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How does the molecular structure of the bent-core molecules affects the occurrence of twist-bend nematic phase?: a mean-field study

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A newly observed γ -helical (twist-bend) nematic phase (NTB) of nanoscale pitch [1] has recently caught much of attention. Initially, the theoretical concept of this phase has been presented by R. B. Meyer [2] in 1973, where he assumed that the director of the molecules precesses on a cone forming an oblique helicoidal structure. Subsequently in 2001 Dozov [3], in 2002 Memmer [4] and in 2004 Lorman et al. [5], suggested that the formation of the N_{TB} can be facilitated by the shape of bent-core molecules.

Here we present theoretical investigations on relation between biaxiality and bend angle on stability of nematic twist-bend phase. We use a generalized Maier-Saupe type of model for NTB [6], with intrinsic molecular biaxiality on both of the arms of the molecule, quantified by a 3×3 second-rank traceless symmetric tensor \mathbf{Q} . Values of bend angle ranging from 130 to 170 degree were investigated. The detailed results show the influence of the molecular biaxiality parameter [7] on the relative stability of the NTB, nematic, isotropic phase and the related phase transitions. For the bend angles equal or larger than 140 degree we observe all five possible phases: uniaxial and biaxial twist-bend nematics, together with uniaxial and biaxial nematics and isotropic phase.

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