

Database name:	TGG Aqueous Solution Database	Database acronym:	AQS2
Database owner:	Theoretical Geochemistry Group	Database version:	2.6
Database segment:	Aqueous Solutions		

Brief Description

AQS2 is a database suitable for calculating thermodynamic properties of complex aqueous solutions.

Applications

Materials corrosion processes; Hydro-metallurgy, Aqueous chemistry, Geochemistry and Environmental chemistry.

Included Elements (82)

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

Included Phases

The database contains an AQUEOUS solution phase which consists of various free cations and anions, inorganic and organic complexes. The hypothetical phase, REFERENCE_ELECTRODE, is introduced to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system. Connected with this database, the non-ideality of the EOS, thermodynamic, electrostatic and transport properties of H₂O is calculated using the comprehensive Johnson-Norton model that is implemented in the Thermo-Calc software. The non-ideality of the AQUEOUS solution phase in this database is described using the complete revised HKF (Helgeson-Kirkham-Flowers) model, i.e., taking into account of the Debye-Hückel Limiting Law term, ionic solvation, ionic association, as well the binary, ternary and higher-order interaction terms.

This database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES, TTNi/Ti/Al/Mg, and GCE databases. Some phases from other appropriate databases, such as gaseous mixtures and stoichiometric solids from SSUB, and solid solutions from SSOL or TCFE, should be appended to make heterogeneous equilibrium calculations in complex systems involving aqueous solutions.

AQS2 can be used in the POURBAIX module in the TCC software, if the multiple database option is chosen with appropriately appended gas and solid phases from other available databases (*e.g.*, SSUB, SSOL, TCFE, TCNI, TCMP, TCES, TTAI/Ti/Ni/Mg, PGEO or GCE, depending upon application fields and investigation interests), for performing calculations of the so-called Pourbaix diagrams (pH-Eh) and related property diagrams, and in normal TCC and TCW calculation routines for conducting other types of stepping or mapping calculations in varied heterogeneous interaction systems.

Assessed Systems

AQS2 contains evaluated thermodynamic data for a large amount of different species (approximately 1600) in the AQUEOUS solution phase.

Limits

This database is developed for calculating thermodynamic properties of aqueous solutions at conditions of temperatures up to 1000°C, pressures up to 5 kbar, and aqueous concentrations up to 6 molality (at room temperature and pressure) or higher (at high temperature and pressure).

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

Scientific Models & References

See the Thermo-Calc Software reference list and reference library at: <http://www.thermocalc.com/resources/>

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