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

Durga Prasad Ojha, Devesh Kumar, and V. G. K. M. Pisipati

Centre for Liquid Crystal Research and Education (CLCRE), Faculty of Physical Sciences, Nagarjuna University, Nagarjuna Nagar (A.P.) 522 510 India

Reprint requests to Prof. V. G. K. M. P.; venkata_pisipata@hotmail.com

Z. Naturforsch. **57a,** 189–193 (2002); received November 6, 2001

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, 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 **CNDO/2** method. An attempt is made to explain the odd-even effects at the molecular level on the basis of these results.

Key words: Mesogens, Odd-even Effects, Pair Potential, Computer Simulation.