sperms and angiosperms are given elsewhere (*1*) and have been used to predict the expected sensitivity to chronic irradiation. Because most of the gymnosperms examined so far have relatively large interphase chromosome volumes compared to most of the angiosperm species, the predicted sensitivities for both groups show very little overlap (Fig. 4). Whereas 94 percent of the gymnosperms have predicted 3rd-year values of 40 r/day or below, only 8 percent of the angiosperms have predicted values this low. Of the predicted gymnosperm values, 75 percent are between 11 and 40 r/day; of the angiosperm values, 63 percent are between 101 and 570 r/day. The ability to make such predictions for previously unirradiated species should be useful in the planning of various kinds of experiments including those in which woody plants of economic importance are irradiated to produce useful mutations.

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Crystal and Molecular Structure of a Thymine Phototrimer

Abstract. *Thymine trimer was isolated from a frozen aqueous solution of thymine which was irradiated with ultraviolet light and was presumably formed through the rearrangement of an initial oxetane photoproduct. X-ray diffraction analysis of a single crystal has confirmed the trimeric diol structure and has established the stereoconfiguration of the molecule. The possible importance of the diol structure in photobiology is pointed out.*

Irradiation of [2-^{14}C]- or [5-methyl-^{3}H]-thymine in frozen aqueous solution with ultraviolet light (254 nm) produced two detectable products (*1–3*). These were designated as photoproduct of thymine No. 1 (PT$_1$) [R_F, 0.15 in a solution of n-butanol, acetic acid, and water (80 : 12 : 30) on a paper chromatogram] and photoproduct of thymine No. 2 [R_F, 0.29] (*2*). The latter was a mixture of *cis-syn*-thymine dimer and thymine-thymine adduct (T-T adduct) (*4*). The characterization of T-T adduct (*4, 5*) was essential for the characterization of PT$_1$ (*6*) with its intriguing properties (*7*). For structural proof, we analyzed a crystal of PT$_1$ by x-ray diffraction.

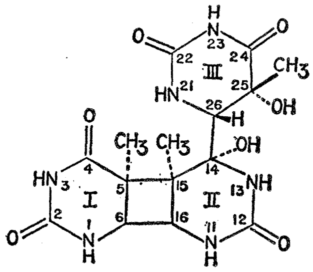


Fig. 1. Stereoconfiguration of the thymine trimer.

X-ray diffraction data for a single crystal of the thymine trimer were collected on a four-circle, fully automated diffractometer (Table 1). Because of the extremely small size of the crystal, only 38 percent of the total data possible within the CuKα 1.5418 Å sphere was obtained. The structure was solved directly by the symbolic addition procedure (*8*). Atomic coordinates and anisotropic thermal parameters were refined by least-squares methods, and all of the hydrogens except those on N-3 and one of the water molecules were located in a difference map. The final *R* factor (agreement between observed and calculated structure factors) for the observed data is 7.9 percent.

The thymine trimer (Fig. 1) shows similarities to both the T-T adduct (*5*) and the cyclobutyl-type dimers. The cyclobutane ring is only slightly puckered with a dihedral angle of 173.5°. This is significantly flatter than the four-membered rings in free dimers of the *cis-syn*-cyclobutyl type—for example, 155° in the uracil dimer (*9*) and 152° to 153° in the dimethylthymine dimer (*10*). However, it is not as flat as the 178° reported for the four-membered ring in the *cis-syn* intramolecular bridged dimer of 1,1′-trimethylenebisthymine (*11*). Rings I and II are rotated with respect to each other by torsion angles of 4.8° and 6.8° about the C-5–C-15 and C-6–C-16 bonds, respectively. Bond distances involving ring III and its substituents in the trimer are very similar to those involving ring I in the T-T adduct. The OH group on C-14 is axial to ring II while the methyl group on C-15 is equatorial to ring II. With respect to ring III, the methyl group on C-25 is axial and the hydroxyl group on the same carbon is equatorial. A water molecule crystallizes with the trimer and is included in the extensive system of hydrogen bonding in the crystal. There are also two intramolecular hy-

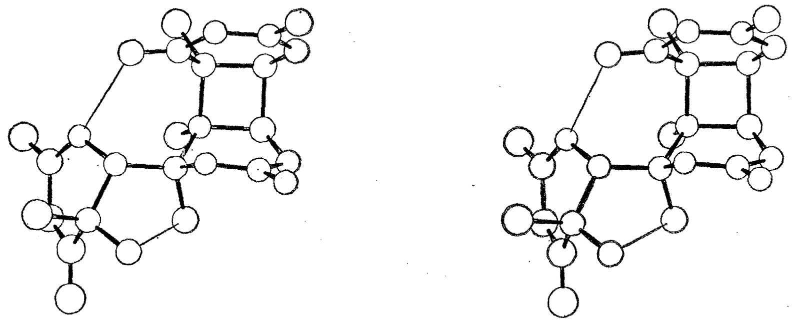


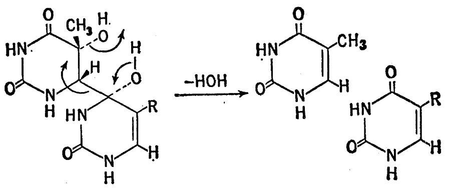
Fig. 2. Stereodiagram of the configuration of the thymine trimer as determined by x-ray analysis. This picture should be seen with a three-dimensional viewer for printed stereophotographs (*12*).

Table 1. Physical constants of PT$_1$.

Molecular formula	$C_{15}H_{20}N_6O_7 \cdot H_2O$
Molecular weight	414.38
Habit	Acicular
Crystal size (mm)	0.44 by 0.06 by 0.03
Space group	$P\bar{1}$
a	9.373 ± .004 Å
b	14.387 ± .004 Å
c	7.201 ± .003 Å
α	103.20°
β	100.00°
γ	91.80°
Molecules/unit cell	2
Density (calc.)	1.48 g/cm^3
No. of independent reflections	1636

drogen bonds, which are illustrated by the light lines in the stereoconfiguration of the molecule shown in Fig. 2.

The reversion of PT$_1$ to thymine has been observed under various conditions (*6*) and conceivably occurs through the following mechanism (*7*). Thus, this diol structure is of particular interest in considering reactivation processes in photobiology. If such a reaction involves cytosine as one of its bases, deamination may occur, resulting in the transformation of a cytosine to a uracil moiety (*7*). Such a change should be examined in relation to biological mutations induced by light. The x-ray data indicate that both OH groups are *trans* to the hydrogen on C-26. This configuration favors *trans* elimination of HOH rather than the rearrangement shown above and explains why the reversion of PT$_1$ to thymine is not a major reaction. Isomeric photoproducts with an all *cis* adduct linkage may also form. Such a configuration, that is, one in which both OH groups are *cis* to the CH, would favor the above rearrangement, and such a reversion to the bases might occur at rather mild acidic or basic conditions. Therefore, even if adducts of this type were present, they could not be detected by assay of the acid hydrolyzates of nucleic acids irradiated with ultraviolet light, a method generally used to analyze photoproducts. Even if undetectable chemically, however, their presence may be manifested by certain biological effects in systems in vivo.



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Deuterium: Natural Variations Used as a Biological Tracer

Abstract. *The suggestion is made that isotope tracing be carried out by monitoring the natural variations in deuterium concentrations. As an example, the natural variations in deuterium concentrations between food and water collected in Illinois and food and water collected in Colorado were used to determine the residence time of water in the blood and urine of rats. We observed not only a 5½-day turnover time of water in the blood and urine, but also evidence for the influx of water vapor from the atmosphere through the lungs into the blood.*

The use of deuterium as D$_2$O, heavy water, in isotope tracing is not new (*1*). The results indicate that rats cannot survive replacement of more than about one-third of the body water by D$_2$O. As the concentration of D$_2$O in the serum of rats approaches 20 percent, the rats show signs of hyperirritability,

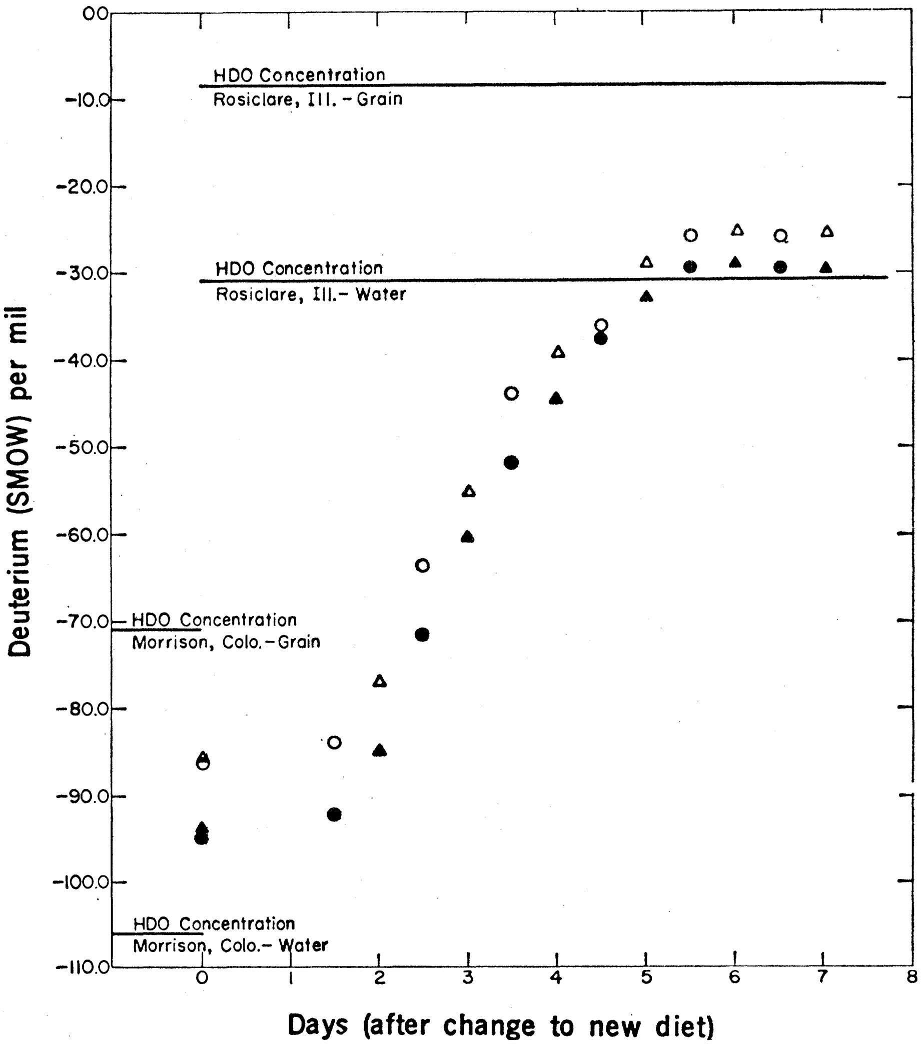

Fig. 1. Relative deuterium concentration in deviation per mil from SMOW standard of blood and urine of rats plotted as a function of time after their diet was changed from one low in deuterium to one relatively enriched in deuterium. ○, blood, rat No. 1; ●, urine, rat No. 1; △, blood, rat No. 2; ▲, urine, rat No. 2.