

Poster Presentation

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Crystal structure of carbon tetrachloride phase Ib

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Carbon tetrachloride forms three solid phases on cooling from the liquid at ambient pressure; an orientationally disordered face-centred cubic phase Ia, an orientationally disordered rhombohedral phase Ib, and an ordered monoclinic phase II [1]. Powder neutron diffraction studies showed that the rhombohedral phase is probably isostructural with phase I of carbon tetrafluoride which solidifies below the melting point before transforming into a distinct ordered monoclinic form [2]. The structure of carbon tetrachloride phase Ib has now been solved and Rietveld refined from powder synchrotron X-ray diffraction studies at 230 K, employing a large medical-imaging detector to record the Debye-Scherrer rings and obtain data of sufficient statistical quality as the orientational disorder leads to a marked decrease in diffracted intensity at higher diffraction angles. The shells of chlorine density resulting from the orientationally disordered molecules were modeled using a spherical-harmonic description.

[1] Silver, L. & Ruddman, R. (1970). *J. Phys. Chem.*, 75, 3134-3139.

[2] Fitch, A. N. & Cockcroft, J. K. (1993). *Z. Krist.*, 203, 29-39.

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