Polar Uniaxial and Biaxial Nematic Phases formed from V-shaped Molecules

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Recent experimental investigations have suggested that V-shaped molecules, with their biaxial shape, may form the elusive biaxial nematic phase [1-3]. There is a problem, however, because the interarm angle is about 140^o which is far from the optimum angle of 109.47^o predicted by theory [4,5]. To explain this difference it has been suggested that electrostatic dipolar interactions can stabilise the biaxial nematic phase since the V-shaped molecules in real systems have large electric dipoles [1-3]. The phase maps calculated by Monte Carlo simulations for a model including an idealised dipolar interaction support this suggestion. Indeed the Landau point predicted for V-shaped molecules at the tetrahedral angle [5] develops into Landau line [6] possibly agreeing with experimental observations [1-3]. There is, however, a potential problem for the alignment of dipoles associated with the molecular V would be expected to lead to polar biaxial nematics but the simulations seem to give just apolar phases.

To explore this unusual result we have extended the molecular field theory developed for V-shaped molecules by the inclusion of a dipolar interaction [7,8] via an idealised dipole parallel to axis bisecting the angle between the two mesogenic arms. The phase maps predicted by this molecular field theory as a function of the interarm angle for different dipole moments show that polar biaxial nematic phases are formed with a rich polymorphism including apolar uniaxial and biaxial nematics. This seems, in part, to agree with the Monte Carlo simulations [6] but it is also in marked contrast to some of the simulation results.

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