

Direct Determination of the Thermodynamic Properties of Melting for Amino Acids

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The properties of melting are used for the prediction of solubility of solid compounds. Unfortunately, by using the conventional DSC or adiabatic calorimetry, direct determination of the melting enthalpy and melting temperature is often not possible for biological compounds due to the decomposition during the measurement. The apparent activation energy of decomposition is at least one order of magnitude smaller than that of melting. This allows shifting of the decomposition process to higher temperature without seriously disturbing the melting by applying very high heating rates. High scanning rates up to $2 \cdot 10^4 \text{ K} \cdot \text{s}^{-1}$ are utilized with fast-scanning calorimeter Mettler Toledo Flash DSC1, which employs thin film chip sensors with sub $\mu\text{J} \cdot \text{K}^{-1}$ addenda heat capacities. With the help of this technique, the melting parameters for L-threonine and glycine were successfully determined, from which the melting temperature of L-threonine and glycine (extrapolated to zero heating rate) were determined. The ultra-fast cooling of the melted samples allows the studied compounds to remain in the liquid state and to determine for the first time its glass transition temperatures. The determined glass transition temperatures agree with the Beaman-Kauzmann rule ($T_g \approx 2/3 T_{\text{fus}}$). At the same time, the entropy of fusion calculated as the ratio of the enthalpy of fusion and melting temperature shows significant deviation between the two amino acids. For L-threonine, it was close to the Walden's rule, while for glycine, it was twice smaller. The results are in reasonable agreement with the simulated PC-SAFT values.