improvement of the refinement can be obtained by eliminating the badly fitted reflections and/or by correcting the model, which could be too inaccurate or involve too subtle features to be modelled depending on the quality of the observations processed. A successfully recognition of the actually influencing reflections is represented by some statistical estimators based on leverage analysis (Belsey et al., 1980, Merli, 2005). Among several exploitable estimators, there are some of them that seem to be particularly suitable in crystallographic calculations: i) Cook distance (Cook, 1977), ii) DFFTIS and iii) DFBETASij (Belsey et al., 1980). In particular, estimator i) can be used to recognize an actual outlier of the refinement, whereas estimator ii) is useful to investigate the effects when a reflection is eliminated from the data set and iii) is able to recognize the variables that are mostly influenced by each reflection. The combined analysis of these diagnostics will be presented. It will be shown how successfully it yields to the recognition of a dangerous reflection and/or the inaccurate estimate of any particular variable.

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MS.88.2

Small-molecule refinement using the computational crystallography toolbox (cctbx) with Olex2

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In recent years, the cctbx[1] (including the macromolecular toolbox, mmtbx) has firmly established itself as a highly flexible, comprehensive and all-encompassing programming tool for macromolecular structure solution and refinement. The program suite PHENIX[2] is based on this framework, and is the most visible part of this long-standing and well-managed framework. As part of an effort to modernise computational tools for small-molecule crystallography, we have been working in collaboration with the cctbx. Our aim is to extend the functionality currently offered by the cctbx to include small molecule solution and refinement. This has resulted in the creation of the Small Molecule Toolbox (smtbx) which is now included with the cctbx framework. In order to make these tools accessible to those chemists and crystallographers who are working with small molecules, the cctbx/smtbx functionality can be accessed via Olex2[2] - a modern Graphical User Interface which is designed to make working with crystal structures as easy as possible for all groups of users. In this presentation we shall elaborate on the areas of the cctbx where modifications and extensions were necessary to achieve `small-molecule functionality' and will outline how we manage the collaboration between the various contributors (in the hope that many may join!). We will also demonstrate how this functionality is accessed from the end-user's point of view. Examples of how structure solution/refinements achieved using the smtbx compare to other solution/refinement programs will be presented.

[1] cctbx: http://cctbx.sourceforge.net/
[2] PHENIX:http://www.phenix-online.org/
[3] Olex2 http://sourceforge.net/projects/olex2 and http://www.olex2.org

MS.88.3

Anisotropic displacement parameters for molecular crystals from periodic HF and DFT calculations

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Accurate X-ray diffraction experiments give information about the thermally averaged charge density in the unit cell. Investigations of the static charge density requires a proper deconvolution of thermal motion and static density. Complementary information about the thermal motion in molecular crystals is seldom available. We present an approach based on periodic HF and DFT calculations using the CRYSTAL06 code [1,2] to estimate both intramolecular and intermolecular vibrational contributions to the anisotropic displacement parameters as applied to molecular crystals. Crystalline urea has been used as case system. We investigate the role of the basis-set and the adopted DFT functional: LDA, GGA and hybrid. The effect of including an empirical dispersion-force correction to B3LYP calculations has also been considered [3]. Finally, at the B3LYP/6-31G(d,p) level, the dispersion of acoustic phonons has been estimated and included through a supercell approach. The results are compared with experimental data from spectroscopy, X-ray and neutron diffraction experiments. On the basis of previous results, work has been extended to urotropine and benzene crystals and preliminary data are reported. These estimates of atomic and molecular motion are especially important for hydrogen atoms because of their low scattering power and intense thermal motion. Recent attempts to estimate hydrogen atom motion show promising results, and we compare the CRYSTAL06 approach with the SHADE [4] procedure.

[1] R. Dovesi et al. CRYSTAL06 User's Manual, University of Torino, 2006. (http://www.crystal.unito.it).
[2] F. Pascale et al. J. Comput. Chem. 25 888 (2004).
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[4] A. O. Madsen, J. Appl. Cryst. 39 757 (2006) (http://shade.ki.ku.dk).

MS.88.4

Joint refinement of single crystal and powder data from X-ray and neutron sources

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The last version of the crystallographic software Jana − a well known tool for structure determination of aperiodic structures - has introduced the generalized data input. In the program Jana2006 data