MS41-02 **Bananas, pears and other fruitful discussions: modelling atomic motions in molecules.** Carole A. Morrison,[a] Anthony M. Reilly,[b] David. W. H. Rankin [a] and K. Robin McLean.[c] [a]*School of Chemisry, University of Edinburgh, UK,* [b]*Fritz-Haber-Institut der Max-Planck-Geselschaft, Berlin, Germany,* [c]*Department of Mathematical Sciences, University of Liverpool, UK.*
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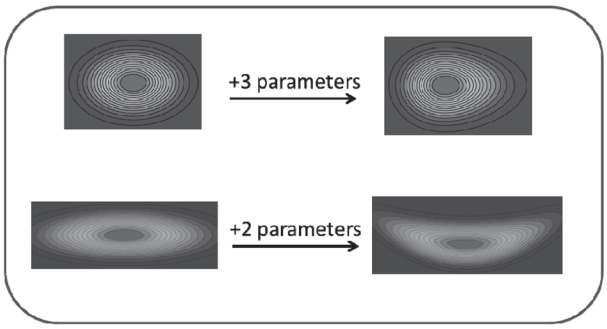

Two new anharmonic forms for the Debye-Waller factor, aimed at modelling curvilinear and asymmetric motion, will be introduced.[1] They permit the refinement of crystallographic data for structures that contain these types of motion using only a small number of additional parameters over what is currenty used in the thermal ellipsoid model. In this presentation the two forms will be assessed using numerical atomic probability density functions derived from molecular dynamics simulations.

[1] Reilly, A. M., Morrison, C. A.,* Rankin, D. W. H. and McLean, K. R. (2011) *Acta Cryst.* **A67**, 346-356.

Keywords: anharmonicity, Debye-Waller factors.

MS41-03 **EVAL15 as a tool for studying crystal properties in detail: dynamic and static disorder.** Loes MJ Kroon-Batenburg, Erik Stronks, Antoine MM Schreurs, Martin Lutz, *Crystal and Structural Chemistry, Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands.*
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X-ray diffraction is routinely used to determine the space and time averaged structure of crystals. Data collection techniques have improved over the years. Recent synchrotron beam lines produce high flux X-ray beams, but also home sources are now available that can compete with 2nd generation synchrotrons. In addition, detectors now have increased sensitivity and low noise, which allows detection of diffuse features with sufficient accuracy. The EVAL15 integration method [1] was developed to accurately determine reflection intensities of single crystals, but especially of problematic crystals like those with multiple lattices, lattice distortion, anisotropic mosaic spread and incommensurate modulation. We found that lattice defects are often accompanied with diffuse scattering. We will give examples of the use of EVAL in cases of packing disorder. Sodium hexafluorosilicate crystalizes in a trigonal lattice with space group P321 [2] and forms a merohedral twin. Strong diffuse scattering is observed, so that apparently the twinning is accompanied with disorder effects. Analysis of the disorder in terms of rigid body motion, anisotropic thermal displacements and temperature dependence will be discussed

[1] Schreurs, A.M.M., Xian, X. & Kroon-Batenburg, L.M.J. (2009). *J. Appl. Cryst.* **43**, 70-82
[2] Zalkin, A., Forrester, J.D. & Templeton, D.H. (1964). *Acta. Cryst.* **17**, 1408-1412.

Keywords: Anisotropic displacement parameters; rigid body motions; EVAL data processing;