Estimation of Fusion Entropy and Fusion Enthalpy of Salts from Crystal Structure

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Fusion enthalpy is an important physical property of the phase change materials (PCM). The magnitude of the fusion enthalpy and melting point influences the actual performance of PCM. Salts have been most preferable high-temperature PCM and they have been widely used for thermal energy storage in the nuclear fuel molten salt reactors or thermal insulation materials in space flight because of their high fusion enthalpy per unit mass. Reliable data of fusion enthalpy are necessary for the process design. However, because of the difficulties in the high temperature of measurement, some of the fusion enthalpy data of salts were derived from phase diagrams or were averaged of widely scattered values. An empirical relationship can be used to estimate fusion enthalpy and a numerical value can be provided when there are no experimental data. Estimations are also useful in selecting the most probable experimental value in cases where two or more values are in significant disagreement. The purpose of this paper is to estimate the fusion entropy of salts based on a uniform model. Fusion enthalpies are calculated from fusion entropies and experimental melting temperature of the solid based on Walden's rule. The physical meaning of total entropy of melting is the sum of all the entropies of transition and the entropy of melting from the crystal to the isotropic liquid. According to Bondi (1968), the total entropy of melting is the sum of its positional, rotational, and conformational contributions. Based on Walden's rule, the entropy of melting for some compounds with little flexibility equals to a constant *C*. Dannenfelser et al. (1993) found that the total entropy of melting for rigid compounds can be predicted by extending Walden's rule to include the effect of molecular rotational symmetry. They related the rotational entropy of melting to the external rotational symmetry number of the molecule. Following equation can be obtained by combining these concepts. In this paper the calculation of entropy of melting is extended further and refined so that it is applicable to chloride and fluoride salts. The molecular symmetry number is refined, and the molecular flexibility is correlated with an empirical relationship. The equation can be used to predict both 1-1 and 1-2 type inorganic salts. Special satisfactory results were obtained for fluoride salts.