Thermodynamic and Kinetic Models of the Appearance and Amplification of Biological Chirality

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Chiral asymmetry choices exhibited by molecules that are present in living organisms constitute a scientifically challenging set of observations. Such geometric preferences favoring one enantiomer over its mirror image are obvious in the observed structures of amino acids, sugars, and the biopolymers that they form. These facts automatically generate fundamental questions about how those chiral asymmetries arose spontaneously in the terrestrial biosphere [1, 2].

We have formulated thermodynamic [3] and kinetic [4] models of chiral amplification. In the thermodynamic case, we model the phase behavior of a ternary mixture composed of two enantiomeric forms of a chiral molecule and a non-chiral liquid solvent. The mean-field solution of the model allows the calculation of a ternary phase diagram, a prominent feature of which is the existence of two symmetric triple points involving coexistence of a liquid phase enriched in one of the enantiomers, a racemic crystal, and an enantiopure crystal. Over broad ranges of initial composition, including liquid mixtures containing almost equal amounts of the two enantiomers, thermodynamic equilibrium results in liquid-phase chiral amplification, in agreement with experimental observations [5].

The kinetic model involves an auto-catalytic reaction leading to the formation of a chiral compound, inhibition, and molecular diffusion. Numerical solution of the model via kinetic Monte Carlo allows the identification of two types of behavior. In one, the system evolves towards a mixture containing equal amounts of the two chiral enantiomers. In the symmetry-broken regime, the system evolves spontaneously towards large excess of one or the other chiral enantiomers. We map the regions of parameter space leading to symmetry breaking.

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