02.12-2 NEUTRON DIFFRACTION STUDY OF γ-CYCLODEXTRIN·14D_2O at 110° K. By V. Zabel, B. E. Hingerty, University of Tennessee-Oak Ridge Graduate School of Biomedical Sciences and Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831; S. A. Mason, Institute Max von Laue-Paul Langevin, 156X, F-38042 Grenoble Cedex, France, and W. Saenger, Institut für Kristallographie, Frei Universität Berlin, D-1000 Berlin 33, FRG.

γ-Cyclodextrin is an octameric oligosaccharide in a cyclically closed torus-like conformation. It consists of 8 residues of α (1-4)-linked glucoses. The biological activity of cyclodextrins has made them of considerable interest to the chemical and agricultural industries because of the inclusion complexes they produce. A low-temperature study of a deuterated crystal has been performed at the Institute Laue-Langevin (ILL) using a new area detector system. The same crystal has been used at low temperature as was used for the room temperature study conducted at the High Flux Isotope Reactor (HFIR) in Oak Ridge. The crystal is monoclinic space group $P2_1$, with cell dimensions of a = 20.226(6), b = 10.891(5), c = 16.899(7) Å, and β = 105.06(2)°. 10,688 reflections were collected at λ = 1.2639 Å on an area detector, yielding 4,907 unique measurements with an R_{merge} = 0.064 on F^2.

The low-temperature structure has the same a-axis as the room-temperature H_2O crystal[1] and 0.25 Å shorter than the room-temperature D_2O crystal. The b-axis is 0.30 Å shorter than the D_2O room-temperature crystal and 0.20 Å shorter than the H_2O (see table below). The H_2O structure is apparently $11H_2O$ while the D_2O room-temperature structure is at least $14D_2O$. The low-temperature D_2O structure is also likely to be different. Results of the refinement and a description of the hydrogen-bonding networks in relation to biological activity will be presented at the meeting.

H_2O(298°K)	D_2O(298°K)	D_2O(110°K)
a=20.287(10)Å	20.520(5)Å	20.226(6)Å
b=11.079(7)Å	11.197(3)Å	10.891(5)Å
c=16.858(12)Å	16.810(3)Å	16.899(7)Å
β=105.07(4)°	105.23(1)°	105.06(2)°

[1]B. Hingerty, Ch. Betzel and W. Saenger, Proc. of the Symp. on "Molecules in Motion" Lexington, Kentucky, May 20-21, 1984; Trans. of the Amer. Cryst. Assoc., Vol. 20, ed. J. J. Stezowski, pp. 159-62 (1984).

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