

Nematogenic Behaviour of EPPV in a Dielectric Medium.

A Theoretical Study

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4-(4'-ethoxyphenylazo) phenyl valerate (**EPPV**) is a nematic liquid crystal, which shows a nematic mesophase at 352 K and becomes an isotropic melt at 401 K. A theoretical study of the molecular ordering has been carried out on the basis of intermolecular interaction energy calculations. The **CNDO/2** method has been employed to compute the net atomic charge and atomic dipole components at each atomic centre of the molecule. Modified Rayleigh-Schrödinger perturbation treatment has been employed to calculate the interaction energy between a molecular pair. The probability of the occurrence of a particular configuration in a dielectric medium has been calculated using the Maxwell-Boltzmann formula. The flexibility of various configurations has been studied in terms of the variation of the probability due to a small departure from the most probable configurations. On the basis of stacking, in-plane and terminal interactions, all possible geometrical arrangements between a molecular pair have been considered, and the most favourable configuration of pairing has been obtained. An attempt has been made to explain the nematogenic behaviour of liquid crystals based on the parameters introduced in this paper.

Key words: CNDO/2 Method; Interaction Energy; Statistical Distribution.