Construction of a Composite-Sphere Model for Molecules of Tetrahedral Symmetry

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We propose a "composite sphere" model for molecules of tetrahedral symmetry. In particular, we choose as an example the hydrocarbon neopentane. We disassemble the molecule into 5 moieties: four methyl groups (species A) and one carbon atom (species B). By imparting pair potentials of spherical symmetry to the A-A (hard sphere type), B-B (hard sphere type), and A-B (square-well type) pairs, we are able to reconstitute the pentamer structure via Monte Carlo simulation. This is demonstrated for four density states: ρ_A^3= 0.03, 0.10, 0.15, and 0.20. We apply two criteria in assessing the percent formation of pentamers: namely the *proximity rule* and the *energy rule*. The proximity rule gives 57% formation of pentamers, while the energy rule is able to give 99% pentamers.