Internally Consistent Thermodynamic Data for Epsomite and Hexahydrite

Grevel, Klaus-Dieter[1] Majzlan, Juraj
[1]Albert-Ludwigs-Universität Freiburg, Mineralogisch-Geochemisches Institut, Albertstr. 23b, D-79104 Freiburg

The magnesium sulfates epsomite ($MgSO_4{\cdot}7H_2O$) and hexahydrite ($MgSO_4{\cdot}6H_2O$) are important constituents of marine evaporite deposits. Results from the most recent Mars missions support the assumption that significant quantities of Mg-sulfate hydrates including epsomite and hexahydrite are present on Mars, too (*cf.* Chipera & Vaniman, 2007). Recently, Chou & Seal (2003) determined epsomite-hexahydrite equilibria along four humidity-buffer curves between 25 and 45°C. Calculated equilibrium curves based on standard enthalpy and entropy values of these two minerals reported in the literature (DeKock, 1986; Wagman et al., 1982) are in poor agreement with the experimental humidity data. Using mathematical programming techniques (Chatterjee, 1991; Grevel, 2004) the following values consistent both with the calorimetric data (DeKock, 1986; Wagman et al., 1982) and the humidity brackets (Chou & Seal, 2003) could be derived:

$\Delta_f H^0{}_{298}$ (epsomite) = –3388.82 kJ mol^{-1}

$S^0{}_{298}$ (epsomite) = 370.08 J mol^{-1} K^{-1}

$\Delta_f H^0{}_{298}$ (hexahydrite) = –3086.55 kJ mol^{-1}

$S^0{}_{298}$ (hexahydrite) = 350.02 J mol^{-1} K^{-1}

For water the equation of state by Grevel & Chatterjee (1992) was used; the standard thermodynamic properties were taken from Robie & Hemingway (1995).

References

Chatterjee, ND (1991) Applied Mineralogical Thermodynamics – Selected Topics. Springer-Verlag, Berlin, Heidelberg, 321 p.

Chipera SJ, Vaniman DT (2007) Experimental stability of magnesium sulfate hydrates that may be present on Mars. Geochim Cosmochim Acta 71: 241-250

Chou IM, Seal, RR II (2003) Determination of epsomite-hexahydrite equilibria by the humidity-buffer technique at 0.1 MPa with implications for phase equilibria in the system $MgSO_4$-H_2O. Astrobiology 3, 619-630

DeKock, CW (1986) Thermodynamic properties of selected metal sulfates and their hydrates. US Bur Mines Inform Circ 9081

Grevel K-D (2004) Intern konsistente thermodynamische Daten für ausgewählte Hochdruckphasen im System CaO-MgO-Al_2O_3-SiO_2-H_2O. Habilitation-Thesis, Ruhr-Universität Bochum, 113 p.

Grevel K-D, Chatterjee ND (1992) A modified Redlich-Kwong-equation of state for H_2-H_2O fluid mixtures at high pressures and at temperatures above 400 °C. Eur J Mineral 4, 1303-1310

Robie, RA, Hemingway, BS (1995) Thermodynamic properties of minerals and related substances at 298.15 K and 1 bar (10^5 Pascals) and at higher temperatures. US Geol Surv Bull 2131: 461 p.

Wagman DD, Evans WH, Parker VB, Schumm RH, Halow I, Bailey SM, Churney KL, Nuttall RL (1982) The NBS tables of chemical thermodynamic properties. Selected values for inorganic and C_1 and C_2 organic substances in SI units: J Phys Chem Ref Data 11, Suppl 2: 371 p.

→

Abs. No. **302**
Meeting: **DMG 2008**
submitted by: **Grevel, Klaus-Dieter**
email: **Klaus-Dieter.Grevel@rub.de**
date: **2008-05-30**
Req. presentation: **Vortrag**
Req. session: **S14**