Molecular Organization in a Nematogen: PBPCN – A Computational Analysis Based on Quantum Mechanics

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A computational analysis has been carried out to determine the configurational preference of a pair of 4'-*n*-pentyloxy-4-biphenylcarbonitrile (**PBPCN**) molecules with respect to translatory and orientational motions. The **CNDO/2** method has been employed to evaluate the net atomic charge and atomic dipole components at each atomic centre of the molecule. Modified Rayleigh-Schrödinger perturbation theory 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. On the basis of stacking, in-plane and terminal interaction energy calculations, all possible geometrical arrangements of molecular pair have been considered. It has been observed that the molecule has a strong preference for stacking through a particular face, while the other configurations, such as stacking through the other face, in-plane and terminal interactions show, in general, an aligned structure along molecular axis. The results are discussed in the light of experimental as well as other theoretical observations.

Key words: PBPCN; Nematogen; Interaction Energy; Computer Simulation.