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Does the Anisotropy of Intermolecular Interactions Determine the Protein Crystal Symmetry? Peter G. Vekilov, Dept. of Chemical Engineering, Univ. of Houston, Houston, Texas 77204-4004.

For insight into the correlation between the anisotropic intermolecular interaction potentials and the crystal symmetry, we compare the thermodynamic characteristics of three phases: normal aqueous solution, the dense liquid that exists in solutions of some proteins under certain conditions, and the crystals of the protein lysozyme. We use independent data on temperature dependence of the second virial coefficient, solution – solid equilibrium, and the binodal and spinodal for liquid-liquid coexistence. We determine the protein chemical potential and osmotic pressure for concentrations as high as 320 mg mL⁻¹ in the above temperature range.

We find that for this protein the enthalpy of the liquid-liquid separation, as expected, vanishes at the critical temperature T_c . At temperatures lower than 5 K from T_c , this enthalpy exceeds the crystallization enthalpy (~ 65 kJ mol⁻¹). The enthalpy of the pair interactions averaged over all polar angles is significantly lower. This comparison suggests structuring of the dense liquid so that pairs of adjacent molecules occupy energetically favored sites in their pair interaction potential, and that in the dense liquid some of the deep minima are also occupied, i.e., in the crystal structure the molecules do not occupy the deepest minima.