

CHIRAL SYMMETRY BREAKING IN THE CRYSTALLIZATION OF 1,1'-BINAPHTHYL AND POLYMORPHISM

A. P. Martín-Islán¹, M. Ester Molina-Montes¹, Julyan H. E. Cartwright² and C. Ignacio Sainz-Díaz²

¹ Estación Experimental del Zaidín, CSIC, C/ Profesor Albareda,1, 18008-Granada (Spain)
E-mail: africam@eez.csic.es

² Laboratorio de Estudios Cristalográficos, Instituto Andaluz de Ciencias de la Tierra (CSIC)
- Universidad de Granada, Av. Fuentenueva s/n, 18002 Granada (Spain)

New approaches on the phenomenon of chiral symmetry breaking are studied in the process of melting crystallization of 1,1'-binaphthyl. We confirm that the chiral symmetry breaking can be observed in crystallization from a melt of 1,1'-binaphthyl by a constant stirring during the crystallization. However, an additional evaporation-crystallization process was found to be produced simultaneously to the melting crystallization. This explains the effect of the reactor shape and initial amount of sample on the enantiomeric excess that justify previous results. Crystallographic studies by Powder X-ray diffraction (PXRD) reveal that two polymorphs of 1,1'-binaphthyl were detected. The chiral crystal corresponds to the trans-1,1'-binaphthyl and the racemic crystal corresponds to the cis-1,1'-binaphthyl conformer. Quantum mechanical calculations of the crystal lattice of 1,1'-binaphthyl polymorphs have been performed, taking into account the rotational barrier between the conformers of this molecule. A good agreement with experiment was found in the crystal lattice parameters and the PXRD pattern.