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Heat capacity and thermodynamic properties for coesite and jadeite, reexamination of the quartz-coesite equilibrium boundary

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Abstract

The heat capacities of synthetic coesite and jadeite were measured between about 15 and 850 K by adiabatic and differential scanning calorimetry. The experimental data were smoothed and estimates were made of heat capacities to 1800 K. The following equations represent our estimate of the heat capacities of coesite and jadeite between 298.15 and 1800 K:

$$C_p^0(\text{coesite}) = 141.35 - 0.01514T + 987190.7T^{-2} - 1780.5T^{-1/2} + 1.029 \times 10^{-6}T^2$$

$$C_p^0(\text{jadeite}) = 259.08 + 0.038032T - 2518908T^{-2} - 1332.57T^{-1/2} - 8.8 \times 10^{-6}T^2.$$

Tables of thermodynamic values for coesite and jadeite to 1800 K are presented. The entropies of coesite and jadeite are 40.38 ± 0.12 and 136.5 ± 0.32 J/(mol·K), respectively, at 298.15 K. The entropy for coesite derived here confirms the value published earlier by Holm et al. (1967).

We have derived an equation to describe the quartz-coesite boundary over the temperature range of 600 to 1500 K, P(GPa) = 1.76 + 0.001T(K). Our results are in agreement with the enthalpy of transition reported by Akaogi and Navrotsky (1984) and yield −907.6 ± 1.4 kJ/mol for the enthalpy of formation of coesite from the elements at 298.15 K and 1 bar, in agreement with the value recommended by CODATA (Khodakovsky et al. 1995). Several sources of uncertainty remain unacceptably high, including: the heat capacities of coesite at temperatures above about 1000 K; the heat capacities and volumetric properties of α quartz at higher pressures and at temperatures above 844 K; the pressure corrections for the piston cylinder apparatus used to determine the quartz-coesite equilibrium boundary.