

Role of Dielectric Medium on a Nematogen. A Statistical Approach Based on Quantum Mechanics and Computer Aided Modelling

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A statistical analysis has been carried out to determine the configurational preferences of a pair of 5-(4-ethylcyclohexyl)-2-(4-cyanophenyl) pyrimidine (**ECCP**) molecules. The **CNDO/2** method has been employed to evaluate the net atomic charge and atomic dipole components at each atomic centre of the molecule. The configurational energy has been computed using the Rayleigh-Schödinger perturbation theory. The total interaction energies obtained by these computations were used to calculate the probability of each configuration in vacuum and in a dielectric medium (benzene) at the phase transition temperature using the Maxwell-Boltzmann formula. On the basis of stacking, in-plane and terminal interaction energy calculations, all possible geometrical arrangements of the molecular pair have been considered. An attempt has been made to explain the nematogenic behavior of liquid crystals and thereby develop a molecular model for liquid crystallinity.

Key words: Liquid Crystal; Quantum Chemistry; Computer Simulation,