Smectogenic Behaviour of 7O.6 at it's Phase Transition Temperature: A Computational Analysis

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 request to Prof. V. G. K. M. P.; E-mail: venkata_pisipati@hotmail.com

Z. Naturforsch. **56a,** 873–878 (2001); received October 12, 2001

A computational analysis has been carried out to determine the configurational preference of a pair of *N*-(4-*n*-heptyloxybenzylidine)-4-hexylaniline **(7O.6)** 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 modified Rayleigh-Schrödinger perturbation method. The obtained energies were used to calculate the probability of each configuration at phase transition temperature, using Maxwell-Boltzmann's formula. The flexibility of various configurations has been studied in terms of variations of the probability due to small departures from the most probable configuration. The results are discussed in the light of experimental as well as other theoretical observations. The smectogenic character of the molecule has been correlated with the parameters introduced in this paper.

Key words: 7O.6, CNDO/2 Method; Quantum Chemistry; Computer Simulation.