

عنوان مقاله:

Calculation of Stability Limit of Isotropic and Uniaxial Nematic Liquid Crystals with Hard Ellipsoid Molecules

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 3

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خلاصه مقاله:

The equilibrium properties of non- isotropic molecular liquids less studied as compared with spherical molecular liquids. In these systems, molecular interactions depend on separation distance and orientation of molecules. Properties of non- spherical molecular liquid crystal have been studied by integral equation, computer simulation and density functional theory (DFT) [1- 4]. Allen [5], Cheng and coworkers [6] calculated phase stability of isotropic and nematic oblate ellipsoids using computer simulation. In this work, Kerr constant [1], phase stability limit and transition density of I-N of hard prolate ellipsoids are calculated by using DFT and new direct correlation (DCF) [7]

کلمات کلیدی:

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