Novel Processes for Chiral Symmetry Breaking

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Abstract:

Macroscopic chiral symmetry breaking refers to as the process in which a mixture of enantiomers departs from 50–50 symmetry to favor one chirality, resulting in either a scalemic mixture or a pure enantiomer. In this domain, crystallization offers various possibilities, from the classical Second Order Asymmetric Transformation (SOAT), Viedma ripening or Temperature Cycle-Induced Deracemization (TCID) to the famous Kondepudi experiment and then to so-called Preferential Enrichment. These processes, together with some variants, will be depicted in terms of Mechanisms, thermodynamic pathways, departure from equilibrium and operating conditions. Influential parameters on the final state will be reviewed as well as the impact of kinetics of the R \Leftrightarrow S equilibrium in solution on chiral symmetry breaking. How one can control the outcome of symmetry breaking is examined. Several open questions are detailed and different interpretations are discussed.

As the system departs more from equilibrium, the mechanical stress imposed on the system has to be softened in order to observe the spontaneous chiral symmetry breaking. Indeed, in Viedma ripening performed close to equilibrium, all sorts of abrasions, breakages, defects induced by shear forces, etc., are beneficial to the advancement of chiral symmetry breaking. In the Kondepudi experiment, the mechanical stress must be softer to avoid primary and secondary heteronucleation in the system. In the case of Preferential Enrichment (PE), the very large departure from equilibrium has to be associated with almost stagnant conditions. Indeed, for the latter case a simple magnetic stirrer is sufficient to return the solution to normal conditions of crystallization without macroscopic chiral symmetry breaking.

References

- Thomas Buhse, Jose-Manuel Cruz, Mar ía E. Noble-Teran, David Hochberg, Josep M. Ribo, Joaquim Crusats, and Jean-Claude Micheau, Spontaneous Deracemizations. Chemical review. https://dx.doi.org/10.1021/acs.chemrev.0c00819
- Leif-Thore Deck, Mercedeh Sadat Hosseinalipour, and Marco Mazzotti, Exact and Ubiquitous Condition for Solid-State Deracemization in Vitro and in Nature, Journal of the American Chemical Society, 2024. 146 (6), 3872-3882; DOI: 10.1021/jacs.3c11332
- Ward, M. R.; Copeland, G. W.; Alexander, A. J., Enantiomorphic symmetry breaking in crystallization of molten sodium chlorate. Chem. Commun. (Cambridge, U. K.) 2010, 46 (40), 7634-7636.
- Intaraboonrod, K.; Lerdwiriyanupap, T.; Hoquante, M.; Coquerel, G.; Flood, A. E., Temperature cycle induced deracemization. Mendeleev Commun. 2020, 30 (4), 395-405.
- Bowen Zhang, Gerard Coquerel, Bum Jun Park, and Woo-Sik Kim, Chiral Symmetry Breaking of Sodium Chlorate in Taylor Vortex Flow, Crystal Growth & Design 2024 24 (3), 1042-1050; DOI: 10.1021/acs.cgd.3c01074

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