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Structural analysis of dye modified, synthetic mordenite single crystals characterising the arrangement and disorder of the organic cationic dves are presented. Microporous materials like zeolites are more and more applied for design and development of new materials. With channel and cavity apertures of several angstroms, they allow stabilisation and incorporation of individual atoms, clusters or molecules. One aspect of modern technology and new materials are onedimensional zeolite host-guest systems and miniaturized electronic devices, e.g. semiconductors organised as quantum dots or chains or luminescent dyes which mimic the natural function of chlorophyll in plants. Different kinds of microcrystalline (< 1µm) synthetic zeolites (zeolite L, zeolite Y, and ZSM-5) have hitherto been used as hosts for this kind of artificial antenna systems [1]. The incorporation of the organic dye molecules is dependent on the aperture of the zeolite channels. The orientation of the molecule in the channel is determined by the shape and size of the dyes and the zeolite channels. Furthermore, the charge distribution on the internal walls of the zeolite channels may influence the orientation of the trapped molecules. Very little is known about geometrical arrangement of the dyes in the zeolite channels. The exact position of the chromophores in the zeolite structure may provide better understanding how the antenna systems work and how the energy transfer can be improved. A suitable method to analyse the modified zeolite structure is single-crystal diffraction applying synchrotron radiation. Single crystals of self-synthesised mordenite-Na were used for incorporation of different cationic dye molecules as thionine blue $(C_{12}H_9N_3S^+)$, methylene blue $(C_{16}H_{18}N_3S^{^+}) \quad \text{and} \quad DAMS \quad (C_{16}H_{19}N_2^{^+}). \quad Mordenite \quad is$ particularly suitable for the structural analysis of dye-zeolite systems, because the anisotropic shape of the channel crosssection limits disorder of the enclosed molecules. The organic, cationic molecules were incorporated by ion exchange in saturated dye solution during 8-12 weeks at 100 °C. Electron microprobe analysis showed that Na⁺ was partially exchanged by the cationic dyes. X-ray data collection of dye-loaded mordenite was performed at 120 K with synchrotron radiation $(\lambda = 0.7995 \text{ Å})$ using the single-crystal diffraction beam line at SNBL (ESRF, Grenoble) where diffracted intensities were registered with a MAR image plate. Possible positions and arrangement of incorporated dye molecules were limited by the ellipsoidal shape of the large 12-membered ring channels $(7.0 \times 6.5 \text{ Å})$ of mordenite. Different low-populated molecule sites were defined which were highly disordered along the channel axis. Arrangement and preferred positions of Scontaining dye molecules (thionine blue, methylene blue) were compared with the structural data of a Se-modified mordenite [2].

^[1] Calzaferri G., Pauchard M., Maas H., Huber S., Khatyr A., Schaafsma T. (2001) J. Mater. Chem., 12(1)

^[2] Simoncic P., and Armbruster T. (2004) Microp. Mesop. Mater. (submitted)