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New experimental melting properties as access for predicting amino-acid solubility

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Abstract

© The Royal Society of Chemistry 2018. The properties of melting are required for the prediction of solubility of solid compounds. Unfortunately, direct determination of the enthalpy of fusion and melting temperature by using conventional DSC or adiabatic calorimetry is often not possible for biological compounds due to decomposition during the measurement. To overcome this, fast scanning calorimetry (FSC) with scanning rates up to 2 × 104 K s-1 was used in this work to measure the melting parameters for l-alanine and glycine. The enthalpy of fusion and melting temperature (extrapolated to zero heating rate) were ΔfusH = (22 ± 5) kJ mol-1 and Tfus = (608 ± 9) K for l-alanine, and ΔfusH = (21 ± 4) kJ mol-1 and Tfus = (569 ± 7) K for glycine. These melting properties were used in the modeling framework PC-SAFT to predict amino-acid solubility in water. The pure-component PC-SAFT parameters and one binary parameter were taken from literature, in which these parameters were fitted to solubility-independent thermodynamic properties such as osmotic coefficients or mixture densities. It was shown that this allowed accurately predicting amino-acid solubility in water over a broad temperature range. The combined methodology of PC-SAFT and FSC proposed in this work opens the door for predicting solubility of molecules that decompose before melting.

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