Poster Presentation

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On the assessment of time-resolved diffraction results

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Dynamic-structure crystallography, and in particular photocrystallography, is a field of great interest because of its numerous applications. The field covers the studies of reactions in crystals including non-reversible reactions, phase transitions and the structure change on excitation leading to short-lifetime species. Data collected during dynamic-structure crystallography experiments require appropriate tools to perform data analysis. The relative scaling of different sets of data recurs in time-resolved pump-probe data collection in which crystals often disintegrate before a full set of data can be collected. We discuss relative scaling and its use with the Ratio method [1], in which ratios of observed intensities collected with and without light-exposure are used as observables. The scaling method has been developed specifically for pump-probe Laue data, but is not limited to polychromatic data sets. The visualization of the externally induced structure changes in the crystal environment is of importance to check the presence of a structural response (see Fig. a) and hence to define a starting point for the structure refinement. For this purpose, ratio-based Fourier difference maps have been defined. After the structure refinement using the software LASER [2], the quality of the light-exposed structure model can be checked in direct space by visualizing the ratio-based Fourier residual maps, and, in a complementary manner, in reciprocal space by performing statistical analysis on the least-squares (LS) residual vector components with respect to the corresponding H-vectors (see Fig. b). The latter allows detection of any outliers or unexpected tendencies such as dependence of the residual vector components on the resolution or the angular direction in the reciprocal space. Application to the complex [Cu(I)-(1,10-phenanthroline-N,N')bis(triphenylphosphine)][BF4] will be presented [3]. Research supported by the National Science Foundation (CHE1213223).

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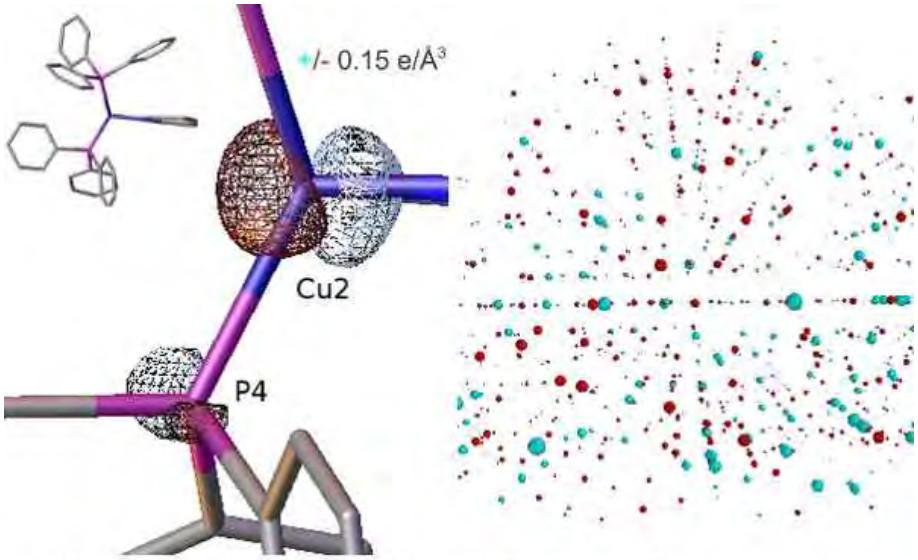

(a) Fourier difference map without temperature increase

(b) Residual vector components plotted at the reciprocal space lattice nodes as positive/negative spheres with radius proportional to their absolute values

Keywords: Dynamic-structure crystallography, Pump-probe method, Data analysis