Structure of Rigid Hard-Ring Fluids

MARIAM NOURI, MARC ROBERT, Department of Chemical and Biomolecular Engineering, Rice University — Structure of fluids of molecules consisting of rigid rings of hard spheres is studied in two, quasi two, and three dimensions, using Monte Carlo computer simulations in the canonical ensemble. For rings of various size and for a wide range of densities, results are reported for the pair distribution function of the ring centers and for the pair distribution of the ring orientations. For dense fluids in two dimensions, a shoulder, precursor of the freezing transition, is observed in the second peak of the pair distribution function of the ring centers, as previously seen in the simple hard-sphere fluid. In quasi two dimensions, where the centers of the rings are confined to a plane but the rings themselves can wobble out of plane, a liquid crystalline nematic phase is observed at sufficiently high densities. Results are also presented for three dimensions.