Phase Transitions in Tetrachlorobenzene Studied by Neutron Powder Diffraction

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Polymorphism and phase transitions are a major issue in the understanding of the organic solid state. The 'Control and Prediction of the Solid State' (CPOSS) project[1] aims to increase our understanding of the polymorphic state using detailed screening to discover 'all' polymorphic forms and solid state phases combined with cutting edge experimental studies and computational studies.

Two polymorphs of tetrachlorobenzene have been reported[2-4]; the room-temperature β form ($P2_1/n$), and a low-temperature α form (P-1), with the phase change occurring at approximately 170K.

The nature of the phase transition, as well as the structure of the two polymorphic forms, has been investigated using the complimentary crystallographic techniques of single-crystal X-ray diffraction and neutron powder diffraction. In particular, the effect of temperature on the lattice parameters is considered, providing insights into the nature and mechanism of the phase transition.

[1] http://www.chem.ucl.ac.uk/basictechorg/index.htm . [2] Herbstein F.H., *Acta Cryst*., 1965, 18, 997-1000.[3] Halac E.B., Burgos E.M., Bonadeo H., D'Alessio E.A., *Acta Cryst* A, 1977, A**33**, 86-89. [4] Anderson D.G., Blake A.J., Blom R., Cradock S., Rankin D.W.H., *Acta Chemica Scandinavica,* 1991, **45,** 158-164.

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