**o.m3.p9** **Adsorption of aromatic molecules in NaX zeolite: trying a structure determination by single crystal X ray diffraction**. E. Aubert[1], F. Porcher[1], M. Souhassou[1], Y. Dusausoy[1], C. Lecomte[1], H.P. Weber[2], S. Capelli[2]. [1]*Laboratoire de Cristallographie et Modélisation de Matériaux Minéraux et Biologiques, Université Henri Poincaré – Nancy I, Vandoeuvre-lès-Nancy, France*. [2]*European Synchrotron Radiation Facility, Grenoble, France.*

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The structural determination and the study of charge density of systems composed by zeolites (or more generally porous materials) and guest molecules have several objectives. Since these porous materials have a great importance in industry, this kind of study may help to improve the understanding of sorption mechanisms and the origin of the selectivity of those "molecular sieves". Also, the charge density modelled from high resolution X ray diffraction experiment allows in principle to derive properties (like, for example, electric field or potential in zeolitic cavities) that can be related with their sorption characteristics.

This research subject is mainly explored by diffraction techniques on powder (by X ray or neutrons[1,2] ) and studies on single crystals are scarce because of the difficulty to obtain large crystals of good crystalline quality.

Octahedral single crystals (150μm) of NaX zeolite (Si/Al ˜ 1.06) were synthesised in our laboratory. Each single crystal, lodged in a quartz capillary, was dehydrated under vacuum and heating according to a well-defined procedure and then exposed to vapours of guest organic compound for one week. After equilibrium, the capillaries were sealed with a torch.

Investigations by X-ray diffraction have been performed at 120K on single crystals of NaX zeolite loaded with dichlorobenzene ($Na_{93}\ Al_{93}\ Si_{99}\ O_{384}\ .\ x\ C_6H_4Cl_2$ ) or benzene ($Na_{93}\ Al_{93}\ Si_{99}\ O_{384}\ .\ x\ C_6H_6$ ).

In the later case, diffraction experiments were done on the same crystal either using a conventional source (Mo(Kα) sealed tube, λ=0.709 Å ( Nonius Kappa CCD diffractometer at LCM[3]B) or using synchrotron radiation with a similar wavelength ( 0.7 Å, ESRF, beamline BM1A, measurement on KUMA KM6 diffractometer equipped with a point detector).

Preliminary results will be presented and discussed in the poster.

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