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Neutron Diffraction from Cyclodextrin Hydrates to Photosystem II. W. Saenger, Inst. of Chemistry and Biochemistry /Crystallography, Free Univ. Berlin, Takustr. 6, 14195 Berlin, Germany.

Cyclodextrins or cycloamyloses consist of 6 to 10 α-1,4 linked D-glucoses with 3 O-H groups in each glucose. The neutron structures of their hydrates show extended networks of ···O-H···O-H···O-H··· hydrogen bonds that are mostly homodromic (in the same direction) and cooperative. These motifs will be illustrated with cyclodeca-amylose • 27 H_2O. In cycloheptaamylose • 12 H_2O, many of the H_2O and O-H groups are disordered, giving rise to flip-flop hydrogen bond disorder that is due to rotation of O-H groups and is dynamic, O-H···O-H ↔ H-O···H-O [1]. The flip-rate was determined by quasi-elastic neutron scattering [2].

Photosystem II is embedded in the thylakoid membrane of plants. The cyanobacterial variety consists of 20 protein subunits and 77 cofactors, the most interesting being a cluster consisting of 4 Mn(III) and Mn(IV) cations and one Ca(II), in short Mn_4Ca, where water is oxidized to atmospheric oxygen [3]. Since X-rays rapidly reduce Mn_4Ca to inactive Mn(II) associated with destruction of the Mn_4Ca architecture, neutron diffraction is the radiation of choice to derive the true architecture of Mn_4Ca.

W. Saenger et al., Chem Rev. *98*, 1787-1802 (1998).
T. Steiner et al., Mol. Phys. *72*, 1211-1232 (1991).
B. Loll et al., Nature 438, 1040-1044 (2005).