CHNOSZ summary

## CHNOSZ database

* <http://chnosz.net/download/alldata.csv>
* (<http://chnosz.net/download/refs.html> ; <http://chnosz.net/>) - R software package
* Python wrapper: pyCHNOSZ <https://zenodo.org/record/5539919>
* **Thermodynamic models in CHNOSZ**: The thermodynamic properties of liquid water are calculated using Fortran code from SUPCRT92 ([Johnson et al., 1992](https://doi.org/10.1016/0098-3004(92)90029-Q)) or an implementation in R of the IAPWS-95 formulation ([Wagner and Pruß, 2002](https://doi.org/10.1063/1.1461829)). Thermodynamic properties of other species are taken from a database for minerals and inorganic and organic aqueous species including biomolecules, or from amino acid group additivity for proteins ([Dick et al., 2006](http://doi.org/10.5194/bg-3-311-2006)). The corresponding high-temperature properties are calculated using the [Berman-Brown (1985)](https://doi.org/10.1007/BF00379451) equations for minerals and the revised [Helgeson-Kirkham-Flowers (1981)](https://doi.org/10.2475/ajs.281.10.1249) equations for aqueous species. The HKF equations are augmented with the Deep Earth Water (DEW) model ([Sverjensky et al., 2014](https://doi.org/10.1016/j.gca.2013.12.019)) and estimates of parameters in the extended Debye-Hückel equation ([Manning et al., 2013](https://doi.org/10.2138/rmg.2013.75.5)) to calculate standard-state properties and activity coefficients for given ionic strength at high pressure (to 6 GPa). Activity coefficients are implemented via adjusted standard Gibbs energies at specified ionic strength ([Alberty, 1996](https://doi.org/10.1111/j.1432-1033.1996.0001h.x)), which converts all activity variables in the workflow to molalities. A related adjustment is available to convert standard Gibbs energies for gases from the 1 bar standard state used in SUPCRT to a variable-pressure standard state ([Anderson and Crerar, 1993, Ch. 12](http://www.worldcat.org/oclc/803272549)).
* From [Dick 2019:](https://www.frontiersin.org/articles/10.3389/feart.2019.00180/full)
  + The default database in the current release version of CHNOSZ contains 3,360 species, and the optional data files (see below) have 641 species. The supplied database provides wide coverage of aqueous species with parameters in the revised Helgeson-Kirkham-Flowers (HKF) equations of state (Tanger and Helgeson, 1988). Unlike SUPCRT92, which is restricted to the 3-term Maier-Kelley equation for the heat capacity of crystalline, liquid, and gas species, parameters can be entered in OBIGT (One BIG Table) for the 5-term Haas-Fisher polynomial equation (Haas and Fisher, 1976; Robie and Hemingway, 1995, p. 2). The T2 term in this equation is also used for organic gases and liquid alcohols (Helgeson et al., 1998). In addition, there is provision for a sixth term that can carry an arbitrary exponent, for instance T3 for the gases Si(OH)4 and As(OH)3 (Akinfiev and Plyasunov, 2014).
  + Although there is considerable overlap with the slop16.dat update for SUPCRT92 (Shock, 2016), OBIGT uses different data sources for aqueous Al species (Tagirov and Schott, 2001), As species (Nordstrom and Archer, 2003), Au, Ag, and Cu species (Akinfiev and Zotov, 2001, 2010), Pd species (Tagirov et al., 2013), Zn species (Akinfiev and Tagirov, 2014), and Pt species (Tagirov et al., 2015). Other notable differences are the inclusion of goethite, other Fe-oxyhydroxides, and evaporite minerals (Majzlan et al., 2003; Grevel and Majzlan, 2009), aqueous phenanthrene and methylphenanthrene isomers (Dick et al., 2013), experimentally derived HKF parameters for aqueous adenine (Lowe et al., 2017), and all of the organic compounds reported by Helgeson et al. (1998) and Richard and Helgeson (1998).
  + 3.1.1. SUPCRT92: This optional data file contains minerals, originally from the SUPCRT92 database, that were present in earlier versions of CHNOSZ but that have been superseded by the Berman (1988) dataset or other sources. The superseded minerals maintained in this file include all of the silicates and Al-bearing minerals from Helgeson et al. (1978), as well as calcite, dolomite, hematite, and magnetite. Additionally, this file contains the SUPCRT92 versions of boehmite, gibbsite, and dawsonite, which were updated following the recommendations of Zimmer et al. (2016), and the 25°C thermodynamic properties of celestite (Reardon and Armstrong, 1987), as recommended by Hörbrand et al. (2018). Other minerals from SUPCRT92, including native elements, sulfides, halides, sulfates, and carbonates and oxides that do not duplicate those in the Berman dataset, are still present in OBIGT.
  + 3.1.2. SLOP98: This file includes data that were compiled in slop98.dat (Shock, 1998), or later versions of the slop files, that were present in earlier versions of CHNOSZ but have been replaced by or are incompatible with subsequent updates to the default database (see above). Data for metal complexes with arsenate and arsenite (Marini and Accornero, 2007, 2010), which are linked to the properties of arsenate and arsenite found in slop98.dat, are also present in this file. Similarly, data for Au(I)-acetate complexes (Shock and Koretsky, 1993) have been moved to this file, but Au+3 (Shock et al., 1997) has been kept in the default database because it is not affected by the updates applied to Au+.
  + 3.1.4. AS04: This file has updates for aqueous SiO2 (Apps and Spycher, 2004) reflecting a higher solubility of quartz in experiments compared to predictions of the SUPCRT92 dataset; see Wolery and Jové Colón (2017) for a review. The updates are not included in OBIGT because the standard Gibbs energy of SiO2 used by Berman (1988) for comparisons with mineral solubilities is much closer to the previous value (Shock et al., 1989), which is also linked to the thermodynamic data of Helgeson et al. (1978).