Different approach in multipole refinement with XD and JANA2006

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In order to compare two computational systems for the multipole refinement accurate data for one simple organic compound (tetrazole (**I**) - $C_1H_2N_4$ - acentric P1, *No. 1*) and one coordination compound (Tetrakis(μ_2-Acetato)-diaqua-di-copper (II) complex (**II**) - centric C 2/c, *No. 15*) were refined at multipolar level by *XD2006* (Volkov *et al.*, 2006) and *JANA2006* (Petříček *et al.*, 2006) software. As the input *xd.hkl* file were used both non averaged data and the data averaged by SADABS (Bruker (2006)). For the second compound different scattering curves (Cu, Cu^+, Cu^{2+}) were used. Moreover, *JANA2006* system allow us to perform anisotropic extinction correction in both computational systems, since the transformation of Sheldrick's direction cosines to the vectors read by *XD2006* software is available. Preliminary results for (**I**) are on Fig. 1a (distances [Å], atomic charges [e] and values of Laplacian in bond critical points [eÅ^{-5}] and the Laplacian for (**II**) on Fig. 1b.

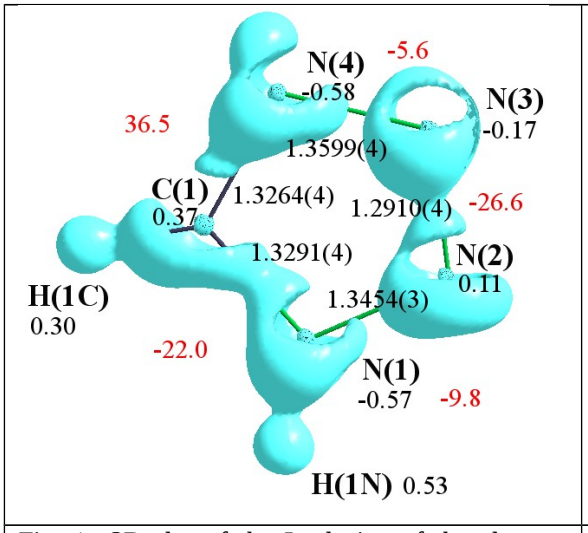

Fig. 1a 3D-plot of the Laplacian of the electron density of tetazole at isosurface value of 10 e Å^{-5}

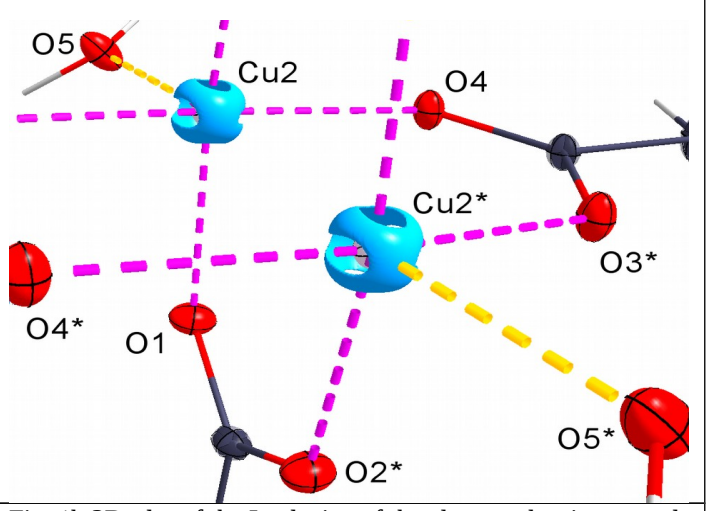

Fig. 1b 3D-plot of the Laplacian of the electron density around Cu at isosurface value of 1500 e Å^{-5}

The topological analysis was performed on the refined densities within the framework of the Quantum Theory of Atoms in Molecules (QTAIM). Atomic charges were obtained from integration of the electron density in the atomic basin. Comparison of bond characteristics, atomic charges, distribution of *d*-electrons in (**II**) and error analysis will be discussed.

A special interactive tool for finding and culling suspicious reflections has been developed in Jana2006 (Friese *et al.*, 2013). This culling procedure is based either on the discrepancies between equivalent reflections during the merging process or on comparison of calculated and observed intensities during the refinement.

References.

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