s2.m9.p4 **Electronic structure of [Cu(dimethylimido-dicarbon-imidate)$_2$] complex.** Jozef Kozísek,[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. E-mail: kozisek@cvt.stuba.sk*

Keywords: Charge density; 3*d*-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(dimethylimido-dicarbonimidate)$_2$] complex [1] was done on F^2 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).

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s2.m9.p5 **Charge separation on pigments of photosystem II reaction centers.** Kutý M.[a,d], Psencík J.[a,c], Vácha F.[a,b], [a]*Institute of Physical Biology, University of South Bohemia, Zámek 136, 373 33 Nové Hrady, Czech Republic,* [b]*Institute of Plant Molecular Biology, AS CR, Branisovská 31, 370 05 Ceské Budejovice, Czech Republic,* [c]*Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 120 00 Prague, Czech Republic,* [d]*Institute of Landscape Ecology, AS CR, Zámek 136, 373 33 Nové Hrady, Czech Republic*. *E-mail: michalk@bf.jcu.cz*

Keywords: Photosystem II; Light absorption; Circular dichroism

Photosystem II (PSII) is a relatively large pigment-protein complex located in thylakoid membrane of cyanobacteria, algae and higher plants. Recently, structure of the PSII complex isolated from cyanobacteria *Synechococcus elongatus* has been presented at the resolution of 3.8Å [1], from *Synechococcus vulkanus* at 3.7Å [2] and from *Thermosynechococcus elongatus* at 3.5Å [3]. PSII complex performs series of light driven reactions, which result in a separation and subsequently in a reduction of an electron-transport chain and water oxidation. Primary site of the energy conversion is located in so-called reaction centre (RC). Time constants of charge distribution and molecules involved in this process are already known, although X-ray and also spectroscopy methods are unfortunatelly not able to give us sufficient explanation of the charge-separation processes. In our last study [4] we have combined the structural homology modelling based model proposed by Svensson et al. [5] (1DOP model), and the experimental structure presented by Zouni et al. [1] and succesfully calculated absorption and circular dichroism spectra using point-dipole approximations [6] and compared them with the experimental results in order to locate accumulated chlorophyll cation during a light treatment of Photosystem II reaction centre in presence of artificial electron acceptor silicomolybdate. Along with the spectra calculations the charge distribution on the primary electron acceptor pheophytine of the combined model in a ground and reduced state and its influence on the surrounding protein environment is studied by using quantum chemistry methods on a semiempirical, density functional and *ab initio* levels.

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