
GCE2: TCS Geochemical/Environmental Database

Database name: TCS Geochemical/Environmental Database *Database acronym:* GCE2

Database owner: Thermo-Calc Software AB *Database version:* 2.3

GCE2 is a database containing about 600 minerals. It is used in applications such as geochemistry, geophysics, hydro-metallurgy, aqueous chemistry and environmental chemistry.

Included Elements (46)

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|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 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 neutral or charged forms).

This database is compatible with almost all other thermodynamic databases available from Thermo-Calc. Especially, when combined with the AQS database, GCE2 can be applied to investigate complex heterogeneous interactions among minerals, aqueous solutions and sub-/super-critical H₂O over a wide temperature - pressure - composition range.

Assessed Systems

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

Limits

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 and References

See the Thermo-Calc Software reference list and reference library at:

<https://www.thermocalc.com/support/resources/>