The cell dimensions used in the calculation of distances, $a = 4.315$ Å., $c = 6.990$ Å., are those of Siegel and Gebert[8] of Argonne National Laboratory, who kindly transmitted them to us. We are grateful to Dr. D. F. Smith of the Oak Ridge Gaseous Diffusion Plant for furnishing the compound and for valuable assistance in its manipulation.

(8) S. Siegel and E. Gebert, J. Am. Chem. Soc., 85, 240 (1963).

(9) This paper is based upon work performed at Oak Ridge National Laboratory, which is operated by Union Carbide Corporation for the Atomic Energy Commission.

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CRYSTAL AND MOLECULAR STRUCTURE OF XENON TETRAFLUORIDE[1]

Sir:

Because of interest in the molecular structure of xenon tetrafluoride[2] we have determined the structure of the crystals by X-ray diffraction at room temperature. The structure consists of a molecular packing of square-planar molecules of XeF_4.

A 4 to 1 molar ratio of F_2 and Xe was passed through a nickel tube at $300°$. With a residence time in the hot zone of 1 minute, essentially all of the xenon reacted, and crystals condensed in the cooler part of the flow system. The solid then was sublimed under vacuum into other Pyrex containers and finally into thin-walled vitreous silica capillaries for X-ray examination.

Preliminary crystal data were obtained from oscillation and Weissenberg photographs of several crystals. The accurate cell dimensions and the intensities of the reflections were measured with a goniostat and scintillation counter with Mo Kα radiation, $\lambda(K\alpha_1) = 0.70926$ A. The well-formed dodecahedral crystal had diameters ranging from 0.13 to 0.24 mm., corresponding to μR. about unity. No correction was made for absorption. Because the crystal grew about 30% during the intensity observations, the data were normalized by repeated measurements of a few reflections.

The monoclinic unit cell has dimensions $a = 5.050$, $b = 5.922$, $c = 5.771$ Å. (each ± 0.003 Å.), $\beta = 99.6°$ $\pm 0.1°$, in reasonable agreement with values found elsewhere.[3,4,5] With 2 molecules per cell the density is 4.04 g./ml. Systematically absent reflections correspond to space group $P2_1/n$. Reflections are strong when $h + k + l$ is even and weak when it is odd, showing that the Xe atoms are at $0,0,0$ and $1/2,1/2,1/2$. Fluorine atoms are in two sets of general positions 4(e): $\pm(x,y,z; 1/2 - x, 1/2 + y, 1/2 - z)$.

Intensities were measured for the 329 independent reflections of the primitive cell with θ less than $25°$. Of these, 36 are absent because of the space group symmetry. Of the other 133 reflections with $h + k + l$ odd, whose intensities depend only on the fluorine scattering, 96 were recorded as non-zero. An extensive search for other weak reflections which would demand a larger unit cell was made by sweeping along many lattice rows and by counting at approximately 100 positions corresponding to reflections of cells with some or all of the axes doubled. No such reflections were found, with the sensitivity about 10^{-4} of the strongest reflection.

A trial structure was derived by simple calculations involving a few reflections. It was refined by least

(1) This work was done in part under the auspices of the U. S. Atomic Energy Commission.

(2) H. H. Claassen, H. Selig and J. G. Malm, J. Am. Chem. Soc., 84, 3593 (1962).

(3) S. Siegel, private communication.

(4) H. A. Levy, private communication.

(5) J. A. Ibers and W. C. Hamilton, private communication.

squares in several series of calculations. With independent isotropic temperature factors and equal weights for 286 reflections (omitting the seven at the lowest angles) the conventional $R = \Sigma \, ||F_0| - |F_c||/\Sigma|F_0|$ was reduced to 0.086 with the parameters

	x	y	z	B, Å.²
Xe	(0)	(0)	(0)	1.6
F_1	0.261	0.147	0.847	3.6
F_2	0.228	0.033	0.295	3.7

Standard deviations are 0.003 for each coördinate. Calculations with anisotropic temperature factors gave the same coördinates within 0.002 or less. Isotropic refinement with the 96 non-zero reflections with $h + k + l$ odd gave the same coördinates within 0.005 or less.

The above coördinates correspond to Xe–F bond distances of 1.92 and 1.90 Å., with standard deviations of 0.02 Å. The F–Xe–F bond angles are $89.7°$ (and $90.3°$) with $\sigma = 0.9°$. The molecule is planar by the symmetry and we find it to be square within the experimental uncertainty.

The thermal motion of the fluorine atoms exceeds that of the xenon atoms. As a result, the average Xe–F distance is greater than that given above. With the assumption that F "rides" on Xe, we estimate (from the anisotropic temperature parameters) that the average corrected distance is 1.93 Å.

The F–F distances within the molecule are 2.69 and 2.71 Å. ($\sigma = 0.03$ Å.). The shortest F–F contact between molecules is 3.02 Å.

Ibers and Hamilton[5] have deduced two structures by refinement of data with $h + k + l$ even. These data do not permit determination of the relative signs of the two y coördinates. One of these two structures is in approximate agreement with our result.

We thank Dr. Henri A. Levy for helpful information concerning the space group.

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RING CLEAVAGE OF PURINE NUCLEOSIDES TO YIELD POSSIBLE BIOGENETIC PRECURSORS OF PTERIDINES AND RIBOFLAVIN[1]

Sir:

The fact that adenine[2,3] and guanine[2-4] may serve as precursors of various pteridines has been amply demonstrated in several biological systems. These purines are all incorporated into the pteridine ring with resultant loss of carbon 8. Based on feeding experiments with radioactive precursors, Brenner-Holzach and Leuthardt[5] in studying the biosynthesis of pteridines in the *Drosophila melanogaster* have postulated that a purine nucleoside (or nucleotide) eliminates C-8 of the purine ring, and atoms 1 and 2 of ribose furnish carbons 6 and 7 of the pteridine nucleus. In the butterfly *Pieris brassiceae L.* it has been shown recently by Weygand, *et al.*,[6] that guanosine (or guanylic acid) serves as the direct precursor of xanthopterin and leucopterin with two of the carbon atoms of the ribosyl

(1) This work was supported by Research Grant No. T-181A from the American Chemical Society.

(2) W. S. McNutt, J. Am. Chem. Soc., 82, 217 (1960).

(3) E. Vieira and E. Shaw, J. Biol. Chem., 236, 2507 (1961).

(4) I. Ziegler-Gunder, H. Simon and A. Wacker, Naturforsch., 11b, 82 (1956).

(5) O. Brenner-Holzach and F. Leuthardt, Helv. Chim. Acta, 42, 2254 (1959); 44, 1480 (1961).

(6) F. Weygand, H. Simon, G. Dahms, M. Waldschmidt, H. J. Schliep and H. Wacker, Angew. Chem., 73, 402 (1961).