Calculation of the Phase Behavior of Lipids

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(September 29, 1997)

The self-assembly of monoacyl lipids in solution is studied employing a model in which the lipid's hydrocarbon tail is described within the Rotational Isomeric State framework and is attached to a simple hydrophilic head. Mean-field theory is employed, and the necessary partition function of a single lipid is obtained via a partial enumeration over a large sample of molecular conformations. The influence of the lipid architecture on the transition between the lamellar and inverted hexagonal phases is calculated, and qualitative agreement with experiment is found.