

s12.m34.p13 **Orientational Ordering in Liquids of Diatomic Molecules.** László Temleitner and László Pusztai, *Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, P.O. Box 49., H-1525, Hungary.* E-mail: temla@szfki.hu

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Diffraction data on the liquid state of N₂, O₂, F₂, Cl₂, Br₂, I₂, CO and NO have been collected from the literature and have been re-analysed by means of the Reverse Monte Carlo (RMC) method [1]. The aim of such a study was to establish whether there is any correlation between the orientations of molecular axes in these simplest molecular liquids. For each material, large structural models, containing 5000 molecules, could be generated that were consistent (within experimental errors) with the measured structure factors. Pair correlation functions (for heteronuclear molecules, partial pair correlation functions) were calculated directly from the particle coordinates. The molecular centre — molecular centre correlation functions could also be evaluated from the models. A purpose-built computer code has been written for determining mutual orientations of molecules as a function of the distance between molecular centres. In this contribution, results for particular orientations such as parallel, T-shaped, cross-shaped and chain-like ordering are presented. It was found that for liquid nitrogen (and to some extent, oxygen, as well) correlations between molecular centres extend surprisingly far, whereas only very weak correlations exist between molecular orientations. For liquid chlorine, bromine and iodine, on the other hand, sizeable short range orientational correlations were detected, with hardly any centre-centre correlations. Liquid fluorine was found to be an intermediate between the other halogens and nitrogen. These findings indicate that it was possible to go beyond results presented in an earlier RMC study [2], by means of a ‘flexible molecule’ algorithm (which is made use here). For liquid carbon monoxide, earlier interpretation of diffraction data indicated that orientational correlations were completely absent [3,4]; in the present study, however, remarkably high level ordering was found for the mutual arrangements of neighbouring molecules. At the contact distance (between molecules), around 0.3 nm, T-shaped arrangements seem to be dominant, whereas around the first maximum of the centre-centre correlation function, around 0.4 nm, molecules clearly prefer parallel and cross-shaped ordering. These tendencies were rather distinct at 83.5 K (higher density) and become less sharp at around 120 K (lower density). In liquid nitric oxide at 120 K, diffraction data were found to be consistent with that about 90 % of the molecules were present in the form of (NO)₂ dimers. However, the ‘cis-planar’ shape of the dimers, that had been generally accepted before [3], could not be confirmed - when such dimers were put in the simulation box, experimental data could not be reproduced satisfactorily. The level of orientational correlations was much closer to that found in a hard sphere reference system than it was for the case of liquid CO.

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s12.m34.p14 **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, UK.* E-mail: lt261@cam.ac.uk

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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.

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