

measurements on a non-deuterated hydroquinone clathrate sample have shown high quality positional and thermal parameters. The obtained atomic displacement parameters are investigated and compared with data from the same compound at the High Flux Isotope Reactor and an X-ray source.

The obtained positional and thermal parameters from the neutron experiment are used in combination with high quality X-ray data for a state-of-the-art charge density refinement. The investigation of these hydroquinone host-guest systems revealed significant charge redistribution of the host structure with the so-called weakly interacting guest solvent molecule.

[1] D.E. Palin, H.M. Powell, *Journal of the Chemical Society* **1948**, 815-821.

Keywords: clathrate, electrostatic, neutron

MS34.P07

Acta Cryst. (2011) **A67**, C446

Comparative study of the electron distribution in 3d-orbitals

Jozef Kožíšek,^a Martin Breza,^a Daniel Věh,^a Kristopher Waynant,^b James D. White,^b ^aDepartment of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, (Slovak Republic). ^bDepartment of Chemistry, Oregon State University, Corvallis, Oregon 97331 (U.S.A.). E-mail: jozef.kozisek@stuba.sk

In tetrakis(μ_2 -Acetato)-diaqua-di-copper(II) complex for the coordinated Cu central atom only Cu-O bonds in the equatorial plane form the coordination bonds [1,2]. Contrary to very small apical Cu-O bond distance of 2.1443(1) Å, this interaction is not a coordination bond. Fully populated d_{z^2} orbital (2.019(5) e) is pointing directly to O(5) atom and accordingly the oxygen O(5) lone electron pair is repelling. The value of the O(5)-Cu-Cu* angle is 173.977(4)°.

Comparing similar crystal structures we have found the crystal structure of Diaqua-bis(2,7-dimethyl-5-oxo-5H-pyrano(4,3-B)pyran-1-ium-4-oxalato-O,O')-copper(II) diperchlorate (YUSNIK) [3] in which the axial Cu-O(5) distance is also very short (2.160 Å), but the O(5)-Cu-O(5)* angle is exactly 180° according to the symmetry. Preliminary B3LYP/G311G* quantum-chemical calculations show highly unusual order of d -orbitals on the hexacoordinated central Cu atom.

In order to explain the electronic structure in YUSNIK the electronic structure study was undertaken.

The GEMINI R diffraction data at 100K will be used for electronic structure study. As the space group is a monoclinic (P 2₁/n) and the whole diffraction sphere was measured, a high redundancy was established. The multipole refinement and the results of both experimental and theoretical topological analysis will be discussed.

This work has been supported by Slovak Grant Agency APVV (APVV-0202-10) and VEGA (1/0679/11).

- [1] J. Kožíšek, L. Perašínová, M. Breza, *Acta Crystallogr.* **2008**, *64*, C128.
[2] L. Perašínová, M. Fronc, L. Bučinsky, M. Gall, M. Breza, J. Kožíšek, submitted to *Inorg. Chem.* [3] K.V. Waynant, J.D. White, L. Zakharov, *Chem. Commun.* **2010**, *46*, 5304-5306.

Keywords: cu-complex, electronic structure, d-orbitals

MS34.P08

Acta Cryst. (2011) **A67**, C446

Electron density studies of magnetic di-nuclear complexes,

Nicolas Claiser,^a Maxime Deutsch,^a Jean-Michel Gillet,^b Claude Lecom

te,^a Hiroshi Sakiyama,^c Katsuya Tone,^c Nabila Mattoussi,^d Dominique Luneau,^d and Mohamed Souhassou,^a ^aCRM2, UMR CNRS 7036, Institut Jean Barriol, Faculté des Sciences et Technologies, Nancy Universités, 54506 Vandœuvre-lès-Nancy (France). ^bS.P.M.S., UMR CNRS 8580, École Centrale Paris, Grande Voie des Vignes, 92295 Chatenay-Malabry (France). ^cFaculty of Science, Yamagata University, 1-4-12 Kojirakawa, Yamagata, 990-8560 (Japan). ^dLMI UMR CNRS 5615 Université Claude Bernard, Campus de la Doua, 22 Avenue Gaston Berger, 69622 Villeurbanne. E-mail: nicolas.claiser@crm2.uhp-nancy.fr

In the aim to rationalise the conception of single molecular magnets the first step is to explore the interactions in molecular magnetic complexes and to understand their role. To this end we modeled the experimental electron density distributions in di-nuclear complexes. For example, we studied a cobalt(II) compound ([Co2(sym-hmp)₂](BPh₄)₂) which was theoretically studied by Tone *et al.* in 2007[1]. When decreasing the temperature, the magnetic susceptibility of this complex deviates from the Curie law (Fig. 1) because of the anti-ferromagnetic exchange interaction, but the susceptibility increases sharply at low temperature (< 20K). The theoretical analysis of Tone *et al.* showed that this behavior is explained by a tilt of local distortion axes around cobalt atoms and not by a paramagnetic impurity. A polarized neutron diffraction experiment was carried out in order to model the spin density and verify this hypothesis (Borta *et al.* (2011), accepted in Phys. Rev. B.)

To support this electronic approach and to better describe the metal-ligand interactions, we determined the charge density of this complex using high resolution X-ray diffraction at 100 K. We will present our multipolar model[2] and its description using various tools (Fig. 2). The different interactions will be described and comparison will be made with spin density results from polarized neutron diffraction experiments. We will finally introduce our project of a new program for joint refinements of a unique electronic model based on X-rays and polarized neutrons diffraction data.

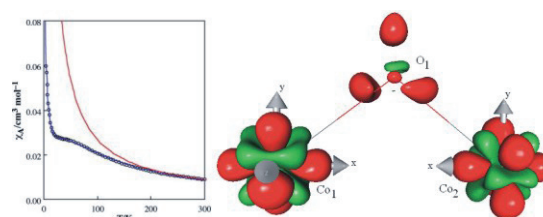


Fig.1. (left) Temperature dependencies of χ_M (O) at 100K. Fig.2. Electron deformation density around each Co atom.

- [1] K. Tone, H. Sakiyama, M. Mikuriya, M. Yamasaki, Y. Nishida, *Inorg. Chem. Commun.* **2007**, *10* (8), 944-947. [2] N. K. Hansen, P. Coppens, *Acta Cryst.* **1978**, *A38*, 905.

Keywords: charge density, interactions, magnetic complexes

MS34.P09

Acta Cryst. (2011) **A67**, C446-C447

Charge density analysis of K₂SO₄

Mette S. Schmökel,^{a,b} Simone Cenedese,^{b,c} Dietmar Stalke,^{b,d} Bo B. Iversen,^{a,b} ^aDepartment of Chemistry and iNano, Aarhus University, Denmark. ^bCMC, Center for Materials Crystallography, Aarhus University, (Denmark). ^cDept. of Physical Chemistry and Electrochemistry, Università degli Studi and CNR-ISTM, Institute of Molecular Sciences and Technology, Milano, (Italy). ^dInstitut für Anorganische Chemie, Georg-August-Universität Göttingen, (Germany). E-mail: mettesch@chem.au.dk.