

# Thermodynamic model for aqueous solutes in low-density fluids: critical assessment of quartz solubility

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Hydrothermal fluids are essential agents of magmatic devolatilization, ore deposit formation and fluid-rock interaction. The modeling of chemical equilibria between minerals, melts and aqueous fluids requires thermodynamic equations of state applicable over wide range of temperature, pressure and composition. Several approaches are available to predict thermodynamic properties of solutes in aqueous fluids: (i) successive hydration of solute, (ii) correlations with H<sub>2</sub>O density, (iii) Helgeson-Kirkham-Flowers (HKF) electrostatic equation of state, (iv) equations of state for solute-solvent mixtures. We have evaluated performance of 16 thermodynamic models for quartz solubility in pure H<sub>2</sub>O up to 1100 °C and 2 GPa. These models generally agree on solubility predictions in the temperature range of 300-700 °C and in the solvent density range of 0.5-1.0 g cm<sup>-3</sup>. By contrast, the individual approaches show large discrepancies at low pressures (< 0.1 GPa) and low densities – experimental data on quartz solubility are best reproduced by hydration, density and virial-based approaches, whereas the electrostatic approaches and calibrations by Holland and Powell (1998) [1] and Gerya et al. (2005) [2] under- or overestimate the quartz solubility. At high pressures (0.5-2 GPa), density models and DEW recalibration accurately predict quartz solubility, whereas the rest of the electrostatic approaches tend to overestimate it. Under high-temperature and high-pressure conditions, the models based on successive hydration or virial expansion perform poorly, partly because they lose their physical meaning. We are developing a new equation of state for aqueous species, which has physically correct limiting behavior at the low-pressure limit of ideal gas, near the critical point of water, and finite hydration coordination at high fluid density. With the complete hydration and formation of the inner sphere around the aqueous solute, the thermodynamic properties of aqueous solute will be function of the combined involvement of intrinsic solute properties, volumetric interaction, and standard-state conversion terms and correlate with the solvent density.

[1] Holland T.J.B. and Powell R. (1998), *Journal of Metamorphic Geology* 16, 309-343.

[2] Gerya T.V. et al. (2005), *European Journal of Mineralogy* 17, 269-283.