | -9.974 |
| H3AsO4 | 7.17E-10 | 7.23E-10 | -9.141 |
| H3PO4 | 2.16E-09 | 2.18E-09 | -8.661 |
| HAsO3-2 | 4.95E-24 | 2.48E-24 | -23.606 |
| HAsO4-2 | 7.94E-09 | 3.97E-09 | -8.401 |
| HCO3- | 0.000111 | 9.37E-05 | -4.028 |
| HCrO4- | 3.38E-07 | 2.84E-07 | -6.546 |
| HF (aq) | 5.16E-08 | 5.21E-08 | -7.283 |
| HF2- | 9.73E-13 | 8.12E-13 | -12.091 |
| Hg(CO3)2-2 | 1.38E-36 | 6.93E-37 | -36.159 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(HS)2 (aq) | 3.7E-106 | 3.7E-106 | -105.427 |
| Hg(N3)2 (aq) | 4.28E-17 | 4.31E-17 | -16.365 |
| Hg(NH3)2+2 | 3.55E-30 | 1.78E-30 | -29.75 |
| Hg(NH3)4+2 | 4.32E-44 | 2.16E-44 | -43.665 |
| Hg(NO2)2 (aq) | 1.77E-75 | 1.79E-75 | -74.748 |
| Hg(NO2)3- | 8.9E-100 | 7.5E-100 | -99.124 |
| Hg(NO2)4-2 | 4.7E-125 | 2.3E-125 | -124.63 |
| Hg(NO3)2 (aq) | 1.5E-104 | 1.5E-104 | -103.816 |
| Hg(OH)2 | 1.02E-29 | 1.03E-29 | -28.987 |
| Hg(SO4)2-2 | 6.86E-35 | 3.44E-35 | -34.464 |
| Hg+2 | 5.25E-33 | 2.63E-33 | -32.581 |
| Hg2OH+3 | 1.36E-63 | 2.86E-64 | -63.544 |
| Hg3(OH)3+3 | 6.58E-90 | 1.39E-90 | -89.858 |
| HgCl+ | 1.51E-27 | 1.27E-27 | -26.895 |
| HgCl2 (aq) | 1.65E-22 | 1.66E-22 | -21.779 |
| HgCl3-1 | 3.36E-23 | 2.82E-23 | -22.549 |
| HgCl4-2 | 4.31E-24 | 2.15E-24 | -23.667 |
| HgClOH (aq) | 8.82E-26 | 8.89E-26 | -25.051 |
| HgCO3 (aq) | 6.98E-31 | 7.03E-31 | -30.153 |
| HgF+ | 4.83E-37 | 4.06E-37 | -36.391 |
| HgHCO3+ | 1.39E-31 | 1.17E-31 | -30.933 |
| HgHS2- | 1.4E-107 | 1.2E-107 | -106.917 |
| HgN3+ | 4.99E-10 | 4.19E-10 | -9.377 |
| HgNO2+ | 1.88E-53 | 1.58E-53 | -52.802 |
| HgNO3+ | 5.57E-69 | 4.68E-69 | -68.33 |
| HgOH+ | 9.35E-32 | 7.86E-32 | -31.105 |
| HgOHCO3- | 9.82E-33 | 8.26E-33 | -32.083 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgS2-2 | 4.7E-111 | 2.4E-111 | -110.627 |
| HgSO4 (aq) | 1.21E-33 | 1.22E-33 | -32.915 |
| HN3 (aq) | 8.57E-06 | 8.64E-06 | -5.063 |
| HNO2 (aq) | 1.7E-28 | 1.71E-28 | -27.766 |
| HPO4-2 | 2.05E-08 | 1.05E-08 | -7.98 |
| HS-1 | 3.7E-56 | 3.09E-56 | -55.511 |
| HSO4- | 2.44E-06 | 2.05E-06 | -5.688 |
| K+1 | 0.000147 | 0.000123 | -3.912 |
| K2HPO4 (aq) | 1.68E-15 | 1.7E-15 | -14.77 |
| K2PO4- | 1.16E-21 | 9.78E-22 | -21.01 |
| KCl (aq) | 1.1E-06 | 1.11E-06 | -5.956 |
| KCr2O7- | 4.6E-15 | 3.87E-15 | -14.412 |
| KCrO4- | 4.89E-12 | 4.11E-12 | -11.386 |
| KF (aq) | 2.3E-10 | 2.32E-10 | -9.634 |
| KH2PO4 (aq) | 3.25E-10 | 3.27E-10 | -9.485 |
| KHPO4- | 9.31E-12 | 7.89E-12 | -11.103 |
| KNO3 (aq) | 7.29E-40 | 7.35E-40 | -39.134 |
| KOH (aq) | 9.73E-14 | 9.81E-14 | -13.008 |
| KPO4-2 | 1.91E-18 | 9.57E-19 | -18.019 |
| KSO4- | 2.36E-06 | 2E-06 | -5.699 |
| Mg DOM1 | 7.74E-07 | 6.93E-07 | -6.159 |
| Mg(NH3)2+2 | 1.1E-18 | 5.49E-19 | -18.261 |
| Mg+2 | 0.002326 | 0.001261 | -2.899 |
| Mg2CO3+2 | 4.32E-12 | 2.16E-12 | -11.666 |
| MgCl+ | 9.62E-05 | 8.09E-05 | -4.092 |
| MgCO3 (aq) | 3.12E-10 | 3.14E-10 | -9.503 |
| MgF+ | 4.11E-07 | 3.46E-07 | -6.461 |
| MgHCO3+ | 1.37E-06 | 1.15E-06 | -5.94 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHPO4 (aq) | 6.98E-09 | 7.04E-09 | -8.152 |
| MgOH+ | 2.29E-10 | 1.96E-10 | -9.708 |
| MgPO4- | 2E-14 | 1.7E-14 | -13.771 |
| MgSO4 (aq) | 0.000579 | 0.000584 | -3.234 |
| Mn+3 | 6.47E-08 | 1.81E-08 | -7.743 |
| N3-1 | 2E-05 | 1.68E-05 | -4.775 |
| Na+1 | 0.006804 | 0.005736 | -2.241 |
| Na2HPO4 (aq) | 2.44E-12 | 2.46E-12 | -11.609 |
| Na2PO4- | 5.45E-18 | 4.58E-18 | -17.339 |
| NaCl (aq) | 5.44E-05 | 5.48E-05 | -4.261 |
| NaCO3- | 5.85E-11 | 4.96E-11 | -10.304 |
| NaCrO4- | 3.06E-10 | 2.57E-10 | -9.589 |
| NaF (aq) | 2.09E-08 | 2.1E-08 | -7.677 |
| NaH2PO4 (aq) | 1.52E-08 | 1.53E-08 | -7.815 |
| NaHCO3 (aq) | 3.16E-07 | 3.19E-07 | -6.497 |
| NaHPO4- | 6.75E-10 | 5.72E-10 | -9.243 |
| NaNO3 (aq) | 1.26E-38 | 1.27E-38 | -37.896 |
| NaOH (aq) | 3.12E-12 | 3.14E-12 | -11.502 |
| NaPO4-2 | 9.87E-17 | 4.94E-17 | -16.306 |
| NaSO4- | 0.000101 | 8.58E-05 | -4.066 |
| NH3 (aq) | 1.58E-08 | 1.6E-08 | -7.796 |
| NH4+1 | 0.000705 | 0.000583 | -3.235 |
| NH4Cr2O7- | 2.54E-14 | 2.14E-14 | -13.67 |
| NH4SO4- | 2.05E-05 | 1.72E-05 | -4.764 |
| Ni DOM1 | 2.28E-08 | 2.04E-08 | -7.69 |
| Ni(N3)2 (aq) | 4.09E-14 | 4.13E-14 | -13.384 |
| Ni(NH3)2+2 | 8.73E-17 | 4.37E-17 | -16.36 |
| Ni(NH3)3+2 | 8.08E-23 | 4.04E-23 | -22.393 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)4+2 | 2.22E-29 | 1.11E-29 | -28.955 |
| Ni(NH3)5+2 | 1.97E-36 | 9.84E-37 | -36.007 |
| Ni(NH3)6+2 | 3.72E-44 | 1.86E-44 | -43.731 |
| Ni(NO2)2 (aq) | 1.33E-56 | 1.34E-56 | -55.872 |
| Ni(OH)2 (aq) | 1.48E-15 | 1.5E-15 | -14.825 |
| Ni(OH)3- | 1.79E-21 | 1.51E-21 | -20.822 |
| Ni(SO4)2-2 | 1.49E-10 | 7.44E-11 | -10.128 |
| Ni+2 | 2.95E-06 | 1.48E-06 | -5.83 |
| NiCl+ | 1.08E-08 | 9.1E-09 | -8.041 |
| NiCl2 (aq) | 5.49E-12 | 5.54E-12 | -11.257 |
| NiCO3 (aq) | 1.9E-11 | 1.92E-11 | -10.717 |
| NiF+ | 1.32E-10 | 1.11E-10 | -9.956 |
| NiH2PO4+ | 1.99E-11 | 1.67E-11 | -10.777 |
| NiHCO3+ | 1.61E-08 | 1.36E-08 | -7.867 |
| NiHPO4 (aq) | 1.12E-11 | 1.13E-11 | -10.947 |
| NiHS+ | 1.68E-56 | 1.41E-56 | -55.851 |
| NiN3+ | 5.56E-10 | 4.68E-10 | -9.33 |
| NiNH3+2 | 3.1E-11 | 1.55E-11 | -10.81 |
| NiNO2+ | 5.11E-31 | 4.3E-31 | -30.366 |
| NiNO3+ | 3.47E-41 | 2.92E-41 | -40.535 |
| NiOH+ | 1.08E-11 | 9.06E-12 | -11.043 |
| NiSO4 (aq) | 7.44E-07 | 7.51E-07 | -6.125 |
| NO2-1 | 1.44E-26 | 1.21E-26 | -25.916 |
| NO3-1 | 9.46E-36 | 7.85E-36 | -35.105 |
| OH- | 5.52E-10 | 4.61E-10 | -9.337 |
| Pb DOM1 | 1.32E-08 | 1.19E-08 | -7.926 |
| Pb(CO3)2-2 | 2.3E-17 | 1.15E-17 | -16.939 |
| Pb(HS)2 (aq) | 1.9E-104 | 1.9E-104 | -103.717 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(HS)3- | 1.4E-158 | 1.2E-158 | -157.928 |
| Pb(NO2)2 (aq) | 2.03E-57 | 2.05E-57 | -56.688 |
| Pb(NO3)2 (aq) | 1.82E-77 | 1.84E-77 | -76.736 |
| Pb(OH)2 (aq) | 8.62E-16 | 8.7E-16 | -15.061 |
| Pb(OH)3- | 1.04E-21 | 8.75E-22 | -21.058 |
| Pb(SO4)2-2 | 4.86E-10 | 2.43E-10 | -9.614 |
| Pb+2 | 2.16E-08 | 1.08E-08 | -7.966 |
| Pb2OH+3 | 2.22E-17 | 4.69E-18 | -17.329 |
| Pb3(OH)4+2 | 6.41E-29 | 3.21E-29 | -28.494 |
| Pb4(OH)4+4 | 8.54E-33 | 5.35E-34 | -33.271 |
| PbCl+ | 7.05E-09 | 5.93E-09 | -8.227 |
| PbCl2 (aq) | 2.09E-10 | 2.11E-10 | -9.675 |
| PbCl3- | 3.4E-12 | 2.86E-12 | -11.544 |
| PbCl4-2 | 3.56E-14 | 1.78E-14 | -13.749 |
| PbCO3 (aq) | 1.27E-11 | 1.28E-11 | -10.893 |
| PbF+ | 7.53E-12 | 6.33E-12 | -11.198 |
| PbF2 (aq) | 3.2E-16 | 3.23E-16 | -15.491 |
| PbH2PO4+ | 5.44E-13 | 4.58E-13 | -12.339 |
| PbHCO3+ | 7.63E-10 | 6.42E-10 | -9.193 |
| PbHPO4 (aq) | 1.15E-13 | 1.16E-13 | -12.937 |
| PbNO2+ | 5.05E-32 | 4.25E-32 | -31.372 |
| PbNO3+ | 1.54E-42 | 1.29E-42 | -41.889 |
| PbOH+ | 2.33E-11 | 1.96E-11 | -10.708 |
| PbSO4 (aq) | 1.45E-08 | 1.46E-08 | -7.835 |
| PO4-3 | 1.63E-15 | 3.58E-16 | -15.446 |
| S-2 | 1.21E-68 | 6.15E-69 | -68.211 |
| SO4-2 | 0.005623 | 0.00276 | -2.559 |
| Zn DOM1 | 2.19E-07 | 1.96E-07 | -6.708 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn(CO3)2-2 | 4.35E-17 | 2.18E-17 | -16.662 |
| Zn(N3)2 (aq) | 2.39E-13 | 2.41E-13 | -12.618 |
| Zn(N3)3- | 2.76E-17 | 2.32E-17 | -16.635 |
| Zn(NH3)2+2 | 2E-16 | 1E-16 | -16 |
| Zn(NH3)3+2 | 9.4E-22 | 4.7E-22 | -21.328 |
| Zn(NH3)4+2 | 2.17E-27 | 1.08E-27 | -26.965 |
| Zn(NO2)2 (aq) | 2.07E-56 | 2.09E-56 | -55.68 |
| Zn(NO3)2 (aq) | 2.74E-76 | 2.77E-76 | -75.558 |
| Zn(OH)2 (aq) | 1.13E-12 | 1.14E-12 | -11.943 |
| Zn(OH)3- | 4.31E-19 | 3.63E-19 | -18.44 |
| Zn(OH)4-2 | 1.16E-26 | 5.78E-27 | -26.238 |
| Zn(SO4)2-2 | 2.6E-07 | 1.3E-07 | -6.886 |
| Zn+2 | 1.7E-05 | 8.95E-06 | -5.048 |
| Zn2OH+3 | 1.57E-14 | 3.3E-15 | -14.482 |
| Zn2S3-2 | 1.1E-161 | 5.3E-162 | -161.278 |
| ZnCl+ | 4.87E-07 | 4.08E-07 | -6.389 |
| ZnCl2 (aq) | 4.42E-09 | 4.45E-09 | -8.351 |
| ZnCl3- | 9.53E-11 | 8.01E-11 | -10.096 |
| ZnCl4-2 | 1.26E-12 | 6.3E-13 | -12.2 |
| ZnCO3 (aq) | 1.78E-10 | 1.8E-10 | -9.745 |
| ZnF+ | 7.54E-10 | 6.34E-10 | -9.198 |
| ZnHCO3+ | 2.51E-08 | 2.11E-08 | -7.676 |
| ZnHPO4 (aq) | 1.56E-10 | 1.57E-10 | -9.805 |
| ZnN3+ | 2.57E-09 | 2.16E-09 | -8.665 |
| ZnNH3+2 | 5.4E-11 | 2.7E-11 | -10.568 |
| ZnNO2+ | 7.78E-31 | 6.54E-31 | -30.184 |
| ZnNO3+ | 2.24E-40 | 1.88E-40 | -39.725 |
| ZnOH+ | 4.9E-10 | 4.12E-10 | -9.385 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnS (aq) | 1.02E-57 | 1.03E-57 | -56.989 |
| ZnSO4 (aq) | 4.91E-06 | 4.95E-06 | -5.305 |

## C1.5 pH 6

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 3.71E-11 | 3.68E-11 | -10.434 |
| Al(OH)2+ | 3.41E-10 | 2.89E-10 | -9.539 |
| Al(OH)3 (aq) | 5.4E-11 | 5.45E-11 | -10.264 |
| Al(OH)4- | 2.89E-11 | 2.43E-11 | -10.614 |
| Al(SO4)2- | 7.02E-11 | 5.91E-11 | -10.229 |
| Al+3 | 1.14E-10 | 3.16E-11 | -10.5 |
| Al2(OH)2+4 | 1.15E-16 | 7.11E-18 | -17.148 |
| Al2(OH)2CO3+2 | 1.02E-12 | 5.08E-13 | -12.294 |
| Al2PO4+3 | 5.78E-16 | 1.21E-16 | -15.917 |
| Al3(OH)4+5 | 4.41E-21 | 5.74E-23 | -22.241 |
| AlCl+2 | 4.4E-13 | 2.2E-13 | -12.658 |
| AlF+2 | 5.53E-09 | 2.85E-09 | -8.545 |
| AlF2+ | 1.25E-08 | 1.06E-08 | -7.976 |
| AlF3 (aq) | 1.15E-09 | 1.16E-09 | -8.936 |
| AlF4- | 6.49E-12 | 5.45E-12 | -11.263 |
| AlHPO4+ | 4.88E-11 | 4.1E-11 | -10.387 |
| AlOH+2 | 3.17E-10 | 1.63E-10 | -9.788 |
| AlSO4+ | 6.05E-10 | 5.09E-10 | -9.293 |
| AsO4-3 | 2.04E-13 | 4.26E-14 | -13.37 |
| AsS(OH)HS- | 1.1E-130 | 9.6E-131 | -130.016 |
| Ca DOM1 | 1.09E-05 | 9.73E-06 | -5.012 |
| Ca(NH3)2+2 | 2.91E-16 | 1.45E-16 | -15.838 |
| Ca(NO3)2 | 3.22E-58 | 3.25E-58 | -57.488 |
| Ca+2 | 0.003139 | 0.001669 | -2.778 |
| CaCl+ | 8.04E-05 | 6.75E-05 | -4.17 |
| CaCO3 (aq) | 5.88E-08 | 5.93E-08 | -7.227 |
| CaCrO4 (aq) | 5.25E-08 | 5.29E-08 | -7.276 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaF+ | 2.1E-07 | 1.78E-07 | -6.75 |
| CaH2PO4+ | 2.27E-08 | 1.92E-08 | -7.716 |
| CaHCO3+ | 1.38E-05 | 1.18E-05 | -4.93 |
| CaHPO4 (aq) | 2.37E-08 | 2.39E-08 | -7.622 |
| CaNH3+2 | 1.77E-09 | 8.86E-10 | -9.053 |
| CaNO3+ | 5.31E-28 | 4.47E-28 | -27.35 |
| CaOH+ | 1.6E-10 | 1.37E-10 | -9.865 |
| CaPO4- | 6E-11 | 5.08E-11 | -10.294 |
| CaSO4 (aq) | 0.000947 | 0.000955 | -3.02 |
| Cd DOM1 | 4.07E-11 | 3.64E-11 | -10.438 |
| Cd(CO3)2-2 | 5.25E-17 | 2.62E-17 | -16.582 |
| Cd(HS)2 (aq) | 4.8E-123 | 4.8E-123 | -122.316 |
| Cd(HS)3- | 1.1E-185 | 9.4E-186 | -185.027 |
| Cd(HS)4-2 | 9.2E-248 | 4.6E-248 | -247.337 |
| Cd(NH3)2+2 | 6.75E-18 | 3.37E-18 | -17.472 |
| Cd(NH3)3+2 | 2.79E-23 | 1.39E-23 | -22.857 |
| Cd(NH3)4+2 | 3.39E-29 | 1.69E-29 | -28.772 |
| Cd(NO2)2 (aq) | 1.59E-41 | 1.61E-41 | -40.794 |
| Cd(NO3)2 (aq) | 2.41E-59 | 2.43E-59 | -58.615 |
| Cd(OH)2 (aq) | 1.25E-17 | 1.26E-17 | -16.899 |
| Cd(OH)3- | 1.48E-24 | 1.24E-24 | -23.905 |
| Cd(OH)4-2 | 2.56E-32 | 1.28E-32 | -31.893 |
| Cd(SO4)2-2 | 1.2E-10 | 5.99E-11 | -10.223 |
| Cd+2 | 4.99E-09 | 2.49E-09 | -8.604 |
| Cd2OH+3 | 6.24E-21 | 1.31E-21 | -20.884 |
| CdCl+ | 4.69E-09 | 3.94E-09 | -8.405 |
| CdCl2 (aq) | 2.67E-10 | 2.7E-10 | -9.569 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCO3 (aq) | 1.44E-12 | 1.45E-12 | -11.838 |
| CdF+ | 4.11E-13 | 3.45E-13 | -12.462 |
| CdHCO3+ | 4.98E-11 | 4.19E-11 | -10.378 |
| CdHPO4 (aq) | 3.76E-13 | 3.79E-13 | -12.422 |
| CdHS+ | 9.35E-66 | 7.86E-66 | -65.105 |
| CdNH3+2 | 3.38E-13 | 1.69E-13 | -12.772 |
| CdNO2+ | 3.61E-25 | 3.04E-25 | -24.518 |
| CdNO3+ | 9.86E-34 | 8.29E-34 | -33.082 |
| CdOH+ | 1.1E-13 | 9.23E-14 | -13.035 |
| CdSO4 (aq) | 1.41E-09 | 1.43E-09 | -8.846 |
| Cl-1 | 0.020517 | 0.017039 | -1.769 |
| CO3-2 | 4.84E-08 | 2.49E-08 | -7.604 |
| Cr2O7-2 | 2.6E-12 | 1.3E-12 | -11.886 |
| CrO3Cl- | 2.22E-14 | 1.87E-14 | -13.729 |
| CrO3H2PO4- | 1.87E-16 | 1.57E-16 | -15.803 |
| CrO3HPO4-2 | 6.55E-13 | 3.27E-13 | -12.486 |
| CrO3SO4-2 | 2.93E-13 | 1.47E-13 | -12.834 |
| CrO4-2 | 1.1E-07 | 5.38E-08 | -7.269 |
| Cu DOM1 | 1.21E-08 | 1.08E-08 | -7.965 |
| Cu(CO3)2-2 | 3.66E-13 | 1.83E-13 | -12.738 |
| Cu(N3)2 (aq) | 3.31E-13 | 3.34E-13 | -12.476 |
| Cu(N3)3- | 4.58E-16 | 3.85E-16 | -15.414 |
| Cu(N3)4-2 | 4.67E-20 | 2.33E-20 | -19.632 |
| Cu(NH3)2+2 | 4.32E-14 | 2.16E-14 | -13.666 |
| Cu(NH3)3+2 | 5.84E-18 | 2.92E-18 | -17.535 |
| Cu(NH3)4+2 | 1.63E-22 | 8.15E-23 | -22.089 |
| Cu(NO2)2 (aq) | 2.9E-41 | 2.93E-41 | -40.533 |
| Cu(NO3)2 (aq) | 4.52E-59 | 4.56E-59 | -58.341 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(OH)2 (aq) | 2.95E-13 | 2.97E-13 | -12.527 |
| Cu(OH)3- | 5.06E-17 | 4.25E-17 | -16.371 |
| Cu(OH)4-2 | 5.68E-25 | 2.84E-25 | -24.547 |
| Cu+2 | 3.55E-08 | 1.86E-08 | -7.73 |
| Cu2(OH)2+2 | 7.95E-15 | 3.97E-15 | -14.402 |
| Cu2OH+3 | 2.21E-16 | 4.62E-17 | -16.335 |
| Cu2S3-2 | 7.2E-194 | 3.6E-194 | -193.443 |
| Cu3(OH)4+2 | 4.73E-21 | 2.36E-21 | -20.626 |
| CuCl+ | 6.73E-10 | 5.63E-10 | -9.249 |
| CuCl2 (aq) | 1.59E-12 | 1.6E-12 | -11.796 |
| CuCl3- | 2.53E-16 | 2.12E-16 | -15.674 |
| CuCl4-2 1 | 5.03E-20 | 2.56E-20 | -19.592 |
| CuCO3 (aq) | 2.7E-09 | 2.73E-09 | -8.564 |
| CuF+ | 8.68E-12 | 7.29E-12 | -11.137 |
| CuHCO3+ | 7.42E-10 | 6.23E-10 | -9.205 |
| CuHPO4 (aq) | 7.39E-12 | 7.45E-12 | -11.128 |
| CuHSO4+ | 1.34E-14 | 1.12E-14 | -13.95 |
| CuN3+ | 3.69E-10 | 3.1E-10 | -9.508 |
| CuNH3+2 | 8.35E-11 | 4.17E-11 | -10.38 |
| CuNO2+ | 2.81E-24 | 2.36E-24 | -23.627 |
| CuNO3+ | 5.82E-33 | 4.89E-33 | -32.311 |
| CuOH+ | 4.28E-10 | 3.59E-10 | -9.445 |
| CuS(aq) | 9.02E-70 | 9.09E-70 | -69.041 |
| CuSO4 (aq) | 1.03E-08 | 1.04E-08 | -7.983 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.474 |
| DOM1 | 1.66E-05 | 4.26E-06 | -5.37 |
| F-1 | 1.13E-05 | 9.38E-06 | -5.028 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe DOM1 | 7.25E-17 | 7.2E-17 | -16.143 |
| Fe(N3)2+ | 4.68E-20 | 3.93E-20 | -19.405 |
| Fe(N3)3 (aq) | 1.92E-22 | 1.94E-22 | -21.712 |
| Fe(NH3)2+2 | 2.43E-22 | 1.22E-22 | -21.915 |
| Fe(NH3)3+2 | 1.18E-28 | 5.92E-29 | -28.228 |
| Fe(NH3)4+2 | 2.46E-35 | 1.23E-35 | -34.911 |
| Fe(NO2)2+ | 1.79E-50 | 1.51E-50 | -49.821 |
| Fe(NO2)3 (aq) | 2.08E-66 | 2.1E-66 | -65.678 |
| Fe(OH)2 (aq) | 1.29E-20 | 1.3E-20 | -19.886 |
| Fe(OH)2+ | 2.42E-13 | 2.05E-13 | -12.688 |
| Fe(OH)3- | 4.45E-25 | 3.76E-25 | -24.425 |
| Fe(OH)3 (aq) | 6.74E-17 | 6.8E-17 | -16.167 |
| Fe(OH)4- | 5.26E-19 | 4.46E-19 | -18.351 |
| Fe(SO4)2- | 3.25E-19 | 2.73E-19 | -18.564 |
| Fe+2 | 4.13E-11 | 2.17E-11 | -10.664 |
| Fe+3 | 7.02E-19 | 1.96E-19 | -18.708 |
| Fe2(OH)2+4 | 3.57E-28 | 2.21E-29 | -28.655 |
| Fe3(OH)4+5 | 1.19E-37 | 1.54E-39 | -38.811 |
| FeCl+ | 2.77E-13 | 2.33E-13 | -12.633 |
| FeCl+2 | 1.44E-19 | 7.3E-20 | -19.137 |
| FeCrO4+ | 4.6E-19 | 3.87E-19 | -18.412 |
| FeF+ | 3.92E-15 | 3.3E-15 | -14.482 |
| FeF+2 | 3.44E-18 | 1.75E-18 | -17.757 |
| FeF2+ | 7.35E-19 | 6.21E-19 | -18.207 |
| FeF3 (aq) | 5.35E-21 | 5.4E-21 | -20.268 |
| FeH2PO4+ | 6.07E-15 | 5.14E-15 | -14.289 |
| FeH2PO4+2 | 3.41E-21 | 1.75E-21 | -20.756 |
| FeHCO3+ | 1.7E-13 | 1.45E-13 | -12.839 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHPO4 (aq) | 2.57E-15 | 2.59E-15 | -14.587 |
| FeHPO4+ | 8.64E-17 | 7.32E-17 | -16.135 |
| FeHS+ | 3.31E-70 | 2.79E-70 | -69.555 |
| FeN3+2 | 1.41E-18 | 7.02E-19 | -18.153 |
| FeNH3+2 | 1.97E-16 | 9.83E-17 | -16.007 |
| FeNO2+2 | 7.53E-34 | 3.76E-34 | -33.425 |
| FeOH+ | 4.71E-15 | 3.97E-15 | -14.401 |
| FeOH+2 | 2.58E-15 | 1.31E-15 | -14.881 |
| FeSO4 (aq) | 1.3E-11 | 1.31E-11 | -10.882 |
| FeSO4+ | 8.01E-18 | 6.77E-18 | -17.17 |
| H DOM1 | 9.55E-08 | 5.44E-08 | -7.264 |
| H+1 | 1.15E-06 | 0.000001 | -6 |
| H2AsO3- | 5.06E-17 | 4.25E-17 | -16.371 |
| H2AsO4- | 4.21E-07 | 3.54E-07 | -6.451 |
| H2CO3* (aq) | 0.001737 | 0.001752 | -2.756 |
| H2CrO4 (aq) | 6.31E-14 | 6.37E-14 | -13.196 |
| H2PO4- | 7.19E-07 | 6.09E-07 | -6.215 |
| H2S (aq) | 4.45E-64 | 4.49E-64 | -63.348 |
| H3AsO3 | 9.18E-14 | 9.26E-14 | -13.033 |
| H3AsO4 | 6.26E-11 | 6.31E-11 | -10.2 |
| H3PO4 | 7.65E-11 | 7.71E-11 | -10.113 |
| HAsO3-2 | 4.34E-25 | 2.16E-25 | -24.665 |
| HAsO4-2 | 6.95E-08 | 3.47E-08 | -7.46 |
| HCO3- | 0.000788 | 0.000668 | -3.175 |
| HCrO4- | 2.02E-07 | 1.69E-07 | -6.771 |
| HF (aq) | 1.17E-08 | 1.18E-08 | -7.929 |
| HF2- | 4.99E-13 | 4.16E-13 | -12.381 |
| Hg(CO3)2-2 | 5.14E-37 | 2.57E-37 | -36.59 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(HS)2 (aq) | 2.7E-128 | 2.7E-128 | -127.564 |
| Hg(N3)2 (aq) | 5.85E-19 | 5.9E-19 | -18.229 |
| Hg(NH3)2+2 | 2.59E-32 | 1.3E-32 | -31.888 |
| Hg(NH3)4+2 | 3.15E-44 | 1.57E-44 | -43.804 |
| Hg(NO2)2 (aq) | 1.29E-63 | 1.3E-63 | -62.886 |
| Hg(NO2)3- | 6.5E-80 | 5.47E-80 | -79.262 |
| Hg(NO2)4-2 | 3.41E-97 | 1.7E-97 | -96.769 |
| Hg(NO3)2 (aq) | 1.1E-88 | 1.11E-88 | -87.954 |
| Hg(OH)2 | 7.46E-32 | 7.53E-32 | -31.123 |
| Hg(SO4)2-2 | 5.02E-39 | 2.5E-39 | -38.601 |
| Hg+2 | 3.84E-37 | 1.92E-37 | -36.717 |
| Hg2OH+3 | 7.27E-71 | 1.52E-71 | -70.817 |
| Hg3(OH)3+3 | 2.6E-99 | 5.4E-100 | -99.268 |
| HgCl+ | 1.1E-31 | 9.28E-32 | -31.032 |
| HgCl2 (aq) | 1.2E-26 | 1.21E-26 | -25.916 |
| HgCl3-1 | 2.45E-27 | 2.06E-27 | -26.687 |
| HgCl4-2 | 3.14E-28 | 1.57E-28 | -27.804 |
| HgClOH (aq) | 6.43E-29 | 6.49E-29 | -28.188 |
| HgCO3 (aq) | 3.63E-33 | 3.66E-33 | -32.437 |
| HgF+ | 7.98E-41 | 6.71E-41 | -40.173 |
| HgHCO3+ | 7.22E-35 | 6.07E-35 | -34.217 |
| HgHS2- | 1E-128 | 8.8E-129 | -128.054 |
| HgN3+ | 4.99E-10 | 4.19E-10 | -9.378 |
| HgNO2+ | 1.37E-49 | 1.15E-49 | -48.939 |
| HgNO3+ | 4.06E-63 | 3.41E-63 | -62.467 |
| HgOH+ | 6.83E-35 | 5.74E-35 | -34.241 |
| HgOHCO3- | 5.11E-34 | 4.3E-34 | -33.367 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgS2-2 | 3.4E-131 | 1.7E-131 | -130.764 |
| HgSO4 (aq) | 8.8E-38 | 8.87E-38 | -37.052 |
| HN3 (aq) | 1.17E-06 | 1.18E-06 | -5.927 |
| HNO2 (aq) | 1.7E-21 | 1.71E-21 | -20.766 |
| HPO4-2 | 7.29E-08 | 3.7E-08 | -7.431 |
| HS-1 | 3.7E-65 | 3.08E-65 | -64.511 |
| HSO4- | 2.44E-07 | 2.05E-07 | -6.688 |
| K+1 | 0.000147 | 0.000122 | -3.912 |
| K2HPO4 (aq) | 5.95E-15 | 6E-15 | -14.222 |
| K2PO4- | 4.11E-20 | 3.45E-20 | -19.462 |
| KCl (aq) | 1.1E-06 | 1.11E-06 | -5.956 |
| KCr2O7- | 1.63E-15 | 1.37E-15 | -14.862 |
| KCrO4- | 2.91E-11 | 2.45E-11 | -10.611 |
| KF (aq) | 5.21E-10 | 5.25E-10 | -9.28 |
| KH2PO4 (aq) | 1.15E-10 | 1.16E-10 | -9.937 |
| KHPO4- | 3.29E-11 | 2.79E-11 | -10.555 |
| KNO3 (aq) | 7.28E-30 | 7.34E-30 | -29.134 |
| KOH (aq) | 9.72E-13 | 9.8E-13 | -12.009 |
| KPO4-2 | 6.77E-17 | 3.38E-17 | -16.471 |
| KSO4- | 2.36E-06 | 2E-06 | -5.7 |
| Mg DOM1 | 8.17E-07 | 7.31E-07 | -6.136 |
| Mg(NH3)2+2 | 1.09E-16 | 5.45E-17 | -16.263 |
| Mg+2 | 0.00232 | 0.001255 | -2.901 |
| Mg2CO3+2 | 3.06E-10 | 1.53E-10 | -9.816 |
| MgCl+ | 9.58E-05 | 8.05E-05 | -4.094 |
| MgCO3 (aq) | 2.21E-08 | 2.23E-08 | -7.652 |
| MgF+ | 9.27E-07 | 7.8E-07 | -6.108 |
| MgHCO3+ | 9.72E-06 | 8.14E-06 | -5.089 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHPO4 (aq) | 2.46E-08 | 2.48E-08 | -7.606 |
| MgOH+ | 2.29E-09 | 1.95E-09 | -8.709 |
| MgPO4- | 7.05E-13 | 5.97E-13 | -12.224 |
| MgSO4 (aq) | 0.000576 | 0.000581 | -3.236 |
| Mn+3 | 6.49E-12 | 1.81E-12 | -11.743 |
| N3-1 | 2.74E-05 | 2.3E-05 | -4.638 |
| Na+1 | 0.006802 | 0.005731 | -2.242 |
| Na2HPO4 (aq) | 8.61E-12 | 8.69E-12 | -11.061 |
| Na2PO4- | 1.92E-16 | 1.62E-16 | -15.791 |
| NaCl (aq) | 5.43E-05 | 5.47E-05 | -4.262 |
| NaCO3- | 4.17E-09 | 3.53E-09 | -8.452 |
| NaCrO4- | 1.82E-09 | 1.53E-09 | -8.814 |
| NaF (aq) | 4.72E-08 | 4.76E-08 | -7.322 |
| NaH2PO4 (aq) | 5.37E-09 | 5.42E-09 | -8.266 |
| NaHCO3 (aq) | 2.25E-06 | 2.27E-06 | -5.644 |
| NaHPO4- | 2.39E-09 | 2.02E-09 | -8.694 |
| NaNO3 (aq) | 1.26E-28 | 1.27E-28 | -27.897 |
| NaOH (aq) | 3.12E-11 | 3.14E-11 | -10.503 |
| NaPO4-2 | 3.5E-15 | 1.75E-15 | -14.758 |
| NaSO4- | 0.000101 | 8.57E-05 | -4.067 |
| NH3 (aq) | 1.58E-07 | 1.6E-07 | -6.797 |
| NH4+1 | 0.000705 | 0.000582 | -3.235 |
| NH4Cr2O7- | 9.03E-15 | 7.59E-15 | -14.12 |
| NH4SO4- | 2.05E-05 | 1.72E-05 | -4.764 |
| Ni DOM1 | 2.35E-08 | 2.1E-08 | -7.677 |
| Ni(N3)2 (aq) | 7.45E-14 | 7.52E-14 | -13.124 |
| Ni(NH3)2+2 | 8.49E-15 | 4.24E-15 | -14.373 |
| Ni(NH3)3+2 | 7.85E-20 | 3.92E-20 | -19.407 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)4+2 | 2.15E-25 | 1.08E-25 | -24.969 |
| Ni(NH3)5+2 | 1.91E-31 | 9.52E-32 | -31.021 |
| Ni(NH3)6+2 | 3.6E-38 | 1.8E-38 | -37.746 |
| Ni(NO2)2 (aq) | 1.29E-40 | 1.3E-40 | -39.886 |
| Ni(OH)2 (aq) | 1.44E-13 | 1.45E-13 | -12.838 |
| Ni(OH)3- | 1.74E-18 | 1.46E-18 | -17.835 |
| Ni(SO4)2-2 | 1.45E-10 | 7.22E-11 | -10.141 |
| Ni+2 | 2.88E-06 | 1.44E-06 | -5.843 |
| NiCl+ | 1.05E-08 | 8.84E-09 | -8.054 |
| NiCl2 (aq) | 5.33E-12 | 5.37E-12 | -11.27 |
| NiCO3 (aq) | 1.32E-09 | 1.33E-09 | -8.877 |
| NiF+ | 2.9E-10 | 2.43E-10 | -9.614 |
| NiH2PO4+ | 6.84E-12 | 5.75E-12 | -11.24 |
| NiHCO3+ | 1.12E-07 | 9.4E-08 | -7.027 |
| NiHPO4 (aq) | 3.85E-11 | 3.89E-11 | -10.41 |
| NiHS+ | 1.63E-65 | 1.37E-65 | -64.864 |
| NiN3+ | 7.4E-10 | 6.22E-10 | -9.206 |
| NiNH3+2 | 3.01E-10 | 1.5E-10 | -9.823 |
| NiNO2+ | 4.97E-23 | 4.18E-23 | -22.379 |
| NiNO3+ | 3.37E-31 | 2.83E-31 | -30.548 |
| NiOH+ | 1.05E-10 | 8.81E-11 | -10.055 |
| NiSO4 (aq) | 7.23E-07 | 7.29E-07 | -6.137 |
| NO2-1 | 1.44E-18 | 1.21E-18 | -17.916 |
| NO3-1 | 9.46E-26 | 7.85E-26 | -25.105 |
| OH- | 5.53E-09 | 4.61E-09 | -8.337 |
| Pb DOM1 | 1.26E-08 | 1.13E-08 | -7.948 |
| Pb(CO3)2-2 | 1.05E-13 | 5.24E-14 | -13.281 |
| Pb(HS)2 (aq) | 1.7E-122 | 1.7E-122 | -121.765 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(HS)3- | 1.3E-185 | 1.1E-185 | -184.976 |
| Pb(NO2)2 (aq) | 1.82E-41 | 1.84E-41 | -40.736 |
| Pb(NO3)2 (aq) | 1.63E-57 | 1.65E-57 | -56.784 |
| Pb(OH)2 (aq) | 7.74E-14 | 7.8E-14 | -13.108 |
| Pb(OH)3- | 9.34E-19 | 7.85E-19 | -18.105 |
| Pb(SO4)2-2 | 4.37E-10 | 2.18E-10 | -9.662 |
| Pb+2 | 1.94E-08 | 9.7E-09 | -8.013 |
| Pb2OH+3 | 1.8E-16 | 3.77E-17 | -16.423 |
| Pb3(OH)4+2 | 4.64E-25 | 2.32E-25 | -24.635 |
| Pb4(OH)4+4 | 5.58E-29 | 3.47E-30 | -29.46 |
| PbCl+ | 6.32E-09 | 5.31E-09 | -8.275 |
| PbCl2 (aq) | 1.88E-10 | 1.89E-10 | -9.723 |
| PbCl3- | 3.05E-12 | 2.56E-12 | -11.592 |
| PbCl4-2 | 3.19E-14 | 1.59E-14 | -13.797 |
| PbCO3 (aq) | 8.12E-10 | 8.19E-10 | -9.087 |
| PbF+ | 1.53E-11 | 1.29E-11 | -10.891 |
| PbF2 (aq) | 1.47E-15 | 1.48E-15 | -14.828 |
| PbH2PO4+ | 1.73E-13 | 1.45E-13 | -12.838 |
| PbHCO3+ | 4.88E-09 | 4.1E-09 | -8.387 |
| PbHPO4 (aq) | 3.64E-13 | 3.67E-13 | -12.436 |
| PbNO2+ | 4.53E-24 | 3.81E-24 | -23.42 |
| PbNO3+ | 1.38E-32 | 1.16E-32 | -31.936 |
| PbOH+ | 2.09E-10 | 1.76E-10 | -9.755 |
| PbSO4 (aq) | 1.3E-08 | 1.31E-08 | -7.882 |
| PO4-3 | 5.8E-14 | 1.27E-14 | -13.898 |
| S-2 | 1.21E-76 | 6.15E-77 | -76.211 |
| SO4-2 | 0.005634 | 0.002759 | -2.559 |
| Zn DOM1 | 2.3E-07 | 2.06E-07 | -6.687 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn(CO3)2-2 | 2.2E-13 | 1.1E-13 | -12.96 |
| Zn(N3)2 (aq) | 4.44E-13 | 4.48E-13 | -12.349 |
| Zn(N3)3- | 7.02E-17 | 5.9E-17 | -16.229 |
| Zn(NH3)2+2 | 1.98E-14 | 9.88E-15 | -14.005 |
| Zn(NH3)3+2 | 9.31E-19 | 4.65E-19 | -18.333 |
| Zn(NH3)4+2 | 2.14E-23 | 1.07E-23 | -22.971 |
| Zn(NO2)2 (aq) | 2.05E-40 | 2.06E-40 | -39.685 |
| Zn(NO3)2 (aq) | 2.71E-56 | 2.73E-56 | -55.563 |
| Zn(OH)2 (aq) | 1.12E-10 | 1.13E-10 | -9.947 |
| Zn(OH)3- | 4.27E-16 | 3.59E-16 | -15.445 |
| Zn(OH)4-2 | 1.15E-22 | 5.73E-23 | -22.242 |
| Zn(SO4)2-2 | 2.57E-07 | 1.29E-07 | -6.891 |
| Zn+2 | 1.69E-05 | 8.86E-06 | -5.052 |
| Zn2OH+3 | 1.54E-13 | 3.23E-14 | -13.49 |
| Zn2S3-2 | 1E-185 | 5.2E-186 | -185.287 |
| ZnCl+ | 4.82E-07 | 4.04E-07 | -6.394 |
| ZnCl2 (aq) | 4.37E-09 | 4.41E-09 | -8.356 |
| ZnCl3- | 9.42E-11 | 7.92E-11 | -10.101 |
| ZnCl4-2 | 1.25E-12 | 6.23E-13 | -12.206 |
| ZnCO3 (aq) | 1.26E-08 | 1.27E-08 | -7.896 |
| ZnF+ | 1.69E-09 | 1.42E-09 | -8.847 |
| ZnHCO3+ | 1.77E-07 | 1.49E-07 | -6.827 |
| ZnHPO4 (aq) | 5.45E-10 | 5.5E-10 | -9.26 |
| ZnN3+ | 3.49E-09 | 2.93E-09 | -8.533 |
| ZnNH3+2 | 5.36E-10 | 2.67E-10 | -9.573 |
| ZnNO2+ | 7.7E-23 | 6.47E-23 | -22.189 |
| ZnNO3+ | 2.22E-30 | 1.86E-30 | -29.73 |
| ZnOH+ | 4.86E-09 | 4.08E-09 | -8.389 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnS (aq) | 1.01E-65 | 1.02E-65 | -64.993 |
| ZnSO4 (aq) | 4.86E-06 | 4.9E-06 | -5.309 |

## C2: Species distribution

### C2.1: pH 2

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 80.107 | HgCl2 (aq) |
| | 16.786 | HgCl3-1 |
| | 2.296 | HgCl4-2 |
| | 0.809 | HgN3+ |
| NH4+1 | 98.64 | NH4+1 |
| | 1.36 | NH4SO4- |
| Cl-1 | 98.758 | Cl-1 |
| | 0.014 | AlCl+2 |
| | 0.418 | CaCl+ |
| | 0.06 | FeCl+ |
| | 0.488 | MgCl+ |
| | 0.253 | NaCl (aq) |
| Fe+2 | 87.152 | Fe+2 |
| | 0.564 | FeCl+ |
| | 12.27 | FeSO4 (aq) |
| | 0.014 | FeH2PO4+ |
| Zn+2 | 86.188 | Zn+2 |
| | 0.02 | Zn DOM1 |
| | 2.377 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 11.091 | ZnSO4 (aq) |
| | 0.302 | Zn(SO4)2-2 |
| F-1 | 0.031 | F-1 |
| | 0.311 | HF (aq) |
| | 99.505 | AlF+2 |
| | 0.15 | AlF2+ |

| Component | % of total concentration | Species name |
|---|---|---|
| SO4-2 | 39.946 | SO4-2 |
| | 16.295 | HSO4- |
| | 25.486 | AlSO4+ |
| | 2.827 | Al(SO4)2- |
| | 0.035 | ZnSO4 (aq) |
| | 3.859 | FeSO4 (aq) |
| | 4.005 | MgSO4 (aq) |
| | 6.721 | CaSO4 (aq) |
| | 0.668 | NaSO4- |
| | 0.016 | KSO4- |
| | 0.136 | NH4SO4- |
| Ni+2 | 89.666 | Ni+2 |
| | 0.013 | Ni DOM1 |
| | 0.314 | NiCl+ |
| | 10.006 | NiSO4 (aq) |
| N3-1 | 0.237 | N3-1 |
| | 99.762 | HN3 (aq) |
| PO4-3 | 39.829 | H2PO4- |
| | 41.538 | H3PO4 |
| | 15.252 | FeH2PO4+ |
| | 1.365 | CaH2PO4+ |
| | 1.705 | AlHPO4+ |
| | 0.015 | Al2PO4+3 |
| | 0.289 | NaH2PO4 (aq) |
| AsO4-3 | 59.312 | H3AsO4 |
| | 40.687 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |

| Component | % of total concentration | Species name |
|---|---|---|
| DOM1 | 19.827 | DOM1 |
| | 64.427 | H DOM1 |
| | 14.909 | Al DOM1 |
| | 0.761 | Ca DOM1 |
| | 0.056 | Mg DOM1 |
| | 0.016 | Zn DOM1 |
| Ca+2 | 86.179 | Ca+2 |
| | 2.138 | CaCl+ |
| | 11.677 | CaSO4 (aq) |
| Mg+2 | 86.796 | Mg+2 |
| | 3.486 | MgCl+ |
| | 9.717 | MgSO4 (aq) |
| K+1 | 98.528 | K+1 |
| | 0.723 | KCl (aq) |
| | 0.749 | KSO4- |
| Na+1 | 98.522 | Na+1 |
| | 0.779 | NaCl (aq) |
| | 0.699 | NaSO4- |
| CO3-2 | 99.995 | H2CO3* (aq) |
| Al+3 | 28.739 | Al+3 |
| | 0.154 | Al DOM1 |
| | 0.471 | AlF+2 |
| | 0.108 | AlCl+2 |
| | 66.813 | AlSO4+ |
| | 3.706 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 48.007 | Cd+2 |
| | 43.235 | CdCl+ |

| Component | % of total concentration | Species name |
|---|---|---|
| | 2.444 | CdCl2 (aq) |
| | 6.044 | CdSO4 (aq) |
| | 0.264 | Cd(SO4)2-2 |
| CrO4-2 | 98.847 | HCrO4- |
| | 0.304 | H2CrO4 (aq) |
| | 0.11 | CrO3Cl- |
| | 0.724 | CrO3SO4-2 |
| Cu+2 | 86.494 | Cu+2 |
| | 0.513 | Cu DOM1 |
| | 1.585 | CuCl+ |
| | 11.254 | CuSO4 (aq) |
| | 0.149 | CuHSO4+ |
| Pb+2 | 61.181 | Pb+2 |
| | 0.684 | Pb DOM1 |
| | 19.072 | PbCl+ |
| | 0.56 | PbCl2 (aq) |
| | 18.176 | PbSO4 (aq) |
| | 0.314 | Pb(SO4)2-2 |
| Fe+3 | 11.984 | Fe+3 |
| | 20.293 | Fe DOM1 |
| | 4.245 | FeOH+2 |
| | 0.038 | Fe(OH)2+ |
| | 0.02 | FeF+2 |
| | 2.38 | FeCl+2 |
| | 59.604 | FeSO4+ |
| | 1.155 | Fe(SO4)2- |
| | 0.056 | FeN3+2 |
| | 0.066 | FeH2PO4+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.158 | FeHPO4+ |
| NO2-1 | 7.975 | NO2-1 |
| | 92.024 | HNO2 (aq) |
| NO3-1 | 99.259 | NO3-1 |
| | 0.603 | CaNO3+ |
| | 0.128 | NaNO3 (aq) |
| HS-1 | 99.655 | H2S (aq) |
| | 0.343 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |

## C2.2: pH 3

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 0.104 | HgCl2 (aq) |
| | 0.022 | HgCl3-1 |
| | 99.868 | HgN3+ |
| NH4+1 | 98.301 | NH4+1 |
| | 1.699 | NH4SO4- |
| Cl-1 | 98.757 | Cl-1 |
| | 0.012 | AlCl+2 |
| | 0.417 | CaCl+ |
| | 0.06 | FeCl+ |
| | 0.489 | MgCl+ |
| | 0.257 | NaCl (aq) |
| Fe+2 | 84.129 | Fe+2 |
| | 0.563 | FeCl+ |
| | 15.289 | FeSO4 (aq) |
| | 0.019 | FeH2PO4+ |
| Zn+2 | 83.251 | Zn+2 |
| | 0.072 | Zn DOM1 |
| | 2.371 | ZnCl+ |
| | 0.022 | ZnCl2 (aq) |
| | 13.828 | ZnSO4 (aq) |
| | 0.454 | Zn(SO4)2-2 |
| F-1 | 0.037 | F-1 |
| | 0.038 | HF (aq) |
| | 99.734 | AlF+2 |
| | 0.187 | AlF2+ |
| SO4-2 | 48.017 | SO4-2 |
| | 2.018 | HSO4- |

| Component | % of total concentration | Species name |
|---|---|---|
| | 26.97 | AlSO4+ |
| | 3.738 | Al(SO4)2- |
| | 0.044 | ZnSO4 (aq) |
| | 4.809 | FeSO4 (aq) |
| | 5.005 | MgSO4 (aq) |
| | 8.368 | CaSO4 (aq) |
| | 0.833 | NaSO4- |
| | 0.019 | KSO4- |
| | 0.169 | NH4SO4- |
| Ni+2 | 87.05 | Ni+2 |
| | 0.045 | Ni DOM1 |
| | 0.316 | NiCl+ |
| | 12.582 | NiSO4 (aq) |
| N3-1 | 2.303 | N3-1 |
| | 97.695 | HN3 (aq) |
| PO4-3 | 52.101 | H2PO4- |
| | 5.486 | H3PO4 |
| | 19.869 | FeH2PO4+ |
| | 1.777 | CaH2PO4+ |
| | 19.048 | AlHPO4+ |
| | 1.307 | Al2PO4+3 |
| | 0.384 | NaH2PO4 (aq) |
| AsO4-3 | 12.832 | H3AsO4 |
| | 0.015 | HAsO4-2 |
| | 87.153 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 29.502 | DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 22.272 | H DOM1 |
| | 45.28 | Al DOM1 |
| | 2.676 | Ca DOM1 |
| | 0.198 | Mg DOM1 |
| | 0.057 | Zn DOM1 |
| Ca+2 | 83.309 | Ca+2 |
| | 0.018 | Ca DOM1 |
| | 2.131 | CaCl+ |
| | 14.54 | CaSO4 (aq) |
| Mg+2 | 84.368 | Mg+2 |
| | 3.488 | MgCl+ |
| | 12.143 | MgSO4 (aq) |
| K+1 | 98.326 | K+1 |
| | 0.738 | KCl (aq) |
| | 0.936 | KSO4- |
| Na+1 | 98.334 | Na+1 |
| | 0.793 | NaCl (aq) |
| | 0.873 | NaSO4- |
| CO3-2 | 0.046 | HCO3- |
| | 99.952 | H2CO3* (aq) |
| Al+3 | 23.286 | Al+3 |
| | 0.467 | Al DOM1 |
| | 0.064 | AlOH+2 |
| | 0.472 | AlF+2 |
| | 0.09 | AlCl+2 |
| | 70.703 | AlSO4+ |
| | 4.9 | Al(SO4)2- |
| | 0.015 | AlHPO4+ |

| Component | % of total concentration | Species name |
|---|---|---|
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 46.296 | Cd+2 |
| | 0.024 | Cd DOM1 |
| | 43.239 | CdCl+ |
| | 2.494 | CdCl2 (aq) |
| | 7.549 | CdSO4 (aq) |
| | 0.397 | Cd(SO4)2-2 |
| CrO4-2 | 0.056 | CrO4-2 |
| | 99.779 | HCrO4- |
| | 0.031 | H2CrO4 (aq) |
| | 0.028 | CaCrO4 (aq) |
| | 0.011 | CrO3Cl- |
| | 0.089 | CrO3SO4-2 |
| Cu+2 | 82.71 | Cu+2 |
| | 1.788 | Cu DOM1 |
| | 1.565 | CuCl+ |
| | 13.891 | CuSO4 (aq) |
| | 0.018 | CuHSO4+ |
| | 0.02 | CuN3+ |
| Pb+2 | 56.584 | Pb+2 |
| | 2.316 | Pb DOM1 |
| | 18.294 | PbCl+ |
| | 0.548 | PbCl2 (aq) |
| | 21.774 | PbSO4 (aq) |
| | 0.453 | Pb(SO4)2-2 |
| | 0.02 | PbHCO3+ |
| Fe+3 | 5.44 | Fe+3 |
| | 34.528 | Fe DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 19.619 | FeOH+2 |
| | 1.788 | Fe(OH)2+ |
| | 0.011 | FeF+2 |
| | 1.112 | FeCl+2 |
| | 35.354 | FeSO4+ |
| | 0.856 | Fe(SO4)2- |
| | 0.254 | FeN3+2 |
| | 0.04 | FeH2PO4+2 |
| | 0.992 | FeHPO4+ |
| NO2-1 | 46.179 | NO2-1 |
| | 53.816 | HNO2 (aq) |
| NO3-1 | 99.259 | NO3-1 |
| | 0.601 | CaNO3+ |
| | 0.13 | NaNO3 (aq) |
| HS-1 | 96.7 | H2S (aq) |
| | 3.286 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |

## C2.3: pH 4

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 100 | HgN3+ |
| NH4+1 | 98.076 | NH4+1 |
| | 1.924 | NH4SO4- |
| Cl-1 | 98.798 | Cl-1 |
| | 0.426 | CaCl+ |
| | 0.5 | MgCl+ |
| | 0.265 | NaCl (aq) |
| Pb+2 | 50.076 | Pb+2 |
| | 9.072 | Pb DOM1 |
| | 16.595 | PbCl+ |
| | 0.497 | PbCl2 (aq) |
| | 23.047 | PbSO4 (aq) |
| | 0.513 | Pb(SO4)2-2 |
| | 0.186 | PbHCO3+ |
| Zn+2 | 80.792 | Zn+2 |
| | 0.306 | Zn DOM1 |
| | 2.343 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 15.961 | ZnSO4 (aq) |
| | 0.56 | Zn(SO4)2-2 |
| | 0.013 | ZnHCO3+ |
| F-1 | 0.203 | F-1 |
| | 0.021 | HF (aq) |
| | 98.674 | AlF+2 |
| | 1.078 | AlF2+ |
| | 0.018 | MgF+ |
| CrO4-2 | 0.531 | CrO4-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 99.156 | HCrO4- |
| | 0.285 | CaCrO4 (aq) |
| Ni+2 | 84.779 | Ni+2 |
| | 0.193 | Ni DOM1 |
| | 0.316 | NiCl+ |
| | 14.656 | NiSO4 (aq) |
| | 0.049 | NiHCO3+ |
| N3-1 | 18.836 | N3-1 |
| | 81.158 | HN3 (aq) |
| PO4-3 | 0.055 | HPO4-2 |
| | 55.181 | H2PO4- |
| | 0.59 | H3PO4 |
| | 0.117 | FeH2PO4+ |
| | 0.021 | MgHPO4 (aq) |
| | 0.02 | CaHPO4 (aq) |
| | 1.917 | CaH2PO4+ |
| | 37.399 | AlHPO4+ |
| | 4.271 | Al2PO4+3 |
| | 0.418 | NaH2PO4 (aq) |
| AsO4-3 | 1.471 | H3AsO4 |
| | 0.16 | HAsO4-2 |
| | 98.369 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 42.914 | DOM1 |
| | 9.014 | H DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 35.5 | Al DOM1 |
| | 11.422 | Ca DOM1 |
| | 0.016 | Cu DOM1 |
| | 0.846 | Mg DOM1 |
| | 0.025 | Ni DOM1 |
| | 0.018 | Pb DOM1 |
| | 0.245 | Zn DOM1 |
| Ca+2 | 81.037 | Ca+2 |
| | 0.078 | Ca DOM1 |
| | 2.107 | CaCl+ |
| | 16.771 | CaSO4 (aq) |
| Mg+2 | 82.492 | Mg+2 |
| | 3.456 | MgCl+ |
| | 14.039 | MgSO4 (aq) |
| K+1 | 98.201 | K+1 |
| | 0.738 | KCl (aq) |
| | 1.061 | KSO4- |
| Na+1 | 98.221 | Na+1 |
| | 0.792 | NaCl (aq) |
| | 0.986 | NaSO4- |
| CO3-2 | 0.449 | HCO3- |
| | 99.534 | H2CO3* (aq) |
| Cu+2 | 75.942 | Cu+2 |
| | 7.227 | Cu DOM1 |
| | 1.463 | CuCl+ |
| | 15.17 | CuSO4 (aq) |
| | 0.158 | CuN3+ |
| | 0.023 | CuHCO3+ |

| Component | % of total concentration | Species name |
|---|---|---|
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.025 | Cd+2 |
| | 0.103 | Cd DOM1 |
| | 43.106 | CdCl+ |
| | 2.485 | CdCl2 (aq) |
| | 8.781 | CdSO4 (aq) |
| | 0.494 | Cd(SO4)2-2 |
| Fe+2 | 81.748 | Fe+2 |
| | 0.557 | FeCl+ |
| | 17.669 | FeSO4 (aq) |
| | 0.02 | FeH2PO4+ |
| NO2-1 | 89.41 | NO2-1 |
| | 10.581 | HNO2 (aq) |
| NO3-1 | 99.242 | NO3-1 |
| | 0.614 | CaNO3+ |
| | 0.134 | NaNO3 (aq) |
| HS-1 | 0.082 | HS-1 |
| | 99.669 | H2S (aq) |
| | 0.041 | NiHS+ |
| | 0.185 | FeHS+ |
| | 0.022 | CdHS+ |
| H3AsO3 | 99.999 | H3AsO3 |
| Fe+3 | 0.881 | Fe+3 |
| | 25.708 | Fe DOM1 |
| | 32.764 | FeOH+2 |
| | 31.09 | Fe(OH)2+ |
| | 0.01 | FeF+2 |
| | 0.183 | FeCl+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 6.95 | FeSO4+ |
| | 0.19 | Fe(SO4)2- |
| | 0.352 | FeN3+2 |
| | 1.852 | FeHPO4+ |
| | 0.011 | FeCrO4+ |
| SO4-2 | 68.645 | SO4-2 |
| | 0.302 | HSO4- |
| | 7.487 | AlSO4+ |
| | 1.174 | Al(SO4)2- |
| | 0.067 | ZnSO4 (aq) |
| | 0.01 | NiSO4 (aq) |
| | 0.041 | FeSO4 (aq) |
| | 7.765 | MgSO4 (aq) |
| | 12.954 | CaSO4 (aq) |
| | 1.264 | NaSO4- |
| | 0.029 | KSO4- |
| | 0.257 | NH4SO4- |
| Al+3 | 19.138 | Al+3 |
| | 1.766 | Al DOM1 |
| | 0.54 | AlOH+2 |
| | 2.252 | AlF+2 |
| | 0.012 | AlF2+ |
| | 0.075 | AlCl+2 |
| | 70.504 | AlSO4+ |
| | 5.526 | Al(SO4)2- |
| | 0.14 | AlHPO4+ |
| | 0.032 | Al2PO4+3 |

## C2.4: pH 5

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 100 | HgN3+ |
| NH4+1 | 97.176 | NH4+1 |
| | 2.822 | NH4SO4- |
| Cl-1 | 98.877 | Cl-1 |
| | 0.389 | CaCl+ |
| | 0.464 | MgCl+ |
| | 0.262 | NaCl (aq) |
| Pb+2 | 37.318 | Pb+2 |
| | 22.876 | Pb DOM1 |
| | 0.04 | PbOH+ |
| | 0.013 | PbF+ |
| | 12.169 | PbCl+ |
| | 0.361 | PbCl2 (aq) |
| | 25.036 | PbSO4 (aq) |
| | 0.839 | Pb(SO4)2-2 |
| | 0.022 | PbCO3 (aq) |
| | 1.317 | PbHCO3+ |
| Zn+2 | 74.232 | Zn+2 |
| | 0.953 | Zn DOM1 |
| | 2.122 | ZnCl+ |
| | 0.019 | ZnCl2 (aq) |
| | 21.413 | ZnSO4 (aq) |
| | 1.132 | Zn(SO4)2-2 |
| | 0.011 | ZnN3+ |
| | 0.109 | ZnHCO3+ |
| F-1 | 37.772 | F-1 |
| | 0.392 | HF (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 18.535 | AlF+2 |
| | 37.03 | AlF2+ |
| | 2.261 | AlF3 (aq) |
| | 3.125 | MgF+ |
| | 0.71 | CaF+ |
| | 0.159 | NaF (aq) |
| CrO4-2 | 5.018 | CrO4-2 |
| | 0.084 | NaCrO4- |
| | 92.47 | HCrO4- |
| | 2.421 | CaCrO4 (aq) |
| Ni+2 | 78.793 | Ni+2 |
| | 0.608 | Ni DOM1 |
| | 0.289 | NiCl+ |
| | 19.855 | NiSO4 (aq) |
| | 0.015 | NiN3+ |
| | 0.431 | NiHCO3+ |
| N3-1 | 69.973 | N3-1 |
| | 30.013 | HN3 (aq) |
| PO4-3 | 0.95 | HPO4-2 |
| | 93.939 | H2PO4- |
| | 0.1 | H3PO4 |
| | 0.323 | MgHPO4 (aq) |
| | 0.311 | CaHPO4 (aq) |
| | 2.982 | CaH2PO4+ |
| | 0.031 | NaHPO4- |
| | 0.637 | AlHPO4+ |
| | 0.015 | KH2PO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.702 | NaH2PO4 (aq) |
| AsO4-3 | 0.146 | H3AsO4 |
| | 1.62 | HAsO4-2 |
| | 98.234 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 57.223 | DOM1 |
| | 3.132 | H DOM1 |
| | 0.122 | Al DOM1 |
| | 35.895 | Ca DOM1 |
| | 0.043 | Cu DOM1 |
| | 2.698 | Mg DOM1 |
| | 0.079 | Ni DOM1 |
| | 0.046 | Pb DOM1 |
| | 0.762 | Zn DOM1 |
| Ca+2 | 75.073 | Ca+2 |
| | 0.246 | Ca DOM1 |
| | 1.926 | CaCl+ |
| | 22.705 | CaSO4 (aq) |
| | 0.046 | CaHCO3+ |
| Mg+2 | 77.437 | Mg+2 |
| | 0.026 | Mg DOM1 |
| | 0.014 | MgF+ |
| | 3.203 | MgCl+ |
| | 19.275 | MgSO4 (aq) |
| | 0.046 | MgHCO3+ |
| K+1 | 97.709 | K+1 |
| | 0.728 | KCl (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 1.563 | KSO4- |
| Na+1 | 97.759 | Na+1 |
| | 0.781 | NaCl (aq) |
| | 1.455 | NaSO4- |
| CO3-2 | 4.332 | HCO3- |
| | 95.524 | H2CO3* (aq) |
| | 0.054 | MgHCO3+ |
| | 0.076 | CaHCO3+ |
| | 0.012 | NaHCO3 (aq) |
| Cu+2 | 60.735 | Cu+2 |
| | 19.59 | Cu DOM1 |
| | 0.073 | CuOH+ |
| | 1.154 | CuCl+ |
| | 17.714 | CuSO4 (aq) |
| | 0.014 | CuNH3+2 |
| | 0.462 | CuN3+ |
| | 0.065 | CuCO3 (aq) |
| | 0.178 | CuHCO3+ |
| SO4-2 | 77.156 | SO4-2 |
| | 0.033 | HSO4- |
| | 0.067 | ZnSO4 (aq) |
| | 0.01 | NiSO4 (aq) |
| | 7.944 | MgSO4 (aq) |
| | 13.068 | CaSO4 (aq) |
| | 1.389 | NaSO4- |
| | 0.032 | KSO4- |
| | 0.281 | NH4SO4- |

| Component | % of total concentration | Species name |
|---|---|---|
| Cd+2 | 43.226 | Cd+2 |
| | 0.334 | Cd DOM1 |
| | 40.72 | CdCl+ |
| | 2.328 | CdCl2 (aq) |
| | 12.288 | CdSO4 (aq) |
| | 1.042 | Cd(SO4)2-2 |
| | 0.061 | CdHCO3+ |
| Fe+2 | 75.563 | Fe+2 |
| | 0.508 | FeCl+ |
| | 23.848 | FeSO4 (aq) |
| | 0.031 | FeH2PO4+ |
| | 0.044 | FeHCO3+ |
| NO2-1 | 98.826 | NO2-1 |
| | 1.164 | HNO2 (aq) |
| NO3-1 | 99.297 | NO3-1 |
| | 0.561 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| HS-1 | 0.819 | HS-1 |
| | 98.576 | H2S (aq) |
| | 0.371 | NiHS+ |
| | 0.208 | CdHS+ |
| | 0.023 | ZnS (aq) |
| H3AsO3 | 99.994 | H3AsO3 |
| Fe+3 | 0.025 | Fe+3 |
| | 2.457 | Fe DOM1 |
| | 9.274 | FeOH+2 |
| | 86.957 | Fe(OH)2+ |
| | 0.055 | FeF+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.288 | FeSO4+ |
| | 0.012 | Fe(SO4)2- |
| | 0.037 | FeN3+2 |
| | 0.878 | FeHPO4+ |
| Al+3 | 1.935 | Al+3 |
| | 0.597 | Al DOM1 |
| | 0.54 | AlOH+2 |
| | 0.058 | Al(OH)2+ |
| | 41.709 | AlF+2 |
| | 41.663 | AlF2+ |
| | 1.696 | AlF3 (aq) |
| | 10.346 | AlSO4+ |
| | 1.202 | Al(SO4)2- |
| | 0.236 | AlHPO4+ |
| Mn+3 | 100 | Mn+3 |

## C2.5: pH 6

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 100 | HgN3+ |
| NH4+1 | 97.158 | NH4+1 |
| | 2.82 | NH4SO4- |
| | 0.022 | NH3 (aq) |
| Cl-1 | 98.882 | Cl-1 |
| | 0.387 | CaCl+ |
| | 0.462 | MgCl+ |
| | 0.262 | NaCl (aq) |
| Pb+2 | 33.562 | Pb+2 |
| | 21.773 | Pb DOM1 |
| | 0.361 | PbOH+ |
| | 0.026 | PbF+ |
| | 10.917 | PbCl+ |
| | 0.324 | PbCl2 (aq) |
| | 22.448 | PbSO4 (aq) |
| | 0.754 | Pb(SO4)2-2 |
| | 1.401 | PbCO3 (aq) |
| | 8.428 | PbHCO3+ |
| Zn+2 | 73.683 | Zn+2 |
| | 1.002 | Zn DOM1 |
| | 0.021 | ZnOH+ |
| | 2.102 | ZnCl+ |
| | 0.019 | ZnCl2 (aq) |
| | 21.196 | ZnSO4 (aq) |
| | 1.122 | Zn(SO4)2-2 |
| | 0.015 | ZnN3+ |
| | 0.055 | ZnCO3 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.772 | ZnHCO3+ |
| F-1 | 90.127 | F-1 |
| | 0.094 | HF (aq) |
| | 0.044 | AlF+2 |
| | 0.2 | AlF2+ |
| | 0.028 | AlF3 (aq) |
| | 0.014 | ZnF+ |
| | 7.424 | MgF+ |
| | 1.685 | CaF+ |
| | 0.378 | NaF (aq) |
| CrO4-2 | 29.985 | CrO4-2 |
| | 0.499 | NaCrO4- |
| | 55.15 | HCrO4- |
| | 14.357 | CaCrO4 (aq) |
| Ni+2 | 76.748 | Ni+2 |
| | 0.627 | Ni DOM1 |
| | 0.281 | NiCl+ |
| | 19.281 | NiSO4 (aq) |
| | 0.02 | NiN3+ |
| | 0.035 | NiCO3 (aq) |
| | 2.985 | NiHCO3+ |
| N3-1 | 95.873 | N3-1 |
| | 0.012 | ZnN3+ |
| | 4.109 | HN3 (aq) |
| Cd+2 | 43.112 | Cd+2 |
| | 0.352 | Cd DOM1 |
| | 40.513 | CdCl+ |
| | 2.313 | CdCl2 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 12.219 | CdSO4 (aq) |
| | 1.038 | Cd(SO4)2-2 |
| | 0.431 | CdHCO3+ |
| | 0.012 | CdCO3 (aq) |
| AsO4-3 | 0.013 | H3AsO4 |
| | 14.173 | HAsO4-2 |
| | 85.814 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 57.961 | DOM1 |
| | 0.333 | H DOM1 |
| | 37.888 | Ca DOM1 |
| | 0.042 | Cu DOM1 |
| | 2.849 | Mg DOM1 |
| | 0.082 | Ni DOM1 |
| | 0.044 | Pb DOM1 |
| | 0.801 | Zn DOM1 |
| Ca+2 | 74.894 | Ca+2 |
| | 0.259 | Ca DOM1 |
| | 1.917 | CaCl+ |
| | 22.591 | CaSO4 (aq) |
| | 0.33 | CaHCO3+ |
| Mg+2 | 77.249 | Mg+2 |
| | 0.027 | Mg DOM1 |
| | 0.031 | MgF+ |
| | 3.189 | MgCl+ |
| | 19.179 | MgSO4 (aq) |
| | 0.324 | MgHCO3+ |

| Component | % of total concentration | Species name |
|---|---|---|
| K+1 | 97.711 | K+1 |
| | 0.727 | KCl (aq) |
| | 1.562 | KSO4- |
| Na+1 | 97.734 | Na+1 |
| | 0.78 | NaCl (aq) |
| | 1.453 | NaSO4- |
| | 0.032 | NaHCO3 (aq) |
| CO3-2 | 30.894 | HCO3- |
| | 68.078 | H2CO3* (aq) |
| | 0.381 | MgHCO3+ |
| | 0.541 | CaHCO3+ |
| | 0.088 | NaHCO3 (aq) |
| Cu+2 | 56.379 | Cu+2 |
| | 19.25 | Cu DOM1 |
| | 0.68 | CuOH+ |
| | 0.014 | CuF+ |
| | 1.069 | CuCl+ |
| | 16.398 | CuSO4 (aq) |
| | 0.133 | CuNH3+2 |
| | 0.586 | CuN3+ |
| | 0.012 | CuHPO4 (aq) |
| | 4.296 | CuCO3 (aq) |
| | 1.178 | CuHCO3+ |
| SO4-2 | 77.312 | SO4-2 |
| | 0.067 | ZnSO4 (aq) |
| | 7.905 | MgSO4 (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 12.995 | CaSO4 (aq) |
| | 1.388 | NaSO4- |
| | 0.032 | KSO4- |
| | 0.281 | NH4SO4- |
| Fe+2 | 75.416 | Fe+2 |
| | 0.506 | FeCl+ |
| | 23.735 | FeSO4 (aq) |
| | 0.011 | FeH2PO4+ |
| | 0.311 | FeHCO3+ |
| NO2-1 | 99.873 | NO2-1 |
| | 0.118 | HNO2 (aq) |
| NO3-1 | 99.3 | NO3-1 |
| | 0.558 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| HS-1 | 7.146 | HS-1 |
| | 85.96 | H2S (aq) |
| | 3.145 | NiHS+ |
| | 1.805 | CdHS+ |
| | 1.945 | ZnS (aq) |
| H3AsO3 | 99.945 | H3AsO3 |
| | 0.055 | H2AsO3- |
| Fe+3 | 0.03 | Fe DOM1 |
| | 1.056 | FeOH+2 |
| | 98.845 | Fe(OH)2+ |
| | 0.028 | Fe(OH)3 (aq) |
| | 0.035 | FeHPO4+ |
| Al+3 | 0.546 | Al+3 |
| | 0.178 | Al DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 1.522 | AlOH+2 |
| | 1.64 | Al(OH)2+ |
| | 0.26 | Al(OH)3 (aq) |
| | 0.139 | Al(OH)4- |
| | 26.605 | AlF+2 |
| | 60.055 | AlF2+ |
| | 5.529 | AlF3 (aq) |
| | 0.031 | AlF4- |
| | 2.909 | AlSO4+ |
| | 0.338 | Al(SO4)2- |
| | 0.234 | AlHPO4+ |
| Mn+3 | 100 | Mn+3 |
| PO4-3 | 8.356 | HPO4-2 |
| | 82.504 | H2PO4- |
| | 2.82 | MgHPO4 (aq) |
| | 2.716 | CaHPO4 (aq) |
| | 2.606 | CaH2PO4+ |
| | 0.274 | NaHPO4- |
| | 0.062 | ZnHPO4 (aq) |
| | 0.013 | KH2PO4 (aq) |
| | 0.616 | NaH2PO4 (aq) |

# C3 Saturation indicies

## C3.1: pH 2

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 2.3 | -9.175 |
| Al(OH)3 (Soil) | 2.3 | -6.628 |
| Al2O3(s) | 4.6 | -16.624 |
| Al4(OH)10SO4(s) | 2.321 | -20.379 |
| AlAsO4:2H2O(s) | -30.341 | -14.541 |
| AlOHF2(s) | -18.665 | -19.072 |
| AlOHSO4(s) | -4.58 | -1.35 |
| Alunite | -8.777 | -8.654 |
| Anglesite | -10.663 | -2.8 |
| Anhydrite | -5.622 | -1.306 |
| Antlerite | -17.596 | -26.384 |
| Aragonite | -18.178 | -9.899 |
| Arsenolite | -12.609 | -11.046 |
| Artinite | -17.185 | -27.516 |
| As2O5(s) | -65.282 | -30.573 |
| As2S3(am) | -105.109 | -58.724 |
| Atacamite | -10.908 | -18.867 |
| Azurite | -49.587 | -32.434 |
| Bianchite | -7.892 | -6.131 |
| Birnessite | 7.352 | -10.739 |
| Bixbyite | 0.21 | 0.098 |
| Boehmite | 2.3 | -6.993 |
| Brochantite | -21.168 | -37.623 |
| Brucite | 1.125 | -16.668 |
| Ca3(AsO4)2:4H2O(s) | -61.508 | -42.608 |
| Ca3(PO4)2 (am1) | -51.879 | -26.95 |
| Ca3(PO4)2 (am2) | -51.879 | -24.158 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(PO4)2 (beta) | -51.879 | -22.631 |
| Ca4H(PO4)3:3H2O(s) | -78.447 | -31.136 |
| CaCO3xH2O(s) | -18.178 | -11.091 |
| CaCrO4(s) | -13.765 | -11.663 |
| CaHPO4(s) | -26.568 | -7.105 |
| CaHPO4:2H2O(s) | -26.568 | -7.434 |
| Calcite | -18.178 | -9.747 |
| CaS(s) | -29.575 | -40.755 |
| Cd metal (alpha) | -19.082 | -33.055 |
| Cd metal (gamma) | -19.082 | -33.162 |
| Cd(OH)2(s) | -4.588 | -18.807 |
| Cd3(OH)4SO4(s) | -20.643 | -43.203 |
| Cd3(PO4)2(s) | -69.416 | -36.816 |
| Cd3OH2(SO4)2(s) | -27.524 | -34.234 |
| Cd4(OH)6SO4(s) | -25.231 | -53.631 |
| CdCl2(s) | -12.116 | -11.57 |
| CdCl2:1H2O(s) | -12.116 | -10.468 |
| CdCl2:2.5H2O(s) | -12.116 | -10.159 |
| CdF2(s) | -25.553 | -24.622 |
| CdOHCl(s) | -8.352 | -12.077 |
| CdSO4(s) | -11.468 | -11.612 |
| CdSO4:1H2O(s) | -11.468 | -9.934 |
| CdSO4:2.67H2O(s) | -11.468 | -9.704 |
| Cerrusite | -23.219 | -9.868 |
| Chalcanthite | -10.452 | -7.775 |
| Chalcopyrite | -64.246 | -28.073 |
| Chloropyromorphite(c) | -106.158 | -21.728 |
| Chloropyromorphite(soil) | -106.158 | -25.758 |
| Cinnabar | -53.443 | -6.62 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Claudetite | -12.609 | -11.096 |
| Cotunnite | -11.311 | -6.372 |
| Covellite | -34.405 | -11.595 |
| Cr(VI)-Ettringite | -32.921 | -96.322 |
| Cr(VI)-Jarosite | -47.119 | -28.603 |
| CrO3(s) | -15.023 | -11.844 |
| Cryolite | -61.333 | -27.262 |
| Cu azide | -22.075 | -14.234 |
| Cu(OH)2(s) | -3.572 | -13.185 |
| Cu2(OH)3NO3(s) | -74.252 | -83.944 |
| Cu3(AsO4)2:2H2O(s) | -75.998 | -40.898 |
| Cu3(PO4)2(s) | -66.369 | -29.519 |
| Cu3(PO4)2:3H2O(s) | -66.369 | -31.249 |
| CuCO3(s) | -23.008 | -11.508 |
| CuCrO4(s) | -18.595 | -13.155 |
| CuF2(s) | -24.537 | -26.059 |
| CuF2:2H2O(s) | -24.537 | -20.08 |
| CuOCuSO4(s) | -14.024 | -25.165 |
| Cupric Ferrite | -13.675 | -20.942 |
| CuSO4(s) | -10.452 | -13.836 |
| Diaspore | 2.3 | -5.199 |
| Dolomite (disordered) | -36.488 | -20.23 |
| Dolomite (ordered) | -36.488 | -19.638 |
| Epsomite | -5.755 | -3.558 |
| Ettringite | -8.492 | -67.68 |
| FCO3-Apatite | -171.093 | -55.691 |
| Fe(OH)2 (am) | 0.993 | -13.054 |
| Fe(OH)2 (c) | 0.993 | -11.897 |
| Fe(OH)2.7Cl.3(s) | -6.181 | -3.141 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe2(SO4)3(s) | -30.744 | -28.481 |
| Fe3(OH)8(s) | -9.111 | -29.333 |
| FeAsO4:2H2O(s) | -37.693 | -17.493 |
| Ferrihydrite | -5.052 | -8.862 |
| Ferrihydrite (aged) | -5.052 | -8.352 |
| FeS (ppt) | -29.841 | -26.957 |
| Fluorite | -19.707 | -9.134 |
| Galena | -34.616 | -19.21 |
| Gibbsite (C) | 2.3 | -6.078 |
| Goethite | -5.052 | -5.911 |
| Goslarite | -7.892 | -5.794 |
| Greenockite | -35.421 | -21.067 |
| Greigite | -132.443 | -87.408 |
| Gypsum | -5.622 | -1.006 |
| Halite | -4.01 | -5.537 |
| Hematite | -10.103 | -9.47 |
| Hercynite | 5.593 | -19.209 |
| Hg(OH)2(s) | -22.609 | -19.113 |
| Hg3O2CO3(s) | -87.264 | -57.684 |
| HgCl2(s) | -30.138 | -8.22 |
| HgSO4(s) | -29.49 | -19.981 |
| Hinsdalite | -31.589 | -29.089 |
| H-Jarosite | -28.915 | -24.883 |
| Huntite | -73.109 | -43.796 |
| Hydrocerrusite | -50.22 | -31.46 |
| Hydromagnesite | -72.116 | -64.678 |
| Hydroxyapatite | -77.189 | -32.856 |
| Hydroxylpyromorphite | -102.394 | -39.604 |
| Hydrozincite | -43.931 | -54.069 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K2Cr2O7(s) | -33.882 | -16.148 |
| K2CrO4(s) | -18.858 | -18.234 |
| K-Alum | -13.378 | -8.024 |
| KCl(s) | -5.682 | -6.582 |
| K-Jarosite | -30.833 | -20.452 |
| Langite | -21.168 | -39.663 |
| Larnakite | -14.446 | -14.144 |
| Laurionite | -7.547 | -8.17 |
| Lepidocrocite | -5.052 | -6.423 |
| Lime | 1.258 | -32.62 |
| Litharge | -3.783 | -16.871 |
| Mackinawite | -29.841 | -26.241 |
| Maghemite | -10.103 | -16.489 |
| Magnesioferrite | -8.978 | -27.534 |
| Magnesite | -18.31 | -10.729 |
| Magnetite | -9.111 | -13.781 |
| Malachite | -26.58 | -21.379 |
| Massicot | -3.783 | -17.079 |
| Matlockite | -18.03 | -8.854 |
| Melanothallite | -11.1 | -17.743 |
| Melanterite | -5.888 | -3.554 |
| Metacinnabar | -53.443 | -7.018 |
| Mg(OH)2 (active) | 1.125 | -17.669 |
| Mg2(OH)3Cl:4H2O(s) | -1.514 | -27.514 |
| Mg3(PO4)2(s) | -52.277 | -28.997 |
| MgCO3:5H2O(s) | -18.31 | -13.77 |
| MgCrO4(s) | -13.898 | -19.819 |
| MgF2(s) | -19.84 | -11.779 |
| MgHPO4:3H2O(s) | -26.701 | -8.526 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| MgS(s) | -29.708 | -47.388 |
| Minium | 3.146 | -72.941 |
| Mirabilite | -7.372 | -5.775 |
| Mn2(SO4)3(s) | -20.43 | -15.713 |
| Montroydite | -22.609 | -18.893 |
| Morenosite | -8.686 | -6.467 |
| Na2Cr2O7(s) | -30.538 | -20.508 |
| Na2CrO4(s) | -15.515 | -18.564 |
| NaF(s) | -10.728 | -10.234 |
| Na-Jarosite | -29.161 | -24.666 |
| Natron | -19.927 | -18.216 |
| Nesquehonite | -18.31 | -13.788 |
| Ni(OH)2 (am) | -1.806 | -15.279 |
| Ni(OH)2 (c) | -1.806 | -12.596 |
| Ni3(AsO4)2:8H2O(s) | -70.7 | -45.2 |
| Ni3(PO4)2(s) | -61.07 | -29.77 |
| Ni4(OH)6SO4(s) | -14.103 | -46.103 |
| NiCO3(s) | -21.242 | -10.294 |
| NiS (alpha) | -32.639 | -27.119 |
| NiS (beta) | -32.639 | -21.619 |
| NiS (gamma) | -32.639 | -19.919 |
| Nsutite | 7.352 | -10.152 |
| Orpiment | -105.109 | -57.209 |
| Otavite | -24.024 | -11.972 |
| Pb azide (alpha) | -22.286 | -13.312 |
| Pb metal | -18.278 | -22.518 |
| Pb(OH)2(s) | -3.783 | -12.289 |
| Pb10(OH)6O(CO3)6(s) | -154.443 | -145.683 |
| Pb2(OH)3Cl(s) | -11.33 | -20.123 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O(OH)2(s) | -7.566 | -33.756 |
| Pb2O3(s) | 6.929 | -54.111 |
| Pb2OCO3(s) | -27.001 | -26.692 |
| Pb3(AsO4)2(s) | -76.631 | -41.131 |
| Pb3(PO4)2(s) | -67.001 | -23.471 |
| Pb3O2CO3(s) | -30.784 | -42.477 |
| Pb3O2SO4(s) | -18.229 | -29.396 |
| Pb4(OH)6SO4(s) | -22.011 | -43.111 |
| Pb4O3SO4(s) | -22.011 | -44.718 |
| PbCrO4(s) | -18.806 | -5.937 |
| PbF2(s) | -24.748 | -17.186 |
| PbHPO4(s) | -31.609 | -7.804 |
| PbO:0.3H2O(s) | -3.783 | -16.763 |
| Periclase | 1.125 | -21.378 |
| Phosgenite | -34.53 | -14.72 |
| Plattnerite | 10.712 | -40.69 |
| Plumbgummite | -52.535 | -19.745 |
| Portlandite | 1.258 | -22.228 |
| Pyrite | -46.179 | -27.368 |
| Realgar | -44.385 | -23.655 |
| Retgersite | -8.686 | -6.618 |
| Siderite | -18.443 | -7.898 |
| Smithsonite | -20.448 | -9.571 |
| Spharelite | -31.845 | -20.843 |
| Spinel | 5.726 | -33.481 |
| Strengite | -32.878 | -6.535 |
| Struvite | -27.94 | -14.68 |
| Sulfur | -16.338 | -14.293 |
| Tenorite(am) | -3.572 | -12.456 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Tenorite(c) | -3.572 | -11.607 |
| Thenardite | -7.372 | -7.749 |
| Thermonatrite | -19.927 | -20.628 |
| Tsumebite | -38.964 | -29.174 |
| Vaterite | -18.178 | -10.341 |
| Vivianite | -52.675 | -14.884 |
| Wurtzite | -31.845 | -23.096 |
| Zincite | -1.012 | -12.787 |
| Zincosite | -7.892 | -12.324 |
| Zn metal | -15.507 | -42.228 |
| Zn(NO3)2:6H2O(s) | -135.227 | -138.393 |
| Zn(OH)2 (am) | -1.012 | -14.006 |
| Zn(OH)2 (beta) | -1.012 | -13.271 |
| Zn(OH)2 (delta) | -1.012 | -12.856 |
| Zn(OH)2 (epsilon) | -1.012 | -13.024 |
| Zn(OH)2 (gamma) | -1.012 | -13.243 |
| Zn2(OH)2SO4(s) | -8.904 | -16.404 |
| Zn2(OH)3Cl(s) | -5.788 | -20.979 |
| Zn3(PO4)2:4H2O(s) | -58.688 | -23.268 |
| Zn3AsO42:2.5H2O(s) | -68.318 | -40.818 |
| Zn3O(SO4)2(s) | -16.796 | -37.278 |
| Zn4(OH)6SO4(s) | -10.927 | -39.327 |
| Zn5(OH)8Cl2(s) | -12.587 | -51.087 |
| Zn-Al LDH(s) | -9.441 | -29.271 |
| ZnCl2(s) | -8.54 | -16.031 |
| ZnCO3(s) | -20.448 | -9.648 |
| ZnCO3:1H2O(s) | -20.448 | -10.188 |
| ZnF2(s) | -21.977 | -21.806 |
| ZnSO4:1H2O(s) | -7.892 | -7.522 |

## C3.2: pH 3

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 5.231 | -6.244 |
| Al(OH)3 (Soil) | 5.231 | -3.698 |
| Al2O3(s) | 10.463 | -10.762 |
| Al4(OH)10SO4(s) | 12.141 | -10.559 |
| AlAsO4:2H2O(s) | -25.413 | -9.613 |
| AlOHF2(s) | -17.566 | -17.973 |
| AlOHSO4(s) | -3.552 | -0.322 |
| Alunite | -2.787 | -2.664 |
| Anglesite | -10.585 | -2.722 |
| Anhydrite | -5.527 | -1.211 |
| Antlerite | -13.518 | -22.306 |
| Aragonite | -16.181 | -7.902 |
| Arsenolite | -12.614 | -11.051 |
| Artinite | -13.189 | -23.52 |
| As2O5(s) | -61.288 | -26.578 |
| As2S3(am) | -134.817 | -88.433 |
| Atacamite | -7.916 | -15.875 |
| Azurite | -43.607 | -26.454 |
| Bianchite | -7.799 | -6.038 |
| Birnessite | 11.375 | -6.716 |
| Bixbyite | 6.255 | 6.143 |
| Boehmite | 5.231 | -4.062 |
| Brochantite | -15.097 | -31.552 |
| Brucite | 3.124 | -14.669 |
| Ca3(AsO4)2:4H2O(s) | -51.522 | -32.622 |
| Ca3(PO4)2 (am1) | -47.645 | -22.716 |
| Ca3(PO4)2 (am2) | -47.645 | -19.924 |
| Ca3(PO4)2 (beta) | -47.645 | -18.396 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca4H(PO4)3:3H2O(s) | -73.096 | -25.785 |
| CaCO3xH2O(s) | -16.181 | -9.094 |
| CaCrO4(s) | -12.759 | -10.658 |
| CaHPO4(s) | -25.45 | -5.987 |
| CaHPO4:2H2O(s) | -25.451 | -6.316 |
| Calcite | -16.181 | -7.75 |
| CaS(s) | -37.479 | -48.659 |
| Cd metal (alpha) | -19.083 | -33.056 |
| Cd metal (gamma) | -19.083 | -33.163 |
| Cd(OH)2(s) | -2.589 | -16.809 |
| Cd3(OH)4SO4(s) | -16.55 | -39.11 |
| Cd3(PO4)2(s) | -65.178 | -32.578 |
| Cd3OH2(SO4)2(s) | -25.333 | -32.043 |
| Cd4(OH)6SO4(s) | -19.14 | -47.54 |
| CdCl2(s) | -12.108 | -11.562 |
| CdCl2:1H2O(s) | -12.108 | -10.46 |
| CdCl2:2.5H2O(s) | -12.109 | -10.151 |
| CdF2(s) | -25.387 | -24.455 |
| CdOHCl(s) | -7.349 | -11.074 |
| CdSO4(s) | -11.372 | -11.516 |
| CdSO4:1H2O(s) | -11.372 | -9.838 |
| CdSO4:2.67H2O(s) | -11.373 | -9.609 |
| Cerrusite | -21.238 | -7.888 |
| Chalcanthite | -10.363 | -7.686 |
| Chalcopyrite | -80.057 | -43.884 |
| Chloropyromorphite(c) | -99.887 | -15.457 |
| Chloropyromorphite(soil) | -99.887 | -19.487 |
| Cinnabar | -64.239 | -17.416 |
| Claudetite | -12.614 | -11.101 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cotunnite | -11.321 | -6.382 |
| Covellite | -42.313 | -19.503 |
| Cr(VI)-Ettringite | -18.061 | -81.462 |
| Cr(VI)-Jarosite | -39.107 | -20.591 |
| CrO3(s) | -16.015 | -12.836 |
| Cryolite | -60.891 | -26.82 |
| Cu azide | -20.101 | -12.259 |
| Cu(OH)2(s) | -1.579 | -11.192 |
| Cu2(OH)3NO3(s) | -61.262 | -70.955 |
| Cu3(AsO4)2:2H2O(s) | -66.023 | -30.923 |
| Cu3(PO4)2(s) | -62.146 | -25.296 |
| Cu3(PO4)2:3H2O(s) | -62.147 | -27.027 |
| CuCO3(s) | -21.014 | -9.514 |
| CuCrO4(s) | -17.593 | -12.153 |
| CuF2(s) | -24.376 | -25.898 |
| CuF2:2H2O(s) | -24.377 | -19.919 |
| CuOCuSO4(s) | -11.939 | -23.08 |
| Cupric Ferrite | -5.686 | -12.953 |
| CuSO4(s) | -10.361 | -13.745 |
| Diaspore | 5.231 | -2.268 |
| Dolomite (disordered) | -32.492 | -16.234 |
| Dolomite (ordered) | -32.492 | -15.643 |
| Epsomite | -5.661 | -3.464 |
| Ettringite | 3.635 | -55.553 |
| FCO3-Apatite | -158.329 | -42.927 |
| Fe(OH)2 (am) | 2.99 | -11.057 |
| Fe(OH)2 (c) | 2.99 | -9.9 |
| Fe(OH)2.7Cl.3(s) | -3.482 | -0.442 |
| Fe2(SO4)3(s) | -30.457 | -28.194 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe3(OH)8(s) | -1.119 | -21.341 |
| FeAsO4:2H2O(s) | -32.699 | -12.499 |
| Ferrihydrite | -2.055 | -5.865 |
| Ferrihydrite (aged) | -2.055 | -5.355 |
| FeS (ppt) | -37.744 | -34.861 |
| Fluorite | -19.542 | -8.969 |
| Galena | -42.537 | -27.13 |
| Gibbsite (C) | 5.231 | -3.148 |
| Goethite | -2.054 | -2.914 |
| Goslarite | -7.799 | -5.702 |
| Greenockite | -43.323 | -28.969 |
| Greigite | -164.056 | -119.021 |
| Gypsum | -5.528 | -0.912 |
| Halite | -4.003 | -5.53 |
| Hematite | -4.108 | -3.474 |
| Hercynite | 13.453 | -11.348 |
| Hg(OH)2(s) | -23.505 | -20.008 |
| Hg3O2CO3(s) | -89.949 | -60.369 |
| HgCl2(s) | -33.023 | -11.105 |
| HgSO4(s) | -32.287 | -22.779 |
| Hinsdalite | -23.598 | -21.098 |
| H-Jarosite | -23.73 | -19.697 |
| Huntite | -65.116 | -35.803 |
| Hydrocerrusite | -44.279 | -25.519 |
| Hydromagnesite | -62.125 | -54.687 |
| Hydroxyapatite | -69.84 | -25.507 |
| Hydroxylpyromorphite | -95.128 | -32.338 |
| Hydrozincite | -33.942 | -44.08 |
| K2Cr2O7(s) | -33.858 | -16.125 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K2CrO4(s) | -17.843 | -17.219 |
| K-Alum | -13.253 | -7.899 |
| KCl(s) | -5.674 | -6.574 |
| K-Jarosite | -24.643 | -14.262 |
| Langite | -15.097 | -33.593 |
| Larnakite | -12.387 | -12.086 |
| Laurionite | -6.562 | -7.185 |
| Lepidocrocite | -2.054 | -3.425 |
| Lime | 3.256 | -30.623 |
| Litharge | -1.802 | -14.89 |
| Mackinawite | -37.744 | -34.144 |
| Maghemite | -4.108 | -10.494 |
| Magnesioferrite | -0.984 | -19.539 |
| Magnesite | -16.312 | -8.73 |
| Magnetite | -1.118 | -5.788 |
| Malachite | -22.593 | -17.393 |
| Massicot | -1.802 | -15.099 |
| Matlockite | -17.96 | -8.785 |
| Melanothallite | -11.097 | -17.74 |
| Melanterite | -5.795 | -3.462 |
| Metacinnabar | -64.239 | -17.814 |
| Mg(OH)2 (active) | 3.124 | -15.67 |
| Mg2(OH)3Cl:4H2O(s) | 1.487 | -24.513 |
| Mg3(PO4)2(s) | -48.038 | -24.758 |
| MgCO3:5H2O(s) | -16.314 | -11.774 |
| MgCrO4(s) | -12.891 | -18.812 |
| MgF2(s) | -19.673 | -11.612 |
| MgHPO4:3H2O(s) | -25.583 | -7.408 |
| MgS(s) | -37.61 | -55.29 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Minium | 11.088 | -64.999 |
| Mirabilite | -7.273 | -5.676 |
| Mn2(SO4)3(s) | -20.094 | -15.376 |
| Montroydite | -23.504 | -19.787 |
| Morenosite | -8.59 | -6.371 |
| Na2Cr2O7(s) | -30.516 | -20.486 |
| Na2CrO4(s) | -14.501 | -17.551 |
| NaF(s) | -10.642 | -10.147 |
| Na-Jarosite | -22.972 | -18.478 |
| Natron | -17.926 | -16.215 |
| Nesquehonite | -16.313 | -11.79 |
| Ni(OH)2 (am) | 0.196 | -13.278 |
| Ni(OH)2 (c) | 0.196 | -10.594 |
| Ni3(AsO4)2:8H2O(s) | -60.703 | -35.203 |
| Ni3(PO4)2(s) | -56.823 | -25.523 |
| Ni4(OH)6SO4(s) | -8 | -40 |
| NiCO3(s) | -19.24 | -8.293 |
| NiS (alpha) | -40.539 | -35.019 |
| NiS (beta) | -40.539 | -29.519 |
| NiS (gamma) | -40.539 | -27.819 |
| Nsutite | 11.375 | -6.129 |
| Orpiment | -134.817 | -86.918 |
| Otavite | -22.025 | -9.974 |
| Pb azide (alpha) | -20.324 | -11.35 |
| Pb metal | -18.296 | -22.537 |
| Pb(OH)2(s) | -1.802 | -10.308 |
| Pb10(OH)6O(CO3)6(s) | -134.639 | -125.879 |
| Pb2(OH)3Cl(s) | -8.364 | -17.157 |
| Pb2O(OH)2(s) | -3.605 | -29.795 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O3(s) | 12.89 | -48.15 |
| Pb2OCO3(s) | -23.04 | -22.731 |
| Pb3(AsO4)2(s) | -66.694 | -31.194 |
| Pb3(PO4)2(s) | -62.818 | -19.288 |
| Pb3O2CO3(s) | -24.842 | -36.535 |
| Pb3O2SO4(s) | -14.189 | -25.357 |
| Pb4(OH)6SO4(s) | -15.993 | -37.093 |
| Pb4O3SO4(s) | -15.991 | -38.698 |
| PbCrO4(s) | -17.817 | -4.948 |
| PbF2(s) | -24.6 | -17.038 |
| PbHPO4(s) | -30.508 | -6.703 |
| PbO:0.3H2O(s) | -1.802 | -14.782 |
| Periclase | 3.124 | -19.379 |
| Phosgenite | -32.559 | -12.749 |
| Plattnerite | 14.692 | -36.709 |
| Plumbgummite | -43.521 | -10.731 |
| Portlandite | 3.255 | -20.231 |
| Pyrite | -61.984 | -43.173 |
| Realgar | -55.289 | -34.559 |
| Retgersite | -8.589 | -6.521 |
| Siderite | -16.446 | -5.9 |
| Smithsonite | -18.45 | -7.573 |
| Spharelite | -39.748 | -28.746 |
| Spinel | 13.587 | -25.62 |
| Strengite | -30.76 | -4.417 |
| Struvite | -25.816 | -12.556 |
| Sulfur | -24.24 | -22.194 |
| Tenorite(am) | -1.578 | -10.463 |
| Tenorite(c) | -1.578 | -9.613 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Thenardite | -7.269 | -7.646 |
| Thermonatrite | -17.923 | -18.623 |
| Tsumebite | -33.89 | -24.1 |
| Vaterite | -16.181 | -8.344 |
| Vivianite | -48.443 | -10.652 |
| Wurtzite | -39.748 | -31 |
| Zincite | 0.986 | -10.789 |
| Zincosite | -7.797 | -12.228 |
| Zn metal | -15.508 | -42.229 |
| Zn(NO3)2:6H2O(s) | -115.226 | -118.392 |
| Zn(OH)2 (am) | 0.986 | -12.009 |
| Zn(OH)2 (beta) | 0.986 | -11.274 |
| Zn(OH)2 (delta) | 0.986 | -10.858 |
| Zn(OH)2 (epsilon) | 0.986 | -11.026 |
| Zn(OH)2 (gamma) | 0.986 | -11.245 |
| Zn2(OH)2SO4(s) | -6.811 | -14.311 |
| Zn2(OH)3Cl(s) | -2.787 | -17.978 |
| Zn3(PO4)2:4H2O(s) | -54.454 | -19.034 |
| Zn3AsO42:2.5H2O(s) | -58.33 | -30.83 |
| Zn3O(SO4)2(s) | -14.607 | -35.09 |
| Zn4(OH)6SO4(s) | -4.839 | -33.239 |
| Zn5(OH)8Cl2(s) | -4.589 | -43.089 |
| Zn-Al LDH(s) | -2.515 | -22.345 |
| ZnCl2(s) | -8.533 | -16.023 |
| ZnCO3(s) | -18.45 | -7.65 |
| ZnCO3:1H2O(s) | -18.45 | -8.19 |
| ZnF2(s) | -21.811 | -21.64 |
| ZnSO4:1H2O(s) | -7.797 | -7.427 |

## C3.3: pH 4

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 7.499 | -3.976 |
| Al(OH)3 (Soil) | 7.499 | -1.429 |
| Al2O3(s) | 14.999 | -6.225 |
| Al4(OH)10SO4(s) | 19.268 | -3.432 |
| AlAsO4:2H2O(s) | -21.894 | -6.094 |
| AlOHF2(s) | -15.799 | -16.206 |
| AlOHSO4(s) | -3.23 | 0 |
| Alunite | 1.131 | 1.255 |
| Anglesite | -10.561 | -2.698 |
| Anhydrite | -5.466 | -1.15 |
| Antlerite | -9.513 | -18.301 |
| Aragonite | -14.175 | -5.896 |
| Arsenolite | -14.113 | -12.55 |
| Artinite | -9.174 | -19.505 |
| As2O5(s) | -58.786 | -24.077 |
| As2S3(am) | -166.156 | -119.771 |
| Atacamite | -4.955 | -12.914 |
| Azurite | -37.66 | -20.507 |
| Bianchite | -7.737 | -5.976 |
| Birnessite | 15.411 | -2.68 |
| Bixbyite | 12.328 | 12.216 |
| Boehmite | 7.5 | -1.794 |
| Brochantite | -9.107 | -25.563 |
| Brucite | 5.133 | -12.66 |
| Ca3(AsO4)2:4H2O(s) | -42.998 | -24.098 |
| Ca3(PO4)2 (am1) | -43.56 | -18.632 |
| Ca3(PO4)2 (am2) | -43.56 | -15.839 |
| Ca3(PO4)2 (beta) | -43.56 | -14.312 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca4H(PO4)3:3H2O(s) | -67.973 | -20.662 |
| CaCO3xH2O(s) | -14.176 | -7.089 |
| CaCrO4(s) | -11.748 | -9.647 |
| CaHPO4(s) | -24.412 | -4.949 |
| CaHPO4:2H2O(s) | -24.413 | -5.278 |
| Calcite | -14.175 | -5.745 |
| CaS(s) | -45.418 | -56.598 |
| Cd metal (alpha) | -19.072 | -33.044 |
| Cd metal (gamma) | -19.072 | -33.151 |
| Cd(OH)2(s) | -0.578 | -14.797 |
| Cd3(OH)4SO4(s) | -12.463 | -35.023 |
| Cd3(PO4)2(s) | -61.083 | -28.483 |
| Cd3OH2(SO4)2(s) | -23.192 | -29.902 |
| Cd4(OH)6SO4(s) | -13.041 | -41.441 |
| CdCl2(s) | -12.11 | -11.564 |
| CdCl2:1H2O(s) | -12.11 | -10.463 |
| CdCl2:2.5H2O(s) | -12.111 | -10.154 |
| CdF2(s) | -23.876 | -22.945 |
| CdOHCl(s) | -6.344 | -10.069 |
| CdSO4(s) | -11.307 | -11.451 |
| CdSO4:1H2O(s) | -11.307 | -9.773 |
| CdSO4:2.67H2O(s) | -11.308 | -9.544 |
| Cerrusite | -19.27 | -5.92 |
| Chalcanthite | -10.326 | -7.649 |
| Chalcopyrite | -98.222 | -62.049 |
| Chloropyromorphite(c) | -93.95 | -9.52 |
| Chloropyromorphite(soil) | -93.95 | -13.55 |
| Cinnabar | -77.098 | -30.275 |
| Claudetite | -14.113 | -12.6 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cotunnite | -11.364 | -6.425 |
| Covellite | -50.275 | -27.466 |
| Cr(VI)-Ettringite | -4.468 | -67.869 |
| Cr(VI)-Jarosite | -37.861 | -19.345 |
| CrO3(s) | -17.012 | -13.833 |
| Cryolite | -57.111 | -23.039 |
| Cu azide | -18.279 | -10.438 |
| Cu(OH)2(s) | 0.405 | -9.208 |
| Cu2(OH)3NO3(s) | -48.288 | -57.98 |
| Cu3(AsO4)2:2H2O(s) | -57.57 | -22.47 |
| Cu3(PO4)2(s) | -58.133 | -21.283 |
| Cu3(PO4)2:3H2O(s) | -58.134 | -23.014 |
| CuCO3(s) | -19.033 | -7.533 |
| CuCrO4(s) | -16.606 | -11.166 |
| CuF2(s) | -22.893 | -24.415 |
| CuF2:2H2O(s) | -22.894 | -18.437 |
| CuOCuSO4(s) | -9.918 | -21.059 |
| Cupric Ferrite | -2.213 | -9.48 |
| CuSO4(s) | -10.324 | -13.707 |
| Diaspore | 7.5 | 0 |
| Dolomite (disordered) | -28.481 | -12.223 |
| Dolomite (ordered) | -28.481 | -11.631 |
| Epsomite | -5.599 | -3.402 |
| Ettringite | 14.379 | -44.809 |
| FCO3-Apatite | -144.251 | -28.849 |
| Fe(OH)2 (am) | 2.734 | -11.313 |
| Fe(OH)2 (c) | 2.734 | -10.156 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -34.808 | -32.545 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe3(OH)8(s) | 0.114 | -20.108 |
| FeAsO4:2H2O(s) | -30.704 | -10.504 |
| Ferrihydrite | -1.31 | -5.121 |
| Ferrihydrite (aged) | -1.31 | -4.611 |
| FeS (ppt) | -47.946 | -45.063 |
| Fluorite | -18.036 | -7.463 |
| Galena | -50.513 | -35.106 |
| Gibbsite (C) | 7.499 | -0.879 |
| Goethite | -1.31 | -2.169 |
| Goslarite | -7.738 | -5.64 |
| Greenockite | -51.259 | -36.904 |
| Greigite | -202.609 | -157.574 |
| Gypsum | -5.467 | -0.851 |
| Halite | -4.004 | -5.532 |
| Hematite | -2.619 | -1.985 |
| Hercynite | 17.734 | -7.067 |
| Hg(OH)2(s) | -26.417 | -22.92 |
| Hg3O2CO3(s) | -98.688 | -69.108 |
| HgCl2(s) | -37.949 | -16.031 |
| HgSO4(s) | -37.146 | -27.638 |
| Hinsdalite | -17.738 | -15.238 |
| H-Jarosite | -25.39 | -21.357 |
| Huntite | -57.092 | -27.779 |
| Hydrocerrusite | -38.373 | -19.613 |
| Hydromagnesite | -52.091 | -44.653 |
| Hydroxyapatite | -62.709 | -18.376 |
| Hydroxylpyromorphite | -88.184 | -25.394 |
| Hydrozincite | -23.907 | -34.045 |
| K2Cr2O7(s) | -33.839 | -16.106 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K2CrO4(s) | -16.827 | -16.203 |
| K-Alum | -13.871 | -8.518 |
| KCl(s) | -5.674 | -6.574 |
| K-Jarosite | -25.297 | -14.916 |
| Langite | -9.108 | -27.603 |
| Larnakite | -10.393 | -10.091 |
| Laurionite | -5.598 | -6.221 |
| Lepidocrocite | -1.31 | -2.681 |
| Lime | 5.263 | -28.615 |
| Litharge | 0.168 | -12.92 |
| Mackinawite | -47.946 | -44.346 |
| Maghemite | -2.619 | -9.005 |
| Magnesioferrite | 2.514 | -16.042 |
| Magnesite | -14.306 | -6.724 |
| Magnetite | 0.116 | -4.555 |
| Malachite | -18.627 | -13.427 |
| Massicot | 0.168 | -13.128 |
| Matlockite | -17.247 | -8.072 |
| Melanothallite | -11.127 | -17.77 |
| Melanterite | -7.997 | -5.664 |
| Metacinnabar | -77.098 | -30.673 |
| Mg(OH)2 (active) | 5.133 | -13.661 |
| Mg2(OH)3Cl:4H2O(s) | 4.498 | -21.502 |
| Mg3(PO4)2(s) | -43.951 | -20.671 |
| MgCO3:5H2O(s) | -14.307 | -9.767 |
| MgCrO4(s) | -11.879 | -17.8 |
| MgF2(s) | -18.166 | -10.104 |
| MgHPO4:3H2O(s) | -24.543 | -6.368 |
| MgS(s) | -45.548 | -63.228 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Minium | 18.999 | -57.087 |
| Mirabilite | -7.209 | -5.612 |
| Mn2(SO4)3(s) | -19.86 | -15.143 |
| Montroydite | -26.416 | -22.7 |
| Morenosite | -8.524 | -6.305 |
| Na2Cr2O7(s) | -30.499 | -20.469 |
| Na2CrO4(s) | -13.487 | -16.537 |
| NaF(s) | -9.887 | -9.392 |
| Na-Jarosite | -23.627 | -19.132 |
| Natron | -15.918 | -14.206 |
| Nesquehonite | -14.307 | -9.784 |
| Ni(OH)2 (am) | 2.208 | -11.266 |
| Ni(OH)2 (c) | 2.208 | -8.582 |
| Ni3(AsO4)2:8H2O(s) | -52.165 | -26.665 |
| Ni3(PO4)2(s) | -52.726 | -21.426 |
| Ni4(OH)6SO4(s) | -1.898 | -33.898 |
| NiCO3(s) | -17.231 | -6.284 |
| NiS (alpha) | -48.473 | -42.953 |
| NiS (beta) | -48.473 | -37.453 |
| NiS (gamma) | -48.473 | -35.753 |
| Nsutite | 15.411 | -2.093 |
| Orpiment | -166.156 | -118.256 |
| Otavite | -20.016 | -7.965 |
| Pb azide (alpha) | -18.517 | -9.542 |
| Pb metal | -18.326 | -22.567 |
| Pb(OH)2(s) | 0.168 | -8.338 |
| Pb10(OH)6O(CO3)6(s) | -114.95 | -106.19 |
| Pb2(OH)3Cl(s) | -5.43 | -14.223 |
| Pb2O(OH)2(s) | 0.336 | -25.854 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O3(s) | 18.831 | -42.209 |
| Pb2OCO3(s) | -19.102 | -18.792 |
| Pb3(AsO4)2(s) | -58.281 | -22.781 |
| Pb3(PO4)2(s) | -58.845 | -15.315 |
| Pb3O2CO3(s) | -18.934 | -30.626 |
| Pb3O2SO4(s) | -10.224 | -21.392 |
| Pb4(OH)6SO4(s) | -10.057 | -31.157 |
| Pb4O3SO4(s) | -10.056 | -32.763 |
| PbCrO4(s) | -16.843 | -3.975 |
| PbF2(s) | -23.131 | -15.569 |
| PbHPO4(s) | -29.507 | -5.702 |
| PbO:0.3H2O(s) | 0.168 | -12.812 |
| Periclase | 5.133 | -17.37 |
| Phosgenite | -30.635 | -10.825 |
| Plattnerite | 18.663 | -32.739 |
| Plumbgummite | -36.684 | -3.894 |
| Portlandite | 5.263 | -18.223 |
| Pyrite | -80.133 | -61.322 |
| Realgar | -66.985 | -46.255 |
| Retgersite | -8.524 | -6.456 |
| Siderite | -16.704 | -6.158 |
| Smithsonite | -16.444 | -5.567 |
| Spharelite | -47.687 | -36.684 |
| Spinel | 20.133 | -19.074 |
| Strengite | -30.985 | -4.642 |
| Struvite | -23.771 | -10.511 |
| Sulfur | -32.187 | -30.141 |
| Tenorite(am) | 0.406 | -8.479 |
| Tenorite(c) | 0.406 | -7.629 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Thenardite | -7.205 | -7.582 |
| Thermonatrite | -15.915 | -16.615 |
| Tsumebite | -28.934 | -19.144 |
| Vaterite | -14.175 | -6.339 |
| Vivianite | -51.149 | -13.358 |
| Wurtzite | -47.687 | -38.938 |
| Zincite | 2.994 | -8.781 |
| Zincosite | -7.735 | -12.167 |
| Zn metal | -15.5 | -42.221 |
| Zn(NO3)2:6H2O(s) | -95.205 | -98.371 |
| Zn(OH)2 (am) | 2.994 | -10.001 |
| Zn(OH)2 (beta) | 2.994 | -9.265 |
| Zn(OH)2 (delta) | 2.994 | -8.85 |
| Zn(OH)2 (epsilon) | 2.994 | -9.018 |
| Zn(OH)2 (gamma) | 2.994 | -9.237 |
| Zn2(OH)2SO4(s) | -4.741 | -12.241 |
| Zn2(OH)3Cl(s) | 0.222 | -14.969 |
| Zn3(PO4)2:4H2O(s) | -50.369 | -14.949 |
| Zn3AsO42:2.5H2O(s) | -49.804 | -22.304 |
| Zn3O(SO4)2(s) | -12.476 | -32.959 |
| Zn4(OH)6SO4(s) | 1.247 | -27.153 |
| Zn5(OH)8Cl2(s) | 3.438 | -35.062 |
| Zn-Al LDH(s) | 3.768 | -16.062 |
| ZnCl2(s) | -8.538 | -16.029 |
| ZnCO3(s) | -16.444 | -5.644 |
| ZnCO3:1H2O(s) | -16.445 | -6.185 |
| ZnF2(s) | -20.305 | -20.133 |
| ZnSO4:1H2O(s) | -7.736 | -7.365 |

## C3.4: pH 5

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 7.499 | -3.976 |
| Al(OH)3 (Soil) | 7.499 | -1.429 |
| Al2O3(s) | 14.999 | -6.225 |
| Al4(OH)10SO4(s) | 17.438 | -5.262 |
| AlAsO4:2H2O(s) | -22.812 | -7.012 |
| AlOHF2(s) | -13.265 | -13.672 |
| AlOHSO4(s) | -5.059 | -1.829 |
| Alunite | -1.531 | -1.408 |
| Anglesite | -10.525 | -2.662 |
| Anhydrite | -5.334 | -1.018 |
| Antlerite | -5.652 | -14.44 |
| Aragonite | -12.232 | -3.953 |
| Arsenolite | -19.948 | -18.385 |
| Artinite | -5.257 | -15.589 |
| As2O5(s) | -60.622 | -25.912 |
| As2S3(am) | -201.479 | -155.094 |
| Atacamite | -2.164 | -10.123 |
| Azurite | -32.006 | -14.852 |
| Bianchite | -7.61 | -5.849 |
| Birnessite | 17.504 | -0.587 |
| Bixbyite | 14.514 | 14.401 |
| Boehmite | 7.5 | -1.794 |
| Brochantite | -3.35 | -19.805 |
| Brucite | 7.1 | -10.693 |
| Ca3(AsO4)2:4H2O(s) | -38.95 | -20.05 |
| Ca3(PO4)2 (am1) | -39.219 | -14.29 |
| Ca3(PO4)2 (am2) | -39.219 | -11.498 |
| Ca3(PO4)2 (beta) | -39.219 | -9.97 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca4H(PO4)3:3H2O(s) | -62.441 | -15.13 |
| CaCO3xH2O(s) | -12.232 | -5.146 |
| CaCrO4(s) | -10.82 | -8.718 |
| CaHPO4(s) | -23.222 | -3.758 |
| CaHPO4:2H2O(s) | -23.222 | -4.088 |
| Calcite | -12.232 | -3.802 |
| CaS(s) | -53.286 | -64.466 |
| Cd metal (alpha) | -19.096 | -33.069 |
| Cd metal (gamma) | -19.096 | -33.176 |
| Cd(OH)2(s) | 1.397 | -12.822 |
| Cd3(OH)4SO4(s) | -8.366 | -30.926 |
| Cd3(PO4)2(s) | -56.698 | -24.098 |
| Cd3OH2(SO4)2(s) | -20.924 | -27.634 |
| Cd4(OH)6SO4(s) | -6.968 | -35.368 |
| CdCl2(s) | -12.138 | -11.592 |
| CdCl2:1H2O(s) | -12.139 | -10.491 |
| CdCl2:2.5H2O(s) | -12.139 | -10.182 |
| CdF2(s) | -19.367 | -18.435 |
| CdOHCl(s) | -5.37 | -9.096 |
| CdSO4(s) | -11.161 | -11.305 |
| CdSO4:1H2O(s) | -11.161 | -9.627 |
| CdSO4:2.67H2O(s) | -11.162 | -9.398 |
| Cerrusite | -17.423 | -4.072 |
| Chalcanthite | -10.258 | -7.581 |
| Chalcopyrite | -116.683 | -80.51 |
| Chloropyromorphite(c) | -87.937 | -3.507 |
| Chloropyromorphite(soil) | -87.937 | -7.537 |
| Cinnabar | -89.497 | -42.674 |
| Claudetite | -19.948 | -18.435 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cotunnite | -11.502 | -6.563 |
| Covellite | -58.208 | -35.398 |
| Cr(VI)-Ettringite | 4.202 | -59.199 |
| Cr(VI)-Jarosite | -38.028 | -19.512 |
| CrO3(s) | -18.044 | -14.865 |
| Cryolite | -46.519 | -12.448 |
| Cu azide | -17.246 | -9.405 |
| Cu(OH)2(s) | 2.302 | -7.311 |
| Cu2(OH)3NO3(s) | -35.5 | -45.193 |
| Cu3(AsO4)2:2H2O(s) | -53.715 | -18.615 |
| Cu3(PO4)2(s) | -53.984 | -17.134 |
| Cu3(PO4)2:3H2O(s) | -53.985 | -18.865 |
| CuCO3(s) | -17.154 | -5.654 |
| CuCrO4(s) | -15.741 | -10.301 |
| CuF2(s) | -18.462 | -19.984 |
| CuF2:2H2O(s) | -18.463 | -14.006 |
| CuOCuSO4(s) | -7.954 | -19.094 |
| Cupric Ferrite | 0.284 | -6.982 |
| CuSO4(s) | -10.256 | -13.64 |
| Diaspore | 7.5 | 0 |
| Dolomite (disordered) | -24.588 | -8.33 |
| Dolomite (ordered) | -24.588 | -7.738 |
| Epsomite | -5.461 | -3.264 |
| Ettringite | 20.657 | -38.531 |
| FCO3-Apatite | -125.918 | -10.516 |
| Fe(OH)2 (am) | 2.035 | -12.012 |
| Fe(OH)2 (c) | 2.035 | -10.855 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -39.694 | -37.431 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe3(OH)8(s) | 0.016 | -20.206 |
| FeAsO4:2H2O(s) | -31.321 | -11.121 |
| Ferrihydrite | -1.01 | -4.82 |
| Ferrihydrite (aged) | -1.01 | -4.31 |
| FeS (ppt) | -58.475 | -55.592 |
| Fluorite | -13.54 | -2.967 |
| Galena | -58.477 | -43.07 |
| Gibbsite (C) | 7.499 | -0.879 |
| Goethite | -1.009 | -1.869 |
| Goslarite | -7.61 | -5.512 |
| Greenockite | -59.112 | -44.758 |
| Greigite | -242.024 | -196.989 |
| Gypsum | -5.335 | -0.719 |
| Halite | -4.01 | -5.537 |
| Hematite | -2.018 | -1.384 |
| Hercynite | 17.035 | -7.767 |
| Hg(OH)2(s) | -28.987 | -25.49 |
| Hg3O2CO3(s) | -106.415 | -76.835 |
| HgCl2(s) | -42.523 | -20.605 |
| HgSO4(s) | -41.545 | -32.037 |
| Hinsdalite | -18.473 | -15.973 |
| H-Jarosite | -28.146 | -24.114 |
| Huntite | -49.301 | -19.988 |
| Hydrocerrusite | -32.812 | -14.052 |
| Hydromagnesite | -42.326 | -34.888 |
| Hydroxyapatite | -55.216 | -10.883 |
| Hydroxylpyromorphite | -81.169 | -18.379 |
| Hydrozincite | -14.157 | -24.295 |
| K2Cr2O7(s) | -33.912 | -16.178 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K2CrO4(s) | -15.868 | -15.243 |
| K-Alum | -16.534 | -11.18 |
| KCl(s) | -5.68 | -6.58 |
| K-Jarosite | -27.058 | -16.677 |
| Langite | -3.35 | -21.845 |
| Larnakite | -8.491 | -8.19 |
| Laurionite | -4.735 | -5.358 |
| Lepidocrocite | -1.009 | -2.38 |
| Lime | 7.224 | -26.654 |
| Litharge | 2.034 | -11.055 |
| Mackinawite | -58.475 | -54.875 |
| Maghemite | -2.018 | -8.404 |
| Magnesioferrite | 5.082 | -13.473 |
| Magnesite | -12.356 | -4.775 |
| Magnetite | 0.017 | -4.653 |
| Malachite | -14.852 | -9.651 |
| Massicot | 2.034 | -11.263 |
| Matlockite | -15.117 | -5.942 |
| Melanothallite | -11.234 | -17.876 |
| Melanterite | -10.526 | -8.192 |
| Metacinnabar | -89.497 | -43.072 |
| Mg(OH)2 (active) | 7.1 | -11.694 |
| Mg2(OH)3Cl:4H2O(s) | 7.43 | -18.57 |
| Mg3(PO4)2(s) | -39.591 | -16.311 |
| MgCO3:5H2O(s) | -12.358 | -7.818 |
| MgCrO4(s) | -10.944 | -16.865 |
| MgF2(s) | -13.664 | -5.603 |
| MgHPO4:3H2O(s) | -23.347 | -5.172 |
| MgS(s) | -53.41 | -71.09 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Minium | 26.595 | -49.491 |
| Mirabilite | -7.045 | -5.448 |
| Mn2(SO4)3(s) | -23.162 | -18.445 |
| Montroydite | -28.986 | -25.269 |
| Morenosite | -8.392 | -6.173 |
| Na2Cr2O7(s) | -30.571 | -20.541 |
| Na2CrO4(s) | -12.527 | -15.577 |
| NaF(s) | -7.624 | -7.129 |
| Na-Jarosite | -25.387 | -20.893 |
| Natron | -13.943 | -12.232 |
| Nesquehonite | -12.357 | -7.835 |
| Ni(OH)2 (am) | 4.169 | -9.304 |
| Ni(OH)2 (c) | 4.169 | -6.621 |
| Ni3(AsO4)2:8H2O(s) | -48.117 | -22.617 |
| Ni3(PO4)2(s) | -48.384 | -17.084 |
| Ni4(OH)6SO4(s) | 4.117 | -27.883 |
| NiCO3(s) | -15.287 | -4.34 |
| NiS (alpha) | -56.341 | -50.821 |
| NiS (beta) | -56.341 | -45.321 |
| NiS (gamma) | -56.341 | -43.621 |
| Nsutite | 17.504 | 0 |
| Orpiment | -201.479 | -153.579 |
| Otavite | -18.059 | -6.007 |
| Pb azide (alpha) | -17.515 | -8.541 |
| Pb metal | -18.461 | -22.701 |
| Pb(OH)2(s) | 2.033 | -6.473 |
| Pb10(OH)6O(CO3)6(s) | -96.402 | -87.642 |
| Pb2(OH)3Cl(s) | -2.701 | -11.494 |
| Pb2O(OH)2(s) | 4.067 | -22.123 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O3(s) | 24.562 | -36.478 |
| Pb2OCO3(s) | -15.389 | -15.079 |
| Pb3(AsO4)2(s) | -54.521 | -19.021 |
| Pb3(PO4)2(s) | -54.79 | -11.26 |
| Pb3O2CO3(s) | -13.355 | -25.048 |
| Pb3O2SO4(s) | -6.458 | -17.625 |
| Pb4(OH)6SO4(s) | -4.425 | -25.525 |
| Pb4O3SO4(s) | -4.424 | -27.131 |
| PbCrO4(s) | -16.01 | -3.142 |
| PbF2(s) | -18.731 | -11.169 |
| PbHPO4(s) | -28.412 | -4.607 |
| PbO:0.3H2O(s) | 2.034 | -10.946 |
| Periclase | 7.1 | -15.403 |
| Phosgenite | -28.925 | -9.115 |
| Plattnerite | 22.528 | -28.873 |
| Plumbgummite | -36.36 | -3.57 |
| Portlandite | 7.224 | -16.262 |
| Pyrite | -98.491 | -79.68 |
| Realgar | -80.731 | -60.001 |
| Retgersite | -8.392 | -6.324 |
| Siderite | -17.421 | -6.875 |
| Smithsonite | -14.505 | -3.628 |
| Spharelite | -55.559 | -44.556 |
| Spinel | 22.1 | -17.107 |
| Strengite | -31.456 | -5.112 |
| Struvite | -21.58 | -8.32 |
| Sulfur | -40.016 | -37.97 |
| Tenorite(am) | 2.303 | -6.582 |
| Tenorite(c) | 2.303 | -5.732 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Thenardite | -7.042 | -7.419 |
| Thermonatrite | -13.94 | -14.641 |
| Tsumebite | -24.077 | -14.287 |
| Vaterite | -12.232 | -4.396 |
| Vivianite | -54.788 | -16.998 |
| Wurtzite | -55.559 | -46.81 |
| Zincite | 4.951 | -6.824 |
| Zincosite | -7.607 | -12.039 |
| Zn metal | -15.543 | -42.264 |
| Zn(NO3)2:6H2O(s) | -75.26 | -78.426 |
| Zn(OH)2 (am) | 4.951 | -8.044 |
| Zn(OH)2 (beta) | 4.951 | -7.308 |
| Zn(OH)2 (delta) | 4.951 | -6.893 |
| Zn(OH)2 (epsilon) | 4.951 | -7.061 |
| Zn(OH)2 (gamma) | 4.951 | -7.28 |
| Zn2(OH)2SO4(s) | -2.656 | -10.156 |
| Zn2(OH)3Cl(s) | 3.134 | -12.057 |
| Zn3(PO4)2:4H2O(s) | -46.039 | -10.619 |
| Zn3AsO42:2.5H2O(s) | -45.768 | -18.268 |
| Zn3O(SO4)2(s) | -10.263 | -30.746 |
| Zn4(OH)6SO4(s) | 7.246 | -21.154 |
| Zn5(OH)8Cl2(s) | 11.219 | -27.281 |
| Zn-Al LDH(s) | 7.673 | -12.157 |
| ZnCl2(s) | -8.585 | -16.076 |
| ZnCO3(s) | -14.505 | -3.705 |
| ZnCO3:1H2O(s) | -14.505 | -4.245 |
| ZnF2(s) | -15.813 | -15.642 |
| ZnSO4:1H2O(s) | -7.608 | -7.238 |

## C3.5: pH 6

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 7.499 | -3.976 |
| Al(OH)3 (Soil) | 7.499 | -1.429 |
| Al2O3(s) | 14.999 | -6.225 |
| Al4(OH)10SO4(s) | 15.438 | -7.262 |
| AlAsO4:2H2O(s) | -23.871 | -8.071 |
| AlOHF2(s) | -14.555 | -14.962 |
| AlOHSO4(s) | -7.059 | -3.829 |
| Alunite | -4.532 | -4.409 |
| Anglesite | -10.572 | -2.709 |
| Anhydrite | -5.337 | -1.021 |
| Antlerite | -1.752 | -10.54 |
| Aragonite | -10.381 | -2.102 |
| Arsenolite | -26.066 | -24.503 |
| Artinite | -1.408 | -11.739 |
| As2O5(s) | -62.739 | -28.03 |
| As2S3(am) | -237.597 | -191.212 |
| Atacamite | 0.77 | -7.189 |
| Azurite | -26.4 | -9.246 |
| Bianchite | -7.614 | -5.853 |
| Birnessite | 17.504 | -0.587 |
| Bixbyite | 12.514 | 12.401 |
| Boehmite | 7.5 | -1.794 |
| Brochantite | 2.517 | -13.938 |
| Brucite | 9.098 | -8.695 |
| Ca3(AsO4)2:4H2O(s) | -35.075 | -16.175 |
| Ca3(PO4)2 (am1) | -36.128 | -11.199 |
| Ca3(PO4)2 (am2) | -36.128 | -8.407 |
| Ca3(PO4)2 (beta) | -36.128 | -6.879 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca4H(PO4)3:3H2O(s) | -58.804 | -11.492 |
| CaCO3xH2O(s) | -10.382 | -3.295 |
| CaCrO4(s) | -10.046 | -7.945 |
| CaHPO4(s) | -22.675 | -3.212 |
| CaHPO4:2H2O(s) | -22.676 | -3.541 |
| Calcite | -10.381 | -1.951 |
| CaS(s) | -61.288 | -72.468 |
| Cd metal (alpha) | -19.099 | -33.071 |
| Cd metal (gamma) | -19.099 | -33.178 |
| Cd(OH)2(s) | 3.395 | -10.824 |
| Cd3(OH)4SO4(s) | -4.373 | -26.933 |
| Cd3(PO4)2(s) | -53.607 | -21.007 |
| Cd3OH2(SO4)2(s) | -18.931 | -25.641 |
| Cd4(OH)6SO4(s) | -0.977 | -29.377 |
| CdCl2(s) | -12.141 | -11.595 |
| CdCl2:1H2O(s) | -12.141 | -10.494 |
| CdCl2:2.5H2O(s) | -12.142 | -10.185 |
| CdF2(s) | -18.659 | -17.728 |
| CdOHCl(s) | -4.373 | -8.098 |
| CdSO4(s) | -11.163 | -11.307 |
| CdSO4:1H2O(s) | -11.164 | -9.629 |
| CdSO4:2.67H2O(s) | -11.164 | -9.401 |
| Cerrusite | -15.617 | -2.266 |
| Chalcanthite | -10.291 | -7.615 |
| Chalcopyrite | -135.416 | -99.244 |
| Chloropyromorphite(c) | -83.527 | 0.903 |
| Chloropyromorphite(soil) | -83.527 | -3.127 |
| Cinnabar | -101.634 | -54.811 |
| Claudetite | -26.066 | -24.553 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cotunnite | -11.55 | -6.611 |
| Covellite | -66.241 | -43.431 |
| Cr(VI)-Ettringite | 12.515 | -50.886 |
| Cr(VI)-Jarosite | -38.577 | -20.061 |
| CrO3(s) | -19.269 | -16.09 |
| Cryolite | -47.391 | -13.32 |
| Cu azide | -17.006 | -9.165 |
| Cu(OH)2(s) | 4.269 | -5.344 |
| Cu2(OH)3NO3(s) | -22.567 | -32.26 |
| Cu3(AsO4)2:2H2O(s) | -49.932 | -14.832 |
| Cu3(PO4)2(s) | -50.986 | -14.136 |
| Cu3(PO4)2:3H2O(s) | -50.987 | -15.867 |
| CuCO3(s) | -15.334 | -3.834 |
| CuCrO4(s) | -14.999 | -9.559 |
| CuF2(s) | -17.786 | -19.307 |
| CuF2:2H2O(s) | -17.786 | -13.329 |
| CuOCuSO4(s) | -6.02 | -17.161 |
| Cupric Ferrite | 2.851 | -4.415 |
| CuSO4(s) | -10.29 | -13.673 |
| Diaspore | 7.5 | 0 |
| Dolomite (disordered) | -20.887 | -4.629 |
| Dolomite (ordered) | -20.887 | -4.037 |
| Epsomite | -5.463 | -3.266 |
| Ettringite | 26.644 | -32.545 |
| FCO3-Apatite | -115.402 | 0 |
| Fe(OH)2 (am) | 1.335 | -12.712 |
| Fe(OH)2 (c) | 1.335 | -11.555 |
| Fe(OH)2.7Cl.3(s) | -3.04 | 0 |
| Fe2(SO4)3(s) | -45.095 | -42.832 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe3(OH)8(s) | -0.084 | -20.306 |
| FeAsO4:2H2O(s) | -32.079 | -11.879 |
| Ferrihydrite | -0.71 | -4.52 |
| Ferrihydrite (aged) | -0.71 | -4.01 |
| FeS (ppt) | -69.175 | -66.292 |
| Fluorite | -12.833 | -2.26 |
| Galena | -66.524 | -51.118 |
| Gibbsite (C) | 7.499 | -0.879 |
| Goethite | -0.709 | -1.569 |
| Goslarite | -7.614 | -5.517 |
| Greenockite | -67.115 | -52.76 |
| Greigite | -282.125 | -237.09 |
| Gypsum | -5.338 | -0.721 |
| Halite | -4.01 | -5.538 |
| Hematite | -1.418 | -0.784 |
| Hercynite | 16.335 | -8.467 |
| Hg(OH)2(s) | -31.123 | -27.627 |
| Hg3O2CO3(s) | -112.973 | -83.393 |
| HgCl2(s) | -46.66 | -24.742 |
| HgSO4(s) | -45.682 | -36.174 |
| Hinsdalite | -19.971 | -17.471 |
| H-Jarosite | -31.246 | -27.214 |
| Huntite | -41.897 | -12.584 |
| Hydrocerrusite | -27.248 | -8.488 |
| Hydromagnesite | -32.924 | -25.486 |
| Hydroxyapatite | -49.581 | -5.248 |
| Hydroxylpyromorphite | -75.758 | -12.968 |
| Hydrozincite | -4.472 | -14.61 |
| K2Cr2O7(s) | -34.362 | -16.628 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| K2CrO4(s) | -15.093 | -14.469 |
| K-Alum | -19.535 | -14.181 |
| KCl(s) | -5.681 | -6.581 |
| K-Jarosite | -29.158 | -18.777 |
| Langite | 2.517 | -15.978 |
| Larnakite | -6.586 | -6.284 |
| Laurionite | -3.782 | -4.405 |
| Lepidocrocite | -0.709 | -2.08 |
| Lime | 9.222 | -24.656 |
| Litharge | 3.987 | -9.102 |
| Mackinawite | -69.175 | -65.575 |
| Maghemite | -1.418 | -7.804 |
| Magnesioferrite | 7.68 | -10.875 |
| Magnesite | -10.505 | -2.924 |
| Magnetite | -0.083 | -4.753 |
| Malachite | -11.065 | -5.865 |
| Massicot | 3.987 | -9.31 |
| Matlockite | -14.809 | -5.634 |
| Melanothallite | -11.267 | -17.91 |
| Melanterite | -13.226 | -10.892 |
| Metacinnabar | -101.634 | -55.209 |
| Mg(OH)2 (active) | 9.098 | -9.696 |
| Mg2(OH)3Cl:4H2O(s) | 10.426 | -15.574 |
| Mg3(PO4)2(s) | -36.499 | -13.219 |
| MgCO3:5H2O(s) | -10.507 | -5.967 |
| MgCrO4(s) | -10.17 | -16.091 |
| MgF2(s) | -12.957 | -4.895 |
| MgHPO4:3H2O(s) | -22.8 | -4.625 |
| MgS(s) | -61.412 | -79.092 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Minium | 34.454 | -41.633 |
| Mirabilite | -7.046 | -5.449 |
| Mn2(SO4)3(s) | -31.163 | -26.446 |
| Montroydite | -31.123 | -27.406 |
| Morenosite | -8.405 | -6.186 |
| Na2Cr2O7(s) | -31.021 | -20.991 |
| Na2CrO4(s) | -11.752 | -14.802 |
| NaF(s) | -7.269 | -6.775 |
| Na-Jarosite | -27.488 | -22.993 |
| Natron | -12.091 | -10.38 |
| Nesquehonite | -10.506 | -5.984 |
| Ni(OH)2 (am) | 6.156 | -7.317 |
| Ni(OH)2 (c) | 6.156 | -4.634 |
| Ni3(AsO4)2:8H2O(s) | -44.272 | -18.772 |
| Ni3(PO4)2(s) | -45.324 | -14.024 |
| Ni4(OH)6SO4(s) | 10.067 | -21.933 |
| NiCO3(s) | -13.447 | -2.5 |
| NiS (alpha) | -64.354 | -58.834 |
| NiS (beta) | -64.354 | -53.334 |
| NiS (gamma) | -64.354 | -51.634 |
| Nsutite | 17.504 | 0 |
| Orpiment | -237.597 | -189.698 |
| Otavite | -16.208 | -4.156 |
| Pb azide (alpha) | -17.289 | -8.315 |
| Pb metal | -18.508 | -22.748 |
| Pb(OH)2(s) | 3.986 | -4.52 |
| Pb10(OH)6O(CO3)6(s) | -77.756 | -68.996 |
| Pb2(OH)3Cl(s) | 0.204 | -8.589 |
| Pb2O(OH)2(s) | 7.973 | -18.217 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb2O3(s) | 30.467 | -30.573 |
| Pb2OCO3(s) | -11.63 | -11.321 |
| Pb3(AsO4)2(s) | -50.78 | -15.28 |
| Pb3(PO4)2(s) | -51.834 | -8.304 |
| Pb3O2CO3(s) | -7.644 | -19.336 |
| Pb3O2SO4(s) | -2.599 | -13.767 |
| Pb4(OH)6SO4(s) | 1.386 | -19.714 |
| Pb4O3SO4(s) | 1.387 | -21.319 |
| PbCrO4(s) | -15.282 | -2.413 |
| PbF2(s) | -18.068 | -10.507 |
| PbHPO4(s) | -27.911 | -4.106 |
| PbO:0.3H2O(s) | 3.986 | -8.994 |
| Periclase | 9.098 | -13.405 |
| Phosgenite | -27.167 | -7.357 |
| Plattnerite | 26.481 | -24.92 |
| Plumbgummite | -37.31 | -4.52 |
| Portlandite | 9.222 | -14.264 |
| Pyrite | -117.191 | -98.38 |
| Realgar | -94.79 | -74.061 |
| Retgersite | -8.404 | -6.336 |
| Siderite | -18.268 | -7.722 |
| Smithsonite | -12.656 | -1.779 |
| Spharelite | -63.563 | -52.561 |
| Spinel | 24.098 | -15.109 |
| Strengite | -32.607 | -6.264 |
| Struvite | -20.034 | -6.774 |
| Sulfur | -48.016 | -45.97 |
| Tenorite(am) | 4.269 | -4.615 |
| Tenorite(c) | 4.269 | -3.765 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Thenardite | -7.043 | -7.42 |
| Thermonatrite | -12.088 | -12.788 |
| Tsumebite | -19.656 | -9.866 |
| Vaterite | -10.381 | -2.545 |
| Vivianite | -59.791 | -22 |
| Wurtzite | -63.563 | -54.815 |
| Zincite | 6.947 | -4.828 |
| Zincosite | -7.612 | -12.044 |
| Zn metal | -15.547 | -42.268 |
| Zn(NO3)2:6H2O(s) | -55.265 | -58.431 |
| Zn(OH)2 (am) | 6.947 | -6.048 |
| Zn(OH)2 (beta) | 6.947 | -5.313 |
| Zn(OH)2 (delta) | 6.947 | -4.897 |
| Zn(OH)2 (epsilon) | 6.947 | -5.065 |
| Zn(OH)2 (gamma) | 6.947 | -5.284 |
| Zn2(OH)2SO4(s) | -0.665 | -8.165 |
| Zn2(OH)3Cl(s) | 6.125 | -9.066 |
| Zn3(PO4)2:4H2O(s) | -42.954 | -7.534 |
| Zn3AsO42:2.5H2O(s) | -41.899 | -14.399 |
| Zn3O(SO4)2(s) | -8.276 | -28.759 |
| Zn4(OH)6SO4(s) | 13.229 | -15.171 |
| Zn5(OH)8Cl2(s) | 19.198 | -19.302 |
| Zn-Al LDH(s) | 11.591 | -8.239 |
| ZnCl2(s) | -8.59 | -16.08 |
| ZnCO3(s) | -12.656 | -1.856 |
| ZnCO3:1H2O(s) | -12.657 | -2.397 |
| ZnF2(s) | -15.108 | -14.936 |
| ZnSO4:1H2O(s) | -7.612 | -7.242 |

# C4 Mass distribution

## C4.1: pH 2

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 5.64E-12 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.004194 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021436 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 2.96E-10 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.01801 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.91E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 2.12E-24 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003003 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.83E-49 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 9.69E-66 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## C4.2: pH 3

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 2.59E-09 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.004194 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021437 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 6.17E-10 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.006447 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.88E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 2.74E-34 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003003 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 3.15E-42 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 9.64E-56 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## C4.3: pH 4

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.000577 | 20.744 | 0 | 0 | 0.002203 | 79.256 |
| AsO4-3 | 4.03E-07 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.004194 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.020753 | 96.81 | 0 | 0 | 0.000684 | 3.19 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 1.25E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.94E-11 | 0 | 0 | 0 | 0.00228 | 100 |
| H+1 | 0.005251 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 8.7E-08 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 3.02E-44 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003003 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.63E-34 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 9.62E-46 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.00543 | 74.517 | 0 | 0 | 0.001857 | 25.483 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## C4.4: pH 5

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 5.85E-06 | 0.21 | 0 | 0 | 0.002774 | 99.79 |
| AsO4-3 | 4.9E-07 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.004194 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.020749 | 96.792 | 0 | 0 | 0.000688 | 3.208 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 2.74E-08 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.39E-12 | 0 | 0 | 0 | 0.002292 | 100 |
| H+1 | 0.00502 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 1.05E-10 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 4.52E-54 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 6.47E-08 | 1.269 | 0 | 0 | 5.03E-06 | 98.731 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.46E-26 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 9.53E-36 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## C4.5: pH 6

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 2.08E-08 | 0.001 | 0 | 0 | 0.00278 | 99.999 |
| AsO4-3 | 4.91E-07 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.004192 | 99.94 | 0 | 0 | 2.51E-06 | 0.06 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.020749 | 96.792 | 0 | 0 | 0.000688 | 3.208 |
| CO3-2 | 0.002552 | 99.987 | 0 | 0 | 3.23E-07 | 0.013 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.25E-05 | 94.929 | 0 | 0 | 6.67E-07 | 5.071 |
| Fe+2 | 5.48E-11 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 2.45E-13 | 0 | 0 | 0 | 0.002292 | 100 |
| H+1 | 0.004295 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 9.19E-14 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 5.18E-64 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 99.999 | 0 | 0 | 3.87E-08 | 0.001 |
| Mn+3 | 6.49E-12 | 0 | 0 | 0 | 5.1E-06 | 100 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 99.999 | 0 | 0 | 9.69E-08 | 0.001 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.44E-18 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 9.53E-26 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 8.72E-07 | 40.299 | 0 | 0 | 1.29E-06 | 59.701 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

# C5 Finite solids

## C5.1: pH 2

No mineral solids precipitate from solution

## C5.2: pH 3

No mineral solids precipitate from solution

## C5.3: pH 4

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.28E-03 |
| AlOHSO4(s) | 1.86E-03 |
| Diaspore | 3.46E-04 |

## C5.4: pH 5

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.29E-03 |
| Diaspore | 2.77E-03 |
| Nsutite | 5.03E-06 |

## C5.5: pH 6

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Fe(OH)2.7Cl.3(s) | 2.29E-03 |
| Diaspore | 2.78E-03 |
| Nsutite | 5.10E-06 |

| Solid | Equilibrium amount (mol/l) |
|---|---|
| FCO3-Apatite | 2.69E-07 |

# **Appendix D** - Anaerobic treatment system for water discharge from Big Swamp into Reach 3 of Boundary Creek

## D1 Aqueous species

## D1.1: Eh 150

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 8.78E-06 | 8.71E-06 | -5.06 |
| Al(OH)2+ | 2.85E-10 | 2.37E-10 | -9.625 |
| Al(OH)3 (aq) | 1.83E-14 | 1.85E-14 | -13.732 |
| Al(OH)4- | 4.11E-18 | 3.42E-18 | -17.466 |
| Al(SO4)2- | 0.000134 | 0.000112 | -3.952 |
| Al+3 | 0.000782 | 0.000152 | -3.819 |
| Al2(OH)2+4 | 5.17E-10 | 2.8E-11 | -10.553 |
| Al2(OH)2CO3+2 | 1.04E-12 | 5.04E-13 | -12.298 |
| Al2PO4+3 | 4.08E-09 | 7.92E-10 | -9.101 |
| Al3(OH)4+5 | 1.77E-14 | 1.86E-16 | -15.731 |
| AlCl+2 | 2.26E-06 | 1.09E-06 | -5.962 |
| AlF+2 | 1.31E-05 | 6.33E-06 | -5.199 |
| AlF2+ | 1.31E-08 | 1.09E-08 | -7.963 |
| AlF3 (aq) | 5.47E-13 | 5.52E-13 | -12.258 |
| AlF4- | 1.44E-18 | 1.2E-18 | -17.92 |
| AlHPO4+ | 1.62E-07 | 1.35E-07 | -6.869 |
| AlOH+2 | 6.71E-07 | 3.24E-07 | -6.49 |
| AlSO4+ | 0.001838 | 0.001532 | -2.815 |
| As3S4(HS)- | 5.59E-40 | 4.66E-40 | -39.332 |
| AsO4-3 | 8.07E-29 | 1.57E-29 | -28.805 |
| AsS(OH)HS- | 4.43E-18 | 3.69E-18 | -17.433 |
| Ca DOM1 | 3.9E-07 | 3.47E-07 | -6.459 |
| Ca(NH3)2+2 | 3.89E-23 | 1.88E-23 | -22.727 |
| Ca(NO3)2 | 5.5E-168 | 5.6E-168 | -167.253 |
| Ca+2 | 0.002503 | 0.001208 | -2.918 |
| CaCl+ | 6.08E-05 | 5.07E-05 | -4.295 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCO3 (aq) | 1.07E-14 | 1.08E-14 | -13.966 |
| CaCrO4 (aq) | 2.81E-11 | 2.84E-11 | -10.547 |
| CaF+ | 7.14E-11 | 5.95E-11 | -10.225 |
| CaH2PO4+ | 2.77E-08 | 2.31E-08 | -7.636 |
| CaHCO3+ | 6.21E-09 | 5.18E-09 | -8.286 |
| CaHPO4 (aq) | 1.18E-11 | 1.19E-11 | -10.925 |
| CaNH3+2 | 5.61E-13 | 2.71E-13 | -12.567 |
| CaNO3+ | 5.97E-83 | 4.98E-83 | -82.303 |
| CaOH+ | 4.91E-14 | 4.09E-14 | -13.388 |
| CaPO4- | 1.25E-17 | 1.05E-17 | -16.981 |
| CaSO4 (aq) | 0.00043 | 0.000434 | -3.363 |
| Cd DOM1 | 2.07E-12 | 1.84E-12 | -11.734 |
| Cd(CO3)2-2 | 3.53E-30 | 1.7E-30 | -29.769 |
| Cd(HS)2 (aq) | 1.45E-20 | 1.47E-20 | -19.833 |
| Cd(HS)3- | 5.9E-32 | 4.92E-32 | -31.308 |
| Cd(HS)4-2 | 8.58E-43 | 4.14E-43 | -42.383 |
| Cd(NH3)2+2 | 1.28E-24 | 6.16E-25 | -24.21 |
| Cd(NH3)3+2 | 2.23E-33 | 1.07E-33 | -32.969 |
| Cd(NH3)4+2 | 1.14E-42 | 5.52E-43 | -42.258 |
| Cd(NO2)2 (aq) | 4.1E-127 | 4.2E-127 | -126.38 |
| Cd(NO3)2 (aq) | 5.8E-169 | 5.9E-169 | -168.229 |
| Cd(OH)2 (aq) | 2.19E-24 | 2.22E-24 | -23.655 |
| Cd(OH)3- | 1.08E-34 | 9.03E-35 | -34.044 |
| Cd(OH)4-2 | 7.96E-46 | 3.84E-46 | -45.416 |
| Cd(SO4)2-2 | 5.02E-11 | 2.42E-11 | -10.616 |
| Cd+2 | 5.29E-09 | 2.55E-09 | -8.593 |
| Cd2OH+3 | 2.93E-24 | 5.68E-25 | -24.246 |
| CdCl+ | 5.02E-09 | 4.19E-09 | -8.378 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl2 (aq) | 2.95E-10 | 2.97E-10 | -9.527 |
| CdCO3 (aq) | 3.71E-19 | 3.75E-19 | -18.426 |
| CdF+ | 1.97E-16 | 1.64E-16 | -15.786 |
| CdHCO3+ | 3.14E-14 | 2.61E-14 | -13.583 |
| CdHPO4 (aq) | 2.64E-16 | 2.67E-16 | -15.574 |
| CdHS+ | 1.66E-14 | 1.39E-14 | -13.858 |
| CdNH3+2 | 1.52E-16 | 7.31E-17 | -16.136 |
| CdNO2+ | 5.94E-68 | 4.95E-68 | -67.305 |
| CdNO3+ | 1.57E-88 | 1.31E-88 | -87.883 |
| CdOH+ | 4.7E-17 | 3.92E-17 | -16.407 |
| CdSO4 (aq) | 9.08E-10 | 9.17E-10 | -9.038 |
| Cl-1 | 0.021205 | 0.017673 | -1.753 |
| CO3-2 | 1.3E-14 | 6.27E-15 | -14.203 |
| Cr2O7-2 | 8.64E-12 | 4.17E-12 | -11.38 |
| CrO3Cl- | 1.01E-10 | 8.39E-11 | -10.076 |
| CrO3H2PO4- | 1.36E-12 | 1.13E-12 | -11.946 |
| CrO3HPO4-2 | 2.02E-12 | 9.72E-13 | -12.012 |
| CrO3SO4-2 | 8.25E-10 | 3.98E-10 | -9.4 |
| CrO4-2 | 8.27E-11 | 3.99E-11 | -10.399 |
| Cu DOM1 | 2.28E-14 | 2.03E-14 | -13.693 |
| Cu(CO3)2-2 | 9.11E-31 | 4.4E-31 | -30.357 |
| Cu(N3)2 (aq) | 1.25E-21 | 1.26E-21 | -20.899 |
| Cu(N3)3- | 1.74E-26 | 1.45E-26 | -25.838 |
| Cu(N3)4-2 | 1.82E-32 | 8.79E-33 | -32.056 |
| Cu(NH3)2+2 | 3.02E-25 | 1.46E-25 | -24.836 |
| Cu(NH3)3+2 | 1.73E-32 | 8.33E-33 | -32.079 |
| Cu(NH3)4+2 | 2.04E-40 | 9.83E-41 | -40.007 |
| Cu(NO2)2 (aq) | 2.8E-131 | 2.8E-131 | -130.552 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO3)2 (aq) | 4.1E-173 | 4.1E-173 | -172.387 |
| Cu(OH)2 (aq) | 1.91E-24 | 1.93E-24 | -23.715 |
| Cu(OH)3- | 1.37E-31 | 1.14E-31 | -30.942 |
| Cu(OH)4-2 | 6.54E-43 | 3.15E-43 | -42.501 |
| Cu+2 | 1.46E-12 | 7.05E-13 | -12.152 |
| Cu2(OH)2+2 | 2.02E-30 | 9.76E-31 | -30.011 |
| Cu2OH+3 | 1.42E-28 | 2.75E-29 | -28.561 |
| Cu2S3-2 | 3.88E-59 | 1.87E-59 | -58.728 |
| Cu3(OH)4+2 | 7.82E-48 | 3.77E-48 | -47.423 |
| CuCl+ | 2.66E-14 | 2.21E-14 | -13.655 |
| CuCl2 (aq) | 6.46E-17 | 6.52E-17 | -16.186 |
| CuCl3- | 1.07E-20 | 8.96E-21 | -20.048 |
| CuCl4-2 1 | 2.32E-24 | 1.12E-24 | -23.95 |
| CuCO3 (aq) | 2.58E-20 | 2.6E-20 | -19.584 |
| CuF+ | 1.54E-19 | 1.28E-19 | -18.893 |
| CuHCO3+ | 1.73E-17 | 1.44E-17 | -16.842 |
| CuHPO4 (aq) | 1.92E-19 | 1.94E-19 | -18.712 |
| CuHSO4+ | 7.75E-16 | 6.46E-16 | -15.19 |
| CuN3+ | 1.41E-16 | 1.17E-16 | -15.93 |
| CuNH3+2 | 1.38E-18 | 6.67E-19 | -18.176 |
| CuNO2+ | 1.71E-71 | 1.42E-71 | -70.847 |
| CuNO3+ | 3.43E-92 | 2.86E-92 | -91.544 |
| CuOH+ | 6.75E-18 | 5.62E-18 | -17.25 |
| CuS(aq) | 2.43E-26 | 2.46E-26 | -25.61 |
| CuSO4 (aq) | 2.45E-13 | 2.48E-13 | -12.606 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.473 |
| DOM1 | 7.76E-06 | 1.86E-06 | -5.73 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| F-1 | 5.21E-09 | 4.34E-09 | -8.362 |
| Fe DOM1 | 3.66E-13 | 3.63E-13 | -12.44 |
| Fe(N3)2+ | 4.81E-19 | 4E-19 | -18.397 |
| Fe(N3)3 (aq) | 1.95E-23 | 1.97E-23 | -22.705 |
| Fe(NH3)2+2 | 1.93E-21 | 9.31E-22 | -21.031 |
| Fe(NH3)3+2 | 3.97E-31 | 1.91E-31 | -30.718 |
| Fe(NH3)4+2 | 3.48E-41 | 1.68E-41 | -40.775 |
| Fe(NO2)2+ | 4.7E-131 | 3.9E-131 | -130.409 |
| Fe(NO2)3 (aq) | 8.5E-190 | 8.6E-190 | -189.064 |
| Fe(OH)2 (aq) | 9.46E-20 | 9.56E-20 | -19.02 |
| Fe(OH)2+ | 4.3E-15 | 3.58E-15 | -14.446 |
| Fe(OH)3- | 1.37E-27 | 1.14E-27 | -26.942 |
| Fe(OH)3 (aq) | 4.88E-22 | 4.92E-22 | -21.308 |
| Fe(OH)4- | 1.6E-27 | 1.33E-27 | -26.875 |
| Fe(SO4)2- | 1.32E-14 | 1.1E-14 | -13.959 |
| Fe+2 | 0.001929 | 0.000931 | -3.031 |
| Fe+3 | 1.03E-13 | 2E-14 | -13.699 |
| Fe2(OH)2+4 | 7.3E-25 | 3.96E-26 | -25.403 |
| Fe3(OH)4+5 | 4.59E-36 | 4.82E-38 | -37.317 |
| FeCl+ | 1.25E-05 | 1.04E-05 | -4.984 |
| FeCl+2 | 1.6E-14 | 7.73E-15 | -14.112 |
| FeCrO4+ | 3.51E-17 | 2.93E-17 | -16.533 |
| FeF+ | 7.87E-11 | 6.56E-11 | -10.183 |
| FeF+2 | 1.72E-16 | 8.28E-17 | -16.082 |
| FeF2+ | 1.63E-20 | 1.36E-20 | -19.867 |
| FeF3 (aq) | 5.42E-26 | 5.48E-26 | -25.262 |
| FeH2PO4+ | 4.4E-07 | 3.67E-07 | -6.436 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeH2PO4+2 | 6.17E-16 | 2.97E-16 | -15.527 |
| FeHCO3+ | 4.54E-09 | 3.79E-09 | -8.422 |
| FeHPO4 (aq) | 7.57E-11 | 7.64E-11 | -10.117 |
| FeHPO4+ | 6.17E-15 | 5.14E-15 | -14.289 |
| FeHS+ | 2.47E-11 | 2.06E-11 | -10.686 |
| FeN3+2 | 1.48E-15 | 7.16E-16 | -15.145 |
| FeNH3+2 | 3.7E-12 | 1.78E-12 | -11.749 |
| FeNO2+2 | 1.27E-71 | 6.11E-72 | -71.214 |
| FeOH+ | 8.47E-11 | 7.06E-11 | -10.151 |
| FeOH+2 | 1.15E-13 | 5.55E-14 | -13.255 |
| FeSO4 (aq) | 0.00035 | 0.000354 | -3.451 |
| FeSO4+ | 5.21E-13 | 4.34E-13 | -12.363 |
| H DOM1 | 1.17E-05 | 6.49E-06 | -5.188 |
| H+1 | 0.002899 | 0.002416 | -2.617 |
| H2AsO3- | 1.13E-13 | 9.41E-14 | -13.026 |
| H2AsO4- | 9.1E-16 | 7.59E-16 | -15.12 |
| H2CO3* (aq) | 0.002552 | 0.002577 | -2.589 |
| H2CrO4 (aq) | 2.73E-10 | 2.76E-10 | -9.56 |
| H2PO4- | 1.21E-06 | 1.01E-06 | -5.995 |
| H2S (aq) | 1.85E-09 | 1.87E-09 | -8.729 |
| H3AsO3 | 4.91E-07 | 4.95E-07 | -6.305 |
| H3AsO4 | 3.24E-16 | 3.27E-16 | -15.485 |
| H3PO4 | 3.06E-07 | 3.09E-07 | -6.509 |
| HAsO3-2 | 4.11E-25 | 1.98E-25 | -24.703 |
| HAsO4-2 | 6.38E-20 | 3.08E-20 | -19.511 |
| HCO3- | 4.88E-07 | 4.06E-07 | -6.391 |
| HCrO4- | 3.64E-07 | 3.03E-07 | -6.518 |
| HF (aq) | 1.31E-08 | 1.32E-08 | -7.88 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HF2- | 2.59E-16 | 2.15E-16 | -15.667 |
| Hg(CO3)2-2 | 7.67E-43 | 3.7E-43 | -42.432 |
| Hg(HS)2 (aq) | 1.82E-18 | 1.84E-18 | -17.736 |
| Hg(N3)2 (aq) | 2.27E-22 | 2.29E-22 | -21.64 |
| Hg(NH3)2+2 | 1.09E-31 | 5.25E-32 | -31.28 |
| Hg(NH3)4+2 | 2.36E-50 | 1.14E-50 | -49.944 |
| Hg(NO2)2 (aq) | 7.4E-142 | 7.5E-142 | -141.126 |
| Hg(NO2)3- | 6E-201 | 5E-201 | -200.301 |
| Hg(NO2)4-2 | 5.1E-261 | 2.5E-261 | -260.606 |
| Hg(NO3)2 (aq) | 5.9E-191 | 6E-191 | -190.221 |
| Hg(OH)2 | 2.9E-31 | 2.93E-31 | -30.533 |
| Hg(SO4)2-2 | 4.65E-32 | 2.24E-32 | -31.649 |
| Hg+2 | 9.03E-30 | 4.36E-30 | -29.361 |
| Hg2OH+3 | 1.68E-59 | 3.26E-60 | -59.487 |
| Hg3(OH)3+3 | 2.31E-87 | 4.49E-88 | -87.348 |
| HgCl+ | 2.63E-24 | 2.19E-24 | -23.66 |
| HgCl2 (aq) | 2.94E-19 | 2.97E-19 | -18.528 |
| HgCl3-1 | 6.26E-20 | 5.21E-20 | -19.283 |
| HgCl4-2 | 8.55E-21 | 4.13E-21 | -20.384 |
| HgClOH (aq) | 6.27E-25 | 6.33E-25 | -24.199 |
| HgCO3 (aq) | 2.07E-32 | 2.09E-32 | -31.679 |
| HgF+ | 8.47E-37 | 7.06E-37 | -36.151 |
| HgHCO3+ | 1.01E-30 | 8.4E-31 | -30.076 |
| HgHS2- | 2.95E-22 | 2.46E-22 | -21.609 |
| HgN3+ | 3.35E-18 | 2.79E-18 | -17.555 |
| HgNO2+ | 4.99E-85 | 4.16E-85 | -84.381 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgNO3+ | 1.4E-110 | 1.2E-110 | -109.923 |
| HgOH+ | 6.48E-31 | 5.4E-31 | -30.268 |
| HgOHCO3- | 1.22E-36 | 1.02E-36 | -35.992 |
| HgS2-2 | 4.11E-28 | 1.98E-28 | -27.702 |
| HgSO4 (aq) | 1.25E-30 | 1.27E-30 | -29.898 |
| HN3 (aq) | 2.83E-05 | 2.86E-05 | -4.544 |
| HNO2 (aq) | 6.52E-61 | 6.58E-61 | -60.182 |
| HPO4-2 | 5.27E-11 | 2.54E-11 | -10.594 |
| HS-1 | 6.37E-14 | 5.31E-14 | -13.275 |
| HSO4- | 0.000374 | 0.000311 | -3.507 |
| K+1 | 0.000148 | 0.000124 | -3.908 |
| K2HPO4 (aq) | 4.16E-18 | 4.2E-18 | -17.377 |
| K2PO4- | 1.2E-26 | 1E-26 | -26 |
| KCl (aq) | 1.15E-06 | 1.16E-06 | -5.937 |
| KCr2O7- | 5.34E-15 | 4.45E-15 | -14.352 |
| KCrO4- | 2.2E-14 | 1.83E-14 | -13.737 |
| KF (aq) | 2.43E-13 | 2.45E-13 | -12.61 |
| KH2PO4 (aq) | 1.92E-10 | 1.94E-10 | -9.713 |
| KHPO4- | 2.32E-14 | 1.93E-14 | -13.714 |
| KNO3 (aq) | 1.13E-84 | 1.14E-84 | -83.943 |
| KOH (aq) | 4.05E-16 | 4.09E-16 | -15.388 |
| KPO4-2 | 2.01E-23 | 9.7E-24 | -23.013 |
| KSO4- | 1.52E-06 | 1.26E-06 | -5.898 |
| Mg DOM1 | 3.98E-08 | 3.54E-08 | -7.451 |
| Mg(NH3)2+2 | 1.98E-23 | 9.54E-24 | -23.021 |
| Mg+2 | 0.002551 | 0.001231 | -2.91 |
| Mg2CO3+2 | 7.66E-17 | 3.7E-17 | -16.432 |
| MgCl+ | 9.82E-05 | 8.19E-05 | -4.087 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgCO3 (aq) | 5.45E-15 | 5.51E-15 | -14.259 |
| MgF+ | 4.25E-10 | 3.54E-10 | -9.451 |
| MgHCO3+ | 5.83E-09 | 4.86E-09 | -8.314 |
| MgHPO4 (aq) | 1.65E-11 | 1.67E-11 | -10.777 |
| MgOH+ | 9.5E-13 | 7.92E-13 | -12.101 |
| MgPO4- | 2E-19 | 1.67E-19 | -18.778 |
| MgSO4 (aq) | 0.000354 | 0.000358 | -3.447 |
| Mn+3 | 5.1E-06 | 9.89E-07 | -6.005 |
| N3-1 | 2.76E-07 | 2.3E-07 | -6.639 |
| Na+1 | 0.00684 | 0.0057 | -2.244 |
| Na2HPO4 (aq) | 5.85E-15 | 5.9E-15 | -14.229 |
| Na2PO4- | 5.46E-23 | 4.55E-23 | -22.342 |
| NaCl (aq) | 5.59E-05 | 5.65E-05 | -4.248 |
| NaCO3- | 1.06E-15 | 8.85E-16 | -15.053 |
| NaCrO4- | 1.36E-12 | 1.13E-12 | -11.947 |
| NaF (aq) | 2.17E-11 | 2.19E-11 | -10.659 |
| NaH2PO4 (aq) | 8.86E-09 | 8.94E-09 | -8.049 |
| NaHCO3 (aq) | 1.36E-09 | 1.37E-09 | -8.862 |
| NaHPO4- | 1.66E-12 | 1.38E-12 | -11.86 |
| NaNO3 (aq) | 1.92E-83 | 1.94E-83 | -82.712 |
| NaOH (aq) | 1.28E-14 | 1.29E-14 | -13.888 |
| NaPO4-2 | 1.02E-21 | 4.94E-22 | -21.306 |
| NaSO4- | 6.42E-05 | 5.35E-05 | -4.272 |
| NH3 (aq) | 6.68E-11 | 6.74E-11 | -10.171 |
| NH4+1 | 0.000713 | 0.000594 | -3.226 |
| NH4Cr2O7- | 2.98E-14 | 2.49E-14 | -13.605 |
| NH4SO4- | 1.32E-05 | 1.1E-05 | -4.958 |
| Ni DOM1 | 1.27E-09 | 1.13E-09 | -8.947 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(N3)2 (aq) | 8.08E-18 | 8.16E-18 | -17.088 |
| Ni(NH3)2+2 | 1.71E-21 | 8.23E-22 | -21.085 |
| Ni(NH3)3+2 | 6.66E-30 | 3.22E-30 | -29.493 |
| Ni(NH3)4+2 | 7.72E-39 | 3.72E-39 | -38.429 |
| Ni(NH3)5+2 | 2.89E-48 | 1.39E-48 | -47.856 |
| Ni(NH3)6+2 | 2.3E-58 | 1.11E-58 | -57.955 |
| Ni(NO2)2 (aq) | 3.5E-126 | 3.6E-126 | -125.446 |
| Ni(OH)2 (aq) | 2.68E-20 | 2.71E-20 | -19.567 |
| Ni(OH)3- | 1.35E-28 | 1.13E-28 | -27.948 |
| Ni(SO4)2-2 | 6.42E-11 | 3.1E-11 | -10.509 |
| Ni+2 | 3.24E-06 | 1.56E-06 | -5.806 |
| NiCl+ | 1.2E-08 | 9.98E-09 | -8.001 |
| NiCl2 (aq) | 6.23E-12 | 6.29E-12 | -11.201 |
| NiCO3 (aq) | 3.61E-16 | 3.64E-16 | -15.439 |
| NiF+ | 1.47E-13 | 1.23E-13 | -12.911 |
| NiH2PO4+ | 1.25E-11 | 1.04E-11 | -10.983 |
| NiHCO3+ | 7.48E-11 | 6.23E-11 | -10.205 |
| NiHPO4 (aq) | 2.88E-14 | 2.91E-14 | -13.536 |
| NiHS+ | 3.08E-14 | 2.57E-14 | -13.591 |
| NiN3+ | 8.12E-12 | 6.77E-12 | -11.17 |
| NiNH3+2 | 1.43E-13 | 6.92E-14 | -13.16 |
| NiNO2+ | 8.68E-66 | 7.23E-66 | -65.141 |
| NiNO3+ | 5.7E-86 | 4.75E-86 | -85.323 |
| NiOH+ | 4.76E-14 | 3.97E-14 | -13.401 |
| NiSO4 (aq) | 4.94E-07 | 4.98E-07 | -6.303 |
| NO2-1 | 2.31E-61 | 1.93E-61 | -60.715 |
| NO3-1 | 1.45E-80 | 1.21E-80 | -79.918 |
| OH- | 2.29E-12 | 1.91E-12 | -11.72 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb DOM1 | 1.01E-09 | 8.99E-10 | -9.046 |
| Pb(CO3)2-2 | 1.11E-26 | 5.36E-27 | -26.271 |
| Pb(HS)2 (aq) | 8.14E-20 | 8.22E-20 | -19.085 |
| Pb(HS)3- | 1.04E-31 | 8.71E-32 | -31.06 |
| Pb(NO2)2 (aq) | 7.4E-127 | 7.5E-127 | -126.125 |
| Pb(NO3)2 (aq) | 6.2E-167 | 6.3E-167 | -166.2 |
| Pb(OH)2 (aq) | 2.13E-20 | 2.16E-20 | -19.666 |
| Pb(OH)3- | 1.08E-28 | 8.97E-29 | -28.047 |
| Pb(SO4)2-2 | 2.87E-10 | 1.39E-10 | -9.858 |
| Pb+2 | 3.25E-08 | 1.57E-08 | -7.805 |
| Pb2OH+3 | 2.09E-19 | 4.06E-20 | -19.391 |
| Pb3(OH)4+2 | 5.91E-38 | 2.85E-38 | -37.545 |
| Pb4(OH)4+4 | 1.27E-41 | 6.89E-43 | -42.162 |
| PbCl+ | 1.07E-08 | 8.89E-09 | -8.051 |
| PbCl2 (aq) | 3.25E-10 | 3.28E-10 | -9.484 |
| PbCl3- | 5.53E-12 | 4.61E-12 | -11.336 |
| PbCl4-2 | 6.17E-14 | 2.98E-14 | -13.526 |
| PbCO3 (aq) | 3.29E-16 | 3.33E-16 | -15.478 |
| PbF+ | 1.15E-14 | 9.61E-15 | -14.017 |
| PbF2 (aq) | 5.09E-22 | 5.14E-22 | -21.289 |
| PbH2PO4+ | 4.67E-13 | 3.89E-13 | -12.41 |
| PbHCO3+ | 4.83E-12 | 4.03E-12 | -11.395 |
| PbHPO4 (aq) | 4.03E-16 | 4.07E-16 | -15.391 |
| PbNO2+ | 1.17E-66 | 9.77E-67 | -66.01 |
| PbNO3+ | 3.45E-87 | 2.88E-87 | -86.541 |
| PbOH+ | 1.41E-13 | 1.17E-13 | -12.931 |
| PbSO4 (aq) | 1.32E-08 | 1.33E-08 | -7.877 |
| PO4-3 | 1.86E-20 | 3.6E-21 | -20.444 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| S-2 | 9.08E-29 | 4.38E-29 | -28.358 |
| SO4-2 | 0.00359 | 0.001732 | -2.761 |
| Zn DOM1 | 1.19E-08 | 1.06E-08 | -7.976 |
| Zn(CO3)2-2 | 1.5E-26 | 7.24E-27 | -26.14 |
| Zn(N3)2 (aq) | 4.6E-17 | 4.65E-17 | -16.333 |
| Zn(N3)3- | 7.33E-23 | 6.11E-23 | -22.214 |
| Zn(NH3)2+2 | 3.8E-21 | 1.84E-21 | -20.736 |
| Zn(NH3)3+2 | 7.55E-29 | 3.64E-29 | -28.439 |
| Zn(NH3)4+2 | 7.34E-37 | 3.54E-37 | -36.451 |
| Zn(NO2)2 (aq) | 5.4E-126 | 5.4E-126 | -125.265 |
| Zn(NO3)2 (aq) | 6.7E-166 | 6.8E-166 | -165.17 |
| Zn(OH)2 (aq) | 1.99E-17 | 2.01E-17 | -16.696 |
| Zn(OH)3- | 3.18E-26 | 2.65E-26 | -25.577 |
| Zn(OH)4-2 | 3.62E-36 | 1.75E-36 | -35.757 |
| Zn(SO4)2-2 | 1.09E-07 | 5.27E-08 | -7.278 |
| Zn+2 | 1.91E-05 | 9.22E-06 | -5.035 |
| Zn2OH+3 | 7.47E-17 | 1.45E-17 | -16.839 |
| Zn2S3-2 | 4.19E-42 | 2.02E-42 | -41.695 |
| Zn4S6-4 | 1.28E-81 | 6.93E-83 | -82.159 |
| ZnCl+ | 5.23E-07 | 4.36E-07 | -6.361 |
| ZnCl2 (aq) | 4.89E-09 | 4.93E-09 | -8.307 |
| ZnCl3- | 1.1E-10 | 9.2E-11 | -10.036 |
| ZnCl4-2 | 1.55E-12 | 7.5E-13 | -12.125 |
| ZnCO3 (aq) | 3.3E-15 | 3.33E-15 | -14.478 |
| ZnF+ | 8.23E-13 | 6.86E-13 | -12.164 |
| ZnHCO3+ | 1.13E-10 | 9.43E-11 | -10.026 |
| ZnHPO4 (aq) | 3.89E-13 | 3.93E-13 | -12.406 |
| ZnN3+ | 3.66E-11 | 3.05E-11 | -10.516 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnNH3+2 | 2.44E-13 | 1.18E-13 | -12.93 |
| ZnNO2+ | 1.29E-65 | 1.07E-65 | -64.97 |
| ZnNO3+ | 3.58E-85 | 2.99E-85 | -84.525 |
| ZnOH+ | 2.11E-12 | 1.76E-12 | -11.755 |
| ZnS (aq) | 7.46E-18 | 7.53E-18 | -17.123 |
| ZnSO4 (aq) | 3.17E-06 | 3.2E-06 | -5.494 |

## D1.2: Eh 200

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 8.77E-06 | 8.71E-06 | -5.06 |
| Al(OH)2+ | 2.85E-10 | 2.37E-10 | -9.625 |
| Al(OH)3 (aq) | 1.83E-14 | 1.85E-14 | -13.733 |
| Al(OH)4- | 4.1E-18 | 3.42E-18 | -17.466 |
| Al(SO4)2- | 0.000134 | 0.000112 | -3.952 |
| Al+3 | 0.000782 | 0.000152 | -3.819 |
| Al2(OH)2+4 | 5.17E-10 | 2.8E-11 | -10.553 |
| Al2(OH)2CO3+2 | 1.04E-12 | 5.04E-13 | -12.298 |
| Al2PO4+3 | 4.08E-09 | 7.92E-10 | -9.101 |
| Al3(OH)4+5 | 1.77E-14 | 1.86E-16 | -15.732 |
| AlCl+2 | 2.26E-06 | 1.09E-06 | -5.962 |
| AlF+2 | 1.31E-05 | 6.33E-06 | -5.199 |
| AlF2+ | 1.31E-08 | 1.09E-08 | -7.963 |
| AlF3 (aq) | 5.47E-13 | 5.52E-13 | -12.258 |
| AlF4- | 1.44E-18 | 1.2E-18 | -17.92 |
| AlHPO4+ | 1.62E-07 | 1.35E-07 | -6.869 |
| AlOH+2 | 6.71E-07 | 3.24E-07 | -6.49 |
| AlSO4+ | 0.001838 | 0.001532 | -2.815 |
| As3S4(HS)- | 5.88E-82 | 4.9E-82 | -81.31 |
| AsO4-3 | 4.53E-27 | 8.79E-28 | -27.056 |
| AsS(OH)HS- | 4.5E-32 | 3.75E-32 | -31.426 |
| Ca DOM1 | 3.9E-07 | 3.47E-07 | -6.459 |
| Ca(NH3)2+2 | 3.89E-23 | 1.88E-23 | -22.727 |
| Ca(NO3)2 | 5.4E-154 | 5.5E-154 | -153.261 |
| Ca+2 | 0.002503 | 0.001208 | -2.918 |
| CaCl+ | 6.08E-05 | 5.07E-05 | -4.295 |
| CaCO3 (aq) | 1.07E-14 | 1.08E-14 | -13.966 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCrO4 (aq) | 2.81E-11 | 2.84E-11 | -10.547 |
| CaF+ | 7.14E-11 | 5.95E-11 | -10.225 |
| CaH2PO4+ | 2.77E-08 | 2.31E-08 | -7.636 |
| CaHCO3+ | 6.21E-09 | 5.18E-09 | -8.286 |
| CaHPO4 (aq) | 1.18E-11 | 1.19E-11 | -10.925 |
| CaNH3+2 | 5.61E-13 | 2.71E-13 | -12.567 |
| CaNO3+ | 5.92E-76 | 4.94E-76 | -75.307 |
| CaOH+ | 4.91E-14 | 4.09E-14 | -13.388 |
| CaPO4- | 1.25E-17 | 1.05E-17 | -16.981 |
| CaSO4 (aq) | 0.00043 | 0.000434 | -3.363 |
| Cd DOM1 | 2.07E-12 | 1.84E-12 | -11.734 |
| Cd(CO3)2-2 | 3.53E-30 | 1.7E-30 | -29.769 |
| Cd(HS)2 (aq) | 1.48E-34 | 1.49E-34 | -33.826 |
| Cd(HS)3- | 6.05E-53 | 5.04E-53 | -52.297 |
| Cd(HS)4-2 | 8.87E-71 | 4.28E-71 | -70.369 |
| Cd(NH3)2+2 | 1.28E-24 | 6.16E-25 | -24.21 |
| Cd(NH3)3+2 | 2.23E-33 | 1.07E-33 | -32.969 |
| Cd(NH3)4+2 | 1.14E-42 | 5.52E-43 | -42.258 |
| Cd(NO2)2 (aq) | 1.3E-116 | 1.3E-116 | -115.886 |
| Cd(NO3)2 (aq) | 5.8E-155 | 5.8E-155 | -154.236 |
| Cd(OH)2 (aq) | 2.19E-24 | 2.22E-24 | -23.655 |
| Cd(OH)3- | 1.08E-34 | 9.03E-35 | -34.044 |
| Cd(OH)4-2 | 7.96E-46 | 3.84E-46 | -45.416 |
| Cd(SO4)2-2 | 5.02E-11 | 2.42E-11 | -10.616 |
| Cd+2 | 5.29E-09 | 2.55E-09 | -8.593 |
| Cd2OH+3 | 2.93E-24 | 5.68E-25 | -24.246 |
| CdCl+ | 5.02E-09 | 4.19E-09 | -8.378 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl2 (aq) | 2.95E-10 | 2.97E-10 | -9.527 |
| CdCO3 (aq) | 3.71E-19 | 3.75E-19 | -18.426 |
| CdF+ | 1.97E-16 | 1.64E-16 | -15.786 |
| CdHCO3+ | 3.14E-14 | 2.61E-14 | -13.583 |
| CdHPO4 (aq) | 2.64E-16 | 2.67E-16 | -15.574 |
| CdHS+ | 1.68E-21 | 1.4E-21 | -20.855 |
| CdNH3+2 | 1.52E-16 | 7.31E-17 | -16.136 |
| CdNO2+ | 1.05E-62 | 8.75E-63 | -62.058 |
| CdNO3+ | 1.56E-81 | 1.3E-81 | -80.887 |
| CdOH+ | 4.7E-17 | 3.92E-17 | -16.407 |
| CdSO4 (aq) | 9.08E-10 | 9.17E-10 | -9.038 |
| Cl-1 | 0.021205 | 0.017673 | -1.753 |
| CO3-2 | 1.3E-14 | 6.27E-15 | -14.203 |
| Cr2O7-2 | 8.64E-12 | 4.17E-12 | -11.38 |
| CrO3Cl- | 1.01E-10 | 8.39E-11 | -10.076 |
| CrO3H2PO4- | 1.36E-12 | 1.13E-12 | -11.946 |
| CrO3HPO4-2 | 2.02E-12 | 9.72E-13 | -12.012 |
| CrO3SO4-2 | 8.25E-10 | 3.98E-10 | -9.4 |
| CrO4-2 | 8.27E-11 | 3.99E-11 | -10.399 |
| Cu DOM1 | 8.17E-10 | 7.27E-10 | -9.139 |
| Cu(CO3)2-2 | 3.26E-26 | 1.57E-26 | -25.803 |
| Cu(N3)2 (aq) | 4.48E-17 | 4.52E-17 | -16.345 |
| Cu(N3)3- | 6.25E-22 | 5.21E-22 | -21.284 |
| Cu(N3)4-2 | 6.52E-28 | 3.15E-28 | -27.502 |
| Cu(NH3)2+2 | 1.08E-20 | 5.22E-21 | -20.282 |
| Cu(NH3)3+2 | 6.18E-28 | 2.98E-28 | -27.525 |
| Cu(NH3)4+2 | 7.3E-36 | 3.52E-36 | -35.453 |
| Cu(NO2)2 (aq) | 3.1E-116 | 3.1E-116 | -115.503 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO3)2 (aq) | 1.4E-154 | 1.4E-154 | -153.84 |
| Cu(OH)2 (aq) | 6.84E-20 | 6.9E-20 | -19.161 |
| Cu(OH)3- | 4.91E-27 | 4.09E-27 | -26.388 |
| Cu(OH)4-2 | 2.34E-38 | 1.13E-38 | -37.947 |
| Cu+2 | 5.24E-08 | 2.53E-08 | -7.598 |
| Cu2(OH)2+2 | 2.59E-21 | 1.25E-21 | -20.903 |
| Cu2OH+3 | 1.82E-19 | 3.52E-20 | -19.453 |
| Cu2S3-2 | 5.1E-71 | 2.46E-71 | -70.609 |
| Cu3(OH)4+2 | 3.59E-34 | 1.73E-34 | -33.761 |
| CuCl+ | 9.51E-10 | 7.93E-10 | -9.101 |
| CuCl2 (aq) | 2.31E-12 | 2.34E-12 | -11.632 |
| CuCl3- | 3.85E-16 | 3.21E-16 | -15.494 |
| CuCl4-2 1 | 8.32E-20 | 4.02E-20 | -19.396 |
| CuCO3 (aq) | 9.24E-16 | 9.33E-16 | -15.03 |
| CuF+ | 5.5E-15 | 4.59E-15 | -14.339 |
| CuHCO3+ | 6.18E-13 | 5.15E-13 | -12.288 |
| CuHPO4 (aq) | 6.88E-15 | 6.95E-15 | -14.158 |
| CuHSO4+ | 2.78E-11 | 2.31E-11 | -10.636 |
| CuN3+ | 5.05E-12 | 4.2E-12 | -11.376 |
| CuNH3+2 | 4.95E-14 | 2.39E-14 | -13.622 |
| CuNO2+ | 1.08E-61 | 9.01E-62 | -61.045 |
| CuNO3+ | 1.22E-80 | 1.01E-80 | -79.994 |
| CuOH+ | 2.42E-13 | 2.01E-13 | -12.696 |
| CuS(aq) | 8.78E-29 | 8.87E-29 | -28.052 |
| CuSO4 (aq) | 8.79E-09 | 8.87E-09 | -8.052 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.473 |
| DOM1 | 7.76E-06 | 1.86E-06 | -5.73 |
| F-1 | 5.21E-09 | 4.34E-09 | -8.362 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Fe DOM1 | 2.74E-12 | 2.72E-12 | -11.566 |
| Fe(N3)2+ | 3.6E-18 | 3E-18 | -17.523 |
| Fe(N3)3 (aq) | 1.46E-22 | 1.48E-22 | -21.831 |
| Fe(NH3)2+2 | 1.93E-21 | 9.31E-22 | -21.031 |
| Fe(NH3)3+2 | 3.97E-31 | 1.91E-31 | -30.718 |
| Fe(NH3)4+2 | 3.48E-41 | 1.68E-41 | -40.775 |
| Fe(NO2)2+ | 1.1E-119 | 9.1E-120 | -119.04 |
| Fe(NO2)3 (aq) | 3.5E-173 | 3.6E-173 | -172.448 |
| Fe(OH)2 (aq) | 9.46E-20 | 9.56E-20 | -19.02 |
| Fe(OH)2+ | 3.22E-14 | 2.68E-14 | -13.571 |
| Fe(OH)3- | 1.37E-27 | 1.14E-27 | -26.942 |
| Fe(OH)3 (aq) | 3.65E-21 | 3.69E-21 | -20.433 |
| Fe(OH)4- | 1.2E-26 | 9.99E-27 | -26 |
| Fe(SO4)2- | 9.88E-14 | 8.24E-14 | -13.084 |
| Fe+2 | 0.001929 | 0.000931 | -3.031 |
| Fe+3 | 7.72E-13 | 1.5E-13 | -12.825 |
| Fe2(OH)2+4 | 4.1E-23 | 2.22E-24 | -23.654 |
| Fe3(OH)4+5 | 1.93E-33 | 2.03E-35 | -34.693 |
| FeCl+ | 1.25E-05 | 1.04E-05 | -4.984 |
| FeCl+2 | 1.2E-13 | 5.79E-14 | -13.237 |
| FeCrO4+ | 2.63E-16 | 2.19E-16 | -15.659 |
| FeF+ | 7.87E-11 | 6.56E-11 | -10.183 |
| FeF+2 | 1.29E-15 | 6.2E-16 | -15.207 |
| FeF2+ | 1.22E-19 | 1.02E-19 | -18.992 |
| FeF3 (aq) | 4.06E-25 | 4.1E-25 | -24.387 |
| FeH2PO4+ | 4.4E-07 | 3.67E-07 | -6.436 |
| FeH2PO4+2 | 4.62E-15 | 2.23E-15 | -14.652 |
| FeHCO3+ | 4.54E-09 | 3.79E-09 | -8.422 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHPO4 (aq) | 7.57E-11 | 7.64E-11 | -10.117 |
| FeHPO4+ | 4.62E-14 | 3.85E-14 | -13.415 |
| FeHS+ | 2.49E-18 | 2.08E-18 | -17.683 |
| FeN3+2 | 1.11E-14 | 5.37E-15 | -14.27 |
| FeNH3+2 | 3.7E-12 | 1.78E-12 | -11.749 |
| FeNO2+2 | 1.68E-65 | 8.08E-66 | -65.092 |
| FeOH+ | 8.47E-11 | 7.06E-11 | -10.151 |
| FeOH+2 | 8.62E-13 | 4.16E-13 | -12.381 |
| FeSO4 (aq) | 0.00035 | 0.000354 | -3.451 |
| FeSO4+ | 3.9E-12 | 3.25E-12 | -11.488 |
| H DOM1 | 1.17E-05 | 6.49E-06 | -5.188 |
| H+1 | 0.002899 | 0.002416 | -2.617 |
| H2AsO3- | 1.13E-13 | 9.41E-14 | -13.026 |
| H2AsO4- | 5.11E-14 | 4.26E-14 | -13.371 |
| H2CO3* (aq) | 0.002552 | 0.002577 | -2.589 |
| H2CrO4 (aq) | 2.73E-10 | 2.76E-10 | -9.56 |
| H2PO4- | 1.21E-06 | 1.01E-06 | -5.995 |
| H2S (aq) | 1.87E-16 | 1.88E-16 | -15.725 |
| H3AsO3 | 4.91E-07 | 4.95E-07 | -6.305 |
| H3AsO4 | 1.82E-14 | 1.84E-14 | -13.736 |
| H3PO4 | 3.06E-07 | 3.09E-07 | -6.509 |
| HAsO3-2 | 4.11E-25 | 1.98E-25 | -24.703 |
| HAsO4-2 | 3.58E-18 | 1.73E-18 | -17.762 |
| HCO3- | 4.88E-07 | 4.06E-07 | -6.391 |
| HCrO4- | 3.64E-07 | 3.03E-07 | -6.518 |
| HF (aq) | 1.31E-08 | 1.32E-08 | -7.88 |
| HF2- | 2.59E-16 | 2.15E-16 | -15.667 |
| Hg(CO3)2-2 | 7.61E-36 | 3.67E-36 | -35.435 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(HS)2 (aq) | 1.83E-25 | 1.85E-25 | -24.732 |
| Hg(N3)2 (aq) | 2.25E-15 | 2.27E-15 | -14.644 |
| Hg(NH3)2+2 | 1.08E-24 | 5.21E-25 | -24.283 |
| Hg(NH3)4+2 | 2.34E-43 | 1.13E-43 | -42.948 |
| Hg(NO2)2 (aq) | 2.3E-124 | 2.3E-124 | -123.635 |
| Hg(NO2)3- | 3.3E-178 | 2.7E-178 | -177.563 |
| Hg(NO2)4-2 | 5E-233 | 2.4E-233 | -232.621 |
| Hg(NO3)2 (aq) | 5.8E-170 | 5.9E-170 | -169.232 |
| Hg(OH)2 | 2.88E-24 | 2.9E-24 | -23.537 |
| Hg(SO4)2-2 | 4.61E-25 | 2.23E-25 | -24.653 |
| Hg+2 | 8.96E-23 | 4.32E-23 | -22.364 |
| Hg2OH+3 | 1.65E-45 | 3.2E-46 | -45.495 |
| Hg3(OH)3+3 | 2.25E-66 | 4.37E-67 | -66.359 |
| HgCl+ | 2.6E-17 | 2.17E-17 | -16.663 |
| HgCl2 (aq) | 2.91E-12 | 2.94E-12 | -11.531 |
| HgCl3-1 | 6.2E-13 | 5.17E-13 | -12.286 |
| HgCl4-2 | 8.48E-14 | 4.09E-14 | -13.388 |
| HgClOH (aq) | 6.22E-18 | 6.28E-18 | -17.202 |
| HgCO3 (aq) | 2.06E-25 | 2.08E-25 | -24.683 |
| HgF+ | 8.4E-30 | 7E-30 | -29.155 |
| HgHCO3+ | 1E-23 | 8.33E-24 | -23.079 |
| HgHS2- | 2.98E-29 | 2.48E-29 | -28.606 |
| HgN3+ | 3.32E-11 | 2.77E-11 | -10.558 |
| HgNO2+ | 8.74E-73 | 7.29E-73 | -72.138 |
| HgNO3+ | 1.41E-96 | 1.18E-96 | -95.93 |
| HgOH+ | 6.42E-24 | 5.35E-24 | -23.272 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgOHCO3- | 1.21E-29 | 1.01E-29 | -28.996 |
| HgS2-2 | 4.15E-35 | 2E-35 | -34.699 |
| HgSO4 (aq) | 1.24E-23 | 1.26E-23 | -22.901 |
| HN3 (aq) | 2.83E-05 | 2.86E-05 | -4.544 |
| HNO2 (aq) | 1.15E-55 | 1.16E-55 | -54.935 |
| HPO4-2 | 5.27E-11 | 2.54E-11 | -10.594 |
| HS-1 | 6.42E-21 | 5.35E-21 | -20.271 |
| HSO4- | 0.000374 | 0.000311 | -3.507 |
| K+1 | 0.000148 | 0.000124 | -3.908 |
| K2HPO4 (aq) | 4.16E-18 | 4.2E-18 | -17.377 |
| K2PO4- | 1.2E-26 | 1E-26 | -26 |
| KCl (aq) | 1.15E-06 | 1.16E-06 | -5.937 |
| KCr2O7- | 5.34E-15 | 4.45E-15 | -14.352 |
| KCrO4- | 2.2E-14 | 1.83E-14 | -13.737 |
| KF (aq) | 2.43E-13 | 2.45E-13 | -12.61 |
| KH2PO4 (aq) | 1.92E-10 | 1.94E-10 | -9.713 |
| KHPO4- | 2.32E-14 | 1.93E-14 | -13.714 |
| KNO3 (aq) | 1.12E-77 | 1.13E-77 | -76.947 |
| KOH (aq) | 4.05E-16 | 4.09E-16 | -15.388 |
| KPO4-2 | 2.01E-23 | 9.7E-24 | -23.013 |
| KSO4- | 1.52E-06 | 1.26E-06 | -5.898 |
| Mg DOM1 | 3.98E-08 | 3.54E-08 | -7.451 |
| Mg(NH3)2+2 | 1.98E-23 | 9.54E-24 | -23.021 |
| Mg+2 | 0.002551 | 0.001231 | -2.91 |
| Mg2CO3+2 | 7.66E-17 | 3.69E-17 | -16.432 |
| MgCl+ | 9.82E-05 | 8.19E-05 | -4.087 |
| MgCO3 (aq) | 5.45E-15 | 5.5E-15 | -14.259 |
| MgF+ | 4.25E-10 | 3.54E-10 | -9.451 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHCO3+ | 5.83E-09 | 4.86E-09 | -8.314 |
| MgHPO4 (aq) | 1.65E-11 | 1.67E-11 | -10.777 |
| MgOH+ | 9.5E-13 | 7.92E-13 | -12.101 |
| MgPO4- | 2E-19 | 1.67E-19 | -18.778 |
| MgSO4 (aq) | 0.000354 | 0.000358 | -3.447 |
| Mn+3 | 5.1E-06 | 9.89E-07 | -6.005 |
| N3-1 | 2.76E-07 | 2.3E-07 | -6.639 |
| Na+1 | 0.00684 | 0.0057 | -2.244 |
| Na2HPO4 (aq) | 5.85E-15 | 5.9E-15 | -14.229 |
| Na2PO4- | 5.46E-23 | 4.55E-23 | -22.342 |
| NaCl (aq) | 5.59E-05 | 5.65E-05 | -4.248 |
| NaCO3- | 1.06E-15 | 8.85E-16 | -15.053 |
| NaCrO4- | 1.36E-12 | 1.13E-12 | -11.947 |
| NaF (aq) | 2.17E-11 | 2.19E-11 | -10.659 |
| NaH2PO4 (aq) | 8.86E-09 | 8.94E-09 | -8.049 |
| NaHCO3 (aq) | 1.36E-09 | 1.37E-09 | -8.862 |
| NaHPO4- | 1.66E-12 | 1.38E-12 | -11.86 |
| NaNO3 (aq) | 1.91E-76 | 1.93E-76 | -75.715 |
| NaOH (aq) | 1.28E-14 | 1.29E-14 | -13.888 |
| NaPO4-2 | 1.02E-21 | 4.94E-22 | -21.306 |
| NaSO4- | 6.42E-05 | 5.35E-05 | -4.272 |
| NH3 (aq) | 6.68E-11 | 6.74E-11 | -10.171 |
| NH4+1 | 0.000713 | 0.000594 | -3.226 |
| NH4Cr2O7- | 2.98E-14 | 2.49E-14 | -13.605 |
| NH4SO4- | 1.32E-05 | 1.1E-05 | -4.958 |
| Ni DOM1 | 1.27E-09 | 1.13E-09 | -8.947 |
| Ni(N3)2 (aq) | 8.08E-18 | 8.16E-18 | -17.088 |
| Ni(NH3)2+2 | 1.71E-21 | 8.23E-22 | -21.085 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)3+2 | 6.66E-30 | 3.22E-30 | -29.493 |
| Ni(NH3)4+2 | 7.72E-39 | 3.72E-39 | -38.429 |
| Ni(NH3)5+2 | 2.89E-48 | 1.39E-48 | -47.856 |
| Ni(NH3)6+2 | 2.3E-58 | 1.11E-58 | -57.955 |
| Ni(NO2)2 (aq) | 1.1E-115 | 1.1E-115 | -114.951 |
| Ni(OH)2 (aq) | 2.68E-20 | 2.71E-20 | -19.567 |
| Ni(OH)3- | 1.35E-28 | 1.13E-28 | -27.948 |
| Ni(SO4)2-2 | 6.43E-11 | 3.1E-11 | -10.509 |
| Ni+2 | 3.24E-06 | 1.56E-06 | -5.806 |
| NiCl+ | 1.2E-08 | 9.98E-09 | -8.001 |
| NiCl2 (aq) | 6.23E-12 | 6.29E-12 | -11.201 |
| NiCO3 (aq) | 3.61E-16 | 3.64E-16 | -15.439 |
| NiF+ | 1.47E-13 | 1.23E-13 | -12.911 |
| NiH2PO4+ | 1.25E-11 | 1.04E-11 | -10.983 |
| NiHCO3+ | 7.48E-11 | 6.23E-11 | -10.205 |
| NiHPO4 (aq) | 2.88E-14 | 2.91E-14 | -13.536 |
| NiHS+ | 3.1E-21 | 2.59E-21 | -20.587 |
| NiN3+ | 8.12E-12 | 6.77E-12 | -11.17 |
| NiNH3+2 | 1.43E-13 | 6.92E-14 | -13.16 |
| NiNO2+ | 1.53E-60 | 1.28E-60 | -59.894 |
| NiNO3+ | 5.65E-79 | 4.71E-79 | -78.327 |
| NiOH+ | 4.76E-14 | 3.97E-14 | -13.401 |
| NiSO4 (aq) | 4.94E-07 | 4.98E-07 | -6.303 |
| NO2-1 | 4.09E-56 | 3.41E-56 | -55.468 |
| NO3-1 | 1.44E-73 | 1.2E-73 | -72.921 |
| OH- | 2.29E-12 | 1.91E-12 | -11.72 |
| Pb DOM1 | 1.01E-09 | 8.99E-10 | -9.046 |
| Pb(CO3)2-2 | 1.11E-26 | 5.36E-27 | -26.271 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(HS)2 (aq) | 8.28E-34 | 8.36E-34 | -33.078 |
| Pb(HS)3- | 1.07E-52 | 8.93E-53 | -52.049 |
| Pb(NO2)2 (aq) | 2.3E-116 | 2.3E-116 | -115.631 |
| Pb(NO3)2 (aq) | 6.1E-153 | 6.2E-153 | -152.208 |
| Pb(OH)2 (aq) | 2.13E-20 | 2.16E-20 | -19.667 |
| Pb(OH)3- | 1.08E-28 | 8.97E-29 | -28.047 |
| Pb(SO4)2-2 | 2.87E-10 | 1.39E-10 | -9.858 |
| Pb+2 | 3.25E-08 | 1.57E-08 | -7.805 |
| Pb2OH+3 | 2.09E-19 | 4.06E-20 | -19.391 |
| Pb3(OH)4+2 | 5.91E-38 | 2.85E-38 | -37.545 |
| Pb4(OH)4+4 | 1.27E-41 | 6.89E-43 | -42.162 |
| PbCl+ | 1.07E-08 | 8.89E-09 | -8.051 |
| PbCl2 (aq) | 3.25E-10 | 3.28E-10 | -9.484 |
| PbCl3- | 5.53E-12 | 4.61E-12 | -11.336 |
| PbCl4-2 | 6.17E-14 | 2.98E-14 | -13.526 |
| PbCO3 (aq) | 3.29E-16 | 3.33E-16 | -15.478 |
| PbF+ | 1.15E-14 | 9.61E-15 | -14.017 |
| PbF2 (aq) | 5.09E-22 | 5.14E-22 | -21.289 |
| PbH2PO4+ | 4.67E-13 | 3.89E-13 | -12.41 |
| PbHCO3+ | 4.83E-12 | 4.03E-12 | -11.395 |
| PbHPO4 (aq) | 4.03E-16 | 4.07E-16 | -15.391 |
| PbNO2+ | 2.07E-61 | 1.73E-61 | -60.763 |
| PbNO3+ | 3.43E-80 | 2.85E-80 | -79.544 |
| PbOH+ | 1.41E-13 | 1.17E-13 | -12.931 |
| PbSO4 (aq) | 1.32E-08 | 1.33E-08 | -7.877 |
| PO4-3 | 1.86E-20 | 3.6E-21 | -20.444 |
| S-2 | 9.16E-36 | 4.42E-36 | -35.355 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| SO4-2 | 0.00359 | 0.001732 | -2.761 |
| Zn DOM1 | 1.19E-08 | 1.06E-08 | -7.976 |
| Zn(CO3)2-2 | 1.5E-26 | 7.24E-27 | -26.141 |
| Zn(N3)2 (aq) | 4.6E-17 | 4.65E-17 | -16.333 |
| Zn(N3)3- | 7.33E-23 | 6.11E-23 | -22.214 |
| Zn(NH3)2+2 | 3.8E-21 | 1.84E-21 | -20.736 |
| Zn(NH3)3+2 | 7.55E-29 | 3.64E-29 | -28.439 |
| Zn(NH3)4+2 | 7.34E-37 | 3.54E-37 | -36.451 |
| Zn(NO2)2 (aq) | 1.7E-115 | 1.7E-115 | -114.771 |
| Zn(NO3)2 (aq) | 6.6E-152 | 6.6E-152 | -151.178 |
| Zn(OH)2 (aq) | 1.99E-17 | 2.01E-17 | -16.696 |
| Zn(OH)3- | 3.18E-26 | 2.65E-26 | -25.577 |
| Zn(OH)4-2 | 3.62E-36 | 1.75E-36 | -35.758 |
| Zn(SO4)2-2 | 1.09E-07 | 5.27E-08 | -7.278 |
| Zn+2 | 1.91E-05 | 9.22E-06 | -5.035 |
| Zn2OH+3 | 7.47E-17 | 1.45E-17 | -16.839 |
| Zn2S3-2 | 4.29E-63 | 2.07E-63 | -62.684 |
| Zn4S6-4 | 1.3E-123 | 7.3E-125 | -124.137 |
| ZnCl+ | 5.23E-07 | 4.36E-07 | -6.361 |
| ZnCl2 (aq) | 4.89E-09 | 4.93E-09 | -8.307 |
| ZnCl3- | 1.1E-10 | 9.2E-11 | -10.036 |
| ZnCl4-2 | 1.55E-12 | 7.5E-13 | -12.125 |
| ZnCO3 (aq) | 3.3E-15 | 3.33E-15 | -14.478 |
| ZnF+ | 8.23E-13 | 6.86E-13 | -12.164 |
| ZnHCO3+ | 1.13E-10 | 9.43E-11 | -10.026 |
| ZnHPO4 (aq) | 3.89E-13 | 3.93E-13 | -12.406 |
| ZnN3+ | 3.66E-11 | 3.05E-11 | -10.516 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnNH3+2 | 2.44E-13 | 1.18E-13 | -12.93 |
| ZnNO2+ | 2.27E-60 | 1.89E-60 | -59.723 |
| ZnNO3+ | 3.55E-78 | 2.96E-78 | -77.528 |
| ZnOH+ | 2.11E-12 | 1.76E-12 | -11.755 |
| ZnS (aq) | 7.52E-25 | 7.59E-25 | -24.12 |
| ZnSO4 (aq) | 3.17E-06 | 3.2E-06 | -5.494 |

## D1.3: Eh 250

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 8.77E-06 | 8.71E-06 | -5.06 |
| Al(OH)2+ | 2.85E-10 | 2.37E-10 | -9.625 |
| Al(OH)3 (aq) | 1.83E-14 | 1.85E-14 | -13.733 |
| Al(OH)4- | 4.1E-18 | 3.42E-18 | -17.466 |
| Al(SO4)2- | 0.000134 | 0.000112 | -3.952 |
| Al+3 | 0.000782 | 0.000152 | -3.819 |
| Al2(OH)2+4 | 5.17E-10 | 2.8E-11 | -10.553 |
| Al2(OH)2CO3+2 | 1.04E-12 | 5.04E-13 | -12.298 |
| Al2PO4+3 | 4.08E-09 | 7.92E-10 | -9.101 |
| Al3(OH)4+5 | 1.77E-14 | 1.86E-16 | -15.732 |
| AlCl+2 | 2.26E-06 | 1.09E-06 | -5.962 |
| AlF+2 | 1.31E-05 | 6.33E-06 | -5.199 |
| AlF2+ | 1.31E-08 | 1.09E-08 | -7.963 |
| AlF3 (aq) | 5.47E-13 | 5.52E-13 | -12.258 |
| AlF4- | 1.44E-18 | 1.2E-18 | -17.92 |
| AlHPO4+ | 1.62E-07 | 1.35E-07 | -6.869 |
| AlOH+2 | 6.71E-07 | 3.24E-07 | -6.49 |
| AlSO4+ | 0.001838 | 0.001532 | -2.815 |
| As3S4(HS)- | 6.2E-124 | 5.1E-124 | -123.288 |
| AsO4-3 | 2.54E-25 | 4.93E-26 | -25.307 |
| AsS(OH)HS- | 4.58E-46 | 3.81E-46 | -45.419 |
| Ca DOM1 | 3.9E-07 | 3.47E-07 | -6.459 |
| Ca(NH3)2+2 | 3.89E-23 | 1.88E-23 | -22.727 |
| Ca(NO3)2 | 5.3E-140 | 5.4E-140 | -139.268 |
| Ca+2 | 0.002503 | 0.001208 | -2.918 |
| CaCl+ | 6.08E-05 | 5.07E-05 | -4.295 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCO3 (aq) | 1.07E-14 | 1.08E-14 | -13.966 |
| CaCrO4 (aq) | 2.81E-11 | 2.84E-11 | -10.547 |
| CaF+ | 7.14E-11 | 5.95E-11 | -10.225 |
| CaH2PO4+ | 2.77E-08 | 2.31E-08 | -7.636 |
| CaHCO3+ | 6.21E-09 | 5.18E-09 | -8.286 |
| CaHPO4 (aq) | 1.18E-11 | 1.19E-11 | -10.925 |
| CaNH3+2 | 5.61E-13 | 2.71E-13 | -12.567 |
| CaNO3+ | 5.88E-69 | 4.9E-69 | -68.31 |
| CaOH+ | 4.91E-14 | 4.09E-14 | -13.388 |
| CaPO4- | 1.25E-17 | 1.05E-17 | -16.981 |
| CaSO4 (aq) | 0.00043 | 0.000434 | -3.363 |
| Cd DOM1 | 2.07E-12 | 1.84E-12 | -11.734 |
| Cd(CO3)2-2 | 3.53E-30 | 1.7E-30 | -29.769 |
| Cd(HS)2 (aq) | 1.5E-48 | 1.52E-48 | -47.819 |
| Cd(HS)3- | 6.2E-74 | 5.17E-74 | -73.287 |
| Cd(HS)4-2 | 9.2E-99 | 4.4E-99 | -98.354 |
| Cd(NH3)2+2 | 1.28E-24 | 6.16E-25 | -24.21 |
| Cd(NH3)3+2 | 2.23E-33 | 1.07E-33 | -32.969 |
| Cd(NH3)4+2 | 1.14E-42 | 5.52E-43 | -42.258 |
| Cd(NO2)2 (aq) | 4E-106 | 4.1E-106 | -105.391 |
| Cd(NO3)2 (aq) | 5.7E-141 | 5.7E-141 | -140.243 |
| Cd(OH)2 (aq) | 2.19E-24 | 2.22E-24 | -23.655 |
| Cd(OH)3- | 1.08E-34 | 9.03E-35 | -34.044 |
| Cd(OH)4-2 | 7.96E-46 | 3.84E-46 | -45.416 |
| Cd(SO4)2-2 | 5.02E-11 | 2.42E-11 | -10.616 |
| Cd+2 | 5.29E-09 | 2.55E-09 | -8.593 |
| Cd2OH+3 | 2.93E-24 | 5.68E-25 | -24.246 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl+ | 5.02E-09 | 4.19E-09 | -8.378 |
| CdCl2 (aq) | 2.95E-10 | 2.97E-10 | -9.527 |
| CdCO3 (aq) | 3.71E-19 | 3.75E-19 | -18.426 |
| CdF+ | 1.97E-16 | 1.64E-16 | -15.786 |
| CdHCO3+ | 3.14E-14 | 2.61E-14 | -13.583 |
| CdHPO4 (aq) | 2.64E-16 | 2.67E-16 | -15.574 |
| CdHS+ | 1.69E-28 | 1.41E-28 | -27.851 |
| CdNH3+2 | 1.52E-16 | 7.31E-17 | -16.136 |
| CdNO2+ | 1.85E-57 | 1.55E-57 | -56.811 |
| CdNO3+ | 1.54E-74 | 1.29E-74 | -73.891 |
| CdOH+ | 4.7E-17 | 3.92E-17 | -16.407 |
| CdSO4 (aq) | 9.08E-10 | 9.17E-10 | -9.038 |
| Cl-1 | 0.021205 | 0.017673 | -1.753 |
| CO3-2 | 1.3E-14 | 6.27E-15 | -14.203 |
| Cr2O7-2 | 8.64E-12 | 4.17E-12 | -11.38 |
| CrO3Cl- | 1.01E-10 | 8.39E-11 | -10.076 |
| CrO3H2PO4- | 1.36E-12 | 1.13E-12 | -11.946 |
| CrO3HPO4-2 | 2.02E-12 | 9.72E-13 | -12.012 |
| CrO3SO4-2 | 8.25E-10 | 3.98E-10 | -9.4 |
| CrO4-2 | 8.27E-11 | 3.99E-11 | -10.399 |
| Cu DOM1 | 8.17E-10 | 7.27E-10 | -9.139 |
| Cu(CO3)2-2 | 3.26E-26 | 1.57E-26 | -25.803 |
| Cu(N3)2 (aq) | 4.48E-17 | 4.52E-17 | -16.345 |
| Cu(N3)3- | 6.25E-22 | 5.21E-22 | -21.284 |
| Cu(N3)4-2 | 6.52E-28 | 3.15E-28 | -27.502 |
| Cu(NH3)2+2 | 1.08E-20 | 5.22E-21 | -20.282 |
| Cu(NH3)3+2 | 6.18E-28 | 2.98E-28 | -27.525 |
| Cu(NH3)4+2 | 7.3E-36 | 3.52E-36 | -35.453 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO2)2 (aq) | 9.7E-106 | 9.8E-106 | -105.008 |
| Cu(NO3)2 (aq) | 1.4E-140 | 1.4E-140 | -139.847 |
| Cu(OH)2 (aq) | 6.84E-20 | 6.9E-20 | -19.161 |
| Cu(OH)3- | 4.91E-27 | 4.09E-27 | -26.388 |
| Cu(OH)4-2 | 2.34E-38 | 1.13E-38 | -37.947 |
| Cu+2 | 5.24E-08 | 2.53E-08 | -7.598 |
| Cu2(OH)2+2 | 2.59E-21 | 1.25E-21 | -20.903 |
| Cu2OH+3 | 1.82E-19 | 3.52E-20 | -19.453 |
| Cu2S3-2 | 5.23E-92 | 2.52E-92 | -91.598 |
| Cu3(OH)4+2 | 3.59E-34 | 1.73E-34 | -33.761 |
| CuCl+ | 9.51E-10 | 7.93E-10 | -9.101 |
| CuCl2 (aq) | 2.31E-12 | 2.34E-12 | -11.632 |
| CuCl3- | 3.85E-16 | 3.21E-16 | -15.494 |
| CuCl4-2 1 | 8.32E-20 | 4.02E-20 | -19.396 |
| CuCO3 (aq) | 9.24E-16 | 9.33E-16 | -15.03 |
| CuF+ | 5.5E-15 | 4.59E-15 | -14.339 |
| CuHCO3+ | 6.18E-13 | 5.15E-13 | -12.288 |
| CuHPO4 (aq) | 6.88E-15 | 6.95E-15 | -14.158 |
| CuHSO4+ | 2.78E-11 | 2.31E-11 | -10.636 |
| CuN3+ | 5.05E-12 | 4.2E-12 | -11.376 |
| CuNH3+2 | 4.95E-14 | 2.39E-14 | -13.622 |
| CuNO2+ | 1.91E-56 | 1.59E-56 | -55.798 |
| CuNO3+ | 1.21E-73 | 1.01E-73 | -72.998 |
| CuOH+ | 2.42E-13 | 2.01E-13 | -12.696 |
| CuS(aq) | 8.86E-36 | 8.94E-36 | -35.049 |
| CuSO4 (aq) | 8.79E-09 | 8.87E-09 | -8.052 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.473 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| DOM1 | 7.76E-06 | 1.86E-06 | -5.73 |
| F-1 | 5.21E-09 | 4.34E-09 | -8.362 |
| Fe DOM1 | 2.05E-11 | 2.04E-11 | -10.691 |
| Fe(N3)2+ | 2.7E-17 | 2.25E-17 | -16.648 |
| Fe(N3)3 (aq) | 1.1E-21 | 1.11E-21 | -20.956 |
| Fe(NH3)2+2 | 1.93E-21 | 9.31E-22 | -21.031 |
| Fe(NH3)3+2 | 3.97E-31 | 1.91E-31 | -30.718 |
| Fe(NH3)4+2 | 3.48E-41 | 1.68E-41 | -40.775 |
| Fe(NO2)2+ | 2.6E-108 | 2.1E-108 | -107.671 |
| Fe(NO2)3 (aq) | 1.5E-156 | 1.5E-156 | -155.831 |
| Fe(OH)2 (aq) | 9.46E-20 | 9.56E-20 | -19.02 |
| Fe(OH)2+ | 2.41E-13 | 2.01E-13 | -12.697 |
| Fe(OH)3- | 1.37E-27 | 1.14E-27 | -26.942 |
| Fe(OH)3 (aq) | 2.74E-20 | 2.76E-20 | -19.559 |
| Fe(OH)4- | 8.98E-26 | 7.49E-26 | -25.126 |
| Fe(SO4)2- | 7.4E-13 | 6.17E-13 | -12.21 |
| Fe+2 | 0.001929 | 0.000931 | -3.031 |
| Fe+3 | 5.78E-12 | 1.12E-12 | -11.95 |
| Fe2(OH)2+4 | 2.3E-21 | 1.25E-22 | -21.904 |
| Fe3(OH)4+5 | 8.11E-31 | 8.52E-33 | -32.069 |
| FeCl+ | 1.25E-05 | 1.04E-05 | -4.984 |
| FeCl+2 | 8.99E-13 | 4.34E-13 | -12.363 |
| FeCrO4+ | 1.97E-15 | 1.64E-15 | -14.784 |
| FeF+ | 7.87E-11 | 6.56E-11 | -10.183 |
| FeF+2 | 9.63E-15 | 4.65E-15 | -14.333 |
| FeF2+ | 9.16E-19 | 7.63E-19 | -18.117 |
| FeF3 (aq) | 3.04E-24 | 3.07E-24 | -23.512 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeH2PO4+ | 4.4E-07 | 3.67E-07 | -6.436 |
| FeH2PO4+2 | 3.46E-14 | 1.67E-14 | -13.777 |
| FeHCO3+ | 4.54E-09 | 3.79E-09 | -8.422 |
| FeHPO4 (aq) | 7.57E-11 | 7.64E-11 | -10.117 |
| FeHPO4+ | 3.46E-13 | 2.88E-13 | -12.54 |
| FeHS+ | 2.51E-25 | 2.09E-25 | -24.679 |
| FeN3+2 | 8.33E-14 | 4.02E-14 | -13.396 |
| FeNH3+2 | 3.7E-12 | 1.78E-12 | -11.749 |
| FeNO2+2 | 2.22E-59 | 1.07E-59 | -58.971 |
| FeOH+ | 8.47E-11 | 7.06E-11 | -10.151 |
| FeOH+2 | 6.46E-12 | 3.12E-12 | -11.506 |
| FeSO4 (aq) | 0.00035 | 0.000354 | -3.451 |
| FeSO4+ | 2.92E-11 | 2.44E-11 | -10.614 |
| H DOM1 | 1.17E-05 | 6.49E-06 | -5.188 |
| H+1 | 0.002899 | 0.002416 | -2.617 |
| H2AsO3- | 1.13E-13 | 9.41E-14 | -13.026 |
| H2AsO4- | 2.87E-12 | 2.39E-12 | -11.622 |
| H2CO3* (aq) | 0.002552 | 0.002577 | -2.589 |
| H2CrO4 (aq) | 2.73E-10 | 2.76E-10 | -9.56 |
| H2PO4- | 1.21E-06 | 1.01E-06 | -5.995 |
| H2S (aq) | 1.88E-23 | 1.9E-23 | -22.722 |
| H3AsO3 | 4.91E-07 | 4.95E-07 | -6.305 |
| H3AsO4 | 1.02E-12 | 1.03E-12 | -11.987 |
| H3PO4 | 3.06E-07 | 3.09E-07 | -6.509 |
| HAsO3-2 | 4.11E-25 | 1.98E-25 | -24.703 |
| HAsO4-2 | 2.01E-16 | 9.7E-17 | -16.013 |
| HCO3- | 4.88E-07 | 4.06E-07 | -6.391 |
| HCrO4- | 3.64E-07 | 3.03E-07 | -6.518 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HF (aq) | 1.31E-08 | 1.32E-08 | -7.88 |
| HF2- | 2.59E-16 | 2.15E-16 | -15.667 |
| Hg(CO3)2-2 | 1.03E-34 | 4.97E-35 | -34.303 |
| Hg(HS)2 (aq) | 2.53E-38 | 2.55E-38 | -37.594 |
| Hg(N3)2 (aq) | 3.05E-14 | 3.08E-14 | -13.512 |
| Hg(NH3)2+2 | 1.46E-23 | 7.05E-24 | -23.152 |
| Hg(NH3)4+2 | 3.16E-42 | 1.53E-42 | -41.816 |
| Hg(NO2)2 (aq) | 9.7E-113 | 9.8E-113 | -112.009 |
| Hg(NO2)3- | 2.5E-161 | 2E-161 | -160.689 |
| Hg(NO2)4-2 | 6.6E-211 | 3.2E-211 | -210.5 |
| Hg(NO3)2 (aq) | 7.7E-155 | 7.8E-155 | -154.108 |
| Hg(OH)2 | 3.9E-23 | 3.93E-23 | -22.405 |
| Hg(SO4)2-2 | 6.25E-24 | 3.01E-24 | -23.521 |
| Hg+2 | 1.21E-21 | 5.85E-22 | -21.233 |
| Hg2OH+3 | 3.03E-43 | 5.87E-44 | -43.231 |
| Hg3(OH)3+3 | 5.6E-63 | 1.09E-63 | -62.964 |
| HgCl+ | 3.53E-16 | 2.94E-16 | -15.532 |
| HgCl2 (aq) | 3.95E-11 | 3.99E-11 | -10.4 |
| HgCl3-1 | 8.4E-12 | 7E-12 | -11.155 |
| HgCl4-2 | 1.15E-12 | 5.54E-13 | -12.256 |
| HgClOH (aq) | 8.42E-17 | 8.5E-17 | -16.071 |
| HgCO3 (aq) | 2.79E-24 | 2.81E-24 | -23.551 |
| HgF+ | 1.14E-28 | 9.49E-29 | -28.023 |
| HgHCO3+ | 1.35E-22 | 1.13E-22 | -21.948 |
| HgHS2- | 4.1E-42 | 3.41E-42 | -41.467 |
| HgN3+ | 4.49E-10 | 3.75E-10 | -9.426 |
| HgNO2+ | 2.09E-66 | 1.74E-66 | -65.758 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgNO3+ | 1.89E-88 | 1.58E-88 | -87.802 |
| HgOH+ | 8.7E-23 | 7.25E-23 | -22.14 |
| HgOHCO3- | 1.64E-28 | 1.37E-28 | -27.864 |
| HgS2-2 | 5.71E-48 | 2.76E-48 | -47.56 |
| HgSO4 (aq) | 1.68E-22 | 1.7E-22 | -21.769 |
| HN3 (aq) | 2.83E-05 | 2.86E-05 | -4.544 |
| HNO2 (aq) | 2.03E-50 | 2.05E-50 | -49.687 |
| HPO4-2 | 5.27E-11 | 2.54E-11 | -10.594 |
| HS-1 | 6.48E-28 | 5.4E-28 | -27.268 |
| HSO4- | 0.000374 | 0.000311 | -3.507 |
| K+1 | 0.000148 | 0.000124 | -3.908 |
| K2HPO4 (aq) | 4.16E-18 | 4.2E-18 | -17.377 |
| K2PO4- | 1.2E-26 | 1E-26 | -26 |
| KCl (aq) | 1.15E-06 | 1.16E-06 | -5.937 |
| KCr2O7- | 5.34E-15 | 4.45E-15 | -14.352 |
| KCrO4- | 2.2E-14 | 1.83E-14 | -13.737 |
| KF (aq) | 2.43E-13 | 2.45E-13 | -12.61 |
| KH2PO4 (aq) | 1.92E-10 | 1.94E-10 | -9.713 |
| KHPO4- | 2.32E-14 | 1.93E-14 | -13.714 |
| KNO3 (aq) | 1.11E-70 | 1.12E-70 | -69.95 |
| KOH (aq) | 4.05E-16 | 4.09E-16 | -15.388 |
| KPO4-2 | 2.01E-23 | 9.7E-24 | -23.013 |
| KSO4- | 1.52E-06 | 1.26E-06 | -5.898 |
| Mg DOM1 | 3.98E-08 | 3.54E-08 | -7.451 |
| Mg(NH3)2+2 | 1.98E-23 | 9.54E-24 | -23.021 |
| Mg+2 | 0.002551 | 0.001231 | -2.91 |
| Mg2CO3+2 | 7.66E-17 | 3.69E-17 | -16.432 |
| MgCl+ | 9.82E-05 | 8.19E-05 | -4.087 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgCO3 (aq) | 5.45E-15 | 5.5E-15 | -14.259 |
| MgF+ | 4.25E-10 | 3.54E-10 | -9.451 |
| MgHCO3+ | 5.83E-09 | 4.86E-09 | -8.314 |
| MgHPO4 (aq) | 1.65E-11 | 1.67E-11 | -10.777 |
| MgOH+ | 9.5E-13 | 7.92E-13 | -12.101 |
| MgPO4- | 2E-19 | 1.67E-19 | -18.778 |
| MgSO4 (aq) | 0.000354 | 0.000358 | -3.447 |
| Mn+3 | 5.1E-06 | 9.89E-07 | -6.005 |
| N3-1 | 2.76E-07 | 2.3E-07 | -6.639 |
| Na+1 | 0.00684 | 0.0057 | -2.244 |
| Na2HPO4 (aq) | 5.85E-15 | 5.9E-15 | -14.229 |
| Na2PO4- | 5.46E-23 | 4.55E-23 | -22.342 |
| NaCl (aq) | 5.59E-05 | 5.65E-05 | -4.248 |
| NaCO3- | 1.06E-15 | 8.85E-16 | -15.053 |
| NaCrO4- | 1.36E-12 | 1.13E-12 | -11.947 |
| NaF (aq) | 2.17E-11 | 2.19E-11 | -10.659 |
| NaH2PO4 (aq) | 8.86E-09 | 8.94E-09 | -8.049 |
| NaHCO3 (aq) | 1.36E-09 | 1.37E-09 | -8.862 |
| NaHPO4- | 1.66E-12 | 1.38E-12 | -11.86 |
| NaNO3 (aq) | 1.89E-69 | 1.91E-69 | -68.719 |
| NaOH (aq) | 1.28E-14 | 1.29E-14 | -13.888 |
| NaPO4-2 | 1.02E-21 | 4.94E-22 | -21.306 |
| NaSO4- | 6.42E-05 | 5.35E-05 | -4.272 |
| NH3 (aq) | 6.68E-11 | 6.74E-11 | -10.171 |
| NH4+1 | 0.000713 | 0.000594 | -3.226 |
| NH4Cr2O7- | 2.98E-14 | 2.49E-14 | -13.605 |
| NH4SO4- | 1.32E-05 | 1.1E-05 | -4.958 |
| Ni DOM1 | 1.27E-09 | 1.13E-09 | -8.947 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(N3)2 (aq) | 8.08E-18 | 8.16E-18 | -17.088 |
| Ni(NH3)2+2 | 1.71E-21 | 8.23E-22 | -21.085 |
| Ni(NH3)3+2 | 6.66E-30 | 3.22E-30 | -29.493 |
| Ni(NH3)4+2 | 7.72E-39 | 3.72E-39 | -38.429 |
| Ni(NH3)5+2 | 2.89E-48 | 1.39E-48 | -47.856 |
| Ni(NH3)6+2 | 2.3E-58 | 1.11E-58 | -57.955 |
| Ni(NO2)2 (aq) | 3.5E-105 | 3.5E-105 | -104.457 |
| Ni(OH)2 (aq) | 2.68E-20 | 2.71E-20 | -19.567 |
| Ni(OH)3- | 1.35E-28 | 1.13E-28 | -27.948 |
| Ni(SO4)2-2 | 6.43E-11 | 3.1E-11 | -10.509 |
| Ni+2 | 3.24E-06 | 1.56E-06 | -5.806 |
| NiCl+ | 1.2E-08 | 9.98E-09 | -8.001 |
| NiCl2 (aq) | 6.23E-12 | 6.29E-12 | -11.201 |
| NiCO3 (aq) | 3.61E-16 | 3.64E-16 | -15.439 |
| NiF+ | 1.47E-13 | 1.23E-13 | -12.911 |
| NiH2PO4+ | 1.25E-11 | 1.04E-11 | -10.983 |
| NiHCO3+ | 7.48E-11 | 6.23E-11 | -10.205 |
| NiHPO4 (aq) | 2.88E-14 | 2.91E-14 | -13.536 |
| NiHS+ | 3.13E-28 | 2.61E-28 | -27.584 |
| NiN3+ | 8.12E-12 | 6.77E-12 | -11.17 |
| NiNH3+2 | 1.43E-13 | 6.92E-14 | -13.16 |
| NiNO2+ | 2.71E-55 | 2.26E-55 | -54.646 |
| NiNO3+ | 5.6E-72 | 4.67E-72 | -71.331 |
| NiOH+ | 4.76E-14 | 3.97E-14 | -13.401 |
| NiSO4 (aq) | 4.94E-07 | 4.98E-07 | -6.303 |
| NO2-1 | 7.22E-51 | 6.02E-51 | -50.22 |
| NO3-1 | 1.43E-66 | 1.19E-66 | -65.925 |
| OH- | 2.29E-12 | 1.91E-12 | -11.72 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb DOM1 | 1.01E-09 | 8.99E-10 | -9.046 |
| Pb(CO3)2-2 | 1.11E-26 | 5.36E-27 | -26.271 |
| Pb(HS)2 (aq) | 8.41E-48 | 8.5E-48 | -47.071 |
| Pb(HS)3- | 1.1E-73 | 9.15E-74 | -73.039 |
| Pb(NO2)2 (aq) | 7.2E-106 | 7.3E-106 | -105.136 |
| Pb(NO3)2 (aq) | 6E-139 | 6.1E-139 | -138.215 |
| Pb(OH)2 (aq) | 2.13E-20 | 2.16E-20 | -19.667 |
| Pb(OH)3- | 1.08E-28 | 8.97E-29 | -28.047 |
| Pb(SO4)2-2 | 2.87E-10 | 1.39E-10 | -9.858 |
| Pb+2 | 3.25E-08 | 1.57E-08 | -7.805 |
| Pb2OH+3 | 2.09E-19 | 4.06E-20 | -19.391 |
| Pb3(OH)4+2 | 5.91E-38 | 2.85E-38 | -37.545 |
| Pb4(OH)4+4 | 1.27E-41 | 6.89E-43 | -42.162 |
| PbCl+ | 1.07E-08 | 8.89E-09 | -8.051 |
| PbCl2 (aq) | 3.25E-10 | 3.28E-10 | -9.484 |
| PbCl3- | 5.53E-12 | 4.61E-12 | -11.336 |
| PbCl4-2 | 6.17E-14 | 2.98E-14 | -13.526 |
| PbCO3 (aq) | 3.29E-16 | 3.33E-16 | -15.478 |
| PbF+ | 1.15E-14 | 9.61E-15 | -14.017 |
| PbF2 (aq) | 5.09E-22 | 5.14E-22 | -21.289 |
| PbH2PO4+ | 4.67E-13 | 3.89E-13 | -12.41 |
| PbHCO3+ | 4.83E-12 | 4.03E-12 | -11.395 |
| PbHPO4 (aq) | 4.03E-16 | 4.07E-16 | -15.391 |
| PbNO2+ | 3.66E-56 | 3.05E-56 | -55.516 |
| PbNO3+ | 3.4E-73 | 2.83E-73 | -72.548 |
| PbOH+ | 1.41E-13 | 1.17E-13 | -12.931 |
| PbSO4 (aq) | 1.32E-08 | 1.33E-08 | -7.877 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| PO4-3 | 1.86E-20 | 3.6E-21 | -20.444 |
| S-2 | 9.23E-43 | 4.45E-43 | -42.351 |
| SO4-2 | 0.00359 | 0.001732 | -2.761 |
| Zn DOM1 | 1.19E-08 | 1.06E-08 | -7.976 |
| Zn(CO3)2-2 | 1.5E-26 | 7.24E-27 | -26.141 |
| Zn(N3)2 (aq) | 4.6E-17 | 4.65E-17 | -16.333 |
| Zn(N3)3- | 7.33E-23 | 6.11E-23 | -22.214 |
| Zn(NH3)2+2 | 3.8E-21 | 1.84E-21 | -20.736 |
| Zn(NH3)3+2 | 7.55E-29 | 3.64E-29 | -28.439 |
| Zn(NH3)4+2 | 7.34E-37 | 3.54E-37 | -36.451 |
| Zn(NO2)2 (aq) | 5.2E-105 | 5.3E-105 | -104.276 |
| Zn(NO3)2 (aq) | 6.5E-138 | 6.5E-138 | -137.185 |
| Zn(OH)2 (aq) | 1.99E-17 | 2.01E-17 | -16.696 |
| Zn(OH)3- | 3.18E-26 | 2.65E-26 | -25.577 |
| Zn(OH)4-2 | 3.62E-36 | 1.75E-36 | -35.758 |
| Zn(SO4)2-2 | 1.09E-07 | 5.27E-08 | -7.278 |
| Zn+2 | 1.91E-05 | 9.22E-06 | -5.035 |
| Zn2OH+3 | 7.47E-17 | 1.45E-17 | -16.839 |
| Zn2S3-2 | 4.4E-84 | 2.12E-84 | -83.673 |
| Zn4S6-4 | 1.4E-165 | 7.7E-167 | -166.116 |
| ZnCl+ | 5.23E-07 | 4.36E-07 | -6.361 |
| ZnCl2 (aq) | 4.89E-09 | 4.93E-09 | -8.307 |
| ZnCl3- | 1.1E-10 | 9.2E-11 | -10.036 |
| ZnCl4-2 | 1.55E-12 | 7.5E-13 | -12.125 |
| ZnCO3 (aq) | 3.3E-15 | 3.33E-15 | -14.478 |
| ZnF+ | 8.23E-13 | 6.86E-13 | -12.164 |
| ZnHCO3+ | 1.13E-10 | 9.43E-11 | -10.026 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnHPO4 (aq) | 3.89E-13 | 3.93E-13 | -12.406 |
| ZnN3+ | 3.66E-11 | 3.05E-11 | -10.516 |
| ZnNH3+2 | 2.44E-13 | 1.18E-13 | -12.93 |
| ZnNO2+ | 4.01E-55 | 3.35E-55 | -54.476 |
| ZnNO3+ | 3.53E-71 | 2.94E-71 | -70.532 |
| ZnOH+ | 2.11E-12 | 1.76E-12 | -11.755 |
| ZnS (aq) | 7.58E-32 | 7.66E-32 | -31.116 |
| ZnSO4 (aq) | 3.17E-06 | 3.2E-06 | -5.494 |

## D1.4: Eh 300

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Al DOM1 | 8.77E-06 | 8.71E-06 | -5.06 |
| Al(OH)2+ | 2.85E-10 | 2.37E-10 | -9.625 |
| Al(OH)3 (aq) | 1.83E-14 | 1.85E-14 | -13.733 |
| Al(OH)4- | 4.1E-18 | 3.42E-18 | -17.466 |
| Al(SO4)2- | 0.000134 | 0.000112 | -3.952 |
| Al+3 | 0.000782 | 0.000152 | -3.819 |
| Al2(OH)2+4 | 5.17E-10 | 2.8E-11 | -10.553 |
| Al2(OH)2CO3+2 | 1.04E-12 | 5.04E-13 | -12.298 |
| Al2PO4+3 | 4.08E-09 | 7.92E-10 | -9.101 |
| Al3(OH)4+5 | 1.77E-14 | 1.86E-16 | -15.732 |
| AlCl+2 | 2.26E-06 | 1.09E-06 | -5.962 |
| AlF+2 | 1.31E-05 | 6.33E-06 | -5.199 |
| AlF2+ | 1.31E-08 | 1.09E-08 | -7.963 |
| AlF3 (aq) | 5.47E-13 | 5.52E-13 | -12.258 |
| AlF4- | 1.44E-18 | 1.2E-18 | -17.92 |
| AlHPO4+ | 1.62E-07 | 1.35E-07 | -6.869 |
| AlOH+2 | 6.71E-07 | 3.24E-07 | -6.49 |
| AlSO4+ | 0.001838 | 0.001532 | -2.815 |
| As3S4(HS)- | 6.5E-166 | 5.4E-166 | -165.268 |
| AsO4-3 | 1.43E-23 | 2.77E-24 | -23.558 |
| AsS(OH)HS- | 4.65E-60 | 3.88E-60 | -59.412 |
| Ca DOM1 | 3.9E-07 | 3.47E-07 | -6.459 |
| Ca(NH3)2+2 | 3.89E-23 | 1.88E-23 | -22.727 |
| Ca(NO3)2 | 5.3E-126 | 5.3E-126 | -125.275 |
| Ca+2 | 0.002503 | 0.001208 | -2.918 |
| CaCl+ | 6.08E-05 | 5.07E-05 | -4.295 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CaCO3 (aq) | 1.07E-14 | 1.08E-14 | -13.966 |
| CaCrO4 (aq) | 2.81E-11 | 2.84E-11 | -10.547 |
| CaF+ | 7.14E-11 | 5.95E-11 | -10.225 |
| CaH2PO4+ | 2.77E-08 | 2.31E-08 | -7.636 |
| CaHCO3+ | 6.21E-09 | 5.18E-09 | -8.286 |
| CaHPO4 (aq) | 1.18E-11 | 1.19E-11 | -10.925 |
| CaNH3+2 | 5.61E-13 | 2.71E-13 | -12.567 |
| CaNO3+ | 5.83E-62 | 4.86E-62 | -61.314 |
| CaOH+ | 4.91E-14 | 4.09E-14 | -13.388 |
| CaPO4- | 1.25E-17 | 1.05E-17 | -16.981 |
| CaSO4 (aq) | 0.00043 | 0.000434 | -3.363 |
| Cd DOM1 | 2.07E-12 | 1.84E-12 | -11.734 |
| Cd(CO3)2-2 | 3.53E-30 | 1.7E-30 | -29.769 |
| Cd(HS)2 (aq) | 1.53E-62 | 1.54E-62 | -61.812 |
| Cd(HS)3- | 6.36E-95 | 5.3E-95 | -94.276 |
| Cd(HS)4-2 | 9.5E-127 | 4.6E-127 | -126.34 |
| Cd(NH3)2+2 | 1.28E-24 | 6.16E-25 | -24.21 |
| Cd(NH3)3+2 | 2.23E-33 | 1.07E-33 | -32.969 |
| Cd(NH3)4+2 | 1.14E-42 | 5.52E-43 | -42.258 |
| Cd(NO2)2 (aq) | 1.26E-95 | 1.27E-95 | -94.896 |
| Cd(NO3)2 (aq) | 5.6E-127 | 5.6E-127 | -126.25 |
| Cd(OH)2 (aq) | 2.19E-24 | 2.22E-24 | -23.655 |
| Cd(OH)3- | 1.08E-34 | 9.03E-35 | -34.044 |
| Cd(OH)4-2 | 7.96E-46 | 3.84E-46 | -45.416 |
| Cd(SO4)2-2 | 5.02E-11 | 2.42E-11 | -10.616 |
| Cd+2 | 5.29E-09 | 2.55E-09 | -8.593 |
| Cd2OH+3 | 2.93E-24 | 5.68E-25 | -24.246 |
| CdCl+ | 5.02E-09 | 4.19E-09 | -8.378 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| CdCl2 (aq) | 2.95E-10 | 2.97E-10 | -9.527 |
| CdCO3 (aq) | 3.71E-19 | 3.75E-19 | -18.426 |
| CdF+ | 1.97E-16 | 1.64E-16 | -15.786 |
| CdHCO3+ | 3.14E-14 | 2.61E-14 | -13.583 |
| CdHPO4 (aq) | 2.64E-16 | 2.67E-16 | -15.574 |
| CdHS+ | 1.7E-35 | 1.42E-35 | -34.848 |
| CdNH3+2 | 1.52E-16 | 7.31E-17 | -16.136 |
| CdNO2+ | 3.28E-52 | 2.73E-52 | -51.564 |
| CdNO3+ | 1.53E-67 | 1.28E-67 | -66.894 |
| CdOH+ | 4.7E-17 | 3.92E-17 | -16.407 |
| CdSO4 (aq) | 9.08E-10 | 9.17E-10 | -9.038 |
| Cl-1 | 0.021205 | 0.017673 | -1.753 |
| CO3-2 | 1.3E-14 | 6.27E-15 | -14.203 |
| Cr2O7-2 | 8.64E-12 | 4.17E-12 | -11.38 |
| CrO3Cl- | 1.01E-10 | 8.39E-11 | -10.076 |
| CrO3H2PO4- | 1.36E-12 | 1.13E-12 | -11.946 |
| CrO3HPO4-2 | 2.02E-12 | 9.72E-13 | -12.012 |
| CrO3SO4-2 | 8.25E-10 | 3.98E-10 | -9.4 |
| CrO4-2 | 8.27E-11 | 3.99E-11 | -10.399 |
| Cu DOM1 | 8.16E-10 | 7.27E-10 | -9.139 |
| Cu(CO3)2-2 | 3.26E-26 | 1.57E-26 | -25.803 |
| Cu(N3)2 (aq) | 4.48E-17 | 4.52E-17 | -16.345 |
| Cu(N3)3- | 6.25E-22 | 5.21E-22 | -21.284 |
| Cu(N3)4-2 | 6.52E-28 | 3.15E-28 | -27.502 |
| Cu(NH3)2+2 | 1.08E-20 | 5.22E-21 | -20.282 |
| Cu(NH3)3+2 | 6.18E-28 | 2.98E-28 | -27.525 |
| Cu(NH3)4+2 | 7.3E-36 | 3.52E-36 | -35.453 |
| Cu(NO2)2 (aq) | 3.03E-95 | 3.06E-95 | -94.514 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Cu(NO3)2 (aq) | 1.4E-126 | 1.4E-126 | -125.854 |
| Cu(OH)2 (aq) | 6.84E-20 | 6.9E-20 | -19.161 |
| Cu(OH)3- | 4.91E-27 | 4.09E-27 | -26.388 |
| Cu(OH)4-2 | 2.34E-38 | 1.13E-38 | -37.947 |
| Cu+2 | 5.24E-08 | 2.53E-08 | -7.598 |
| Cu2(OH)2+2 | 2.59E-21 | 1.25E-21 | -20.903 |
| Cu2OH+3 | 1.82E-19 | 3.52E-20 | -19.453 |
| Cu2S3-2 | 5.4E-113 | 2.6E-113 | -112.587 |
| Cu3(OH)4+2 | 3.59E-34 | 1.73E-34 | -33.761 |
| CuCl+ | 9.51E-10 | 7.93E-10 | -9.101 |
| CuCl2 (aq) | 2.31E-12 | 2.34E-12 | -11.632 |
| CuCl3- | 3.85E-16 | 3.21E-16 | -15.494 |
| CuCl4-2 1 | 8.32E-20 | 4.02E-20 | -19.396 |
| CuCO3 (aq) | 9.24E-16 | 9.33E-16 | -15.03 |
| CuF+ | 5.5E-15 | 4.59E-15 | -14.339 |
| CuHCO3+ | 6.18E-13 | 5.15E-13 | -12.288 |
| CuHPO4 (aq) | 6.88E-15 | 6.95E-15 | -14.158 |
| CuHSO4+ | 2.78E-11 | 2.31E-11 | -10.636 |
| CuN3+ | 5.05E-12 | 4.2E-12 | -11.376 |
| CuNH3+2 | 4.95E-14 | 2.39E-14 | -13.622 |
| CuNO2+ | 3.38E-51 | 2.81E-51 | -50.551 |
| CuNO3+ | 1.2E-66 | 9.97E-67 | -66.001 |
| CuOH+ | 2.42E-13 | 2.01E-13 | -12.696 |
| CuS(aq) | 8.93E-43 | 9.02E-43 | -42.045 |
| CuSO4 (aq) | 8.79E-09 | 8.87E-09 | -8.052 |
| DOC (Gaussian DOM) | 0.000333 | 0.000336 | -3.473 |
| DOM1 | 7.76E-06 | 1.86E-06 | -5.73 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| F-1 | 5.21E-09 | 4.34E-09 | -8.362 |
| Fe DOM1 | 1.54E-10 | 1.53E-10 | -9.817 |
| Fe(N3)2+ | 2.02E-16 | 1.68E-16 | -15.774 |
| Fe(N3)3 (aq) | 8.21E-21 | 8.29E-21 | -20.082 |
| Fe(NH3)2+2 | 1.93E-21 | 9.31E-22 | -21.031 |
| Fe(NH3)3+2 | 3.97E-31 | 1.91E-31 | -30.718 |
| Fe(NH3)4+2 | 3.48E-41 | 1.68E-41 | -40.775 |
| Fe(NO2)2+ | 5.99E-97 | 4.99E-97 | -96.302 |
| Fe(NO2)3 (aq) | 6E-140 | 6.1E-140 | -139.215 |
| Fe(OH)2 (aq) | 9.46E-20 | 9.56E-20 | -19.02 |
| Fe(OH)2+ | 1.81E-12 | 1.51E-12 | -11.822 |
| Fe(OH)3- | 1.37E-27 | 1.14E-27 | -26.942 |
| Fe(OH)3 (aq) | 2.05E-19 | 2.07E-19 | -18.684 |
| Fe(OH)4- | 6.73E-25 | 5.61E-25 | -24.251 |
| Fe(SO4)2- | 5.55E-12 | 4.62E-12 | -11.335 |
| Fe+2 | 0.001929 | 0.000931 | -3.031 |
| Fe+3 | 4.33E-11 | 8.4E-12 | -11.076 |
| Fe2(OH)2+4 | 1.29E-19 | 6.99E-21 | -20.155 |
| Fe3(OH)4+5 | 3.41E-28 | 3.58E-30 | -29.446 |
| FeCl+ | 1.25E-05 | 1.04E-05 | -4.984 |
| FeCl+2 | 6.74E-12 | 3.25E-12 | -11.488 |
| FeCrO4+ | 1.48E-14 | 1.23E-14 | -13.91 |
| FeF+ | 7.87E-11 | 6.56E-11 | -10.183 |
| FeF+2 | 7.21E-14 | 3.48E-14 | -13.458 |
| FeF2+ | 6.86E-18 | 5.72E-18 | -17.243 |
| FeF3 (aq) | 2.28E-23 | 2.3E-23 | -22.638 |
| FeH2PO4+ | 4.4E-07 | 3.67E-07 | -6.436 |
| FeH2PO4+2 | 2.59E-13 | 1.25E-13 | -12.903 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| FeHCO3+ | 4.54E-09 | 3.79E-09 | -8.422 |
| FeHPO4 (aq) | 7.57E-11 | 7.64E-11 | -10.117 |
| FeHPO4+ | 2.59E-12 | 2.16E-12 | -11.665 |
| FeHS+ | 2.53E-32 | 2.11E-32 | -31.675 |
| FeN3+2 | 6.24E-13 | 3.01E-13 | -12.521 |
| FeNH3+2 | 3.7E-12 | 1.78E-12 | -11.749 |
| FeNO2+2 | 2.94E-53 | 1.42E-53 | -52.849 |
| FeOH+ | 8.47E-11 | 7.06E-11 | -10.151 |
| FeOH+2 | 4.84E-11 | 2.33E-11 | -10.632 |
| FeSO4 (aq) | 0.00035 | 0.000354 | -3.451 |
| FeSO4+ | 2.19E-10 | 1.82E-10 | -9.739 |
| H DOM1 | 1.17E-05 | 6.49E-06 | -5.188 |
| H+1 | 0.002899 | 0.002416 | -2.617 |
| H2AsO3- | 1.13E-13 | 9.41E-14 | -13.026 |
| H2AsO4- | 1.61E-10 | 1.34E-10 | -9.873 |
| H2CO3* (aq) | 0.002552 | 0.002577 | -2.589 |
| H2CrO4 (aq) | 2.73E-10 | 2.76E-10 | -9.56 |
| H2PO4- | 1.21E-06 | 1.01E-06 | -5.995 |
| H2S (aq) | 1.9E-30 | 1.91E-30 | -29.718 |
| H3AsO3 | 4.9E-07 | 4.95E-07 | -6.305 |
| H3AsO4 | 5.72E-11 | 5.78E-11 | -10.238 |
| H3PO4 | 3.06E-07 | 3.09E-07 | -6.509 |
| HAsO3-2 | 4.11E-25 | 1.98E-25 | -24.703 |
| HAsO4-2 | 1.13E-14 | 5.44E-15 | -14.264 |
| HCO3- | 4.88E-07 | 4.06E-07 | -6.391 |
| HCrO4- | 3.64E-07 | 3.03E-07 | -6.518 |
| HF (aq) | 1.31E-08 | 1.32E-08 | -7.88 |
| HF2- | 2.59E-16 | 2.15E-16 | -15.667 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Hg(CO3)2-2 | 1.03E-34 | 4.97E-35 | -34.303 |
| Hg(HS)2 (aq) | 2.57E-52 | 2.59E-52 | -51.586 |
| Hg(N3)2 (aq) | 3.05E-14 | 3.08E-14 | -13.512 |
| Hg(NH3)2+2 | 1.46E-23 | 7.05E-24 | -23.152 |
| Hg(NH3)4+2 | 3.16E-42 | 1.53E-42 | -41.816 |
| Hg(NO2)2 (aq) | 3E-102 | 3.1E-102 | -101.514 |
| Hg(NO2)3- | 1.4E-145 | 1.1E-145 | -144.947 |
| Hg(NO2)4-2 | 6.4E-190 | 3.1E-190 | -189.51 |
| Hg(NO3)2 (aq) | 7.6E-141 | 7.7E-141 | -140.115 |
| Hg(OH)2 | 3.9E-23 | 3.93E-23 | -22.405 |
| Hg(SO4)2-2 | 6.25E-24 | 3.01E-24 | -23.521 |
| Hg+2 | 1.21E-21 | 5.85E-22 | -21.233 |
| Hg2OH+3 | 3.03E-43 | 5.87E-44 | -43.231 |
| Hg3(OH)3+3 | 5.6E-63 | 1.09E-63 | -62.964 |
| HgCl+ | 3.53E-16 | 2.94E-16 | -15.532 |
| HgCl2 (aq) | 3.95E-11 | 3.99E-11 | -10.4 |
| HgCl3-1 | 8.4E-12 | 7E-12 | -11.155 |
| HgCl4-2 | 1.15E-12 | 5.54E-13 | -12.256 |
| HgClOH (aq) | 8.42E-17 | 8.5E-17 | -16.071 |
| HgCO3 (aq) | 2.79E-24 | 2.81E-24 | -23.551 |
| HgF+ | 1.14E-28 | 9.49E-29 | -28.023 |
| HgHCO3+ | 1.35E-22 | 1.13E-22 | -21.948 |
| HgHS2- | 4.16E-56 | 3.47E-56 | -55.46 |
| HgN3+ | 4.49E-10 | 3.75E-10 | -9.426 |
| HgNO2+ | 3.7E-61 | 3.08E-61 | -60.511 |
| HgNO3+ | 1.88E-81 | 1.57E-81 | -80.805 |
| HgOH+ | 8.7E-23 | 7.25E-23 | -22.14 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| HgOHCO3- | 1.64E-28 | 1.37E-28 | -27.864 |
| HgS2-2 | 5.8E-62 | 2.8E-62 | -61.553 |
| HgSO4 (aq) | 1.68E-22 | 1.7E-22 | -21.769 |
| HN3 (aq) | 2.83E-05 | 2.86E-05 | -4.544 |
| HNO2 (aq) | 3.6E-45 | 3.63E-45 | -44.44 |
| HPO4-2 | 5.27E-11 | 2.54E-11 | -10.594 |
| HS-1 | 6.53E-35 | 5.44E-35 | -34.264 |
| HSO4- | 0.000374 | 0.000311 | -3.507 |
| K+1 | 0.000148 | 0.000124 | -3.908 |
| K2HPO4 (aq) | 4.16E-18 | 4.2E-18 | -17.377 |
| K2PO4- | 1.2E-26 | 1E-26 | -26 |
| KCl (aq) | 1.15E-06 | 1.16E-06 | -5.937 |
| KCr2O7- | 5.34E-15 | 4.45E-15 | -14.352 |
| KCrO4- | 2.2E-14 | 1.83E-14 | -13.737 |
| KF (aq) | 2.43E-13 | 2.45E-13 | -12.61 |
| KH2PO4 (aq) | 1.92E-10 | 1.94E-10 | -9.713 |
| KHPO4- | 2.32E-14 | 1.93E-14 | -13.714 |
| KNO3 (aq) | 1.1E-63 | 1.11E-63 | -62.954 |
| KOH (aq) | 4.05E-16 | 4.09E-16 | -15.388 |
| KPO4-2 | 2.01E-23 | 9.7E-24 | -23.013 |
| KSO4- | 1.52E-06 | 1.26E-06 | -5.898 |
| Mg DOM1 | 3.98E-08 | 3.54E-08 | -7.451 |
| Mg(NH3)2+2 | 1.98E-23 | 9.54E-24 | -23.021 |
| Mg+2 | 0.002551 | 0.001231 | -2.91 |
| Mg2CO3+2 | 7.66E-17 | 3.69E-17 | -16.432 |
| MgCl+ | 9.82E-05 | 8.19E-05 | -4.087 |
| MgCO3 (aq) | 5.45E-15 | 5.5E-15 | -14.259 |
| MgF+ | 4.25E-10 | 3.54E-10 | -9.451 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| MgHCO3+ | 5.83E-09 | 4.86E-09 | -8.314 |
| MgHPO4 (aq) | 1.65E-11 | 1.67E-11 | -10.777 |
| MgOH+ | 9.5E-13 | 7.92E-13 | -12.101 |
| MgPO4- | 2E-19 | 1.67E-19 | -18.778 |
| MgSO4 (aq) | 0.000354 | 0.000358 | -3.447 |
| Mn+3 | 5.1E-06 | 9.89E-07 | -6.005 |
| N3-1 | 2.76E-07 | 2.3E-07 | -6.639 |
| Na+1 | 0.00684 | 0.0057 | -2.244 |
| Na2HPO4 (aq) | 5.85E-15 | 5.9E-15 | -14.229 |
| Na2PO4- | 5.46E-23 | 4.55E-23 | -22.342 |
| NaCl (aq) | 5.59E-05 | 5.65E-05 | -4.248 |
| NaCO3- | 1.06E-15 | 8.85E-16 | -15.053 |
| NaCrO4- | 1.36E-12 | 1.13E-12 | -11.947 |
| NaF (aq) | 2.17E-11 | 2.19E-11 | -10.659 |
| NaH2PO4 (aq) | 8.86E-09 | 8.94E-09 | -8.049 |
| NaHCO3 (aq) | 1.36E-09 | 1.37E-09 | -8.862 |
| NaHPO4- | 1.66E-12 | 1.38E-12 | -11.86 |
| NaNO3 (aq) | 1.88E-62 | 1.89E-62 | -61.723 |
| NaOH (aq) | 1.28E-14 | 1.29E-14 | -13.888 |
| NaPO4-2 | 1.02E-21 | 4.94E-22 | -21.306 |
| NaSO4- | 6.42E-05 | 5.35E-05 | -4.272 |
| NH3 (aq) | 6.68E-11 | 6.74E-11 | -10.171 |
| NH4+1 | 0.000713 | 0.000594 | -3.226 |
| NH4Cr2O7- | 2.98E-14 | 2.49E-14 | -13.605 |
| NH4SO4- | 1.32E-05 | 1.1E-05 | -4.958 |
| Ni DOM1 | 1.27E-09 | 1.13E-09 | -8.947 |
| Ni(N3)2 (aq) | 8.08E-18 | 8.16E-18 | -17.088 |
| Ni(NH3)2+2 | 1.71E-21 | 8.23E-22 | -21.085 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Ni(NH3)3+2 | 6.66E-30 | 3.22E-30 | -29.493 |
| Ni(NH3)4+2 | 7.72E-39 | 3.72E-39 | -38.429 |
| Ni(NH3)5+2 | 2.89E-48 | 1.39E-48 | -47.856 |
| Ni(NH3)6+2 | 2.3E-58 | 1.11E-58 | -57.955 |
| Ni(NO2)2 (aq) | 1.08E-94 | 1.09E-94 | -93.962 |
| Ni(OH)2 (aq) | 2.68E-20 | 2.71E-20 | -19.567 |
| Ni(OH)3- | 1.35E-28 | 1.13E-28 | -27.948 |
| Ni(SO4)2-2 | 6.43E-11 | 3.1E-11 | -10.509 |
| Ni+2 | 3.24E-06 | 1.56E-06 | -5.806 |
| NiCl+ | 1.2E-08 | 9.98E-09 | -8.001 |
| NiCl2 (aq) | 6.23E-12 | 6.29E-12 | -11.201 |
| NiCO3 (aq) | 3.61E-16 | 3.64E-16 | -15.439 |
| NiF+ | 1.47E-13 | 1.23E-13 | -12.911 |
| NiH2PO4+ | 1.25E-11 | 1.04E-11 | -10.983 |
| NiHCO3+ | 7.48E-11 | 6.23E-11 | -10.205 |
| NiHPO4 (aq) | 2.88E-14 | 2.91E-14 | -13.536 |
| NiHS+ | 3.16E-35 | 2.63E-35 | -34.58 |
| NiN3+ | 8.12E-12 | 6.77E-12 | -11.17 |
| NiNH3+2 | 1.43E-13 | 6.92E-14 | -13.16 |
| NiNO2+ | 4.79E-50 | 3.99E-50 | -49.399 |
| NiNO3+ | 5.56E-65 | 4.63E-65 | -64.334 |
| NiOH+ | 4.76E-14 | 3.97E-14 | -13.401 |
| NiSO4 (aq) | 4.94E-07 | 4.98E-07 | -6.303 |
| NO2-1 | 1.28E-45 | 1.06E-45 | -44.973 |
| NO3-1 | 1.41E-59 | 1.18E-59 | -58.928 |
| OH- | 2.29E-12 | 1.91E-12 | -11.72 |
| Pb DOM1 | 1.01E-09 | 8.99E-10 | -9.046 |
| Pb(CO3)2-2 | 1.11E-26 | 5.36E-27 | -26.271 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Pb(HS)2 (aq) | 8.55E-62 | 8.64E-62 | -61.064 |
| Pb(HS)3- | 1.13E-94 | 9.38E-95 | -94.028 |
| Pb(NO2)2 (aq) | 2.26E-95 | 2.28E-95 | -94.642 |
| Pb(NO3)2 (aq) | 5.9E-125 | 6E-125 | -124.222 |
| Pb(OH)2 (aq) | 2.13E-20 | 2.16E-20 | -19.667 |
| Pb(OH)3- | 1.08E-28 | 8.97E-29 | -28.047 |
| Pb(SO4)2-2 | 2.87E-10 | 1.39E-10 | -9.858 |
| Pb+2 | 3.25E-08 | 1.57E-08 | -7.805 |
| Pb2OH+3 | 2.09E-19 | 4.06E-20 | -19.391 |
| Pb3(OH)4+2 | 5.91E-38 | 2.85E-38 | -37.545 |
| Pb4(OH)4+4 | 1.27E-41 | 6.89E-43 | -42.162 |
| PbCl+ | 1.07E-08 | 8.89E-09 | -8.051 |
| PbCl2 (aq) | 3.25E-10 | 3.28E-10 | -9.484 |
| PbCl3- | 5.53E-12 | 4.61E-12 | -11.336 |
| PbCl4-2 | 6.17E-14 | 2.98E-14 | -13.526 |
| PbCO3 (aq) | 3.29E-16 | 3.33E-16 | -15.478 |
| PbF+ | 1.15E-14 | 9.61E-15 | -14.017 |
| PbF2 (aq) | 5.09E-22 | 5.14E-22 | -21.289 |
| PbH2PO4+ | 4.67E-13 | 3.89E-13 | -12.41 |
| PbHCO3+ | 4.83E-12 | 4.03E-12 | -11.395 |
| PbHPO4 (aq) | 4.03E-16 | 4.07E-16 | -15.391 |
| PbNO2+ | 6.47E-51 | 5.39E-51 | -50.268 |
| PbNO3+ | 3.37E-66 | 2.81E-66 | -65.552 |
| PbOH+ | 1.41E-13 | 1.17E-13 | -12.931 |
| PbSO4 (aq) | 1.32E-08 | 1.33E-08 | -7.877 |
| PO4-3 | 1.86E-20 | 3.6E-21 | -20.444 |
| S-2 | 9.31E-50 | 4.49E-50 | -49.348 |
| SO4-2 | 0.00359 | 0.001732 | -2.761 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| Zn DOM1 | 1.19E-08 | 1.06E-08 | -7.976 |
| Zn(CO3)2-2 | 1.5E-26 | 7.24E-27 | -26.141 |
| Zn(N3)2 (aq) | 4.6E-17 | 4.65E-17 | -16.333 |
| Zn(N3)3- | 7.33E-23 | 6.11E-23 | -22.214 |
| Zn(NH3)2+2 | 3.8E-21 | 1.84E-21 | -20.736 |
| Zn(NH3)3+2 | 7.55E-29 | 3.64E-29 | -28.439 |
| Zn(NH3)4+2 | 7.34E-37 | 3.54E-37 | -36.451 |
| Zn(NO2)2 (aq) | 1.64E-94 | 1.65E-94 | -93.781 |
| Zn(NO3)2 (aq) | 6.4E-124 | 6.4E-124 | -123.192 |
| Zn(OH)2 (aq) | 1.99E-17 | 2.01E-17 | -16.696 |
| Zn(OH)3- | 3.18E-26 | 2.65E-26 | -25.577 |
| Zn(OH)4-2 | 3.62E-36 | 1.75E-36 | -35.758 |
| Zn(SO4)2-2 | 1.09E-07 | 5.27E-08 | -7.278 |
| Zn+2 | 1.91E-05 | 9.22E-06 | -5.035 |
| Zn2OH+3 | 7.47E-17 | 1.45E-17 | -16.839 |
| Zn2S3-2 | 4.5E-105 | 2.2E-105 | -104.662 |
| Zn4S6-4 | 1.5E-207 | 8E-209 | -208.095 |
| ZnCl+ | 5.23E-07 | 4.36E-07 | -6.361 |
| ZnCl2 (aq) | 4.89E-09 | 4.93E-09 | -8.307 |
| ZnCl3- | 1.1E-10 | 9.2E-11 | -10.036 |
| ZnCl4-2 | 1.55E-12 | 7.5E-13 | -12.125 |
| ZnCO3 (aq) | 3.3E-15 | 3.33E-15 | -14.478 |
| ZnF+ | 8.23E-13 | 6.86E-13 | -12.164 |
| ZnHCO3+ | 1.13E-10 | 9.43E-11 | -10.026 |
| ZnHPO4 (aq) | 3.89E-13 | 3.93E-13 | -12.406 |
| ZnN3+ | 3.66E-11 | 3.05E-11 | -10.516 |
| ZnNH3+2 | 2.44E-13 | 1.18E-13 | -12.93 |

| Species | Concentration | Activity | Log activity |
|---|---|---|---|
| ZnNO2+ | 7.1E-50 | 5.91E-50 | -49.228 |
| ZnNO3+ | 3.5E-64 | 2.91E-64 | -63.536 |
| ZnOH+ | 2.11E-12 | 1.76E-12 | -11.755 |
| ZnS (aq) | 7.64E-39 | 7.72E-39 | -38.112 |
| ZnSO4 (aq) | 3.17E-06 | 3.2E-06 | -5.494 |

## D2 Species distribution

### D2.1: Eh 150

| Component | % of total concentration | Species name |
|---|---|---|
| Pb+2 | 56.037 | Pb+2 |
| | 1.744 | Pb DOM1 |
| | 18.428 | PbCl+ |
| | 0.562 | PbCl2 (aq) |
| | 22.714 | PbSO4 (aq) |
| | 0.496 | Pb(SO4)2-2 |
| NH4+1 | 98.178 | NH4+1 |
| | 1.822 | NH4SO4- |
| Cl-1 | 98.92 | Cl-1 |
| | 0.011 | AlCl+2 |
| | 0.284 | CaCl+ |
| | 0.058 | FeCl+ |
| | 0.458 | MgCl+ |
| | 0.261 | NaCl (aq) |
| Fe+2 | 84.153 | Fe+2 |
| | 0.543 | FeCl+ |
| | 15.284 | FeSO4 (aq) |
| | 0.019 | FeH2PO4+ |
| Zn+2 | 83.335 | Zn+2 |
| | 0.052 | Zn DOM1 |
| | 2.28 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 13.834 | ZnSO4 (aq) |
| | 0.476 | Zn(SO4)2-2 |
| F-1 | 0.04 | F-1 |
| | 0.099 | HF (aq) |

| Component | % of total concentration | Species name |
|---|---|---|
| | 99.658 | AlF+2 |
| | 0.198 | AlF2+ |
| Cu+2 | 83.173 | Cu+2 |
| | 1.297 | Cu DOM1 |
| | 1.512 | CuCl+ |
| | 13.961 | CuSO4 (aq) |
| | 0.044 | CuHSO4+ |
| Ni+2 | 86.476 | Ni+2 |
| | 0.034 | Ni DOM1 |
| | 0.32 | NiCl+ |
| | 13.166 | NiSO4 (aq) |
| N3-1 | 0.966 | N3-1 |
| | 99.034 | HN3 (aq) |
| PO4-3 | 56.106 | H2PO4- |
| | 14.166 | H3PO4 |
| | 20.339 | FeH2PO4+ |
| | 1.282 | CaH2PO4+ |
| | 7.492 | AlHPO4+ |
| | 0.189 | Al2PO4+3 |
| | 0.409 | NaH2PO4 (aq) |
| AsO4-3 | 26.248 | H3AsO4 |
| | 73.746 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 27.058 | DOM1 |
| | 40.807 | H DOM1 |
| | 30.586 | Al DOM1 |
| | 1.361 | Ca DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.139 | Mg DOM1 |
| | 0.041 | Zn DOM1 |
| Ca+2 | 83.604 | Ca+2 |
| | 0.013 | Ca DOM1 |
| | 2.031 | CaCl+ |
| | 14.351 | CaSO4 (aq) |
| Mg+2 | 84.934 | Mg+2 |
| | 3.271 | MgCl+ |
| | 11.793 | MgSO4 (aq) |
| K+1 | 98.235 | K+1 |
| | 0.76 | KCl (aq) |
| | 1.006 | KSO4- |
| Na+1 | 98.274 | Na+1 |
| | 0.804 | NaCl (aq) |
| | 0.922 | NaSO4- |
| CO3-2 | 0.019 | HCO3- |
| | 99.98 | H2CO3* (aq) |
| Al+3 | 28.146 | Al+3 |
| | 0.316 | Al DOM1 |
| | 0.024 | AlOH+2 |
| | 0.472 | AlF+2 |
| | 0.081 | AlCl+2 |
| | 66.134 | AlSO4+ |
| | 4.82 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.717 | Cd+2 |
| | 0.018 | Cd DOM1 |
| | 43.432 | CdCl+ |

| Component | % of total concentration | Species name |
|---|---|---|
| | 2.547 | CdCl2 (aq) |
| | 7.852 | CdSO4 (aq) |
| | 0.434 | Cd(SO4)2-2 |
| CrO4-2 | 0.023 | CrO4-2 |
| | 99.636 | HCrO4- |
| | 0.075 | H2CrO4 (aq) |
| | 0.028 | CrO3Cl- |
| | 0.226 | CrO3SO4-2 |
| Fe+3 | 8.99 | Fe+3 |
| | 31.886 | Fe DOM1 |
| | 10.043 | FeOH+2 |
| | 0.375 | Fe(OH)2+ |
| | 0.015 | FeF+2 |
| | 1.398 | FeCl+2 |
| | 45.417 | FeSO4+ |
| | 1.151 | Fe(SO4)2- |
| | 0.13 | FeN3+2 |
| | 0.054 | FeH2PO4+2 |
| | 0.538 | FeHPO4+ |
| NO2-1 | 26.197 | NO2-1 |
| | 73.801 | HNO2 (aq) |
| NO3-1 | 99.448 | NO3-1 |
| | 0.41 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| SO4-2 | 49.268 | SO4-2 |
| | 5.126 | HSO4- |
| | 25.227 | AlSO4+ |
| | 3.678 | Al(SO4)2- |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.044 | ZnSO4 (aq) |
| | 4.808 | FeSO4 (aq) |
| | 4.861 | MgSO4 (aq) |
| | 5.897 | CaSO4 (aq) |
| | 0.881 | NaSO4- |
| | 0.021 | KSO4- |
| | 0.182 | NH4SO4- |
| H3AsO3 | 100 | H3AsO3 |
| Hg(OH)2 | 5.313 | HgCl2 (aq) |
| | 1.131 | HgCl3-1 |
| | 0.155 | HgCl4-2 |
| | 32.88 | Hg(HS)2 (aq) |
| | 60.512 | HgN3+ |
| HS-1 | 98.676 | H2S (aq) |
| | 1.319 | FeHS+ |

## D2.2: Eh 200

| Component | % of total concentration | Species name |
|---|---|---|
| Pb+2 | 56.037 | Pb+2 |
| | 1.744 | Pb DOM1 |
| | 18.428 | PbCl+ |
| | 0.562 | PbCl2 (aq) |
| | 22.714 | PbSO4 (aq) |
| | 0.496 | Pb(SO4)2-2 |
| NH4+1 | 98.178 | NH4+1 |
| | 1.822 | NH4SO4- |
| Cl-1 | 98.92 | Cl-1 |
| | 0.011 | AlCl+2 |
| | 0.284 | CaCl+ |
| | 0.058 | FeCl+ |
| | 0.458 | MgCl+ |
| | 0.261 | NaCl (aq) |
| Fe+2 | 84.153 | Fe+2 |
| | 0.543 | FeCl+ |
| | 15.285 | FeSO4 (aq) |
| | 0.019 | FeH2PO4+ |
| Zn+2 | 83.335 | Zn+2 |
| | 0.052 | Zn DOM1 |
| | 2.28 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 13.834 | ZnSO4 (aq) |
| | 0.476 | Zn(SO4)2-2 |
| F-1 | 0.04 | F-1 |
| | 0.099 | HF (aq) |
| | 99.658 | AlF+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.198 | AlF2+ |
| SO4-2 | 49.268 | SO4-2 |
| | 5.126 | HSO4- |
| | 25.227 | AlSO4+ |
| | 3.678 | Al(SO4)2- |
| | 0.044 | ZnSO4 (aq) |
| | 4.808 | FeSO4 (aq) |
| | 4.861 | MgSO4 (aq) |
| | 5.897 | CaSO4 (aq) |
| | 0.881 | NaSO4- |
| | 0.021 | KSO4- |
| | 0.182 | NH4SO4- |
| Ni+2 | 86.476 | Ni+2 |
| | 0.034 | Ni DOM1 |
| | 0.32 | NiCl+ |
| | 13.166 | NiSO4 (aq) |
| N3-1 | 0.966 | N3-1 |
| | 99.034 | HN3 (aq) |
| PO4-3 | 56.106 | H2PO4- |
| | 14.166 | H3PO4 |
| | 20.339 | FeH2PO4+ |
| | 1.282 | CaH2PO4+ |
| | 7.492 | AlHPO4+ |
| | 0.189 | Al2PO4+3 |
| | 0.409 | NaH2PO4 (aq) |
| AsO4-3 | 26.249 | H3AsO4 |
| | 73.746 | H2AsO4- |

| Component | % of total concentration | Species name |
|---|---|---|
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 27.057 | DOM1 |
| | 40.806 | H DOM1 |
| | 30.585 | Al DOM1 |
| | 1.361 | Ca DOM1 |
| | 0.139 | Mg DOM1 |
| | 0.041 | Zn DOM1 |
| Ca+2 | 83.603 | Ca+2 |
| | 0.013 | Ca DOM1 |
| | 2.031 | CaCl+ |
| | 14.351 | CaSO4 (aq) |
| Mg+2 | 84.934 | Mg+2 |
| | 3.271 | MgCl+ |
| | 11.794 | MgSO4 (aq) |
| K+1 | 98.235 | K+1 |
| | 0.76 | KCl (aq) |
| | 1.006 | KSO4- |
| Na+1 | 98.274 | Na+1 |
| | 0.804 | NaCl (aq) |
| | 0.922 | NaSO4- |
| CO3-2 | 0.019 | HCO3- |
| | 99.98 | H2CO3* (aq) |
| Al+3 | 28.146 | Al+3 |
| | 0.316 | Al DOM1 |
| | 0.024 | AlOH+2 |
| | 0.472 | AlF+2 |
| | 0.081 | AlCl+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 66.134 | AlSO4+ |
| | 4.82 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |
| Cd+2 | 45.717 | Cd+2 |
| | 0.018 | Cd DOM1 |
| | 43.432 | CdCl+ |
| | 2.547 | CdCl2 (aq) |
| | 7.852 | CdSO4 (aq) |
| | 0.434 | Cd(SO4)2-2 |
| CrO4-2 | 0.023 | CrO4-2 |
| | 99.636 | HCrO4- |
| | 0.075 | H2CrO4 (aq) |
| | 0.028 | CrO3Cl- |
| | 0.226 | CrO3SO4-2 |
| Cu+2 | 83.173 | Cu+2 |
| | 1.297 | Cu DOM1 |
| | 1.512 | CuCl+ |
| | 13.961 | CuSO4 (aq) |
| | 0.044 | CuHSO4+ |
| Fe+3 | 8.99 | Fe+3 |
| | 31.885 | Fe DOM1 |
| | 10.043 | FeOH+2 |
| | 0.375 | Fe(OH)2+ |
| | 0.015 | FeF+2 |
| | 1.398 | FeCl+2 |
| | 45.419 | FeSO4+ |
| | 1.151 | Fe(SO4)2- |
| | 0.13 | FeN3+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 0.054 | FeH2PO4+2 |
| | 0.538 | FeHPO4+ |
| NO2-1 | 26.196 | NO2-1 |
| | 73.801 | HNO2 (aq) |
| NO3-1 | 99.448 | NO3-1 |
| | 0.41 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| HS-1 | 98.676 | H2S (aq) |
| | 1.319 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |
| Hg(OH)2 | 7.918 | HgCl2 (aq) |
| | 1.686 | HgCl3-1 |
| | 0.23 | HgCl4-2 |
| | 90.16 | HgN3+ |

## D2.3: Eh 250

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 7.918 | HgCl2 (aq) |
| | 1.686 | HgCl3-1 |
| | 0.23 | HgCl4-2 |
| | 90.16 | HgN3+ |
| NH4+1 | 98.178 | NH4+1 |
| | 1.822 | NH4SO4- |
| Cl-1 | 98.92 | Cl-1 |
| | 0.011 | AlCl+2 |
| | 0.284 | CaCl+ |
| | 0.058 | FeCl+ |
| | 0.458 | MgCl+ |
| | 0.261 | NaCl (aq) |
| Fe+2 | 84.153 | Fe+2 |
| | 0.543 | FeCl+ |
| | 15.285 | FeSO4 (aq) |
| | 0.019 | FeH2PO4+ |
| Zn+2 | 83.335 | Zn+2 |
| | 0.052 | Zn DOM1 |
| | 2.28 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 13.834 | ZnSO4 (aq) |
| | 0.476 | Zn(SO4)2-2 |
| F-1 | 0.04 | F-1 |
| | 0.099 | HF (aq) |
| | 99.658 | AlF+2 |
| | 0.198 | AlF2+ |
| SO4-2 | 49.268 | SO4-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 5.126 | HSO4- |
| | 25.227 | AlSO4+ |
| | 3.678 | Al(SO4)2- |
| | 0.044 | ZnSO4 (aq) |
| | 4.808 | FeSO4 (aq) |
| | 4.861 | MgSO4 (aq) |
| | 5.897 | CaSO4 (aq) |
| | 0.881 | NaSO4- |
| | 0.021 | KSO4- |
| | 0.182 | NH4SO4- |
| Ni+2 | 86.476 | Ni+2 |
| | 0.034 | Ni DOM1 |
| | 0.32 | NiCl+ |
| | 13.166 | NiSO4 (aq) |
| N3-1 | 0.966 | N3-1 |
| | 99.033 | HN3 (aq) |
| PO4-3 | 56.106 | H2PO4- |
| | 14.166 | H3PO4 |
| | 20.339 | FeH2PO4+ |
| | 1.282 | CaH2PO4+ |
| | 7.492 | AlHPO4+ |
| | 0.189 | Al2PO4+3 |
| | 0.409 | NaH2PO4 (aq) |
| AsO4-3 | 26.249 | H3AsO4 |
| | 73.746 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 27.057 | DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 40.806 | H DOM1 |
| | 30.585 | Al DOM1 |
| | 1.361 | Ca DOM1 |
| | 0.139 | Mg DOM1 |
| | 0.041 | Zn DOM1 |
| Ca+2 | 83.603 | Ca+2 |
| | 0.013 | Ca DOM1 |
| | 2.031 | CaCl+ |
| | 14.351 | CaSO4 (aq) |
| Mg+2 | 84.934 | Mg+2 |
| | 3.271 | MgCl+ |
| | 11.794 | MgSO4 (aq) |
| K+1 | 98.235 | K+1 |
| | 0.76 | KCl (aq) |
| | 1.006 | KSO4- |
| Na+1 | 98.274 | Na+1 |
| | 0.804 | NaCl (aq) |
| | 0.922 | NaSO4- |
| CO3-2 | 0.019 | HCO3- |
| | 99.98 | H2CO3* (aq) |
| Al+3 | 28.146 | Al+3 |
| | 0.316 | Al DOM1 |
| | 0.024 | AlOH+2 |
| | 0.472 | AlF+2 |
| | 0.081 | AlCl+2 |
| | 66.134 | AlSO4+ |
| | 4.82 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |

| Component | % of total concentration | Species name |
|---|---|---|
| Cd+2 | 45.717 | Cd+2 |
| | 0.018 | Cd DOM1 |
| | 43.432 | CdCl+ |
| | 2.547 | CdCl2 (aq) |
| | 7.852 | CdSO4 (aq) |
| | 0.434 | Cd(SO4)2-2 |
| CrO4-2 | 0.023 | CrO4-2 |
| | 99.636 | HCrO4- |
| | 0.075 | H2CrO4 (aq) |
| | 0.028 | CrO3Cl- |
| | 0.226 | CrO3SO4-2 |
| Cu+2 | 83.173 | Cu+2 |
| | 1.297 | Cu DOM1 |
| | 1.512 | CuCl+ |
| | 13.961 | CuSO4 (aq) |
| | 0.044 | CuHSO4+ |
| Pb+2 | 56.037 | Pb+2 |
| | 1.744 | Pb DOM1 |
| | 18.428 | PbCl+ |
| | 0.562 | PbCl2 (aq) |
| | 22.714 | PbSO4 (aq) |
| | 0.496 | Pb(SO4)2-2 |
| Fe+3 | 8.99 | Fe+3 |
| | 31.885 | Fe DOM1 |
| | 10.043 | FeOH+2 |
| | 0.375 | Fe(OH)2+ |
| | 0.015 | FeF+2 |
| | 1.398 | FeCl+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 45.419 | FeSO4+ |
| | 1.151 | Fe(SO4)2- |
| | 0.13 | FeN3+2 |
| | 0.054 | FeH2PO4+2 |
| | 0.538 | FeHPO4+ |
| NO2-1 | 26.196 | NO2-1 |
| | 73.801 | HNO2 (aq) |
| NO3-1 | 99.448 | NO3-1 |
| | 0.41 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| HS-1 | 98.676 | H2S (aq) |
| | 1.319 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |

## D2.4: Eh 300

| Component | % of total concentration | Species name |
|---|---|---|
| Hg(OH)2 | 7.918 | HgCl2 (aq) |
| | 1.686 | HgCl3-1 |
| | 0.23 | HgCl4-2 |
| | 90.16 | HgN3+ |
| NH4+1 | 98.178 | NH4+1 |
| | 1.822 | NH4SO4- |
| Cl-1 | 98.92 | Cl-1 |
| | 0.011 | AlCl+2 |
| | 0.284 | CaCl+ |
| | 0.058 | FeCl+ |
| | 0.458 | MgCl+ |
| | 0.261 | NaCl (aq) |
| Fe+2 | 84.153 | Fe+2 |
| | 0.543 | FeCl+ |
| | 15.285 | FeSO4 (aq) |
| | 0.019 | FeH2PO4+ |
| Zn+2 | 83.335 | Zn+2 |
| | 0.052 | Zn DOM1 |
| | 2.28 | ZnCl+ |
| | 0.021 | ZnCl2 (aq) |
| | 13.834 | ZnSO4 (aq) |
| | 0.476 | Zn(SO4)2-2 |
| F-1 | 0.04 | F-1 |
| | 0.099 | HF (aq) |
| | 99.658 | AlF+2 |
| | 0.198 | AlF2+ |
| SO4-2 | 49.268 | SO4-2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 5.126 | HSO4- |
| | 25.227 | AlSO4+ |
| | 3.678 | Al(SO4)2- |
| | 0.044 | ZnSO4 (aq) |
| | 4.808 | FeSO4 (aq) |
| | 4.861 | MgSO4 (aq) |
| | 5.897 | CaSO4 (aq) |
| | 0.881 | NaSO4- |
| | 0.021 | KSO4- |
| | 0.182 | NH4SO4- |
| Ni+2 | 86.476 | Ni+2 |
| | 0.034 | Ni DOM1 |
| | 0.32 | NiCl+ |
| | 13.166 | NiSO4 (aq) |
| N3-1 | 0.966 | N3-1 |
| | 99.033 | HN3 (aq) |
| PO4-3 | 56.106 | H2PO4- |
| | 14.166 | H3PO4 |
| | 20.339 | FeH2PO4+ |
| | 1.282 | CaH2PO4+ |
| | 7.492 | AlHPO4+ |
| | 0.189 | Al2PO4+3 |
| | 0.409 | NaH2PO4 (aq) |
| AsO4-3 | 26.249 | H3AsO4 |
| | 73.746 | H2AsO4- |
| DOC (Gaussian DOM) | 100 | DOC (Gaussian DOM) |
| DOM1 | 27.057 | DOM1 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 40.806 | H DOM1 |
| | 30.584 | Al DOM1 |
| | 1.361 | Ca DOM1 |
| | 0.139 | Mg DOM1 |
| | 0.041 | Zn DOM1 |
| Ca+2 | 83.603 | Ca+2 |
| | 0.013 | Ca DOM1 |
| | 2.031 | CaCl+ |
| | 14.351 | CaSO4 (aq) |
| Mg+2 | 84.934 | Mg+2 |
| | 3.271 | MgCl+ |
| | 11.794 | MgSO4 (aq) |
| K+1 | 98.235 | K+1 |
| | 0.76 | KCl (aq) |
| | 1.006 | KSO4- |
| Na+1 | 98.274 | Na+1 |
| | 0.804 | NaCl (aq) |
| | 0.922 | NaSO4- |
| CO3-2 | 0.019 | HCO3- |
| | 99.98 | H2CO3* (aq) |
| Al+3 | 28.146 | Al+3 |
| | 0.316 | Al DOM1 |
| | 0.024 | AlOH+2 |
| | 0.472 | AlF+2 |
| | 0.081 | AlCl+2 |
| | 66.134 | AlSO4+ |
| | 4.82 | Al(SO4)2- |
| Mn+3 | 100 | Mn+3 |

| Component | % of total concentration | Species name |
|---|---|---|
| Cd+2 | 45.717 | Cd+2 |
| | 0.018 | Cd DOM1 |
| | 43.432 | CdCl+ |
| | 2.547 | CdCl2 (aq) |
| | 7.852 | CdSO4 (aq) |
| | 0.434 | Cd(SO4)2-2 |
| CrO4-2 | 0.023 | CrO4-2 |
| | 99.636 | HCrO4- |
| | 0.075 | H2CrO4 (aq) |
| | 0.028 | CrO3Cl- |
| | 0.226 | CrO3SO4-2 |
| Cu+2 | 83.173 | Cu+2 |
| | 1.297 | Cu DOM1 |
| | 1.512 | CuCl+ |
| | 13.961 | CuSO4 (aq) |
| | 0.044 | CuHSO4+ |
| Pb+2 | 56.037 | Pb+2 |
| | 1.744 | Pb DOM1 |
| | 18.428 | PbCl+ |
| | 0.562 | PbCl2 (aq) |
| | 22.714 | PbSO4 (aq) |
| | 0.496 | Pb(SO4)2-2 |
| Fe+3 | 8.99 | Fe+3 |
| | 31.885 | Fe DOM1 |
| | 10.043 | FeOH+2 |
| | 0.375 | Fe(OH)2+ |
| | 0.015 | FeF+2 |
| | 1.398 | FeCl+2 |

| Component | % of total concentration | Species name |
|---|---|---|
| | 45.419 | FeSO4+ |
| | 1.151 | Fe(SO4)2- |
| | 0.13 | FeN3+2 |
| | 0.054 | FeH2PO4+2 |
| | 0.538 | FeHPO4+ |
| NO2-1 | 26.196 | NO2-1 |
| | 73.801 | HNO2 (aq) |
| NO3-1 | 99.448 | NO3-1 |
| | 0.41 | CaNO3+ |
| | 0.132 | NaNO3 (aq) |
| HS-1 | 98.676 | H2S (aq) |
| | 1.319 | FeHS+ |
| H3AsO3 | 100 | H3AsO3 |

## D3 Saturation indicies

## D3.1: Eh 150

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 4.03 | -7.444 |
| Al(OH)3 (Soil) | 4.03 | -4.898 |
| Al2O3(s) | 8.062 | -13.162 |
| Al4(OH)10SO4(s) | 8.127 | -14.573 |
| AlAsO4:2H2O(s) | -32.625 | -16.825 |
| AlOHF2(s) | -17.926 | -18.333 |
| AlOHSO4(s) | -3.964 | -0.734 |
| Alunite | -5.189 | -5.066 |
| Anglesite | -10.567 | -2.704 |
| Anhydrite | -5.679 | -1.363 |
| Antlerite | -28.751 | -37.539 |
| Aragonite | -17.121 | -8.842 |
| Arsenolite | -12.609 | -11.046 |
| Artinite | -14.791 | -25.122 |
| As2O5(s) | -73.31 | -38.601 |
| As2S3(am) | -60.283 | -13.898 |
| Atacamite | -18.207 | -26.166 |
| Azurite | -59.627 | -42.474 |
| Bianchite | -7.799 | -6.038 |
| Birnessite | 7.085 | -11.006 |
| Bixbyite | 3.69 | 3.577 |
| Boehmite | 4.031 | -5.263 |
| Brochantite | -35.669 | -52.125 |
| Brucite | 2.323 | -15.47 |
| Ca3(AsO4)2:4H2O(s) | -66.366 | -47.466 |
| Ca3(PO4)2 (am1) | -49.642 | -24.713 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(PO4)2 (am2) | -49.642 | -21.921 |
| Ca3(PO4)2 (beta) | -49.642 | -20.393 |
| Ca4H(PO4)3:3H2O(s) | -75.622 | -28.31 |
| CaCO3xH2O(s) | -17.121 | -10.034 |
| CaCrO4(s) | -13.317 | -11.215 |
| CaHPO4(s) | -25.979 | -6.515 |
| CaHPO4:2H2O(s) | -25.98 | -6.845 |
| Calcite | -17.121 | -8.691 |
| CaS(s) | -13.576 | -24.756 |
| Cd metal (alpha) | -13.841 | -27.813 |
| Cd metal (gamma) | -13.841 | -27.92 |
| Cd(OH)2(s) | -3.361 | -17.58 |
| Cd3(OH)4SO4(s) | -18.076 | -40.636 |
| Cd3(PO4)2(s) | -66.667 | -34.067 |
| Cd3OH2(SO4)2(s) | -26.07 | -32.78 |
| Cd4(OH)6SO4(s) | -21.436 | -49.836 |
| CdCl2(s) | -12.099 | -11.553 |
| CdCl2:1H2O(s) | -12.099 | -10.451 |
| CdCl2:2.5H2O(s) | -12.1 | -10.143 |
| CdF2(s) | -25.317 | -24.386 |
| CdOHCl(s) | -7.73 | -11.455 |
| CdSO4(s) | -11.355 | -11.499 |
| CdSO4:1H2O(s) | -11.355 | -9.821 |
| CdSO4:2.67H2O(s) | -11.356 | -9.592 |
| Cerrusite | -22.008 | -8.657 |
| Chalcanthite | -14.915 | -12.239 |
| Chalcopyrite | -36.499 | -0.327 |
| Chloropyromorphite(c) | -102.11 | -17.68 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Chloropyromorphite(soil) | -102.11 | -21.71 |
| Cinnabar | -46.424 | 0.399 |
| Claudetite | -12.609 | -11.096 |
| Cotunnite | -11.311 | -6.372 |
| Covellite | -22.81 | 0 |
| Cr(VI)-Ettringite | -24.958 | -88.359 |
| Cr(VI)-Jarosite | -50.105 | -31.589 |
| CrO3(s) | -15.632 | -12.453 |
| Cryolite | -60.723 | -26.652 |
| Cu azide | -25.429 | -17.588 |
| Cu(OH)2(s) | -6.919 | -16.532 |
| Cu2(OH)3NO3(s) | -96.372 | -106.064 |
| Cu3(AsO4)2:2H2O(s) | -94.066 | -58.966 |
| Cu3(PO4)2(s) | -77.342 | -40.492 |
| Cu3(PO4)2:3H2O(s) | -77.344 | -42.224 |
| CuCO3(s) | -26.354 | -14.854 |
| CuCrO4(s) | -22.551 | -17.111 |
| CuF2(s) | -28.876 | -30.397 |
| CuF2:2H2O(s) | -28.877 | -24.419 |
| CuOCuSO4(s) | -21.831 | -32.972 |
| Cupric Ferrite | -18.617 | -25.883 |
| CuSO4(s) | -14.913 | -18.297 |
| Diaspore | 4.031 | -3.469 |
| Dolomite (disordered) | -34.233 | -17.975 |
| Dolomite (ordered) | -34.233 | -17.383 |
| Epsomite | -5.674 | -3.478 |
| Ettringite | -2.045 | -61.233 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| FCO3-Apatite | -164.322 | -48.92 |
| Fe(OH)2 (am) | 2.202 | -11.845 |
| Fe(OH)2 (c) | 2.202 | -10.688 |
| Fe(OH)2.7Cl.3(s) | -7.161 | -4.121 |
| Fe2(SO4)3(s) | -35.683 | -33.42 |
| Fe3(OH)8(s) | -9.498 | -29.72 |
| FeAsO4:2H2O(s) | -42.505 | -22.305 |
| Ferrihydrite | -5.85 | -9.66 |
| Ferrihydrite (aged) | -5.85 | -9.15 |
| FeS (ppt) | -13.689 | -10.806 |
| Fluorite | -19.642 | -9.069 |
| Galena | -18.463 | -3.057 |
| Gibbsite (C) | 4.03 | -4.348 |
| Goethite | -5.85 | -6.709 |
| Goslarite | -7.8 | -5.702 |
| Greenockite | -19.251 | -4.897 |
| Greigite | -73.062 | -28.027 |
| Gypsum | -5.68 | -1.064 |
| Halite | -3.997 | -5.524 |
| Hematite | -11.699 | -11.065 |
| Hercynite | 10.264 | -14.537 |
| Hg(OH)2(s) | -30.533 | -27.037 |
| Hg3O2CO3(s) | -111.035 | -81.455 |
| HgCl2(s) | -39.272 | -17.354 |
| HgSO4(s) | -38.528 | -29.019 |
| Hinsdalite | -26.768 | -24.268 |
| H-Jarosite | -33.539 | -29.507 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Huntite | -68.458 | -39.146 |
| Hydrocerrusite | -46.588 | -27.828 |
| Hydromagnesite | -66.129 | -58.691 |
| Hydroxyapatite | -73.305 | -28.972 |
| Hydroxylpyromorphite | -97.741 | -34.951 |
| Hydrozincite | -37.882 | -48.02 |
| K2Cr2O7(s) | -33.847 | -16.114 |
| K2CrO4(s) | -18.215 | -17.591 |
| K-Alum | -13.255 | -7.902 |
| KCl(s) | -5.661 | -6.561 |
| K-Jarosite | -34.83 | -24.449 |
| Langite | -35.67 | -54.165 |
| Larnakite | -13.139 | -12.837 |
| Laurionite | -6.942 | -7.565 |
| Lepidocrocite | -5.85 | -7.221 |
| Lime | 2.315 | -31.563 |
| Litharge | -2.572 | -15.66 |
| Mackinawite | -13.689 | -10.089 |
| Maghemite | -11.699 | -18.085 |
| Magnesioferrite | -9.375 | -27.931 |
| Magnesite | -17.113 | -9.531 |
| Magnetite | -9.497 | -14.167 |
| Malachite | -33.273 | -28.073 |
| Massicot | -2.572 | -15.868 |
| Matlockite | -17.92 | -8.745 |
| Melanothallite | -15.657 | -22.3 |
| Melanterite | -5.796 | -3.462 |
| Metacinnabar | -46.424 | 0 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Mg(OH)2 (active) | 2.323 | -16.471 |
| Mg2(OH)3Cl:4H2O(s) | 0.275 | -25.725 |
| Mg3(PO4)2(s) | -49.617 | -26.337 |
| MgCO3:5H2O(s) | -17.115 | -12.575 |
| MgCrO4(s) | -13.309 | -19.23 |
| MgF2(s) | -19.634 | -11.573 |
| MgHPO4:3H2O(s) | -25.972 | -7.797 |
| MgS(s) | -13.568 | -31.248 |
| Minium | 2.764 | -73.322 |
| Mirabilite | -7.254 | -5.657 |
| Mn2(SO4)3(s) | -20.294 | -15.577 |
| Montroydite | -30.533 | -26.816 |
| Morenosite | -8.57 | -6.351 |
| Na2Cr2O7(s) | -30.519 | -20.489 |
| Na2CrO4(s) | -14.887 | -17.937 |
| NaF(s) | -10.606 | -10.111 |
| Na-Jarosite | -33.166 | -28.671 |
| Natron | -18.695 | -16.984 |
| Nesquehonite | -17.114 | -12.591 |
| Ni(OH)2 (am) | -0.573 | -14.046 |
| Ni(OH)2 (c) | -0.573 | -11.363 |
| Ni3(AsO4)2:8H2O(s) | -75.031 | -49.531 |
| Ni3(PO4)2(s) | -58.305 | -27.005 |
| Ni4(OH)6SO4(s) | -10.286 | -42.286 |
| NiCO3(s) | -20.009 | -9.061 |
| NiS (alpha) | -16.464 | -10.944 |
| NiS (beta) | -16.464 | -5.444 |
| NiS (gamma) | -16.464 | -3.744 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Nsutite | 7.085 | -10.419 |
| Orpiment | -60.283 | -12.384 |
| Otavite | -22.796 | -10.745 |
| Pb azide (alpha) | -21.083 | -12.108 |
| Pb metal | -13.053 | -17.293 |
| Pb(OH)2(s) | -2.572 | -11.078 |
| Pb10(OH)6O(CO3)6(s) | -142.337 | -133.577 |
| Pb2(OH)3Cl(s) | -9.514 | -18.307 |
| Pb2O(OH)2(s) | -5.145 | -31.335 |
| Pb2O3(s) | 5.337 | -55.703 |
| Pb2OCO3(s) | -24.58 | -24.27 |
| Pb3(AsO4)2(s) | -81.026 | -45.526 |
| Pb3(PO4)2(s) | -64.303 | -20.773 |
| Pb3O2CO3(s) | -27.152 | -38.844 |
| Pb3O2SO4(s) | -15.711 | -26.878 |
| Pb4(OH)6SO4(s) | -18.284 | -39.384 |
| Pb4O3SO4(s) | -18.283 | -40.99 |
| PbCrO4(s) | -18.204 | -5.336 |
| PbF2(s) | -24.529 | -16.968 |
| PbHPO4(s) | -30.866 | -7.061 |
| PbO:0.3H2O(s) | -2.572 | -15.552 |
| Periclase | 2.323 | -20.18 |
| Phosgenite | -33.319 | -13.509 |
| Plattnerite | 7.909 | -43.493 |
| Plumbgummite | -47.068 | -14.278 |
| Portlandite | 2.315 | -21.171 |
| Pyrite | -19.1 | -0.289 |
| Realgar | -27.436 | -6.706 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Retgersite | -8.57 | -6.502 |
| Siderite | -17.234 | -6.688 |
| Smithsonite | -19.238 | -8.361 |
| Spharelite | -15.693 | -4.691 |
| Spinel | 10.386 | -28.821 |
| Strengite | -34.144 | -7.801 |
| Struvite | -26.58 | -13.32 |
| Sulfur | -5.411 | -3.365 |
| Tenorite(am) | -6.918 | -15.803 |
| Tenorite(c) | -6.918 | -14.953 |
| Thenardite | -7.25 | -7.627 |
| Thermonatrite | -18.691 | -19.392 |
| Tsumebite | -40.358 | -30.568 |
| Vaterite | -17.121 | -9.284 |
| Vivianite | -49.985 | -12.194 |
| Wurtzite | -15.693 | -6.944 |
| Zincite | 0.198 | -11.577 |
| Zincosite | -7.797 | -12.228 |
| Zn metal | -10.282 | -37.004 |
| Zn(NO3)2:6H2O(s) | -164.873 | -168.039 |
| Zn(OH)2 (am) | 0.198 | -12.797 |
| Zn(OH)2 (beta) | 0.198 | -12.062 |
| Zn(OH)2 (delta) | 0.198 | -11.646 |
| Zn(OH)2 (epsilon) | 0.198 | -11.814 |
| Zn(OH)2 (gamma) | 0.198 | -12.034 |
| Zn2(OH)2SO4(s) | -7.599 | -15.099 |
| Zn2(OH)3Cl(s) | -3.974 | -19.165 |
| Zn3(PO4)2:4H2O(s) | -55.994 | -20.574 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn3AsO42:2.5H2O(s) | -72.717 | -45.217 |
| Zn3O(SO4)2(s) | -15.395 | -35.877 |
| Zn4(OH)6SO4(s) | -7.203 | -35.603 |
| Zn5(OH)8Cl2(s) | -7.75 | -46.25 |
| Zn-Al LDH(s) | -5.292 | -25.122 |
| ZnCl2(s) | -8.54 | -16.031 |
| ZnCO3(s) | -19.238 | -8.438 |
| ZnCO3:1H2O(s) | -19.238 | -8.978 |
| ZnF2(s) | -21.759 | -21.588 |
| ZnSO4:1H2O(s) | -7.797 | -7.427 |

## D3.2: Eh 200

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 4.03 | -7.445 |
| Al(OH)3 (Soil) | 4.03 | -4.898 |
| Al2O3(s) | 8.062 | -13.163 |
| Al4(OH)10SO4(s) | 8.127 | -14.573 |
| AlAsO4:2H2O(s) | -30.876 | -15.076 |
| AlOHF2(s) | -17.926 | -18.333 |
| AlOHSO4(s) | -3.964 | -0.734 |
| Alunite | -5.189 | -5.066 |
| Anglesite | -10.567 | -2.704 |
| Anhydrite | -5.679 | -1.363 |
| Antlerite | -15.089 | -23.877 |
| Aragonite | -17.121 | -8.842 |
| Arsenolite | -12.609 | -11.046 |
| Artinite | -14.791 | -25.122 |
| As2O5(s) | -69.812 | -35.103 |
| As2S3(am) | -81.272 | -34.887 |
| Atacamite | -9.099 | -17.058 |
| Azurite | -45.965 | -28.812 |
| Bianchite | -7.799 | -6.038 |
| Birnessite | 7.96 | -10.131 |
| Bixbyite | 3.69 | 3.577 |
| Boehmite | 4.031 | -5.263 |
| Brochantite | -17.453 | -33.909 |
| Brucite | 2.323 | -15.47 |
| Ca3(AsO4)2:4H2O(s) | -62.868 | -43.968 |
| Ca3(PO4)2 (am1) | -49.642 | -24.713 |
| Ca3(PO4)2 (am2) | -49.642 | -21.921 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(PO4)2 (beta) | -49.642 | -20.393 |
| Ca4H(PO4)3:3H2O(s) | -75.622 | -28.31 |
| CaCO3xH2O(s) | -17.121 | -10.034 |
| CaCrO4(s) | -13.317 | -11.215 |
| CaHPO4(s) | -25.979 | -6.515 |
| CaHPO4:2H2O(s) | -25.98 | -6.845 |
| Calcite | -17.121 | -8.691 |
| CaS(s) | -20.573 | -31.753 |
| Cd metal (alpha) | -15.59 | -29.562 |
| Cd metal (gamma) | -15.59 | -29.669 |
| Cd(OH)2(s) | -3.361 | -17.58 |
| Cd3(OH)4SO4(s) | -18.076 | -40.636 |
| Cd3(PO4)2(s) | -66.667 | -34.067 |
| Cd3OH2(SO4)2(s) | -26.07 | -32.78 |
| Cd4(OH)6SO4(s) | -21.436 | -49.836 |
| CdCl2(s) | -12.099 | -11.553 |
| CdCl2:1H2O(s) | -12.099 | -10.451 |
| CdCl2:2.5H2O(s) | -12.1 | -10.143 |
| CdF2(s) | -25.317 | -24.386 |
| CdOHCl(s) | -7.73 | -11.455 |
| CdSO4(s) | -11.355 | -11.499 |
| CdSO4:1H2O(s) | -11.355 | -9.821 |
| CdSO4:2.67H2O(s) | -11.356 | -9.592 |
| Cerrusite | -22.008 | -8.657 |
| Chalcanthite | -10.361 | -7.685 |
| Chalcopyrite | -45.938 | -9.765 |
| Chloropyromorphite(c) | -102.11 | -17.68 |
| Chloropyromorphite(soil) | -102.11 | -21.71 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cinnabar | -46.424 | 0.399 |
| Claudetite | -12.609 | -11.096 |
| Cotunnite | -11.311 | -6.372 |
| Covellite | -25.252 | -2.442 |
| Cr(VI)-Ettringite | -24.958 | -88.359 |
| Cr(VI)-Jarosite | -47.482 | -28.966 |
| CrO3(s) | -15.632 | -12.453 |
| Cryolite | -60.723 | -26.652 |
| Cu azide | -20.875 | -13.034 |
| Cu(OH)2(s) | -2.365 | -11.978 |
| Cu2(OH)3NO3(s) | -80.267 | -89.96 |
| Cu3(AsO4)2:2H2O(s) | -76.906 | -41.806 |
| Cu3(PO4)2(s) | -63.68 | -26.83 |
| Cu3(PO4)2:3H2O(s) | -63.682 | -28.562 |
| CuCO3(s) | -21.8 | -10.3 |
| CuCrO4(s) | -17.997 | -12.557 |
| CuF2(s) | -24.322 | -25.843 |
| CuF2:2H2O(s) | -24.323 | -19.865 |
| CuOCuSO4(s) | -12.723 | -23.864 |
| Cupric Ferrite | -12.314 | -19.58 |
| CuSO4(s) | -10.359 | -13.743 |
| Diaspore | 4.031 | -3.469 |
| Dolomite (disordered) | -34.233 | -17.975 |
| Dolomite (ordered) | -34.233 | -17.383 |
| Epsomite | -5.674 | -3.478 |
| Ettringite | -2.045 | -61.233 |
| FCO3-Apatite | -164.322 | -48.92 |
| Fe(OH)2 (am) | 2.202 | -11.846 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe(OH)2 (c) | 2.202 | -10.688 |
| Fe(OH)2.7Cl.3(s) | -6.286 | -3.246 |
| Fe2(SO4)3(s) | -33.934 | -31.671 |
| Fe3(OH)8(s) | -7.749 | -27.971 |
| FeAsO4:2H2O(s) | -39.882 | -19.682 |
| Ferrihydrite | -4.975 | -8.786 |
| Ferrihydrite (aged) | -4.975 | -8.276 |
| FeS (ppt) | -20.686 | -17.803 |
| Fluorite | -19.642 | -9.069 |
| Galena | -25.46 | -10.053 |
| Gibbsite (C) | 4.03 | -4.348 |
| Goethite | -4.975 | -5.834 |
| Goslarite | -7.8 | -5.702 |
| Greenockite | -26.248 | -11.893 |
| Greigite | -99.298 | -54.263 |
| Gypsum | -5.68 | -1.064 |
| Halite | -3.997 | -5.524 |
| Hematite | -9.95 | -9.316 |
| Hercynite | 10.264 | -14.538 |
| Hg(OH)2(s) | -23.537 | -20.041 |
| Hg3O2CO3(s) | -90.046 | -60.466 |
| HgCl2(s) | -32.275 | -10.358 |
| HgSO4(s) | -31.531 | -22.023 |
| Hinsdalite | -26.769 | -24.269 |
| H-Jarosite | -30.916 | -26.883 |
| Huntite | -68.458 | -39.146 |
| Hydrocerrusite | -46.589 | -27.829 |
| Hydromagnesite | -66.129 | -58.691 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Hydroxyapatite | -73.305 | -28.972 |
| Hydroxylpyromorphite | -97.741 | -34.951 |
| Hydrozincite | -37.882 | -48.02 |
| K2Cr2O7(s) | -33.847 | -16.114 |
| K2CrO4(s) | -18.215 | -17.591 |
| K-Alum | -13.255 | -7.902 |
| KCl(s) | -5.661 | -6.561 |
| K-Jarosite | -32.207 | -21.826 |
| Langite | -17.454 | -35.949 |
| Larnakite | -13.139 | -12.837 |
| Laurionite | -6.942 | -7.565 |
| Lepidocrocite | -4.975 | -6.346 |
| Lime | 2.315 | -31.563 |
| Litharge | -2.572 | -15.66 |
| Mackinawite | -20.686 | -17.086 |
| Maghemite | -9.95 | -16.336 |
| Magnesioferrite | -7.626 | -26.182 |
| Magnesite | -17.113 | -9.531 |
| Magnetite | -7.748 | -12.418 |
| Malachite | -24.165 | -18.965 |
| Massicot | -2.572 | -15.868 |
| Matlockite | -17.92 | -8.745 |
| Melanothallite | -11.103 | -17.746 |
| Melanterite | -5.796 | -3.462 |
| Metacinnabar | -46.424 | 0 |
| Mg(OH)2 (active) | 2.323 | -16.471 |
| Mg2(OH)3Cl:4H2O(s) | 0.275 | -25.725 |
| Mg3(PO4)2(s) | -49.617 | -26.337 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| MgCO3:5H2O(s) | -17.115 | -12.575 |
| MgCrO4(s) | -13.309 | -19.23 |
| MgF2(s) | -19.634 | -11.573 |
| MgHPO4:3H2O(s) | -25.972 | -7.797 |
| MgS(s) | -20.564 | -38.244 |
| Minium | 4.514 | -71.573 |
| Mirabilite | -7.254 | -5.657 |
| Mn2(SO4)3(s) | -20.294 | -15.577 |
| Montroydite | -23.537 | -19.82 |
| Morenosite | -8.57 | -6.351 |
| Na2Cr2O7(s) | -30.519 | -20.489 |
| Na2CrO4(s) | -14.887 | -17.937 |
| NaF(s) | -10.606 | -10.111 |
| Na-Jarosite | -30.543 | -26.048 |
| Natron | -18.695 | -16.984 |
| Nesquehonite | -17.114 | -12.591 |
| Ni(OH)2 (am) | -0.573 | -14.046 |
| Ni(OH)2 (c) | -0.573 | -11.363 |
| Ni3(AsO4)2:8H2O(s) | -71.533 | -46.033 |
| Ni3(PO4)2(s) | -58.305 | -27.005 |
| Ni4(OH)6SO4(s) | -10.286 | -42.286 |
| NiCO3(s) | -20.009 | -9.061 |
| NiS (alpha) | -23.46 | -17.94 |
| NiS (beta) | -23.46 | -12.44 |
| NiS (gamma) | -23.46 | -10.74 |
| Nsutite | 7.96 | -9.544 |
| Orpiment | -81.272 | -33.373 |
| Otavite | -22.796 | -10.745 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb azide (alpha) | -21.083 | -12.108 |
| Pb metal | -14.802 | -19.042 |
| Pb(OH)2(s) | -2.573 | -11.078 |
| Pb10(OH)6O(CO3)6(s) | -142.338 | -133.578 |
| Pb2(OH)3Cl(s) | -9.514 | -18.307 |
| Pb2O(OH)2(s) | -5.145 | -31.335 |
| Pb2O3(s) | 7.086 | -53.954 |
| Pb2OCO3(s) | -24.58 | -24.27 |
| Pb3(AsO4)2(s) | -77.528 | -42.028 |
| Pb3(PO4)2(s) | -64.303 | -20.773 |
| Pb3O2CO3(s) | -27.152 | -38.844 |
| Pb3O2SO4(s) | -15.711 | -26.878 |
| Pb4(OH)6SO4(s) | -18.284 | -39.384 |
| Pb4O3SO4(s) | -18.283 | -40.99 |
| PbCrO4(s) | -18.204 | -5.336 |
| PbF2(s) | -24.529 | -16.968 |
| PbHPO4(s) | -30.866 | -7.061 |
| PbO:0.3H2O(s) | -2.572 | -15.552 |
| Periclase | 2.323 | -20.18 |
| Phosgenite | -33.319 | -13.509 |
| Plattnerite | 9.658 | -41.744 |
| Plumbgummite | -47.068 | -14.278 |
| Portlandite | 2.315 | -21.171 |
| Pyrite | -31.344 | -12.533 |
| Realgar | -35.307 | -14.577 |
| Retgersite | -8.57 | -6.502 |
| Siderite | -17.234 | -6.688 |
| Smithsonite | -19.238 | -8.361 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Spharelite | -22.69 | -11.687 |
| Spinel | 10.385 | -28.821 |
| Strengite | -33.269 | -6.926 |
| Struvite | -26.58 | -13.32 |
| Sulfur | -10.658 | -8.612 |
| Tenorite(am) | -2.364 | -11.249 |
| Tenorite(c) | -2.364 | -10.399 |
| Thenardite | -7.25 | -7.627 |
| Thermonatrite | -18.691 | -19.392 |
| Tsumebite | -35.804 | -26.014 |
| Vaterite | -17.121 | -9.284 |
| Vivianite | -49.985 | -12.194 |
| Wurtzite | -22.69 | -13.941 |
| Zincite | 0.198 | -11.577 |
| Zincosite | -7.797 | -12.228 |
| Zn metal | -12.032 | -38.753 |
| Zn(NO3)2:6H2O(s) | -150.88 | -154.046 |
| Zn(OH)2 (am) | 0.198 | -12.797 |
| Zn(OH)2 (beta) | 0.198 | -12.062 |
| Zn(OH)2 (delta) | 0.198 | -11.646 |
| Zn(OH)2 (epsilon) | 0.198 | -11.814 |
| Zn(OH)2 (gamma) | 0.198 | -12.034 |
| Zn2(OH)2SO4(s) | -7.599 | -15.099 |
| Zn2(OH)3Cl(s) | -3.974 | -19.165 |
| Zn3(PO4)2:4H2O(s) | -55.994 | -20.574 |
| Zn3AsO42:2.5H2O(s) | -69.219 | -41.719 |
| Zn3O(SO4)2(s) | -15.395 | -35.877 |
| Zn4(OH)6SO4(s) | -7.203 | -35.603 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn5(OH)8Cl2(s) | -7.75 | -46.25 |
| Zn-Al LDH(s) | -5.292 | -25.122 |
| ZnCl2(s) | -8.54 | -16.031 |
| ZnCO3(s) | -19.238 | -8.438 |
| ZnCO3:1H2O(s) | -19.238 | -8.978 |
| ZnF2(s) | -21.759 | -21.588 |
| ZnSO4:1H2O(s) | -7.797 | -7.427 |

## D3.3: Eh 250

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 4.03 | -7.445 |
| Al(OH)3 (Soil) | 4.03 | -4.898 |
| Al2O3(s) | 8.062 | -13.163 |
| Al4(OH)10SO4(s) | 8.127 | -14.573 |
| AlAsO4:2H2O(s) | -29.127 | -13.327 |
| AlOHF2(s) | -17.926 | -18.333 |
| AlOHSO4(s) | -3.964 | -0.734 |
| Alunite | -5.189 | -5.066 |
| Anglesite | -10.567 | -2.704 |
| Anhydrite | -5.679 | -1.363 |
| Antlerite | -15.089 | -23.877 |
| Aragonite | -17.121 | -8.842 |
| Arsenolite | -12.609 | -11.046 |
| Artinite | -14.791 | -25.122 |
| As2O5(s) | -66.314 | -31.605 |
| As2S3(am) | -102.261 | -55.877 |
| Atacamite | -9.099 | -17.058 |
| Azurite | -45.965 | -28.812 |
| Bianchite | -7.799 | -6.038 |
| Birnessite | 8.834 | -9.257 |
| Bixbyite | 3.69 | 3.577 |
| Boehmite | 4.031 | -5.263 |
| Brochantite | -17.453 | -33.909 |
| Brucite | 2.323 | -15.47 |
| Ca3(AsO4)2:4H2O(s) | -59.37 | -40.47 |
| Ca3(PO4)2 (am1) | -49.642 | -24.713 |
| Ca3(PO4)2 (am2) | -49.642 | -21.921 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(PO4)2 (beta) | -49.642 | -20.393 |
| Ca4H(PO4)3:3H2O(s) | -75.622 | -28.31 |
| CaCO3xH2O(s) | -17.121 | -10.034 |
| CaCrO4(s) | -13.317 | -11.215 |
| CaHPO4(s) | -25.979 | -6.515 |
| CaHPO4:2H2O(s) | -25.98 | -6.845 |
| Calcite | -17.121 | -8.691 |
| CaS(s) | -27.569 | -38.749 |
| Cd metal (alpha) | -17.339 | -31.312 |
| Cd metal (gamma) | -17.339 | -31.418 |
| Cd(OH)2(s) | -3.361 | -17.58 |
| Cd3(OH)4SO4(s) | -18.076 | -40.636 |
| Cd3(PO4)2(s) | -66.667 | -34.067 |
| Cd3OH2(SO4)2(s) | -26.07 | -32.78 |
| Cd4(OH)6SO4(s) | -21.436 | -49.836 |
| CdCl2(s) | -12.099 | -11.553 |
| CdCl2:1H2O(s) | -12.099 | -10.451 |
| CdCl2:2.5H2O(s) | -12.1 | -10.143 |
| CdF2(s) | -25.317 | -24.386 |
| CdOHCl(s) | -7.73 | -11.455 |
| CdSO4(s) | -11.355 | -11.499 |
| CdSO4:1H2O(s) | -11.355 | -9.821 |
| CdSO4:2.67H2O(s) | -11.356 | -9.592 |
| Cerrusite | -22.008 | -8.657 |
| Chalcanthite | -10.361 | -7.685 |
| Chalcopyrite | -59.931 | -23.758 |
| Chloropyromorphite(c) | -102.11 | -17.68 |
| Chloropyromorphite(soil) | -102.11 | -21.71 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cinnabar | -52.289 | -5.466 |
| Claudetite | -12.609 | -11.096 |
| Cotunnite | -11.311 | -6.372 |
| Covellite | -32.249 | -9.439 |
| Cr(VI)-Ettringite | -24.958 | -88.359 |
| Cr(VI)-Jarosite | -44.858 | -26.342 |
| CrO3(s) | -15.632 | -12.453 |
| Cryolite | -60.723 | -26.652 |
| Cu azide | -20.875 | -13.034 |
| Cu(OH)2(s) | -2.365 | -11.978 |
| Cu2(OH)3NO3(s) | -73.271 | -82.963 |
| Cu3(AsO4)2:2H2O(s) | -73.408 | -38.308 |
| Cu3(PO4)2(s) | -63.68 | -26.83 |
| Cu3(PO4)2:3H2O(s) | -63.682 | -28.562 |
| CuCO3(s) | -21.8 | -10.3 |
| CuCrO4(s) | -17.997 | -12.557 |
| CuF2(s) | -24.322 | -25.843 |
| CuF2:2H2O(s) | -24.323 | -19.865 |
| CuOCuSO4(s) | -12.723 | -23.864 |
| Cupric Ferrite | -10.565 | -17.831 |
| CuSO4(s) | -10.359 | -13.743 |
| Diaspore | 4.031 | -3.469 |
| Dolomite (disordered) | -34.233 | -17.975 |
| Dolomite (ordered) | -34.233 | -17.383 |
| Epsomite | -5.674 | -3.478 |
| Ettringite | -2.045 | -61.233 |
| FCO3-Apatite | -164.322 | -48.92 |
| Fe(OH)2 (am) | 2.202 | -11.846 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe(OH)2 (c) | 2.202 | -10.688 |
| Fe(OH)2.7Cl.3(s) | -5.412 | -2.372 |
| Fe2(SO4)3(s) | -32.184 | -29.922 |
| Fe3(OH)8(s) | -6 | -26.222 |
| FeAsO4:2H2O(s) | -37.258 | -17.058 |
| Ferrihydrite | -4.101 | -7.911 |
| Ferrihydrite (aged) | -4.101 | -7.401 |
| FeS (ppt) | -27.682 | -24.799 |
| Fluorite | -19.642 | -9.069 |
| Galena | -32.456 | -17.05 |
| Gibbsite (C) | 4.03 | -4.348 |
| Goethite | -4.1 | -4.96 |
| Goslarite | -7.8 | -5.702 |
| Greenockite | -33.244 | -18.89 |
| Greigite | -125.535 | -80.5 |
| Gypsum | -5.68 | -1.064 |
| Halite | -3.997 | -5.524 |
| Hematite | -8.2 | -7.567 |
| Hercynite | 10.264 | -14.538 |
| Hg(OH)2(s) | -22.405 | -18.909 |
| Hg3O2CO3(s) | -86.65 | -57.07 |
| HgCl2(s) | -31.143 | -9.226 |
| HgSO4(s) | -30.399 | -20.891 |
| Hinsdalite | -26.769 | -24.269 |
| H-Jarosite | -28.292 | -24.259 |
| Huntite | -68.458 | -39.146 |
| Hydrocerrusite | -46.589 | -27.829 |
| Hydromagnesite | -66.129 | -58.691 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Hydroxyapatite | -73.305 | -28.972 |
| Hydroxylpyromorphite | -97.741 | -34.951 |
| Hydrozincite | -37.882 | -48.02 |
| K2Cr2O7(s) | -33.847 | -16.114 |
| K2CrO4(s) | -18.215 | -17.591 |
| K-Alum | -13.255 | -7.902 |
| KCl(s) | -5.661 | -6.561 |
| K-Jarosite | -29.583 | -19.202 |
| Langite | -17.454 | -35.949 |
| Larnakite | -13.139 | -12.837 |
| Laurionite | -6.942 | -7.565 |
| Lepidocrocite | -4.1 | -5.471 |
| Lime | 2.315 | -31.563 |
| Litharge | -2.572 | -15.66 |
| Mackinawite | -27.682 | -24.082 |
| Maghemite | -8.2 | -14.586 |
| Magnesioferrite | -5.877 | -24.433 |
| Magnesite | -17.113 | -9.531 |
| Magnetite | -5.999 | -10.669 |
| Malachite | -24.165 | -18.965 |
| Massicot | -2.572 | -15.868 |
| Matlockite | -17.92 | -8.745 |
| Melanothallite | -11.103 | -17.746 |
| Melanterite | -5.796 | -3.462 |
| Metacinnabar | -52.289 | -5.865 |
| Mg(OH)2 (active) | 2.323 | -16.471 |
| Mg2(OH)3Cl:4H2O(s) | 0.275 | -25.725 |
| Mg3(PO4)2(s) | -49.617 | -26.337 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| MgCO3:5H2O(s) | -17.115 | -12.575 |
| MgCrO4(s) | -13.309 | -19.23 |
| MgF2(s) | -19.634 | -11.573 |
| MgHPO4:3H2O(s) | -25.972 | -7.797 |
| MgS(s) | -27.561 | -45.241 |
| Minium | 6.263 | -69.824 |
| Mirabilite | -7.254 | -5.657 |
| Mn2(SO4)3(s) | -20.294 | -15.577 |
| Montroydite | -22.405 | -18.688 |
| Morenosite | -8.57 | -6.351 |
| Na2Cr2O7(s) | -30.519 | -20.489 |
| Na2CrO4(s) | -14.887 | -17.937 |
| NaF(s) | -10.606 | -10.111 |
| Na-Jarosite | -27.919 | -23.424 |
| Natron | -18.695 | -16.984 |
| Nesquehonite | -17.114 | -12.591 |
| Ni(OH)2 (am) | -0.573 | -14.046 |
| Ni(OH)2 (c) | -0.573 | -11.363 |
| Ni3(AsO4)2:8H2O(s) | -68.035 | -42.535 |
| Ni3(PO4)2(s) | -58.305 | -27.005 |
| Ni4(OH)6SO4(s) | -10.286 | -42.286 |
| NiCO3(s) | -20.009 | -9.061 |
| NiS (alpha) | -30.457 | -24.937 |
| NiS (beta) | -30.457 | -19.437 |
| NiS (gamma) | -30.457 | -17.737 |
| Nsutite | 8.834 | -8.67 |
| Orpiment | -102.261 | -54.362 |
| Otavite | -22.796 | -10.745 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb azide (alpha) | -21.083 | -12.108 |
| Pb metal | -16.551 | -20.791 |
| Pb(OH)2(s) | -2.573 | -11.078 |
| Pb10(OH)6O(CO3)6(s) | -142.338 | -133.578 |
| Pb2(OH)3Cl(s) | -9.514 | -18.307 |
| Pb2O(OH)2(s) | -5.145 | -31.335 |
| Pb2O3(s) | 8.835 | -52.205 |
| Pb2OCO3(s) | -24.58 | -24.27 |
| Pb3(AsO4)2(s) | -74.03 | -38.53 |
| Pb3(PO4)2(s) | -64.303 | -20.773 |
| Pb3O2CO3(s) | -27.152 | -38.844 |
| Pb3O2SO4(s) | -15.711 | -26.878 |
| Pb4(OH)6SO4(s) | -18.284 | -39.384 |
| Pb4O3SO4(s) | -18.283 | -40.99 |
| PbCrO4(s) | -18.204 | -5.336 |
| PbF2(s) | -24.529 | -16.968 |
| PbHPO4(s) | -30.866 | -7.061 |
| PbO:0.3H2O(s) | -2.572 | -15.552 |
| Periclase | 2.323 | -20.18 |
| Phosgenite | -33.319 | -13.509 |
| Plattnerite | 11.407 | -39.995 |
| Plumbgummite | -47.068 | -14.278 |
| Portlandite | 2.315 | -21.171 |
| Pyrite | -43.588 | -24.776 |
| Realgar | -43.178 | -22.448 |
| Retgersite | -8.57 | -6.502 |
| Siderite | -17.234 | -6.688 |
| Smithsonite | -19.238 | -8.361 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Spharelite | -29.686 | -18.684 |
| Spinel | 10.385 | -28.821 |
| Strengite | -32.395 | -6.052 |
| Struvite | -26.58 | -13.32 |
| Sulfur | -15.905 | -13.86 |
| Tenorite(am) | -2.364 | -11.249 |
| Tenorite(c) | -2.364 | -10.399 |
| Thenardite | -7.25 | -7.627 |
| Thermonatrite | -18.691 | -19.392 |
| Tsumebite | -35.804 | -26.014 |
| Vaterite | -17.121 | -9.284 |
| Vivianite | -49.985 | -12.194 |
| Wurtzite | -29.686 | -20.937 |
| Zincite | 0.198 | -11.577 |
| Zincosite | -7.797 | -12.228 |
| Zn metal | -13.781 | -40.502 |
| Zn(NO3)2:6H2O(s) | -136.888 | -140.053 |
| Zn(OH)2 (am) | 0.198 | -12.797 |
| Zn(OH)2 (beta) | 0.198 | -12.062 |
| Zn(OH)2 (delta) | 0.198 | -11.646 |
| Zn(OH)2 (epsilon) | 0.198 | -11.814 |
| Zn(OH)2 (gamma) | 0.198 | -12.034 |
| Zn2(OH)2SO4(s) | -7.599 | -15.099 |
| Zn2(OH)3Cl(s) | -3.974 | -19.165 |
| Zn3(PO4)2:4H2O(s) | -55.994 | -20.574 |
| Zn3AsO42:2.5H2O(s) | -65.72 | -38.22 |
| Zn3O(SO4)2(s) | -15.395 | -35.877 |
| Zn4(OH)6SO4(s) | -7.203 | -35.603 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn5(OH)8Cl2(s) | -7.75 | -46.25 |
| Zn-Al LDH(s) | -5.292 | -25.122 |
| ZnCl2(s) | -8.54 | -16.031 |
| ZnCO3(s) | -19.238 | -8.438 |
| ZnCO3:1H2O(s) | -19.238 | -8.978 |
| ZnF2(s) | -21.759 | -21.588 |
| ZnSO4:1H2O(s) | -7.797 | -7.427 |

## D3.4: Eh 300

| Mineral | log IAP | Sat. index |
|---|---|---|
| Al(OH)3 (am) | 4.03 | -7.445 |
| Al(OH)3 (Soil) | 4.03 | -4.898 |
| Al2O3(s) | 8.062 | -13.163 |
| Al4(OH)10SO4(s) | 8.127 | -14.573 |
| AlAsO4:2H2O(s) | -27.378 | -11.578 |
| AlOHF2(s) | -17.926 | -18.333 |
| AlOHSO4(s) | -3.964 | -0.734 |
| Alunite | -5.189 | -5.066 |
| Anglesite | -10.567 | -2.704 |
| Anhydrite | -5.679 | -1.363 |
| Antlerite | -15.089 | -23.877 |
| Aragonite | -17.121 | -8.842 |
| Arsenolite | -12.609 | -11.047 |
| Artinite | -14.791 | -25.122 |
| As2O5(s) | -62.816 | -28.107 |
| As2S3(am) | -123.251 | -76.866 |
| Atacamite | -9.099 | -17.058 |
| Azurite | -45.965 | -28.812 |
| Bianchite | -7.799 | -6.038 |
| Birnessite | 9.709 | -8.382 |
| Bixbyite | 3.69 | 3.577 |
| Boehmite | 4.031 | -5.263 |
| Brochantite | -17.453 | -33.909 |
| Brucite | 2.323 | -15.47 |
| Ca3(AsO4)2:4H2O(s) | -55.872 | -36.972 |
| Ca3(PO4)2 (am1) | -49.642 | -24.713 |
| Ca3(PO4)2 (am2) | -49.642 | -21.921 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Ca3(PO4)2 (beta) | -49.642 | -20.393 |
| Ca4H(PO4)3:3H2O(s) | -75.622 | -28.31 |
| CaCO3xH2O(s) | -17.121 | -10.034 |
| CaCrO4(s) | -13.317 | -11.215 |
| CaHPO4(s) | -25.979 | -6.515 |
| CaHPO4:2H2O(s) | -25.98 | -6.845 |
| Calcite | -17.121 | -8.691 |
| CaS(s) | -34.565 | -45.745 |
| Cd metal (alpha) | -19.088 | -33.061 |
| Cd metal (gamma) | -19.088 | -33.168 |
| Cd(OH)2(s) | -3.361 | -17.58 |
| Cd3(OH)4SO4(s) | -18.076 | -40.636 |
| Cd3(PO4)2(s) | -66.667 | -34.067 |
| Cd3OH2(SO4)2(s) | -26.07 | -32.78 |
| Cd4(OH)6SO4(s) | -21.436 | -49.836 |
| CdCl2(s) | -12.099 | -11.553 |
| CdCl2:1H2O(s) | -12.099 | -10.451 |
| CdCl2:2.5H2O(s) | -12.1 | -10.143 |
| CdF2(s) | -25.317 | -24.386 |
| CdOHCl(s) | -7.73 | -11.455 |
| CdSO4(s) | -11.355 | -11.499 |
| CdSO4:1H2O(s) | -11.355 | -9.821 |
| CdSO4:2.67H2O(s) | -11.356 | -9.592 |
| Cerrusite | -22.008 | -8.657 |
| Chalcanthite | -10.361 | -7.685 |
| Chalcopyrite | -73.924 | -37.751 |
| Chloropyromorphite(c) | -102.11 | -17.68 |
| Chloropyromorphite(soil) | -102.11 | -21.71 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Cinnabar | -59.285 | -12.463 |
| Claudetite | -12.609 | -11.096 |
| Cotunnite | -11.311 | -6.372 |
| Covellite | -39.245 | -16.435 |
| Cr(VI)-Ettringite | -24.958 | -88.359 |
| Cr(VI)-Jarosite | -42.234 | -23.718 |
| CrO3(s) | -15.632 | -12.453 |
| Cryolite | -60.723 | -26.652 |
| Cu azide | -20.875 | -13.034 |
| Cu(OH)2(s) | -2.365 | -11.978 |
| Cu2(OH)3NO3(s) | -66.274 | -75.967 |
| Cu3(AsO4)2:2H2O(s) | -69.91 | -34.81 |
| Cu3(PO4)2(s) | -63.68 | -26.83 |
| Cu3(PO4)2:3H2O(s) | -63.682 | -28.562 |
| CuCO3(s) | -21.8 | -10.3 |
| CuCrO4(s) | -17.997 | -12.557 |
| CuF2(s) | -24.322 | -25.843 |
| CuF2:2H2O(s) | -24.323 | -19.865 |
| CuOCuSO4(s) | -12.723 | -23.864 |
| Cupric Ferrite | -8.816 | -16.082 |
| CuSO4(s) | -10.359 | -13.743 |
| Diaspore | 4.031 | -3.469 |
| Dolomite (disordered) | -34.233 | -17.975 |
| Dolomite (ordered) | -34.233 | -17.383 |
| Epsomite | -5.674 | -3.478 |
| Ettringite | -2.045 | -61.233 |
| FCO3-Apatite | -164.322 | -48.92 |
| Fe(OH)2 (am) | 2.202 | -11.846 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Fe(OH)2 (c) | 2.202 | -10.688 |
| Fe(OH)2.7Cl.3(s) | -4.537 | -1.497 |
| Fe2(SO4)3(s) | -30.435 | -28.173 |
| Fe3(OH)8(s) | -4.251 | -24.473 |
| FeAsO4:2H2O(s) | -34.635 | -14.435 |
| Ferrihydrite | -3.226 | -7.037 |
| Ferrihydrite (aged) | -3.226 | -6.527 |
| FeS (ppt) | -34.679 | -31.796 |
| Fluorite | -19.642 | -9.069 |
| Galena | -39.453 | -24.046 |
| Gibbsite (C) | 4.03 | -4.348 |
| Goethite | -3.226 | -4.085 |
| Goslarite | -7.8 | -5.702 |
| Greenockite | -40.241 | -25.886 |
| Greigite | -151.772 | -106.737 |
| Gypsum | -5.68 | -1.064 |
| Halite | -3.997 | -5.524 |
| Hematite | -6.451 | -5.818 |
| Hercynite | 10.264 | -14.538 |
| Hg(OH)2(s) | -22.405 | -18.909 |
| Hg3O2CO3(s) | -86.65 | -57.07 |
| HgCl2(s) | -31.143 | -9.226 |
| HgSO4(s) | -30.399 | -20.891 |
| Hinsdalite | -26.769 | -24.269 |
| H-Jarosite | -25.668 | -21.636 |
| Huntite | -68.458 | -39.146 |
| Hydrocerrusite | -46.589 | -27.829 |
| Hydromagnesite | -66.129 | -58.691 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Hydroxyapatite | -73.305 | -28.972 |
| Hydroxylpyromorphite | -97.741 | -34.951 |
| Hydrozincite | -37.882 | -48.02 |
| K2Cr2O7(s) | -33.847 | -16.114 |
| K2CrO4(s) | -18.215 | -17.591 |
| K-Alum | -13.255 | -7.902 |
| KCl(s) | -5.661 | -6.561 |
| K-Jarosite | -26.959 | -16.578 |
| Langite | -17.454 | -35.949 |
| Larnakite | -13.139 | -12.837 |
| Laurionite | -6.942 | -7.565 |
| Lepidocrocite | -3.226 | -4.597 |
| Lime | 2.315 | -31.563 |
| Litharge | -2.572 | -15.66 |
| Mackinawite | -34.679 | -31.079 |
| Maghemite | -6.451 | -12.837 |
| Magnesioferrite | -4.128 | -22.683 |
| Magnesite | -17.113 | -9.531 |
| Magnetite | -4.249 | -8.92 |
| Malachite | -24.165 | -18.965 |
| Massicot | -2.572 | -15.868 |
| Matlockite | -17.92 | -8.745 |
| Melanothallite | -11.103 | -17.746 |
| Melanterite | -5.796 | -3.462 |
| Metacinnabar | -59.285 | -12.861 |
| Mg(OH)2 (active) | 2.323 | -16.471 |
| Mg2(OH)3Cl:4H2O(s) | 0.275 | -25.725 |
| Mg3(PO4)2(s) | -49.617 | -26.337 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| MgCO3:5H2O(s) | -17.115 | -12.575 |
| MgCrO4(s) | -13.309 | -19.23 |
| MgF2(s) | -19.634 | -11.573 |
| MgHPO4:3H2O(s) | -25.972 | -7.797 |
| MgS(s) | -34.557 | -52.237 |
| Minium | 8.012 | -68.075 |
| Mirabilite | -7.254 | -5.657 |
| Mn2(SO4)3(s) | -20.294 | -15.577 |
| Montroydite | -22.405 | -18.688 |
| Morenosite | -8.57 | -6.351 |
| Na2Cr2O7(s) | -30.519 | -20.489 |
| Na2CrO4(s) | -14.887 | -17.937 |
| NaF(s) | -10.606 | -10.111 |
| Na-Jarosite | -25.295 | -20.8 |
| Natron | -18.695 | -16.984 |
| Nesquehonite | -17.114 | -12.591 |
| Ni(OH)2 (am) | -0.573 | -14.046 |
| Ni(OH)2 (c) | -0.573 | -11.363 |
| Ni3(AsO4)2:8H2O(s) | -64.537 | -39.037 |
| Ni3(PO4)2(s) | -58.305 | -27.005 |
| Ni4(OH)6SO4(s) | -10.286 | -42.286 |
| NiCO3(s) | -20.009 | -9.061 |
| NiS (alpha) | -37.453 | -31.933 |
| NiS (beta) | -37.453 | -26.433 |
| NiS (gamma) | -37.453 | -24.733 |
| Nsutite | 9.709 | -7.795 |
| Orpiment | -123.251 | -75.352 |
| Otavite | -22.796 | -10.745 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Pb azide (alpha) | -21.083 | -12.108 |
| Pb metal | -18.3 | -22.541 |
| Pb(OH)2(s) | -2.573 | -11.078 |
| Pb10(OH)6O(CO3)6(s) | -142.338 | -133.578 |
| Pb2(OH)3Cl(s) | -9.514 | -18.307 |
| Pb2O(OH)2(s) | -5.145 | -31.335 |
| Pb2O3(s) | 10.584 | -50.456 |
| Pb2OCO3(s) | -24.58 | -24.27 |
| Pb3(AsO4)2(s) | -70.532 | -35.032 |
| Pb3(PO4)2(s) | -64.303 | -20.773 |
| Pb3O2CO3(s) | -27.152 | -38.844 |
| Pb3O2SO4(s) | -15.711 | -26.878 |
| Pb4(OH)6SO4(s) | -18.284 | -39.384 |
| Pb4O3SO4(s) | -18.283 | -40.99 |
| PbCrO4(s) | -18.204 | -5.336 |
| PbF2(s) | -24.529 | -16.968 |
| PbHPO4(s) | -30.866 | -7.061 |
| PbO:0.3H2O(s) | -2.572 | -15.552 |
| Periclase | 2.323 | -20.18 |
| Phosgenite | -33.319 | -13.509 |
| Plattnerite | 13.156 | -38.246 |
| Plumbgummite | -47.068 | -14.278 |
| Portlandite | 2.315 | -21.171 |
| Pyrite | -55.831 | -37.02 |
| Realgar | -51.049 | -30.319 |
| Retgersite | -8.57 | -6.502 |
| Siderite | -17.234 | -6.688 |
| Smithsonite | -19.238 | -8.361 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Spharelite | -36.682 | -25.68 |
| Spinel | 10.385 | -28.821 |
| Strengite | -31.52 | -5.177 |
| Struvite | -26.58 | -13.32 |
| Sulfur | -21.153 | -19.107 |
| Tenorite(am) | -2.364 | -11.249 |
| Tenorite(c) | -2.364 | -10.399 |
| Thenardite | -7.25 | -7.627 |
| Thermonatrite | -18.691 | -19.392 |
| Tsumebite | -35.804 | -26.014 |
| Vaterite | -17.121 | -9.284 |
| Vivianite | -49.985 | -12.194 |
| Wurtzite | -36.682 | -27.934 |
| Zincite | 0.198 | -11.577 |
| Zincosite | -7.797 | -12.228 |
| Zn metal | -15.53 | -42.251 |
| Zn(NO3)2:6H2O(s) | -122.895 | -126.061 |
| Zn(OH)2 (am) | 0.198 | -12.797 |
| Zn(OH)2 (beta) | 0.198 | -12.062 |
| Zn(OH)2 (delta) | 0.198 | -11.646 |
| Zn(OH)2 (epsilon) | 0.198 | -11.814 |
| Zn(OH)2 (gamma) | 0.198 | -12.034 |
| Zn2(OH)2SO4(s) | -7.599 | -15.099 |
| Zn2(OH)3Cl(s) | -3.974 | -19.165 |
| Zn3(PO4)2:4H2O(s) | -55.994 | -20.574 |
| Zn3AsO42:2.5H2O(s) | -62.223 | -34.723 |
| Zn3O(SO4)2(s) | -15.395 | -35.877 |
| Zn4(OH)6SO4(s) | -7.203 | -35.603 |

| Mineral | log IAP | Sat. index |
|---|---|---|
| Zn5(OH)8Cl2(s) | -7.75 | -46.25 |
| Zn-Al LDH(s) | -5.292 | -25.122 |
| ZnCl2(s) | -8.54 | -16.031 |
| ZnCO3(s) | -19.238 | -8.438 |
| ZnCO3:1H2O(s) | -19.238 | -8.978 |
| ZnF2(s) | -21.759 | -21.588 |
| ZnSO4:1H2O(s) | -7.797 | -7.427 |

## D4 Mass distribution

## D4.1: Eh 150

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 1.23E-15 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.002994 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021437 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 1.76E-12 | 0.001 | 0 | 0 | 1.56E-07 | 99.999 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 1.15E-12 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.008421 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.91E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 5.53E-18 | 0 | 0 | 0 | 4.99E-10 | 100 |
| HS-1 | 1.87E-09 | 1.182 | 0 | 0 | 1.57E-07 | 98.818 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 8.83E-61 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.46E-80 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## D4.2: Eh 200

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 6.93E-14 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.002994 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021437 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 8.59E-12 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.008421 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.91E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 3.68E-11 | 7.383 | 0 | 0 | 4.62E-10 | 92.617 |
| HS-1 | 1.89E-16 | 0 | 0 | 0 | 4.62E-10 | 100 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 1.56E-55 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.45E-73 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## D4.3: Eh 250

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 3.89E-12 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.002994 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021437 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 6.43E-11 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.008421 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.91E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.91E-23 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 2.76E-50 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.43E-66 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

## D4.4: Eh 300

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| Al+3 | 0.00278 | 100 | 0 | 0 | 0 | 0 |
| AsO4-3 | 2.18E-10 | 100 | 0 | 0 | 0 | 0 |
| Ca+2 | 0.002994 | 100 | 0 | 0 | 0 | 0 |
| Cd+2 | 1.16E-08 | 100 | 0 | 0 | 0 | 0 |
| Cl-1 | 0.021437 | 100 | 0 | 0 | 0 | 0 |
| CO3-2 | 0.002552 | 100 | 0 | 0 | 0 | 0 |
| CrO4-2 | 3.65E-07 | 100 | 0 | 0 | 0 | 0 |
| Cu+2 | 6.29E-08 | 100 | 0 | 0 | 0 | 0 |
| DOC (Gaussian DOM) | 0.000333 | 100 | 0 | 0 | 0 | 0 |
| DOM1 | 2.87E-05 | 100 | 0 | 0 | 0 | 0 |
| F-1 | 1.32E-05 | 100 | 0 | 0 | 0 | 0 |
| Fe+2 | 0.002292 | 100 | 0 | 0 | 0 | 0 |
| Fe+3 | 4.82E-10 | 100 | 0 | 0 | 0 | 0 |
| H+1 | 0.008421 | 100 | 0 | 0 | 0 | 0 |
| H3AsO3 | 4.9E-07 | 100 | 0 | 0 | 0 | 0 |
| Hg(OH)2 | 4.99E-10 | 100 | 0 | 0 | 0 | 0 |
| HS-1 | 1.92E-30 | 100 | 0 | 0 | 0 | 0 |
| K+1 | 0.000151 | 100 | 0 | 0 | 0 | 0 |
| Mg+2 | 0.003004 | 100 | 0 | 0 | 0 | 0 |
| Mn+3 | 5.1E-06 | 100 | 0 | 0 | 0 | 0 |
| N3-1 | 2.86E-05 | 100 | 0 | 0 | 0 | 0 |
| Na+1 | 0.00696 | 100 | 0 | 0 | 0 | 0 |
| NH4+1 | 0.000726 | 100 | 0 | 0 | 0 | 0 |
| Ni+2 | 3.75E-06 | 100 | 0 | 0 | 0 | 0 |
| NO2-1 | 4.87E-45 | 100 | 0 | 0 | 0 | 0 |
| NO3-1 | 1.42E-59 | 100 | 0 | 0 | 0 | 0 |
| Pb+2 | 5.79E-08 | 100 | 0 | 0 | 0 | 0 |

| Component | Total dissolved | % dissolved | Total sorbed | % sorbed | Total precipitated | % precipitated |
|---|---|---|---|---|---|---|
| PO4-3 | 2.16E-06 | 100 | 0 | 0 | 0 | 0 |
| SO4-2 | 0.007287 | 100 | 0 | 0 | 0 | 0 |
| Zn+2 | 2.29E-05 | 100 | 0 | 0 | 0 | 0 |

# D5 Finite solids

## D5.1: Eh 150

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Metacinnabar | 4.99E-10 |
| Covellite | 1.56E-07 |

## D5.2: Eh 200

| Solid | Equilibrium amount (mol/l) |
|---|---|
| Metacinnabar | 4.62E-10 |

## D5.3: Eh 250

No soils precipitate are predicted by the model.

## D5.4: Eh 300

No soils precipitate are predicted by the model.

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Document Status

| Revision | Author | Reviewer | | Approved for Issue | | |
|---|---|---|---|---|---|---|
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