MS9-P9 Crystal structure comparison methods

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Crystal structures can be compared by many ways – by chemical composition, unit cell parameters, atomic positions, by positions of fragments or by other properties or values describing the crystal structure. Comparison of different properties give us a different results. The basic question is, what we would like to compare? We developed several crystal structure comparison methods, which can be divided into two basic approaches - (i) comparing of fingerprints and (ii) comparing of atomic positions. In the first case we selected pair-distribution function and powder diffraction pattern as fingerprints and we tested their sensitivity for small (e.g. change of one atom) and large (e.g. change of several atoms) changes. In the case of the second approach, it is obvious, that crystal structures has to be overlapped before comparing of atomic positions. This is the most difficult task of these methods. The success or failure of these methods depends on success or failure of the overlapping algorithm. In general, the situation is complicated by different atom labelling and, in the case of different space group, it is also complicated by different content of the asymmetric part of the unit cell and the situation can be also complicated by presence of special positions. We developed two algorithms for crystal structure overlapping - one of them is slow but it finds the overlay automatically and the second one is much faster but it needs the user definition of the similar fragment. We developed a testing code for this purpose, which we called CrystalCMP and which can be freely downloaded from this link (http://sourceforge.net/projects/crystalcmp/). We will show success or failures and also strengths and weakness of suggested methods.

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MS9-P10 Light-atom structures: absolute configuration determination and beyond

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The determination of the absolute configuration for light-atom structures is central to research in pharmaceuticals and natural-product synthesis [1]. In the absence of elements heavier than silicon, it is often problematic to make a significant assignment of absolute configuration. Traditionally, heavy-atom derivatives were prepared which have a stronger anomalous signal compared to the native compound. However, this is not always feasible.

The assignment of the absolute structure of pure organic compounds has become somewhat easier with the advent of high-intensity microfocus sources [2], as the increased flux density improves the anomalous signal through improvements in counting statistics. In order to maximize the anomalous signal, X-ray sources with Cu anodes are usually used for the absolute structure determination. However, these data are usually limited to a maximum resolution of about 0.80 Å. High-brilliance microfocus X-ray sources with Mo targets enable the collection of high quality data beyond 0.40 Å within a reasonable amount of time. This allows not only a more accurate modelling of the electron density by using aspherical scattering factors, but also enables a reliable determination of the absolute structure, despite the significantly lower anomalous signal obtained with Mo-K_α radiation.

With the recently introduced liquid-Gallium-jet X-ray source unprecedented beam intensities can be achieved [3]. The shorter wavelength of Ga-K_α compared to Cu-K_α slightly weakens the anomalous signal of a typical light-atom structure. However, due to the shorter wavelength, the highest resolution for the liquid metal-jet source is typically at about 0.70 Å, compared to about 0.80 Å for Cu-K_α. Hence, about 50% more unique reflections can be recorded. This clearly improves the structural model and the quality of the Flack parameter.

Selected results on the absolute structure and charge density determinations for light-atom structures will be presented.

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