Molecular Ordering of 4-Acetyl-2′-Nitrobiphenyl – A Computational Analysis

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The molecular ordering of some biphenyl derivatives like 4-acetyl-2′-nitrobiphenyl (**ANBP**), 4-nitro-2-biphenylamine (**NBPA**) and 4-acetyl-3′-chlorobiphenyl (**ACBP**) has been examined using basic concepts of quantum mechanics and intermolecular forces. The CNDO/2 method has been employed to compute the net atomic charge and atomic dipole components at each atomic centre. The modified Rayleigh-Schrödinger perturbation theory along with the multicentred-multipole expansion method has been employed to evaluate long-range interactions while a '6-exp' potential function has been assumed for short-range interactions. Accuracies upto 0.1 Å in translation and 1° in rotation have been achieved. Probability of occurrence of a particular configuration has been calculated using MB-statistics. On the basis of stacking and in-plane interaction energy calculations, all possible geometrical arrangements between molecular pairs have been considered and a most favorable configuration of pairing has been obtained. A comparative picture of molecular parameters like total energy, binding energy, total dipole moment etc. has been given. An attempt has been made to develop a molecular model correlated with the liquid crystalline property exhibited by this class of molecules.

Key words: Biphenyl Derivatives; CNDO/2 Method; Interaction Energy; MB-Statistics.