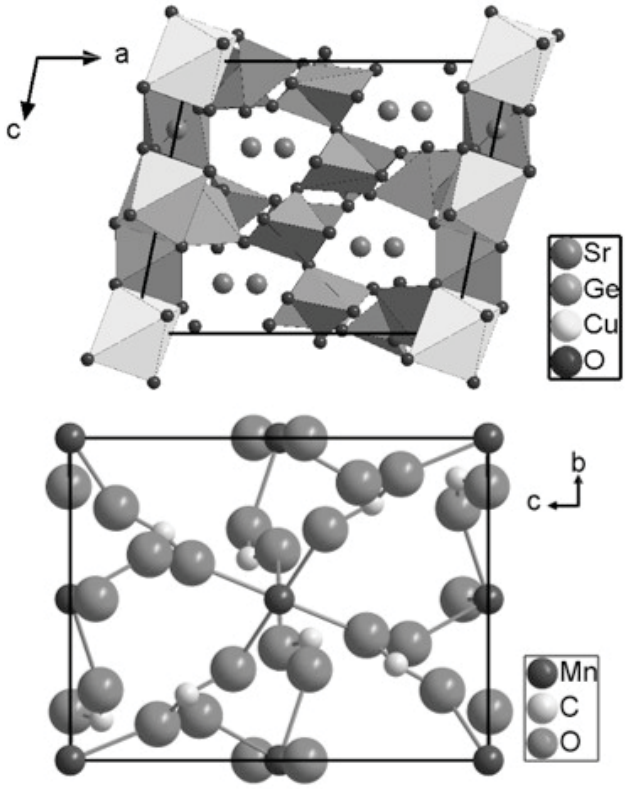

Keywords: Low dose, Electron diffraction tomography, Structure solution

MS23-P08

First preliminary results from TAAM-UBDB refinement on electron diffraction data

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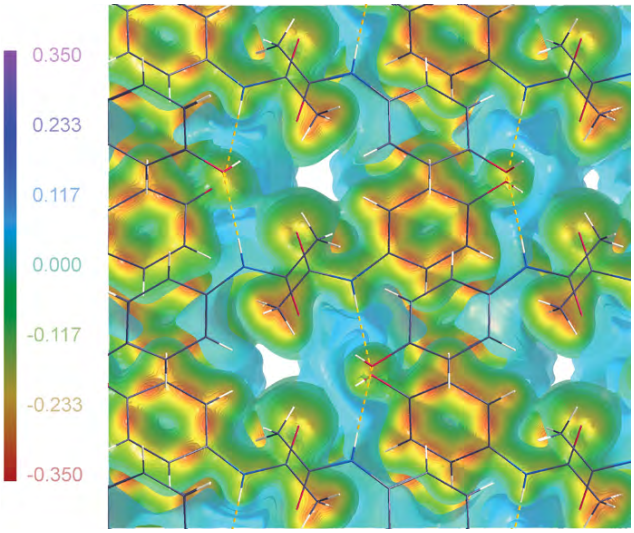
Cryo-electron microscopy and electron diffraction methods have made enormous progress in the last years and an increasing number of atomic and near atomic resolution structures are becoming available. At present, interpretation of collected data relay on a very approximate scattering model. The model is based on spherical independent atoms (IAM), ignoring the charge redistribution due to chemical bonding. This approximation may lead to unnecessary loss of information. We propose to base interpretation of data from cryo-electron microscopy and from electron diffraction methods on more realistic electron scattering models.

We are developing Transferable Aspherical Atom Models (TAAMs) from detailed electron densities of molecules and crystals. To build TAAMs we use a databank of aspherical atomic electron densities called UBDB [1]. Currently UBDB allow to reconstruct electron density of any protein, nucleic acid or other biologically important molecule. Thus, it gives also fast access to electrostatic potential.

It has been shown already [2] that replacement of the IAM by TAAM in x-ray crystallography leads to more accurate geometrical information and provide access to quantitative estimation of the electron density distribution and properties derived from it for molecules in a crystalline environment.

Given the fact that electron diffraction is more sensitive to charge density redistribution than x-ray we expect to see even more pronounced improvement after introduction of TAAM to analysis of electron diffraction/scattering.

We will present our first preliminary results of TAAM-UBDB refinements against electron diffraction data collected for paracetamol[3]. The figure illustrates the difference in crystal electrostatic potential (e/bohr) resulting from the differences between the IAM and the TAAM-UBDB electron scattering models.



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Keywords: electron crystallography, UBDB, electrostatic potential modelling

MS23-P09

Riding the camel: the double-peaked rocking curve and its use in the processing of precession electron diffraction data

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Data collected by the precession electron diffraction (PED) technique can be successfully used for solution and also accurate refinement of unknown crystal structures. Especially efficient in this respect is the technique of PED tomography (PEDT), where a series of PED patterns are collected on a crystal progressively tilted by small steps around a rotation axis [1].

Such PEDT data have certain special characteristics that make it different from standard rotation data. The most prominent is the rocking curve of a reflection in PEDT data, i.e. the reflection intensity as a function of the tilt angle. While the rocking curve of non-precession data is a narrow single peaked function, the rocking curve of a reflection in PED is a broad function with two maxima. Typically, each reflection is measured several times. The precession angle is usually much larger than the angular width of the non-precession rocking curve of the reflections, and therefore the width and shape of the rocking curve is determined mostly by the precession angle and not so much by the crystal itself. Because of the specific shape of the curve, we call the plot of the precession rocking curve colloquially “the camel plot”.

This feature can be exploited in several way during the analysis of the PEDT data. One of the applications is the refinement of the crystal orientation. The crystals are often not steady during the PEDT experiment, but they turn. Ignoring this rotation leads to distorted data sets and very inaccurate lattice parameters. Using the knowledge of the rocking curve shape allows an accurate refinement of the crystal orientation during the experiment and substantial improvement of the data.

The knowledge of the rocking curve can also be exploited in the intensity extraction. The typical approach to the determination of the total intensity of certain reflection is the integration of intensity accross all frames on which the reflection is measured. However, this provides inaccurate rresults for partially covered reflections and it is also sensitive to intensity variations due to dynamical diffraction. Knowng the rocking curve allows the total intensity to be determined more accurately by fitting the rocking curve profile to the reflection intesities.

Implementation of these features in the computer program PETS 2.0 [2] and their application to a number of practical examples shows that “riding the camel” can lead to significantly improved data quality and sometimes make a difference between a solved and unsolved structure.

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Keywords: precession electron diffraction, intensity extraction,