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The Crystal Structure of $[(UO_2)_2(OH)_2Cl_2(H_2O)_4]$

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The structure of the uranyl hydroxide chloride $[(UO_2)_2(OH)_2Cl_2(H_2O)_4]$ has been determined from three-dimensional X-ray data. The crystals are monoclinic and the space group is No. 14: $P2_1/n$. The unit cell contains four formula units (eight uranium atoms) and has the dimensions

$a=17.743$ Å, $b=6.136$ Å, $c=10.725$ Å and $\beta=95.52°$

The structure is built up from discrete, uncharged molecules containing two linear uranyl groups, each of which is surrounded by one chlorine and four oxygen atoms forming an irregular planar pentagon. The two uranium atoms in a molecule are linked through a double OH bridge and the dimers are held together by hydrogen bonds.

The hydrolysis of the uranyl ion, UO_2^{2+}, has been studied repeatedly by means of, *e.g.*, emf methods and a list of papers on the subject published before 1964 is given in the IUPAC *Tables of Stability Constants*.[1] The results indicate that a series of polynuclear complexes is formed. Two complexes, $(UO_2)_2(OH)_2^{2+}$ and $(UO_2)_3(OH)_5^{+}$, have come out with well-defined equilibrium constants in all ionic media, but additional complexes have also been suggested.

Emf data can at most give the charge and the number of metal atoms in the complex but cannot give any information about its atomic structure. A preliminary investigation of some hydroxide salts of uranium(VI), made by the author using X-ray methods, indicated that the compound $UO_3 \cdot HCl \cdot 2H_2O$, and the isomorphous bromide, both of which have previously been described in the literature,[2,3] contain discrete dimers with a U—U distance of about 3.9 Å. It seemed likely that this dinuclear complex would be similar to the one found in solution and a complete crystal structure determination has been performed.

EXPERIMENTAL

Preparation of crystals. The synthesis of $UO_3 \cdot HCl \cdot 2H_2O$ described by Mylius and Dietz [2] was slightly modified. A solution of uranyl chloride was prepared by dissolving UO_3 in concentrated hydrochloric acid. Sodium hydroxide was added until a precipitate

was formed. After filtration the solution was allowed to crystallize at room temperature. Thin yellow tabular crystals which were not quite stable outside the mother liquor appeared after some weeks.

Analysis. A weighed amount of the compound was dissolved in water and uranium was determined by precipitation with 8-hydroxyquinoline according to a method described by Hecht and Donau.[4] The amount of chloride was obtained by passing a measured volume of the solution of the dissolved crystals through a H^+-saturated cation exchanger (Dowex 50 × 8) and titrating the eluate with standardized NaOH. The water content was estimated by difference and was confirmed by the results of the structure investigation. The density was determined by comparison of the weight of a sample in benzene and in air. The results of the analysis are given in Table 1 and are also compared with calculated values for $UO_3 \cdot HCl \cdot 2H_2O$ assuming eight formula units in the unit cell.

Table 1.

	Found	Calculated for $UO_3 \cdot HCl \cdot 2H_2O$
% UO_3	79.8	79.8
% HCl	10.4	10.2
% H_2O	9.8 (by difference)	10.0
Density	4.05	4.11

Crystals of the corresponding bromide, $UO_3 \cdot HBr \cdot 2H_2O$, were prepared according to a method described by Peterson.[3] By comparison of Weissenberg photographs of the first five layer lines taken around the *b* axis of both the chloride and bromide, the compounds were found to be isomorphous. Because of the lower atomic number of chlorine as compared with bromine, and a better stability, the compound $UO_3 \cdot HCl \cdot 2H_2O$ was chosen for the structure determination.

The calculations in connection with this investigation have been carried out on the CD 3600 computer in Uppsala and the IBM 7090 of FOA, Stockholm, using the programs described in Table 2.

Table 2. Computer programs used in the structure investigation.

Program	Authors
CELSIUS: Least squares refinement of unit cell dimensions	J. Tegenfeldt, Uppsala, Sweden
DATAP2: Lorentz-polarization and absorption corrections	P. Coppens, L. Leiserowitz and D. Rabinovich, revised by M. Elfström and O. Olofsson, Uppsala, Sweden
DRF: Fourier summations and structure factor calculations	A. Zalkin, Berkeley, USA, modified by R. Liminga and J.-O. Lundgren, Uppsala, Sweden
LALS: Least squares refinements of positional parameters and temperature factors	P. K. Gantzel, R. A. Sparks and K. N. Trueblood, Los Angeles, USA, modified by A. Zalkin, Berkeley, USA and by C.-I. Brändén, R. Liminga and J.-O. Lundgren, Uppsala, Sweden
DISTAN: Interatomic distances and angles	A. Zalkin, Berkeley, USA
PLANE: Least squares fit of a plane to a set of points	C.-I. Brändén, Uppsala, Sweden
LISTFC: Listing structure factor data (for IBM 7090)	J. M. Stewart and R. L. Braun, University of Maryland, USA

UNIT CELL AND SPACE GROUP

Rotation and Weissenberg photographs around the *b* axis and precession photographs around the *a* and *c* axes showed that the crystals were monoclinic and gave approximate unit cell dimensions. In order to obtain more precise

Table 3. Powder photograph of $UO_3 \cdot HCl \cdot 2H_2O$ taken in a Guinier camera with Cu$K\alpha$ radiation. Values are given for the first lines only.

hkl	$10^4 \sin^2\theta_{calc}$	$10^4 \sin^2\theta_{obs}$	I_{obs}
200	76	77	s
002	208	210	vs
011	210		
210	234	234	vs
$\bar{2}02$	260	260	vw
211	298	298	w
400	304	305	s
202	309	309	vs
012	366	366	s
$\bar{1}12$	373	373	vw
$\bar{2}12$	418	417	vs
410	462	464	vs
$\bar{4}02$	464		
$\bar{2}12$	466		
$\bar{4}11$	490	489	w
013	626	626	w
020	630		
113	663	665	vvw
$\bar{2}13$	666		
600	685	685	w
$\bar{1}21$	695	694	w
220	706	706	vvw
121	707		
$\bar{4}12$	719	720	vw
$\bar{2}21$	746	746	s
221	771	771	w
$\bar{6}02$	820	820	m
004	833	834	m
$\bar{3}21$	835		
$\bar{4}13$	858	858	m
$\bar{6}11$	858		
$\bar{2}04$	861		
122	870	872	vvw
321	872		
222	939	940	vvw
204	958	958	m
$\bar{4}21$	963	965	w
602	966		
$\bar{6}12$	978	977	m
014	991	990	s
$\bar{5}13$	1011	1013	m
421	1011		
$\bar{4}04$	1040	1039	s
023	1099	1098	s
$\bar{1}23$	1100		
$\bar{2}23$	1139	1137	s

values of the lattice parameters, a powder photograph was taken with Cu$K\alpha$ radiation (λ=1.5405 Å) in a Guinier focusing camera with KCl (a=6.29294 Å at 25°C) as internal standard (Table 3). By means of a least squares refinement (unit weights) the unit cell was found to have the following dimensions with maximum errors 3σ.*

$a=17.743\pm7$ Å, $b=6.136\pm2$ Å, $c=10.725\pm3$ Å and $\beta=95.52\pm3°$

The corresponding values for the bromide were approximately

$$a=18.1_7 \text{ Å}, \quad b=6.3_7 \text{ Å}, \quad c=10.9_1 \text{ Å} \text{ and } \beta=97°$$

Using the multiple film technique, Weissenberg photographs were taken around the b axis (0 to 6th layer line) with Mo$K\alpha$ radiation (λ=0.7107 Å) and around the c axis (0 to 6th layer line) with Cu$K\alpha$ radiation (λ=1.5418 Å). Because the crystals were found to be slightly deliquescent, they had to be placed in thin-walled glass capillaries for these experiments.

The systematic absences were such that

$h0l$ occurred only for $h+l=2n$
$0k0$ » » » $k=2n$

This is characteristic of space group No. 14: $P2_1/n$ (the setting differs from that given in the *International Tables* [5]).

Intensities were estimated visually by comparison with calibrated intensity scales and were corrected for Lorentz and polarization factors and for absorption. The data which were used for the absorption corrections are summarized in Table 4. The number of independent reflections observed with Mo$K\alpha$ radiation was 2474, corresponding to about 60 % of those with sin $\theta/\lambda \lesssim 1$. Reflections with a value of sin $\theta/\lambda \gtrsim 1$ were generally too weak to be observed. The number of intensity values recorded around the c axis was 1112, which were about 70 % of those within the Cu$K\alpha$ sphere.

Table 4. Data used for the absorption corrections of $UO_3 \cdot HCl \cdot 2H_2O$. The b axis is orientated in the long direction of the crystal plate and the c axis along the diagonal of the cross section.

Rotation axis	Radiation	Crystal length (mm)	Cross section (mm × mm)	Absorption coefficient (cm^{-1})
b	Mo$K\alpha$	0.324	0.051 × 0.122	338
c	Cu$K\alpha$	0.113	0.021 × 0.055	1104

STRUCTURE DETERMINATION

The structure determination was based on the data taken with Mo$K\alpha$ radiation around the b axis.

* All standard deviations and maximum errors are given as errors in the last figure of the corresponding value.

Preliminary scale factors for putting the intensities of the reflections of the seven layers on an absolute scale were obtained using Wilson's method.[6] In order to find the positions of the uranium atoms, a three-dimensional Patterson function, $P(u,v,w)$, was then calculated. Table 5 lists those peaks

Table 5. Peaks (> 100) in the three-dimensional Patterson function (expected height for a single U—U vector is 120).

u	v	w	Peak height	Number of vectors U—U
0.50	0.09	0	492	4
0.50	0.12	0.50	249	2
0.31	0.195	0.095	119	1
0	0.215	0.50	468	4
0.185	0.285	0.905	222	2
0.50	0.31	0.50	259	2
0.32	0.375	0.09	115	1
0.315	0.40	0.595	228	2
0.185	0.50	0.405	418	4

which have a height larger than 100 on a scale where the expected height is 120 for a single U—U vector.

From the values of u, v, and w in Table 5 it is obvious that the eight uranium atoms must occupy two of the general fourfold positions: $\pm(x,y,z)$; $\pm(\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z)$ in space group $P2_1/n$.

On the $h0l$ photographs all reflections with l odd are extremely weak and it seems likely that the uranium atoms make very small contributions to the intensities of these reflections. Accordingly the two independent sets of uranium atoms must be approximately related by a glide plane perpendicular to the b axis and with the glide direction parallel to the c axis. This leads to the following relations between the parameters for the two sets of uranium atoms

4 U(1) in 4(*e*): $\pm(x,\ y_1,\ z)$; $\pm(\frac{1}{2}+x,\ \frac{1}{2}-y_1,\ \frac{1}{2}+z)$;
4 U(2) in 4(*e*): $\pm(x,\ y_2,\ \frac{1}{2}+z)$; $\pm(\frac{1}{2}+x,\ \frac{1}{2}-y_2,\ z)$;

The vectors between these positions are

$\frac{1}{2},\ \frac{1}{2}-2y_1,\ \frac{1}{2}$	weight 2	within the fourfold positions
$\frac{1}{2},\ \frac{1}{2}-2y_2,\ \frac{1}{2}$	» 2	
$\frac{1}{2}-2x,\ \frac{1}{2},\ \frac{1}{2}-2z$	» 4	
$2x,\ \pm 2y_1,\ 2z$	» 1	
$2x,\ \pm 2y_2,\ 2z$	» 1	
$0,\ \pm(y_1-y_2),\ \frac{1}{2}$	weight 4	between the fourfold positions
$\frac{1}{2},\ \frac{1}{2}\pm(y_1+y_2),\ 0$	» 4	
$2x,\ \pm(y_1+y_2),\ \frac{1}{2}+2z$	» 2	
$\frac{1}{2}+2x,\ \frac{1}{2}+(y_1-y_2),\ 2z$	» 2	

When comparing these vectors with the values of u, v and w in Table 5 it can be shown that the only possible combinations of x-, y- and z-parameters

($0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq 1$) are $x=0.16$; $y=0.09$, 0.19, 0.31 or 0.41; $z=0.05$ or 0.55 or $x=0.34$; $y=0.09$, 0.19, 0.31 or 0.41; $z=0.45$ or 0.95.

The parameters of the first set of uranium atoms which can be chosen arbitrarily from the above combinations have been given the following values $x_1=0.16$; $y_1=0.31$; $z_1=0.05$.

Now the choice of the parameters of the second set of uranium atoms is restricted to the values $x_2=0.16$; $y_2=0.09$; $z_2=0.55$ by the approximate glide plane relation and by the peaks in the Patterson function. Thus the glide plane perpendicular to the b axis is situated at $y \approx 0.20$.

All vectors within and between these two fourfold positions are present as peaks in the three-dimensional Patterson function and have approximately the heights expected from the weights of the corresponding vectors (Table 5).

The parameters of the uranium atoms were now subjected to a full-matrix least squares refinement. Individual scale factors for the seven layers and isotropic temperature factors were also refined. The following values were obtained: $x_1=0.1606$; $y_1=0.3150$; $z_1=0.0468$ and $x_2=0.1543$; $y_2=0.1009$; $z_2=0.5487$.

The reliability index, defined by $R=\sum||F_o|-|F_c||/\sum|F_o|$, was lowered from 0.292 to 0.189 in four cycles.

To locate the light atoms, an electron density map based on $F_o-F_c^U$ was calculated. The F_o values were given the signs of the structure factors for the uranium atoms obtained from the above coordinates (F_c^U). All the chlorine and oxygen atoms which occupy the general fourfold position 4(*e*) were found

Table 6. Final positional and thermal parameters based on the Mo$K\alpha$ data. The positional parameters given belong to atoms in the same dimer. Standard deviations (σ) are given in parentheses. All atoms are in the positions 4(*e*) ($\pm(x,y,z)$; $\pm(\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z)$;) in space group No. 14:$P2_1/n$.

Atom	x	y	z	B or B_{11}
U(1)	0.33919(5)	0.31520(16)	0.45281(8)	0.49(2)
U(2)	0.15424(5)	0.60167(16)	0.54829(8)	0.55(2)
Cl(1)	0.4170(4)	0.5963(13)	0.3113(7)	1.5(2)
Cl(2)	0.0787(4)	0.3241(14)	0.6943(7)	2.1(2)
O(1)	0.2659(12)	0.6293(39)	0.4411(20)	1.7(3)
O(2)	0.2282(11)	0.2834(35)	0.5623(18)	1.3(3)
O(3)	0.2842(11)	0.2022(36)	0.3157(19)	1.6(3)
O(4)	0.3897(8)	0.4222(29)	0.5874(14)	0.6(2)
O(5)	0.1012(11)	0.4895(37)	0.4102(18)	1.5(3)
O(6)	0.2073(11)	0.7171(36)	0.6790(18)	1 4(3)
O(7)	0.3478(10)	−0.0400(35)	0.5390(17)	1.2(3)
O(8)	0.4520(11)	0.1044(36)	0.3897(19)	1.5(3)
O(9)	0.1517(9)	0.9617(33)	0.4591(16)	0.9(2)
O(10)	0.0425(18)	0.7995(53)	0.6082(30)	3.7(6)

	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
U(1)	0.65(5)	0.81(3)	0.09(4)	0.23(4)	0.03(5)
U(2)	0.65(5)	0.74(3)	−0.05(5)	0.21(4)	−0.25(5)
Cl(1)	2.1(4)	2.3(3)	−0.2(4)	0.9(4)	0.8(4)
Cl(2)	2.5(4)	1.7(3)	−1.1(4)	1.4(4)	0.1(4)

Table 7. Final observed and calculated structure factors of $UO_3{\cdot}HCl{\cdot}2H_2O$. The columns are h, $10|F_o|$, and $10F_c$. Unobserved reflections are marked with an asterisk and have been given F_o values corresponding to the estimated minimum observable intensity. Values marked with a plus have been taken from the Cu$K\alpha$ data. All other values are Mo$K\alpha$ data.

h	10|Fo|	10Fc
H,0,0		
2	3117+	-2548
4	3515	-4541
6	3337	3846
8	689	-679
10	4388	-4024
12	4280	3482
14	1936	1409
16	4798	-3814
18	2086	1426
20	2057	1521
22	2444	-2280
24	747*	522
26	2037	1733
28	1559	-1366
H,0,1		
-21	1403	-1265
-19	757*	341
-17	864	839
-15	1196	-1030
-13	577*	92
-11	891	850
-9	636	-670
-7	331	-352
-5	684	562
-3	110+	-215
-1	73+	-96
1	74+	-138
3	124+	17
5	438*	329
7	514*	-309
9	585*	-176
11	1031	972
13	810	-712
15	759	-693
17	1364	1284
H,0,2		
-32	996	1194
-30	827	-869
-28	832*	-599
-26	2422	2090
-24	1053	-1078
-22	2553	-1992
-20	2987	2566
-18	694*	265
-16	3046	-2789
-14	2698	2697
-12	509	481
-10	4470	-5277
-8	2800	2731
-6	4837	5326
-4	4642	-5116
-2	1321	1128
0	5036	5111
2	6604	-6126
4	1944	-1419
6	5341	4399
8	2066	-1798
10	2561	-2562
12	4047	4160
14	1743	-1557
16	2946	-2627
18	3395	2806
20	673*	490
22	2168	-1961
24	1313	1109
26	730*	509
28	1508	-1601
H,0,3		
-25	1085	1193
-23	822*	-285
-21	1077	-1051
-19	855	911
-17	636*	343
-15	1032	-1027
-13	518	612
-11	324	366
-9	1063	-1107
-7	346*	234
-5	746	673
-3	284*	-244
-1	286*	-29
1	310*	-42
3	365*	94
5	442*	175
7	673	-648
9	573*	282
11	731	797
13	951	-966
15	616*	128
17	896	926
19	657	-693
21	679*	-404
23	852	692
H,0,4		
-30	1552	-1529
-28	901*	70
-26	1568	1549
-24	1682	-1648
-22	773*	-152
-20	2647	2513
-18	2042	-1753
-16	2411	-2267
-14	3315	3527
-12	1073	-980
-10	2492	-2657
-8	4477	4980
-6	877	719
-4	4955	-5493
-2	2013	1932
0	1490	1584
2	4095	-4208
4	2654	2424
6	3401	3050
8	4821	-4607
10	600*	-212
12	3212	3519
14	2087	-2142
16	634*	-266
18	2514	2277
20	1349	-1285
22	1388	-1331
24	1929	1716
26	718*	-337
28	900	-1045
H,0,5		
-25	1051	1013
-23	796*	-703
-21	734*	-310
-19	952	1135
-17	612*	-534
-15	968	-1014
-13	1154	1088
-11	456*	-15
-9	585	-609
-7	652	625
-5	351*	198
-3	572	-517
-1	340*	23
1	361*	-16
3	396*	295
5	447*	-27
7	511	-518
9	731	633
11	633*	207
13	732	-722
15	714*	431
H,0,6		
-30	1206	-1356
-28	1158	1172
-26	880*	789
-24	1923	-1810
-22	758*	634
-20	1419	1310
-18	2804	-2757
-16	589*	525
-14	3854	3798
-12	2789	-2624
-10	1051	-1001
-8	2540	2584
-6	2356	-2237
-4	2273	-2254
-2	4554	4790
0	1136	-1029
2	3649	-3881
4	3542	3494
6	489*	240
8	2848	-3132
10	2488	2531
12	1745	1577
14	2752	-2789
16	685	733
18	1371	1294
20	1882	-1975
22	699*	174
24	1446	1679
26	1151	-1151
H,0,7		
-23	968	-1084
-21	729*	120
-19	828	875
-17	1077	-1029
-15	569*	-91
-13	1139	1209
-11	485	-466
-9	451	-417
-7	517	436
-5	406*	-216
-3	397*	-289
-1	394*	261
1	398*	64
3	408*	195
5	424*	-223
7	444*	-115
9	468	445
11	495*	-276
H,0,8		
-28	1142	1388
-26	880*	-639
-24	1518	-1683
-22	1925	1869
-20	710*	664
-18	2129	-2154
-16	1968	1906
-14	944	800
-12	3455	-3429
-10	1174	1123
-8	2403	2436
-6	2594	-2972
-4	432*	117
-2	3420	3696
0	3470	-3815
2	1030	-916
4	3279	3779
6	1063	-1039
8	1566	-1650
10	2786	2599
12	890	-877
14	2912	-2407
16	2336	2189
18	732*	465
20	1465	-1800
22	893	968
24	737	730
26	1388	-1319
H,0,9		
-17	918	-882
-15	602*	418
-13	558*	453
-11	810	-924
-9	499*	-1
-7	581	592
-5	461*	-237
-3	455*	-76
-1	453*	195
1	457*	-45
3	466*	-23
5	479*	-155
7	496*	86
9	517*	314
H,0,10		
-28	1326	1253
-26	1092	-1154
-24	837*	-286
-22	2058	2113
-20	901	-1058
-18	1877	-1692
-16	2039	2092
-14	596	-534
-12	2169	-2015
-10	2581	2901
-8	513	540
-6	3424	-3832
-4	1767	1812
-2	1822	1918
0	2795	-2855
2	1325	1396
4	2124	2105
6	2908	-2810
8	643	-583
10	2631	2636
12	1982	-1776
14	832	-773
16	2274	2168
18	795	-737
20	1213	-1181
22	1319	1298
H,0,11		
-21	942	1014
-19	719*	-180
-17	826	-895
-15	639	608
-13	610*	62
-11	584	-612
-9	561*	521
-7	542*	325
-5	475	-488
-3	529*	-25
-1	528*	190
1	532*	-23
3	540*	-5
5	552*	-207
7	567*	219
H,0,12		
-22	982	1031
-20	1533	-1743
-18	716*	-30
-16	2385	2492
-14	1819	-1666
-12	1234	-1238
-10	2513	2454
-8	1158	-1112
-6	1968	-1764
-4	2749	2909
-2	578*	75
0	2360	-2525
2	1777	1767
4	636*	538
6	2695	-2628
8	1443	1294
10	1696	1661
12	2180	-2039
14	854*	231
16	1273	1290
18	1023	-1140
H,0,13		
-7	623*	-55
-5	616*	-331
-3	612*	256
-1	612*	96
1	616*	-51
3	624*	-111
5	635*	-134
7	650*	264
H,0,14		
-20	1368	-1568
-18	756	873
-16	882	1119
-14	2095	-2262
-12	672*	343
-10	1748	1951
-8	1476	-1381
-6	639*	-406
-4	2299	2044
-2	1898	-1672
0	1546	-1327
2	2248	2356
4	720*	-386
6	1519	-1508
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4	2918	-3797
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7	1065	-1039
8	3830	4286
9	771	707
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11	906	797
12	2009	-1602
13	834	-807
14	2646	2168
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16	763	-720
17	959	849
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-19	803	-861
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-8	718	774
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4	3069	-2818
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6	1850	1282
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21	713*	69
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23	735*	586
24	1057	-942
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9	998	-889
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18	681*	255
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24	737*	25
25	749*	-634
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-13	659	703
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-9	958	-996
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13	738*	-57
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21	727	719

Table 7. Continued.

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12	727*	437
13	757*	-21
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18	697	893
19	733*	-31
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10	684	-583
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12	694	-573
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11	790*	332
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11	577*	321
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7	1620	-1393
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15	1177	1312
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9	792	-816
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15	674	-658
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18	912	-839
19	653*	450
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14	707	825
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Table 7. Continued.

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19	899	816
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22	896	-859
23	734	-598
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10	613*	-370
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13	653*	-369
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-4	2256	2474
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-2	2390	-2548
-1	1058	-1039
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1	1798	-1805
2	1907	1979
3	1876	1840
4	1511	-1444
5	757	-624
6	486	-513
7	1885	-1736
8	2390	2292
9	1880	1715
10	944	-815
11	709	681
12	1401	-1353
13	1688	-1842
14	1600	1681
15	933	837
16	662*	-394
17	814	847
18	1060	-1027
19	1133	-1268
20	1082	1087
21	694*	190
22	700*	137
23	1000	1003
24	1010	-987
H,3,6		
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-22	770*	-339
-21	665	-731
-20	876	1046
-19	686*	-376
-18	655*	-394
-17	1162	1084
-16	738	-685
-15	578*	-293
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-13	645	-631
-12	503*	46
-11	951	1064
-10	1070	-1158
-9	542	-543
-8	427	529
-7	956	-962
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-5	1195	1289
-4	1103	-1082
-3	374*	-241
-2	374*	213
-1	567	-534
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2	1142	-1019

Table 7. Continued.

H,3,6		
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6	1172	1127
7	698	846
8	572*	343
9	608*	131
10	990	-1025
11	659	-836
12	523	559
13	740	920
14	715*	428
15	697*	-67
16	839	-365
17	838	-902
H,3,7		
-24	1260	1300
-23	983	966
-22	773*	-451
-21	747*	-397
-20	879	-864
-19	845	-791
-18	1358	1340
-17	1584	1552
-16	609*	-516
-15	587*	-110
-14	1303	-1407
-13	1721	-1971
-12	1589	1965
-11	1242	1465
-10	476*	271
-9	916	967
-8	1642	-1557
-7	1559	-1821
-6	1211	1219
-5	695	776
-4	621	565
-3	1464	1539
-2	2291	-2469
-1	2356	-2496
0	1307	1306
1	424*	-93
2	1379	1429
3	1643	1851
4	1742	-1615
5	1235	-1237
6	527	515
7	555	-576
8	1563	1428
9	2009	1937
10	2177	-1811
11	654	-775
12	732*	-93
13	1693	-1321
14	1973	1568
15	1605	1542
16	1614	-957
17	712*	98
18	709*	-412
19	1004	-1062
20	1008	1032
21	721	613
22	725	-556
23	727*	367
24	728*	-569
25	1039	-336
26	899	926
27	735*	332
H,3,8		
-20	647	746
-19	698*	239
-18	822	-734
-17	791	839
-16	624*	-304
-15	1152	-1049
-14	967	967
-13	557*	-247
-12	558*	-446
-11	926	912
-10	612	-527
-9	796	-709
-8	1395	1233
-7	459*	243
-6	452*	-107
-5	1007	917
-4	1160	-1249
-3	997	-921
-2	445	454
-1	447	-428
0	715	665
1	910	882
2	792	-774
3	487	-514
4	485*	-37
5	434*	-244
6	926	1041
7	1144	1010
8	609	-601
9	637	-690
10	560	-564
11	705*	-377
12	745	803
13	959	848
14	770*	-68
15	761*	-477
16	674	-616
17	661	-354
18	738*	491
19	654	725
H,3,9		
-27	914	-934
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-25	864*	369
-24	751	794
-23	997	977
-22	965	-1173
-21	933	-998
-20	735*	-126
-19	712*	-331
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-17	1357	1389
-16	1010	-1037
-15	933	-1041
-14	594*	-344
-13	812	-755
-12	1587	1766
-11	1351	2046
-10	1177	-1249
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-7	1512	-1759
-6	1728	1857
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1	1459	1557
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3	1034	1067
4	1693	-1943
5	1877	-1955
6	1151	1291
7	604*	208
8	693	711
9	1643	1572
10	1717	-1553
11	1478	-1281
12	926	767
13	789*	-208
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15	1434	1255
16	1372	-1345
17	780	-766
18	768*	269
19	760	-643
20	921	877
21	916	934
H,3,10		
-18	855	-887
-17	672*	254
-16	651*	496
-15	892	-797
-14	864	790
-13	724	721
-12	812	-913
-11	562*	441
-10	546*	-100
-9	985	-863
-8	830	769
-7	518*	221
-6	458	-547
-5	427	377
-4	664	-629
-3	855	-846
-2	866	922
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0	529*	256
1	775	710
2	1036	-877
3	886	-342
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5	595*	272
6	614*	367
7	634*	420
8	810	-733
9	641	-836
10	712*	126
11	746*	224
12	694	720
13	727	604
14	841*	-488
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-19	736*	535
-18	709	857
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-16	1567	-1645
-15	1330	-1237
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-13	615*	46
-12	1001	1092
-11	1198	1180
-10	1344	-1385
-9	1356	-1397
-8	554*	182
-7	672	-629
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-5	2040	1958
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-2	676	-714
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1	1693	1684
2	977	-931
3	596*	-68
4	867	-861
5	1828	-1503
6	1884	1559
7	1374	1107
8	691*	-256
9	880	677
10	1368	-1251
11	1576	-1416
12	1338	1124
13	828*	417
14	855*	32
15	791	705
16	1061	-1001
17	1018	-970
18	725	781
H,3,12		
-19	668	791
-18	725*	-604
-17	706*	-25
-16	842	808
-15	669*	-455
-14	652*	36
-13	570	556
-12	862	-856
-11	611*	-251
-10	603*	274
-9	726	-721
-8	583	621
-7	713	693
-6	580	-562
-5	582*	223
-4	580*	-72
-3	584	-575
-2	722	754
-1	602	616
0	542	-557
1	600*	-161
2	597*	-408
3	779	-693
4	798	727
5	666	599
6	686*	38
7	706*	161
8	650	-651
H,3,13		
-19	933	991
-18	748*	-68
-17	736*	164
-16	1122	-1234
-15	1421	-1402
-14	1071	1135
-13	593	678
-12	654*	542
-11	785	706
-10	1166	-1333
-9	1153	-1273
-8	555	675
-7	615*	393
-6	753	795
-5	1418	1362
-4	1540	-1637
-3	1497	-1381
-2	639*	391
-1	630*	-400
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1	1578	1469
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3	606	-645
4	693*	-162
5	632	-687
6	1024	1087
7	1369	1111
8	934	-907
9	784*	-304
10	807*	-416
11	1173	-1025
12	1353	1204
13	1085	952
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-9	662*	-114
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-6	582	-728
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-1	602	554
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3	720*	-217
4	731	577
5	743	575
6	763*	-310
7	783*	-210
8	797*	-481
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-14	1034	1117
-13	1248	1213
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-7	690	713
-6	687*	210
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3	1078	-1057
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5	790*	-57
6	803	665
7	1003	940
8	1023	-909
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-6	724*	-374
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-2	720*	76
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2	727*	156
3	731*	-44
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5	739*	358
6	744*	-419
7	749*	-420
8	755*	30
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-7	928	934
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2	820*	-596
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6	857*	47
7	861*	534
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7	1623	-1886
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13	1181	-1055
14	736	-760
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16	1244	1147
17	2358	1703
18	793*	-107
19	786*	-133
20	785	-792
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22	699	756
23	1358	1268
24	788*	155
25	791*	198
26	797	-886
27	1262	-1292
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-18	786*	-439
-17	1174	-994
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-14	993	1016
-13	1243	1133
-12	589*	-179
-11	555	-722
-10	840	-891
-9	814	-846
-8	956	1001
-7	1461	1686
-6	373	-335
-5	332	-388
-4	482	-626
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2	637*	-519
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8	801	-771
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11	690*	-54
12	696*	-265
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15	501	-454
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17	599	-557
18	724*	-123
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20	734	-751
21	742*	-336
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23	758	-680
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-25	1082	-1033
-24	875*	736
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-20	1235	-1054
-19	776	-743
-18	745*	390
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-15	1949	2088
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-13	882	-862
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-6	931	-923
-5	1984	-2427
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-1	501	524
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1	3716	-3623
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3	1856	1940
4	515	490
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6	2379	-1865
7	3206	-2841
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10	926	792
11	1570	1806
12	1057	-1253
13	1625	-1973
14	651*	280
15	665*	-61
16	1167	1110
17	2349	2050
18	982	-899
19	1178	-1168
20	716*	-547
21	647	-761
22	897	978
23	1240	1400
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-20	698	847
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-16	651*	-124
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-14	934	986
-13	848	893
-12	646	-786
-11	993	-967
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-9	434*	-123
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6	788	-662
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9	1361	-1161
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11	636	658
12	635	-614
13	641	564
14	651*	-147
15	1212	-1054
16	596	740
17	676*	-76
18	686	-640
19	852	884
20	704*	-302
21	635	-601
22	887	869
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-8	1613	-1756
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17	963	1091
18	974	-1171
19	1707	-1945
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21	714*	221
22	833	883
23	1156	1278
24	661	-622
25	913	-932
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-19	723*	-372
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-14	629	570
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-11	1252	-1335
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-8	687	665
-7	817	767
-6	940	-982
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-2	574	522
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3	773	-648
4	626	602
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6	725	-732
7	675	-566
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9	789	-743
10	652*	347
11	909	861
12	903	-844
13	717*	-21
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16	692	521
17	619	665
18	624	-712
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20	715*	165
21	880	-749
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-22	837	-752
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-20	743*	-224
-19	1477	-1539
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-17	1357	1380
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-14	1189	-1152
-13	2253	-2455
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9	2601	2494
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15	1475	1616
16	719*	99
17	719*	215
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21	892	936
22	736*	307
23	739	531
24	666	-804
25	918	-1113
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-18	695	-685
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-15	754	748
-14	591*	134
-13	569	-673
-12	711	-869
-11	743	-790
-10	621	756
-9	1274	1484
-8	471*	48
-7	456*	123
-6	833	-885
-5	1107	-1215
-4	655	613
-3	718	772
-2	432*	246
-1	433	466
0	537	-590

Table 7. Continued.

	H,5,11		-1 821* 128	0 600* 38	0 377* 38	14 911* -458	-4 633* -296	0 805* -77
			0 822* -29	1 665* 511	1 739 -681	15 1268 -1354	-3 891 -783	1 999 -649
1 669* 423			1 825* 156	2 605* -38	2 435* -142	16 897* 62	-2 632* 23	2 828* 118
2 673* -107			2 828* -136	3 2152 -2144	3 1688 -1899	17 1275 1379	-1 1487 1600	3 1912 1653
3 678* -96			3 832* -347	4 648* -70	4 543* -0		0 646* 97	4 871* 110
4 685* -199			4 836* -2	5 1499 1637	5 1831 1840	H,6,6	1 466 -447	5 887* -391
5 693 -448			5 841* 96	6 776* 270	6 673* 181		2 680* -49	6 912* -202
6 701* 159				7 1364 1419	7 734* 42	-19 1181 1065	3 1168 -1258	7 843 -901
7 711* 512			H,5,16	8 864* -166	8 804* -281	-18 926* 267	4 722* -46	8 973* 66
				9 2222 -2352	9 1991 -1856	-17 887 -823	5 1260 1199	9 1224 1180
	H,5,12		-15 819 -1073	10 882* -328	10 850* -51	-16 856* -537	6 785* -110	10 1031* 186
			-14 907* -16	11 891* 74	11 1389 1533	-15 733 -840	7 819* 261	11 1069* -213
-19 1103 -1319			-13 902* -403	12 903* 440	12 832* 474	-14 787* 257	8 854* 139	12 1107* -307
-18 677* 443			-12 888* 457	13 1799 1638	13 649 702	-13 1364 1404	9 1270 -1215	13 1025 -1042
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-16 835* 71			-10 878* -285	15 1455 -1323	15 1802 -1741	-11 689* -213	11 885 964	H,6,12
-15 815* 176			-9 781 -795	16 927* -454	16 871* -313	-10 663 -541	12 1000* -219	
-14 795* -407			-8 879* -168	17 933* -85	17 881 631	-9 1001 -1022	13 1011* 391	-15 834 1066
-13 1093 -1607			-7 867 -605	18 935* 402	18 896* 526	-8 608* 117	14 1022* 130	-14 873* 324
-12 758* 381			-6 873* 403	19 1334 1397	19 902 795	-7 1368 1414	15 1033 -1131	-13 870* -122
-11 1132 1126			-5 1237 1343	20 949* 219	20 913* -113	-6 572* 338		-12 859* -464
-10 732* 159			-4 878* -199	21 857 -976	21 1133 -1261	-5 554* 54	H,6,9	-11 767 -938
-9 1214 1245			-3 885* -410	22 967* -580		-4 545* -182		-10 848* -10
-8 716 -622			-2 894* -258	23 969 -648	H,6,4	-3 1604 -1748	-19 1214 -1281	-9 839 907
-7 1784 -1892			-1 1112 -1096	24 976* 249		-2 533* -19	-18 960* 389	-8 831* 333
-6 712* 240			0 912* 366	25 980 1104	-21 944 -872	-1 1247 1305	-17 925* 260	-7 824* 378
-5 708* 436			1 1311 1138		-20 1011* 187	0 543* 135	-16 898* -317	-6 818* -214
-4 712* 545			2 941* -38	H,6,2	-19 1197 1189	1 594 491	-15 1777 1574	-5 1679 -1402
-3 1582 1520			3 950* 145		-18 939* 460	2 581* -9	-14 838* -55	-4 842* -80
-2 724 -598			4 972* -292	-25 1001 871	-17 897* 114	3 1405 -1489	-13 1358 -1155	-3 1166 693
-1 2137 -1824			5 1216 -1198	-24 1119* 502	-16 862* -547	4 636* -27	-12 783* 362	-2 832* 202
0 746* 157			6 998* 324	-23 1129* 270	-15 1516 -1374	5 478 536	-11 680 -659	-1 754 817
1 750* -225			7 1232 927	-22 1117* -445	-14 780* -25	6 716* -164	-10 739* -178	0 857* -93
2 767* 473			8 1009* 30	-21 1116 -1131	-13 1126 1096	7 833 983	-9 1392 1492	1 1372 -1196
3 2273 1943			9 1015* 472	-20 1072* -63	-12 702 554	8 809* 64	-8 707* -161	2 881* -59
4 858* -443			10 1021* -327	-19 1033* 532	-11 664* 288	9 1562 -1342	-7 851 -850	3 902* 340
5 1300 -1152			11 1452 -1005	-18 993 636	-10 627* -325	10 890* 171	-6 688* 127	4 916* 78
6 837* -86				-17 954 851	-9 1339 -1616	11 923* 132	-5 1097 -949	5 840 850
7 789 -813			H,5,17	-16 909* -355	-8 558* -206	12 956* -298	-4 676* 39	6 965* 37
8 886* 362				-15 1577 -1585	-7 647 749	13 1405 1240	-3 1566 1932	7 883 -933
9 1875 1458			-3 879* -135	-14 825* -388	-6 495* 267	14 962* 3	-2 684* -15	8 1017* 21
10 936* -259			-2 880* 77	-13 781 615	-5 1296 1553	15 836 -959	-1 690* -342	9 1045* -272
11 970* -532			-1 880* 166	-12 738 523	-4 454* -127	16 931* 404	0 699* -49	10 1074* -127
12 947* -167			0 881* -88	-11 1060 1353	-3 1535 -1747	17 928* -118	1 1755 -1562	11 987 1011
13 923 -989			1 883* -68	-10 652* -28	-2 437* -82	18 929* -231	2 728* -31	12 1140* 15
14 1054* 384			2 885* -52	-9 1469 -1401	-1 436* 178	19 831 799	3 1548 1366	13 1170* -536
15 1317 1350			3 898* -195	-8 559* -307	0 441* 135		4 770* 154	
				-7 513* -314	1 1457 1490	H,6,7	5 794* 173	H,6,13
	H,5,13		H,5,18	-6 468* 232	2 484* 7		6 826* -178	
				-5 1454 1793	3 1519 -1624	-21 1273 1290	7 1759 -1592	-13 824 -856
-7 761* 66			-1 996* -294	-4 383* 2	4 564* 87	-20 1003* -143	8 888* -36	-12 909* 83
-6 756* -218			0 997* 342	-3 930 -1043	5 616* -116	-19 965 -865	9 931 1015	-11 1095 1137
-5 753* 296			1 1223 1237	-2 321* -166	6 675* -81	-18 934* 475	10 967* 363	-10 883* -152
-4 750* -179				-1 1674 -944	7 1690 1498	-17 803 -976	11 1008 913	-9 875* 174
-3 749* -409			H,6,0	0 309* 20	8 812* -47	-16 866* -156	12 1055* -198	-8 868* 37
-2 748* 156				1 2038 2330	9 894 -833	-15 1641 1482	13 1552 -1330	-7 1448 -1507
-1 749* -138			0 501* -52	2 591* -21	10 897* 258	-14 801* -342		-6 866* 55
0 750* 69			1 2385* 1963	3 881 -816	11 1106 -975	-13 766* -487	H,6,10	-5 862 647
1 751* 466			2 619* -96	4 558* 139	12 882* -286	-12 739* 366		-4 868* -39
2 753* -142			3 772 601	5 1527 -1429	13 1439 1342	-11 1353 -1181	-17 944 -1058	-3 875 839
3 755* -160			4 493* 145	6 748* 8	14 870* -256	-10 689* 30	-16 911* -60	-2 882* -22
4 757* -53			5 1276 -1870	7 1687 1661	15 876* -322	-9 1580 1924	-15 791 807	-1 1259 -1262
5 774* -141			6 607* 126	8 817* -242	16 886* 455	-8 645* -201	-14 862* 633	0 901* 20
6 781* 177			7 1044 1049	9 814* 0	17 894 -744	-7 625* 210	-13 835* 370	1 920* 359
7 787* 363			8 710* -379	10 811* 320	18 900* -23	-6 607* 100	-12 817* -228	2 932* 125
			9 1148 969	11 1357 -1459	19 1110 977	-5 1859 -2184	-11 1325 -1400	3 1165 1028
	H,5,14		10 801* 131	12 827* 77		-4 589* -25	-10 775* -277	4 968* -45
			11 2114 -1903	13 1354 1124	H,6,5	-3 1120 1088	-9 764 554	5 1208 -1108
-17 1097 1300			12 892* 372	14 852* -416		-2 586* -70	-8 746* 326	6 1008* -220
-16 878* -226			13 663 625	15 869* 339	-21 1275 1300	-1 985 948	-7 1161 1057	7 1033* -168
-15 869* -352			14 971* -423	16 878* 283	-20 1004* -471	0 598* -10	-6 725* -79	8 1059* 144
-14 852* -241			15 1231 1204	17 1410 -1326	-19 963* 276	1 1786 -1771	-5 1488 -1250	9 967 1059
-13 1024 -737			16 1023* 66	18 901* 123	-18 928* 418	2 626* -18	-4 726* -218	
-12 867* 444			17 1276 -1278	19 915* 510	-17 1091 -1335	3 1028 965	-3 790* -155	H,6,14
-11 1363 1538			18 1023* 472	20 923* -562	-16 854* 102	4 680* 183	-2 736* 161	
-10 804* -121			19 1016* -140	21 935 747	-15 1363 1156	5 1371 1209	-1 1523 1355	-5 813 -787
-9 806* -142			20 1010* -484	22 944* 227	-14 776* -471	6 748* -49	0 752* 11	-4 916* 45
-8 830* -426			21 1007 955	23 852 -816	-13 738* 339	7 1961 -1960	1 1276 -1114	-3 923 1073
-7 1626 -1733					-12 702* 215	8 830* -310	2 781* -76	-2 931* 206
-6 792* 507			H,6,1	H,6,3	-11 1887 -2163	9 874* -57	3 802* -337	-1 941* -9
-5 1280 1297					-10 638* 178	10 925* 323	4 817* 32	0 959* -110
-4 794* 68			-23 1076 -1023	-23 1419 -1233	-9 1019 1022	11 1639 1566	5 1666 1412	1 868 -965
-3 801 628			-22 1076* 464	-22 1122* 293	-8 579* -231	12 1020* 78	6 866* -21	2 982* -39
-2 808* -461			-21 1072* 79	-21 1078* 674	-7 1383 1519	13 1064 -1056	7 900 -573	3 995 572
-1 1574 -1514			-20 1071* -417	-20 1041* -519	-6 532* 61	14 1028* -375	8 928* 105	4 1018* 66
0 833* 272			-19 1521 1463	-19 997 741	-5 1593 -1930	15 998* -384	9 861 -812	5 1033* 411
1 843 658			-18 1042* -173	-18 959* 159	-4 500* 630	16 973* 299	10 1001* -47	6 1056* 32
2 852* 143			-17 1434 -1312	-17 1694 -1693	-3 490* 328	17 1351 1337	11 928 1070	7 963 -873
3 782 870			-16 969* 571	-16 878* 404	-2 484* -63			
4 887* -417			-15 922 -859	-15 835* 489	-1 1511 1912	H,6,8	H,6,11	H,6,15
5 1518 -1533			-14 881* -232	-14 793* -496	0 492* -57			
6 943* 191			-13 1886 1954	-13 1774 1889	1 1788 -1973	-17 1116 -1035	-13 1443 -1486	-5 954 1138
7 945* 258			-12 792* -252	-12 715* 23	2 530* -117	-16 878* -493	-12 843* 164	-4 961* -17
8 962* 260			-11 747 -708	-11 1475 -1611	3 688 -630	-15 850* 205	-11 831* 423	-3 969* 81
9 1206 1279			-10 705* 420	-10 630* 305	4 600* 154	-14 823* 483	-10 811* -219	-2 978* -18
10 1010* -345			-9 1098 -1302	-9 719 -528	5 2016 2161	-13 1227 1337	-9 1258 1213	-1 987 -1014
11 1035 -1020			-8 636* -127	-8 549* -229	6 691* 135	-12 764* 3	-8 784* -13	0 989* -20
			-7 1731 2273	-7 1538 1727	7 910 -919	-11 1067 -1167	-7 1300 -1243	1 992 759
	H,5,15		-6 497* -233	-6 477* -98	8 800* -301	-10 710* -373	-6 778* 145	2 995* 56
			-5 438* -145	-5 1533 -1686	9 946 -920	-9 696* -361	-5 773* 39	3 993* 220
-5 823* 178			-4 383* 106	-4 418* 165	10 918* 97	-8 676* 361	-4 776* -19	4 1004* -90
-4 821* 1			-3 2036 -2475	-3 872 -847	11 1810 1707	-7 1263 1327	-3 1588 1344	5 1427 -1042
-3 820* -169			-2 602* 37	-2 377* 26	12 953* 320	-6 648* 156	-2 780* -62	
-2 820* 189			-1 2117* 1632	-1 2586 2821	13 927 -683	-5 900 -881	-1 1629 -1371	

Table 7. Continued.

H,4,7		
1	1168	-1058
2	462	447
3	455	308
4	454*	55
5	1053	928
6	783	-724
7	1394	-1227
8	754	676
9	652*	-206
10	687*	-16
11	1179	1039

H,4,8		
-23	1408	1513
-22	613	-940
-21	782*	-264
-20	757*	116
-19	1160	-1213
-18	630	725
-17	1392	1425
-16	801	-927
-15	629*	-310
-14	608*	-233
-13	1955	-2050
-12	1430	1533
-11	1714	2009
-10	645	-646
-9	954	984
-8	928	-1093
-7	1957	-2345
-6	1165	1260
-5	940	1009
-4	467*	-73
-3	1110	1116
-2	1120	-1173
-1	2047	-2278
0	1137	1090
1	813	805
2	705	561
3	1946	2093
4	1432	-1501
5	1304	-2020
6	579*	199
7	610	-383
8	967	965
9	1794	1824
10	994	-999
11	1515	-1481
12	769*	-25
13	602	-573
14	1018	1043
15	1652	1698

H,4,9		
-19	910	-1045
-18	718*	-252
-17	696*	352
-16	620	664
-15	792	777
-14	626	-532
-13	739	-712
-12	582	-611
-11	565*	-104
-10	950	910
-9	1167	1100
-8	524*	-255
-7	779	-759
-6	358	-304
-5	504	-544
-4	580	635
-3	1121	1000
-2	506*	-245
-1	511*	-159
0	632	-446
1	1048	-992
2	758	637
3	872	803
4	567*	-295
5	591*	330
6	610*	-332
7	1274*	-1098
8	594	646
9	692	479
10	722*	-249
11	676	686
12	790*	-263
13	743	-632

H,4,10		
-22	744	-773
-21	1141	-1277
-20	778*	653
-19	756*	-543
-18	734*	456
-17	1450	1752
-16	837	-964
-15	811	-793
-14	639*	382
-13	878	-755
-12	739	766
-11	1861	1749
-10	1178	-1118
-9	795	-786
-8	554*	-83
-7	1755	-1522
-6	1105	1174
-5	1900	1827
-4	612	-532
-3	542*	254
-2	621	-701
-1	1941	-1732
0	1229	1079
1	1426	1563
2	576*	-337
3	592*	338
4	1134	-1039
5	2112	-2134
6	1081	961
7	945	921
8	695*	416
9	1138	1067
10	916	-655
11	1595	-1356
12	805*	360
13	832*	390
14	860*	474
15	1093	939
16	857	-775
17	1168	-1161

H,4,11		
-9	591	558
-8	521	-591
-7	1079	-902
-6	573*	-77
-5	575*	200
-4	572	496
-3	613	834
-2	519	-487
-1	722	-736
0	594*	-56
1	540	-584
2	612	583
3	1088	1041
4	634	-412
5	642*	-151
6	650*	-67
7	659	-593
8	669*	367
9	690	641

H,4,12		
-17	904	1000
-16	644	-784
-15	1405	-1449
-14	613	722
-13	669*	-9
-12	652*	225
-11	1074	1168
-10	773	-823
-9	1042	-1110
-8	551	530
-7	610*	-116
-6	545	586
-5	1929	1834
-4	1253	-1118
-3	1257	-1254
-2	621*	-35
-1	1260	-1077
0	1066	959
1	1757	1615
2	654	-619
3	670*	-533
4	682*	-203
5	1063	-895
6	882	883
7	1517	1403
8	763*	-345
9	786*	-82
10	809	-686
11	1396	-1253
12	864	668
13	801	999

H,4,13		
-9	658*	114
-8	653	-667
-7	916	-895
-6	650*	325
-5	654	480
-4	658*	365
-3	663*	414
-2	669*	-485
-1	828	-738
0	683*	108
1	692*	113
2	702*	286
3	873	756
4	725*	-403
5	663	-590
6	751*	184
7	759*	-179
8	768*	163
9	778	601

H,4,14		
-15	917	-1099
-14	657	838
-13	885	1059
-12	715*	-331
-11	629	688
-10	694	-684
-9	1416	-1473
-8	841	735
-7	686*	474
-6	683*	-2
-5	838	841
-4	615	-805
-3	1565	-1494
-2	624	679
-1	704*	336
0	719*	458
1	1497	1259
2	908	-814
3	1068	-1057
4	767*	127
5	785*	-244
6	799*	598
7	1154	1195
8	746	-645
9	856	-840
10	878*	-163
11	901*	-543
12	924	718
13	1163	1226

H,4,15		
-8	728*	-447
-7	724*	-528
-6	721*	411
-5	718	682
-4	717*	51
-3	716*	62
-2	716*	-404
-1	717*	-524
0	718*	260
1	720*	421
2	723*	56
3	727*	245
4	731*	-274
5	736	-703
6	742*	334
7	748*	204
8	754*	-68

H,4,16		
-9	929	-1118
-8	756	810
-7	925	1072
-6	758*	-327
-5	763*	237
-4	762*	-419
-3	942	-1034
-2	776	681
-1	784	834
0	792*	-99
1	808*	395
2	818	-709
3	1447	-1277
4	840*	520
5	844*	491
6	849*	309
7	1050	849
8	861	-652

H,5,0		
1	1985*	1558
2	973*	-702
3	2003	-3114
4	743	773
5	962	1056
6	529*	293
7	2571	3092
8	870	-975
9	2831	-3060
10	695*	404
11	737	-605
12	778*	358
13	2562	2242
14	601	-704
15	1764	-1521
16	899*	257
17	916	-827
18	911*	506
19	2733	2162
20	899*	-472
21	899*	-562
22	895*	-3
23	1443	-1251
24	897*	317
25	1452	1272

H,5,1		
-18	918	845
-17	876*	-452
-16	839*	-40
-15	565	480
-14	932	-853
-13	724*	67
-12	683*	475
-11	1043	-934
-10	606*	349
-9	565*	441
-8	525	-547
-7	731	737
-6	435*	67
-5	746	-758
-4	336	341
-3	429	387
-2	492*	-151
-1	490*	338
0	485*	-241
1	1231*	-946
2	497*	60
3	573*	0
4	643	477
5	1022	899
6	686*	-227
7	721	-651
8	769	-558
9	817*	-3
10	864*	550
11	910*	645
12	955*	89
13	1000*	-446
14	1044*	-679
15	1087*	-354
16	1131*	497
17	1174*	522
18	1217*	496

H,5,2		
-29	1167	-1207
-28	962*	283
-27	975*	651
-26	984*	134
-25	897	855
-24	1010*	-458
-23	1643	-1411
-22	991*	195
-21	962*	587
-20	932*	309
-19	1565	1547
-18	866	-658
-17	2452	-2375
-16	790*	266
-15	751*	-492
-14	715	660
-13	2146	2715
-12	783	-680
-11	1363	-1567
-10	564*	-104
-9	1052	-1127
-8	688	654
-7	2384	3088
-6	655	-673
-5	1299	-1457
-4	330*	-183
-3	2032	-2291
-2	1127	990
-1	3426	3228
0	419	-401
1	438	371
2	636	-585
3	2951	-3229
4	1000	882
5	2752	2443
6	695*	-384
7	726	649
8	698	-671
9	2837	-3280
10	859	786
11	1194	1327
12	726*	106
13	1478	1741
14	749*	-530
15	1526	-1866
16	774*	401
17	786*	233
18	796*	81
19	1656	1599
20	818*	-553
21	1699	-1636
22	841*	299
23	850*	-277
24	857*	246
25	1492	1478

H,5,3		
-18	745	857
-17	796*	-483
-16	758	-586
-15	720*	570
-14	683*	-434
-13	651*	101
-12	617	712
-11	580	-497
-10	545*	-6
-9	852	726
-8	474	-490
-7	439*	-92
-6	289	269
-5	842	-782
-4	357*	154
-3	514	486
-2	328*	-157
-1	325*	98
0	331*	-78
1	569	-547
2	373*	106
3	419	470
4	470*	259
5	533	509
6	604	-472
7	844	-787
8	722*	-138
9	757*	141
10	793	606
11	828*	212
12	864*	-171
13	899*	-391
14	935*	-461
15	970*	246
16	1006*	707
17	1041*	381
18	1077*	-9

H,5,4		
-27	1337	1305
-26	1068*	-153
-25	1045*	22
-24	1020*	-407
-23	1986	-1714
-22	955*	547
-21	1127	1236
-20	889*	106
-19	856*	539
-18	812*	-586
-17	1958	-2152
-16	743*	466
-15	1348	1412
-14	677*	118
-13	1503	1679
-12	607	-744
-11	1979	-2598
-10	542*	378
-9	511*	159
-8	589	566
-7	2155	2502
-6	720	-790
-5	2095	-2513
-4	392	269
-3	376*	-256
-2	600	665
-1	3140	3424
0	981	-972
1	2147	-2227
2	414*	-101
3	2162	-2233
4	980	850
5	2682	2849
6	588	-495
7	645	-622
8	708*	-132
9	1763	-1649
10	829	658
11	2310	2348
12	784*	-369
13	777*	124
14	771*	-420
15	2221	-2286
16	776	564
17	1308	1346
18	791*	-147
19	979	863
20	805*	-342
21	1675	-1640
22	828*	447
23	833	609
24	844*	-1
25	758	808
26	853*	-334
27	1048	-1064

H,5,5		
-16	651	-707
-15	630	562
-14	610*	76
-13	589*	-293
-12	569	583
-11	550*	-321
-10	531	-452
-9	512	399
-8	495*	-223
-7	586	-502
-6	565	523
-5	446*	-45
-4	431*	-68
-3	701	695
-2	422*	-184
-1	432*	-77
0	441*	-72
1	562	-475
2	478*	102
3	501*	338
4	531*	38
5	563*	-191
6	602*	-251
7	647*	-311
8	694*	223
9	749	644
10	774*	413
11	801*	-154
12	829*	-517
13	857*	-319
14	886*	-204
15	915*	359
16	944	725

H,5,6		
-25	924	-1008
-24	1000*	-155
-23	867	-922
-22	934*	531
-21	1808	1973
-20	867*	-324
-19	837*	-375
-18	802*	-391
-17	1582	-1431
-16	750*	593
-15	1662	1711
-14	677*	-118
-13	646*	-40
-12	620*	-489
-11	2123	-2450
-10	696	749
-9	1952	2223
-8	525*	33
-7	1470	1475
-6	979	-934
-5	2761	-3228
-4	660	567
-3	922	920
-2	460*	250
-1	1517	1614
0	754	-708
1	2358	-2635
2	497	451
3	521*	323
4	550*	493
5	2729	2728
6	757	-712
7	2161	-1949
8	698*	77
9	746	-757
10	796*	445
11	2680	2267
12	865*	-562
13	1243	-1183
14	848*	20
15	1167	-1196
16	818*	571
17	1675	1914
18	819*	-358
19	827*	-280
20	826*	-159
21	1178	-1293
22	834*	318
23	1032	996

H,5,7		
-16	747	-726
-15	721*	-60
-14	689*	441
-13	513	-488
-12	641*	341
-11	612*	281
-10	592	-633
-9	403	466
-8	552*	178
-7	378	-431
-6	368	396
-5	515*	176
-4	509	-360
-3	509*	155
-2	506*	-170
-1	505	-509
0	516*	157
1	530*	65
2	541*	165
3	559	504
4	584*	-56
5	610*	-490
6	639*	-181
7	674*	159
8	711*	281
9	755*	458
10	800*	93
11	601	-547
12	674*	-545
13	899*	-159
14	924*	234
15	949*	462
16	974*	385

H,5,8		
-21	1290	1369
-20	877*	-455
-19	1371	-1562
-18	817*	43
-17	790*	-593
-16	765*	646
-15	1972	2158
-14	709*	-495
-13	968	-917
-12	657*	-325
-11	1423	-1394
-10	615	680
-9	2198	2508
-8	579	-397
-7	913	-882
-6	560*	-409
-5	2027	-2327
-4	825	778
-3	1967	2137
-2	546*	-69
-1	675	645
0	394	-535
1	2058	-2146
2	412	520
3	1511	1594
4	626*	-16
5	1483	1146
6	681	-672
7	3153	-2716
8	742	509
9	780	796
10	815*	257
11	1761	1687
12	898*	-520
13	1934	-1631
14	921*	213
15	903*	-165
16	887*	233
17	1385	1373
18	867*	-389
19	1058	-1073
20	867*	81
21	868*	-452
22	868*	239
23	1056	1265

H,5,9		
-11	660	482
-10	641	-604
-9	629*	-102
-8	613*	323
-7	502	-580
-6	596*	150
-5	415	408
-4	591*	-364
-3	594*	-25
-2	598*	93
-1	603*	-315
0	611*	257
1	625	554
2	636*	41
3	654*	151
4	668*	-250
5	842	-759
6	700*	-80
7	713*	288
8	727*	313
9	741*	275
10	757*	-151
11	773*	-442

H,5,10		
-21	930*	637
-20	906*	-546
-19	1466	-1597
-18	850*	257
-17	734	804
-16	796*	298
-15	1577	1563
-14	744	-638
-13	2009	-2020
-12	703*	119
-11	691*	-359
-10	673*	562
-9	1916	1853
-8	647*	-469
-7	1595	-1478
-6	632*	-20
-5	627	-436
-4	560	556
-3	2465	2406
-2	638	-512
-1	1217	-1026
0	652*	-285
1	2073	-1792
2	672	659
3	2240	2204
4	710*	-260
5	731*	-171
6	754*	-310
7	1957	-1741
8	809*	536
9	1715	1542
10	868*	-116
11	903*	335
12	939*	-384
13	1643	-1651
14	964*	309
15	951	724
16	935*	41
17	1134	877
18	918*	-275
19	1113	-1257

H,5,11		
-7	682*	-27
-6	676*	18
-5	671	655
-4	667*	-230
-3	665*	-289
-2	664*	132
-1	664*	-385
0	666*	117

as peaks of average heights 47 and 17 electrons/Å^3, respectively. The highest electron density of the background was about 10 electrons/Å^3 but peaks of the height 30 electrons/Å^3 were found close to the uranium atoms.

All atoms were now included for a new series of least squares refinement. The scattering factors were those given by Cromer and Waber [7] for uranium and chlorine and by Berghuis *et al.*[8] for oxygen. For the uranium and chlorine atoms the real part of the dispersion correction was introduced.[9] Hughes' weighting scheme was used.[10] In addition to the positional parameters, individual scale factors for the seven layers and isotropic temperature factors for all atoms were refined. The R factor was lowered from 0.257 to 0.095 in four cycles.

In the difference Fourier map mentioned above, indications of anisotropic vibrations of the uranium and chlorine atoms were observed. Thus a refinement including anisotropic temperature factors for these atoms was carried out. At this stage an overall scale factor was introduced because of the risk of degeneracy between interlayer scale factors and anisotropic temperature factors expressed by, *e.g.*, Lingafelter and Donohue.[11] This refinement gave a final R factor of 0.091 after three cycles. In the last cycle all shifts in the parameters were less than 0.1 % of the calculated standard deviations. The final parameters and temperature factors based on the Mo$K\alpha$ data are given in Table 6 and observed and calculated structure factors obtained in the last cycle of the refinement are listed in Table 7.

A new difference Fourier map indicated that the accuracy of the experimental data was not sufficient to make an anisotropic refinement of the oxygen positions meaningful. Nevertheless an attempt was made to include anisotropic temperature factors for all atoms in a refinement which, however, resulted in some of the thermal parameters of five of the oxygen atoms being negative. In another refinement the imaginary part of the dispersion correction for the uranium and chlorine atoms [9] was included. No significant differences in the parameters and no change in the R factor were obtained.

To check the results of the least squares refinement and to confirm that no other atoms except hydrogen atoms were present in the unit cell, a final three-dimensional electron density map and a three-dimensional difference map were calculated using the parameters obtained in the last cycle of the least squares refinement and with all observed reflections included. All peaks in the difference map were less than 6 electrons/Å^3 (the average height of an oxygen peak was 20 electrons/Å^3) except for some spurious peaks close to the uranium atoms which had a height of about 10 electrons/Å^3. These are most probably due to the uncertainty in the absorption correction.

The Cu$K\alpha$ data were refined in the same way as described above for the Mo$K\alpha$ data. The final R factor was 0.099. The differences in the positional parameters between the two sets of data were for all values within three times the standard deviations with an average root mean square deviation of 0.05 Å for the oxygen atoms. However, the temperature factors calculated from the Cu$K\alpha$ data were about three times larger than those from the Mo$K\alpha$ data. This is probably due to a decomposition of the crystal during the investigation and the significance of the B values given in Table 6 may, therefore, be doubtful.

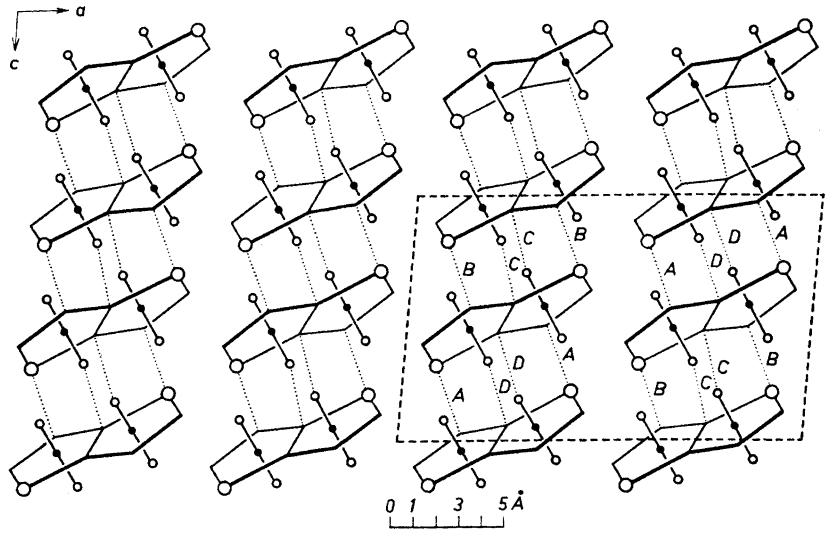

Fig. 1. Projection of the structure along the *b* axis. Uranium atoms are indicated by filled circles, uranyl oxygen atoms by small and chlorine atoms by large open circles. Other atoms are not marked. Those edges which are at a higher level are drawn as thick lines. The unit cell is indicated by dashed and possible hydrogen bonds by dotted lines. The letters refer to hydrogen bonds discussed in the text.

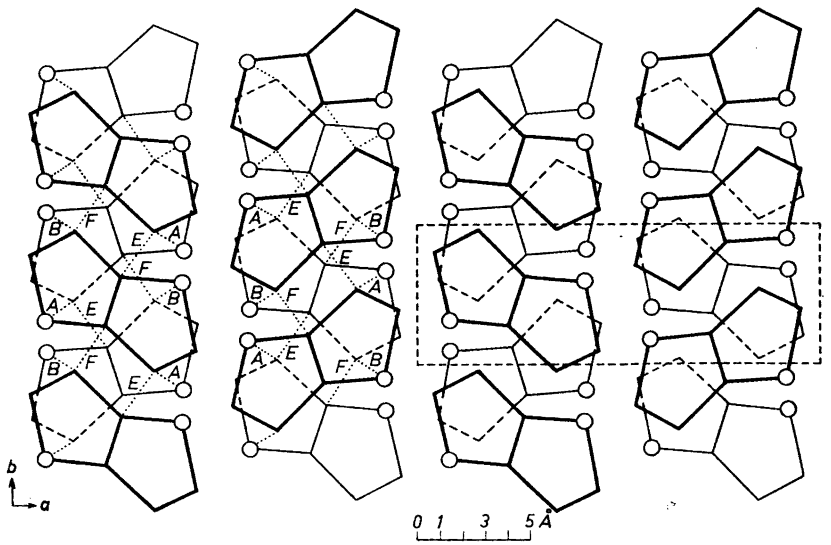

Fig. 2. Projection of the structure along the *c* axis. Designations as before except that the uranyl groups are left out for clarity.

DESCRIPTION OF THE STRUCTURE

Projections of the structure along the two shortest axes of the unit cell, the *b* and *c* axes, are shown in Figs. 1 and 2. The structure can be viewed as being built up from dimers of uranium atoms bonded by double oxygen bridges. The U(1)—U(2) distance within the dimer is 3.94 Å. The shortest distances between uranium atoms belonging to different dimers are 5.61 Å in the *a* axis direction, 5.62 Å in the *b* axis direction, and 5.50 and 5.54 Å in the *c* axis direction.

The structure of one dimer is shown in Fig. 3. Some important bond lengths and angles within the dimer are given in Table 8. Each of the two uranium atoms is surrounded by one chlorine and six oxygens at the vertices of a pentagonal bipyramid. Since two oxygens are shared between the uraniums

Table 8. Some important interatomic distances and angles. Standard deviations are given in parentheses.

	Distance (Å)		Distance (Å)
U(1)—U(2)	3.944(1)		
—Cl(1)	2.754(8)	U(2)—Cl(2)	2.748(8)
—O(1)	2.321(23)	—O(1)	2.391(21)
—O(2)	2.396(19)	—O(2)	2.349(21)
—O(3)	1.821(21)	—O(5)	1.812(20)
—O(4)	1.752(15)	—O(6)	1.760(20)
—O(7)	2.366(21)	—O(9)	2.406(20)
—O(8)	2.533(21)	—O(10)	2.462(32)
Cl(1)—O(1)	3.143(22)	Cl(2)—O(2)	3.134(21)
—O(3)	3.379(22)	—O(5)	3.271(21)
—O(4)	3.228(17)	—O(6)	3.334(22)
—O(8)	3.179(23)	—O(10)	3.108(33)
O(1)—O(2)	2.61(3)		
—O(3)	2.98(3)	O(2)—O(5)	2.94(3)
—O(4)	2.87(3)	—O(6)	2.98(3)
—O(9)	2.90(3)	—O(7)	2.93(3)
O(7)—O(3)	2.95(3)	O(9)—O(5)	3.06(3)
—O(4)	2.97(3)	—O(6)	2.89(3)
—O(8)	2.71(3)	—O(10)	2.81(4)
O(8)—O(3)	3.07(3)	O(10)—O(5)	3.10(4)
—O(4)	3.16(3)	—O(6)	2.99(4)
	Angle (°)		Angle (°)
Cl(1)—U(1)—O(1)	76.0(6)	Cl(2)—U(2)—O(2)	75.4(5)
O(1)— —O(2)	67.2(7)	O(2)— —O(1)	66.8(7)
O(2)— —O(7)	76.0(7)	O(1)— —O(9)	74.3(7)
O(7)— —O(8)	67.1(7)	O(9)— —O(10)	70.5(9)
O(8)— —Cl(1)	73.8(5)	O(10)— —Cl(2)	73.0(8)
O(3)— —O(4)	178.3(8)	O(5)— —O(6)	178.0(9)
U(1)—O(1)—U(2)	113.6(9)		
—O(2)—	112.4(8)		

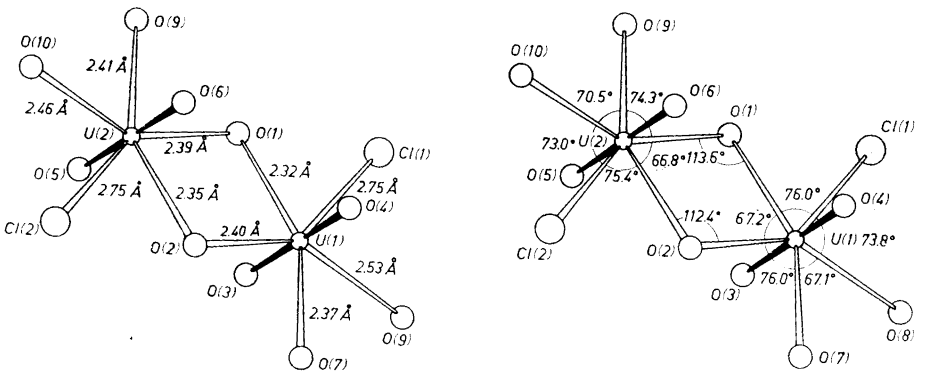

Fig. 3. The discrete group $[(UO_2)_2(OH)_2Cl_2(H_2O)_4]$ viewed along the *b* axis. O(1) and O(2) form a double oxygen bridge. O(3), O(4), O(5), and O(6) are the uranyl oxygen atoms whose bonds to the uranium atoms are filled in the figures. O(7), O(8), O(9), and O(10) are water oxygen atoms.

the dimer contains in total two chlorine and ten oxygen atoms. Four of these oxygens, O(3), O(4), O(5), and O(6), are more strongly bonded to the uranium atoms than the others. The distances vary between 1.75 and 1.82 Å with an average value of 1.79 Å. These oxygens form together with the uranium atoms two uranyl groups. The angles O(3)—U(1)—O(4) and O(5)—U(2)—O(6) are both 178° which is not significantly different from 180°, and the uranyl groups are thus linear. They also lie in the same plane. The deviations of the six atoms from the mean plane $0.267x+0.894y-0.531z-0.461=0$ obtained by the method of least squares are not significant (Fig. 4a).

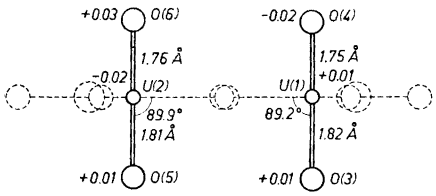

Fig. 4a. Plane through the linear uranyl groups. The dashed lines and circles indicate the rings. The figures give the deviations in Å (with sign) from the best mean plane obtained by the method of least squares.

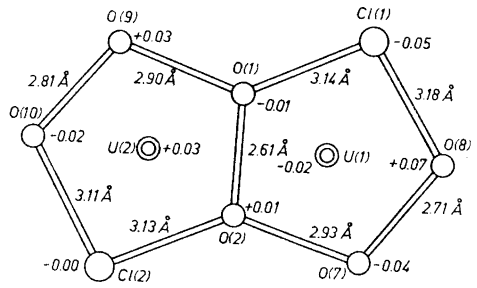

Fig. 4b. Plane through the two coplanar five-membered rings and the uranium atoms. The figures give the deviations in Å (with sign) from the least squares plane.

Table 9. Review of known uranyl compounds with sevenfold coordination of uranium(VI).

Compound	Five-ring members	U–O distance in UO_2^{2+} (Å)	Other U–O distances (Å)	Other distances (Å)	Reference
$K_3UO_2F_5$	5F	1.76		U–F = 2.24	12
$Cu(UO_2)_2(OH)_2(SO_4)_2 \cdot 6H_2O$	O in $3SO_4$ + 2OH				13
$[Ca(H_3O)_2](UO_2)_2(SiO_4)_2 \cdot 3H_2O$	O in $4SiO_4$				14
$Cs_2(UO_2)_2(SO_4)_3$	O in $5SO_4$	1.74	2.43		15
$Cs_x(UO_2)OCl_x$ ($x \approx 0.9$)	2Cl + 3O	1.82 and 1.85	2.26	U–Cl = 2.98 U–U = 3.704	16
$K_2(UO_2)_2V_2O_8$ $Cs_2(UO_2)_2V_2O_8$	O in $3V_2O_8$	1.77	2.32	U–U = 3.882	17
UO_3	5O	1.80 and 1.85	2.20–2.56	U–U = 3.690–4.279	18
$UO_2(C_9H_6NO)_2C_9H_7NO$	O + N in 2 oxine groups O in 1 oxine group	1.50 and 1.54	2.24–2.33		19
UO_2Cl_2 $UO_2Cl_2 \cdot H_2O$	4 Cl + O				20
$UO_2Cl_2 \cdot 3H_2O$	2 Cl + 3O				
$[(UO_2)_2(OH)_2Cl_2(H_2O)_4]$	1 Cl + 4O	1.79	2.32–2.53	U–U = 3.944 U–Cl = 2.75	

The U—O distances within the bridge formed by O(1) and O(2) are 2.32, 2.35, 2.39, and 2.40 Å which give an average value of 2.37 Å. The remaining oxygens, O(7), O(8), O(9), and O(10), are only coordinated to one uranium atom. Here the U—O distances vary between 2.37 and 2.53 Å. The U—Cl distances are both 2.75 Å. The difference in size between chlorine and oxygen atoms, in addition to the stronger U—O bonds within the uranyl groups, make the coordination polyhedra distorted. The two five-membered rings around the uranyl groups are coplanar. The least squares plane through all atoms in the dimer except the uranyl oxygens has the equation $-0.444x-0.349y-0.826z+7.112=0$. None of the ten atoms deviates significantly from this plane (Fig. 4b). The uranyl groups are perpendicular to the plane; the calculated angles are 89.2° and 89.9°.

The sevenfold coordination of uranium(VI) described here, with five atoms in the equatorial plane and the linear uranyl group perpendicular to the plane, has earlier been found in a great many compounds (Table 9). Comparison between the bond lengths given in Table 9 and those obtained in the present determination show good agreement with one exception. Such a high value as that of 2.53 Å for the distance U(1)—O(8) has only been found in a high-pressure form of UO_3.[18]

A review of the crystal structures, containing the uranyl group, known up to 1963 has been made by Evans.[21] He found that the uranyl group can coordinate four, five, or six oxygen atoms about its equator with a strong tendency to make these atoms coplanar. Fourfold and fivefold coordinations are geometrically stable. The oxygens can approach at an optimum distance in a plane without overcrowding. Stable planar sixfold coordination can occur when highly polarized, bidentate anionic groups donate the oxygen atoms which then can be drawn very close together. When oxygen atoms or hydroxide groups are brought into six-coordination around the uranyl group, they are forced out of the equatorial plane forming a puckered ring. Thus the stability of the structure tends to be reduced.

Crystal structure determinations published after 1963 show that some of the oxygens around the uranyl group can be replaced by other atoms, mainly chlorine atoms as in $Cs_x(UO_2)OCl_x$($x\approx0.9$),[16] the uranyl chlorides [20] and the present compound, without changing the coordination polyhedron except for some distortion due to the difference in size between oxygen and chlorine atoms.

Table 10. Short O—O (<3.0 Å) and O—Cl (<3.2 Å) distances and corresponding angles

	Distance (Å)	Letter in Figs. 1 and 2		Angle (°)
O(1)—O(3)	2.85(3)	C	O(3) —O(1)—O(7)	111.8(10)
—O(7)	2.65(3)	E		
O(2)—O(6)	2.93(3)	D	O(6) —O(2)—O(9)	116.2(9)
—O(9)	2.58(3)	F		
O(7)—Cl(2)	3.14(2)	A	Cl(2)—O(7)—O(1)	108.7(8)
O(9)—Cl(1)	3.15(2)	B	Cl(1)—O(9)—O(2)	109.6(8)

The dimers are arranged in sheets perpendicular to the $\vec{a}$ direction (Figs. 1 and 2). Since they are uncharged they must be held together by bonds of a different type than ionic, probably hydrogen bonds. In Table 10 short O—O and O—Cl distances are listed. These indicate the presence of hydrogen bonds. This assumption is supported by the size of the corresponding angles which are all rather close to the tetrahedron angle of 109°.

Four of the hydrogen bonds are extended mainly in the $\vec{c}$ direction, namely those joining an oxygen atom coordinated to only one uranium atom and a chlorine atom, O(7)—H···Cl(2) (A in Figs. 1 and 2) and O(9)—H···Cl(1) (B in Figs. 1 and 2), which are 3.14 and 3.16 Å, respectively, and those directed from a bridge oxygen atom toward a uranyl oxygen atom, O(1)—H···O(3) (C in Fig. 1) and O(2)—H···O(6) (D in Fig. 1), whose lengths are 2.85 and 2.93 Å, respectively.

The two remaining hydrogen bonds, which are the strongest ones, are extended in the $\vec{b}$ direction joining a bridge oxygen atom and the same singly coordinated oxygen atom as above, O(7)—H···O(1) (E in Fig. 2) and O(9)—H···O(2) (F in Fig. 2). Their lengths are 2.65 and 2.58 Å, respectively.

In all known crystal structures of uranyl compounds it has been found that water molecules never form bridges between the uranyl groups. Accordingly, two hydroxide groups most probably constitute the bridge and the O(7), O(8), O(9), and O(10) atoms, which are bonded to only one uranium atom, belong to water molecules. The formula of the compound should then be written as $[(UO_2)_2(OH)_2Cl_2(H_2O)_4]$ to be in agreement with the structure.

All the hydrogen atoms of O(1), O(2), O(7), and O(9) have been indicated by the presence of hydrogen bonds. The remaining water oxygen atoms, O(8) and O(10), have in total four hydrogen atoms which are difficult to locate. No distances are short enough to give evidence for hydrogen bonds. Possibly the hydrogens are directed towards the chlorine atoms with the following distances

O(8) —H ⟶	Cl(1)	3.27 Å
⟶	Cl(2)	3.25 Å
O(10)—H ⟶	Cl(1)	3.32 Å
⟶	Cl(2)	3.39 Å

According to Pimentel and McClellan[23] the upper limit of an O—H···Cl bond is 3.25 Å. The angles Cl(1)—O(8)—Cl(2) and Cl(1)—O(10)—Cl(2) are 95° and 76°, respectively, which is quite different from the tetrahedron angle.

The forces between the sheets of dimers must be rather weak as no short distances have been found indicating hydrogen bonds in the $\vec{a}$ direction. This is verified by the perfect cleavage of the crystals perpendicular to the a axis.

In conclusion it can be said that the group $(UO_2)_2(OH)_2$ which has been found in hydrolyzed solution seems to be retained on forming the crystalline state. Work is in progress on an investigation of hydrolyzed solutions of uranyl chloride using X-ray diffraction in order to compare distances and coordination in the crystalline and liquid states.

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