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

Thiamin methyl asethyllphosphonate is monoclinic, $P2_1/c$, $a=9.918(8)$, $b=16.840(1)$, $c=15.786(1)$ $\text{Å}$, $\beta=119.45(4)^{\circ}$, $\omega=299.5^{\circ}$ $z=4$. The structure was solved using direct methods and refined by full-matrix least squares to an $R$ value of .037 for 1587 observed structure factor amplitudes measured with $K_a$ radiation on a Nonius automatic diffractometer. Various biosynthetic pathways involve thiamin (Vitamin B$_1$) but there exists a great deal of debate as to conformation and mechanism of action of this coenzyme. Thiamin C(2) adducts are intermediates in the reaction mechanism, many of which are stable under mildly acidic conditions. Substitution occurring on the C(2) changes the conformation of the molecule with respect to free thiamin. The structure of this inhibitor intermediate was analyzed by X-ray diffraction to investigate whether or not conformational change or retention of configuration is occurring at a specific step in the reaction mechanism. There seem to be many interesting contacts occurring with the phosphate side chain of this molecule. In particular, one contact from the terminal oxygens seems to have created energetically equal sites causing disorder of one water molecule.

03.4-05 THE CRYSTAL STRUCTURE OF THIAMINE DINITRATE. By D.S.C. Yang, C.S. Yoo, W. Furey, Jr., B.C. Wang, J. Fletcher and M. Sax, Biocystallography 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 $a=8.938$, $b=10.200$, $c=10.410$ $\text{Å}$, $\alpha=92.50^{\circ}$, $\beta=104.0^{\circ}$, $\gamma=113.50^{\circ}$. The space group is $P_{2_1}2_12$. The molecule crystallizes with an internal hydrogen bond between the hydroxyl and aperoxide oxygen atoms. This forces 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(g)pyrene.

The structure of a covalent adduct of deoxyadenosine with the carcinogen 7-choloromethyl-12-methylbenz[a]anthracene (5'- (12-methylbenz[a]anthracenyl-7-methyl) deoxyadenosine, $\alpha=15.815$, $b=17.965$, $c=8.871$, space group $P_{2_1}2_12$) has been determined. 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) 14, 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-05339 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.

03.4-06 TWO STRUCTURES RELEVANT TO POLYCYCLIC AROHEL CARCINOGENESIS. By J. P. Glusker, H. L. Carroll and D. E. Zacharias, The Institute For Cancer Research, The Fox Chase Cancer Center, 7701 Burholme Avenue, Philadelphia, Pa. 19111, USA.

The structure of a syn monol epoxide (3,4-epoxy-2-methyl-1,2,3,4-tetrahydro-1-naphthyl) has been determined ($\alpha=8.151(1)$, $b=10.007(1)$, $c=6.324(1)$ $\text{Å}$, $\beta=92.80(1)$, $\gamma=104.35(1)^{\circ}$, space group $P_{2_1}2_12$). The molecule crystallizes with an internal hydrogen bond between the hydroxyl and aperoxide oxygen atoms. This forces 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(g)pyrene.

The structure of a covalent adduct of deoxyadenosine with the carcinogen 7-choloromethyl-12-methylbenz[a]anthracene (5'- (12-methylbenz[a]anthracenyl-7-methyl) deoxyadenosine, $\alpha=15.815$, $b=17.965$, $c=8.871$, space group $P_{2_1}2_12$) has been determined. 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) 14, 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-05339 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.