Generalized Maier-Saupe Theory for Flexible Nematogens*

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We have applied a generalized Maier-Saupe approximation appropriate for flexible molecules [1] to the calculation of nematic-isotropic transition temperatures for a variety of liquid crystals. The goal of this work is to develop a tool for the routine pre-synthesis prediction of clearing temperatures for new materials. We report our initial attempts to calibrate the model by fitting calculated transition temperatures to observed values for a representative ensemble of nematogens to fix the adjustable parameter(s) in the model. These calculations involve detailed quantum chemical studies of conformational energy surfaces for flexible mesogenic molecules, from which rotational isomeric state (RIS) models are derived. Within the RIS approximation, numerical solutions of the Maier-Saupe mean field theory can be obtained. The results of this study provide information about the relative importance of steric and dispersion interactions and conformational entropy in determining the clearing temperature.

[1] D.J. Photinos, E.T. Samulski, and H. Toriumi, *J. Chem. Phys.* **94**, 2758 (1991).

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