Molecular Ordering in Non-Liquid Crystalline versus Liquid Crystalline Materials with Special Reference to DADMBP – A Computational Analysis

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Z. Naturforsch. **57a,** 194–198 (2002); received February 8, 2002

A computational analysis of the molecular ordering of the non-liquid crystalline biphenyl derivative 4,4′-diamino-3,3′-dimethylbiphenyl (**DADMBP**) has been performed. The **CNDO/2** method has been employed to compute the net atomic charge and atomic dipole components at each atomic centre. The modified Rayleigh-Schrödinger perturbation theory along with the multicentered-multipole expansion method has been employed to evaluate the long-range interactions, while a "*6-exp*" potential function has been assumed for short-range interactions. On the basis of stacking, in-plane and terminal interaction energy calculations, all possible arrangements of a molecular pair have been considered. It is found that, if a suitable functional group is attached to **DADMBP**, so that the length to breadth ratio is increased, the molecule will show a change in the long-range order, the phase transition temperature and other liquid crystalline properties. The results are compared with those for the liquid crystalline compounds 4-(*4′*-ethoxyphenylazo)phenyl valerate (**EPPV**) and 4,4′-di-*n*-propoxy-azoxybenzene (**DPAB**).

Key words: DADMBP; CNDO/2 Method; Quantum Chemistry; Computer Simulation.