GCE2

Database name: TGG Geochemical/Environmental Database
Database acronym: GCE2 **Database version:** 2.3
Database owner: Theoretical Geochemistry Group
Database segment: Geochemistry and Environment

Brief description
GCE2 is a database containing about 600 minerals.

Applications
Geochemistry, geophysics, hydro-metallurgy, aqueous chemistry and environmental chemistry.

Included Elements

Ag	Al	Ar	As	Au	B	Ba	Be	Br	C	Ca	Cd	Cl	Co	Cr	Cs	Cu
F	Fe	Ga	Gd	H	Hg	I	K	Li	Mg	Mn	Mo	N	Na	Ni	O	P
Pb	Rb	S	Se	Si	Sn	Sr	Ti	U	V	W	Zn					

Included Phases
This database contains critically assessed temperature-, pressure- and composition-dependent data for minerals (silicates, oxides, hydroxides, halides, carbonates, sulfides, sulfates, nitrates, phosphates, etc.). The Birch-Murnaghan model for the pressure dependence of EOS is used. The applicable temperatures range from 298.15 K to about 6000 K and pressures from 1 bar to 1000 kbar (100 GPa). The compounds are treated as either stoichiometric or solution phases. A metallic liquid solution phase is included, but currently there is no data for melt mixture phases with e.g., oxide/silicate/carbonate/sulfide/sulphate/... species (of neutrial or charged forms).

This database is compatible with PURE, SSUB, SSOL, TCFE, SLAG, ION, TCNI, TCMP, TCES and AQS databases. For simulations of complex heterogeneous interactions among minerals, aqueous solutions and sub-/super-critical fluids over a wide temperature-pressure-composition range, the AQS database and the SUPERFLUID model (which is implemented into the Thermo-Calc GES system) can be appended.

Assessed Systems
All phases have been critically assessed and treated by appropriate thermodynamic models.

Limits
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

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