The conformational polymorphism of 1,1,2,2-tetrachloroethane (C₂H₂Cl₄)

Ph. Negrier¹, M. Barrio+, M. Zuriaga³, S.C. Pérez³, J.Ll. Tamarit², and D. Mondieig¹

¹Laboratoire Ondes et Matière d’Aquitaine, UMR 5798 au CNRS-Université Bordeaux I, 351, cours de la Libération, 33405 Talence Cedex, France.
²Grup de Caracterització de Materials, Department de Física I Enginyeria Nuclear, ETSEIB, Diagonal 647, 08028 Barcelona, Universitat Politècnica de Catalunya, Catalonia
³Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba and IFEG-CONICET, Ciudad Universitaria, X5016LAE Córdoba, Argentina

The molecule of 1,1,2,2-tetrachloroethane can appear in two different conformations: trans (antiperiplanar) and gauche (synclinal). The slight energy difference between both conformers (<1 kcal mol⁻¹) [1, 2] means that the polymorphic phases appearing at different temperature and pressure conditions would mainly depend on the intermolecular interactions.

At normal pressure, the stable phase β is known to be orthorhombic (P2₁2₁2₁, Z=8, Z'=2) with only one gauche conformation. At high-pressure (ca. 0.65 GPa) the structure of a second polymorph was found to be monoclinic (P2₁/c, Z=2, Z'=0.5) and formed by only molecules with trans conformation [3].

The present work presents a new solid phase in which both gauche conformers coexist. This phase is reached by means of recrystallization of the supercooled melt into a new metastable α phase, which on heating transforms irreversibly to the stable β phase. The thermodynamic relationships between the different condensed phases as well as the structural details of the new phase will be detailed in the present communication.

References