

Uniform phases in fluids of hard isosceles triangles

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Two dimensional fluids of hard anisotropic particles are paradigms of systems where liquid-crystal phases can be stabilized solely by entropy [1, 2, 3]. Hard-rod particles such as hard rectangles, discorightangles or ellipses, exhibit the completely disordered isotropic (I) phase, but also a nematic (N) phase at higher densities where particle axes point, on average, along a common director. In two dimensions the N phase does not possess true long-range orientational order, and the N-I transition is usually continuous via a Kosterlitz-Thouless disclination unbinding mechanism. The N phase is stable for high enough aspect ratios and its stability region (in the density-aspect ratio phase diagram) is bounded below by the I phase, and above by other liquid-crystal nonuniform phases such as the smectic or completely ordered crystal phases. At low aspect ratios the I phase can exhibit a direct transition to a plastic crystal or to a more complex crystalline phase in which particle shapes, orientations and lattice structures are coupled in a complex fashion.

In the present work we formulate the scaled particle theory for a general mixture of hard isosceles triangles and calculate different phase diagrams for the one-component fluid and for certain binary mixtures [4]. The fluid of hard triangles exhibits a complex phase behavior: (i) the presence of a triatic (TR) phase with sixfold symmetry, (ii) the I-N transition is of first order for certain ranges of aspect ratios, and (iii) the one-component system exhibits N-N transitions ending in critical points. We found the TR phase to be stable not only for equilateral triangles but also for triangles of similar aspect ratios.

We focused the study of binary mixtures on the case of symmetric mixtures: equal particle areas with aspect ratios κ_i symmetric with respect to the equilateral one $\kappa_1\kappa_2 = 3$. For these mixtures we found, aside from first-order I-N and N-N transitions (the latter ending in a critical point): (i) a region of TR phase stability even for mixtures made of particles that do not form this phase at the one-component limit, and (ii) the presence of a Landau point at which two TR-N first-order transitions and a N-N demixing transition coalesce. This phase behavior is analogous to that of a symmetric three-dimensional mixture of rods and plates. In Fig. 1

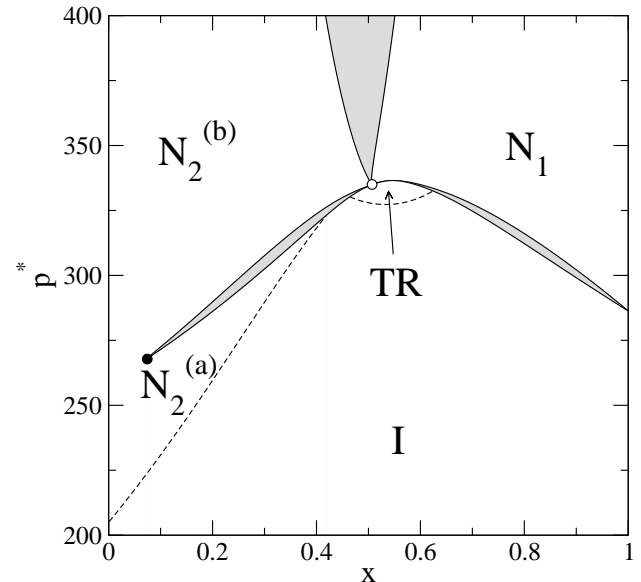


Fig. 1. Phase diagram of a symmetric binary mixture of hard isosceles triangles (see the text for the mixture description).

we show the phase diagram (reduced pressure $p^* = \beta p a_1$ vs. composition $x \equiv x_1$) of a symmetric ($\kappa_1\kappa_2 = 3$) binary mixture with $\kappa_1 = 2.52$, equal particle areas $a_1 = a_2$ and the ratio between the bases of triangles is fixed to $b_2/b_1 = 1.453$.

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- [1] M. A. Bates and D. Frenkel, *J. Chem. Phys.* **122**, 10034 (2000).
 [2] Y. Martínez-Ratón, E. Velasco, and L. Mederos, *J. Chem. Phys.* **122**, 064903 (2005).
 [3] R. Wittmann, C. E. Sitta, F. Smalenburg, and H. Löwen, *J. Chem. Phys.* **147**, 134908 (2017).
 [4] Y. Martínez-Ratón, A. Díaz-De Armas, and E. Velasco, *Phys. Rev. E* **97**, 052703 (2008).