

Two-dimensional model for mixtures of enantiomers, *hard bent needles*: a Monte Carlo simulation

Raúl A. Perusquía and Jacqueline Quintana

Instituto de Química,
Universidad Nacional Autónoma de México,
México 04510 D.F., México.

Abstract

We study the statistical mechanical conditions under which segregation of racemic mixtures of chiral molecules is possible in a 2-dimensional fluid model. Motivated by experimental evidence suggesting that chiral heads of amphiphilic molecules lying in a monolayer can cristalize undergoing a chiral phase separation, we propose a 2-dimensional system to model the projection of the chiral head of amphiphilic molecules in a monolayer. The molecules of our model are infinitely hard and infinitely thin. We consider only infinitely repulsive interactions where molecules have no effective area (2-dimensional volume) and no attractive interactions. As a consequence all effects we found are due to excluded area. The Monte Carlo Gibbs ensemble is used to study phase separation whereas simulations at constant pressure are performed to obtain the equations of state of pure and racemic systems. We find that for this simple model segregation is generally possible in the very high density regime. However, for some specific molecular geometries excluded area is not sufficient to generate segregation.