Pressure and Isotropic-Nematic Transition Temperature of Model Liquid Crystals

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Z. Naturforsch. **54 a,** 559–569 (1999); received June 1, 1999

The pressure in the gaseous, the isotropic liquid and nematic liquid crystalline states, as well as the isotropic–nematic transition temperature are calculated for a model system composed of non–spherical particles. The potential is a generalization of the Lennard–Jones interaction where the attractive part depends on the relative orientations of the particles and the vector joining their centers of mass. Point of departure is an augmented van der Waals approach. It involves a modified Carnahan–Starling expression associated with the repulsive part of the interaction, and an orientation dependent second virial coefficient, as well as the orientational distribution functions of a pair of particles, linked with the attractive part of the potential. In a high temperature approximation, and for a special choice of model parameters, results are presented and displayed graphically.

PACS: 05.20.-y, 61.30.by, 64.70.-p, 64.70.Md

Key words: Nematic Liquid Crystal; Interaction Potential; Equation of State.