

EVOLUTION OF HOMOCHIRALITY IN A SYSTEM OF COUPLED CHIRAL BIOMOLECULES

M. BABINCOVÁ, P. BABINEC

*Department of Biophysics, Math. and Phys. Faculty, Comenius University,
Mlynská dolina, 842 15 Bratislava, Slovak Republic*

Received 14 September 1993

Possible explanation of the origin of homochirality of biomolecules at the prebiological stage of evolution is presented, based on the chiral symmetry breaking in a racemic mixture of long-range coupled chiral biomolecules.

Since the Pasteur [1] discovery of mirror asymmetry of living things (proteins are constructed from "left-handed" L-amino acids, whereas nucleic acids contain only "right-handed" D-sugars) many attempts have been made to understand its origin [2-6].

Our aim is to show, that in the presence of the long-range stereospecific coupling between chiral biomolecules, system has similar properties like previously studied cooperative chemical systems.

Let us consider a system of N chiral biomolecules (numbered $i = 1, \dots, N$). Each molecule fluctuate between L and D states, with transition rates r_i^L and r_i^D . The dynamics of i -th molecule is described by two-state master equation for probabilities p_i^L and p_i^D of being in L and D states, respectively. Let each molecule for simplicity is coupled to all others by the same coupling constant C . Transition rates are given by equations

$$r_i^D = r_0 \exp \left(\frac{C}{kT} \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N (p_j^D - p_j^L) + \frac{S}{kT} \right), \quad (1)$$

$$r_i^L = r_0 \exp \left(\frac{C}{kT} \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N (p_j^L - p_j^D) - \frac{S}{kT} \right), \quad (2)$$

where $r_0 = \nu \exp(-\Delta U/kT)$ is transition rate in an isolated biomolecule, with energy barrier ΔU between enantiomers, S/kT is an advantage factor conditioned by, e.g., weak neutral currents induced lowering of the energy of one kind of the enantiomer [2].

The nonlinear Master equations for this system are

$$\frac{dp_i^L}{dt} = r_i^D p_i^L - r_i^L p_i^D, \quad (3)$$

$$\frac{dp_i^D}{dt} = r_i^L p_i^D - r_i^D p_i^L. \quad (4)$$

In the mean field approximation ($N \rightarrow \infty$) we have

$$\frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N (p_j^L - p_j^D) = p_i^L - p_i^D \equiv \eta. \quad (5)$$

The equation of motion for the chiral polarization η is then

$$\frac{d\eta}{dt} = -2r_0 \sinh(\rho\eta + g) + 2r_0\eta \cosh(\rho\eta + g) \quad (6)$$

where $\rho = C/kT$ and $g = S/kT$. The bifurcation equation is then given by the stationary solution of Eq. (6)

$$\eta_0 = \tanh(\rho\eta_0 + g). \quad (7)$$

For $g = 0$ and $g > 0$ bifurcation diagrams are given in Figs. 1a and b, respectively.

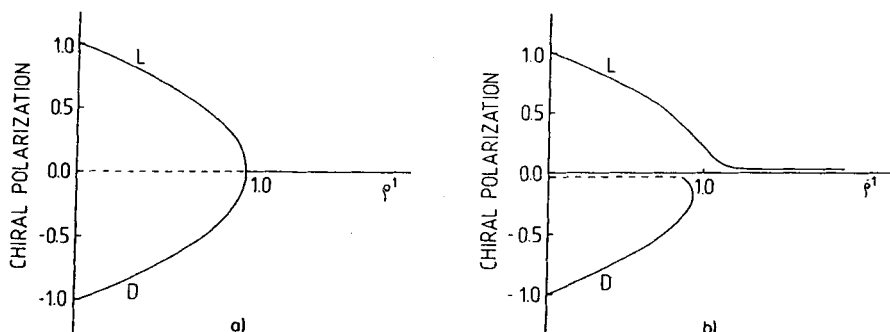


Fig. 1. Bifurcation diagram of the stationary solution of Eq. (6) with the advantage factor a) $g = 0$ and b) $g > 0$.

The dashed lines represent unstable solution and solid lines are for stable solutions. Analogously like in the cooperative chemical systems at $1/\rho = 1$ spontaneous symmetry breaking occurs. The order parameter $1/\rho$ is in this system proportional to the temperature and has much simpler meaning then in previously studied systems. Breaking of chiral symmetry may be realized simply by lowering temperature, which may correspond to one glacial era. For $g > 0$ the branch with $\eta > 0$ polarization is preferred. Open is the question about realization of a very long-range biomolecular coupling. According to some opinions [7,8] the prebiological evolution takes place at a thin layer on the ocean surface. Components of this layer, like lipids and cholesterol, form the liquid crystal structures which can realize long-range forces between molecules [9]. Embedding a racemic mixture in such a model of the liquid crystal system, lowering temperature followed by chiroptic methods, it may be a test of this mechanism expressed by the change in the chiral polarization.

References

- [1] Pasteur L.: *Recherches sur la Dissymetrie Moleculaire*. Masson, Paris, 1860.
- [2] Kondepudi D. K. and Nelson G. W.: *Nature* **314** (1985) 438.
- [3] Klemm A.: *Z. Nat.forsch. A* **40** (1985) 1231.
- [4] Salam A.: *J. Mol. Evol.* **33** (1991) 105.
- [5] Martell E. A.: *J. Mol. Evol.* **35** (1985) 346.
- [6] Krempaský J. and Krejčiová E.: *Gen. Physiol. Biophys.* **12** (1993) 85.
- [7] Onsager L.: *in Quantum Statistical Mechanics in Natural Sciences* (Ed. B. Kursunoglu). Plenum Press, New York, p. 1.
- [8] Lasaga A. C., Holland H. D., and Dwyer M. O.: *Science* **174** (1972) 53.
- [9] Goulian M., Bruinsma R., and Pincus P.: *Europhys. Lett.* **22** (1993) 145.