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A presumable mechanism of the separation of diastereomeric- and enantiomeric mixtures

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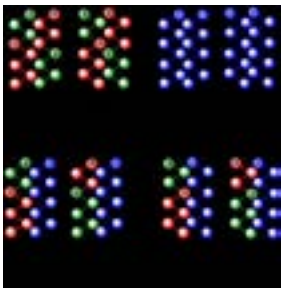
Based on our and others experimental observations we can declare that the distribution between two phases of enantiomeric- and diastereomeric mixtures can be identical (in melt-solid, solution-solid, solid-gas, liquid- liquid phases). The stoichiometry of distribution of enantiomers and diastereomers between phases is determined by the eutectic composition of enantiomeric mixtures of chiral compounds present in the mixture. The distribution of chiral compounds can be different in different solvents. According to the kinetic or thermodynamic control the composition of phases may change during the distribution (i.e. crystallization time) in the same solvent. The molecules in solution (not in solid state) form polymers, associates having P and M helicity, forming double helices (with parallel and antiparallel arrangement). Thus, mirror-image crystals will be formed during the crystallization. Crystals precipitating from the supramolecular associates having P and M helicity formed according to the self-disproportionation (SDE) of chiral compounds are crystallizing in the ratio of the eutectic composition (eeEu) of chiral compounds. Diastereomeric mixtures are separated when the mixture has no mirror-image relation. In this case, the ratio of mirror-image compounds will correlate with the eutectic composition of one of the chiral molecules present in the mixture. The solvent and the time (time of the distribution, time of crystallization) will determine that which one of the chiral compounds will influence the composition of the diastereomeric According to these principles, we have proposed a possible mechanism for distribution of enantiomeric and diastereomeric mixtures , justified by our earlier and recent experimental results.



Biography

Emese Pálovics graduated from the University of Technology "Traian Vuia" of Timisoara in 1990 as a chemical engineer. Since 1994, she has been a scientific assistant at the Budapest University of Technology and Economics in a research group of the Hungarian Academy of Sciences at the Department of Organic Chemical Technology working on crown ethers and organophosphorus compounds. Since 2004, she has been working with Prof. Elemér Fogassy as senior research fellow, in the field of optical resolution. She earned her PhD in 2009, which studied structurally related compounds with common skeleton in the resolution processes. She is the co-author of 45 papers (the majority of which appeared in international journals), and three patents.

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