Molecular Ordering in Liquid Crystalline EMBAC. A Quantum Mechanical Study

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Molecular ordering in a liquid crystal, ethyl 4-(4′-methoxybenzylidene amino) cinnamate (EMBAC) has been studied by intermolecular interaction energy calculations. The CNDO/2 method has been employed to compute the atomic charge and atomic dipole at each atomic centre. The modified Rayleigh-Schrödinger perturbation theory along with the multicentered-multipole expansion method have been employed to evaluate the long-range intermolecular interactions, while a '6-exp' potential function has been assumed for the short-range interactions. On the basis of stacking, in-plane, and terminal interaction energy calculations all possible geometrical arrangements of a molecular pair have been considered, and the most favourable configuration of the pair has been obtained. Molecular parameters like total energy, binding energy and total dipole moment have been given. Results are discussed in the light of those obtained for the nematogens 4-(4′-ethoxyphenylazo) phenyl valerate (EPPV) and 4,4′-di-*n*-propoxyazoxybenzene (DPAB). An attempt is made to explain the liquid crystalline behavior of these liquid crystals and thereby develop a molecular model for liquid crystallinity.

Key words: Liquid Crystal; Multicentered-multipole; CNDO/2 Method; Intermolecular Interactions; EMBAC.