Chiral symmetry breaking in a chemical network
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Introduction

Interestingly, among the biomolecules, there are certain classes that are enantiomerically pure, like the amino acids and the nucleic acids. Whether this purity is a consequence of the dynamic activity of living matter, or the life originated in a chirally pure ambient, remains to be understood. Here, the dynamic properties of a simple chemical network, containing enantiomeric species, are investigated. Basically, modifications were introduced to a model proposed by Plasson et al., aiming at exploring the consequences of autocatalysis, the flow of matter, and the sensibility to statistical molecular fluctuations on the chiral symmetry breaking processes, see Fig. 1.

**Figure 1** – Illustration of the model reaction network. The blue arrows correspond to the original APED model. A is a prochiral species, P is an inert product, LD and DL are heterochiral dimers and the other species are chiral ones. The rate constants are indicated in lower case.

From the reaction network considered in Fig. 1 one can write the rate law for each species yielding the set of differential equations of the model. The fluctuations were only considered for the initiation steps \( A \rightarrow D, A \rightarrow D \), by considering a random perturbation in its rate constants: \( \tau = \tau_0 (1 + \xi \text{ ran}) \), where \( \xi = <\text{N}>^{-1/2} \) is the relative amplitude order of statistical fluctuations, with N the number of particles, and \(-1 < \text{ ran } < 1\) is a number that follows a random sequence. It is opportune to define here the enantiomeric excess, \( EE \), a normalized measure of the degree of dominance of one enantiomeric family over the other:

\[
EE = \left( \frac{[L] + [L^*] + 2[LL]}{[D] + [D^*] + 2[DD]} \right)^{1/2}
\]

where \( c \) is the sum of the concentration of all chiral species in the system.

Results and Discussion

A stability diagram was obtained in the \((a-\omega)\)-parameter space, where one can identify domains corresponding to the different dynamic regimes: racemic, \( R (EE = 0) \), homochiral, \( H (|EE| = 1) \), and chiral oscillatory, \( O (-1 < EE < 1) \), see Fig. 2.

**Figure 2** – The parameter space \( \alpha \) vs. \( \omega \), showing the stable attractors: racemic (R), oscillatory (O) and homochiral (H). \( b = \beta = \gamma = 0, a = p = h = 1, \tau_0 = \tau = 10^{-1}, e = 1 \) (black) and \( e = 0.5 \) (red). Initial condition: racemic.

Conclusions

The fluctuations allow the dynamic chemical network to break the chiral symmetry autonomously, even starting from a strictly racemic initial state.

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1 Podlech, J. CMLS. 2001, 58(1), 44.