Nematic Behaviour of a Compound EBBA – A Compuational Analysis

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A computational analysis has been carried out to determine the configurational preferences of a pair of *p*-ethoxybenzylidine-*p*-*n*-butylaniline (**EBBA**) 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. The configurational energy has been computed using the Rayleigh-Schrödinger perturbation method. The interaction energies obtained through these computations were used to calculate the probability of each configuration at 300 K. The energy of a molecular pair during stacking, in-plane, and terminal interaction has been calculated. The results are discussed in the light of other experimental and theoretical results.

Key words: EBBA, CNDO/2 Method; Quantum Chemistry; Computer Simulation.