Table 2. *Powder data for* BPO_4 *and* $BAsO_4$ *(Quartz forms)*

	BPO_4					$BAsO_4$				
	Mackenzie *et al.*		Present work			Mackenzie *et al.*		Present work		
Index	d_o	I	d_o	I	d_c	d_o	I	d_o	I	d_c
10·0	3·895 Å	*s*	3·878 Å	50	3·871 Å	3·964 Å	*m*	3·960 Å	25	3·951 Å
10·1	3·626	*m*	*		3·607	3·699	*s*	3·694	55	3·690
	3·363	*vvw*								
00·3	3·318	*w*	*		3·309	3·452	*w*	3·440	40	3·443
	3·204	*vvw*								
10·2	3·060	*vs*	3·051	100	3·052	3·145	*vs*	3·143	100	3·138
10·3	2·519	*vvw*	2·515	5	2·515	2·598	*vw*	2·600	5	2·596
11·0	2·239	*m*	2·244	30	2·235	2·281	*w*	2·281	20	2·281
11·1	2·183	*vw*	2·180	7	2·181	2·228	*w*	2·228	10	2·227
10·4	2·092	*m*	2·088	15	2·089	2·162	*m*	2·161	20	2·162
11·2	2·040	*w*	2·037	15	2·038	2·087	*vw*	2·088	10	2·087
20·0	1·936	*vvw*	1·938	10	1·935	1·976	*w*	1·975	20	1·975
20·1						1·941	*vvw*	1·941	3	1·940
11·3	1·852	*vvw*			1·852	1·901	*vw*	1·903	7	1·902
20·2	1·805	*vw*	$1·800_5$	20	1·803					
10·5	1·768	*vvw*	1·764	10	1·766	1·831	*w*	1·831	8	1·831
00·6								1·722	13	1·722
20·3	1·671	*w*			1·671			1·713	20	1·713
11·4	1·662	*m*	$1·659_3$	30	1·661	1·710	*m*	1·710	25	1·710
10·6								1·578	8	1·579
20·4	1·527	*w*	$1·526_6$	10	1·526	1·568	*vw*	1·570	5	1·569
11·5	1·485	*vvw*			1·484	1·530	*vw*	1·530	5	1·531
21·1	1·448	*vw*			1·447	1·476	*vw*	1·477	13	1·478
21·2	1·403	*w*	$1·402_4$	50	1·403	1·433	*w*	1·434	15	1·434

* Obscured in our patterns by presence of some cristobalite form, which gives peaks in this region.

guished. The two extra lines included by Mackenzie *et al.* (1959) appear to be due to such causes; their inclusion necessitated the adoption of the larger unit cell by Mackenzie *et al.* (1959), and obscured the relationship to quartz.

Refractive indices and density have also been determined directly. Except for the indices of $BAsO_4$ they differ only slightly from those obtained by Mackenzie *et al.* (1959), and very kindly communicated to us personally. Both sets of results are given in Table 1.

The study of the silica phases conducted in this laboratory has been supported by the Chemical Physics branch of the U.S. Army Signal Corps over a period of years. Experimentation at high pressures is done under contract to the Office of Naval Research, Contract N(onr) 656 (20). We are indebted to Prof. Rustum Roy for reading the manuscript.

References

Dachille, F. & Roy, R. (1957). Work reported at Amer. Mineralogical Soc. Meeting, Atlantic City, N. J. (Nov. 4, 1957). *Z. Kristallogr.* (In press).
Huttenlocher, H. F. (1935). *Z. Kristallogr.* **90**, 508.
Machatschki, F. (1935). *Z. Kristallogr.* **90**, 314.
Machatschki, F. (1936). *Z. Kristallogr.* **94**, 222.
Mackenzie, J. D., Roth, W. L. & Wentorf, R. H. (1959). *Acta Cryst.* **12**, 79.
Schulze, G. E. (1934). *Z. phys. Chem.* B, **24**, 215.
Shafer, E. C., Shafer, M. W. & Roy, R. (1956). *Z. Kristallogr.* **108**, 263.

Acta Cryst. (1959). **12**, 821

Unit cell and space group of uranyl acetate dihydrate, $UO_2(CH_3COO)_2.2H_2O$.

By V. Amirthalingam, D. V. Chandran and V. M. Padmanabhan, *Chemistry Division, Atomic Energy Establishment, Trombay, Bombay, India.*

(*Received 5 June* 1959)

Uranyl acetate dihydrate crystallises as plates and prisms from dilute acetic acid, and belongs to the orthorhombic system. The exposed crystals loose their transparency and become amorphous in one or two days. Its crystal structure has not been reported.

Rotation and Weissenberg layer photographs with Cu $K\alpha$ radiation are taken about the b and the c axes. The cell dimensions thus obtained were checked by indexing the powder pattern obtained with a Philips counter diffractometer. The lattice parameters are

$$a = 14·95, \quad b = 9·61, \quad c = 6·93 \text{ Å}.$$

The ratio $a : 2b : c = 0·78 : 1 : 0·36$ agrees with the Groth's value $a : b : c = 0·7817 : 1 : 0·3550$ indicating that the true b-axis is half the morphological b-axis. Taking the den-

sity* to be 2·893 g.cm.$^{-3}$ the number of molecules per unit cell is found to be $Z = 4·092$ i.e. 4. Absent spectra were found to be $(0kl)$ for k odd and $(h0l)$ for $h+l$ odd. Hence the space group is $Pbn2_1$. This can be converted to space group $Pna2_1$ by interchanging the a and b axes. The complete structure analysis is in progress.

* Handbook of chemistry and physics, 39th edition, p.630. Ohio: Chemical Rubber Publishing Co.

We are grateful to Dr Jagdish Shankar for his interest during the progress of the work.

Reference

GROTH, P. (1906–19). *Chemische Crystallographie*, Vol. III, p. 72. Leipzig: Engelmann.

Acta Cryst. (1959). **12**, 822

The structure of crystals containing a hydrogen-bonded complex of 1-methylthymine and 9-methyladenine.*

By KARST HOOGSTEEN, *Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena, California, U.S.A.*

(*Received* 11 *May* 1959)

Introduction

A fundamental structural feature of the two-strand helical configuration proposed by Watson & Crick (1953) for deoxyribose nucleic acid (DNA) is the arrangement of the purine and pyrimidine bases in hydrogen-bonded pairs of adenine–thymine and guanine–cytosine. As part of a program of research on the structure of the nucleic acids in progress at this Institute, we have been interested in the possibility of preparing and determining the structure of crystals containing hydrogen-bonded pairs of these bases as a means of establishing the existence of such arrangements and of providing a direct experimental determination of the dimensions of the molecules and the manner of hydrogen bonding. Even if crystals could be obtained containing the nucleosides thymidine and adenosine in hydrogen-bonded pairs, they would undoubtedly be so complicated that a satisfactory determination of their structure would not be feasible. Use of the simple bases, thymine and adenine, would not be satisfactory because in them the nitrogen atoms 1 and 9, respectively, which in the nucleosides are attached to the sugar deoxyribose, are free for the formation of other hydrogen bonds that might lead to structures very different from the particular hydrogen-bonded structure that may be present in DNA. The most desirable crystal appeared to be one composed of derivatives of thymine and adenine in which the respective 1 and 9 nitrogen positions are blocked by the simplest possible organic radical, namely, methyl. We have now prepared crystals containing hydrogen-bonded pairs of the two compounds, 1-methylthymine and 9-methyladenine, and have definitely established the molecular arrangement and the manner of the hydrogen bonding.

A preparation of 1-methylthymine was made available to us by Prof. James English of the Department of Chemistry, Yale University; through the courtesy of Dr C. P. Rhodes and Dr G. B. Brown of the Sloan-Kettering Institute for Cancer Research and Dr G. H. Hutchings of the Welcome Research Laboratories, we were supplied with crystals of 9-methyladenine.

* Contribution No. 2466 from the Gates and Crellin Laboratories of Chemistry. This investigation was supported, in part, by a grant, CVRE 121, from The National Foundation.

1-Methylthymine and 9-methyladenine

Crystals of 1-methylthymine were obtained by evaporation of an aqueous solution at room temperature. The crystals were prismatic in shape with forms {100} and {111} predominating. Crystals of 9-methyladenine grown under similar conditions appeared as needles with forms {010}, {110}, and {001} well developed, the c axis being parallel to the needle axis of the crystal. The space groups and unit-cell dimensions of both compounds were determined from rotation and Weissenberg photographs taken with Cu $K\alpha$ ($\lambda = 1·5418$) radiation. The crystallographic data are tabulated below.

1-Methylthymine	9-Methyladenine
$a = 7·11 \pm 0·03$ Å	$a = 7·67 \pm 0·03$ Å
$b = 11·96 \pm 0·04$	$b = 12·24 \pm 0·04$
$c = 7·52 \pm 0·03$	$c = 8·47 \pm 0·03$
$\beta = 90° 0' \pm 10'$	$\beta = 123° 26' \pm 10'$
Space group: $P2_1/c$	Space group: $P2_1/c$
Density: 1·415 g.cm.$^{-3}$ (meas.)	Density: 1·471 g.cm.$^{-3}$ (meas.)
$Z = 4$	$Z = 4$

Systematic absences (both crystals):

$h0l$ absent for $l = 2n+1$, $0k0$ absent for $k = 2n+1$.

1-Methylthymine-9-methyladenine complex

Equimolecular quantities of 1-methylthymine and 9-methyladenine were dissolved in hot water. Upon cooling and evaporating to dryness at room temperature, good crystals were obtained in the form of monoclinic needles with the needle axis parallel to the b crystallographic axis. Forms {001} and {100} predominated. The crystallographic data as determined from rotation and Weissenberg photographs are:

Systematic absences: $0k0$ absent for $k = 2n+1$

$a = 8·28 \pm 0·03$, $b = 6·51 \pm 0·03$, $c = 12·75 \pm 0·05$ Å;
$\beta = 106° 48' \pm 10'$.

Space group: $P2_1$ or $P2_1/m$.
Density: 1·433 g.cm.$^{-3}$ (meas.).