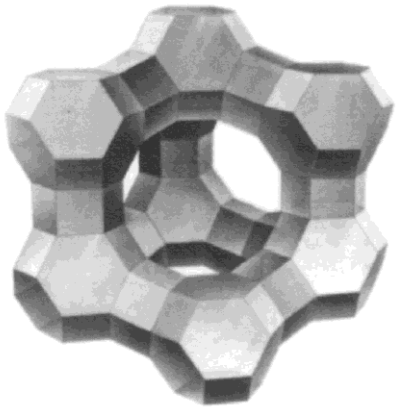
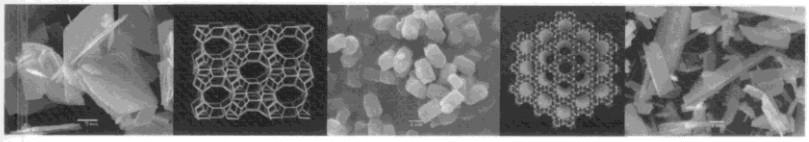
School of Molecular Sieves

Prague, April 1-3, 2012





Program and Book of Abstracts

P1

CRYSTAL STRUCTURE AND SORPTION PROPERTIES OF COMPLEX $\{[Zn_2(MTB)(H_2O)_2]\cdot 6DMF\cdot 5H_2O\}_n$

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Porous metal-organic frameworks (MOFs) have attracted great attention because of their potential applications in gas storage and separation processes, ion exchange, catalysis, sensor technology and fabrication of metal nanoparticles[1].

In our work we have focused on the preparation of novel MOF using Zn(II) and carboxylate anion methanetetrabenzoate (MTB^{4-}). Complex with formula $\{[Zn_2(MTB)(H_2O)_2]\cdot 6DMF\cdot 5H_2O\}_n$ was prepared by solvothermal route.

The crystal structure of complex (see Fig. 1a) is formed by SBU: the paddle-wheel cluster in which a zinc dimmer is bridged by four syn-syn carboxylate bridges with water ligands occupying the axial positions on Zn. Complex shows a PtS-like structure that is quite rare in MOFs, although it is frequently encountered in minerals. The central C of MTB can be considered the S vertex, and the square arranged carboxylate C atoms at the corners of the SBU decorate the Pt positions in PtS. The benzene units space apart the vertexes to give an overall expanded PtS network with 3D pores of dimensions of 20.5 x 5.4 $Å^2$, 5.4 x 5.4 $Å^2$and 9.2 x 8.3 $Å^2$. The pores are filled with five water and six DMF guests per formula unit. Since the guest molecules could not be defined by the X-ray diffraction data due to the high thermal disorder, they were characterized by the elemental analysis, IR spectroscopy as well as TGA data.

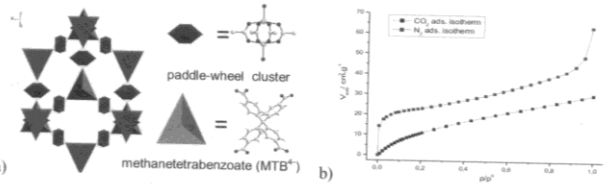

Fig. 1 a) View of the structure. b) N_2 and CO_2 adsorption isotherms.

To check the porosity of complex, gas sorption was measured for N_2 and CO_2 gases (see Fig 1b). The activated compound adsorb N_2 gas up to 22.0 wt.% (10.05 $mmol.g^{-1}$, 63.5 $cm^3.g^{-1}$ at STP) at 77K and 1 atm, and CO_2 up to 5.6 wt.% (1.35 $mmol.g^{-1}$, 30.35 $cm^3.g^{-1}$at STP) at 273K and 1 atm.

Acknowledgements:

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References:

[1]Furukawa, H.; et al. Science **2010**, 329, 424-428.