

Disorder in Chloronitrobenzene Derivatives. L. H. Thomas^a, J. M. Cole^a, and C. C. Wilson^{b,c}. ^a*Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW*, ^b*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxon, OX11 0QX* and ^c*Department of Chemistry, University of Glasgow, Joseph Black Building, University Avenue, Glasgow, G12 8QQ*.

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Chloronitrobenzene derivatives are of interest as they have interesting physical properties, which may be linked to structural effects. They exhibit anomalous dielectric properties, which are often attributed to their disordered nature and associated phase transitions. Single crystal x-ray diffraction studies have failed to fully characterise many of these materials because of their highly disordered nature. A previous study of pentachloronitrobenzene had suggested three possible models for the disorder with one being tentatively assigned [1]. The single crystal structure of *p*-chloronitrobenzene had previously only been partially characterised [2] and is also reported to undergo an order-disorder phase transition at 282 K [3]. We have revisited these two materials and will present completed structures with accompanying models of their disorder from conventional single crystal x-ray diffraction. Measurements have been taken at several temperatures to probe whether the disorder is static or dynamic in nature. The results give some clarity to the likely models of disorder and will be the platform leading to studies of the diffuse scattering arising from these materials.

[1] I. Tanaka, F. Iwasaki, and A. Aihara (1974), *Acta Cryst.*, B30, 1546-1549.

[2] T.C.W. Mak, and J. Trotter (1962), *Acta Cryst.*, 15, 1078-1080.

[3] C.A. Meriles, J.F. Schneider, Y.P. Mascarenhas, and A.H. Brunetti (2000), *J. Appl. Cryst.*, 33, 71-81.