LOW AND HIGH TEMPERATURE HEAT CAPACITIES OF DEERITE, HOWIEITE AND ZUSSMANITE

Bertoldi, C.[1,2], Dachs, E.[1] & Lattard, D.[3]

[1]Abteilung Mineralogie und Materialwissenschaften, Universität Salzburg, Hellbrunnerstr. 34, 5020, Österreich
[2]Institut für Geowissenschaften, Universität Kiel, Ludwig-Meyn-Strasse 10, 24118 Kiel, Deutschland
[3]Mineralogisches Institut, Universität Heidelberg, INF 236, 69120 Heidelberg, Deutschland
e-mail: christian.bertoldi@sbg.ac.at

Deerite, howieite and zussmanite are iron-rich hydrated silicates that occur in ferruginous metasediments and typically form under blueschist-facies conditions. The three samples studied here are from the type locality, the Laytonville quarry, Mendocino Co., California, USA [1]. The heat capacities of these minerals were measured applying differential scanning calorimetry (DSC: 250--650K) and low-temperature heat-pulse calorimetry (HPC: 5–300 K) using the heat capacity option of the Physical Properties Measurement System (PPMS) produced by Quantum Design [2]. The chemical compositions of the three minerals were determined on pure concentrates with the electron microprobe (major elements), with inductively coupled plasma mass spectrometry (minor and trace elements), and through coulometric titration (H_2O). The standard entropies (S^o_{298}) were calculated by numerical integration of the HPC-data and are given in Table 1. The DSC-data were fitted with a least-squares method using the C_p-polynomial $C_p = k_o + k_1 T^{-0.5} + k_2 T^{-2} + k_3 T^{-3}$ [3] (Table 1). The heat capacities normalized to one atom at 3000 K is a measure for the reliability for extrapolating C_p to higher temperatures, and the calculated values are well within 28.3 ± 2.0 J/(apfu K) reported by [2].

Table 1: Standard entropy, coefficients of the Berman and Brown C_p polynomial and the heat capacity normalized to one atom at 3000 K of deerite, howieite and zussmanite.

	S^o_{298} [J/(mol K)]	k_o [J/(mol K)]	k_1*10^{-3} [J/(mol K)]	k_2*10^{-7} [J/(mol K)]	k_3*10^{-9} [J/(mol K)]	C_p(3000K) [J/(apfu K)]
[1]Deerite	784(±1)	1225.1	-12.908	–5.6734	7.3766	26.6
[2]Howieite	1333(±2)	3070.5	-35.179	5.8947	–10.469	29.7
[3]Zussmanite	1669(±2)	2801.1	-7.9120	-10.444	12.252	26.5

[1] $(Fe^{2+}_{5.30(03)}Mn_{0.59(05)}Mg_{0.03(01)})(Fe^{3+}_{2.98(02)}Al_{0.01(03)})[Si_{6.03(03)}O_{20}](OH)_{5.04(02)}$
[2] $Na_{1.04(04)}(Fe^{2+}_{5.55(16)}Fe^{3+}_{2.99(08)}Mn_{2.43(16)}Mg_{0.40(11)}Al_{0.14(06)})[Si_{11.94(05)}O_{31}](OH)_{13.05(09)}$
[3] $K_{0.93(02)}Na_{0.06(01)}(Fe^{2+}_{10.90(29)}Mn_{0.56(10)}Mg_{1.07(18)}Al_{0.37(04)})[Si_{16.78(12)}Al_{1.22(12)}O_{42}](OH)_{13.97(10)}$

[1] AGRELL, S.O., BROWN, M.G. & MCKIE, D. (1965) Am. Mineral., 50, 278.
[2] DACHS, E. & BERTOLDI, C. (2005) Eur. J. Mineral., 17, 251-261.
[3] BERMAN, R.G. & BROWN, T.H. (1985) Contrib. Mineral. Petrol., 89.168-183.