

P14.03.07*Acta Cryst.* (2008). A64, C567**Experimental and theoretical charge density analysis of new charge-neutral rhodium (I) complexes**El-Eulmi Bendeif¹, Cherif Matta², Mark Stradiotto², Claude Lecomte³, Pierre Fertey¹¹Synchrotron SOLEIL, L'Orme des Merisiers - Saint Aubin B.P. 48, Gif sur Yvette, Essonne, 91192, France, ²Department of chemistry, Dalhousie University, Halifax- Canada, ³LCM3B, Nancy- Universite, Nancy, France., E-mail: el-eulmi.bendeif@synchrotron-soleil.fr

The development of cationic square-planar complexes of the heavier metals has emerged as an important theme in modern organometallic research, since such species are among the most active and widely used classes of homogeneous catalysts [1]. However, the range of experimental conditions under which such cationic species can be employed is limited. Furthermore, the systematic design of cationic catalysts is complicated and can influence catalytic performance in a negative manner. In this context, a new class of neutral, cationic, and formally zwitterionic Rh(I) complexes featuring organic ligands have been prepared and structurally characterized [2]. We will present here the accurate analysis of the charge density based on higher-intensity synchrotron radiation at 100 K for both Rh zwitterion (C₂₅H₃₇NPRh) and its analogous cation (C₂₆H₃₈F₃NO₃PRhS). Experimental deformation densities allow a first qualitative view of the non-spherical density and reveal fine details, coherent with the chemistry of the molecules. The topological analysis of the total electron density will be discussed. The accurate analysis of the charge density gives a better insight into the subtle electronic variations between the Rh cation and zwitterions as well as the specific origins of the differing reactivity properties of the structurally related cationic and zwitterionic Rh complexes. Experimental electron densities will be then compared to theoretical quantum chemistry calculations, in order to quantify the effects of polarization on the electron density and their contribution to intermolecular interaction energies.

[1] Gavrilov, K. N. & Polosukhin, A. I. (2000). *Russ. Chem. Rev.* 69, 661-682.[2] Stradiotto, M.; Cipot, J. & McDonald, R. (2003). *J. Am. Chem. Soc.* 125(19); 5618-5619.

Keywords: charge density, metal complexes, topological analysis

P14.03.08*Acta Cryst.* (2008). A64, C567 **β -hydroquinone acetonitrile clathrate: Insight into host-guest chemistry**Henrik F. Clausen¹, Mark A. Spackman², Bo B. Iversen¹¹University of Aarhus, Department of Chemistry, Langelandsgade 140, Aarhus C, Oestjylland, DK-8000, Denmark, ²Department of Biomedical, Biomolecular and Chemical Sciences, University of Western Australia, Crawley WA 6009, Australia, E-mail: hfano@chem.au.dk

Supramolecular chemistry is the foundation of design and development of materials with a vast number of potential applications such as catalysis, targeted drug delivery and gas storage. This research is part of a project that aims to make a novel contribution to understanding of intermolecular interactions, with special focus on crystalline guest-host systems such as the β -hydroquinone clathrates, 3C₆H₄(OH)₂ · xS with S being the enclathrated solvent. Analysis of an experimental determined charge distribution of the clathrates provides information such as the electrostatic properties of the host lattice as well as the guest molecules, from which an

estimation of the formation energies can be given. In the structure of β -hydroquinone acetonitrile clathrate reported by Chan et al. [1] three symmetry independent acetonitrile molecules fit inside the voids of the rhombohedral hydroquinone framework with one guest molecule orientated in the opposite direction to the two other. Data obtained using synchrotron X-ray radiation at 15(2)K from the D3 beamline at the DESY, Germany and the ChemMatCARS beamline at the APS, USA was used to model the electron density distribution using the multipole formalism. Examination of the preliminary models obtained however revealed additional disorder of the solvent molecules. Neutron data was collected at IPNS, Chicago, USA to obtain high accuracy unbiased structural parameters (e.g. thermal and positional) and the preliminary model again suggests that the solvent is more disordered than previously reported. Preliminary analysis of the charge distributions and the neutron structural model in the β -hydroquinone clathrates with the solvent CH₃CN will be presented here.

[1] T.-L. Chan, T. C. W. Mak, *J. Chem. Soc. Perkin Trans. II* (1983), 777-781

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P14.06.09*Acta Cryst.* (2008). A64, C567**Electronic situation in the oxirane ring-charge density and ELF study on several oxirane derivatives**Simon Grabowsky¹, Thomas Pfeuffer², Manuela Weber¹, Stefan Mebs¹, Juergen Buschmann¹, Carsten Paulmann³, Tanja Schirmeister², Peter Luger¹¹Freie Universitaet Berlin, Institut fuer Chemie und Biochemie/ Kristallographie, Fabeckstr. 36a, Berlin, Berlin, 14195, Germany, ²Universitaet Wuerzburg, Am Hubland, Bayern, Wuerzburg, 97074, Germany, ³HasyLab at Desy, Notkestr. 85, Hamburg, Hamburg, 22607, Germany, E-mail: vongrabo@chemie.fu-berlin.de

The electronic situation in ethylene oxide (oxirane, epoxide) is very special in chemistry due to its high ring strain. We synthesised and crystallised a row of oxirane derivatives (compounds I-IV, see Figure). Single-crystal X-ray diffraction experiments at low temperatures (25K to 100K) were carried out at the synchrotron beamline F1 of HASYLAB/ DESY and at a conventional Mo source. From the experimental structure factors we determined the electron-density (ED) distribution (multipolar modelling, programme XD2006) and the electron localization function (ELF) (constrained wavefunction fitting, programme TONTO) and analysed them with respect to the bonding situation in the three-membered ring. In addition, quantum chemical ab-initio calculations were carried out in the gas phase and with periodical boundaries (programmes GAUSSIAN 03 and CRYSTAL 06) to obtain ED and ELF from theory, too. In recent pharmaceutical research, oxirane derivatives have been found to be of potential anticancer activity. Cpd. IV serves as a model compound for protease inhibitors which makes it even more important to investigate the bonding situation of oxiranes in detail.

Keywords: electron localization function, electron density, oxirane