Heat capacity measurements of CaAlSiO$_4$F from 5 to 850 K and its standard entropy

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ABSTRACT

Heat capacity (C_P) data of Al-F-bearing titanite are presented that yield the standard entropy $S_{298.15}^{\circ}$ of F-Al-titanite CaAlFSiO$_4$ (FAT). C_P of synthetic FAT was measured with relaxation calorimetry and differential scanning calorimetry between 5 and 764 K. The results constrain $S_{298.15}^{\circ}$ to be 115.4 ± 2.0 J/(mol·K) and subsequently the standard Gibbs free energy of formation from the elements, $\Delta_f G^{\circ}$, of CaAlSiO$_4$F to be between –2583 ± 3.0 and –2588 ± 3.0 kJ/mol, and the standard enthalpy of formation from the elements, $\Delta_f H^{\circ}$, to lie between –2728 ± 3.0 and –2733 ± 3.0 kJ/mol depending on the thermodynamic data retrieval approach. These data, in turn, can be used to quantitatively model high-grade and UHP fluid-rock interaction. The calculation of future petrogenetic grids involving F-bearing minerals and titanite solid solutions in the system CaTiSiO$_4$O–CaAlSiO$_4$F will only be possible by expanding existing internally consistent thermodynamic databases to the F-system.

Keywords: F-Al titanite, PPMS, DSC, standard entropy