conference abstracts

s2.m1.p25 **Can we observe the position of protons from high resolution X-ray diffraction in the oxovanadate Na$_{10}$ [N$_3 \subset$H$_3$V$_{18}$O$_{44}$], 30 H$_2$O?** N. Claiser[§], V. Pichon-Pesme[§], C. Lecomte[§], M.-M. Rohmer[#], M. Bénard[#], T.B. Pedersen[#], (#) Laboratoire de Chimie Quantique, UMR 7551, CNRS and Université Louis Pasteur, Strasbourg, France; (§) LCM³B, Université Henri Poincaré Nancy-1, Vandoeuvre-lès-Nancy, France.

Keywords: polyoxovanadate, electron density, electrostatic potential.

The complex Na$_{10}$ [N$_3 \subset$H$_3$V$_{18}$O$_{44}$], 30 H$_2$O (1) is an electronically inverse host-guest system. It means that a central guest anion is surrounded by a negative shell of metal oxide polyhedra. In this case, 18 VO$_5$ square pyramids form an ellipsoidal cage around the central azid ion N$_3^-$. 10 sodium ions allow the electroneutrality of the structure.

In order to determine the electron density, accurate X-ray measurements were performed at room temperature with molybdenum radiation on a Nonius Kappa CCD diffractometer. 456330 intensities were integrated in a resolution range from 0.01 to 1.23^{-1}, reduced in 49941 unique corrected from absorption (R$_{int}$= 6%).

The quality of our measurements permits to determine the complex's structure and the position of the Na$^+$ cations and the solvent molecules. Furthermore, the weak thermal displacement parameters allows to study the electronic density. MOLLY program (2) was used for modelling electron density. In this poster we will particularly focus on vanadium atoms To this aim, different electron density maps at every stages of the refinement were carried out. The first results, at the end of the spherical refinement, shows an important charge accumulation near the vanadium atoms, in the extension of the double V=O bond. We compare our results to the ab-initio study work out at Strasbourg and we notice a quite good correspondence. We are actually trying to locate the three missing protons of the shell.

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s2.m1.p26 **Electrostatic properties of zeolites from charge density modelling: Succes after pitfalls?** F. Porcher, E. Aubert, M. Souhassou, Y. Dusausoy, C. Lecomte., *L.C.M.³ B., Université H. Poincaré- Nancy I, Nancy, France.*

Keywords: charge density, zeolites, microporous materials.

The peculiar physico-chemical properties of zeolites are based on the existence of large cavities in their structure that can lodge neutral or charged hosts molecules. The sorption properties are related to the structure of the flexible TO$_4$ framework (T = Al, Si, P, Ga)and to the distribution of the exchangeable charge compensating cations inside the pores.

As a first approximation, the interaction between cations and guest molecules is limited to the long range electrostatic interactions, the dispersion term being negligible for cation-sorbant distances greater than two angströms. It is therefore possible to evaluate the sorption energies from the electrostatic potential of empty dehydrated zeolites. This later can also be derived from the electron density distribution of the material that can be obtained by *ab initio* calculations[1,2] (though these systems are often very large for accurate studies) or charge density modelling from high resolution X ray diffraction measurements[3,4].

This later method also is difficult because of the weak diffracting power of synthetic zeolites, the existence of superstructure and the difficulty to synthesise single crystals large enough for charge density studies, even when using synchrotron radiation. Structural disorder in the framework (substitution of Si by Al on tetrahedral sites for instance) and in cations distribution and large "thermal displacement parameters" also preclude any accurate modelling[5].

Despite all these pitfalls, can we obtain however the charge density distribution in molecular sieves and use it for their subsequent modelling ?

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