Computer Simulation of Chiral Liquid Crystal Phases IX. Chiral Induction in Guest-host Systems – Calculation of the Helical Twisting Power

Reiner Memmer and Folkert Janssen

Fachbereich Chemie, Universität Kaiserslautern, D-67663 Kaiserslautern

Reprint requests to Dr. R. M.; E-mail: memmer@rhrk.uni-kl.de.

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The chiral induction in liquid crystalline phases was studied by Monte Carlo simulation of the chiral Lebwohl-Lasher model. Binary guest-host systems composed of achiral and chiral molecules as well as of different chiral molecules were investigated in dependence on the composition. A cholesteric phase was induced by dissolving a small fraction of chiral molecules in a nematic phase. For dilute solutions the equilibrium pitch was found to be a linear function of the chiral dopant concentration. Independent of system size effects the application of self-determined boundary conditions enabled the determination of the symmetry adapted quantities for the chiral induction, the helical twisting power (HTP) and the achiral helical twisting power (AHTP). Additionally, a different orientational behaviour of enantiomeric dopants in the chiral surroundings of a cholesteric host phase has been determined.

Key words: Chirality; Liquid Crystals; Computer Simulation; Induced Cholesteric Phases; Helical Twisting Power.