Computer Simulations of Ordering in a Nematogen – The Role of Dielectric Medium

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Z. Naturforsch. **65a,** 555 – 560 (2010); received June 29, 2009 / revised October 7, 2009

Computer simulations of ordering in a nematic liquid crystal propyl 4-(4′-methoxybenzylidene amino)-α-methyl cinnamate (MBA2C3) was carried out with respect to translatory and orientational motions. The evaluation of atomic charges and dipole moment at each atomic center was carried out through the complete neglect differential overlap (CNDO/2) method. The modified Rayleigh-Schrödinger perturbation method along with 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. The total interaction energy values obtained through these computations were used to calculate the probability of each configuration in a dielectric medium (i. e., non-interacting and non-mesogenic solvent, e. g. benzene) at room temperature (300 K) using the Maxwell-Boltzmann formula. On the basis of stacking, in-plane, and terminal interaction energy calculations, all possible geometrical arrangements of pairs have been considered. The most favourable configuration of pairing has been obtained. An attempt has been made to develop a new and interesting molecular model of nematogen in dielectric medium.

Key words: Computer Simulations; Nematogen; Quantum Chemistry; Dielectric Medium.