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<b>Database name:</b>	TCS Aqueous Solution Database	<b>Database version:</b>	2.5
<b>Database acronym:</b>	TCAQ2		
<b>Database owner:</b>	Thermo-Calc Software AB		
<b>Database segment:</b>	Aqueous Solutions		

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### Brief description

TCAQ2 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

Ag	Al	Ar	As	Au	B	Ba	Be	Bi	Br	C	Ca	Cd	Ce	Cl	Co	Cr
Cs	Cu	Dy	Er	Eu	F	Fe	Ga	Gd	Ge	H	He	Hg	Ho	I	In	Ir
K	Kr	La	Li	Lu	Mg	Mn	Mo	N	Na	Nb	Nd	Ne	Ni	O	Os	P
Pb	Pd	Pr	Pt	Ra	Rb	Re	Rh	Ru	S	Sb	Sc	Se	Si	Sm	Sn	Sr
Ta	Tb	Te	Th	Ti	Tl	Tm	U	W	V	Xe	Y	Yb	Ze	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 and thermodynamic properties of H<sub>2</sub>O is calculated, using an empirical expression of the simplified HGK model. The non-ideality of the AQUEOUS solution phase in this database is described using the extended SIT model, i.e., taking into account of the Debye-Hückel Limiting Law term, 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.

The TCAQ2 database can be used in the POURBAIX module in the TCC software, if the multiple database option is chosen with appended gas and solid phases from other available databases (e.g., SSUB and SSOL).

### Assessed Systems

TCAQ2 contains evaluated thermodynamic data for a large amount of different species in the AQUEOUS solution phase.

### Limits

TCAQ2 can be applied to low PTX conditions (up to 100 bar, 350 °C and 3 molality). However, if investigated heterogeneous interaction processes occur at high PTX (up to 5 kbar, 1000 °C, and 6 molality of equivalent NaCl at room PT conditions and higher concentrations at higher PT), the other aqueous solution database (i.e., AQS2) is required, which implies the complete revised HKF (Helgeson-Kirkham-Flowers) model.

Combinations of several critically-assessed systems can calculate and extrapolate higher-order multicomponent systems. Such extrapolations require experience and understanding and the producer or vendor should be contacted if problems occur. Critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software 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 available at:

[http://www.thermocalc.com/DOWNLOAD\\_AREA/References.html](http://www.thermocalc.com/DOWNLOAD_AREA/References.html)