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Weighted Random Mixing and Exact Finite Lattice Descriptions of Molecular Aggregation Equilibria[1]

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Entropic and energetic contributions to a broad class of molecular aggregation and self-assembly processes are described by performing a mean field Boltzmann average over aggregate size distributions pertaining to an idealized random mixture. Predictions obtained using the resulting weighted random mixing (WRM) model are compared with exact finite lattice and fluid molecular dynamics simulation results for systems in which each aggregate resembles a central molecule with multiple ligand binding sites. Good agreement between the exact and WRM results is found for systems with interaction energies of various magnitudes (and signs), both in the large and small cohesive interaction energy regimes (or at low and high temperature, respectively). The latter two regimes are separated by a critical point on either side of which qualitatively different aggregation behavior is predicted and observed. More specifically, both the WRM model and exact finite lattice aggregation results reveal that when half the ligand binding sites are filled, the corresponding aggregate size distributions are bimodal below and unimodal above the corresponding critical temperature, whose value depends on the ligand-ligand interaction energy, but is independent of the binding energy of each ligand to the central molecule.

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