Odd-even Effect in a Homologous Series of 4-n-Alkylbenzoic Acids: Role of Anisotropic Pair Potential

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A computational analysis based on quantum mechanics has been carried out to determine the association energy of seven homologues of the 4-n-alkylbenzoic acid series \((n = 3, 4, 5, 6, 7, 8, \text{ and } 9)\), using the Rayleigh-Schrödinger perturbation method for various nearest neighbour configurations of interacting pairs. The net atomic charges and dipoles have been computed using the \textit{CNDO/2} method. An attempt is made to explain the odd-even effects at the molecular level on the basis of these results.

\textit{Key words:} Mesogens, Odd-even Effects, Pair Potential, Computer Simulation.