Acknowledgments.—This work was supported by a grant to C. J. H. from the Australian Research Grants Committee and in part by a grant to J. K. B. from the National Institutes of Health, GM 16168. We thank Professor Reilley for making his results available prior to publication.

CONTRIBUTION FROM ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS, AND THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF TEXAS, AUSTIN, TEXAS

A Neutron Diffraction Study of Uranyl Nitrate Dihydrate[1a]

BY N. KENT DALLEY,[1b] M. H. MUELLER,*,[1b] AND S. H. SIMONSEN[1c]

Received November 24, 1969

The crystal structure of uranyl nitrate dihydrate, $UO_2(H_2O)_2(NO_3)_2$, has been determined by neutron diffraction. The structure is monoclinic with a = 14.124 (13), b = 8.432 (8), c = 7.028 (7) Å, β = 108.0 (1)°, and space group $P2_1/c$ with 4 formula weights per unit cell. This is in disagreement with a previously reported X-ray study. In the present study the structure was solved with three-dimensional data by applying Patterson and Fourier techniques. The four uranium atoms per unit cell are located on special positions (a) and (b) of the space group. Each uranyl group is surrounded by a nearly perpendicular planar oxygen hexagon. This hexagon consists of two oxygen atoms from each of two equivalent bidentate nitrate groups and two oxygen atoms from equivalent water molecules. This arrangement is similar to that reported for the uranyl nitrate hexahydrate. The structural units are bound together by hydrogen bonds from the oxygen of the water molecule to the uncoordinated oxygen atom of the nitrate group and to the oxygen atom of the uranyl group.

Introduction

An X-ray diffraction study of $UO_2(H_2O)_2(NO_3)_2$ has been reported by Vdovenko, *et al.*,[2] but the U–O bond lengths they reported are not in agreement with the lengths of similar bonds found in other compounds. Table I lists the U–O distances determined by Vdovenko, *et al.*,[2] in $UO_2(H_2O)_2(NO_3)_2$, by Taylor and Mueller[3] in a neutron investigation of $[UO_2(H_2O)_2(NO_3)_2]\cdot 4H_2O$, and by Zachariasen and Plettinger[4] in an X-ray study of $Na[UO_2(C_2H_3O_2)_3]$. Since all three compounds exhibit sixfold oxygen coordination about the linear uranyl ion, the chemically similar bonds should be about equal in length.

TABLE I

U–O BOND DISTANCES[a] FOUND IN SIXFOLD-COORDINATED URANYL ION COMPLEXES (Å)

Bond type	Vdovenko[2] $UO_2(H_2O)_2(NO_3)_2$	Taylor and Mueller[3] $[UO_2(H_2O)_2(NO_3)_2]\cdot 4H_2O$	Zachariasen and Plettinger[4] $Na[UO_2(C_2H_3O_2)_3]$
U–O (uranyl)	1.9 (1)	1.770 (7)	1.74 (4)
		1.749 (7)	1.70 (4)
U–O (ligand)	2.0 (1)	2.504 (5)	2.47 (2)
	2.1 (1)	2.547 (6)	2.51 (2)
		2.397 (3)	

[a] Values in parentheses are standard errors that occur in the last recorded decimal place. (This system will be used throughout the paper.)

The present neutron study of $UO_2(H_2O)_2(NO_3)_2$ was instigated in order to (1) determine if the differences revealed in Table I are real and (2) obtain the positions of all atoms in the complex, including hydrogen atoms, and thereby ascertain the role of the hydrogen bonding in the compound.

Experimental Section

Large flat crystals of uranyl nitrate dihydrate were grown in a uranyl nitrate–nitric acid–water solution with the following composition (by weight): 28.8% uranyl nitrate, 54.5% nitric acid, and 16.7% water. This composition is dictated by the phase diagram established by Gaunt, *et al.*[5] Two samples were analyzed by the Karl Fischer method, which established the water content in the samples to be 8.44 and 9.20%. The analysis clearly showed the material was the dihydrate because the calculated water content is 8.34% for the dihydrate and 12.05% for the trihydrate. One of the analyzed samples was stored in a desiccator, and the other was exposed to humid air prior to the titration, which may account for the difference in percentages of water content. Therefore, some protection for the crystal was considered necessary during data collection.

A crystal, 10.5 × 5.1 × 4.8 mm (approximately a parallelepiped), weighing 0.740 g, was coated with a thin layer of silicone oil, encapsulated in a vanadium can, and mounted on the Argonne automated four-circle diffractometer along a nonmajor axis. A beam of neutrons with a wavelength of 1.063 Å was produced making use of the (110) plane of a beryllium single crystal to monochromate the beam. The wavelength was obtained by measuring several known reflections of a standard sodium chloride crystal and calculating the wavelength by a least-squares technique. Preliminary investigation of the reciprocal lattice revealed monoclinic symmetry with the following systematic extinctions: $h0l$, $l = 2n + 1$, and $0k0$, $k = 2n + 1$. These data uniquely determined the space group as $P2_1/c$. Lattice parameters were obtained at the room temperature, 25 ± 3°, from neutron diffractometer measurements of 15 reflections. Results from a least-squares refinement, using a computer program written by Heaton and Gvildys,[6] were a = 14.124 (13), b = 8.432 (8), c =

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* To whom correspondence should be addressed.

(1) (a) Research supported by the U. S. Atomic Energy Commission. (b) Argonne National Laboratory. (c) University of Texas.

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TABLE II

POSITIONAL AND THERMAL[a] PARAMETERS ($\times 10^4$) FOR $UO_2(H_2O)_2(NO_3)_2$

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
U(1)	0	0	0	19 (1)	52 (2)	84 (2)	−1 (1)	14 (1)	−2 (2)
O(1)	−367 (1)	1994 (2)	−165 (3)	36 (1)	62 (2)	159 (4)	6 (1)	31 (1)	4 (2)
N(1)	1692 (1)	790 (1)	3546 (2)	24 (1)	72 (1)	114 (2)	−4 (1)	15 (1)	−3 (1)
O(11)	858 (1)	339 (3)	3682 (2)	27 (1)	105 (3)	105 (3)	−8 (1)	21 (1)	−8 (2)
O(12)	2369 (1)	1188 (3)	5009 (3)	30 (1)	146 (4)	130 (3)	−19 (2)	12 (1)	−29 (3)
O(13)	1755 (1)	822 (3)	1805 (3)	29 (1)	115 (3)	131 (3)	−13 (1)	25 (1)	−7 (3)
O(2)	1052 (1)	629 (2)	−2104 (2)	24 (1)	121 (3)	113 (3)	−1 (1)	24 (1)	8 (2)
H(21)	1744 (3)	341 (7)	−1680 (8)	39 (2)	203 (8)	257 (10)	17 (3)	38 (4)	22 (8)
H(22)	837 (3)	582 (8)	−3526 (6)	53 (2)	261 (11)	152 (7)	−26 (4)	30 (3)	1 (7)
U(2)	5000	5000	5000	21 (1)	52 (2)	120 (3)	−1 (1)	19 (1)	1 (2)
O(3)	5047 (1)	4958 (3)	7535 (3)	40 (1)	100 (3)	130 (3)	−3 (1)	29 (1)	5 (3)
N(2)	6872 (1)	3243 (1)	5799 (2)	26 (1)	73 (1)	225 (3)	4 (1)	24 (1)	−4 (2)
O(21)	6841 (1)	4756 (2)	5803 (4)	25 (1)	73 (2)	231 (5)	−4 (1)	26 (1)	−12 (3)
O(22)	7627 (2)	2532 (4)	5998 (7)	35 (1)	115 (4)	561 (15)	19 (2)	60 (3)	5 (6)
O(23)	6039 (1)	2574 (3)	5539 (4)	30 (1)	70 (2)	303 (7)	−2 (1)	31 (2)	−1 (3)
O(4)	4088 (1)	2485 (2)	4331 (4)	30 (1)	62 (3)	250 (5)	−7 (1)	35 (2)	−5 (3)
H(41)	3453 (3)	2201 (6)	4468 (9)	41 (2)	143 (6)	364 (14)	−16 (3)	56 (4)	−16 (8)
H(42)	4413 (4)	1536 (6)	4267 (15)	56 (3)	97 (7)	719 (33)	1 (4)	74 (8)	−14 (11)

[a] The thermal parameters are of the form: $T = \exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$.

7.028 (7) Å, and β = 108.0 (1)°. The observed density, measured by a volume displacement procedure, was 3.5 g/cm^3 and the calculated density, assuming four formula weights per unit cell, was 3.6 g/cm^3. Obviously this crystal was a different modification from that of Vdovenko, *et al.*,[2] who reported the crystal to be of space group C_m, with a = 10.52 (3), b = 5.93 (3), c = 6.95 (2) Å, β = 72.0 (5)°, and Z = 2 formula weights per unit cell.

Integrated intensities were measured on the automated diffractometer using a θ–2θ step scan mode, with a step interval of 0.1°. The counting time on each step was regulated by a fission counter in order to compensate for the fluctuation of the neutron beam. The takeoff angle of 55° gave the best resolution near a 2θ angle of 55°. Reflections with 2θ values below 15° and above 90° were scanned in 50 steps or 2.5° while reflections between these limits were scanned in 40 steps or 2.0°. Scans required from 13 to 15 min. Backgrounds were measured for each reflection at both the beginning and the end of a scan with the time of each background reading being equivalent to five steps of a scan. The total background counting time for each reflection amounted to about 3 min. A 1-in. diamater Reuter–Stoakes BF_3 counter with active length of 6 in. was used as a detector. Each reflection was recorded on a strip chart and was checked to see that adequate resolution was maintained and that there were no counting irregularities. When irregularities from electronic noise were observed, the data were retaken. No resolution problems were encountered. Two standard reflections were checked every 25 reflections. No drift in the electronics or change in orientation of the crystal was observed throughout the data collection period. A total of 2050 reflections was systematically collected out to a $(\sin \theta)/\lambda$ limit of 0.67 (d = 0.75 Å). An additional 271 reflections were collected beyond that limit, but because the intensities were small, data collection was terminated. These 2321 independent reflections were used in the structure analysis with a resulting observation:variable parameter ratio of about 15:1. These data were scaled to nearly absolute values by comparison with the (400) reflection from a standard sodium chloride crystal. Absorption corrections were applied to the observed intensities using the ORABS program,[7] μ_{obsd} = 1.08 cm^{-1}. The calculated transmission factors varied from 0.48 to 0.63 because of the difference in path length.

Solution and Refinement of the Structure

A three-dimensional Patterson map revealed uranium atoms on centers of inversion at special positions (a) and (b) of space group $P2_1/c$. A molecule with the uranium atom U(1) at site (a) will be designated molecule I and a molecule with the uranium atom U(2) at site (b) will be called molecule II.

The vectors from the uranium atom to the atoms of the nitrate group of molecule I were obvious in the y = 0 level of the Patterson map. A peak located about 1.8 Å from the origin almost directly along the y direction was identified as a uranium–uranyl oxygen vector. The position for the uranyl oxygen of molecule II was also determined from the Patterson map.

Structure factors were calculated with the Busing, Martin, and Levy least-squares program[8] with the positional parameters found in the Patterson map for the uranium, uranyl oxygen, and the atoms of the nitrate group of molecule I, and, in addition, the uranium and uranyl oxygen atoms of molecule II. Isotropic temperature factors similar to those found in the hexahydrate study[3] were assigned. The neutron scattering amplitudes used were as follows: $b_N = 0.94$, $b_U = 0.85$, $b_O = 0.577$, and $b_H = -0.37$ (all $\times 10^{-12}$ cm/atom).[9] An F_o Fourier map phased by these atoms revealed the positions of the remainder of the nonhydrogen atoms. The next Fourier map revealed the positions of the hydrogen atoms.

Refinement was carried out with unit weights and isotropic temperature factors by using the full-matrix least-squares program of Busing, *et al.*, to an R value of 15% where

$$R = \frac{\sum |F_o - s_q F_c|}{\sum |F_o|}$$

where s_q is the scale factor. By including anisotropic temperature factors and a weighting scheme similar to

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[7] D. J. Wehe, W. R. Busing, and H. A. Levy, "A Fortran Program for Calculating Single Crystal Absorption Corrections," Report No. ORNL-TM-229, U. S. Atomic Energy Commission, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962.

[8] W. R. Busing, K. O. Martin, and H. A. Levy, "A Fortran Crystallographic Least-Squares Program," Report No. ORNL-TM-305, U. S. Atomic Energy Commission, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962.

[9] "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1962, p 229.

that used by Corfield, Doedens, and Ibers[10] ($p = 0.03$) an R value of 8.1% and R_w of 6.4% was obtained where

$$R_w = \sqrt{\frac{\sum(wF_o - s_qF_c)^2}{\sum wF_o^2}}$$

A total of 145 reflections, with $|F_o| < \sigma|F_o|$, were not used in the refinement. Only one of these reflections had an F_c greater than $2\sigma|F_o|$. Approximately 37 reflections appeared to be strongly affected by extinction. An additional two cycles were carried out including an isotropic extinction parameter with the LINUS program.[11] The following results were obtained: $R = 6.6\%$; $R_w = 7.4\%$; $g' = 0.35$ (2); $\eta = 16.6''$. All shifts in positional parameters were considerably less than one standard deviation. At the conclusion of the refinement a unit weight of 0.2 was obtained, which suggested a slightly smaller p value possibly should have been used in the weighting. The final parameters are listed in Table II. A difference Fourier map calculated using these parameters was featureless, which substantiated the model. Bond lengths and angles calculated with the ORFFE program[12] are listed in Table III, and the calculated and observed structure factors are given in Table IV.

TABLE III

INTERATOMIC DISTANCES (Å) AND ANGLES (DEG) IN $UO_2(H_2O)_2(NO_3)_2$

Distances

U–O (Uranyl)		N–O (Nitrate Groups)	
U(1)–O(1)	1.754 (4)	N(1)–O(11)	1.269 (4)
U(2)–O(3)	1.763 (5)	N(1)–O(12)	1.213 (4)
		N(1)–O(13)	1.253 (4)
U–O (Coordination)		N(2)–O(21)	1.275 (5)
U(1)–O(2)	2.457 (4)	N(2)–O(22)	1.190 (5)
U(1)–O(11)	2.513 (5)	N(2)–O(23)	1.262 (4)
U(1)–O(13)	2.508 (4)		
U(2)–O(4)	2.446 (4)	**O–H (Water)**	
U(2)–O(21)	2.491 (5)	O(2)–H(21)	0.957 (8)
U(2)–O(23)	2.477 (5)	O(2)–H(22)	0.956 (8)
		O(4)–H(41)	0.960 (8)
O–O (Contacts in Hexagon)		O(4)–H(42)	0.931 (10)
O(11)–O(13)	2.131 (5)		
O(13)–O(2)	2.621 (6)	**O–O (Possible H Bonds)**	
O(11)–O(2)	2.710 (5)	O(4)–O(12)	2.833 (6)
O(21)–O(23)	2.132 (5)	O(4)–O(3)	2.959 (6)
O(21)–O(4)	2.654 (6)	O(2)–O(22)	3.160 (7)
O(23)–O(4)	2.625 (6)	O(2)–O(1)	3.164 (6)

Angles

In Nitrate Groups		In Water	
O(13)–N(1)–O(12)	123.0 (3)	H(21)–O(2)–H(22)	105.4 (8)
O(12)–N(1)–O(11)	121.7 (3)	H(41)–O(4)–H(42)	106.0 (9)
O(11)–N(1)–O(13)	115.3 (3)		
O(23)–N(2)–O(22)	123.5 (4)	**In Possible Hydrogen Bonds**	
O(22)–N(2)–O(21)	122.1 (4)	O(2)–H(21)···O(22)	124.7 (8)
O(21)–N(2)–O(23)	114.4 (3)	O(2)–H(22)···O(1)	111.5 (8)
		O(4)–H(41)···O(12)	166.2 (8)
		O(4)–H(42)···O(3)	146.3 (1.4)

Discussion of the Structure

The coordination of the uranium atom is shown in Figure 1. Two uranyl oxygen atoms together with the uranium atom form a linear group that is perpendicular to the nearly planar hexagon formed by the six other oxygen atoms. The hexagon is composed of four oxygen atoms from the two equivalent bidentate nitrate groups and two oxygen atoms from the equivalent water molecules. Such a coordination was proposed by Jezowska-Trzebiatowska, *et al.*,[13] from their infrared investigation of uranyl nitrate dihydrate and is identical to the basic coordination found in the hexahydrate. The infrared study also indicated that no evidence existed for loosely bound water molecules outside the first coordination sphere and that the nitrate groups were bidentate since their symmetry was C_{2v}. Both structural features were substantiated by our diffraction study.

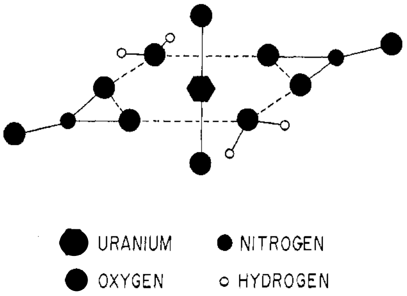

Figure 1.—The coordination of the uranium atom in $UO_2(H_2O)_2(NO_3)_2$.

The U–O bond lengths of the crystallographic nonequivalent molecules I and II are listed in Table IV; there is good agreement between these values and similar U–O bond lengths determined by Taylor and Mueller[3] and by Zachariasen and Plettinger,[4] as listed in Table I. The bond lengths reported by Vdovenko, *et al.*,[2] are very different from those found in the present investigation.

The hexagonal planes of the oxygen atoms in molecules I and II are nearly perpendicular to each other. Equations of least-squares planes for the hexagons and the deviations of the atoms from these planes are listed in Table V. These results were calculated by using the program of Norment.[14] The dihedral angle between the planes is 85°.

The O(4)–H(42) bond length in Table III appears to be unusually short. This is most likely caused by the large thermal motion of the H(42) atom[15] (see Table II). When corrections for thermal motion were made using the riding model the following bond lengths (Å) were calculated: O(2)–H(21), 0.992 (9); O(2)–H(22), 0.997 (9); O(4)–H(41), 0.993 (14); O(4)–H(42), 0.988 (10).

Nitrate Groups.—Bond lengths and angles found in the nitrate groups are shown in Table III. In both nonequivalent nitrate groups, the nitrogen–uncoordinated oxygen bonds are considerably shorter

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(11) P. Coppens and W. C. Hamilton, *Acta Crystallogr., Sect. A*, **26**, 71 (1970).

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TABLE IV

OBSERVED AND CALCULATED STRUCTURE FACTORS ($\times 10^2$)

H	K	FO	FC
** H K 0 **			
0	2	360	342
0	4	865	889
0	6	208	198
0	8	276	252
0	10	201	195
-1	1	367	362
-1	2	136	123
-1	3	1024	1002
-1	4	580	587
-1	5	116	116
-1	6	128	134
-1	7	422	451
-1	8	573	573
-1	9	306	316
-1	10	157	142
-1	11	112	101
-2	0	158	152
-2	1	712	679
-2	2	411	416
-2	3	671	653
-2	4	960	960
-2	5	288	273
-2	6	450	461
-2	7	231	238
-2	8	350	349
-2	9	135	127
-2	10	332	328
-2	11	122	132
-3	0	112	106
-3	1	047	004
-3	2	582	554
-3	3	136	127
-3	4	200	196
-3	5	518	527
-3	6	715	741
-3	8	093	068
-3	9	223	223
-3	10	129	118
-3	11	132	125
-4	0	404	400
-4	1	737	721
-4	2	223	210
-4	3	216	205
-4	4	340	343
-4	6	711	724
-4	7	068	080
-4	8	392	393
-4	9	420	432
-4	10	468	476
-5	0	084	095
-5	1	208	208
-5	2	913	872
-5	3	153	162
-5	4	043	050
-5	5	139	149
-5	6	1113	1083
-5	7	161	171
-5	8	286	276
-5	9	346	347
-5	10	150	138
-6	0	384	397
-6	1	061	062
-6	2	1047	1025
-6	3	357	349
-6	4	282	272
-6	5	398	406
-6	6	753	743
-6	7	205	203
-6	8	294	289
-6	9	112	094
-6	10	601	611
-7	0	056	009
-7	1	362	364
-7	2	349	344
-7	3	031	009
-7	4	081	070
-7	5	262	275
-7	6	344	345
-7	7	742	730
-7	8	181	185
-7	9	172	163
-7	10	034	015
-8	0	192	192
-8	1	125	122
-8	2	195	204
-8	3	025	029
-8	4	484	474
-8	5	169	173
-8	6	083	085
-8	7	358	358
-8	8	742	730
-8	9	305	085
-8	10	075	055
-9	0	361	371
-9	1	138	131
-9	2	165	151
-9	3	293	288
-9	4	079	068
-9	5	504	500
-9	6	366	362
-9	7	232	226
-9	8	057	041
-9	9	012	009
-10	0	1024	998
-10	1	452	453
-10	2	297	291
-10	3	214	210
-10	4	760	758
-10	5	173	167
-10	6	422	427
-10	7	274	266
-10	8	324	314
-10	9	254	266
-11	0	834	827
-11	1	202	207
-11	2	628	614
-11	3	213	207
-11	4	487	475
-11	5	030	010
-11	6	377	377
-11	7	056	044
-11	8	330	327
-12	0	939	931
-12	1	294	299
-12	2	534	556
-12	3	098	095
-12	4	310	307
-12	5	338	341
-12	6	114	118
-12	7	204	210
-12	8	350	343
-13	0	469	464
-13	1	129	130
-13	2	218	200
-13	3	541	541
-13	4	055	025
-13	5	138	132
-13	6	068	019
-13	7	191	181
-14	0	750	716
-14	1	095	108
-14	2	434	419
-14	3	448	434
-14	4	203	220
-14	5	071	049
-14	6	508	496
-15	0	668	662
-15	1	285	268
-15	2	261	250
-15	3	276	268
-15	4	190	198
-15	5	027	004
-15	6	075	105
-16	0	294	282
-16	1	238	234
-16	2	340	337
-16	3	399	390
-16	4	146	158
-17	0	147	138
-17	1	142	132
-17	2	145	139
-17	3	310	313
-18	0	194	202
-18	1	157	153
-18	2	358	362
-18	3	186	173
-19	0	082	065
-19	1	122	137
-19	2	109	098
-19	3	171	174
-20	0	102	104
-20	1	137	112
-20	2	057	073
-21	0	235	239
-21	1	012	051
** H K 1 **			
0	1	464	479
0	2	550	554
0	3	210	201
0	4	447	443
0	5	1007	1042
0	6	291	294
0	7	143	162
0	8	013	023
0	9	144	137
0	10	082	074
0	11	236	244
1	1	584	568
-1	1	060	037
1	2	401	382
-1	2	740	748
1	3	279	278
-1	3	216	211
1	4	224	223
-1	4	225	228
1	5	345	344
-1	5	417	422
1	6	184	178
-1	6	162	157
1	7	058	052
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-4	2	126	104
4	3	369	392
-4	3	214	187
4	4	097	081
-4	4	115	099
4	5	107	115
-4	5	414	410
-4	6	074	033
-4	7	070	025
5	1	172	195
-5	1	00	010
5	2	119	108
-5	2	196	194
5	3	103	105
-5	3	275	057
5	4	283	281
-5	4	083	090
-5	5	397	387
-5	6	108	103
-5	7	072	052
6	1	086	096
-6	1	173	179
6	2	049	018
-6	2	250	243
6	3	191	214
-6	3	254	225
6	4	292	271
-6	4	046	034
-6	5	212	213
-6	6	069	034
-6	7	229	215
7	1	216	203
-7	1	320	314
7	2	082	078
-7	2	077	022
7	3	025	018
-7	3	051	051
7	4	026	015
-7	4	061	059
-7	5	052	085
-7	6	054	059
-7	7	039	065
8	1	154	149
-8	1	565	554
8	2	00	054
-8	2	056	037
8	3	197	194
-8	3	231	233
8	4	106	096
-8	4	167	210
-8	5	325	317
-8	6	055	037
-8	7	026	063
9	1	059	001
-9	1	079	083
9	2	161	175
-9	2	049	007
9	3	00	030
-9	3	129	097
9	4	069	046
-9	4	399	391
-9	5	099	070
-9	6	00	031
10	1	157	136
-10	1	069	051
10	2	078	069
-10	2	177	152
10	3	149	140
-10	3	087	087
-10	4	255	268
-10	5	165	171
-10	6	128	127
-11	1	136	133
-11	2	053	033
-11	3	136	161
-11	4	00	024
-11	5	222	209
-11	6	101	125
-12	1	131	126
-12	2	324	327
-12	3	161	172
-12	4	036	055
-12	5	120	116
-13	1	078	026
-13	2	245	225
-13	3	188	159
-13	4	227	228
-13	5	174	166
-14	1	548	522
-14	2	088	097
-14	3	162	167
-14	4	084	064
-15	1	201	189
-15	2	00	019
-15	3	262	256
-16	1	00	007
-16	2	250	260
-16	3	268	262
-17	1	00	044
-17	2	098	118
-17	3	128	124
-18	1	119	082
-18	2	186	185
-18	3	182	208
-19	1	00	023
-19	2	084	046
-20	1	221	226
-20	2	143	152
-21	1	026	029
** H K 8 **			
0	0	324	341
0	1	136	142
0	2	339	352
0	3	072	054
0	4	186	195
1	0	084	064
-1	0	198	189
1	1	00	033
-1	1	184	181
1	2	073	053
-1	2	198	168
1	3	088	101
-1	3	070	060
1	4	063	011
-1	4	135	116
-1	5	056	006
2	0	362	367
-2	0	183	184
2	1	045	020
-2	1	102	067
2	2	281	302
-2	2	250	255
2	3	088	078
-2	3	00	023
2	4	295	294
-2	4	384	374
-2	5	046	050
3	0	115	125
-3	0	193	180
3	1	140	159
-3	1	093	074
3	2	072	063
3	3	062	046
-3	3	085	093
3	4	061	034
-3	4	103	104
-3	5	355	322
4	0	170	169
-4	0	729	705
4	1	045	028
-4	1	115	101
4	2	179	157
-4	2	155	144
4	3	075	045
-4	3	079	070
4	4	175	184
-4	4	184	179
-4	5	106	078
5	0	063	059
-5	0	050	024
5	1	041	007
-5	1	092	076
5	2	051	022
-5	2	142	126
5	3	00	023
-5	3	226	221
5	4	112	108
-5	4	273	269
-5	5	00	028
6	0	184	178
-6	0	141	121
6	1	138	126
-6	1	082	074
6	2	170	154
-6	2	049	046
6	3	043	044
-6	3	153	165
6	4	226	225
-6	4	380	382
-6	5	086	085
7	0	169	144
-7	0	270	241
7	1	078	044
-7	1	040	010
7	2	081	058
-7	2	221	215
7	3	00	037
-7	3	00	001
-7	4	073	039
-7	5	00	00
8	0	308	293
-8	0	356	346
8	1	047	030
-8	1	302	292
8	2	210	214
-8	2	190	179
-8	3	097	079
-8	4	235	239
-8	5	050	088
-9	0	063	073
-9	1	089	085
-9	2	210	195
-9	3	178	168
-9	4	061	055
-9	5	132	125
-10	0	361	344
-10	1	054	073
-10	2	472	481
-10	3	037	016
-10	4	277	278
-11	0	301	275
-11	1	160	165
-11	2	056	051
-11	3	00	061
-11	4	065	084
-12	0	362	357
-12	1	136	133
-12	2	497	498
-12	3	109	085
-13	0	032	015
-13	1	113	094
-13	2	082	075
-13	3	197	226
-14	0	314	312
-14	1	065	072
-14	2	227	218
-14	3	185	184
-15	0	459	461
-15	1	172	159
-15	2	114	095
-15	3	096	144
-16	0	071	032
-16	1	059	093
-16	2	139	135
-16	3	085	051
-17	0	105	099
-17	1	079	016
-17	2	043	080
-17	3	053	023
-18	0	074	033
-18	1	00	047
-18	2	114	120
-19	0	312	313
-19	1	105	066
-19	2	00	031
-20	0	168	195
-20	1	044	085
** H K 9 **			
0	1	103	099
0	2	094	082
0	3	161	159
0	4	272	272
1	1	168	139
-1	1	290	279
1	2	065	052
-1	2	171	163
1	3	041	011
-1	3	063	017
1	4	172	181
-1	4	175	153
2	1	028	006
-2	1	408	400
2	2	008	024
-2	2	047	029
2	3	052	050
-2	3	132	133
2	4	091	101
-2	4	043	006
3	1	118	130
-3	1	177	180
3	2	083	072
-3	2	279	263
3	3	085	080
-3	3	088	067
3	4	037	009
-3	4	115	091
4	1	055	071
-4	1	254	229
4	2	002	086
-4	2	142	148
4	3	102	109
-4	3	155	167
-4	4	145	130
-5	1	057	031
-5	2	100	092
-5	3	052	029
-6	1	129	138
-6	2	073	043
-6	3	136	105
-6	4	025	008
-7	1	132	118
-7	2	054	043
-7	3	118	113
-7	4	00	039
-8	1	132	103
-8	2	062	051
-8	3	105	072
-8	4	121	119
-9	1	200	188
-9	2	021	031
-9	3	089	043
-9	4	115	109
-10	1	135	135
-10	2	069	040
-10	3	083	042
-11	1	121	001
-11	2	144	114
-11	3	061	066
-12	1	117	092
-12	2	067	089
-12	3	190	245
-13	1	028	080
-13	2	044	030
-13	3	123	096
-14	1	331	314
-14	2	219	071
-14	3	175	183
-15	1	00	029
-15	2	00	042
-15	3	021	060
-16	1	108	086
-17	1	058	036
-17	2	080	082
-18	1	097	130
-18	2	139	150
** H K 10 **			
0	0	128	121
0	1	134	141
0	2	075	048
-1	0	067	041
-1	1	082	095
-1	2	057	068
-1	3	076	077
-1	4	095	114
-2	0	227	199
-2	1	047	024
-2	2	048	063
-2	3	051	033
-3	0	078	090
-3	1	009	009
-3	2	071	045
-3	3	111	108
-4	0	250	244
-4	1	035	003
-4	2	028	012
-4	3	073	030
-5	1	032	009
-5	2	061	028
-5	3	135	125
-5	4	071	044
-6	1	068	071
-6	2	080	069
-6	3	00	008
-6	4	193	226
-7	1	146	154
-7	2	097	083
-7	4	182	202
-8	0	284	287
-8	1	238	221
-8	2	129	122
-8	3	218	221
-8	4	102	110
-9	0	453	434
-9	1	117	011
-9	2	278	285
-9	3	00	022
-9	4	076	051
-10	0	398	378
-10	1	045	035
-10	2	240	249
-10	3	210	248
-11	0	078	110
-11	1	048	035
-11	2	057	064
-11	3	245	263
-12	0	245	243
-12	1	00	08
-12	2	00	049
-13	0	144	126
-13	1	031	008
-13	2	142	115
-14	0	128	123
-14	1	141	138
-14	2	085	034
-15	0	062	049
-15	1	099	128
-15	2	093	098
-16	0	160	186
-16	1	00	012
-16	2	109	150
** H K 11 **			
-1	1	00	010
-2	1	00	013
-2	2	088	079
-3	1	106	100
-3	2	036	004
-4	1	075	099
-4	2	129	158
-5	1	081	099
-5	2	106	148
-6	2	065	055
-7	1	058	075
-7	2	127	141
-8	1	00	047
-8	2	00	058
-9	1	110	109
-9	2	072	085
-10	1	164	191
-10	2	118	159
-11	1	130	149
-11	2	00	058
-12	1	104	152

than the nitrogen–coordinated oxygen bonds. Also, the coordinated oxygen–nitrogen–coordinated oxygen angles are smaller in both nonequivalent nitrate groups than the angles involving coordinated oxygen–nitrogen–uncoordinated oxygen. This is in agreement with other studies of compounds with bidentate nitrate groups (see Table VI). The observation that the N–O uncoordinated bond length in molecule II is shorter than in molecule I will be discussed in connection with the hydrogen bonding. Equations were calculated for the least-squares planes of both nonequivalent nitrate groups. The groups are planar within ±0.006 Å, which is within the limits of error of the data.

Hydrogen Bonding.—The O–O distances and O–H–O angles are listed in Table III and identified in Figure 2.[16] These results indicate that the water hydrogen atoms in molecule I are not involved in hydrogen bonding.

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[16] C. K. Johnson, "A Fortran Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations," Report No. ORNL-3794, U. S. Atomic Energy Commission, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1965.

TABLE V

LEAST-SQUARES PLANES OF URANIUM AND THE HEXAGONS OF MOLECULES I AND II

Equations of Planes

Molecule I $-4.0957x + 7.9902y - 0.2610z = 3.8646$

Molecule II $-3.5230x + 0.2918y - 7.0094z = 1.5973$

Deviations from Planes

Molecule I		Molecule II	
Atom	Dist from plane,[a] Å	Atom	Dist from plane,[a] Å
U(1)	0.0000	U(2)	0.0000
O(11)	0.0200	O(21)	0.0768
O(13)	0.0196	O(23)	0.0775
O(2)	0.0171	O(4)	0.0670

[a] Deviations stated in absolute values because U is at the center of inversion.

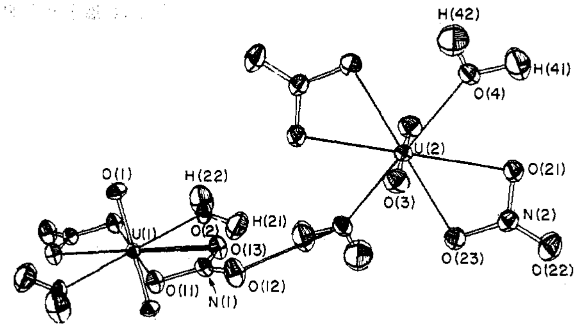

Figure 2.—Thermal motion and atom designations by means of the ORTEP program of Johnson.[16] This view is looking down the *c* axis.

TABLE VI

INTERATOMIC DISTANCES AND ANGLES[a] FOUND IN OTHER BIDENTATE NITRATE GROUPS

Compound	Distances, Å			Angles, deg		
	r_1	r_2	r_3	α_1	α_2	α_3
Uranyl nitrate dihydrate, $NO_3(1)$	1.269 (4)	1.253 (4)	1.213 (4)	121.7 (3)	123.0 (3)	115.3 (3)
$NO_3(2)$	1.275 (5)	1.262 (4)	1.190 (5)	122.1 (4)	123.5 (4)	114.4 (3)
Thorium nitrate pentahydrate,[b] $NO_3(1)$	1.250 (3)	1.270 (3)	1.202 (3)	123.2 (2)	121.7 (2)	115.2 (2)
$NO_3(2)$	1.264 (3)	1.275 (3)	1.206 (3)	123.0 (2)	122.5 (2)	114.5 (2)
Uranyl nitrate hexahydrate,[c] $NO_3(1)$	1.271 (4)	1.271 (4)	1.208 (8)	122.7 (2)	122.7 (2)	114.6 (5)
$NO_3(2)$	1.260 (4)	1.260 (4)	1.231 (7)	122.2 (2)	122.2 (2)	115.6 (5)
Rubidium uranyl nitrate,[d] $NO_3(1)$	1.26	1.26	1.21	121.2	121.2	117.5
Cerium magnesium nitrate hydrate,[e] $NO_3(1)$	1.259	1.268	1.220	122.8	121.2	116.1
$NO_3(2)$	1.262	1.257	1.225	120.8	121.8	117.4

[a] r_i and α_i are the distances and angles formed by the NO_3 group. The distances r_1 and r_2 and the included angle, α_3, are associated with the metal–oxygen bond. [b] J. C. Taylor, M. H. Mueller, and R. L. Hitterman, *Acta Crystallogr.*, **20,** 842 (1966). [c] J. C. Taylor and M. H. Mueller, *ibid.*, **19,** 536 (1965). [d] G. A. Barclay, T. M. Sabine, and J. C. Taylor, *ibid.*, **19,** 205 (1965). [e] A. Zalkin, J. D. Forrester, and D. H. Templeton, *J. Chem. Phys.*, **39,** 2881 (1963).

O(2)–O(1) and O(2)–O(22) are each at a distance of 3.162 (9) Å and their O–H–O angles deviate considerably from 180° (namely, 124 (1) and 111 (1)°). These values are highly unfavorable for hydrogen bonding.

The hydrogen atoms of molecule II, that is the hydrogen atoms of O(4), shown in Figure 3, participate in two distinctly different types of hydrogen bonds. The O(4)–H(41)···O(12) interaction involves the uncoordinated nitrate oxygen O(12) of molecule I. This is a medium-strength hydrogen bond as indicated by the O(4)–O(12) distance of 2.833 (6) Å. The O(4)–H(42)···O(3) bond of 2.959 (6) Å is weaker and involves the uranyl oxygen atom of molecule II, O(3). The stronger bond links a molecule I to a molecule II while the weaker bond joins a molecule II to a molecule II, as shown in Figure 3. In this manner the basic structural units are held together. The fact that neither of the hydrogen bonds is very strong probably accounts for the instability of the compound.

It is interesting to note in Figure 2 that the N–O bond of the uncoordinated oxygen of molecule II, N(2)–O(22), is shorter than the corresponding bond N(1)–O(12) of molecule I by 0.023 Å, which is approximately 4 times the standard error. The difference in the N–O distances perhaps can be correlated with the fact that O(12) is involved in hydrogen bonding while the O(22) is not. An alternative explanation is that the larger thermal motion (see Table VII) of the O(22) atom, which is partially a result of not being involved in hydrogen bonding, causes the N–O distance to appear shorter.[15]

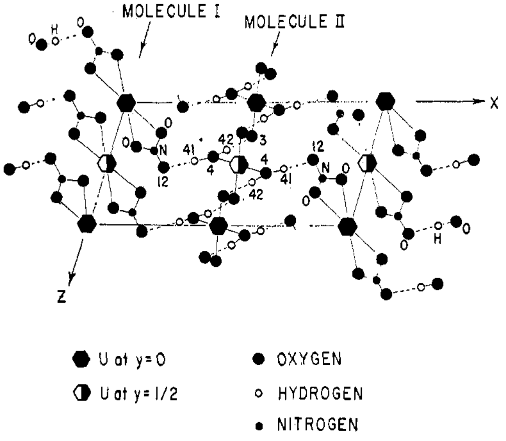

Figure 3.—The hydrogen-bonding network linking molecules I and II. Atoms not involved in the network are not shown.

Thermal Motion

The rms radial displacement and the rms components of displacement along the principal axes of the vibrational ellipsoids are listed in Table VII. The anisotropic motion of the atoms is also illustrated in Figure 2. The motion of the uranium atom is the smallest, and the motion of the other atoms is a function of their role in the intra- and intermolecular bonding, as expected. The thermal motion also illustrates that O(22) does not

TABLE VII

RMS RADIAL THERMAL DISPLACEMENTS AND COMPONENTS ALONG THE PRINCIPAL AXES R_1, R_2, AND R_3 OF THE VIBRATIONAL ELLIPSOIDS

Atom	Rms radial displacements, Å	Principal axes, Å		
		R_1	R_2	R_3
U(1)	0.228	0.124	0.132	0.138
U(2)	0.245	0.156	0.137	0.159
O(1)	0.293	0.136	0.174	0.193
O(3)	0.311	0.160	0.185	0.192
N(1)	0.263	0.138	0.155	0.162
O(11)	0.284	0.140	0.153	0.194
O(12)	0.327	0.140	0.179	0.235
O(13)	0.299	0.142	0.163	0.207
N(2)	0.311	0.145	0.164	0.222
O(21)	0.309	0.138	0.156	0.229
O(22)	0.440	0.142	0.213	0.358
O(23)	0.343	0.152	0.160	0.262
O(2)	0.291	0.131	0.159	0.205
H(21)	0.400	0.180	0.237	0.268
H(22)	0.413	0.180	0.206	0.310
O(4)	0.314	0.131	0.166	0.233
H(41)	0.401	0.172	0.226	0.283
H(42)	0.493	0.182	0.212	0.406

participate in hydrogen bonding since it is much larger than the motion of the corresponding oxygen of the other molecule.

Conclusion

All attempts to resolve the differences between this study and the X-ray study of Vdovenko, *et al.*,[2] have failed. The neutron study does indicate a face-centered symmetry with respect to the uranium atoms, and the β angles are similar when the usual convention is applied to the X-ray results, but the large differences with respect to the unique "*b*" axis cannot be reconciled. Also, the bond lengths are considerably different. It must be concluded, in light of the neutron study, that the abnormal U–O distances found by Vdovenko, *et al.*,[2] are in error and that the correct distances for such a structure are near those predicted by Zachariasen and Plettinger.[4]

Acknowledgments.—We wish to thank Drs. L. Heaton and J. Taylor, Materials Science Division of Argonne National Laboratory, for assistance in this study and for helpful discussions. We also appreciate the technical and programming assistance of R. Hitterman and J. Gvildys of this Laboratory. Thanks are due to Dr. J. Ferraro of the Chemistry Division of ANL for helpful discussions of infrared studies of nitrate ligands and for his work in establishing the water content of the compounds.

CONTRIBUTION FROM THE RESEARCH DEPARTMENT,
MOBIL RESEARCH AND DEVELOPMENT CORPORATION, PAULSBORO LABORATORY, PAULSBORO, NEW JERSEY 08066

The Crystal and Molecular Structure of the Polymeric Complex Mercuric *O,O'*-Diisopropylphosphorodithioate, $Hg[(i\text{-}C_3H_7O)_2PS_2]_2$

BY STEPHEN L. LAWTON

Received March 9, 1970

Mercuric *O,O'*-diisopropylphosphorodithioate, $Hg[(i\text{-}C_3H_7O)_2PS_2]_2$, crystallizes in the monoclinic space group $C2/c$ with unit cell parameters $a = 31.70 \pm 0.02$, $b = 8.66 \pm 0.01$, $c = 22.34 \pm 0.01$ Å, and $\beta = 129.34 \pm 0.02°$. The observed and calculated densities are 1.74 ± 0.02 and 1.758 ± 0.004 g/cm^3 (for $Z = 8$ molecules/unit cell), respectively. The structure was refined by least-squares methods to a final conventional R index of 0.057 using three-dimensional X-ray diffraction counter data. Unlike the zinc(II) and cadmium(II) *O,O'*-diisopropylphosphorodithioate complexes which exist as dimers, this complex polymerizes into helical chains around the unit cell twofold screw axis aligned parallel with the crystal needle axis. One of the $(RO)_2PS_2$ groups functions as a chelating group and the other as a bridging group linking two mercury atoms together. Each mercury atom is surrounded by five sulfur atoms: two at relatively short distances of 2.388 ± 0.005 and 2.391 ± 0.006 Å, two at intermediate distances of 2.748 ± 0.005 (the polymeric bridge) and 2.888 ± 0.005 Å, and one making a van der Waals contact at 3.408 ± 0.006 Å. The –S–Hg–S– angle involving the two short Hg–S bonds is $149.7 \pm 0.2°$. There are no Hg–S interactions with neighboring chains. The P–S bonds within each ligand are unequal in length, averaging 2.01 ± 0.01 and 1.94 ± 0.01 Å; sulfur atoms forming the shorter bonds are associated with the longer (and weaker) Hg–S interactions. The P–O bonds within the nonbridging ligand average 1.62 ± 0.03 Å and those within the bridging ligand average 1.54 ± 0.02 Å.

Introduction

Recently the structures of zinc *O,O'*-diisopropylphosphorodithioate, $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$, and of cadmium *O,O'*-diisopropylphosphorodithioate, $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$, were reported.[1] These two complexes were found to exist in the crystalline state as isomorphous dimers in which each metal atom is coordinated with four sulfur atoms in a somewhat distorted tetrahedral environment. The two phosphorodithioate groups per metal were found to serve two independent functions: one acting as a chelating group and the other as a bridging group linking two metal atoms together to form the dimer. The four phosphorus–sulfur bonds were found to be essentially equivalent.

It is well known that mercury, the third member of

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[1] S. L. Lawton and G. T. Kokotailo, *Inorg. Chem.*, **8**, 2410 (1969).