Poster Presentations

[MS13-P04] Comparative study of the electron distribution in *3d*-orbitals: J. Kožišek, P. Herich, and M. Breza

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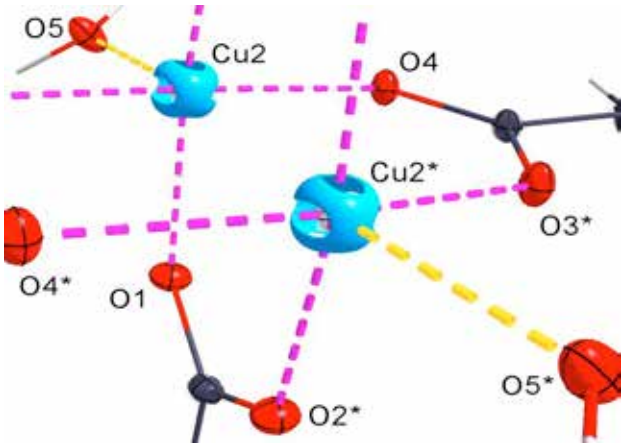
The bonding properties of transition metals in coordination compounds are of great importance for inorganic as well as bio-inorganic chemistry. In enzymes, metal centres are important for their activity. In order to understand the kinetics and thermodynamics of the reactions of biological systems, knowledge of the structure and bonding properties of the active site is essential. For this purpose it is useful to study simple model compounds for which accurate data can be obtained. Experimental electronic structure of *3d*-complexes is still a challenge, particularly in the sense of determination the *d*-orbital population. Very accurate data for Tetrakis(μ2-Acetato)-diaqua-di-copper (II) [1] and Tetrakis(μ2-Acetato)-diaqua-di-chromium (II) [2] complexes were obtained with Oxford Diffraction CCD GEMINI R diffractometer at 100K. Multipolar refinement and consecutive topological analysis was performed using XD package.



3D-plot of the Laplacian of the electron density around Cu at isosurface value of 1500 e A-5

Population of the *d*-orbitals

M	orbital	d_{x2-y2}	d_{xz}	d_{xy}	d_{z2}	d_{yz}	Σ
Cr	[e]	0.27(1)	0.89(1)	1.00(1)	0.91(1)	0.94(1)	4.01
Cu	[e]	1.28(1)	1.92(1)	1.94(1)	1.97(1)	2.02(1)	9.13

Theoretical calculations were done using GAUSSIAN03 and AIM2000 software at B3LYP/6-311+G* level of theory. In conclusion could be said that:
1) electron density distribution corresponds to the oxidation state MII
2) spin density is totally different for both compounds
3) M-M interaction is comparable with M-H2O interaction.

Keywords: charge density; chemical bonding; metal-metal bond