

Electronic structure of [Cu(dimethylimidodicarbonimidate)₂] complex. Jozef Kožišek,^{a*} Ingrid Svoboda^b, and Hartmut Fuess^b, ^a*Department of Physical Chemistry, Slovak University of Technology, Bratislava, Slovakia,* ^b*Materials Science, Darmstadt University of Technology, Darmstadt, Germany.*

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Keywords: charge density; 3d-elements; d-orbital population

Electronic structure obtained by topological analysis of experimental electron density is reported. Comparison with the results of quantum chemical calculations in solid state gives us an additional information of a new quality which cannot be obtained from the routine monocrystal structure analysis. In spite of the great progress in experimental technique for X-ray single crystal data collection, the papers on charge density studies of 3d-coordination compounds are still rare. It could be due to not fully straightforward way for extracting the high quality data set of Bragg intensities. In our contribution we report an attempt to combine Xcalibur CCD and STOE point detector data. Multipole refinement of [Cu(dimethylimidodicarbonimidate)₂] complex [1] was done on F² using 22 853 diffractions from the first and 14 938 from the second set. Preliminary calculations gave R(F) = 0.0267 and Rw(F) = 0.0191 as well. The population of d-orbitals were as follows: d_{z²} = 2.14(2), d_{xz} = 1.96(2), d_{yz} = 1.93(2), d_{x²-y²} = 1.11(2) and d_{xy} = 1.93(2).

[1] Boča R., Hvastijová M., Kožišek J. & Valko M.; *Inorg.Chem.*, **35**, No. 16 4794-4797 (1996).