

s12.m34.p15 **Diffuse Neutron Scattering from Flexible Molecules.** T.R. Welberry^a, D.J. Goossens^a, A.P. Heerdegen^a, W.I.F. David^b, M.J. Gutmann^b and M.J. Bull^b, ^aResearch School of Chemistry, Australian National University, Canberra, ACT 0200, Australia, and ^bISIS, Rutherford Appleton Laboratory, Milton, Didcot, Oxfordshire, UK. E-mail: welberry@rsc.anu.edu.au

Keywords: Diffuse scattering; Neutron scattering; Flexible molecules

Diffuse neutron scattering data have been recorded for the molecular crystal d-benzil, C₁₄D₁₀O₂, using time-of-Flight Laue diffraction on SXD and PRISMA at ISIS. Using SXD it was possible to access a large fraction of the total three-dimensional reciprocal space out to a Q value of 15 Å⁻¹, using only four individual exposures and by making use of the -3m Laue symmetry of the crystal. By binning the scattered data according to incident neutron energy, patterns were obtained using neutrons in the range of ~20 meV to 150 meV, which showed little sign of inelastic effects and so could be compared with previously analysed X-ray data. For neutron energies of <20 meV, inelastic effects were observed, which have been used to obtain an estimate for the energy of phonons associated with a particular vibrational mode. A model previously derived from analysis of X-ray data observed over a limited range of Q has been used to calculate neutron patterns over the full Q range. Comparison with the neutron data showed that while the model obtained by fitting to the X-ray data gives a good description of the form of the diffuse neutron patterns, the magnitudes of the atomic displacements were underestimated by a factor of ~2.25. This has prompted a re-refinement of the original model.

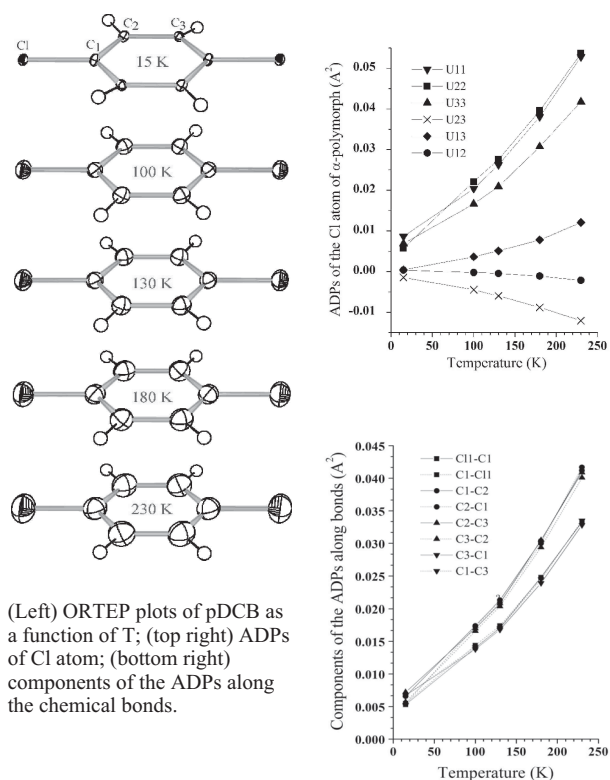
We will further discuss our latest results that test our model by using new SXD data to explore the temperature dependence of the diffuse scattering. In addition PRISMA has been used to measure phonon energies directly, allowing comparison with those energies inferred from the diffuse scattering.

- [1] Welberry, T.R., Goossens, D.J., David, W.I.F., Gutmann, M.J., Bull, M.J. and Heerdegen, A.P. *J. Applied Crystallogr.* **36**, 1440-1447.

s13.m35.p1 **Atomic Displacement Parameters of the α -Polymorph of p-Dichlorobenzene Measured between 15 and 300 K.** Thammarat Aree, Marc Hostettler, Dmitry Chernyshov and Hans-Beat Bürgi, Laboratory for Chemical and Mineralogical Crystallography, University of Berne, Freiestr. 3, CH-3012 Bern, Switzerland. E-mail: thammarat.aee@krist.unibe.ch

Keywords: p-Dichlorobenzene; Polymorphism; Atomic displacement parameters

Synchrotron diffraction data to 0.5 Å resolution of the α -polymorph of p-dichlorobenzene (pDCB) [1] were collected at 15, 100, 130, 180 and 230 K (Swiss-Norwegian Beam Lines at ESRF, Grenoble, France). The data were processed with programs CRYCALIS, SADABS, and SHELXTL and refined with spherical atom and multipole models using XD to deconvolute thermal motion from valence electron density. The increase of the atomic displacement parameters (ADPs) becomes steeper and steeper with increasing temperature indicating anharmonicity and consistent with sublimation of pDCB at room temperature (Figure). The simultaneous analysis of ADPs measured between 15 and 230 K allows separation of the temperature dependent part of the ADPs from the temperature independent contributions [2]. The temperature dependent part determines rigid-body libration and translation, their frequencies, their anharmonicities, low frequency deformation motions and corresponding vibrational entropies. The experimental study was endorsed by *ab initio* calculations of the molecular deformation vibrations.



(Left) ORTEP plots of pDCB as a function of T; (top right) ADPs of Cl atom; (bottom right) components of the ADPs along the chemical bonds.

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 [2] Bürgi, H. -B. Capelli, S. C. & Birkedal, H. (2000). *Acta Cryst.* **A56**, 425-435.