03.4-04 CRYSTAL STRUCTURE OF THIAMIN METHYL ACETYLPHOSPHONATE. By J. Fletcher, A. Turano, W. Furey, M. Sax, Biocrytallography Laboratory, VA Medical Center, Pittsburgh, Pa. 15240, Department of Crystallography, University of Pittsburgh, Pittsburgh, Pa. 15260 and R. Kluger, Department of Chemistry, University of Toronto, Toronto, Ontario.

Thiamin methyl phosphonate is monochlorine, P2_1/c. 

03.4-05 THE CRYSTAL STRUCTURE OF THIAMINE DINITRATE. By D. C. Yang, C. S. Yoo, W. Furey, Jr., B. C. Wang, J. Fletcher and M. Sax, Biocrytallography Laboratory, VA Medical Center, Pittsburgh, Pa. 15240 and the Department of Crystallography, University of Pittsburgh, Pittsburgh, Pa. 15260.

The structure of the compound was determined by X-ray diffraction. It crystallizes in P2_1 with z=2 in a unit cell of dimensions a=8.238, b=10.208, c=10.419, \( \beta = 119.45^\circ \), \( \gamma = 119.45^\circ \). It was prepared by titrating thiamine mononitrate with dilute nitric acid. The structure of the compound was determined by X-ray diffraction. It crystallizes in P2_1/c, \( a = 8.93 \), \( b = 10.20 \), \( c = 10.41 \), \( \beta = 119.45^\circ \), \( \gamma = 119.45^\circ \).

03.4-06 TWO STRUCTURES RELEVANT TO POLYCYCLIC ARO­

The structure of a sym monoclinic (3,4-epoxy-2-methyl-1,2,3,4-tetrahydro-1-phenyl) has been determined (\( a = 8.151 \), \( b = 10.007 \), \( c = 6.324 \) \( \AA \), \( \beta = 92.80 \), \( \beta = 104.35 \), \( \gamma = 113.30^\circ \)), space group P2_1. The molecule crystallizes with an internal hydrogen bond between the hydroxyl and epoxide oxygen atoms. This forms the conformation of the methyl group to be axial. The crystal shows extensive radiation damage during data collection. This structure is a model for the syn diol epoxide of carcinogenic polycyclic aromatic hydrocarbons such as benzo[alpha]pyrene.

The structure of a covalent adduct of deoxycadenosine with the carcinogen 7-chloromethyl-1,2-dimethylbenz[a]­thracene (8'-[12-methylbenz[a]anthracenyl-7-methyl]deoxycadenosine, \( a = 15.815 \), \( b = 17.965 \), \( c = 8.971 \), space group P2_1/c). The molecule lies with the hydrocarbon and sugar groups each perpendicular to the adenine group. The glycosidic torsion angle is \(-124^\circ\) indicating that the compound exists in this structure in the syn conformation with a hydrogen bond between the hydrogen atom on O(5') of the ribose and N(3) of adenine (unlike deoxyadenosine which has the anti-conformation in the crystals studied (Acta Cryst. (1969) 15, 111)). The molecules pack with alternate adenine and hydrocarbon groups from different molecules stacking in columns throughout the crystal. The buckled portion of the hydrocarbon group is not involved in the stacking. This research was supported by grants CA-10925, CA-22780, CA-06627 and RR-05399 from the National Institutes of Health, U.S. Public Health Service, a grant BC-242 from the American Cancer Society and by an appropriation from the Commonwealth of Pennsylvania.

03.4-07 CRYSTAL STRUCTURE OF A BUILDING UNIT OF THE FORSSMAN ANTIGEN. By K. Vangehr, P. Luger and H. Paulsen; Institut für Kristallographie der Freien Universität Berlin and Institut für Organische Chemie und Biochemie der Universität Hamburg; West Germany.

The carbohydrate component of the Forssman antigen consists of the pentasaccharide D-GalNAc-(1-3)-D-GalNAc-\( \beta -(1-3)-D-Gal-a(1-4)-D-Gal-\beta -(1-4)-D-Glc \) (I) which was recently synthesized (Paulsen, H. & Bünzsch, A., Angew. Chem. (1980) 92, 219).

We have investigated the crystal structure of 2-acet­amido-3-O-[2-acetamido-3,4,6-tri-0-acetyl-2-deoxy-a-D-galactopyranosyl]-1,4,6-tri-0-acetyl-2-deoxy-a-D-galac­to-pyranose (II) which is a model compound of the terminal disaccharide of (I). Moreover (II) is a building unit of human blood group determinants. The conformation of (II) is of special interest to study interactions with receptor sites in biological activity and may serve as an approach to the structure of the above mentioned biological molecules. Single crystals of (II) are only stable if held in solvent and they are extremely sensitive against mechanical contacts. The structure determination and refinement was complicated by disorder of two solvent water molecules and of both N-acetyl groups. The result of structure analysis shows that along the glycosidic (1-3) linkage atom C-1 deviates by 38° from a trans position to atom C-2 while as C-3' deviates by 23° from a trans position to C-2.