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Generic Natural Systems Evaluation - Thermodynamic Database Development and Data Management

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Used Fuel Disposition Campaign

**Generic Natural System Evaluation
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***LLNL input to SNL milestone M41UF034002:
Initiating natural system database design***

**GENERIC NATURAL SYSTEMS EVALUATION
- THERMODYNAMIC DATABASE DEVELOPMENT AND DATA MANAGEMENT -**

Lawrence Livermore National Laboratory

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Uses of Thermodynamic Data in Repository Studies

Thermodynamic data are essential for understanding and evaluating geochemical processes, as by speciation-solubility calculations, reaction-path modeling, or reactive transport simulation. These data are required to evaluate both equilibrium states and the kinetic approach to such states (via the affinity term or its equivalent in commonly used rate laws). These types of calculations and the data needed to carry them out are a central feature of geochemistry in many applications, including water-rock interactions in natural systems at low and high temperatures. Such calculations are also made in engineering studies, for example studies of interactions involving man-made materials such as metal alloys and concrete. They are used in a fairly broad spectrum of repository studies where interactions take place among water, rock, and man-made materials (e.g., usage on YMP and WIPP). Waste form degradation, engineered barrier system performance, and near-field and far-field transport typically incorporate some level of thermodynamic modeling, requiring the relevant supporting data.

Typical applications of thermodynamic modeling involve calculations of aqueous speciation (which is of great importance in the case of most radionuclides), solubilities of minerals and related solids, solubilities of gases, and stability relations among the various possible phases that might be present in a chemical system at a given temperature and pressure. If a phase can have a variable chemical composition, then a common calculational task is to determine that composition. Thermodynamic modeling also encompasses ion exchange and surface complexation processes. Any and all of these processes may be important in a geochemical process or reactive transport calculation.

Such calculations are generally carried out using computer codes. For geochemical modeling calculations, codes such as EQ3/6 and PHREEQC, are commonly used. These codes typically provide “full service” geochemistry, meaning that they use a large body of thermodynamic data, generally from a supporting database file, to sort out the various important reactions from a wide spectrum of possibilities, given specified inputs. Usually codes of this kind are used to construct models of initial aqueous solutions that represent initial conditions for some process, although sometimes these calculations also represent a desired end point. Such a calculation might be used to determine the major chemical species of a dissolved component, the solubility of a mineral or mineral-like solid, or to quantify deviation from equilibrium in the form of saturation indices. Reactive transport codes such as TOUGHREACT and NUFT generally require the user to determine which chemical species and reactions are important, and to provide the requisite set of information including thermodynamic data in an input file. Usually this information is abstracted from the output of a geochemical modeling code and its supporting thermodynamic data file.

The Yucca Mountain Project (YMP) developed two qualified thermodynamic databases to model geochemical processes, including ones involving repository components such as spent fuel. The first of the two (BSC, 2007a) was for systems containing dilute aqueous solutions only, the other (BSC, 2007b) for systems involving concentrated aqueous solutions and incorporating a model for such based on Pitzer’s (1991) equations. A 25°C-only database with similarities to the latter was also developed for the Waste Isolation Pilot Plant (WIPP, cf. Xiong, 2005). The

NAGRA/PSI database (Hummel et al., 2002) was developed to support repository studies in Europe. The YMP databases are often used in non-repository studies, including studies of geothermal systems (e.g., Wolery and Carroll, 2010) and CO₂ sequestration (e.g., Aines et al., 2011).

Types of Thermodynamic Data

Thermodynamic data generally appear in one of two forms: standard state Gibbs energies for chemical species or equilibrium constants for reactions. If one has all the necessary standard state Gibbs energies for the chemical species, one can readily calculate the equilibrium constants for an appropriate (independent) set of reactions involving these species.. The reverse is also true, and in some instances Gibbs energies are obtained from solubility data, which equates to measurement of an equilibrium constant. In other instances, Gibbs energies are obtained by calorimetric measurements, which give standard enthalpies and standard entropies, as well as heat capacities. Gibbs energies of mineral species are also sometimes derived using phase equilibrium data (cf. Helgeson et al., 1978).

Operationally, most database development starts with standard state Gibbs energies of individual chemical species. Generally values are obtained for conditions of 25°C and 1 bar pressure. Temperature dependence is dealt with by obtaining values for additional thermodynamic parameters, usually the standard state entropy at 25°C and 1 bar pressure and three or four coefficients describing the standard state heat capacity at 1 bar. The pressure dependence to low order requires the standard state molar volume at 25°C and 1 bar (for more accurate work, thermal expansibilities and compressibilities are needed). In some instances, temperature and/or pressure dependence is dealt with using equation of state (EOS) models, which have their own sets of parameters. Once one has the standard state Gibbs energies of all the relevant species at any temperature and pressure of interest, one can calculate equilibrium constants for appropriate reactions (usually in log K format) at the same temperature and pressure. For an explanation of the methodologies used in such calculations, see Helgeson et al. (1978) and Johnson et al. (1992).

In general, the Gibbs energy of a species at 25°C and 1 bar pressure is technically the Gibbs energy of formation from the chemical elements in their standard reference forms. For other temperatures and pressures, the Gibbs energy is usually dealt with as the *apparent* Gibbs energy of formation at the specified temperature and pressure (cf. Helgeson et al., 1978). Most recent tabulations of Gibbs energies of species as a function of temperature and/or pressure use this formalism (e.g., Barin and Platzki, 1995). Some older literature follows other conventions. Also, in some older literature, there may be issues with the appropriate thermodynamic properties of the chemical elements in their standard reference forms (the reference forms of certain elements may be different).

For solution phases, including aqueous solutions, standard state thermodynamic data are not enough. Thermodynamic models also require data needed to calculate thermodynamic activity coefficients. In the case of dilute aqueous solutions, the familiar Debye-Hückel equation (with some empirical extension) may suffice. Because this model depends on the ionic strength of the

solution (in addition to two Debye-Hückel parameters and possibly a third empirical parameter), calculations of activity coefficients are sometimes called “ionic strength corrections.” However, this is misleading, as the dependence on aqueous solution composition is in reality more complex. A more sophisticated model for aqueous solutions is represented by Pitzer’s equations (cf. Pitzer, 1991), which contains additional dependency on specific interactions represented by terms containing interaction coefficients. These coefficients represent an additional type of thermodynamic data. Other types of activity coefficient or “solution models” exist for aqueous solutions, solid solutions, and gas mixtures. Equation of state (EOS) models for chemical mixtures incorporate aspects of both standard state thermodynamic data and activity coefficient data.

Issues with Thermodynamic Data

Experimentally, thermodynamic data can be obtained by various means. The most common methods are based on calorimetry, solubility, and phase equilibrium (which technically encompasses solubility). The actual calculation of the data from the direct experimental data may require various corrections, including model-dependent corrections and extrapolations. Original measurements may be re-interpreted to yield somewhat different results, and re-evaluations of older data are not uncommon in the literature. In some instances, thermodynamic data are specific to a given model (e.g., interaction coefficients for Pitzer’s equations). Sometimes thermodynamic data are estimated from correlation relations (cf. Helgeson et al., 1978; Tardy and Garrels, 1974) when experimental data are lacking or experimental results are complicated by an inability to separate out various controlling factors.

There is always some uncertainty associated with thermodynamic data, regardless of how the data are obtained. In general, estimated uncertainties are not carried in thermodynamic data files intended to support thermodynamic calculations. In part, this is because uncertainties are not always provided by the sources and because when they are provided, they may not result from application of a consistent methodology. However, a larger factor is that it is difficult to carry uncertainties through complex calculations because the input uncertainties would often be correlated. It is nevertheless important to have some notion as to the magnitude of uncertainties in the data at whatever level this is practicable.

A larger issue in the treatment of thermodynamic data is that of consistency. For example, to develop a consistent set of Gibbs energies of formation for various species, it is necessary to have a consistent set of reference forms for the chemical elements. In general, consistency problems arise when either data are combined which depend on other data for which inconsistent values were used or when a correction is made to some data, but other data whose values depend on those data are not corrected. For example, in the development of the YMP dilute systems database, different values were found to be extant for the standard Gibbs energy of formation of the key aqueous phosphate species (cf. Rard and Wolery, 2007). For the sake of consistency, one set of key values had to be chosen. Then all values depending on these key data needed to be made consistent with the chosen set of key values. Another example discussed in BSC (2007a) concerned the appropriate Gibbs energy for the key species $\text{SiO}_{2(\text{aq})}$.

In building a thermodynamic database, it is easy to introduce inconsistencies, because one may not know how certain adopted data were obtained by the sources. There is a particular problem with older tabulations of thermodynamic data (e.g., Wagman et al., 1982) that simply give “recommended data” without identifying the actual sources, let alone the logic leading to the “recommendations.”

Sources of Thermodynamic Data

The development of thermodynamic databases has a long history in geochemistry (e.g., Garrels and Christ, 1965; Helgeson et al., 1969; Helgeson et al., 1978, Johnson et al., 1992; Robie and Hemingway, 1995), paralleled by related and applicable work in the larger scientific community (e.g., Wagman et al., 1982, 1989; Cox et al., 1989; Barin and Platzki, 1995; Binneweis and Milke, 1999). Unfortunately, the National Bureau of Standards (now the National Institutes of Science and Technology) no longer generally addresses thermodynamic data pertaining to aqueous, mineral, and gas species, its last work being the compilation of Wagman et al. (1982) and the errata published in 1989. IUPAC, whose efforts in this area were generally limited to data pertaining to key species only (a small subset), has not done much in this area since the publication of the Cox et al. (1989) report. The standards organizations have been basically inactive regarding thermodynamic data of interest to geochemical and repository studies for over twenty years. For radionuclide elements, much of this void has been filled by the European Nuclear Energy Agency (NEA), which has sponsored a series of review volumes (e.g., Grenthe et al., 1992 [1 uranium]; Silva et al., 1995 [2 americium]; Rard et al., 1999 [3 technetium]; Lemire et al., 2001 [4 neptunium and plutonium]; Guillaumont et al., 2003 [5 update on uranium, neptunium, plutonium americium, and technetium]; Gamsjäger et al., 2005 [6 nickel]; and Olin et al., 2005 [7 selenium]).

The YMP dilute systems database is widely used in the geochemistry community for a variety of applications involving rock/water interactions. It builds on the work of Prof. Helgeson and his students (see BSC, 2007a for many applicable references), and covers a significant range of temperature (25-300°C). The last version (data0.ymp.R5) covers 86 chemical elements, 1219 aqueous species, 1156 minerals and other solids species, and 128 gas species, detailed in Appendix A. Many data for actinide species have been adopted from the Nuclear Energy Agency (NEA) series of volumes on actinide thermodynamics (see references given in BSC, 2007a), and the appropriate temperature extrapolations have been applied. The YMP concentrated systems database (data0.ypf.R2) covers a smaller chemical system (40 chemical elements, 237 aqueous species, 470 minerals and other solids, and 11 gas species), detailed in Appendix B. It includes temperature dependence, which for many species extends to 200°C, but for others extends to 250°C, to 110°C, or is restricted to 25°C. It is based on many sources (see BSC, 2007b), but draws in particular from the work of Pabalan and Pitzer (1987) and Greenberg and Møller (1989). In addition to their other characteristics, these databases have a regulatory cachet as qualified products of YMP and have already undergone peer-review and QA review.

Data Gaps

The purpose of the present task is to improve these databases for use in the Used Fuel Disposition Campaign and maintain some semblance of order that will support qualification in support of the development of future underground high-level nuclear waste disposal. The work is presently supported by THCM, EBS, and Natural Systems, with the THCM support being incorporated into the EBS work package for FY12. The YMP design was based on disposal in volcanic tuff, in a thick vadose zone in which oxidizing conditions were expected to prevail. A 50-year period of tunnel ventilation was planned to limit maximum temperature. Concentrated solutions were not originally expected at Yucca Mountain. Later concerns about dust deliquescence and evaporative concentration led to the development of the YMP concentrated solutions thermodynamic database (see BSC, 2007b). The YMP design scenario was very different from those for planned repositories in other countries, which envision disposal below the water table (generally under reducing conditions) in clay, salt, granite or other hard rock, usually incorporating relatively low maximum temperature in the designs. The Used Fuel Disposition program is investigating potential disposal in mined repositories in these three rock types, plus a deep borehole option (which appears to imply in granite or other hard rock). The UFD may consider higher maximum temperatures than are presently being considered in other countries, although at present it is focusing on similar design options.

Although the YMP thermodynamic databases incorporated many data of value to generic geochemistry applications, in some areas development was limited owing to the expected generally oxidizing conditions and limited maximum temperatures associated with the YMP design scenario. Consequently, these databases need some additional development to adequately address the different design scenarios being addressed by the Used Fuel Disposition program. There is a need to address a somewhat wider range of mineralogy because of the different rock types. There is a need to fill some gaps arising due to the expectation of reducing instead of oxidizing conditions. There is also a need to address some other things that were not addressed because they were not relevant to the YMP design scenario. Finally, in any effort using thermodynamic data, there is the ever-present factor of flaws being discovered in existing data, and the potential impact of new data reported elsewhere. Errors (and the suspicion of errors) generally come to light in the application of the data.

The following areas are now of concern for thermodynamic database development under UFD:

- Data (and mixing models) for complex clays, including illites and smectites, and certain related sheet silicates (being addressed during FY11-12 in THCM/EBS work packages). Clay minerals play various roles in the geologic disposal of nuclear waste (for an overview of clays from the perspective of the UFD Natural Systems department, see Chapter 4 of *Natural System Evaluation and Tool Development – FY11 Progress Report*: Wang et al., 2011). Clay minerals are nearly ubiquitous at some level in nearly all rock types, ranging from minor alteration components in igneous rocks to major components in sedimentary rocks, notably shales and claystones. Clays may be used as components (often with modification) in an engineered repository, usually in an attempt to limit the access of water to waste containers and/or waste forms. Clays may form (or transform,

potentially to other minerals) in a repository, in response to water circulation and the thermal field that decaying waste may generate.

- Data for certain zeolites, particularly ones for which the data do not trace to Helgeson et al. (1978). Geothermal systems modeling (Wolery and Carroll, 2010) suggested that the data in question here may not be consistent with proper stable mineral assemblages in the geologic systems of interest.
- Data that continue to come out of the NEA review program (or which have come out but were not incorporated into the YMP databases).
- Other new data from other sources not previously incorporated into the database (e.g., the Fe^{2+} and Fe^{3+} data recommended by Parker and Khodakovskii, 1995, which are likely to be adopted by the NEA).
- Additional data for sulfide minerals (which may be very important in UFD disposal systems but were not important to YMP). The mineral pyrite (nominal composition FeS_2) allows many chemical substitutions and could be a sink for some important radionuclides.
- Isolated errors discovered since the termination of the YMP (example: the Gibbs energy and related calorimetric data for $\text{NaHCO}_3(\text{c})$ in the YMP concentrated systems database were found to be inaccurate in the course of a CO_2 air capture project).
- Data for ion exchange and surface complexation processes. For surface complexation, one or more specific models need to be chosen (a fair number are extant).

The last YMP dilute systems thermodynamic database (data0.ymp.R5) contains data derived by such means for some clay compositions shown below in Table 1. A detailed description of the methods and derivation of the corresponding thermodynamic data is given in the Analysis/Model Report ANL-WIS-GS-000003 Rev. 1 (BSC, 2007a). The development follows that of Tardy and Garrels (1974), except that the more recent work includes updated values for the Gibbs energy data used to regress the values for the silicate oxides and also (in the case of subsequent calculation of equilibrium constants) updated values for the Gibbs energies of the relevant aqueous species. Data were obtained for idealized clays with implicitly fully-hydrated smectite end-members, including five beidellites, five saponites, five montmorillonites and five nontronites. These data were intended to be used in solid solution models in modeling software. Data were also obtained by the same process for an illite and three celadonites, and some chlorite and chlorite-related sheet silicates, which will not be noted here.

The Tardy and Garrels (1974) approach does not account for the water of hydration present in the smectite interlayer. In reality, a sodium beidellite for example would have a formula represented by $\text{Na}_{0.33}\text{Al}_2\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2.n\text{H}_2\text{O}$, where n might potentially be as high as 7. However, a key point is that the amount of interlayer water is variable, depending on temperature, pressure, water activity (or pressure), and which cations are in the interlayer. We are looking at models for variable hydration that can be combined with the Tardy-Garrels approach to achieve more accurate models and data for the smectites. Interesting approaches are suggested by Ransom and Helgeson (1993, 1994ab, 1995), Tardy and Duplay 1992, Viellard (1994ab, 2000), Vidal and Dubacq (2011), and others.

Table 1. Gibbs energy data for 20 idealized clays.

Name	Formula	ΔG_f° , cal/mol	Reference Reaction
H-Beidellite	$H_{0.33}Al_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1260419.6	H-Beidellite = Pyrophyllite + 0.165 H_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Na-Beidellite	$Na_{0.33}Al_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1279691.6	Na-Beidellite = Pyrophyllite + 0.165 Na_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
K-Beidellite	$K_{0.33}Al_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1281777.2	K-Beidellite = Pyrophyllite + 0.165 K_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Ca-Beidellite	$Ca_{0.165}Al_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1280912.6	Ca-Beidellite = Pyrophyllite + 0.165 CaO_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Mg-Beidellite	$Mg_{0.165}Al_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1277068.1	Mg-Beidellite = Pyrophyllite + 0.165 MgO_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
H-Saponite	$H_{0.33}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1324610.6	H-Saponite = Talc + 0.165 H_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Na-Saponite	$Na_{0.33}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1343882.6	Na-Saponite = Talc + 0.165 Na_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
K-Saponite	$K_{0.33}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1345968.2	K-Saponite = Talc + 0.165 K_2O_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Ca-Saponite	$Ca_{0.165}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1345103.6	Ca-Saponite = Talc + 0.165 CaO_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
Mg-Saponite	$Mg_{0.165}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1341259.1	Mg-Saponite = Talc + 0.165 MgO_{ex} + 0.165 Al_2O_3 - 0.33 SiO_2
H-Montmorillonite	$H_{0.33}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	-1251321.9	H-Montmorillonite = Pyrophyllite + 0.165 H_2O_{ex} + 0.33 MgO - 0.165 Al_2O_3
Na-Montmorillonite	$Na_{0.33}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	-1270593.9	Na-Montmorillonite = Pyrophyllite + 0.165 Na_2O_{ex} + 0.33 MgO - 0.165 Al_2O_3
K-Montmorillonite	$K_{0.33}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	-1272679.5	K-Montmorillonite = Pyrophyllite + 0.165 K_2O_{ex} + 0.33 MgO - 0.165 Al_2O_3
Ca-Montmorillonite	$Ca_{0.165}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	-1271814.9	Ca-Montmorillonite = Pyrophyllite + 0.165 CaO_{ex} + 0.33 MgO - 0.165 Al_2O_3
Mg-Montmorillonite	$Mg_{0.165}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	-1267970.4	Mg-Montmorillonite = Pyrophyllite + 0.165 MgO_{ex} + 0.33 MgO - 0.165 Al_2O_3
H-Nontronite	$H_{0.33}Fe_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1058235.0	H-Nontronite = Pyrophyllite + 0.165 H_2O_{ex} + Fe_2O_3 - Al_2O_3 + 0.165 Al_2O_3 - 0.33 SiO_2
Na-Nontronite	$Na_{0.33}Fe_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1077507.0	Na-Nontronite = Pyrophyllite + 0.165 Na_2O_{ex} + Fe_2O_3 - Al_2O_3 + 0.165 Al_2O_3 - 0.33 SiO_2
K-Nontronite	$K_{0.33}Fe_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1079592.6	K-Nontronite = Pyrophyllite + 0.165 K_2O_{ex} + Fe_2O_3 - Al_2O_3 + 0.165 Al_2O_3 - 0.33 SiO_2
Ca-Nontronite	$Ca_{0.165}Fe_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1078728.0	Ca-Nontronite = Pyrophyllite + 0.165 CaO_{ex} + Fe_2O_3 - Al_2O_3 + 0.165 Al_2O_3 - 0.33 SiO_2
Mg-Nontronite	$Ca_{0.165}Fe_2Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-1074883.5	Mg-Nontronite = Pyrophyllite + 0.165 MgO_{ex} + Fe_2O_3 - Al_2O_3 + 0.165 Al_2O_3 - 0.33 SiO_2

Note: The data shown here were derived in the YMP work described in BSC (2007a), except that the results for montmorillonites and nontronites that were originally obtained by oxide summation are here updated to correspond to the reference reactions shown here.

We intend to improve the existing data/models for complex clays by:

- Explicitly accounting for water in the exchange layers of smectites and vermiculites
- Accounting for a broader spectrum of physical measurements (e.g., basal spacing studies of clay dehydration, swelling pressure data, ion exchange data over a wide range of temperature)
- Including insights from molecular dynamics (MD) modeling regarding dehydration

Data Management Requirements

The types of thermodynamic data have been discussed previously. We are planning to continue the methods and formats used previously for YMP. For the product data files, we will follow the general EQ3/6 format. This consists of a human-readable text file on which log K data are given on a temperature grid. Underlying this will be a SUPCRT92 data file, which is also human-readable, and various types of Excel files that include standard methods for processing thermodynamic data into the desired log K grid form. One of the functions of the Excel files is to carry out the extrapolation of Gibbs energies to higher temperatures and pressures, and to compute the equilibrium constant values for the chosen chemical reactions. Another tool worth noting is the EQPT code from the EQ3/6 package, which is a database file preprocessor that runs many error checks. Basically, all the necessary data management tools run on a Windows PC, although most or all of them can be ported to other operating systems.

An EQ3/6 data file contains the following main elements: a title (descriptive text), a chemical elements block containing elemental symbols and atomic weights, a “superblock” of blocks for aqueous species, a superblock for pure mineral species, a superblock for gas species, a superblock for solid solutions, and a block or superblock of parameters for calculating the activity coefficients of aqueous species. Here a “superblock” is a sequence of data-blocks. An EQ3/6 data-block for an aqueous complex species is illustrated by the following one for $\text{NpO}_2(\text{OH})_2^-$ (from the data file data0.ymp.R5):

```
+-----
NpO2(OH)2-
  sp.type =  aqueous
  [ ]
  charge  = -1.0
****
  3 element(s):
    2.0000 H           1.0000 Np           4.0000 O
****
  4 species in reaction:
-1.0000 NpO2(OH)2-      -2.0000 H+
  1.0000 NpO2+          2.0000 H2O
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
    25.5045   23.6147   21.4199   19.4099
    17.4475   15.9411   14.7957   13.9864
*
*   P-T extrapolation method: isocoulombic/isoelectric method
*   Data workup source: AqueousSpecies_j_TJW_1.xls
*   Reference-state data source: 01lem/nea
+-----
```

The information includes the species name, the electrical charge number, the chemical composition, the associated chemical reaction, the log K grid for that reaction, and information concerning the provenance of the data. A data-block for a mineral species is very similar, but includes a molar volume (V_0^{PrTr}) instead of an electrical charge number. The following example is also from data0.ymp.R5.

```

+-----
Np2O5
  sp.type =  solid
  [ ]
  V0PrTr =      0.000 cm^3/mol [source:      ]
****
  2 element(s):
    2.0000 Np      5.0000 O
****
  4 species in reaction:
    -1.0000 Np2O5      -2.0000 H+
     1.0000 H2O       2.0000 NpO2+
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
      4.9214      3.7031      2.1757      0.6695
      -0.9387     -2.3319     -3.5852     -4.7609
*
*   P-T extrapolation method: Mixed Cp integration + SUPCRT calc
*   Data workup source: Minerals_j_PVB_Np.xls
*   Reference-state data source: 01lem/nea
+-----

```

A data-block for a gas species is very similar. For Pitzer interaction coefficients, a data-block exists for each species pair or triplet. The following example is the data-block for the Na⁺-Cl⁻ pair from data0.ypf.R2.

```

+-----
Na+      Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0):
    a1 = 7.45618073E-02
    a2 = -4.70789056E+02
    a3 = -1.85114134E+00
    a4 = 1.65564633E-03
  beta(1):
    a1 = 2.75240690E-01
    a2 = -5.21117635E+02
    a3 = -2.88035999E+00
    a4 = 4.71462791E-03
  beta(2):
    a1 = 0
    a2 = 0
    a3 = 0
    a4 = 0
  Cphi:
    a1 = 1.53693372E-03
    a2 = 4.80725476E+01
    a3 = 1.74679979E-01
    a4 = -1.56268596E-04
* Source: refit of 89Gre/Mol [FitPitzerNC_MX_NaCl.xls]
+-----

```

Presently the EQ3/6 format does not include data-blocks for surface complexation model species, but ones analogous to those for aqueous or pure mineral species will be included for future UFD use. The same is true for ion exchange species.

We note that a conversion program was written on YMP to convert data0.ymp.R5 from EQ3/6 to PHREEQC format, and that some other conversion programs may exist or can be written. Thus, it should be possible to provide the data developed under UFD for use in other codes.

For YMP, the thermodynamic databases were documented under the Analysis/Model Report system and kept for download on the Technical Data Management system (TDMS). Generally, for each version of a data file, two data packages (“DTNs”) were prepared, one containing the data file itself, the other containing materials used to construct it (usually SUPCRT92 runs and Excel spreadsheets). In terms of download capability for UFD, we envision something similar using the Sandia Sharepoint system or some other system to be developed.

Because of the general applicability of these databases in geochemistry and allied fields, it would be highly desirable to make them downloadable to the public on a web page. The advantage of this is that it would allow researchers working in areas like geothermal, underground carbon sequestration, and environmental management to exercise the data and provide useful feedback.

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Appendix A: Minerals and Species Included in the Dilute Systems Database

Table A1. Elements in data0.ymp.R5

Ag	Mg	W
Al	Mn	Y
Am	Mo	Yb
Ar	N	Zn
As	Na	Zr
Au	Nb	
B	Nd	
Ba	Ne	
Be	Ni	
Bi	Np	
Br	O	
C	P	
Ca	Pb	
Cd	Pd	
Ce	Pm	
Cl	Pr	
Co	Pt	
Cr	Pu	
Cs	Ra	
Cu	Rb	
Dy	Re	
Er	Rh	
Eu	Rn	
F	Ru	
Fe	S	
Fr	Sb	
Ga	Sc	
Gd	Se	
H	Si	
He	Sm	
Hf	Sn	
Hg	Sr	
Ho	Tb	
I	Tc	
In	Th	
K	Ti	
Kr	Tl	
La	Tm	
Li	U	
Lu	V	

Table A2. Aqueous species in data0.ymp.R5

H2O	Mg++	Zn++
Ag+	Mn++	ZrO++
Al+++	MoO4--	O2(g)
Am++++	NH3(aq)	HS-
Ar(aq)	Na+	Acetic_acid(aq)
Au+	NbO3-	Formic_acid(aq)
B(OH)3(aq)	Nd+++	S2--
Ba++	Ne(aq)	Ag++
Be++	Ni++	Am++
Bi+++	NpO2+	Am++++
Br-	Pb++	AmO2+
Ca++	Pd++	AmO2++
Cd++	Pm+++	Au+++
Ce+++	Pr+++	BH4-
Cl-	Pt++	Br3-
Co++	PuO2+	BrO-
CrO4--	Ra++	BrO3-
Cs+	Rb+	BrO4-
Cu++	ReO4-	CN-
Dy+++	Rh+++	Ce++
Er+++	Rn(aq)	Ce++++
Eu+++	RuO4--	ClO-
F-	SO4--	ClO2-
Fe++	SbO2-	ClO3-
Fr+	Sc+++	ClO4-
Ga+++	SeO3--	Co+++
Gd+++	SiO2(aq)	Cr++
H+	Sm+++	Cr+++
H2AsO4-	Sn++	CrO4---
HCO3-	Sr++	Cu+
HPO4--	Tb+++	Dy++
He(aq)	TcO4-	Er++
Hf++++	Th++++	Ethane(aq)
Hg++	Ti(OH)4(aq)	Eu++
Ho+++	Tl+	Fe+++
I-	Tm+++	Formaldehyde(aq)
In+++	UO2++	Gd++
K+	VO2+	H2(aq)
Kr(aq)	WO4--	H2O2(aq)
La+++	Xe(aq)	H2AsO3-
Li+	Y+++	H2P2O7--
Lu+++	Yb+++	H2PO2-

Note: Tabulated as basis species followed by auxiliary basis species

Table A2. Aqueous species in data0.ymp.R5 (cont.)

HPO3--	S4O6--	Ag(CO3)2---
HSO5-	S5--	Ag(HS)2-
HSe-	S5O6--	AgCO3-
Hg2++	SCN-	AgCl(aq)
Ho++	SO3--	AgCl2-
I3-	SeO4--	AgCl3--
IO-	Sm++	AgCl4---
IO3-	Sn++++	AgF(aq)
IO4-	Tb++	AgNO3(aq)
La++	TcO++	AgO-
Methane(aq)	TcO4--	AgOH(aq)
Methanol(aq)	Tl+++	Al(SO4)2-
Mn+++	Tm++	Al13O4(OH)24(7+)
MnO4--	U+++	Al2(OH)2++++
N2(aq)	U++++	Al3(OH)4(5+)
N2O2--	UO2+	AlF++
N3-	V++	AlF2+
NO2-	V+++	AlF3(aq)
NO3-	VO++	AlF4-
Nd++	Yb++	AlH2PO4++
Np+++	Zr++++	AlHPO4+
Np++++	(NH4)2Sb2S4(aq)	AlO+
NpO2++	(NpO2)2(OH)2++	AlO2-
O2(aq)	(NpO2)2CO3(OH)3-	AlOH++
Pm++	(NpO2)3(CO3)6(-6)	AlSO4+
Pr++	(NpO2)3(OH)5+	Am(CO3)2-
Pu+++	(PuO2)2(OH)2++	Am(CO3)3---
Pu++++	Pu(CO3)5-----	Am(CO3)5(6-)
PuO2++	(PuO2)3(CO3)6(6-)	AmO2(CO3)3----
Rh++	(UO2)11(CO3)6(OH)12--	Am(OH)2+
Ru(OH)2++	(UO2)2(OH)2++	Am(OH)3(aq)
Ru++	(UO2)2(PuO2)(CO3)6(6-)	Am(SO4)2-
Ru+++	(UO2)2CO3(OH)3-	AmCO3+
RuO4-	(UO2)2NpO2(CO3)6(6-)	AmCl++
RuO4(aq)	(UO2)2OH+++	AmF++
S2O3--	(UO2)3(CO3)6(6-)	AmF2+
S2O4--	(UO2)3(OH)4++	AmH2PO4++
S2O6--	(UO2)3(OH)5+	AmN3++
S2O8--	(UO2)3(OH)7-	AmNO2++
S3--	(UO2)3O(OH)2(HCO3)+	AmNO3++
S3O6--	(UO2)4(OH)7+	AmOH++
S4--	(VO)2(OH)2++	AmSO4+

Table A2. Aqueous species in data0.ympr.R5 (cont.)

AsO3F--	CaHSiO3+	CdP2O7--
AsO4---	CaNO3+	CdSCN+
Au(HS)2-	CaOH+	CdSO4(aq)
AuCl(aq)	CaP2O7--	CdSeO4(aq)
AuCl2-	CaPO4-	Ce(CO3)2-
AuCl3--	CaSO4(aq)	Ce(HPO4)2-
AuCl4-	Cd(CN)2(aq)	Ce(OH)2+
B2O(OH)5-	Cd(CN)3-	Ce(OH)2++
BF2(OH)2-	Cd(CN)4--	Ce(OH)3(aq)
BF3OH-	Cd(CO3)2--	Ce(PO4)2---
BF4-	Cd(N3)2(aq)	Ce2(OH)2(6+)
BO2-	Cd(N3)3-	Ce3(OH)5++++
BaB(OH)4+	Cd(N3)4--	CeCO3+
BaCO3(aq)	Cd(NH3)++	CeCl++
BaCl+	Cd(NH3)2++	CeF++
BaF+	Cd(NH3)4++	CeF2+
BaHCO3+	Cd(OH)Cl(aq)	CeH2PO4++
BaNO3+	Cd(SCN)2(aq)	CeHCO3++
BaOH+	Cd(SCN)3-	CeHPO4+
BeCl+	Cd2OH+++	CeNO3++
BeCl2(aq)	Cd4(OH)4++++	CeOH++
BeF+	CdBr+	CeOH+++
BeF2(aq)	CdBr2(aq)	CePO4(aq)
BeF3-	CdBr3-	CeSO4+
BeF4--	CdCN+	Co2(OH)3+
BeO(aq)	CdCO3(aq)	Co4(OH)4++++
BeO2--	CdCl+	CoBr2(aq)
BeOH+	CdCl2(aq)	CoCl+
BiO+	CdCl3-	CoF+
BiO2-	CdCl4--	CoI2(aq)
BiOH++	CdF+	CoNO3+
Br2(aq)	CdF2(aq)	CoO(aq)
CO2(aq)	CdHCO3+	CoO2--
CO3--	CdI+	CoOH+
CaB(OH)4+	CdI2(aq)	CoOH++
CaCO3(aq)	CdI3-	CoSO4(aq)
CaCl+	CdI4--	CoSeO4(aq)
CaCl2(aq)	CdN3+	Cr2O7--
CaCrO4(aq)	CdNO2+	CrOH++
CaF+	CdO(aq)	Cr(OH)3(aq)
CaHCO3+	CdO2--	CrBr++
CaHPO4(aq)	CdOH+	CrCl++

Table A2. Aqueous species in data0.ympr.R5 (cont.)

CrCl ₂ ⁺	Er(OH) ₂ ⁺	Fe ₂ (OH) ₂ ⁺⁺⁺⁺
CrO ⁺	Er(OH) ₃ (aq)	Fe ₃ (OH) ₄ (5 ⁺)
CrO ₂ ⁻	Er(OH) ₄ ⁻	FeCO ₃ (aq)
CrO ₃ Cl ⁻	Er(PO ₄) ₂ ⁻⁻⁻	FeCl ⁺
CsBr(aq)	Er(SO ₄) ₂ ⁻	FeCl ⁺⁺
CsCl(aq)	ErCO ₃ ⁺	FeCl ₂ (aq)
CsI(aq)	ErCl ⁺⁺	FeF ⁺
CsOH(aq)	ErF ⁺⁺	FeF ⁺⁺
Cu(NH ₃) ₂ ⁺⁺	ErH ₂ PO ₄ ⁺⁺	FeF ₂ ⁺
Cu(NH ₃) ₃ ⁺⁺	ErHCO ₃ ⁺⁺	FeH ₂ PO ₄ ⁺
CuCl(aq)	ErHPO ₄ ⁺	FeH ₂ PO ₄ ⁺⁺
CuCl ⁺	ErNO ₃ ⁺⁺	FeHCO ₃ ⁺
CuCl ₂ (aq)	ErOH ⁺⁺	FeNO ₂ ⁺⁺
CuCl ₂ ⁻	ErPO ₄ (aq)	FeNO ₃ ⁺⁺
CuCl ₃ ⁻	ErSO ₄ ⁺	FeO(aq)
CuCl ₃ ⁻⁻	Eu(CO ₃) ₂ ⁻	FeO ⁺
CuCl ₄ ⁻⁻	Eu(HPO ₄) ₂ ⁻	FeO ₂ ⁻
CuF ⁺	Eu(OH) ₂ ⁺	FeOH ⁺
CuNH ₃ ⁺⁺	Eu(OH) ₃ (aq)	FeOH ⁺⁺
CuO(aq)	Eu(PO ₄) ₂ ⁻⁻⁻	FeSO ₄ (aq)
CuO ₂ ⁻⁻	Eu(SO ₄) ₂ ⁻	FeSO ₄ ⁺
CuOH ⁺	EuBr ⁺⁺	Formate
CuSO ₄ (aq)	EuBr ₂ ⁺	GaO ⁺
Dy(CO ₃) ₂ ⁻	EuBrO ₃ ⁺⁺	GaO ₂ ⁻
Dy(HPO ₄) ₂ ⁻	EuCO ₃ ⁺	GaOH ⁺⁺
Dy(OH) ₂ ⁺	EuCl ⁺⁺	Gd(CO ₃) ₂ ⁻
Dy(OH) ₃ (aq)	EuCl ₂ ⁺	Gd(HPO ₄) ₂ ⁻
Dy(OH) ₄ ⁻	EuF ⁺⁺	Gd(OH) ₂ ⁺
Dy(PO ₄) ₂ ⁻⁻⁻	EuF ₂ ⁺	Gd(OH) ₃ (aq)
Dy(SO ₄) ₂ ⁻	EuF ₃ (aq)	Gd(OH) ₄ ⁻
DyCO ₃ ⁺	EuH ₂ PO ₄ ⁺⁺	Gd(PO ₄) ₂ ⁻⁻⁻
DyCl ⁺⁺	EuHCO ₃ ⁺⁺	Gd(SO ₄) ₂ ⁻
DyF ⁺⁺	EuHPO ₄ ⁺	GdCO ₃ ⁺
DyH ₂ PO ₄ ⁺⁺	EuIO ₃ ⁺⁺	GdCl ⁺⁺
DyHCO ₃ ⁺⁺	EuNO ₃ ⁺⁺	GdF ⁺⁺
DyHPO ₄ ⁺	EuOH ⁺⁺	GdF ₂ ⁺
DyNO ₃ ⁺⁺	EuPO ₄ (aq)	GdH ₂ PO ₄ ⁺⁺
DyOH ⁺⁺	EuSO ₄ ⁺	GdHCO ₃ ⁺⁺
DyPO ₄ (aq)	Fe(CO ₃) ₂ ⁻⁻	GdHPO ₄ ⁺
DySO ₄ ⁺	Fe(OH) ₃ ⁻	GdNO ₃ ⁺⁺
Er(CO ₃) ₂ ⁻	Fe(OH) ₄ ⁻⁻	GdOH ⁺⁺
Er(HPO ₄) ₂ ⁻	Fe(SO ₄) ₂ ⁻	GdPO ₄ (aq)

Table A2. Aqueous species in data0.ymp.R5 (cont.)

GdSO4+	HHfO2+	HfO++
H2CrO4(aq)	HHfO3-	HfO2(aq)
H2MoO4(aq)	HHgO2-	HfOH+++
H2N2O2(aq)	HIO(aq)	HgCl+
H2PO3-	HIO3(aq)	HgCl2(aq)
H2PO3F(aq)	HInO2(aq)	HgCl3-
H2PO4-	HMnO2-	HgCl4--
H2S(aq)	HMoO4-	HgF+
H2S2O3(aq)	HN2O2-	HgO(aq)
H2S2O4(aq)	HN3(aq)	HgOH+
H2SO3(aq)	HNO2(aq)	Ho(CO3)2-
H2SO4(aq)	HNO3(aq)	Ho(HPO4)2-
H2Se(aq)	HNbO3(aq)	Ho(OH)2+
H2SeO3(aq)	HNiO2-	Ho(OH)3(aq)
H2VO4-	HO2-	Ho(PO4)2---
H3AsO4(aq)	HP2O7---	Ho(SO4)2-
H3P2O7-	HPO2F2(aq)	HoCO3+
H3PO2(aq)	PO2F2-	HoF++
H3PO3(aq)	HPO3F-	HoH2PO4++
H3PO4(aq)	HPbO2-	HoHCO3++
H3VO4(aq)	HRuO5-	HoHPO4+
H4P2O7(aq)	HS2O3-	HoNO3++
HAIO2(aq)	HS2O4-	HoOH++
HAsO2(aq)	HSO3-	HoPO4(aq)
HAsO3F-	HSO4-	HoSO4+
HAsO4--	HSbO2(aq)	InCl++
HAsS2(aq)	HScO2(aq)	InF++
HBeO2-	HSeO3-	InO+
HBiO2(aq)	HSeO4-	InO2-
HBrO(aq)	CaSeO4(aq)	InOH++
HCdO2-	HSiO3-	KBr(aq)
HClO(aq)	HSnO2-	KCl(aq)
HClO2(aq)	HTlO2(aq)	KHSO4(aq)
HCoO2-	HUO2(aq)	KI(aq)
HCrO2(aq)	HUO2+	KOH(aq)
HCrO4-	HUO3-	KP2O7---
HCuO2-	HUO4-	KSO4-
HF(aq)	HVO4--	La(CO3)2-
HF2-	HWO4-	La(HPO4)2-
HFeO2(aq)	HZnO2-	La(OH)2+
HFeO2-	HZrO2+	La(OH)3(aq)
HGaO2(aq)	HZrO3-	La(PO4)2---

Table A2. Aqueous species in data0.ympr.R5 (cont.)

La(SO4)2-	MgOH+	Nd2(OH)2++++
La2(OH)2++++	MgP2O7--	NdCO3+
La5(OH)9(6+)	MgSO4(aq)	NdCl++
LaCO3+	Mn(NO3)2(aq)	NdF++
LaCl++	Mn2(OH)3+	NdH2PO4++
LaF++	Mn2OH+++	NdHCO3++
LaF2+	MnCl+	NdHPO4+
LaF3(aq)	MnCl3-	NdNO3++
LaH2PO4++	MnF+	NdOH++
LaHCO3++	MnHCO3+	NdPO4(aq)
LaHPO4+	MnNO3+	NdSO4+
LaNO3++	MnO(aq)	NiCO3(aq)
LaOH++	MnO2--	NiCrO4(aq)
LaPO4(aq)	MnO4-	Ni(NH3)2++
LaSO4+	MnOH+	Ni(NH3)6++
LiCl(aq)	MnSO4(aq)	Ni(NO3)2(aq)
LiOH(aq)	MnSeO4(aq)	Ni(OH)2(aq)
LiSO4-	N2H5+	Ni(OH)3-
Lu(CO3)2-	N2H6++	NiBr+
Lu(HPO4)2-	NH4+	NiCl+
Lu(OH)2+	NH4SO4-	NiF+
Lu(OH)3(aq)	NH4SbO2(aq)	NiHP2O7-
Lu(PO4)2---	Na2P2O7--	NiNO3+
Lu(SO4)2-	NaB(OH)4(aq)	NiO(aq)
LuCO3+	NaBr(aq)	NiO2--
LuCl++	NaCO3-	NiOH+
LuF++	NaCl(aq)	NiP2O7--
LuH2PO4++	NaF(aq)	NiSeO4(aq)
LuHCO3++	NaHCO3(aq)	Np(CO3)3---
LuHPO4+	NaHP2O7--	Np(CO3)4----
LuNO3++	NaHSiO3(aq)	Np(CO3)5(6-)
LuOH++	NaI(aq)	Np(OH)4(aq)
LuPO4(aq)	NaOH(aq)	Np(SO4)2(aq)
LuSO4+	NaP2O7---	Np(SCN)+++
Mg4(OH)4++++	NaSO4-	Np(SCN)2++
MgB(OH)4+	Nd(CO3)2-	Np(SCN)3+
MgCO3(aq)	Nd(HPO4)2-	NpCl+++
MgCl+	Nd(OH)2+	NpF+++
MgF+	Nd(OH)3(aq)	NpF2++
MgHCO3+	Nd(OH)4-	NpI+++
MgHPO4(aq)	Nd(PO4)2---	NpNO3+++
MgHSiO3+	Nd(SO4)2-	NpO2(CO3)2--

Table A2. Aqueous species in data0.ympr.R5 (cont.)

NpO2(CO3)2---	PbBr2(aq)	PmNO3++
NpO2(CO3)2OH----	PbBr3-	PmOH++
NpO2(CO3)3(5-)	PbBrO3+	PmPO4(aq)
NpO2(CO3)3----	PbCl+	PmSO4+
NpO2(HPO4)2--	PbCl2(aq)	Pr(CO3)2-
NpO2(OH)2-	PbCl3-	Pr(HPO4)2-
NpO2(SO4)2--	PbCl4--	Pr(OH)2+
NpO2Cl+	PbClO3+	Pr(OH)3(aq)
NpO2CO3-	PbF+	Pr(PO4)2---
NpO2CO3(aq)	PbF2(aq)	Pr(SO4)2-
NpO2F(aq)	PbH2PO4+	PrCO3+
NpO2F+	PbHPO4(aq)	PrCl++
NpO2F2(aq)	PbI+	PrF++
NpO2H2PO4+	PbI2(aq)	PrH2PO4++
NpO2HPO4-	PbI3-	PrHCO3++
NpO2HPO4(aq)	PbI4--	PrHPO4+
NpO2IO3(aq)	PbNO3+	PrNO3++
NpO2IO3+	PbO(aq)	PrOH++
NpO2OH(aq)	PbOH+	PrPO4(aq)
NpO2OH+	PbP2O7--	PrSO4+
NpO2SO4(aq)	PbSCN+	Pt(SO4)2--
NpO2SO4-	Pd(SO4)2--	Pt(SO4)3----
NpOH++	Pd(SO4)3----	PtCl+
NpOH+++	PdCl+	PtCl2(aq)
NpSO4++	PdCl2(aq)	PtCl3-
OH-	PdCl3-	PtCl4--
P2O7----	PdCl4--	PtO(aq)
PH4+	PdO(aq)	PtOH+
PO3F--	PdOH+	PtSO4(aq)
PO4---	PdSO4(aq)	Pu(SO4)2(aq)
Pb(BrO3)2(aq)	Pm(CO3)2-	Pu(SO4)2-
Pb(ClO3)2(aq)	Pm(HPO4)2-	PuBr+++
Pb(HS)2(aq)	Pm(OH)2+	PuCl+++
Pb(HS)3-	Pm(OH)3(aq)	PuF+++
Pb(OH)2(aq)	Pm(PO4)2---	PuF2++
Pb(OH)3-	Pm(SO4)2-	PuH3PO4++++
Pb(SCN)2(aq)	PmCO3+	PuI++
Pb2OH+++	PmCl++	PuNO3+++
Pb3(OH)4++	PmF++	PuO2(CO3)2--
Pb4(OH)4++++	PmH2PO4++	PuO2(CO3)3----
Pb6(OH)8++++	PmHCO3++	PuO2(CO3)3(5-)
PbBr+	PmHPO4+	PuO2(OH)2(aq)

Table A2. Aqueous species in data0.ymp.R5 (cont.)

PuO ₂ (SO ₄) ₂ --	Ru(OH) ₂ Cl ₂ (aq)	SmF ⁺⁺
PuO ₂ Cl ⁺	Ru(OH) ₂ Cl ₃ -	SmH ₂ PO ₄ ⁺⁺
PuO ₂ Cl ₂ (aq)	Ru(OH) ₂ Cl ₄ --	SmHCO ₃ ⁺⁺
PuO ₂ CO ₃ (aq)	Ru(OH) ₂ SO ₄ (aq)	SmHPO ₄ ⁺
PuO ₂ CO ₃ -	Ru(OH) ₄ (aq)	SmNO ₃ ⁺⁺
PuO ₂ F ⁺	Ru(SO ₄) ₂ -	SmOH ⁺⁺
PuO ₂ F ₂ (aq)	Ru(SO ₄) ₂ --	SmPO ₄ (aq)
PuO ₂ OH(aq)	Ru(SO ₄) ₃ ---	SmSO ₄ ⁺
PuO ₂ OH ⁺	Ru(SO ₄) ₃ ----	Sn(OH) ₂ ⁺⁺
PuO ₂ SO ₄ (aq)	Ru ₄ (OH) ₁₂ ++++	Sn(OH) ₃ ⁺
PuOH ⁺⁺	RuCl ⁺	Sn(OH) ₄ (aq)
PuOH ⁺⁺⁺	RuCl ⁺⁺	Sn(OH) ₅ -
PuSCN ⁺⁺	RuCl ₂ (aq)	Sn(OH) ₆ --
PuSO ₄ ⁺	RuCl ₂ ⁺	Sn(SO ₄) ₂ (aq)
PuSO ₄ ⁺⁺	RuCl ₃ (aq)	SnCl ⁺
RbBr(aq)	RuCl ₃ -	SnCl ₂ (aq)
RbCl(aq)	RuCl ₄ -	SnCl ₃ -
RbF(aq)	RuCl ₄ --	SnF ⁺
RbI(aq)	RuCl ₅ --	SnF ₂ (aq)
RbOH(aq)	RuCl ₆ ---	SnF ₃ -
Rh(SO ₄) ₂ -	RuO(aq)	SnO(aq)
Rh(SO ₄) ₂ --	RuO ⁺	SnOH ⁺
Rh(SO ₄) ₃ ---	RuOH ⁺	SnOH ⁺⁺⁺
Rh(SO ₄) ₃ ----	RuOH ⁺⁺	SnSO ₄ ⁺⁺
RhCl ⁺	RuSO ₄ (aq)	SrCO ₃ (aq)
RhCl ⁺⁺	RuSO ₄ ⁺	SrCl ⁺
RhCl ₂ (aq)	S--	SrF ⁺
RhCl ₂ ⁺	S ₂ O ₅ --	SrHCO ₃ ⁺
RhCl ₃ (aq)	SO ₂ (aq)	SrHPO ₄ (aq)
RhCl ₃ -	ScO ⁺	SrNO ₃ ⁺
RhCl ₄ -	ScO ₂ -	SrOH ⁺
RhCl ₄ --	ScOH ⁺⁺	SrP ₂ O ₇ --
RhO(aq)	SiF ₆ --	SrSO ₄ (aq)
RhO ⁺	Sm(CO ₃) ₂ -	Tb(CO ₃) ₂ -
RhOH ⁺	Sm(HPO ₄) ₂ -	Tb(HPO ₄) ₂ -
RhOH ⁺⁺	Sm(OH) ₂ ⁺	Tb(OH) ₂ ⁺
RhSO ₄ (aq)	Sm(OH) ₃ (aq)	Tb(OH) ₃ (aq)
RhSO ₄ ⁺	Sm(OH) ₄ -	Tb(PO ₄) ₂ ---
Ru(Cl) ₂ ⁺	Sm(PO ₄) ₂ ---	Tb(SO ₄) ₂ -
Ru(Cl) ₃ (aq)	Sm(SO ₄) ₂ -	TbCO ₃ ⁺
Ru(OH) ₂ ⁺	SmCO ₃ ⁺	TbCl ⁺⁺
Ru(OH) ₂ Cl ⁺	SmCl ⁺⁺	TbF ⁺⁺

Table A2. Aqueous species in data0.ympr.R5 (cont.)

TbH ₂ PO ₄ ++	TlO ₂ -	UO ₂ (N ₃) ₂ (aq)
TbHCO ₃ ++	TlOH(aq)	UO ₂ (N ₃) ₃ -
TbHPO ₄ +	TlOH++	UO ₂ (N ₃) ₄ --
TbNO ₃ ++	Tm(CO ₃) ₂ -	UO ₂ (SCN) ₂ (aq)
TbOH++	Tm(HPO ₄) ₂ -	UO ₂ (SCN) ₃ -
TbPO ₄ (aq)	Tm(OH) ₂ +	UO ₂ (SO ₄) ₂ --
TbSO ₄ +	Tm(OH) ₃ (aq)	UO ₂ (aq)
TcCO ₃ (OH) ₂ (aq)	Tm(PO ₄) ₂ ---	UO ₂ -
TcCO ₃ (OH) ₃ -	Tm(SO ₄) ₂ -	UO ₂ Br+
TcO(OH) ₂ (aq)	TmCO ₃ +	UO ₂ BrO ₃ +
TcO(OH) ₃ -	TmCl++	UO ₂ CO ₃ (aq)
TcOOH+	TmF++	UO ₂ Cl+
Th(OH) ₂ ++	TmH ₂ PO ₄ ++	UO ₂ Cl ₂ (aq)
Th(OH) ₃ +	TmHCO ₃ ++	UO ₂ ClO ₃ +
Th(OH)(CO ₃) ₄ (5-)	TmHPO ₄ +	UO ₂ F+
Th(OH) ₂ CO ₃ (aq)	TmNO ₃ ++	UO ₂ F ₂ (aq)
Th(OH) ₂ (CO ₃) ₂ --	TmOH++	UO ₂ F ₃ -
Th(OH) ₃ CO ₃ -	TmPO ₄ (aq)	UO ₂ F ₄ --
Th(OH) ₄ CO ₃ --	TmSO ₄ +	UO ₂ H ₂ PO ₄ +
Th(OH) ₄ (aq)	U(CO ₃) ₄ ----	UO ₂ H ₃ PO ₄ ++
Th(OH) ₄ PO ₄ ---	U(CO ₃) ₅ (6-)	UO ₂ HPO ₄ (aq)
Th(SO ₄) ₂ (aq)	U(NO ₃) ₂ ++	UO ₂ IO ₃ +
Th(SO ₄) ₃ --	U(SCN) ₂ ++	UO ₂ N ₃ +
Th(SO ₄) ₄ ----	U(SO ₄) ₂ (aq)	UO ₂ NO ₃ +
Th ₂ (OH) ₂ (6+)	UBr+++	UO ₂ OH(aq)
Th ₂ (OH) ₃ (5+)	UCl+++	UO ₂ OH+
ThCl+++	UF+++	UO ₂ OSi(OH) ₃ +
ThCl ₂ ++	UF ₂ ++	UO ₂ PO ₄ -
ThCl ₃ +	UF ₃ +	UO ₂ S ₂ O ₃ (aq)
ThCl ₄ (aq)	UF ₄ (aq)	UO ₂ SCN+
ThF+++	UF ₅ -	UO ₂ SO ₃ (aq)
ThF ₂ ++	UF ₆ --	UO ₂ SO ₄ (aq)
ThF ₃ +	UI+++	UO ₃ (aq)
ThF ₄ (aq)	UNO ₃ +++	UO ₃ -
Th(OH)+++	UO+	UO ₄ --
ThSO ₄ ++	UO++	UOH++
Ti(OH) ₃ +	UO ₂ (CO ₃) ₂ --	UOH+++
Ti(OH) ₅ -	UO ₂ (CO ₃) ₃ (5-)	USCN+++
TlCl(aq)	UO ₂ (CO ₃) ₃ ----	USO ₄ ++
TlCl++	UO ₂ (H ₂ PO ₄)(H ₃ PO ₄)+	V(OH) ₂ +
TlF(aq)	UO ₂ (H ₂ PO ₄) ₂ (aq)	V ₂ (OH) ₂ ++++
TlO+	UO ₂ (IO ₃) ₂ (aq)	VO(OH) ₃ (aq)

Table A2. Aqueous species in data0.ymp.R5 (cont.)

VO+	YbCl++	
VO ₂ (HPO ₄) ₂ ---	YbF++	
VO ₂ F(aq)	YbH ₂ PO ₄ ++	
VO ₂ F ₂ -	YbHCO ₃ ++	
VO ₂ H ₂ PO ₄ (aq)	YbHPO ₄ +	
VO ₂ HPO ₄ -	YbNO ₃ ++	
VO ₂ SO ₄ -	YbOH++	
VO ₄ ---	YbPO ₄ (aq)	
VOF+	YbSO ₄ +	
VOF ₂ (aq)	Zn(CN) ₄ --	
VOH+	Zn(N ₃) ₂ (aq)	
VOH++	Zn(NH ₃)++	
VOOH+	Zn(NH ₃) ₂ ++	
VOSO ₄ (aq)	Zn(NH ₃) ₃ ++	
VSO ₄ +	Zn(NH ₃) ₄ ++	
Y(CO ₃) ₂ -	Zn(OH)Cl(aq)	
Y(HPO ₄) ₂ -	Zn(SCN) ₂ (aq)	
Y(OH) ₂ +	Zn(SCN) ₄ --	
Y(OH) ₃ (aq)	ZnBr+	
Y(OH) ₄ -	ZnBr ₂ (aq)	
Y(PO ₄) ₂ ---	ZnBr ₃ -	
Y(SO ₄) ₂ -	ZnCO ₃ (aq)	
Y ₂ (OH) ₂ ++++	ZnCl+	
YCO ₃ +	ZnCl ₂ (aq)	
YCl++	ZnCl ₃ -	
YF++	ZnClO ₄ +	
YF ₂ +	ZnF+	
YF ₃ (aq)	ZnH ₂ PO ₄ +	
YH ₂ PO ₄ ++	ZnHCO ₃ +	
YHCO ₃ ++	ZnHPO ₄ (aq)	
YHPO ₄ +	ZnI+	
YNO ₃ ++	ZnI ₂ (aq)	
YOH++	ZnI ₃ -	
YPO ₄ (aq)	ZnI ₄ --	
YSO ₄ +	ZnN ₃ +	
Yb(CO ₃) ₂ -	ZnO(aq)	
Yb(HPO ₄) ₂ -	ZnO ₂ --	
Yb(OH) ₂ +	ZnOH+	
Yb(OH) ₃ (aq)	ZnSO ₄ (aq)	
Yb(OH) ₄ -	ZnSeO ₄ (aq)	
Yb(PO ₄) ₂ ---	ZrO ₂ (aq)	
Yb(SO ₄) ₂ -	ZrOH+++	
YbCO ₃ +		

Table A3. Mineral phases in data0.ymp.R5

(C4AF)	Am ₂ O ₃	Barium
(C4AH13)	AmBr ₃	Ba(OH) ₂ ·8H ₂ O
(CAH10)	AmCl ₃	Ba ₂ Si ₃ O ₈
(C2AH8)	AmF ₃	Ba ₂ SiO ₄
(C4AH19)	AmF ₄	Ba ₂ U ₂ O ₇
(CA2)	AmH ₂	Ba ₃ UO ₆
(CA)	AmI ₃	BaBr ₂
(C3A)	AmO ₂	BaBr ₂ ·2H ₂ O
(C12A7)	AmOBr	BaCl ₂
(NH ₄) ₄ NpO ₂ (CO ₃) ₃	AmOCl	BaCl ₂ ·2H ₂ O
(UO ₂) ₂ As ₂ O ₇	AmOHCO ₃	BaCl ₂ ·H ₂ O
(UO ₂) ₂ Cl ₃	AmPO ₄ (am)	BaCrO ₄
(UO ₂) ₂ P ₂ O ₇	Amesite-14A	BaHPO ₄
(UO ₂) ₃ (AsO ₄) ₂	Amesite-7A	BaI ₂
(UO ₂) ₃ (PO ₄) ₂	Analcime	BaMnO ₄
(UO ₂) ₃ (PO ₄) ₂ ·4H ₂ O	Analcime-dehy	BaO
(UO ₂) ₃ (PO ₄) ₂ ·6H ₂ O	Anatase	BaS
(VO) ₃ (PO ₄) ₂	Andalusite	BaSeO ₃
Acanthite	Andradite	BaSeO ₄
Afwillite	Anglesite	BaSiF ₆
Silver	Anhydrite	BaU ₂ O ₇
Ag ₃ PO ₄	Annite	BaUO ₄
AgTcO ₄	Anorthite	Baddeleyite
Akermanite	Antarcticite	Barite
Aluminum	Anthophyllite	Barytocalcite
Al ₂ (SO ₄) ₃	Antigorite	Bassanite
Al ₂ (SO ₄) ₃ ·6H ₂ O	Antigorite(am)	Beryllium
AlF ₃	Antlerite	Be ₁₃ U
Alabandite	Aphthitalite	Becquerelite
Alamosite	Aragonite	Beidellite-Ca
Albite	Arcanite	Beidellite-H
Albite_high	Arsenolite	Beidellite-K
Albite_low	Arsenopyrite	Beidellite-Mg
Allite	Artinite	Beidellite-Na
Alstonite	Arsenic	Bellite
Alum-K	As ₂ O ₅	Berlinite
Alunite	As ₄ O ₆ (cubi)	Berndtite
Americium	As ₄ O ₆ (mono)	Bieberite
Am(OH) ₃	Gold	Bischofite
Am(OH) ₃ (am)	Azurite	Bixbyite
Am ₂ (CO ₃) ₃	Boron	Bloedite
Am ₂ C ₃	B ₂ O ₃	Boehmite

Table A3. Mineral phases in data0.ymp.R5 (cont.)

Boltwoodite	Cd(IO ₃) ₂	Chamosite-7A
Boltwoodite-Na	Cd(OH) ₂	Chlorargyrite
Borax	Cd(OH)Cl	Chloromagnesite
Boric_acid	Cd ₃ (AsO ₄) ₂	Chromite
Bornite	Cd ₃ (PO ₄) ₂	Chrysotile
Brezinaite	Cd ₃ (SO ₄)(OH) ₄	Cinnabar
Bromellite	Cd ₃ (SO ₄) ₂ (OH) ₂	Claudetite
Brucite	CdBr ₂	Clausthalite
Brushite	CdBr ₂ ·4H ₂ O	Clinochlore-14A
Bunsenite	CdCl ₂	Clinochlore-7A
Burkeite	CdCl ₂ (NH ₃) ₂	Clinoptilolite
Graphite	CdCl ₂ (NH ₃) ₄	Clinoptilolite-Ca
Calcium	CdCl ₂ (NH ₃) ₆	Clinoptilolite-Cs
Ca-Al_Pyroxene	CdCl ₂ ·H ₂ O	Clinoptilolite-K
Ca ₂ Al ₂ O ₅ ·8H ₂ O	CdCr ₂ O ₄	Clinoptilolite-NH ₄
Ca ₂ Cl ₂ (OH) ₂ ·H ₂ O	CdF ₂	Clinoptilolite-Na
Ca ₂ V ₂ O ₇	CdI ₂	Clinoptilolite-Sr
Ca ₃ (AsO ₄) ₂	CdS	Clinoptilolite-dehy
Ca ₃ Al ₂ O ₆	CdSO ₄	Clinozoisite
Ca ₃ V ₂ O ₈	CdSO ₄ ·2.667H ₂ O	Cobalt
Ca ₄ Al ₂ Fe ₂ O ₁₀	CdSO ₄ ·H ₂ O	Co(OH) ₂
Ca ₄ Al ₂ O ₇ ·13H ₂ O	CdSeO ₃	Co ₂ SiO ₄
Ca ₄ Al ₂ O ₇ ·19H ₂ O	CdSeO ₄	Co ₃ (AsO ₄) ₂
Ca ₄ Cl ₂ (OH) ₆ ·13H ₂ O	CdSiO ₃	Co ₃ (PO ₄) ₂
CaAl ₂ O ₄	Cerium	CoCl ₂
CaAl ₂ O ₄ ·10H ₂ O	Ce(OH) ₃	CoCl ₂ ·2H ₂ O
CaAl ₄ O ₇	Ce(OH) ₃ (am)	CoCl ₂ ·6H ₂ O
CaHfO ₃	Ce ₂ (CO ₃) ₃ ·8H ₂ O	CoCr ₂ O ₄
CaSO ₄ ·0.5H ₂ O(beta)	Ce ₂ O ₃	CoF ₂
CaSeO ₄ ·2H ₂ O	Ce ₃ (PO ₄) ₄	CoF ₃
CaUO ₄	CeF ₃ ·.5H ₂ O	CoFe ₂ O ₄
CaV ₂ O ₆	CeO ₂	CoHPO ₄
CaZrO ₃	CePO ₄ ·H ₂ O	CoO
Cadmoselite	Celadonite	CoSO ₄
Calcite	Celestite	CoSO ₄ ·3Co(OH) ₂
Calomel	Cerussite	CoSO ₄ ·6H ₂ O
Carnallite	Chabazite	CoSeO ₃
Cassiterite	Chalcanthite	CoTiO ₃
SnO ₂ (am)	Chalcedony	CoWO ₄
Cattierite	Chalcocite	Coesite
Cadmium	Chalcocyanite	Coffinite
Cd(BO ₂) ₂	Chalcopyrite	Colemanite

Table A3. Mineral phases in data0.ymp.R5 (cont.)

Compreignacite	Dawsonite	EuCl ₂
Cordierite_anhyd	Diaspore	EuCl ₃ :6H ₂ O
Cordierite_hydr	Dicalcium_silicate	EuF ₃ :0.5H ₂ O
Corundum	Diopside	EuO
Cotunnite	Dolomite	EuOCl
Covellite	Dolomite-dis	EuOHCO ₃
Chromium	Dolomite-ord	EuPO ₄ :H ₂ O
CrCl ₃	Downeyite	EuS
CrF ₃	Dysprosium	EuSO ₄
CrF ₄	Dy(OH) ₃	Eucryptite
CrI ₃	Dy(OH) ₃ (am)	Fayalite
CrO ₂	Dy ₂ (CO ₃) ₃	Iron
CrO ₃	Dy ₂ O ₃	Fe(OH) ₂
CrS	DyF ₃ :.5H ₂ O	Fe(OH) ₃
Cr-ettringite	DyPO ₄ :2H ₂ O	Fe ₂ (MoO ₄) ₃
Cr-ferrihydrite	Enstatite	Fe ₂ (SO ₄) ₃
Cristobalite(alpha)	Epidote	FeF ₂
Cristobalite(beta)	Epidote-ord	FeF ₃
Crocoite	Epsomite	FeO
Cronstedtite-7A	Erbium	FeSO ₄
Cesium	Er(OH) ₃	FeV ₂ O ₄
Cs ₂ NaAmCl ₆	Er(OH) ₃ (am)	Ferrite-Ca
Cs ₂ NaPuCl ₆	Er ₂ (CO ₃) ₃	Ferrite-Cu
Cs ₂ NpBr ₆	Er ₂ O ₃	Ferrite-Dicalcium
Cs ₂ NpCl ₆	ErF ₃ :.5H ₂ O	Ferrite-Mg
Cs ₂ PuBr ₆	ErPO ₄ :2H ₂ O	Ferrite-Ni
Cs ₂ PuCl ₆	Erionite	Ferrite-Zn
Cs ₂ U ₂ O ₇	Eskolaite	Ferroaluminoceladonite
Cs ₂ U ₄ O ₁₂	Cr(OH) ₃ (am)	Ferroceldonite
Cs ₂ UO ₄	Ettringite	Ferroselite
Cs ₃ PuCl ₆	Europium	Ferrosilite
CsPu ₂ Cl ₇	Eu(IO ₃) ₃ :2H ₂ O	Fluorapatite
CsTcO ₄	Eu(NO ₃) ₃ :6H ₂ O	Fluorite
CSH:1.7	Eu(OH) ₂ 5Cl.5	Forsterite
Copper	Eu(OH) ₂ Cl	Foshagite
Cu ₃ (PO ₄) ₂	Eu(OH) ₃	Frankdicksonite
CuCl ₂	Eu ₂ (CO ₃) ₃ :3H ₂ O	Frebaldite
CuCr ₂ O ₄	Eu ₂ (SO ₄) ₃ :8H ₂ O	Friedl_salt
CuSeO ₃	Eu ₂ O ₃ (cubic)	Gallium
Cuprite	Eu ₂ O ₃ (monoclinic)	Galena
Daphnite-14A	Eu ₃ O ₄	Gaylussite
Daphnite-7A	EuBr ₃	Gadolinium

Table A3. Mineral phases in data0.ymp.R5 (cont.)

Gd(OH)3	HfS3	KTcO4
Gd(OH)3(am)	Hg2SO4	Kainite
Gd2(CO3)3	Hg2SeO3	Kalicinite
Gd2O3	HgSeO3	Kalsilite
GdF3·.5H2O	Hillebrandite	Kaolinite
GdPO4·2H2O	Holmium	Karelianite
Gehlenate_Hydrate	Ho(OH)3	Katoite
Gehlenite	Ho(OH)3(am)	Kieserite
Gibbsite	Ho2(CO3)3	Klockmannite
Gismondine-Na	Ho2O3	Krutaite
Gismondine-Ca	HoF3·.5H2O	Kyanite
Glauberite	HoPO4·2H2O	Lanthanum
Goethite	Hopeite	La(OH)3
Greenalite	Huntite	La(OH)3(am)
Grossular	Hydroboracite	La2(CO3)3·8H2O
Gypsum	Hydrogarnet	La2O3
Gyrolite	Hydromagnesite	LaCl3
Halite	Hydrophilite	LaCl3·7H2O
Hatrurite	Hydrotalcite	LaF3·.5H2O
Hausmannite	Hydroxylapatite	LaPO4·H2O
Heazlewoodite	Hydrozincite	Lammerite
Hedenbergite	Iodine	Lanarkite
Hematite	Ice	Lansfordite
Hemicarboaluminate	Illite	Larnite
Hercynite	Ilmenite	Laumontite
Herzenbergite	Indium	Laurite
Heulandite	Jadeite	Lawrencite
Hexahydrite	Jarosite	Lawsonite
Hafnium	Jarosite-Na	Leonite
HfB2	Potassium	Lithium
HfBr2	K-Feldspar	Li2Se
HfBr4	K2CO3·1.5H2O	Li2UO4
HfC	K2O	Lime
HfCl2	K2Se	Linnaeite
HfCl4	K2UO4	Litharge
HfF2	K3H(SO4)2	Lopezite
HfF4	K4NpO2(CO3)3	Lutetium
HfI2	K8H4(CO3)6·3H2O	Lu(OH)3
HfI4	KAl(SO4)2	Lu(OH)3(am)
HfN	KBr	Lu2(CO3)3
HfO2	KMgCl3·2H2O	Lu2O3
HfS2	KNaCO3·6H2O	LuF3·.5H2O

Table A3. Mineral phases in data0.ymp.R5 (cont.)

LuPO ₄ :0.5H ₂ O	MnV ₂ O ₆	NaBr
Magnesiochromite	Molybdenum	NaBr:2H ₂ O
Magnesite	MoO ₂ Cl ₂	NaFeO ₂
Magnetite	MoSe ₂	NaNpO ₂ CO ₃
Malachite	Molysite	NaNpO ₂ CO ₃ :3.5H ₂ O
Manganite	Monocarboaluminate	NaTcO ₄ :4H ₂ O
Manganosite	Monohydrocalcite	NaUO ₃
Margarite	Monosulphate	Nahcolite
Massicot	Monteponite	Nantokite
Maximum Microcline	Monticellite	Natrolite
Mayenite	Montmorillonite-Ca	Natron
Melanterite	Montmorillonite-H	Natrosilite
Mercallite	Montmorillonite-K	Naumannite
Merwinite	Montmorillonite-Mg	Neodymium
Mesolite	Montmorillonite-Na	Nd(OH) ₃
Metacinnabar	Montroydite	Nd(OH) ₃ (am)
Magnesium	Mordenite	Nd(OH) ₃ (c)
Mg ₂ V ₂ O ₇	Mordenite-dehy	Nd ₂ (CO ₃) ₃
MgBr ₂	Morenosite	Nd ₂ O ₃
MgBr ₂ :6H ₂ O	Muscovite	NdF ₃ :.5H ₂ O
MgCl ₂ :2H ₂ O	NH ₄ HSe	NdOHCO ₃
MgCl ₂ :4H ₂ O	NH ₄ TcO ₄	NdPO ₄ :H ₂ O
MgCl ₂ :H ₂ O	Sodium	Nepheline
MgOHCl	Na ₂ CO ₃	Nesquehonite
MgSO ₄	Na ₂ CO ₃ :7H ₂ O	Nickel
MgSeO ₃	Na ₂ Cr ₂ O ₇	NiCO ₃
MgUO ₄	Na ₂ CrO ₄	NiCO ₃ :5.5H ₂ O
MgV ₂ O ₆	Na ₂ O	Ni(OH) ₂
Millerite	Na ₂ Se	Ni ₂ P ₂ O ₇
Minium	Na ₂ Se ₂	Ni ₃ (PO ₄) ₂
Minnesotaite	Na ₂ SiO ₃	NiCl ₂
Mirabilite	Na ₂ U ₂ O ₇	NiCl ₂ :2H ₂ O
Misenite	Na ₂ UO ₄ (alpha)	NiCl ₂ :4H ₂ O
Manganese	Na ₃ H(SO ₄) ₂	NiCr ₂ O ₄
Mn(OH) ₂ (am)	Kogarkoite	NiF ₂
MnCl ₂ :2H ₂ O	Na ₃ NpF ₈	NiF ₂ :4H ₂ O
MnCl ₂ :4H ₂ O	Na ₃ NpO ₂ (CO ₃) ₂	NiSO ₄
MnCl ₂ :H ₂ O	Na ₃ UO ₄	NiSO ₄ :6H ₂ O(alpha)
MnO ₂ (gamma)	Na ₄ Ca(SO ₄) ₃ :2H ₂ O	NiTio ₃
MnSO ₄	Na ₄ SiO ₄	NiWO ₄
MnSe	Na ₄ UO ₂ (CO ₃) ₃	Nickelbischofite
MnSeO ₃	Na ₆ Si ₂ O ₇	NiMoO ₄

Table A3. Mineral phases in data0.ymp.R5 (cont.)

Niter	Pb(IO3)2	Pm(OH)3(am)
Nitrobarite	Pb(N3)2(mono)	Pm2(CO3)3
Nontronite-Ca	Pb(N3)2(orth)	Pm2O3
Nontronite-H	Pb2Cl2CO3	PmF3:.5H2O
Nontronite-K	Pb2Cl5NH4	PmPO4:1.5H2O
Nontronite-Mg	Pb2O(N3)2	Polydymite
Nontronite-Na	Pb2SiO4	Polyhalite
Neptunium	Pb3(PO4)2	Portlandite
Np(OH)4(am)	Pb3SO6	Powellite
Np2C3	Pb4Cl2(OH)6	Praseodymium
Np2O5	Pb4O(PO4)2	Pr(OH)3
NpBr3	Pb4SO7	Pr(OH)3(am)
NpBr4	PbBr2	Pr2(CO3)3
NpC0.91	PbBrF	Pr2O3
NpCl3	PbCO3.PbO	PrF3:.5H2O
NpCl4	PbF2	PrPO4:H2O
NpF3	PbFCl	Prehnite
NpF4	PbHPO4	Pseudowollastonite
NpF5	PbI2	Platinum
NpF6	PbSO4(NH3)2	PtS
NpI3	PbSO4(NH3)4	PtS2
NpN	PbSeO4	Plutonium
NpO2	Palladium	Pu(HPO4)2(am)
NpO2(am)	Pd(OH)2	Pu(OH)3
NpO2(NO3)2:6H2O	Pd4S	Pu2C3
NpO2CO3	PdO	Pu2O3
NpO2OH(am)	PdS	Pu3C2
NpO2OH(am)	PdS2	PuAs
NpO3:H2O	Penroseite	PuBi
NpOBr2	Pentahydrite	PuBi2
NpOCl2	Periclase	PuBr3
Okenite	Perovskite	PuC0.84
Orpiment	Petalite	PuCl3
Otavite	Phillipsite	PuCl3:6H2O
Ottemannite	Phlogopite	PuCl4
Oxychloride-Mg	Phosgenite	PuF3
Phosphorus	Picromerite	PuF6
Paragonite	Pirssonite	PuI3
Paralaurionite	Plattnerite	PuN
Pargasite	Plombierite	PuO1.61
Lead	Promethium	PuO2
Pb(H2PO4)2	Pm(OH)3	PuO2(hyd

Table A3. Mineral phases in data0.ymp.R5 (cont.)

PuO ₂ (NO ₃) ₂ ·6H ₂ O	RuO ₄	Sm ₂ (SO ₄) ₃
PuO ₂ (OH) ₂ ·H ₂ O	RuSe ₂	Sm ₂ O ₃
PuO ₂ CO ₃	Rutherfordine	SmF ₃ ·.5H ₂ O
PuO ₂ OH(am)	Rutile	SmPO ₄ ·H ₂ O
PuOBr	Sulfur	Smectite-high-Fe-Mg
PuOCl	Sanbornite	Smectite-low-Fe-Mg
PuOF	Sanidine_high	Smectite_Reykjanes
PuOI	Saponite-Ca	Smithsonite
PuP	Saponite-H	Studtite
PuPO ₄ (s)	Saponite-K	Tin
PuSb	Saponite-Mg	Sn(OH) ₂
Pyrite	Saponite-Na	Sn(SO ₄) ₂
Pyrolusite	Antimony	Sn ₃ S ₄
Pyromorphite	Sb(OH) ₃	SnBr ₂
Pyromorphite-OH	Sb ₂ O ₄	SnBr ₄
Pyrophyllite	Sb ₂ O ₅	SnCl ₂
Pyrrhotite	Sb ₄ O ₆ (cubic)	SnSO ₄
Quartz	Sb ₄ O ₆ (orthorhombic)	SnSe
Radium	SbBr ₃	SnSe ₂
Ra(NO ₃) ₂	SbCl ₃	Soddyite
RaCl ₂ ·2H ₂ O	Scandium	Sphaerocobaltite
RaSO ₄	Scacchite	Sphalerite
Rankinite	Schoepite	Spinel
Rubidium	Scolecite	Spinel-Co
Rb ₂ UO ₄	Selenium	Spodumene
Rhenium	Se ₂ O ₅	Strontium
Realgar	SeCl ₄	Sr(NO ₃) ₂
Rhodium	SeO ₃	Sr(NO ₃) ₂ ·4H ₂ O
Rh ₂ O ₃	Sellaite	Sr(OH) ₂
Rhodochrosite	Sepiolite	Sr ₂ SiO ₄
Rhodonite	Sepiolite(am)	Sr ₃ (AsO ₄) ₂
Ripidolite-14A	Palygorskite	SrBr ₂
Ripidolite-7A	Shcherbinaite	SrBr ₂ ·6H ₂ O
Riversideite	Silicon	SrBr ₂ ·H ₂ O
Romarchite	SiO ₂ (am)	SrCl ₂
Ruthenium	Siderite	SrCl ₂ ·2H ₂ O
Ru(OH) ₃ ·H ₂ O(am)	Sillimanite	SrCl ₂ ·6H ₂ O
RuBr ₃	Sklodowskite	SrCl ₂ ·H ₂ O
RuCl ₃	Samarium	SrCrO ₄
RuI ₃	Sm(OH) ₃	SrF ₂
RuO ₂	Sm(OH) ₃ (am)	SrHPO ₄
RuO ₂ ·2H ₂ O(am)	Sm ₂ (CO ₃) ₃	SrI ₂

Table A3. Mineral phases in data0.ymp.R5 (cont.)

SrO	ThO ₂ :2H ₂ O(am)	U(SO ₃) ₂
SrS	ThO ₂ (am)	U(SO ₄) ₂
SrSeO ₄	ThS	U(SO ₄) ₂ :4H ₂ O
SrSiO ₃	ThS ₂	U(SO ₄) ₂ :8H ₂ O
SrUO ₄ (alpha)	Thenardite	U ₂ C ₃
Starkeyite	Thermonatrite	U ₂ F ₉
Stellerite	Thorianite	U ₂ O ₂ Cl ₅
Stilbite	Titanium	U ₂ O ₃ F ₆
Stilleite	Ti ₂ O ₃	U ₂ S ₃
Strengite	Ti ₃ O ₅	U ₂ Se ₃
Strontianite	TiB ₂	U ₃ As ₄
Sylvite	TiBr ₃	U ₃ O ₅ F ₈
Syngenite	TiBr ₄	U ₃ P ₄
Tachyhydrite	TiC	U ₃ S ₅
Talc	TiCl ₂	U ₃ Sb ₄
Tarapacaite	TiCl ₃	U ₃ Se ₄
Terbium	TiF ₃	U ₃ Se ₅
Tb(OH) ₃	TiF ₄ (am)	U ₄ F ₁₇
Tb(OH) ₃ (am)	TiI ₄	U ₅ O ₁₂ Cl
Tb ₂ (CO ₃) ₃	TiN	UAs
Tb ₂ O ₃	TiO	UAs ₂
TbF ₃ :.5H ₂ O	TiO(alpha)	UBr ₂ Cl
TbPO ₄ :2H ₂ O	Tiemannite	UBr ₂ Cl ₂
Technetium	Titanite	UBr ₃
Tc ₂ O ₇	Thallium	UBr ₃ Cl
Tc ₂ O ₇ :H ₂ O	TiTeO ₄	UBr ₄
TcO ₂	Thulium	UBr ₅
TcO ₂ :1.6H ₂ O	Tm(OH) ₃	UBrCl ₂
Tenorite	Tm(OH) ₃ (am)	UBrCl ₃
Tephroite	Tm ₂ (CO ₃) ₃	UC
Thorium	Tm ₂ O ₃	UC _{1.94} (alpha)
Th(NO ₃) ₄ :5H ₂ O	TmF ₃ :.5H ₂ O	UC ₁₂ F ₂
Th(SO ₄) ₂	TmPO ₄ :2H ₂ O	UC ₁₂ I ₂
Th.75PO ₄	Tobermorite	UCI ₃
Th ₂ S ₃	Tremolite	UCI ₃ F
Th ₂ Se ₃	Trevorite	UCI ₃ I
Th ₇ S ₁₂	Tridymite	UCI ₄
ThBr ₄	Troilite	UCI ₅
ThCl ₄	Trona-K	UCI ₆
ThF ₄	Uranium	UCIF ₃
ThF ₄ :2.5H ₂ O	U(HPO ₄) ₂ :4H ₂ O	UCII ₃
ThI ₄	U(OH) ₂ SO ₄	UF ₃

Table A3. Mineral phases in data0.ymp.R5 (cont.)

UF4	UO3(alpha)	WO2Cl2(s)
UF4:2.5H2O	UO3(beta)	WOC14(s)
UF5(alpha)	UO3(gamma)	WOF4(s)
UF5(beta)	Schoepite(dehyd	Wairakite
UF6	Schoepite(dehyd	Weeksite-K
UH3(beta)	UOBr2	Weeksite-Na
UI3	UOBr3	Whitlockite
UI4	UOCl	Wilkmanite
UN	UOCl2	Witherite
UN1.59(alpha)	UOCl3	Wollastonite
UN1.73(alpha)	UOF2	Wurtzite
UO2(AsO3)2	UOF2:H2O	Wustite
UO2(IO3)2	UOF4	Xonotlite
UO2(NO3)2	UOFOH	Yttrium
UO2(NO3)2:2H2O	UOFOH:.5H2O	Ytterbium
UO2(NO3)2:3H2O	UP	Yb(OH)3
UO2(NO3)2:6H2O	UP2	Yb(OH)3(am)
UO2(NO3)2:H2O	UP2O7	Yb2(CO3)3
UO2(OH)2(beta)	UPO5	Yb2O3
UO2.25	US	YbF3:.5H2O
UO2.25(beta)	US1.9	YbPO4:2H2O
UO2.3333(beta)	US2	Zincite
UO2.6667	US3	Zircon
UO2Br2	USb	Zinc
UO2Br2:3H2O	USb2	Zn(BO2)2
UO2Br2:H2O	USe	Zn(ClO4)2:6H2O
UO2BrOH:2H2O	USe2(alpha)	Zn(IO3)2
UO2Cl	USe2(beta)	Zn(NO3)2:6H2O
UO2Cl2	USe3	Zn(OH)2(beta)
UO2Cl2:3H2O	Umangite	Zn(OH)2(epsilon)
UO2Cl2:H2O	Uraninite	Zn(OH)2(gamma)
UO2ClOH:2H2O	Uranophane(alpha)	Zn2(OH)3Cl
UO2F2	Vanadium	Zn2SO4(OH)2
UO2F2:3H2O	V2O4	Zn2SiO4
UO2FOH:2H2O	V3O5	Zn2TiO4
UO2FOH:H2O	V4O7	Zn3(AsO4)2
UO2HPO4:4H2O	Vaesite	Zn3O(SO4)2
UO2SO3	Tungsten	Zn5(NO3)2(OH)8
UO2SO4	WCl2(s)	ZnBr2
UO2SO4:2.5H2O	WCl4(s)	ZnBr2:2H2O
UO2SO4:3.5H2O	WCl5(s)	ZnCO3:H2O
UO2SO4:3H2O	WCl6(s)	ZnCl2

Table A3. Mineral phases in data0.ymp.R5 (cont.)

ZnCl2(NH3)2		
ZnCl2(NH3)4		
ZnCl2(NH3)6		
ZnCr2O4		
ZnF2		
ZnI2		
ZnSO4		
ZnSO4:6H2O		
ZnSO4:7H2O		
ZnSO4:H2O		
ZnSeO3:H2O		
Zoisite		
Zirconium		
ZrB2		
ZrC		
ZrCl		
ZrCl2		
ZrCl3		
ZrCl4		
ZrF4(beta)		
ZrH2		
ZrN		

Table A4. Liquids and gases in data0.ympr.R5

Liquids			
Bromine	Quicksilver (mercury)		
Gases			
Ag(g)	HCl(g)	SO ₂ (g)	UCl ₃ (g)
Al(g)	HF(g)	Si(g)	UCl ₄ (g)
Am(g)	HI(g)	SiF ₄ (g)	UCl ₅ (g)
AmF ₃ (g)	HNO ₃ (g)	Sn(g)	UCl ₆ (g)
Argon	Helium	Tc(g)	UF(g)
B(g)	Hf(g)	Tc ₂ O ₇ (g)	UF ₂ (g)
BF ₃ (g)	Hg(g)	TcC(g)	UF ₃ (g)
Be(g)	I ₂ (g)	TcO(g)	UF ₄ (g)
Br ₂ (g)	K(g)	TcS(g)	UF ₅ (g)
C(g)	Krypton	Th(g)	UF ₆ (g)
CH ₄ (g)	Li(g)	Ti(g)	UI(g)
CO(g)	Mg(g)	TiBr ₄ (g)	UI ₂ (g)
CO ₂ (g)	Nitrogen	TiCl(g)	UI ₃ (g)
Ca(g)	NH ₃ (g)	TiCl ₂ (g)	UI ₄ (g)
Cd(g)	NO(g)	TiCl ₃ (g)	UO(g)
Chlorine	NO ₂ (g)	TiCl ₄ (g)	UO ₂ (g)
CoCl ₂ (g)	NO ₃ (g)	TiF(g)	UO ₂ Cl ₂ (g)
CoCl ₃ (g)	N ₂ O(g)	TiF ₂ (g)	UO ₂ F ₂ (g)
CoF ₂ (g)	N ₂ O ₃ (g)	TiF ₃ (g)	UO ₃ (g)
CrCl ₄ (g)	N ₂ O ₄ (g)	TiF ₄ (g)	UOF ₄ (g)
Cs(g)	N ₂ O ₅ (g)	TiO(g)	WCl ₂ (g)
Cu(g)	Na(g)	U(g)	WCl ₄ (g)
Fluorine	Neon	U ₂ Cl ₁₀ (g)	WCl ₆ (g)
FeCl ₂ (g)	NiCl ₂ (g)	U ₂ Cl ₈ (g)	WF(g)
FeCl ₃ (g)	NiF ₂ (g)	U ₂ F ₁₀ (g)	WF ₆ (g)
FeF ₂ (g)	O ₂ (g)	UBr(g)	WO ₂ Cl ₂ (g)
FeF ₃ (g)	Pb(g)	UBr ₂ (g)	WOCl ₄ (g)
H ₂ (g)	Rb(g)	UBr ₃ (g)	WOF ₄ (g)
H ₂ O(g)	Radon	UBr ₄ (g)	Xenon
H ₂ O ₂ (g)	RuCl ₃ (g)	UBr ₅ (g)	Zn(g)
H ₂ S(g)	RuO ₃ (g)	UCl(g)	Zr(g)
HBr(g)	S ₂ (g)	UCl ₂ (g)	ZrF ₄ (g)

Appendix B: Minerals and Species Included in the Concentrated Systems Database

Table B1. Elements in data0.ypf.R2

Al	Mg
Am	Mn
B	Mo
Ba	N
Br	Na
C	Nd
Ca	Ni
Cl	Np
Cm	O
Co	P
Cr	Pu
Cs	Rb
Cu	S
F	Si
Fe	Sr
Gd	Tc
H	Th
I	U
K	Zn
Li	Zr

Table B2. Aqueous species in data0.ypf.R2

H2O	CrO4--	Cm(OH)3(aq)
Al+++	Fe+++	CaCl+
Ba++	H2(aq)	CaCl2(aq)
Br-	HPO3--	CO2(aq)
HCO3-	HS-	Cr2O7--
Ca++	Mn+++	FeCl+
Cl-	MnO4--	FeHCO3+
Cr+++	NH4+	FeCO3(aq)
Cs+	NO2-	Fe(CO3)2--
F-	SO3--	FeOH+
Fe++	Am++	Fe(OH)2(aq)
H+	Am++++	FeOH++
I-	AmO2+	Fe(OH)2+
K+	AmO2++	Fe(OH)3(aq)
Li+	BH4-	Fe(OH)4-
Mg++	Np+++	FeSO4+
Mn++	Np++++	Fe(SO4)2-
MoO4--	NpO2++	FeCl++
NO3-	PO4---	FeCl2+
Na+	Pu+++	FeF+
HPO4--	Pu++++	FeF++
Rb+	PuO2++	FeF2+
SO4--	TcO++	HSO4-
SiO2(aq)	U++++	HSiO3-
Sr++	O2(aq)	H2PO4-
B(OH)3(aq)	OH-	H3PO4(aq)
Am++++	CO3--	MgCO3(aq)
Cm+++	AlO2-	MgHCO3+
Gd+++	AlOH++	MgOH+
Nd+++	AlO+	NH3(aq)
NpO2+	HALO2(aq)	MgB(OH)4+
PuO2+	AlF++	Am(CO3)+
TcO4-	AlF2+	Am(CO3)2-
Th++++	AlF3(aq)	Am(CO3)3---
UO2++	AlF4-	Am(CO3)4(5-)
Co++	B(OH)4-	Am(OH)2+
Cu++	B3O3(OH)4-	Am(OH)++
Ni++	B4O5(OH)4--	Am(SO4)2-
Zn++	CaB(OH)4+	Am(SO4)+
Zr++++	CaCO3(aq)	AmCl++
O2(g)	CaOH+	AmCl2+
ClO4-	CaSO4(aq)	Am(OH)3(aq)

Table B2. Aqueous species in data0.yypf.R2 (cont.)

AmF ⁺⁺	Pu(OH) ³⁺	NpO ₂ (OH) ²⁻
AmF ₂ ⁺	Pu(OH) ₄ (aq)	NpO ₂ (CO ₃) ₃ (5-)
AmH ₂ PO ₄ ⁺⁺	ThOH ⁺⁺⁺	NpO ₂ (CO ₃) ₂ ⁻⁻⁻
AmNO ₃ ⁺⁺	Th(OH) ₂ ⁺⁺	NpO ₂ CO ₃ ⁻
Cm(CO ₃) ⁺	Th(OH) ³⁺	PuO ₂ (CO ₃) ₃ ⁻⁻⁻⁻
Cm(CO ₃) ₂ ⁻	Th(OH) ₄ (aq)	PuO ₂ (CO ₃) ₂ ⁻⁻
Cm(CO ₃) ₃ ⁻⁻⁻	Th ₂ (OH) ₂ (6+)	PuO ₂ CO ₃ (aq)
Cm(CO ₃) ₄ (5-)	Th ₄ (OH) ₈ (8+)	UO ₂ CO ₃ (aq)
Cm(OH) ₂ ⁺	Th ₄ (OH) ₁₂ ⁺⁺⁺⁺	UO ₂ (CO ₃) ₂ ⁻⁻
Cm(OH) ⁺⁺	Th ₆ (OH) ₁₅ (9+)	UO ₂ (CO ₃) ₃ ⁻⁻⁻
Cm(SO ₄) ₂ ⁻	Th(CO ₃) ₅ (6-)	(UO ₂) ₂ CO ₃ (OH) ₃ ⁻
Cm(SO ₄) ⁺	Th(SO ₄) ₂ (aq)	(UO ₂) ₁₁ (CO ₃) ₆ (OH) ₁₂ ⁻⁻
CmCl ⁺⁺	Th(SO ₄) ₃ ⁻⁻	(UO ₂) ₃ (CO ₃) ₆ (6-)
CmCl ₂ ⁺	Th(SO ₄) ₄ ⁻⁻⁻⁻	(UO ₂) ₃ O(OH) ₂ (HCO ₃) ⁺
NpOH ⁺⁺⁺	UOH ⁺⁺⁺	(UO ₂) ₂ NpO ₂ (CO ₃) ₆ (6-)
Np(OH) ₂ ⁺⁺	U(OH) ₂ ⁺⁺	(UO ₂) ₂ (PuO ₂)(CO ₃) ₆ (6-)
Nd(CO ₃) ⁺	U(OH) ³⁺	UO ₂ OH ⁺
Nd(CO ₃) ₂ ⁻	U(OH) ₄ (aq)	(UO ₂) ₂ (OH) ₂ ⁺⁺
Nd(CO ₃) ₃ ⁻⁻⁻	NiCrO ₄ (aq)	(UO ₂) ₃ (OH) ₄ ⁺⁺
Nd(CO ₃) ₄ (5-)	H ₂ CrO ₄ (aq)	(UO ₂) ₂ OH ⁺⁺⁺
Nd(OH) ₃ (aq)	HCrO ₄ ⁻	(UO ₂) ₃ (OH) ₅ ⁺
Nd(OH) ₂ ⁺	CrBr ⁺⁺	(UO ₂) ₃ (OH) ₇ ⁻
Nd(OH) ⁺⁺	CrOH ⁺⁺	(UO ₂) ₄ (OH) ₇ ⁺
Nd(SO ₄) ₂ ⁻	Cr(OH) ₂ ⁺	UO ₃ (aq)
Nd(SO ₄) ⁺	Cr(OH) ₃ (aq)	HUO ₄ ⁻
NdCl ⁺⁺	Cr(OH) ₄ ⁻	UO ₄ ⁻⁻
NdCl ₂ ⁺	Cr ₂ O ₂ (OH) ₄ ⁻⁻	UO ₂ Cl ⁺
Np(OH) ₃ ⁺	NiOH ⁺	
Np(OH) ₄ (aq)	Ni(OH) ₂ (aq)	
Pu(CO ₃) ⁺	Ni(OH) ₃ ⁻	
Pu(CO ₃) ₂ ⁻	Ni(OH) ₄ ⁻⁻	
Pu(CO ₃) ₃ ⁻⁻⁻	NiBr ⁺	
Pu(CO ₃) ₄ (5-)	NiCO ₃ (aq)	
Pu(OH) ₃ (aq)	NiF ⁺	
Pu(OH) ₂ ⁺	NiHCO ₃ ⁺	
Pu(OH) ⁺⁺	NiHPO ₄ (aq)	
Pu(SO ₄) ₂ ⁻	NiH ₂ PO ₄ ⁺	
Pu(SO ₄) ⁺	NiPO ₄ ⁻	
PuCl ⁺⁺	NiHP ₂ O ₇ ⁻	
PuCl ₂ ⁺	NiP ₂ O ₇ ⁻⁻	
PuOH ⁺⁺⁺	NiNO ₃ ⁺	
Pu(OH) ₂ ⁺⁺	NpO ₂ OH(aq)	

Table B3. Mineral phases in data0.ypf.R2

Albite	Carnallite	Hexahydrite
Alunite	Carobbite	Huntite
Amesite-7A	Celadonite	Hydroxylapatite
Amesite-14A	Celestite	Hydromagnesite
Analcime	Chabazite	Illite
Analcime-dehy	Chamosite-7A	Jarosite
Anhydrite	Chloromagnesite	Jarosite-Na
Antarcticite	Clinoptilolite	K-Feldspar
Antigorite(am)	Clinoptilolite-dehy	K ₂ CO ₃
Aragonite	Clinoptilolite-Ca	K ₂ CO ₃ :1.5H ₂ O
Arcanite	Clinoptilolite-Cs	K ₂ O
Artinite	Clinoptilolite-K	K ₂ Si ₄ O ₉
Barite	Clinoptilolite-NH ₄	K ₃ H(SO ₄) ₂
Beidellite-Mg	Clinoptilolite-Na	K ₈ H ₄ (CO ₃) ₆ :3H ₂ O
Beidellite-Ca	Clinoptilolite-Sr	Kainite
Beidellite-K	Cristobalite(alpha)	KAlCl ₄
Beidellite-Na	Cronstedtite-7A	K ₂ HPO ₄
Beidellite-H	Cryolite	K ₃ AlCl ₆
Bischofite	Daphnite-14A	K ₃ AlF ₆
Bloedite	Daphnite-7A	K ₃ PO ₄
Boehmite	Dawsonite	Kalicinite
Borax	Dolomite	KAl(SO ₄) ₂
Boric_acid	Epsomite	KAl(SO ₄) ₂ :3H ₂ O
KB ₅ O ₈ :4H ₂ O	Erionite	KAl(SO ₄) ₂ :12H ₂ O
K ₂ B ₄ O ₇ :4H ₂ O	Ferroaluminoceladonite	Kaolinite
NaBO ₂ :4H ₂ O	Ferroceldonite	KBr
NaB ₅ O ₈ :5H ₂ O	Fe ₂ (MoO ₄) ₃	KClO ₄
NaBO ₂ :NaCl:2H ₂ O	FeF ₃	KH ₂ PO ₄
Brushite	Fe ₂ (SO ₄) ₃	KI
Burkeite	Fluorapatite	Kieserite
CaBr ₂	Fluorite	KMgCl ₃ :2H ₂ O
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	Gaylussite	KNaCO ₃ :6H ₂ O
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	Gibbsite	KOH
CaCl ₂	Glaserite	Labile_Salt
CaCl ₂ :2H ₂ O	Glauberite	Lansfordite
CaCl ₂ :4H ₂ O	Goethite	Laumontite
CaI ₂	Greenalite	Leonhardtite
Calcite	Gypsum	Leonite
Ca(NO ₃) ₂	Halite	Lime
Ca(NO ₃) ₂ :2H ₂ O	Hematite	Magnesite
Ca(NO ₃) ₂ :3H ₂ O	Hemihydrate	Magnetite
Ca(NO ₃) ₂ :4H ₂ O	Heulandite	Maximum_Microcline

Table B3. Mineral phases in data0.ypf.R2 (cont.)

Mercallite	(NH ₄) ₂ SO ₄	Sr(OH) ₂
Mesolite	Niter	Stellerite
MgBr ₂	Nontronite-Mg	Stilbite
MgCl ₂ :H ₂ O	Nontronite-Ca	Sylvite
MgCl ₂ :2H ₂ O	Nontronite-K	Syngenite
MgCl ₂ :4H ₂ O	Nontronite-Na	Tachyhydrite
MgI ₂	Nontronite-H	Talc
MgMoO ₄	Oxychloride-Mg	Thenardite
Mg(NO ₃) ₂	Pentahydrite	Thermonatrite
MgOHCl	Pentasalt	Trona
MgSO ₄	Periclase	Trona-K
Minnesotaite	Phillipsite	Villiaumite
Mirabilite	Picromerite	Whitlockite
Misenite	Pirssonite	Americium
Molysite	Polyhalite	Am(OH) ₃
Montmorillonite-H	Portlandite	Am(OH) ₃ (am)
Montmorillonite-Na	Pyrolusite	Am ₂ (CO ₃) ₃
Montmorillonite-K	Pyrophyllite	Am ₂ O ₃
Montmorillonite-Ca	Quartz	AmCl ₃
Montmorillonite-Mg	Ripidolite-7A	AmF ₃
Mordenite	Ripidolite-14A	AmF ₄
NaBr	Saponite-H	AmO ₂
NaClO ₄	Saponite-Na	AmOCl
NaI	Saponite-K	AmOHCO ₃
NaNO ₂	Saponite-Ca	AmPO ₄ (am)
NaOH	Saponite-Mg	Brucite
Na ₂ CO ₃ :7H ₂ O	Scolecite	Chromium
Na ₂ CrO ₄	Sellaite	Eskolaite
Na ₂ MoO ₄	Sepiolite	Cr(OH) ₃ (am)
Na ₂ O	Sepiolite(am)	CrCl ₃ :6H ₂ O
Na ₂ SO ₄ (Sol-3)	Palygorskite	CrF ₃
Na ₃ H(SO ₄) ₂	SiO ₂ (am)	KFe ₃ (CrO ₄) ₂ (OH) ₆
Kogarkoite	Smectite-high-Fe-Mg	Na ₂ CrO ₄ :4H ₂ O
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	Smectite-low-Fe-Mg	Tarapacaite
Nahcolite	Soda Niter	Lopezite
Natrite	Strontianite	CrO ₃
Natron	SrBr ₂	CuCr ₂ O ₄
Natrolite	SrCl ₂	Copper
Nesquehonite	SrF ₂	CuCl ₂ :2H ₂ O
NH ₄ Cl	SrI ₂	CuSO ₄ :5H ₂ O
NH ₄ ClO ₄	SrMoO ₄	CuSO ₄ .Na ₂ SO ₄ :2H ₂ O
NH ₄ I	SrO	CuSO ₄ .K ₂ SO ₄ :6H ₂ O

Table B3. Mineral phases in data0.ypf.R2 (cont.)

Cu ₃ (PO ₄) ₂	Manganite	NpO ₂ CO ₃
Iron	Manganosite	NpO ₂ OH(am)
Fe(OH) ₂	MgUO ₄	NpO ₂ OH(am, aged)
Fe(OH) ₃	Manganese	NpO ₃ :H ₂ O
Siderite	Mn(OH) ₂ (am)	Na ₃ NpF ₈
FeF ₂	Rhodochrosite	Na ₃ NpO ₂ (CO ₃) ₂
FeO	MnCl ₂ :4H ₂ O	NaNpO ₂ CO ₃
FeSO ₄	MnSO ₄	NaNpO ₂ CO ₃ :3.5H ₂ O
Melanterite	Molybdate	KNpO ₂ CO ₃
Ferrite-Ca	Powellite	K ₃ NpO ₂ (CO ₃) ₂
Ferrite-Cu	MoO ₂ Cl ₂	Plutonium
Ferrite-Dicalcium	Sodium	PuO ₂ (cr)
Ferrite-Mg	Neodymium	Pu(OH) ₄ (am)
Ferrite-Ni	Nd(OH) ₃	Pu(HPO ₄) ₂ (am, hyd)
Ferrite-Zn	Nd(OH) ₃ (am)	Pu(OH) ₃
Gadolinium	Nd(OH) ₃ (c)	Pu ₂ O ₃
Gd(OH) ₃	Nd ₂ (CO ₃) ₃	Pu ₂ C ₃
Gd(OH) ₃ (am)	Nd ₂ O ₃	Pu ₃ C ₂
Gd ₂ (CO ₃) ₃	NdF ₃ :.5H ₂ O	PuC _{0.84}
Gd ₂ O ₃	NdOHCO ₃	PuCl ₃ :6H ₂ O
GdF ₃ :.5H ₂ O	NdPO ₄ :10H ₂ O	PuCl ₄
GdPO ₄ :10H ₂ O	Nickel	PuF ₃
Hausmannite	NiCO ₃	PuF ₆
Hydrozincite	NiCl ₂ :4H ₂ O	PuO _{1.61}
Lawrencite	Nickelbischofite	PuO ₂ (NO ₃) ₂ :6H ₂ O
Cobalt	NiMoO ₄	PuO ₂ (OH) ₂ :H ₂ O
Co(OH) ₂	Ni(OH) ₂	PuO ₂ CO ₃
Co ₂ SiO ₄	Ni ₂ P ₂ O ₇	PuOCl
Co ₃ (PO ₄) ₂	Ni ₃ (PO ₄) ₂	PuOF
CoCl ₂	Ni ₄ CrO ₄ (OH) ₆	PuPO ₄ (s, hyd)
CoCl ₂ :2H ₂ O	NiSO ₄ :7H ₂ O	Technetium
CoCl ₂ :6H ₂ O	NiCr ₂ O ₄	Tc ₂ O ₇
CoCr ₂ O ₄	NiF ₂ :4H ₂ O	Tc ₂ O ₇ :H ₂ O
CoF ₂	Neptunium	TcO ₂
CoFe ₂ O ₄	NpO ₂ (cr)	TcO ₂ :1.6H ₂ O
CoHPO ₄	Np ₂ O ₅	NaTcO ₄ :4H ₂ O
CoO	Np(OH) ₄ (am)	KTcO ₄
CoSO ₄ :3Co(OH) ₂	NpOCl ₂	CsTcO ₄
CoSO ₄ :6H ₂ O	NpCl ₄	CsClO ₄
Bieberite	NpF ₄	Thorium
Malachite	NpF ₅	Th(OH) ₄ (am)
Mg ₂ (OH) ₃ Cl:4H ₂ O	NpO ₂ (NO ₃) ₂ :6H ₂ O	ThO ₂ (cr)

Table B3. Mineral phases in data0.yypf.R2 (cont.)

ThO ₂ (am)	UO ₂ F ₂ ·3H ₂ O	
Th(SO ₄) ₂	UO ₂ FOH·2H ₂ O	
Th ₇₅ PO ₄	UO ₂ FOH·H ₂ O	
ThF ₄	UO ₂ HPO ₄ ·4H ₂ O	
ThF ₄ ·2.5H ₂ O	UO ₂ SO ₃	
Uranium	UO ₂ SO ₄	
UO ₂ (cr)	UO ₂ SO ₄ ·2.5H ₂ O	
U(OH) ₄ (am)	UO ₂ SO ₄ ·3.5H ₂ O	
Schoepite	UO ₂ SO ₄ ·3H ₂ O	
Ca(UO ₂) ₆ O ₄ (OH) ₆ ·8H ₂ O	UO ₃ (alpha)	
Boltwoodite-Na	UO ₃ (beta)	
UO ₂ CO ₃	UO ₃ (gamma)	
U(HPO ₄) ₂ ·4H ₂ O	UO ₃ ·.9H ₂ O(alpha)	
U(OH) ₂ SO ₄	UOCl ₂	
U(SO ₃) ₂	UOF ₂	
U(SO ₄) ₂	UOF ₂ ·H ₂ O	
U(SO ₄) ₂ ·4H ₂ O	UOFOH	
U(SO ₄) ₂ ·8H ₂ O	UOFOH·.5H ₂ O	
U ₂ O ₃ F ₆	UP ₂ O ₇	
U ₃ O ₅ F ₈	US ₂	
UCl ₂ F ₂	US ₃	
UCl ₃ F	Uranophane(alpha)	
UCl ₄	Na ₂ U ₂ O ₇	
UCl ₆	Na ₂ UO ₄ (alpha)	
UClF ₃	Na ₄ UO ₂ (CO ₃) ₃	
UF ₄	Witherite	
UF ₄ ·2.5H ₂ O	Zinc	
UF ₆	Zincite	
UI ₄	Zn(BO ₂) ₂	
UO ₂ (NO ₃) ₂	Zn(ClO ₄) ₂ ·6H ₂ O	
UO ₂ (NO ₃) ₂ ·2H ₂ O	Zn(NO ₃) ₂ ·6H ₂ O	
UO ₂ (NO ₃) ₂ ·3H ₂ O	Zn(OH) ₂ (beta)	
UO ₂ (NO ₃) ₂ ·6H ₂ O	Zn(OH) ₂ (epsilon)	
UO ₂ (NO ₃) ₂ ·H ₂ O	Zn(OH) ₂ (gamma)	
UO ₂ (OH) ₂ (beta)	Zn ₂ (OH) ₃ Cl	
UO ₂ .3333(beta)	Zn ₂ SO ₄ (OH) ₂	
UO ₂ .6667	Zn ₃ O(SO ₄) ₂	
UO ₂ Cl ₂	Zn ₅ (NO ₃) ₂ (OH) ₈	
UO ₂ Cl ₂ ·3H ₂ O	ZnBr ₂ ·2H ₂ O	
UO ₂ Cl ₂ ·H ₂ O	ZnCO ₃ ·H ₂ O	
UO ₂ ClOH·2H ₂ O	ZnCl ₂	
UO ₂ F ₂	ZnCl ₂ (NH ₃) ₂	

Table B4. Gases in data0.ypf.R2

CH ₄ (g)
CO ₂ (g)
H ₂ (g)
H ₂ O(g)
HBr(g)
HCl(g)
HF(g)
HNO ₃ (g)
N ₂ O ₅ (g)
NO ₃ (g)
O ₂ (g)

There are no liquid compounds or elements included in the concentrated systems database.