Molecular Ordering of a Nematic Liquid Crystal in a Dielectric Medium

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A computational analysis of the molecular ordering of 4-(4′-ethoxyphenylazo) phenyl hexanoate (**EPPH**) has ben carried out on the basis of intermolecular interaction energy calculations. The **CNDO/2** method has been employed to evaluate the net atomic charge ad atomic dipole moment components at each atomic centre of the molecule. A modified Rayleigh-Schrödinger perturbation theory alongwith a multicentered-multipole expansion method has been employed to evaluate long-range intermolecular interactions, while a "6-exp" potential function has been assumed for short-range interactions, and corresponding probabilities have been calculated in a dielectric medium (benzene) using the Maxwell-Boltzmann formula. Further, the flexibility of various configurations has been studied in terms of variations of the probability due to departure from the most probable configuration. All possible geometrical arrangements between molecular pairs have been considered during stacking, in-plane and terminal interactions, and the most favourable configuration of the paring has been obtained. It has been observed that in a dielectric medium the probabilities are redistributed and there is a considerable rise in the probability of interactions although the order of preference remains the same. An attempt has been made to explain the nematogenic behaviour of liquid crystals and thereby develop a molecular model for liquid crystallinity. Results have been discussed in the light of those obtained for other nematogens like **EPPV** [4-(4′-ethoxyphenylazo) phenyl valerate] and **DPAB** [4-4′-di-*n*-propoxy-azoxybenzene].

Key words: CNDO/2 Method; Intermolecular Interactions; Statistical Analysis; Computer Simulation.