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Chemistry of the Uranyl Group. III. Preparation, Properties, and Crystal Structure of the Isomorphous Pair $UO_2((C_2H_5)_2NCS_2)_2(C_6H_5)_3AsO$ and $UO_2((C_2H_5)_2NCS_2)_2(C_6H_5)_3PO$

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Two monomeric complexes of formula $UO_2((C_2H_5)_2NCS_2)_2 \cdot L$ with L = $(C_6H_5)_3AsO$ and $(C_6H_5)_3PO$ were synthesized from $K\{UO_2((C_2H_5)_2NCS)_3\} \cdot H_2O$ and triphenylarsine and triphenylphosphine oxides, respectively. Infrared and electronic spectra are reported. The crystals are isomorphous and monoclinic and belong to space group $P2_1/n$, with $Z = 4$. Cell dimensions are $a = 18.28 \pm 0.01$, $b = 9.128 \pm 0.005$, $c = 20.95 \pm 0.01$ Å, and $\beta = 111° 18' \pm 10'$ for $UO_2((C_2H_5)_2NCS_2)_2(C_6H_5)_3AsO$ and $a = 18.32 \pm 0.01$, $b = 9.16 \pm 0.01$, $c = 20.97 \pm 0.01$ Å, and $\beta = 111° 39' \pm 10'$ for $UO_2((C_2H_5)_2NCS_2)_2(C_6H_5)_3PO$. The structures have been solved by the heavy-atom method using three-dimensional film data and refined by least squares to final R values of 9.4 and 9.3% for the arsine and the phosphine analogs. The uranium atom is in a seven-coordinate, pentagonal-bipyramidal environment. The linear uranyl group is perpendicular to the plane which contains four sulfur atoms of two carbamate groups and the oxygen atom of the ligand at the corners of an irregular pentagon.

Introduction

The actinyl ions, as UO_2^{2+}, are typical Chatt–Ahrland A group ions and therefore have a weak tendency to form complexes with ligands of low electronegativity by addition to their equatorial plane. In contrast uranyl complexes with oxygen-containing ligands are very common, ligands as acetate or nitrate ions generally acting as bidentate chelating groups. Previous investigations[2] on mixed complexes of these ions with triphenylphosphine oxide or triphenylarsine oxide showed that monomeric or dimeric species are easy to obtain, and the oxygen-donor ionic ligands are bidentate. Proceeding in a planned program, we have turned our attention to a sulfur-containing ligand, less electronegative than the acetate, but with a similar skeleton. The diethyldithiocarbamate (DTC) ion is known to form stable complexes with UO_2^{2+} [3–5] and appears to be a good substrate for study of the effect of the introduced phosphine or arsine oxide and also to investigate the possible existence of dimeric entities. Therefore compounds of formula $UO_2(DTC)_2 \cdot (C_6H_5)_3PO$ and $UO_2(DTC)_2 \cdot (C_6H_5)_3AsO$ have been prepared and characterized by ir and uv spectroscopy and X-ray structural analysis.

Experimental Section

In order to prepare $UO_2(DTC)_2$ as starting material, the method of Jones, *et al.*,[6] was employed. However only the known[3] product $K[UO_2(DTC)_3] \cdot H_2O$ was obtained, analogous to those reported by Zil'berman and Peshchevitskii.[4] Recrystallizing $K[UO_2(DTC)_3] \cdot H_2O$ from hot ethyl alcohol yielded brilliant dark red crystals[6] but no evidence of solvated ethanol molecules arose from ir spectral measurements. Therefore the uranyl diethyldithiocarbamate complexes with triphenylphosphine or triphenylarsine oxide (L) were prepared according to the reaction

$$K[UO_2(DTC)_3] \cdot H_2O + L \longrightarrow UO_2(DTC)_2 \cdot L + KDTC + H_2O$$

Preparation of Potassium Tris(diethyldithiocarbamate)dioxouranium(VI) Monohydrate (A).—To a mixture of 1.8 ml (0.03 mol) of carbon disulfide and 8 ml of water containing 1.68 g (0.03 mol) of potassium hydroxide was added dropwise with stirring 3.1 ml (0.03 mol) of diethylamine in an ice bath. After 30 min a clear yellow solution of potassium diethyldithiocarbamate was obtained and added slowly to a solution of 4.24 g (0.01 mol) of uranyl acetate dihydrate in 150 ml of water. The color became dark red immediately and then $K[UO_2(DTC)_3] \cdot H_2O$ precipitated as a dark red powder. The compound was collected and washed with water and ether successively. Dried over $CaCl_2$ under vacuum, the complex decomposed at about 230°.

The ir spectrum showed that this product contains at least one water molecule of crystallization, with broad absorption at 3600–3400 and 1600–1550 cm^{-1}, respectively.

Anal. Calcd for $C_{15}H_{32}KN_3O_3S_6U$: C, 23.4; H, 4.1; N, 5.5; S, 24.9. Found: C, 23.9; H, 4.1; N, 5.7; S, 23.8.

Bis(diethyldithiocarbamate)dioxo(triphenylphosphine oxide)uranium(VI) (B).—A solution of 385 mg of potassium tris(diethyldithiocarbamate)dioxouranium(VI) monohydrate (0.5 m*M*) and 140 mg of triphenylphosphine oxide (0.5 m*M*) in 15 ml of acetone was stirred at room temperature for 20 min. On addition of 200 ml of water a yellow suspension was observed and the mixture was allowed to stand overnight. A red precipitate of B had formed, which was filtered by suction and dried over $CaCl_2$ under vacuum. The complex recrystallized from hot acetone as brilliant red crystals, mp 243–244° dec.

Anal. Calcd for $C_{28}H_{35}N_2O_3PS_4U$: C, 39.8; H, 4.1; N, 3.3; S, 15.1; U, 28.2. Found: C, 39.6; H, 4.3; N, 3.4; S, 15.3; U, 28.4.

Bis(diethyldithiocarbamate)dioxo(triphenylarsine oxide)uranium(VI) (C).—The preparative method was similar to that described above for B, using 160 mg of triphenylarsine oxide (0.5 m*M*). Compound C recrystallized from hot acetone as brilliant orange-red crystals, mp 231–232° dec.

Anal. Calcd for $C_{28}H_{35}AsN_2O_3S_4U$: C, 37.8; H, 3.9; N, 3.1; S, 14.4; U, 26.8. Found: 38.9; H, 3.8; N, 3.1; S, 14.6; U, 26.5.

From the ir spectra B and C appeared to be anhydrous complexes.

Compound C can be obtained also by addition of triphenylarsine oxide to a solution of B in *sym*-dichloroethane. This reaction appeared to be immediate from spectral measurements.

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[3] R. A. Zingaro, *J. Amer. Chem. Soc.*, **78**, 3568 (1956).

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TABLE I

SOME PHYSICAL DATA OF THE EXAMINED COMPOUNDS

Compound	Λ^a	$\nu_{as}(UO_2)^b$	ν(X–O) (X = P, As)^b	Band maxima^c
$K[UO_2(S_2CN(C_2H_5)_2)_3]\cdot H_2O$	55	888, 860	...	21.0 (1800), 26.3 (4000)
$UO_2(S_2CN(C_2H_5)_2)_2(C_6H_5)_3PO$	4	910, 905	1130, 1117 (P–O)	24.4 (2700), 30.5 (3400)
$UO_2(S_2CN(C_2H_5)_2)_2(C_6H_5)_3AsO$	6	901	880 sh, (As–O)	25.0 (2700), 31.2 sh (3900)

[a] Molar conductivity (cm^2 ohm^{-1} mol^{-1}) of 10^{-3} *M* solutions in nitromethane at 25°. [b] Infrared frequencies in cm^{-1}. [c] Position of bands in electronic spectrum in kK (= 1000 cm^{-1}); molar extinction coefficients are given in parentheses.

TABLE II

ATOMIC PARAMETERS OF $UO_2(DTC)_2(C_6H_5)_3AsO^a$

Atom	*x*	*y*	*z*	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
U	−397 (1)	1665 (2)	1888 (1)	22 (1)	88 (2)	24 (1)	4 (1)	9 (1)	5 (1)
As	1168 (2)	3036 (5)	3582 (2)	26 (1)	100 (8)	23 (1)	1 (3)	9 (1)	3 (2)
S(1)	−1300 (5)	506 (12)	2626 (5)	29 (4)	143 (19)	22 (3)	−5 (6)	10 (2)	3 (6)
S(2)	−1864 (6)	318 (15)	1118 (5)	27 (4)	216 (24)	28 (3)	−30 (8)	9 (3)	−3 (7)
S(3)	−575 (6)	1926 (14)	483 (5)	36 (4)	163 (21)	24 (3)	−12 (8)	8 (3)	9 (6)
S(4)	790 (6)	3139 (16)	1591 (5)	32 (4)	221 (25)	30 (3)	−19 (9)	8 (3)	9 (8)
O(1)	431 (14)	2266 (27)	2977 (11)	11 (10)	156 (45)	17 (7)	−24 (17)	−5 (8)	−18 (13)

Atom	*x*	*y*	*z*	*B*, Å^2	Atom	*x*	*y*	*z*	*B*, Å^2
O(2)	76 (18)	28 (36)	1948 (14)	5.5 (6)	C(13)	2895 (35)	1657 (75)	2834 (27)	7.9 (13)
O(3)	−871 (18)	3298 (38)	1839 (14)	5.2 (6)	C(14)	3415 (34)	2843 (63)	3065 (28)	7.4 (13)
N(1)	−2772 (19)	−65 (39)	1853 (15)	4.8 (7)	C(15)	3338 (34)	3859 (64)	3449 (28)	7.6 (13)
N(2)	643 (25)	3223 (51)	304 (20)	7.5 (9)	C(16)	2667 (32)	3979 (60)	3632 (26)	6.3 (12)
C(1)	−2033 (24)	258 (48)	1879 (20)	4.6 (8)	C(17)	1394 (35)	2282 (66)	4473 (29)	3.4 (13)
C(2)	332 (24)	2825 (45)	746 (20)	5.0 (9)	C(18)	2090 (27)	1836 (60)	4885 (22)	5.1 (10)
C(3)	−2967 (32)	−209 (62)	2484 (26)	7.2 (12)	C(19)	2218 (35)	1043 (66)	5441 (29)	7.6 (13)
C(4)	−3486 (41)	13 (83)	1215 (33)	10.8 (17)	C(20)	1596 (33)	696 (62)	5694 (27)	7.0 (12)
C(5)	354 (42)	2619 (79)	−410 (35)	11.6 (17)	C(21)	857 (36)	1097 (66)	5249 (29)	8.7 (14)
C(6)	1374 (30)	4176 (57)	525 (24)	6.3 (11)	C(22)	703 (30)	1860 (63)	4590 (24)	5.5 (11)
C(7)	−3155 (32)	1233 (61)	2736 (26)	7.0 (13)	C(23)	940 (25)	5024 (52)	3638 (20)	4.3 (8)
C(8)	−3485 (40)	−1424 (83)	970 (33)	12.5 (17)	C(24)	1247 (28)	5882 (56)	4249 (24)	4.9 (10)
C(9)	557 (40)	3471 (81)	−947 (32)	12.0 (16)	C(25)	1038 (32)	7411 (62)	4223 (27)	5.2 (11)
C(10)	2121 (33)	3106 (67)	727 (27)	9.8 (13)	C(26)	549 (32)	8025 (61)	3671 (27)	7.2 (12)
C(11)	2074 (26)	2932 (50)	3350 (21)	4.1 (9)	C(27)	236 (32)	7264 (57)	3050 (26)	5.3 (11)
C(12)	2219 (30)	1828 (66)	3009 (24)	6.6 (10)	C(28)	468 (31)	5765 (62)	3013 (26)	4.9 (12)

[a] Coordinates × 10^4. Standard deviations from the least-squares refinement in parentheses. Anisotropic thermal parameters are defined by $T = \exp\{-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)\}$, and each β_{ij} is multiplied by 10^4.

Physical Measurements.—Conductivities were determined on an LKB Model 3216-B conductivity bridge. Molecular weights were determined on a Mechrolab, Inc., Model 302 vapor pressure osmometer (25°). The ir spectra were recorded on a Perkin-Elmer Model 621 infrared spectrophotometer, using Nujol mulls between KBr plates. Spectra were recorded at room temperature using a Beckman Model DK2A spectrophotometer using quartz cells of 1-cm thickness. The results are summarized in Table I.

Crystal Structure of $UO_2(DTC)_2(C_6H_5)_3AsO$

Crystal Data.—Regular orange-red *b*-prismatic crystals of $UO_2(DTC)_2(C_6H_5)_3AsO$ were grown from acetone solutions. The density was measured by flotation in a mixture of *sym*-tetrabromoethane and *sym*-dichloroethane. Cell dimensions and space group were determined from precession photographs taken with Cu Kα radiation (λ 1.5418 Å). Systematic absences 0*k*0 with $k = 2n + 1$ and *h*0*l* with $h + l = 2n + l$ served to indicate the probable space group. Crystal data obtained are as follows: formula weight 888.85; monoclinic, space group $P2_1/n$; $a = 18.28 \pm 0.01$, $b = 9.128 \pm 0.005$, $c = 20.95 \pm 0.01$ Å; $\beta = 111° 18' \pm 10'$; $V = 3256$ Å^3; $D_m = 1.807$, $D_x = 1.812$ g cm^{-3}; μ(Cu Kα) = 211.6 cm^{-1}; $Z = 4$; $F(000) = 1720$. (The errors reported for the parameters of this compound, as well as for those of the following compound, are the standard deviations calculated from a series of measurements, the actual errors being probably larger.)

Intensity Data.—A single crystal of dimensions 0.1 × 0.55 × 0.2 mm elongated in the *b* direction was chosen for the X-ray work. The specimen was mounted about the long axis and a series of photographs was taken with a Buerger precession camera. From these the unit cell dimensions and the space group were derived (λ(Cu Kα) 1.5418 Å). The crystal was then aligned on a Weissenberg camera. With Cu Kα radiation a series of photographs of the layers $k = 0$–7 was taken by the multifilm equiinclination Weissenberg technique. A total of 2802 intensities were measured with the use of a Joyce and Loebl Flying Spot microdensitometer, the very weak being neglected. They were corrected for Lorentz and polarization factors and initially connected to a single scale by comparison with the *hk*0 and 0*kl* reflections, but separate scale factors for each layer were adjusted during the least-squares calculations.

Because of the appreciable linear absorption coefficient for Cu Kα radiation, absorption correction was applied as for a cylindrical specimen[7] asssuming $\mu R = 1.48$.

Accordingly the observed structure factors were

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(7) "International Tables for X-Ray Crystallography," Vol. II, The Kynoch Press, Birmingham, England, 1962.

TABLE III

OBSERVED AND CALCULATED STRUCTURE FACTORS (×10) OF $UO_2(DTC)_2(C_6H_5)_3AsO$

H,0,0		
4	434	275
6	608	-413
8	1352	-1278
10	1536	-1452
12	2803	-2520
14	1328	-1373
16	519*	-388
H,0,1		
3	2774	2787
-3	1874	1495
-5	496	-404
7	2073	1922
-7	3780	-3905
-9	2817	-2940
-11	948	-766
13	599	-617
15	871	-887
17	692	-851
19	796	-967
-19	778	839
-21	698	905
H,0,2		
2	1113	1101
-2	4628	-4231
4	1440	1340
6	1613	1259
-6	2816	-2393
8	1607	1366
-8	1226	-1019
10	2205	2001
-10	662	-526
12	2067	2104
-12	394*	630
-14	2254	2275
16	294*	-407
-16	1666	1700
-18	794	816
H,0,3		
-1	1010	-1125
3	2999	-3135
5	1768	-1738
-5	1628	-1434
7	1339	1169
-7	461	396
9	700	606
-9	2938	2797
-11	1726	1612
13	928	875
-13	654	493
15	1161	1019
-15	675	671
17	834	900
-17	667	580
-21	719	-810
H,0,4		
0	903	-1002
2	1310	-1241
-2	1836	1728
4	1192	-1078
-4	3390	3447
6	2119	-2210
-6	3354	3185
8	1947	-2071
-8	1935	1959
10	2011	-1981
-10	1289	1280
12	780	-642
-12	547	455
14	975	762
16	558	747
-16	1252	-1377
18	708	826
-18	1286	-1397
-20	729	-701
H,0,5		
1	3499	3945
-1	2018	1010
3	2137	2261
-3	822	853
5	1040	-837
-5	562	542
7	1238	-1191
-7	1890	1064
9	1287	-1247
-9	629	-664
11	1059	-1043
-11	1310	-1303
13	1215	-1089
-13	1304	-1146
-15	1119	-1024
19	371	510
-19	512	-502
H,0,6		
0	2124	2374
2	1958	2247
-2	1559	1739
4	3003	3198
-4	1122	-1359
6	1802	1853
-6	3979	-4053
8	1146	1072
-8	2793	-2930
-10	1316	-1120
12	966	-1001
-12	671	-599
14	593	-763
-14	935	-815
16	805	-891
18	566	-692
-18	1096	1071
-20	750	828
-22	313*	498
H,0,7		
1	1785	-1945
-1	1090	-1276
3	385*	632
-3	1749	-2094
5	2226	2282
-5	3210	-3369
7	1491	1352
-7	1491	-1354
9	1175	1065
-9	1429	-1507
11	959	899
13	732	699
-13	1356	1393
-15	1208	1183
17	726	-789
-17	1268	1312
-19	731	567
-21	313*	469
H,0,8		
0	2676	-3047
2	2573	-2414
-2	3199	-3372
4	2256	-2116
-4	2431	-2293
6	798	-783
-6	975	940
8	1037	936
-8	1536	1542
10	1876	1884
-10	1361	1337
12	995	959
-12	1510	1557
-14	1507	1500
-16	1352	1373
-20	564	-753
-22	530	-560
H,0,9		
1	2175	-2236
-1	506	-489
3	2474	-2649
-3	614	834
5	1195	-1100
-5	2571	2433
7	654	-618
-7	1281	1415
-9	1967	1859
-11	1655	1670
-15	874	-682
17	498	605
-17	816	-783
-19	830	-743
-21	590	-644
-23	446	-742
H,0,10		
0	643	733
2	619	714
-2	1449	1660
4	730	721
-4	3379	3629
-6	2127	2110
8	1613	-1590
10	1086	-1207
12	458	-494
-12	1203	-1072
14	486	-491
-14	1589	-1516
-16	1665	-1446
-18	1117	-1113
H,0,11		
1	2416	2741
-1	1550	1611
3	1416	1334
5	415*	265
-5	827	-832
7	527	600
-9	660	-478
11	495	-500
-11	1756	-1763
13	885	-750
-13	2099	-1962
-15	527	-438
-19	472*	333
-21	491	569
-23	517*	703
H,0,12		
0	600	-656
2	390*	246
-2	939	-1172
4	760	714
-4	1348	-1570
6	1979	1694
-6	2578	-2686
8	1302	1298
-8	1760	-1555
10	509	574
-10	485*	-267
-14	816	643
-16	533	442
-18	941	871
-20	1077	1060
-22	445	453
H,0,13		
1	1238	-1148
-1	2593	-2753
-3	1265	-1439
-5	470*	-334
9	806	772
11	1132	1036
-11	594	584
13	746	770
-13	2025	1980
-15	1191	1175
-17	418	380
H,0,14		
0	772	-735
2	1603	-1727
-2	534	600
4	2035	-1988
-4	832	726
6	1170	-1126
-6	1123	1147
-8	2468	2352
-10	1703	1500
-12	680	549
-20	920	-928
-22	768	-911
H,0,15		
1	798	-749
-1	1246	1298
3	607	-599
-3	1587	1908
5	617	-571
-5	2112	1965
7	704	-615
-7	1369	1240
9	682	-593
-13	603	-612
-15	1248	-1176
-17	1195	-1120
-19	612	-607
H,0,16		
0	1346	1391
2	1397	1350
4	770	852
-4	511	500
-6	1123	968
-10	1083	-1934
12	432	-485
-12	1612	-1522
-14	850	-759
-16	496	-410
-22	547	759
H,0,17		
1	687	625
-1	525	466
3	670	601
-3	435	-417
5	694	694
-5	1132	-1109
7	438	486
-7	1250	-1311
9	364*	261
-9	856	-820
-13	601	-554
-17	873	773
-19	848	955
-21	516	667
H,0,18		
0	1068	-1015
2	593	-670
-2	1092	-978
-4	683	-725
6	501	480
-6	527*	-675
-8	683	-610
10	240	276
-10	533	487
-12	770	878
-14	932	857
-16	774	739
-18	339*	449
-20	267*	327
H,0,19		
-1	597	-490
-3	736	-737
5	860	-765
-7	816	808
-9	902	881
-11	667	704
-13	405	469
-15	822	791
-19	620	-618
-21	408	-547
H,0,20		
0	396	453
-2	812	814
4	880	-719
-4	1132	1093
6	541	-442
-6	791	655
-8	667	576
-10	513*	287
-14	470*	-334
-16	601	-600
-18	626	-578
-20	264*	-354
H,0,21		
1	560	389
-1	666	515
3	496	481
-3	1130	964
-5	945	728
-9	695	-633
-11	737	-613
-13	522	-544
-15	643	-536
-17	556	-566
H,0,22		
0	522	423
-4	455	-514
-6	821	-799
-8	610	-440
-10	644	-733
-12	902	-740
-16	415	352
-18	493	555
H,0,23		
-1	377*	-292
-3	687	-558
-5	1146	-959
-7	614	-570
-13	447	396
-15	614	424
-17	512	573
H,0,24		
0	641	-541
-2	619	-536
-4	301*	-200
-10	440	322
-12	778	744
-14	560	652
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-5	751	-777
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TABLE III (*Continued*)

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10	809	-846
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-11	664	632
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-14	736	-670
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-10	523	-552
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-4	529	-507
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7	1339	1146
-7	1516	-1363
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6	882	-818
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10	748	-775
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12	1042	-1012
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2	925	-897
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-16	599	-723
	H,6,5	
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9	793	-726
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13	605	-803
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	H,6,9	
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	H,6,10	
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3	435	-487
-3	524	453
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5	559	-509
-6	1513	1286
-7	376	-342
8	747	-788
-8	596	572
10	570	-657
-12	635	-635
-14	673	-739
-16	638	-836
	H,6,11	
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3	1115	1096
5	660	555
-5	446	-420
-7	898	-741
-9	818	-895
-10	599	-604
-11	878	-859
-13	963	-955
	H,6,12	
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4	750	770
-4	740	-859
6	975	886
-6	1397	-1313
8	472	618
-8	1037	-995
-18	484	599
	H,6,13	
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-1	1098	-1213
-2	510	498
3	541	-525
-3	899	-1076
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-11	557	574
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-15	798	856
	H,6,14	
0	559	-635
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6	442	-590
-6	608	743
-8	1035	1022
-10	863	884
-18	290*	-341
	H,6,15	
-1	599	695
-3	1061*	1095
-5	908	1094
-7	707	771
-15	586	-710
	H,6,16	
0	642	767
2	577	633
-2	414*	604
-10	623	-704
-12	744	-835
-14	560	-696
	H,6,17	
-5	688	-845
-7	527	-726
	H,6,18	
-2	607	-674
-4	658	-583
	H,6,19	
-9	421	565
	H,6,20	
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	H,7,0	
1	800	854
2	560	512
3	651	548
4	1001	868
6	1694	1446
8	1295	1185
	H,7,1	
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-1	1820	-2025
-3	1118	-999
4	742	791
6	1092	962
-6	759	-665
	H,7,2	
0	725	-877
-1	764	-975
2	1317	-1250
-3	850	-900
4	1399	-1332
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-6	988	654
-8	1648	1426
	H,7,3	
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-3	1326	1201
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-5	1157	995
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-7	1058	925
	H,7,4	
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-3	868	870
4	897	831
-5	785*	915
7	664	-631
-7	684	501
	H,7,5	
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3	593	651
5	1141	1032
-5	1299	-1217
7	959	913
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	H,7,6	
0	907	-989
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2	946	-944
-2	1105	-1024
-4	911	-950
6	827	690
-6	908	-801
	H,7,7	
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-1	910	-1085
3	988	-1118
-3	576*	-704
5	751	-866
-7	1453	1153
-8	671*	-790
-9	814	829
	H,7,8	
2	664	-581
4	751	-885
-4	749	1021
-6	1121	1102
-8	966	924
	H,7,9	
-3	1162	1293
-5	800	883
	H,7,10	
2	759*	969
-6	807	-681
	H,7,11	
-5	946	-1124
	H,7,13	
-7	824	999

multiplied by the square root of the extrapolated absorption factors $\sqrt{A^*}$. Using a mean crystal radius value of 0.0075 cm, $\sqrt{A^*}$(max) and $\sqrt{A^*}$(min) were 3.23 and 2.28. The corresponding calculated corrections should be 2.51 and 1.91 for $R = 0.005$ cm and, respectively, 4.27 and 2.67 for $R = 0.01$ cm.

Atomic form factors were taken from ref 8, and correction for the real part of anomalous dispersion was applied for the uranium and arsenic atoms.[8] The calculations were performed with an Olivetti Elea 6001 3k computer except the full-matrix least-squares refinement which was carried out on the IBM 7040–7094 system using the version of ORFLS included in X-ray 63.[9] The reliability index is defined as $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ where the summation is over the observed unique reflections only.

Solution and Refinement.—Inspection of the peaks which appeared on the Harker line $^1/_2, v, ^1/_2$ and on the section $u, ^1/_2, w$ of the Patterson function permitted the location of the uranium and arsenic atoms. After a least-squares cycle of refinement the approximate coordinates of the remaining nonhydrogen atoms were found from two successive difference Fourier syntheses. The standard R factor was 21%.

A first refinement of the structure was performed with Cruickschank's weighting scheme[10] using the block-diagonal approximation and individual isotropic thermal parameters. After two cycles R dropped to 14%. Further refinement, in which the layer scale factors were first refined separately, and later the positional parameters and the isotropic temperature factors, was made with full-matrix least squares. The R value dropped to 10.9%. A difference synthesis was now calculated which showed characteristic dumbbell-formed peaks, indicating thermal anisotropy. Anisotropic refinement of the heavy atoms reduced R to the final value of 9.4%. The final weighting scheme used is

$$w = 1/(15.1 - 0.085|F_o| + 0.0004|F_o|^2)$$

derived following Mills and Rollett.[11] Atomic parameters with their standard deviations are given in Table II. In Table III the observed and the calculated structure factors are compared. Bond lengths, bond angles, and the best mean planes are given in Tables IV–VI. The molecular geometry is illustrated in Figure 1 together with the numbering scheme used.

Crystal Structure of $UO_2(DTC)_2(C_6H_5)_3PO$

Crystal Data.—Red b-prismatic crystals of $UO_2(DTC)_2(C_6H_5)_3PO$ were grown from acetone solution. The density was measured by flotation. Cell dimensions and space group were determined from precession photographs (λ(Cu Kα) 1.5418 Å). The observed systematic absences are the same as in the arsine compound. Crystal data obtained are as follows: formula weight 844.90; monoclinic, space group $P2_1/n$; $a = 18.32 \pm 0.01$, $b = 9.16 \pm 0.01$, $c = 20.97 \pm 0.01$ Å; $\beta = 111° 39' \pm 10'$; $V = 3270$ Å^3; $D_m = 1.72$, $D_x = 1.73$ g cm^{-3}; μ(Cu Kα) = 203.3 cm^{-1}; $Z = 4$; F(000) = 1648.

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(8) Reference 7, Vol. III.

(9) W. R. Busing, K. O. Martin, and H. A. Levy, "Fortran Crystallographic Least Squares Program, ORNL-TM-305," Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962.

(10) D. W. J. Cruickshank and D. E. Pilling in "Computing Methods and the Phase Problem in X-ray Crystal Analysis," Pergamon Press, London, 1961, p 32.

(11) O. S. Mills and J. S. Rollett in "Computing Methods and the Phase Problem in X-ray Crystal Analysis," Pergamon Press, London, 1961, p 107.

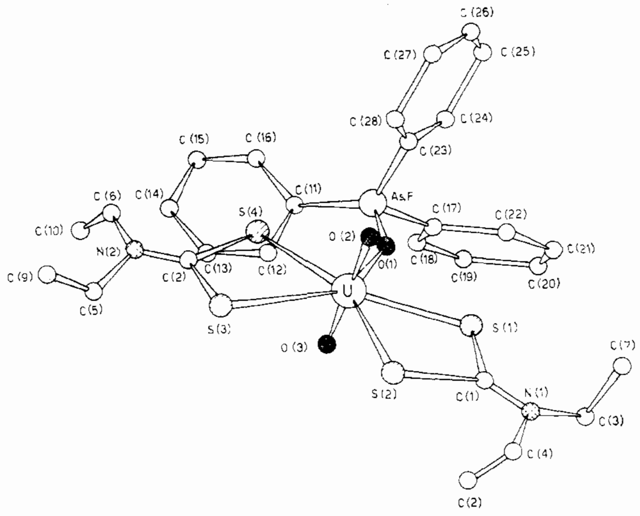

Figure 1.—A perspective view of the molecule.

TABLE IV

BOND LENGTHS AND STANDARD DEVIATIONS (Å)

$UO_2(DTC)_2(C_6H_5)_3AsO$			$UO_2(DTC)_2(C_6H_5)_3PO$		
Uranyl Group			Uranyl Group		
U–O(2)	1.71	0.03	U–O(2)	1.67	0.03
U–O(3)	1.71	0.03	U–O(3)	1.72	0.03
Equatorial Plane			Equatorial Plane		
U–O(1)	2.30	0.02	U–O(1)	2.34	0.02
U–S(1)	2.84	0.01	U–S(1)	2.85	0.01
U–S(2)	2.86	0.01	U–S(2)	2.86	0.01
U–S(3)	2.83	0.01	U–S(3)	2.84	0.01
U–S(4)	2.80	0.01	U–S(4)	2.84	0.01
DTC Groups			DTC Groups		
S(1)–C(1)	1.66	0.04	S(1)–C(1)	1.71	0.04
S(2)–C(1)	1.73	0.04	S(2)–C(1)	1.72	0.04
C(1)–N(1)	1.36	0.06	C(1)–N(1)	1.34	0.05
N(1)–C(3)	1.49	0.08	N(1)–C(3)	1.47	0.06
N(1)–C(4)	1.49	0.06	N(1)–C(4)	1.50	0.07
C(3)–C(7)	1.50	0.08	C(3)–C(7)	1.59	0.07
C(4)–C(8)	1.41	0.09	C(4)–C(8)	1.51	0.10
S(3)–C(2)	1.75	0.04	S(3)–C(2)	1.73	0.04
S(4)–C(2)	1.69	0.04	S(4)–C(2)	1.68	0.04
C(2)–N(2)	1.30	0.06	C(2)–N(2)	1.36	0.06
N(2)–C(5)	1.50	0.08	N(2)–C(5)	1.56	0.07
N(2)–C(6)	1.52	0.07	N(2)–C(6)	1.51	0.07
C(5)–C(9)	1.52	0.10	C(5)–C(9)	1.52	0.09
C(6)–C(10)	1.61	0.08	C(6)–C(10)	1.50	0.08
Triphenylarsine Oxide Group			Triphenylphosphine Oxide Group		
As–O(1)	1.64	0.02	P–O(1)	1.49	0.03
As–C(11)	1.89	0.05	P–C(11)	1.87	0.04
As–C(17)	1.89	0.06	P–C(17)	1.80	0.05
As–C(23)	1.88	0.05	P–C(23)	1.79	0.05
Minimum and Maximum Distances in the Two sets of Phenyl Groups and the Means[a]					
C–C(min)	1.27		C–C(min)	1.27	
C–C(max)	1.48		C–C(max)	1.59	
C–C(mean)	1.395	0.01	C–C(mean)	1.396	0.02

[a] The standard deviation of the mean is calculated from $(\Sigma_i \Delta_i^2/m(m-1))^{1/2}$. The esd's of the carbon–carbon distances are about 0.08 Å.

TABLE V

BOND ANGLES AND STANDARD DEVIATIONS (DEG)

$UO_2(DTC)_2(C_6H_5)_3AsO$			$UO_2(DTC)_2(C_6H_5)_3PO$		
O(2)–U–O(3)	179	1	O(2)–U–O(3)	177	2
O(2)–U–O(1)	90	1	O(2)–U–O(1)	90	1
O(2)–U–S(1)	91	1	O(2)–U–S(1)	91	1
O(2)–U–S(2)	91	1	O(2)–U–S(2)	93	1
O(2)–U–S(3)	91	1	O(2)–U–S(3)	87	1
O(2)–U–S(4)	91	1	O(2)–U–S(4)	88	1
O(3)–U–O(1)	89	1	O(3)–U–O(1)	89	1
O(3)–U–S(1)	89	1	O(3)–U–S(1)	88	1
O(3)–U–S(2)	89	1	O(3)–U–S(2)	90	1
O(3)–U–S(3)	90	1	O(3)–U–S(3)	91	1
O(3)–U–S(4)	89	1	O(3)–U–S(4)	89	1
S(1)–U–S(2)	62.3	0.3	S(1)–U–S(2)	61.9	0.3
S(2)–U–S(3)	73.8	0.3	S(2)–U–S(3)	74.7	0.3
S(3)–U–S(4)	62.6	0.4	S(3)–U–S(4)	62.6	0.4
S(4)–U–O(1)	79.8	0.7	S(4)–U–O(1)	78.4	0.6
O(1)–U–S(1)	81.5	0.7	O(1)–U–S(1)	82.5	0.6
U–S(1)–C(1)	88	2	U–S(1)–C(1)	90	1
U–S(2)–C(1)	87	2	U–S(2)–C(1)	89	2
U–S(3)–C(2)	89	1	U–S(3)–C(2)	88	2
U–S(4)–C(2)	91	2	U–S(4)–C(2)	89	2
U–O(1)–As	159	1	U–O(1)–P	162	2
S(1)–C(1)–S(2)	121	2	S(1)–C(1)–S(2)	119	3
S(1)–C(1)–N(1)	121	2	S(1)–C(1)–N(1)	119	2
S(2)–C(1)–N(1)	118	2	S(2)–C(1)–N(1)	123	4
C(1)–N(1)–C(3)	122	4	C(1)–N(1)–C(3)	124	3
C(1)–N(1)–C(4)	124	4	C(1)–N(1)–C(4)	117	4
C(3)–N(1)–C(4)	113	4	C(3)–N(1)–C(4)	118	4
N(1)–C(3)–C(7)	113	4	N(1)–C(3)–C(7)	109	3
N(1)–C(4)–C(8)	99	5	N(1)–C(4)–C(8)	108	4
S(3)–C(2)–S(4)	117	2	S(3)–C(2)–S(4)	120	2
S(3)–C(2)–N(2)	122	3	S(3)–C(2)–N(2)	119	3
S(4)–C(2)–N(2)	121	3	S(4)–C(2)–N(2)	120	3
C(2)–N(2)–C(5)	121	5	C(2)–N(2)–C(5)	118	4
C(2)–N(2)–C(6)	120	4	C(2)–N(2)–C(6)	119	4
C(5)–N(2)–C(6)	118	4	C(5)–N(2)–C(6)	121	4
N(2)–C(5)–C(9)	117	5	N(2)–C(5)–C(9)	112	4
N(2)–C(6)–C(10)	108	4	N(2)–C(6)–C(10)	118	4
O(1)–As–C(11)	109	2	O(1)–P–C(11)	113	2
O(1)–As–C(17)	116	2	O(1)–P–C(17)	117	2
O(1)–As–C(23)	109	2	O(1)–P–C(23)	112	2
C(11)–As–C(17)	110	3	C(11)–P–C(17)	106	2
C(11)–As–C(23)	107	2	C(11)–P–C(23)	104	2
C(17)–As–C(23)	105	2	C(17)–P–C(23)	104	2
As–C(11)–C(12)	123	4	P–C(11)–C(12)	112	3
As–C(11)–C(16)	118	3	P–C(11)–C(16)	124	4
As–C(17)–C(18)	125	4	P–C(17)–C(18)	126	3
As–C(17)–C(22)	112	3	P–C(17)–C(22)	112	3
As–C(23)–C(24)	124	3	P–C(23)–C(24)	126	3
As–C(23)–C(28)	118	3	P–C(23)–C(28)	111	3
Phenyl Groups[a]					
Max angle	126		Max angle	129	
Min angle	112		Min angle	113	
Mean	119.8	1	Mean	120	1

[a] The standard deviation of the mean is calculated from $(\Sigma_i \Delta_i^2/m(m-1))^{1/2}$. The esd's for the angles in the phenyl groups are about 4°.

Intensity Data.—The specimen chosen for the X-ray work was 0.15 × 0.60 × 0.20 mm in dimensions, with the largest value in the [010] direction. The crystal was rotated about the b axis and equiinclination Weissenberg photographs of $h0l$ to $h6l$ layers were taken with the use of Cu Kα radiation and the multifilm technique. A total of 2801 intensities above background were observed and were corrected for Lorentz and polarization effects and for absorption using the cyclindrical approximation. The assumed R for the crystal was the average value 0.0087 cm. Correction for the real part of anomalous dispersions was applied to the form factors of the uranium atom. The calculations were

TABLE VI
SELECTED LEAST-SQUARES PLANES OF $UO_2(DTC)_2(C_6H_5)_3AsO$ AND $UO_2(DTC)_2(C_6H_5)_3PO$[a]

	$UO_2(DTC)_2(C_6H_5)_3AsO$					$UO_2(DTC)_2(C_6H_5)_3PO$			
Plane	P	Q	R	S	Plane	P	Q	R	S
α	8.816	−7.976	−2.444	−2.169	α	8.930	−7.964	−2.229	−2.150
β	−3.573	8.932	0.220	0.980	β	−4.454	8.850	0.242	1.122
γ	−8.360	8.064	1.484	2.108	γ	8.689	−7.988	−1.333	−2.076
δ	11.298	−7.176	−4.630	−2.517	δ	11.538	−7.096	−4.844	−2.570
ε	2.888	−4.862	15.028	4.256	ε	2.840	−4.442	15.574	4.538
ζ	−1.634	7.863	10.437	6.190	ζ	−0.865	8.037	9.662	5.927
η	17.146	2.417	−11.503	−1.322	η	17.456	2.300	−10.706	−1.112

Distances (Å) of Atoms from the Planes

α		β		γ		δ		α		β		γ		δ	
Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ
U	−0.030	S(1)	0.006	S(3)	0.001	U	0.000	U	−0.026	S(1)	−0.008	S(3)	0.001	U	0.000
S(1)	0.022	S(2)	0.005	S(4)	0.001	O(1)	0.000	S(1)	0.024	S(2)	−0.008	S(4)	0.001	O(1)	0.000
S(2)	0.001	N(1)	0.007	N(2)	0.001	As	0.000	S(2)	0.007	N(1)	−0.011	N(2)	0.001	P	0.000
S(3)	−0.006	C(1)	−0.018	C(2)	−0.003			S(3)	−0.020	C(1)	0.028	C(2)	−0.002		
S(4)	0.027	C(3)^b	0.052	C(5)^b	0.353			S(4)	0.042	C(3)^b	0.037	C(5)^b	−0.225		
O(1)	−0.014	C(4)^b	−0.304	C(6)^b	−0.188			O(1)	−0.026	C(4)^b	−0.315	C(6)^b	0.029		
N(1)^b	0.676							N(1)^b	0.599						
N(2)^b	−0.091							N(2)^b	−0.071						
C(1)^b	0.288							C(1)^b	0.212						
C(2)^b	−0.026							C(2)^b	−0.023						

ε		ζ		η		ε		ζ		η	
Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ	Atom	Δ
C(11)	0.049	C(17)	−0.045	C(23)	0.036	C(11)	0.049	C(17)	−0.049	C(23)	0.011
C(12)	−0.016	C(18)	−0.010	C(24)	0.006	C(12)	−0.009	C(18)	−0.005	C(24)	−0.023
C(13)	−0.032	C(19)	0.054	C(25)	−0.035	C(13)	−0.037	C(19)	0.051	C(25)	0.013
C(14)	0.048	C(20)	−0.039	C(26)	0.020	C(14)	0.047	C(20)	−0.043	C(26)	0.009
C(15)	−0.013	C(21)	−0.011	C(27)	0.026	C(15)	−0.010	C(21)	−0.012	C(27)	−0.022
C(16)	−0.036	C(22)	0.052	C(28)	−0.052	C(16)	−0.041	C(22)	0.057	C(28)	0.012

Angles between the Planes, Deg

∠αβ	17.6	∠εζ	86.7	∠αβ	15.1	∠εζ	88.7
∠αγ	2.7	∠εη	79.7	∠αγ	2.4	∠εη	83.0
∠αδ	9.9	∠ζη	88.1	∠αδ	10.9	∠ζη	84.6

[a] Equations of the least-squares planes are in the form $PX + QY + RZ = S$, and X, Y, Z refer to crystallographic coordinates.
[b] Atoms not included in the least-squares calculation.

TABLE VII
ATOMIC PARAMETERS OF $UO_2(DTC)_2(C_6H_5)_3PO$[a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
U	−381 (1)	1709 (2)	1892 (1)	23 (1)	102 (2)	21 (1)	5 (1)	8 (1)	6 (1)
P	1148 (5)	3069 (12)	3556 (4)	31 (3)	74 (18)	26 (3)	3 (6)	8 (2)	−3 (5)
S(1)	−1270 (5)	565 (12)	2645 (4)	31 (3)	166 (21)	20 (2)	−5 (6)	8 (2)	−4 (5)
S(2)	−1849 (5)	315 (13)	1143 (5)	34 (4)	166 (22)	24 (3)	−20 (7)	10 (3)	3 (6)
S(3)	−561 (6)	1908 (15)	488 (5)	39 (4)	179 (24)	30 (3)	−25 (8)	11 (3)	−5 (7)
S(4)	806 (6)	3212 (15)	1584 (5)	40 (4)	193 (23)	31 (3)	−25 (9)	15 (3)	12 (8)
O(1)	487 (13)	2375 (29)	2992 (10)	43 (9)	154 (46)	12 (6)	31 (16)	8 (6)	8 (13)

Atom	x	y	z	B, Å^2	Atom	x	y	z	B, Å^2
O(2)	128 (16)	173 (35)	1931 (13)	6.7 (6)	C(13)	2831 (22)	1678 (53)	2900 (18)	5.9 (7)
O(3)	−862 (16)	3339 (35)	1847 (13)	6.4 (6)	C(14)	3354 (28)	2827 (55)	3078 (24)	7.5 (10)
N(1)	−2733 (18)	−148 (38)	1910 (15)	5.7 (7)	C(15)	3288 (30)	3998 (57)	3461 (25)	6.1 (12)
N(2)	629 (20)	3238 (44)	276 (16)	6.6 (7)	C(16)	2612 (31)	4072 (60)	3625 (25)	7.2 (12)
C(1)	−2024 (21)	165 (45)	1895 (18)	4.7 (8)	C(17)	1397 (28)	2298 (54)	4398 (23)	4.1 (11)
C(2)	326 (24)	2825 (46)	752 (20)	6.0 (9)	C(18)	2070 (23)	1847 (52)	4788 (19)	5.9 (8)
C(3)	−2891 (26)	−299 (53)	2546 (22)	6.9 (10)	C(19)	2220 (29)	1035 (54)	5419 (24)	6.7 (11)
C(4)	−3415 (35)	−130 (79)	1241 (29)	14.1 (15)	C(20)	1544 (31)	861 (60)	5601 (26)	7.6 (12)
C(5)	234 (36)	2650 (68)	−472 (31)	9.0 (15)	C(21)	826 (35)	1276 (66)	5159 (29)	7.2 (14)
C(6)	1396 (31)	4070 (60)	503 (26)	8.1 (13)	C(22)	696 (26)	1920 (54)	4540 (22)	5.5 (9)
C(7)	−3169 (29)	1236 (57)	2735 (24)	8.1 (12)	C(23)	957 (23)	4945 (51)	3672 (19)	4.8 (8)
C(8)	−3546 (35)	−1675 (77)	964 (29)	13.3 (15)	C(24)	1236 (27)	5701 (56)	4257 (24)	6.8 (10)
C(9)	575 (35)	3336 (73)	−964 (29)	12.8 (14)	C(25)	986 (31)	7369 (59)	4242 (26)	8.1 (12)
C(10)	2146 (34)	3209 (70)	763 (28)	10.6 (14)	C(26)	550 (26)	7956 (52)	3653 (22)	7.4 (10)
C(11)	2081 (21)	3109 (45)	3389 (17)	4.0 (7)	C(27)	295 (29)	7183 (54)	3042 (24)	7.4 (11)
C(12)	2184 (24)	1793 (56)	3033 (20)	5.9 (9)	C(28)	475 (28)	5616 (56)	3031 (24)	5.6 (11)

[a] Coordinates × 10^4. Standard deviations from the least-squares refinement are in parentheses. Anisotropic thermal parameters are defined by $T = \exp\{-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)\}$, and each β_{ij} is multiplied by 10^4.

TABLE VIII

OBSERVED AND CALCULATED STRUCTURE FACTORS (×10) OF $UO_2(DTC)_2(C_6H_5)_3PO$

H,0,0		
2	3227	3144
4	1127	1040
6	337	-270
8	1290	-1511
10	1269	-1471
12	2039	-2109
14	1376	-1308
16	677	-663
H,0,1		
3	3037	2913
-3	937	946
5	2516	2343
7	1615	2011
-7	3359	-3330
9	328	489
-9	2699	-2928
-11	1189	-1177
13	649	-609
15	1032	-996
17	860	-749
-17	501	475
19	859	-843
-19	681	653
21	449	-471
-21	677	801
H,0,2		
2	738	843
-2	2929	-3839
4	1034	827
-4	4041	-3993
6	1631	1749
-6	2573	-2830
8	1363	1577
-8	1170	-1326
10	1645	1581
12	1724	1912
-12	567	693
-14	1899	1882
-16	1446	1496
-18	934	941
-20	639	551
H,0,3		
1	3830	-3702
-1	1420	-1425
3	2313	-2585
5	1715	-1703
-5	1091	-1055
7	698	550
-9	1992	2195
-11	1279	1472
13	1123	1002
-13	893	970
15	1114	1050
-15	940	943
17	936	889
-17	736	587
19	559	522
-21	614	-576
H,0,4		
0	583	-439
2	1115	-1143
-2	1499	1899
4	1517	-1245
-4	2325	2537
6	2268	-2511
-6	2820	3057
8	1697	-1870
-8	2349	2665
10	1680	-1700
-10	1221	1292
12	905	-871
14	587	435
16	730	654
-16	876	-951
18	857	828
-18	1219	-1150
-20	853	-787
-22	553	-537
H,0,5		
1	3553	3459
-1	1968	2116
3	2205	2059
-3	1452	1537
-5	600	539
7	946	-931
-7	1475	1597
9	1227	-1304
11	1200	-1205
-11	889	-1080
13	1152	-1126
-13	1109	-1120
15	834	-845
-15	1141	-1273
-17	1087	-1089
H,0,6		
0	1960	2196
2	2799	2750
-2	1189	1025
4	3182	3358
-4	1124	-937
6	1805	1774
-6	3299	-3396
8	828	912
-8	3168	-3168
-10	1316	-1362
12	652	-642
-12	663	-716
14	869	-786
16	949	-927
18	643	-714
-18	706	675
-20	732	673
-22	559	548
H,0,7		
1	1846	-1473
-1	715	-920
-3	2359	-2449
5	1792	1636
-5	3634	-3602
7	1636	1642
-7	1430	-1460
9	1701	1453
-9	1315	-1433
11	997	921
13	755	698
-13	838	867
-15	1066	1104
17	426	-487
-17	1180	1407
-19	721	694
-21	531	459
H,0,8		
0	3122	-3384
2	2637	-2812
-2	2831	-2911
4	2172	-1973
-4	1809	-2010
6	565	-589
-6	544	493
8	773	601
-8	1099	1149
10	1769	1657
-10	1185	1219
12	927	1041
-12	1649	1830
14	719	555
-14	1368	1492
16	680	687
-16	1257	1292
-20	559	-437
-22	434	-410
H,0,9		
1	1957	-1932
-1	869	-683
3	2427	-2322
-3	543	457
5	1266	-1221
-5	2419	2521
7	1092	-1119
-7	1659	1765
9	615	-499
-9	1797	1702
-11	1246	1292
15	435	433
-17	633	-666
-19	818	-841
-21	755	-649
-23	595	-664
H,0,10		
0	1020	1182
2	638	565
-2	1999	2133
4	464	400
-4	3015	3338
-6	1564	1632
8	1328	-1388
-8	361	329
10	1423	-1327
12	738	-649
-12	1227	-1205
-14	1474	-1576
-16	1418	-1358
-18	1022	-998
H,0,11		
1	2320	2584
-1	1292	1282
3	1368	1510
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H,4,7		
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-1	720	583
2	1830	1979
-2	539	479
3	460	-321
-3	728	720
4	1426	1398
5	524	-481
-5	728	708
6	965	953
7	821	-720
-7	790	693
-8	1498	-1278
9	618	-539
-9	312	324
-10	1776	-2009
11	419	-407
12	690	-756
-12	1595	-1714
14	806	-910
-14	748	-641
-15	441	-448
H,4,8		
0	787	671
1	339	363
-1	844	-817
2	651	592
3	928	893
-3	1162	-1298
5	1588	1500
-5	1276	-1430
7	1525	1470
-7	1703	-1755
-8	496	-327
9	1057	1009
-9	1365	-1273
-10	386	-395
11	478	509
-11	624	-589
-12	568	-432
-14	643	-595
-15	541	548
-17	659	759
-19	694	850
H,4,9		
0	1902	-1827
1	602	461
2	1253	-1167
-2	1649	-1770
3	753	622
-3	587	-700
-4	1122	-1292
5	780	685
-5	699	-698
6	743	635
-6	1074	-1014
7	714	588
-7	933	-951
8	406	422
-9	1030	-907
-10	1129	1063
12	745	852
-12	1379	1274
14	555	622

TABLE VIII (*Continued*)

H,4,9		
-14	1121	1119
-16	727	737
H,4,10		
1	680	-543
-1	743	-818
-2	792	-825
3	1347	-1168
4	365	311
-4	568	-500
5	1399	-1265
6	561	569
-6	468	-505
7	688	-666
-7	1400	1350
-9	1932	1980
-11	986	903
-13	905	840
-16	497	514
-19	451	-526
H,4,11		
0	1130	1004
1	516	-403
-1	456	-581
-2	1000	1179
3	811	-800
4	453	-452
-4	990	1151
5	563	-509
6	1057	-983
-6	969	962
-7	569	462
8	699	-670
-8	1203	1156
-9	704	596
10	541	-747
-10	637	624
-11	495	540
12	558	-673
-14	521	-439
-16	1005	-1007
-18	765	-812
-20	462	-592
H,4,12		
1	875	796
-1	906	1059
3	1512	1444
-3	1056	1084
4	565	-438
-4	692	602
5	675	570
6	441	-382
-6	549	451
-8	708	649
-9	1482	-1402
-10	698	499
11	499	-472
-11	833	-891
-13	758	-620
-15	797	-711
-16	249	-320
-17	538	-539
H,4,13		
1	498	439
2	543	554
3	552	465
-3	747	685
4	1015	1059
-4	1049	-1034
6	1020	995
-6	1106	-1217
8	729	776
-8	1268	-1212
10	399	472
-10	690	-953
-11	731	-597
-12	610	-536
-16	552	505
-18	631	693
H,4,14		
1	725	-921
-1	738	-896
2	453	474
-2	351	486
3	647	-654
-3	1232	-1367
4	550	393
-5	963	-1131
-6	568	-478
7	678	763
-7	572	-425
9	607	760
-11	704	596
-12	354	-360
-13	698	667
-15	651	763
-17	647	828
-19	392	424
H,4,15		
0	887	-1105
2	603	-876
-2	873	-1115
-3	344	-461
4	517	-613
-5	395	-534
6	554	-496
-6	896	998
-8	978	917
-10	1211	1115
-12	1171	1090
-14	479	658
H,4,16		
2	438	-372
-3	498	586
5	469	-635
-5	949	995
7	599	-704
-7	1006	1076
-9	1004	969
-11	462	532
-12	501	424
-15	635	-588
-17	581	-667
-19	462	-589
H,4,17		
0	649	802
-2	670	904
-4	654	796
-5	482	474
-12	676	-708
-14	919	-885
-16	805	-796
H,4,18		
1	573	596
3	640	661
5	319	412
-5	440	-523
-7	678	-695
-9	853	-860
-11	694	-874
H,4,19		
-2	563	-654
-4	616	-682
-6	605	-644
-9	413	-246
-14	511	566
-16	536	558
H,4,20		
1	662	-840
-1	544	-663
3	313	-485
-11	650	704
-13	697	701
H,4,21		
-6	719	751
-3	692	799
H,4,22		
-1	472	630
-3	444	455
-13	525	-586
H,4,23		
-8	478	-595
H,5,0		
1	1199	1002
3	1293	1220
4	1595	-1490
5	944	891
6	1246	-1395
8	1449	-1502
9	1036	-970
10	698	-737
11	816	-730
13	709	-711
16	397	512
H,5,1		
0	860	779
1	1476	1322
-1	1579	1511
2	1236	1224
-2	526	-601
3	865	848
-3	2211	1919
4	1009	883
-4	862	-824
5	513	-414
-5	872	865
6	998	1094
-6	979	-794
7	652	-677
8	632	601
-8	866	-761
9	1106	-1214
-10	646	-643
11	969	-1026
-11	614	-478
-12	793	-787
13	596	-619
-13	739	-688
14	377	-394
15	590	-528
-15	761	-830
16	436	-379
-17	656	-656
18	228	-269
-18	339	358
H,5,2		
0	974	975
-1	1199	-1369
2	1368	1529
-2	910	902
3	481	-420
-3	1284	-1237
4	1430	1539
-4	447	-488
5	567	359
-5	1449	-1560
6	975	959
-6	1313	-1358
7	946	985
-7	1136	-1259
8	451	420
-8	1067	-1045
9	736	717
10	437	-452
-10	1064	-1082
11	496	345
-11	474	487
-12	666	-777
13	443	475
-13	563	503
14	417	-430
-14	444	-405
15	298	355
-15	626	583
16	581	-671
-17	418	489
H,5,3		
0	1217	-1332
-1	654	-703
2	944	-813
-2	853	-760
3	491	355
-3	1326	-1482
4	814	-655
-4	429	-362
5	771	705
-5	1579	-1548
6	884	-696
-6	273	-162
7	1045	1097
-7	879	-916
8	485	-448
-8	592	520
9	1290	1411
-9	732	-648
-10	662	569
11	716	588
-11	532	-410
12	728	678
-12	902	886
14	603	553
-14	694	763
-15	656	659
-17	712	741
H,5,4		
0	1670	-1708
1	362	272
-1	712	637
2	1410	-1383
-2	1476	-1433
3	578	-439
-3	479	309
4	593	-471
-4	535	-518
5	1162	-1078
-5	806	655
6	366	-265
-6	357	329
7	1021	-932
-7	850	915
8	438	428
-8	466	554
9	479	-511
-9	894	902
10	931	894
-10	739	681
11	395	-380
-11	470	376
12	658	620
-12	933	969
14	652	633
-14	841	838
16	315	396
-16	470	434
-17	358	-405
-19	[illegible]	-405
H,5,5		
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1	1482	-1376
2	543	285
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3	1111	-971
-3	617	653
4	865	760
-4	828	909
5	1162	-932
-5	1192	1305
6	365	257
7	1060	-1107
-7	1171	1321
9	820	-666
-9	935	989
10	909	-777
-10	356	-299
-11	1100	1008
12	803	-783
-12	596	-487
14	410	-432
-14	578	-509
-16	523	-501
-18	305	-327
-19	323	-404
H,5,6		
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1	992	937
2	595	404
-2	1476	1605
3	1433	1400
-4	932	1049
5	1376	1367
-5	424	-388
6	572	-496
-6	804	897
-7	640	-518
8	958	-977
-8	403	393
-9	1020	-952
10	992	-987
-11	1115	-1052
12	836	-780
12	731	-780
-12	487	-562
13	457	-442
14	358	-312
-14	877	-981
15	432	-400
-16	491	-632
-18	407	-495
H,5,7		
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3	1290	1138
4	568	393
-4	1437	-1534
5	969	876
-5	358	-222
6	834	644
-6	1077	-1009
-7	783	-815
8	925	921
-8	451	-433
-9	1187	-1121
10	694	717
11	400	-424
-11	1108	-1065
13	498	-668
-13	971	-970
-14	444	168
-15	369	-366
-16	416	472
-18	502	577
H,5,8		
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2	1065	957
-2	839	-1013
3	953	-659
-3	742	-813
4	1121	981
-4	863	-954
-5	462	-385
6	1059	967
-6	1269	-1369
8	810	740
-8	1475	-1567
-9	703	687
10	643	578
-10	872	-683
11	412	289
-11	1260	1229
13	374	453
-13	771	776
-14	397	432
-16	557	491
-18	346	461
H,5,9		
0	445	-206
1	1084	-991
-1	1288	-1323
3	642	-451
-3	819	-829
4	843	-710
-4	392	215
-5	776	-771
6	817	-786
-6	1186	1150
7	581	518
-7	659	-673
8	716	-679
-8	1062	999
9	559	486
-9	546	330
-10	937	796
11	644	671
-11	653	599
-12	753	624
13	531	589
-13	798	772
-15	802	916
-17	637	592
-18	462	-540
H,5,10		
0	872	-776
1	987	807
-1	1124	987
2	1171	-1081
-3	774	708
4	1278	-1214
-4	573	321
-5	846	747
6	581	-617
-6	660	591
-7	492	337
-8	1131	1221
9	323	-350
-9	541	448
-10	1016	969
11	419	-413
-12	706	529
13	252	-438
-13	560	-594
-14	486	369
-15	666	-626
-17	479	-545
-19	232	-381
H,5,11		
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2	672	570
-2	514	478
-3	870	1002
4	722	708
-4	575	532
5	877	-732
-5	1158	1137
6	397	489
7	656	-617
-7	1138	1202
-8	952	-922
9	480	-514
-9	474	432
-10	718	-687
11	424	-493
-11	451	-277
-15	420	-524
-17	621	-683
-19	362	-488
H,5,12		
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-1	546	-788
2	1110	1052
-2	735	814
-3	619	-565
4	774	728
-4	618	399
5	506	391
-5	761	-683
7	593	581
-7	529	-465
-8	432	-413
9	460	532
10	262	-343
-10	933	-863
11	231	417
-11	578	-510
-12	692	-620
-14	779	-733
-16	591	-612
-17	466	475
-19	289	359
H,5,13		
0	849	-912
2	796	-659
-2	536	-601
3	788	693
4	544	-453
-4	637	-595
5	948	916
-5	1021	-1033
-6	479	-377
7	655	559
-7	1083	-1069
8	335	405
9	263	291
-9	826	-904
-10	677	532
-11	343	-379
-12	486	436
-14	567	474
-17	279	403
-19	332	464
H,5,14		
1	779	-725
2	421	-397
-2	753	-856
3	506	-399
-4	1011	-1158
5	542	-533
-5	511	603
-6	440	-563
7	374	-450
-7	820	811
8	263	509
-9	641	678
-11	465	430
-12	506	496
-14	697	627
-16	724	762
-18	200	405
H,5,15		
1	599	-678
-2	599	527
3	624	-801
-4	579	527
5	323	-523
6	309	-483
-6	679	700
-7	590	564
-8	542	572
-9	746	641
-11	779	772
-13	662	666
-14	533	-493
-15	436	517
-16	595	-505
-18	260	-382
H,5,16		
1	443	574
-1	693	744
-3	397	481
-4	879	1002
-6	876	837
-8	421	470
-9	344	-493
-10	442	397
-11	518	-476
-15	405	-470
-16	357	-375
H,5,17		
1	448	525
-1	531	603
-3	559	746
-6	443	-384
-8	767	-796
-10	624	-608
-11	491	-515
-13	801	-760
-15	535	-592
H,5,18		
-1	385	-400
-3	347	-499
-6	374	-541
-8	349	-457
-10	366	-500
-12	567	-629
-15	310	457
H,5,19		
-1	406	-519
2	320	-448
-3	456	-590
-5	443	-569
-7	443	-488
-10	417	433
-13	388	372
H,5,20		
0	349	-573
-5	438	530
-10	359	421
-12	418	596
-13	246	-189
-14	334	457
H,5,21		
0	499	468
-7	351	524
H,5,22		
-7	264	-469
H,6,0		
1	418	384
2	1348	1513
3	722	555
4	1146	988
8	746	-751
10	648	-650
12	961	-930
14	767	-801
16	587	-552
H,6,1		
0	503*	-393
1	999	1165
-1	497	507
-2	544	-483
3	1443	1441
-3	440	-340
-4	432	-378
5	1661	1586
-5	1402	-1268
-6	619	-658
7	1344	1333
-7	1592	-1784
9	541	528
-9	1287	-1495
-11	875	-771
15	540	-599
17	479	-632
-17	337	432
H,6,2		
0	1087	-1305
1	415	-335
2	296	-176
-2	1479	-1568
3	99	-92
-3	239	285
-4	1425	-1470
-5	517	-365
6	917	837
-6	1082	-1121
8	1051	997
-8	748	-659
-9	412	216
10	996	978
12	750	852
-12	418	347
-14	689	709
-16	925	967
-18	489	596
H,6,3		
1	1894	-1617
-1	1499	-1553
2	436	450
-2	328	217
3	1653	-1628
-3	943	-948
-4	99	40
5	1347	-1203
6	470	-366
-6	494	365
-7	941	803
-8	654	511
9	520	440
-9	1186	1075
11	556	477
-11	999	1023
13	644	652
-13	898	865
15	589	593
-15	530	528
17	361	561
H,6,4		
0	312	-264
-1	646	437
2	988	-746
-2	751	721
4	770	-654
-4	1449	1457
6	1076	-1017
-6	1265	1179
8	1127	-1088
-8	1081	1055
10	931	-870
-10	831	853
-16	592	-542
-18	456	-588
H,6,5		
0	641	-533
1	1741	1539
-1	1790	1812
3	1279	1171
-3	1294	1286
4	849	763
-5	939	783
6	650	533
7	864	-658
-7	366	411
-9	455	-364
9	919	-905
11	909	-898
-11	862	-850
13	721	-750
-13	933	-909
15	372	-417
-15	801	-790
-17	582	-604
H,6,6		
0	1405	1426
2	1473	1346
-2	517	518
3	371	-355
-3	817	-715
4	1217	1113
-4	742	-578
-5	332	-181
6	986	871
-6	1112	-1150
8	726	613
-8	1169	-1107
-10	1023	-999
12	482	-469
-12	773	-816
14	409	-489
H,6,7		
1	701	-641
-1	1410	-1181
2	799	-600
3	688	579
-3	1251	-1292
4	732	-593
5	1065	871
-5	1384	-1393
7	1037	947
-7	1203	-1155
-8	347	246
9	965	959
-9	937	-914
-10	621	477
11	796	792
-13	784	698
-15	744	772
-17	565	689
-19	316	534
H,6,8		
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-1	427	-332
2	1290	-1095
-2	1117	-1262
4	1102	-987
-4	741	-820
-5	722	540
7	418	-315
-8	719	565
10	700	668
-10	725	693
12	614	689
-12	1039	1036
14	329	465
-14	846	843
-16	650	662
H,6,9		
1	1095	-944
3	1466	-1423
-3	777	824
-4	508	393
5	1125	-1028
-5	1076	1253
7	706	-682
-7	1268	1247
9	392	-453
-9	1187	1171
-11	802	854
-15	411	-198
-19	369	-533
H,6,10		
0	1047	935
2	388	356
-2	785	782
-4	1304	1299
6	515	-425
-6	1214	1286
-7	299	-338
8	622	-652
-8	717	629
10	615	-667
12	375	-502
-12	648	-566
-14	796	-741
-16	753	-786
-18	581	-671
H,6,11		
0	507	-430
1	1325	1275
-1	728	862
3	1208	1161
5	698	653
-7	804	-679
-9	740	-827
-10	529	-511
-11	825	-802
-13	928	-858
-15	470	-461
H,6,12		
4	648	-654
-4	924	-877
6	805	806
-6	1159	-1293
8	566	632
-8	908	-921
-10	554	-415
-18	456	532
H,6,13		
1	931	-920
-1	849	-1091
3	605	-571
-3	943	-959
-5	773	-689
9	342	475
-9	512	455
-11	629	576
-13	925	863
-15	837	772
H,6,14		
0	470	-618
2	602	-811
4	810	-913
6	547	-676
-6	754	717
-8	1047	966
-10	779	778
-12	595	572
-14	364	394
H,6,15		
-1	551	713
-3	856	1026
-5	1013	1109
7	276	-549
-7	848	784
-13	429	-434
-15	617	-603
-17	546	-626
H,6,16		
0	552	706
-2	614	704
-4	449	485
-10	500	-641
-12	819	-805
-14	752	-785
-16	368	-461
H,6,17		
5	499	568
-5	711	-793
-7	694	-647
-9	626	-591
-11	461	-473
H,6,18		
0	419	-512
-2	471	-678
-4	547	-683
-6	484	-523
-12	396	478
-14	378	508
H,6,19		
-1	310	-408
-9	493	521
-11	496	605
-13	383	504
H,6,20		
-2	400	449
-8	309	472
H,6,22		
-8	267	-449

performed on the IBM 7040–7094 system using the programs included in X-ray 63.

Solution and Refinement.—The structure of $UO_2(DTC)_2(C_6H_5)_3AsO$ was used for a starting model. The structure factor calculation with the coordinates taken from the results of the arsine analog yielded an R of 16%. Refinement proceeded by full-matrix least squares in which the same weighting scheme was used as for the refinement of the isomorphous compound. Two final cycles in which anisotropy was introduced for some atoms as revealed by a difference synthesis dropped the R index to the final value of 9.3% for the observed reflections. Final atomic parameters are given in Table VII. Observed and calculated structure factors are listed in Table VIII. Bond lengths, bond angles, and the best mean planes are given in Tables IV–VI. The molecular geometry and the numbering scheme used are the same as for $UO_2(DTC)_2(C_6H_5)_3AsO$.

Results and Discussion

Molecular weight determination showed the B and C to be monomeric species (B: found, 794; calcd, 844. C: found, 880; calcd, 888), and the molar conductance in nitromethane showed A to be a uni-univalent electrolyte according to its salt-type formulation.

Some physical data of the examined compounds are reported in Table I. Spectral behavior similar to that of the acetato complexes[2b] in regard to the asymmetric stretching of the U–O (uranyl) bond and of the As–O and P–O vibration modes can be seen from the ir absorption bands. The P–O stretching absorption shifts largely toward the lower frequencies while the corresponding As–O bond vibration appears not to be significantly influenced by the complex formation. On the other hand in these compounds as well as in the previously reported acetato complexes[2b] the lowering of the U–O asymmetric stretching frequency is larger in the arsine than in the phosphine oxide complexes. This systematic feature could be explained[12] assuming a larger donation effect of the arsine oxide with respect to the phosphine oxide.

The probable assignments of the most interesting absorption bands of the diethyldithiocarbamate group were made on the basis of the published spectral studies.[13] The absorption around 1000 cm^{-1} (A, 1005 cm^{-1}; B, 995 cm^{-1}; C, 992 cm^{-1}) is related to the C–S group vibration and the strong absorption band at 1480 cm^{-1} (A, 1485 cm^{-1}; B, 1480 cm^{-1}; C, 1479 cm^{-1}) determined in chloroform solution is assigned to the C–N bond.

The electronic spectra of such complexes, called "anisotropic" because of the large equatorial bond distances in comparison with the short uranyl bond lengths, are characterized in the semiempirical approach of optical electronegativity[14] by two different electronegativity values (χ) for the uranium atom, dealing with the uranyl or with the uranium–equatorial ligand system.[15] Thus for $K[UO_2(DTC)_3]$ $\chi_{DTC^-} = 2.5$ and $\chi_{U(VI)} = 1.8$. The electronic absorption spectra of these compounds are characterized by two intense bands deriving from electronic transitions localized in the uranyl system, corresponding to charge-transfer

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transitions from the equatorial ligands to the uranium atom, which cover the extremely weak band centered around 24 kK. The red uranyl dithiocarbamate phosphine or arsine oxides show two band maxima (or shoulders), whose energy difference is about 6 kK. A similar energy increment was found in the electronic spectrum of UO_2^{2+}, by Bell and Biggers,[16] with bands at 31, 37, and so on up to 60 kK. According to these authors this energy difference is too large to be associated to perturbing molecular vibrations and is assumed to represent a regular energy increment between the nonbonding orbitals of uranium.

In our case a comparison with some transition metal atom complexes as such $Ni(DTC)_2$ or $Co(DTC)_3$,[17] whose charge-transfer electronic transitions differ in energy by about 6 kK, induces us to believe that the two electronic transitions arise from two molecular orbitals mainly localized on the sulfur atoms to the same empty molecular orbital of uranium, thus corresponding to $\pi(\text{ligand}) \rightarrow f(\text{uranium})$ transitions.

The crystal structures of the isomorphous pair are composed of discrete molecules. In each complex molecule two dithiocarbamate ligands are planarly chelated to the uranium atom through the sulfur atoms. In the same plane the ligand L (L = $(C_6H_5)_3AsO$ or $(C_6H_5)_3PO$) is coordinated through the oxygen atom. The uranyl group is normal to the equatorial plane. The geometry of the coordination polyhedron is thus a slightly irregular pentagonal bipyramid, the uranium atom having coordination number 7. The uranyl groups are linear. The U–O bond lengths of 1.71 ± 0.03 Å for the arsine and of 1.67 ± 0.03 and 1.72 ± 0.03 Å for the phosphine compound are normal and within error limits equal to the values of 1.72 ± 0.04 and 1.69 ± 0.05 Å found in $[(CH_3)_4N]^+[UO_2(DTC)_3]^-$,[5] the first DTC uranyl complex for which structural information is available. The U–S distances, averaging 2.84 ± 0.02 Å, are equal in the two molecules. However they are larger by about 0.04 Å than the mean value of 2.80 ± 0.01 Å reported for the U–S distances in the above-mentioned ionic complex in which six sulfur atoms are equatorially linked to uranium. The S–C distances are in general close to those found in several DTC complexes and their average value S–C = 1.71 ± 0.07 Å in both the structures seems to be normal. The N–C bond lengths confirm their high double-bond character. The angles S–U–S agree very well in both of the structures with a mean value of 62.2 ± 0.04°. A review[18] of the available structures of DTC complexes suggests that some connection exists between the values of the S–M–S angles (M = metal) and the M–S bond lengths, the tendency being that the angles decrease as the distances increase. This is especially evident in the structures here reported in which the mean M–S distance of 2.84 Å, being the longest of the series, corresponds to S–M–S angles of about 62°, the smallest. This fact appears to be consistent with the rigid structure of the chelating group. (The M–S–C angles are all in the range 83–88°, irrespective of the nature of the metal M, and the S–C distances are constant.) The fact that in $[(CH_3)_4N]^+[UO_2(DTC)_3]^-$ a large U–S distance (2.80 ± 0.01 Å) coincides with S–U–S angles of 73.5 ± 0.05°, which are about 10° larger than we would expect on the basis of the observed tendency, seems to be due reasonably to the different coordination geometry. In fact the presence of six sulfur atoms equatorially coordinated implies very short contacts between sulfur atoms of adjacent carbamate groups. The resulting steric repulsion appears to be responsible both for the staggered structure and for a decrease in the S–C–S angle (110°), the increase of the S–U–S angle being a consequence of the former feature. The U–O (ligand) distances of 2.30 ± 0.02 and 2.34 ± 0.02 Å as well as the As–O and P–O distances of 1.64 ± 0.02 and 1.49 ± 0.03 Å agree with the corresponding values found in the nitrate[2a] and in the acetate[2b] complexes, confirming the strong π contribution to the As–O and P–O bonds.

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