Nematogenic Behaviour of a Cyano-Compound Using Quantum Mechanics and Computer Simulations

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Using quantum mechanics and intermolecular forces, the molecular ordering of a nematogenic cyano-compound, 5-(*trans*-4-ethylcyclohexyl)-2-(4-cyanophenyl)-pyrimidine (**ECCPP**), has been examined. The **CNDO/2** method has been employed to evaluate the net atomic charge and the dipole moment components at each atomic centre of the molecule. The configuration energy has been computed using the modified Rayleigh-Schrödinger perturbation method at intervals of 1Å in translation and 10^0 in rotations, and corresponding probabilities have been calculated using Maxwell-Boltzmann statistics. The flexibility of various configurations has been studied in terms of the variation of the probability due to small departures from the most probable configuration. All possible geometrical arrangements between a molecular pair have been considered during stacking, in-plane and terminal interactions, and the most favourable configuration of pairing has been obtained. An attempt has been made to understand the behaviour of the molecules in terms of their relative order. The results have been compared with those obtained for other nematogens like **DPAB** [4,4′-di-n-propoxy-azoxybenzene] and **EMBAC** [ethyl 4-(4′-methoxybenzylidene amino) cinnamate].

Key words: ECCPP; CNDO/2 Method; Intermolecular Forces; Computer Simulation.