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IMIDAZOLIUM TETRACHLORODIOXOURANIUM(VI), & 3N2H5 ^2 #UO2C147~ 2

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IMIDAZOLIUM TETRACHLORODIOXOURANIUM(VI),
 $[\text{C}_3\text{N}_2\text{H}_5]^+]_2 [\text{UO}_2\text{Cl}_4]^{-2}$

Dale L. Perry, Derek P. Freyberg, and Allan Zalkin

January 1979

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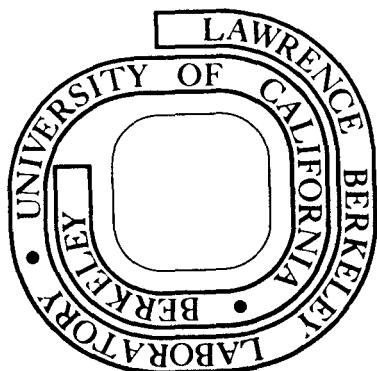
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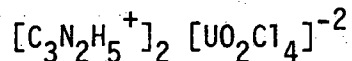


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IMIDAZOLIUM TETRACHLORODIOXOURANIUM(VI),



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JANUARY 1979

Imidazole forms complexes and salts with metal atoms in a variety of ways. A novel example is a ruthenium complex with a carbon-ruthenium bond.^{2a} We studied the reaction of imidazole with uranyl chloride to see if a similar derivative^{2b} could be made; instead, the resultant product was a hydrogen-bonded salt of the imidazolium cation with the uranyl chloride anion, $UO_2Cl_4^{-2}$.

The coordination chemistry of the uranyl ion, UO_2^{+2} , is governed by the ability of the uranium atom to achieve a high equatorial coordination number, most commonly five or six, about the linear uranyl axis; consequently, UO_2^{+} exhibits a wide variety of structures in its complexes when it forms adducts with organic donor molecules.³ Such compounds include mixed bridging and terminal ligands such as are found in uranyl acetate hydrates,⁴ "small bite" ligands such as peroxy groups,⁵ and mixed sulfur-oxygen chelates of alkoxides.⁶ The $UO_2X_4^{-2}$ (where X =

Cl, Br, I) series of complexes,⁷ however, has not received so much attention with respect to hydrogen-bonding as have other compounds involving more complex organic ligands; these compounds exhibit the smallest equatorial coordination number (four) known for the UO_2^+ ion and, as a result of the electronegative halide ligands, should be capable of accepting hydrogen bonds. The present report provides an example of such bonding to the imidazolium cation,⁸ which is stable and readily prepared. The parent imidazole molecule is known to undergo extensive hydrogen bonding⁹ in many of its metal complexes, with hydrogen-bonding playing a major role in its bioinorganic chemistry.¹⁰

EXPERIMENTAL

The title compound was prepared by dissolving 0.122 g. (2 mmoles) of imidazole (Aldrich Chemicals, 99% purity) and 0.341 g (1 mmole) of $UO_2Cl_2 \cdot 3H_2O$ (Alfa Chemicals, reagent grade) in hydrochloric acid which was maintained at a pH of ~ 2.5-3.0 followed by stirring for two hours. The reaction solution was allowed to evaporate slowly over a period of several days, yielding a batch of yellow, crystalline product. The crystals were filtered on a Buchner funnel and allowed to dry in air. Anal. Calcd. for $[C_3N_2H_5^+]_2[UO_2Cl_4]^{-2}$: C, 13.10; H, 1.82; N, 10.18. Found: C, 13.18; H, 1.74; N, 10.31.

A small yellow crystal, approximately $0.15 \times 0.13 \times 0.06$ mm in size, was glued to a glass fiber in air. Preliminary cell dimensions and the space group, $P2_1/n$, were obtained from Weissenberg photography. The crystal was placed on a Nonius CAD-4 automated diffractometer equipped with a Mo tube and a graphite monochromator, ($\lambda(K\alpha_1)$ 0.70930 Å). The setting angles of 22 reflections were used to determine by least-squares the following cell parameters: $a = 9.838(5)$ Å, $b = 10.891(5)$ Å, $c = 6.966(4)$ Å, $\beta = 104.56(5)^\circ$ and $V = 722.41$ Å³. For $Z = 2$ and a molecular weight of 550.01 the calculated density is 2.53 g/cm³.

Intensity data were collected at room temperature using the θ - 2θ scan technique with the scan angle calculated as $(0.60 + 0.35 \tan \theta)^\circ$ and variable scan times up to a maximum of 80 seconds. The counter aperture was 173 mm from the crystal and had a height of 4 mm and a variable width of $(2.50 + 0.50 \tan \theta)$ mm. Background was estimated from an extended scan of 25% on either side of the intensity scan. For reflections where $I > 50,000$ cps, an attenuator was inserted in the diffracted beam that reduced the intensity by a factor of 18.17.

Three standard reflections were measured every 5400 seconds. A total of 4539 scans, including standards, was processed to yield 2810 data which resulted in 1577 unique data after processing and averaging. Data that were space group extinctions, or too weak to be observed, or whose background ratios were greater than 4.0, were deleted from the data set. An absorption correction ($\mu = 114$ cm⁻¹) was applied¹¹ which ranged from 1.8 to 4.5. The crystal decay factor

based on the variations of the three standard reflections ranged from 0.99 to 1.02.

With two formula units in the unit cell, the uranium atom must be on a center of symmetry. A 3-dimensional Fourier calculated with all phases positive (U on the origin) indicated the positions of two chlorines, one oxygen and one nitrogen. Subsequent least-squares refinements and difference Fourier's revealed the rest of the structure. Some of the hydrogen atoms could be observed in the difference maps, but were neither the major peaks nor well resolved. Hydrogen atoms were included at their calculated positions (0.96 Å from N and C) in the final least-squares refinements, but not refined. Least-squares refinements in which the function $\sum w(|F_o| - |F_c|)^2 / \sum w F_o^2$ was minimized converged rapidly to the final structure. The expressions that were used in processing the data and estimating weights are given in the supplementary material; the "ignorance factor", p was set to 0.02. Scattering factors from Doyle and Turner¹² were used, and anomalous dispersion corrections¹³ were applied. Anisotropic thermal parameters were applied to all but the hydrogen atoms. No extinction correction was indicated and, none was made. Because of a few large discrepancies all 5 data below two-theta of 7.6° were zero weighted.

The discrepancy indices for 1494 data where $F^2 > \sigma$ and $7.6^\circ < 2\theta < 60^\circ$ are:

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.034$$

$$R_w = [\sum (|F_o| - |F_c|)^2 / \sum |F_o|^2]^{1/2} = 0.024$$

R for all 1577 data is 0.039. The error in an observation of unit weight is 1.02. In the last cycle, no parameter changed more than 0.005 σ . The largest peak in the final difference Fourier was 1.0 $e/\text{\AA}^3$ and is a ripple near the uranium atom.

RESULTS AND DISCUSSION

Atomic parameters, distances and angles are listed in Tables I-III. Figure 1 shows an ORTEP view of a formula unit with the numbering scheme used for the atoms in the tables.

The compound is a salt consisting of discrete planar imidazolium cations and octahedral tetrachlorodioxouranate anions. The closest non-hydrogen atom approaches between the two ions are 3.20 \AA between O and N(1), 3.33 \AA between Cl(1) and N(1), and 3.26 \AA between Cl(2) and N(2). The H(1)-Cl(1) and H(2)-Cl(2) distances are 2.51 \AA and 2.46 \AA respectively, and the angles N(1)-H(1)-Cl(1) and N(2)-H(2)-Cl(2) are 144° and 140° respectively; these values are consistent with the criteria for N-H...Cl hydrogen bond.¹⁴ Hydrogen bonding distances in $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ between O and Cl are 3.17 to 3.32, and for N to Cl they should be slightly larger.¹⁵

The imidazolium cation is a planar five membered ring. The geometry reported here is in good agreement with other determinations,^{16,17} with bond angles and distances within 4 σ of the literature values.

The tetrachloro dioxouranium(IV) anion is a tetragonally distorted octahedron, with four chlorine atoms in the equatorial positions and

the two uranyl oxygen atoms at the apices. The anion has been well characterized by other structure determinations.¹⁸⁻²⁴ The U-O distances reported for this ion²⁰⁻²⁴ range from 1.72 Å to 1.78 Å which compares to the 1.770 Å value reported here. The U-Cl distances reported for this ion²⁰⁻²⁴ range from 2.62 to 2.70 Å and span the two values reported here.

ACKNOWLEDGEMENT

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SUPPLEMENTARY MATERIAL AVAILABLE

Data processing formulas, and a list of observed structure factors (8 pages). Ordering information is given on any current masthead.

REFERENCES AND NOTES

1. National Science Foundation Postdoctoral Fellow, 1976-1977; Miller Fellow, 1977-79.
2. (a) Sundberg, R.J.; Bryan, R.F.; Taylor, I.F.; Taube, H. J. Amer. Chem. Soc. 1974, 96, 381; (b) The reaction of uranyl salts with imidazole in low pH solutions would be one obvious route to uranium-imidazole complexes with the imidazole ligand coordinated through the C-2 carbon. Any success in preparing such complexes will depend on the choice of other ligands around the UO_2^{+2} species utilized to stabilize the complex as a whole, especially in light of recent comments^{3a} regarding π -bonding ligands with the uranyl ion.
3. Two excellent reviews which address the coordination chemistry and concomitant structural phenomena of the uranyl ion are: (a) Cattalini, L.; Croatto, U.; Degetto, S.; Tondello, E. Inorg. Chim. Acta Rev. 1971, 5, 19 and (b) Casellato, U.; Vidali, M.; Vigato, P.A. Inorg. Chim. Acta Rev. 1976, 18, 77.
4. Howatson, J.; Grev, D.M. J. Inorg. Nucl. Chem. 1975, 37, 1933.
5. Alcock, N.W. J. Chem. Soc. (A) 1968, 1588.
6. Perry, D.L.; Templeton, D.H.; Zalkin, A. Inorg. Chem. 1978, 17, 3699.
7. Bailar, J.C.; Emeleus, H.J.; Nyholm, R.; Trotman-Dickenson, A.F. (Eds.) "Comprehensive Inorganic Chemistry," Vol. 5; Pergamon Press: New York, 1973.
8. Sundberg, R.J.; Martin, R.B. Chem. Rev. 1974, 74, 471.

9. (a) Prince, E.; Mighell, A.D.; Reimann, C.W.; Santoro, A. Cryst. Struc. Comm. 1972, 1, 247; (b) Strandberg, R.; Lundberg, B.K.S. Acta Chem. Scand. 1971, 25, 1767.
10. Matuszak, C.A.; Matuszak, A.J. J. Chem. Ed. 1976, 53, 280 and references therein.
11. Templeton, L.K.; Templeton, D.H. Abstracts, American Crystallographic Proceedings, Series 2, Vol. 1, 1973, p. 143.
12. Doyle, P.A.; Turner, P.S. Acta Crystallogr. 1968, Sect. A, 24, 390.
13. Cromer, D.T.; Liberman, D. J. Chem. Phys. 1970, 53, 1891.
14. Hamilton, W.C.; Ibers, J.A. "Hydrogen Bonding in Solids", W. A. Benjamin Inc: New York, 1968; Chapter 1.
15. (a) Zalkin, A.; Forrester, J.D.; and Templeton D. H. Inorg. Chem. 1964, 3, 529; (b) Baur, W.H. Inorg. Chem. 1965, 4, 1840.
16. James, M. N. G.; Matsushima, M. Acta Crystallogr. 1976, Sect. B, 32, 1708.
17. Freeman, H. C.; Huq, F.; Rosalky, J. M.; Taylor Jr., I. F. Acta Crystallogr. 1975, Sect. B, 31, 2833.
18. Clemente, D. A.; Bandoli, G.; Binetollo, F.; Marzotto, A. J. Cryst. Mol. Struct. 1974, 4, 1.
19. Bois, C.; Dao, N. Q.; Rodier, N. Acta Crystallogr. 1976, Sect. B, 32, 1541.
20. Bois, C.; Dao, N. Q.; Rodier, N. Inorg. Nucl. Chem. 1976, 38, 755.

21. Bombieri, G.; Forsellini, E.; Graziani, R. Acta Crystallogr. 1978, Sect. B, 34, 2622.
22. Di Sipio, L.; Tondello, E.; Pelizzi, G.; Ingletto, G.; Montenero, A. Cryst. Struct. Comm. 1974, 3, 297.
23. Graziani, R.; Bombieri, G.; Forsellini, E.; Paloucci, G. J. Cryst. Mol. Struct. 1975, 5, 1.
24. Di Sipio, L.; Tondello, E.; Pelizzi, G.; Ingletto, G.; Montenero, A. Cryst. Struct. Comm. 1974, 3, 527 and ibid. 1974, 3, 731.

Table I. Positional and Thermal Parameters^a with Estimated Deviations^b

ATOM	X	Y	Z
U	0	0	0
CL(1)	.0150(1)	-.1292(1)	.3341(2)
CL(2)	.1845(1)	.1632(1)	.1948(2)
O(1)	-.1389(3)	.0881(3)	.0483(5)
N(1)	.2980(5)	.0228(5)	-.3568(8)
N(2)	.4930(5)	-.0663(6)	-.2626(8)
C(1)	.3940(7)	.1117(6)	-.291(1)
C(2)	.5183(7)	.0542(8)	-.231(1)
C(3)	.3594(7)	-.0833(6)	-.3405(9)
H(1)	.1992	.0367	-.4092
H(2)	.5626	-.1311	-.2325
H(3)	.3775	.1994	-.2841
H(4)	.6100	.0909	-.1777
H(5)	.3139	-.1619	-.3782

ATOM	B11	B22	B33	B12	B13	B23
U	1.695(8)	2.079(9)	3.44(1)	.15(1)	.557(6)	-.06(1)
CL(1)	3.14(5)	2.85(5)	3.71(6)	.23(4)	.78(4)	.10(4)
CL(2)	2.79(4)	2.94(5)	4.61(6)	-.44(4)	-.01(4)	-.17(5)
O(1)	2.3(1)	2.9(2)	4.6(2)	.8(1)	1.2(1)	.1(1)
N(1)	2.7(2)	5.2(4)	4.9(2)	.7(2)	.7(2)	.8(2)
N(2)	3.9(2)	4.5(3)	4.3(3)	1.8(2)	.8(2)	.3(2)
C(1)	6.3(4)	2.8(2)	5.1(3)	.4(3)	2.0(3)	.3(2)
C(2)	3.4(3)	5.9(3)	4.0(3)	-1.3(3)	.5(2)	.1(3)
C(3)	4.4(3)	3.7(3)	4.0(3)	-.5(2)	.8(2)	.1(2)

^aThe anisotropic temperature factor has the form $\exp(-0.25(B_{11}h^2a^2 + 2B_{12}hka^*b^* + \dots))$. The hydrogen atoms were all assigned an isotropic thermal parameter of 6.0 \AA^2 .

^bHere and in the following tables the number in parentheses is the estimated standard deviation for the least significant figures.

Table II. Distances (Å)

			Corr. ^a
U	-2 O	1.770(3)	1.779
	-2 C1(1)	2.692(2)	2.697
	-2 C1(2)	2.657(2)	2.665
N(1)-	C(1)	1.350(7)	
	- C(3)	1.296(8)	
N(2)-	C(3)	1.303(9)	
	- C(2)	1.343(9)	
C(1)-	C(2)	1.344(8)	

^aCorrected for thermal motion assuming a "riding" model.

Table III. Selected Angles (deg.)

O	-U	-O	180.0
O	-U	-C1(1)	90.2(2)
O	-U	-C1(2)	90.1(2)
C1(1)-U		-C1(1)	180.0
C1(1)-U		-C1(2)	91.5(1)
C1(2)-U		-C1(2)	180.0
C(1)	-N(1)	-C(3)	109.8(5)
C(2)	-N(2)	-C(3)	109.4(6)
N(1)	-C(1)	-C(2)	106.0(6)
N(2)	-C(2)	-C(1)	106.8(6)
N(1)	-C(3)	-N(2)	108.0(5)

FIGURE CAPTION

Fig. 1. ORTEP drawing of one formula unit.

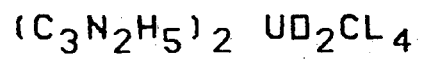
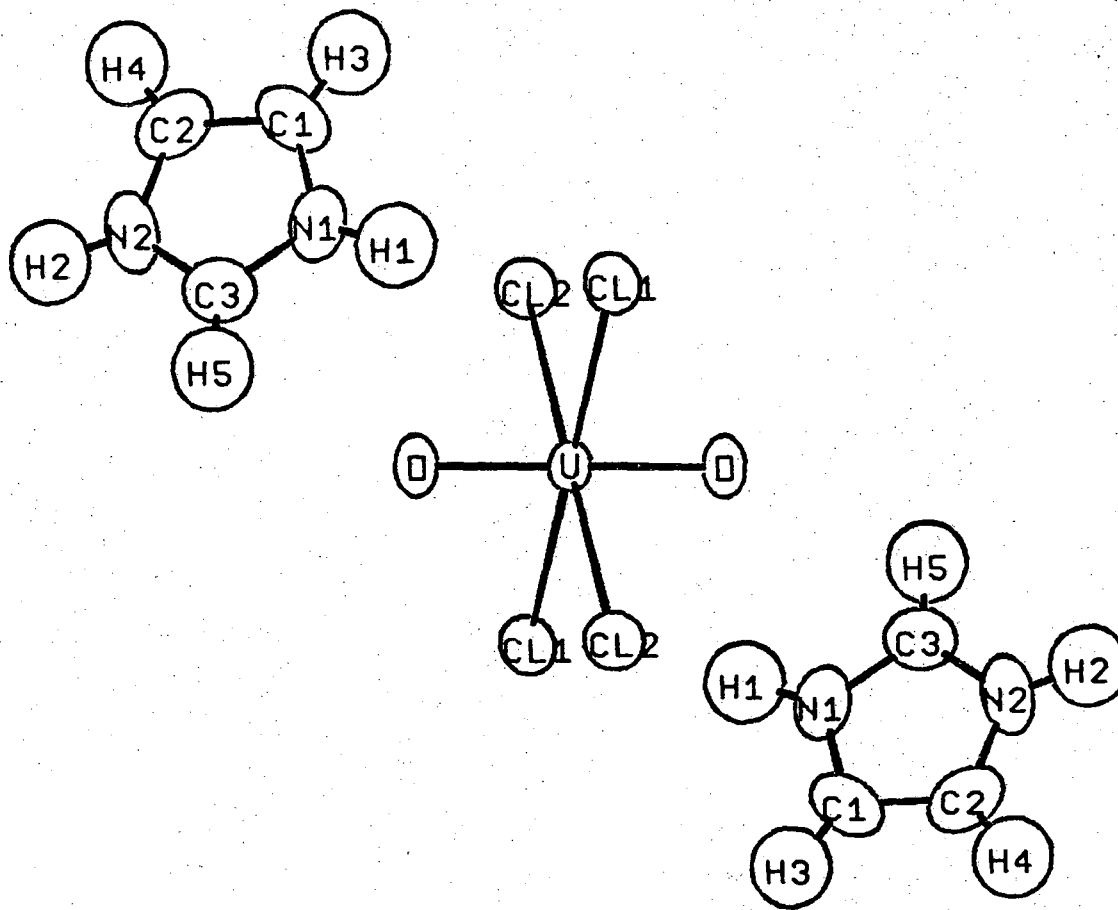
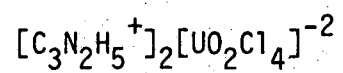


Fig. 1

XBL 789-10683

Supplementary materials for the paper

Imidazolium Tetrachlorodioxouranium(VI),



by Dale L. Perry, Derek P. Freyberg, and Allan Zalkin*

-16-
DATA PROCESSING FORMULAE

$$I = C - (t_c/2t_b)(B_1+B_2)$$

$$\sigma(B) = \text{Max}[(t_c/2t_b)(B_1+B_2)^{\frac{1}{2}}, (t_c/2t_b)|B_1-B_2|]$$

$$\sigma(I) = [C + \sigma^2(B)]^{\frac{1}{2}}$$

$$F^2 = (D \cdot A / L_p) I$$

$$\sigma(F^2) = (D \cdot A / L_p) \sigma(I)$$

$$F_a^2 = \Sigma F^2 / n$$

$$\sigma(F_a^2) = [\Sigma \sigma^2(F^2) / n]^{\frac{1}{2}} \quad \text{When } S(F_a^2) > 4\sigma(F_a^2), \sigma(F_a^2) \text{ is replaced by } S(F_a^2).$$

$$S(F_a^2) = [\Sigma |F^2 - F_a^2|^2 / n(n-1)]^{\frac{1}{2}}$$

$$\sigma(F_o^2) = [\sigma^2(F_a^2) + (pF_a^2)^2 + q^2]^{\frac{1}{2}}$$

$$F_o = (F_a^2)^{\frac{1}{2}}$$

$$\sigma(F) = F_o - [F_a^2 - \sigma(F_o^2)]^{\frac{1}{2}} \text{ when } \sigma(F_o^2) \leq F_a^2 \text{ or } [\sigma(F_a^2)]^{\frac{1}{2}} \text{ when } \sigma(F_a^2) > F_a^2$$

$$L_p = [\cos^2 2\theta_m + \cos^2 2\theta] / [\sin 2\theta (1 + \cos^2 2\theta_m)]$$

$$\text{wtg} = 1/\sigma^2(F)$$

C = counts recorded during a scan

θ_m = monochromater angle

I = individual raw intensity,
background removed.

θ = crystal diffraction angle

t_c = scan count time

S = scatter

t_b = background count time

a = average

B_1 = individual background count

q = additional uncertainty that
affects the weak intensities

$\sigma(B)$ = estimated standard deviation of the total background count

p = estimate of non-statistical errors

F = structure factor

wtg = weighting factors in least squares

D = decay correction; an empirically applied correction obtained from the fluctuations of the standard reflections.

A = absorption correction

L_p = Lorentz and polarization corrections

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 5.0)
 IMIDAZOLIUM URANYL CHLORIDE F(0,0,0) = 2481

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
 SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
 * INDICATES ZERO WEIGHTED DATA.

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
	K,L=	0,	0	-4	561	9	7	-5	125	9	3	3	637	9	5	-10	186	5	16
2	892	9	-20	-2	450	7	12	-3	128	10	-2	4	281	3	0	-8	167	5	3
4	735	9	-3	0	440	6	6	-1	98	9	12	5	444	6	7	-6	277	5	-8
8	405	6	2	2	451	6	-2	1	118	8	5	6	80	7	-2	-4	343	6	1
10	368	5	2	4	183	4	2		K,L=	1,	0	7	367	5	-4	-3	68	13	-1
12	220	5	7	6	256	4	-3	1	724	0	-16*	9	343	6	4	-2	197	4	3
	K,L=	0,	1	8	178	4	-3	2	58	4	-2	10	75	10	3	-1	28	31	15
-13	215	5	-6	10	97	8	6	3	625	7	-4	11	168	5	3	8	336	5	0
-11	273	4	1		K,L=	0,	5	4	225	3	1		K,L=	1,	3	1	136	4	1
-9	299	5	3	-13	137	11	30	5	603	10	-4	-12	201	5	1	2	295	4	-3
-7	603	9	-7	-11	189	6	6	6	65	6	4	-10	283	6	-5	4	222	5	-3
-5	683	8	0	-9	161	5	9	7	468	7	-7	-9	34	36	5	6	227	6	-2
-3	239	3	-8	-7	227	4	6	9	299	4	1	-8	427	7	1	7	72	16	-14
-1	891	0	56*	-5	306	5	-6	10	80	7	-1	-7	144	4	3	8	136	7	-6
1	748	8	-5	-3	164	4	6	11	262	4	6	-6	541	12	8		K,L=	1,	6
3	337	4	2	-1	342	5	4	13	171	6	7	-5	68	5	1	-11	187	7	5
5	432	6	3	1	328	6	-2		K,L=	1,	1	-4	595	12	14	-9	205	5	9
7	217	3	6	3	185	4	-4	-12	247	5	-2	-3	65	8	1	-7	273	5	1
9	277	4	-1	5	256	5	3	-10	259	5	-1	-2	596	8	20	-5	324	6	-6
11	169	5	-2	7	178	4	6	-9	68	9	12	-1	131	3	2	-4	0	57	-12*
	K,L=	0,	2	9	128	7	2	-8	392	6	2	0	764	9	7	-3	358	6	7
-12	184	5	1		K,L=	0,	6	-7	159	3	2	1	165	3	0	-2	75	6	18
-10	116	5	2	-12	169	8	13	-6	555	11	-19	2	652	11	-9	-1	328	6	-2
-8	341	4	1	-10	174	6	12	-5	46	5	1	3	52	7	-3	1	290	6	-2
-6	319	6	-5	-8	282	6	1	-4	365	5	-1	4	418	6	3	3	261	5	-4
-4	298	4	0	-6	348	5	0	-3	342	4	6	6	332	5	-8	4	56	18	-2
-2	327	4	15	-4	231	7	5	-2	869	9	-22	7	54	14	-18	5	211	5	3
0	151	3	6	-2	292	5	5	-1	111	8	7*	8	309	5	-10	6	28	39	9
2	587	8	0	0	339	6	-4	0	667	8	4*	9	57	13	44	7	142	6	9
4	439	7	0	2	215	5	1	2	395	5	1	10	177	5	-1		K,L=	1,	7
6	247	4	-3	4	259	5	-6	3	363	4	10	11	0	40	-40*	-10	135	11	3
8	363	5	-2	6	156	6	1	4	571	8	14		K,L=	1,	4	-9	62	18	17
10	227	5	-9	8	116	11	2	5	17	31	-14	-13	162	7	-3	-8	166	6	-4
12	135	9	-2		K,L=	0,	7	6	354	5	0	-12	16	57	-27	-6	173	5	4
	K,L=	0,	3	-11	121	9	-3	7	0	29	-19*	-11	284	5	3	-5	52	17	32
-13	216	6	4	-9	141	6	10	8	314	5	1	-10	85	8	20	-4	177	6	5
-11	200	5	-6	-7	190	6	-1	10	234	5	3	-9	274	5	7	-3	67	16	-18
-9	377	6	-1	-5	176	7	-8	12	150	6	8	-7	290	4	4	-2	213	5	8
-7	449	7	-4	-3	171	6	-2		K,L=	1,	2	-6	151	5	9	0	126	5	1
-5	548	9	10	-1	162	6	1	-13	173	6	-6	-5	453	8	2	1	61	13	33
-1	503	7	18	1	110	8	-4	-11	210	4	-1	-4	88	6	2	2	147	5	6
1	763	10	8	3	153	5	3	-9	276	6	-2	-3	255	4	1	4	127	9	3
3	722	11	-1	5	114	9	27	-7	498	7	-1	-1	217	3	2	6	75	13	8
5	310	4	-4		K,L=	0,	8	-6	131	4	-5	0	164	4	-3		K,L=	1,	8
7	432	8	-3	-10	100	13	16	-5	410	6	3	1	456	6	0	-9	96	13	12
9	254	4	-2	-8	100	13	4	-4	85	3	4	3	227	4	1	-7	92	13	-3
11	145	7	2	-4	155	6	3	-3	560	7	10	5	195	5	-3	-5	108	10	20
	K,L=	0,	4	-2	109	7	-7	-2	174	4	10	7	203	5	-3	-3	127	6	12
-12	203	6	-4	0	89	13	3	-11	023	11	0	9	138	5	10	-1	94	8	-1
-10	312	5	7	2	132	6	-3	0	321	4	15	10	68	18	40	0	0	43	-15*
-8	327	6	0		K,L=	0,	9	1	680	7	1		K,L=	1,	5	1	95	8	3
-6	403	7	19	-7	87	15	5	2	67	4	4	-12	154	9	9	3	105	8	-1

STRUCTURE FACTORS CONTINUED FOR
INDAZOLIUM URANYL CHLORIDE

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
4	69	17	28	-1	557	7	28	6	230	5	-4	K _p L=	2,	8	-2	131	3	3	
	K _p L=	1,	9	0	615	7	-1	8	209	4	-6	-10	107	11	2	-1	731	9	22
-8	70	20	-15	1	101	3	1	10	153	6	-2	-8	122	8	13	0	155	3	2
-7	0	64	-9*	2	570	7	-6		K _p L=	2,	5	-6	142	7	1	3	458	6	6
-6	96	11	-8	3	51	7	10	-13	157	8	11	-4	144	6	-5	4	95	4	4
-5	0	57	-1*	4	323	5	2	-12	0	69	-34*	-3	39	43	29	5	504	8	2
-4	113	9	1	5	266	4	-2	-11	184	6	3	-2	124	8	1	6	53	12	-17
-2	115	12	16	6	416	6	-5	-9	227	5	1	0	141	6	2	7	347	5	-1
0	104	19	6	7	66	6	-7	-7	296	6	-8	2	114	7	9	9	184	4	1
	K _p L=	2,	0	8	254	5	-5	-6	44	18	30	3	27	47	-1	11	194	5	-2
0	888	0	-113*	9	69	11	-10	-5	285	5	-5	4	105	9	13	12	0	47	-11*
1	131	2	3	10	204	4	0	-4	111	7	-5		K _p L=	2,	9		K _p L=	3,	3
2	776	9	-16	11	47	30	-1	-3	360	15	6	-8	37	47	16	-12	204	6	1
3	184	3	4	12	160	6	-5	-1	345	5	-2	-7	96	13	14	-10	251	6	-1
4	633	8	3		K _p L=	2,	3	0	90	4	-4	-5	77	17	-8	-8	208	4	0
5	66	4	-1	-13	170	8	-3	1	268	4	-3	-3	85	14	-5	-7	74	9	5
6	485	7	0	-11	242	5	9	2	150	3	-2	-1	80	12	-1	-6	441	7	-4
8	421	6	-1	-10	0	41	-10*	3	307	5	-3	1	84	17	16	-4	334	5	10
9	164	5	-6	-9	254	6	2	5	186	4	-2		K _p L=	3,	0	-3	24	30	-6
10	275	4	6	-8	108	5	-3	6	78	10	-4	1	342	4	-5	-2	354	6	9
11	0	46	-26*	-7	387	6	-7	7	166	5	-1	2	111	3	8	-1	81	5	6
12	183	5	1	-6	42	11	-15	8	56	58	11	3	638	8	-1	0	530	8	1
13	51	28	50	-5	444	8	-11	9	148	8	4	4	0	23	-10*	1	29	9	12
	K _p L=	2,	1	-4	145	4	5		K _p L=	2,	6	5	196	3	1	2	159	3	-2
-13	180	6	2	-3	488	7	16	-12	119	10	-1	7	365	6	-1	3	54	6	3
-12	53	15	-3	-2	213	3	12	-10	164	7	2	9	291	5	-3	4	377	6	6
-11	223	4	2	-1	535	8	12	-8	173	5	-5	11	160	7	3	5	31	23	17
-9	378	6	0	0	0	24	-10*	-7	36	21	19	13	192	7	11	6	283	4	-1
-8	130	4	2	1	526	7	-1	-6	213	5	2		K _p L=	3,	1	8	134	4	-1
-7	390	6	-2	2	120	3	3	-5	80	10	2	-12	149	7	-2	10	199	5	1
-6	92	3	2	3	419	7	-3	-4	232	5	-5	-10	275	5	-3		K _p L=	3,	4
-5	604	8	2	5	371	5	-5	-2	200	4	-8	-8	349	5	-5	-13	151	7	2
-4	187	3	7	6	121	4	1	-1	31	40	17	-7	111	4	1	-11	178	7	-6
-3	646	8	-14	7	268	4	-9	0	223	5	5	-6	373	6	6	-9	215	5	2
-2	334	4	10	8	0	45	-2*	1	46	15	5	-5	167	3	-1	-7	336	7	0
-1	575	7	33	9	218	5	11	2	213	4	-3	-4	661	9	-24	-6	74	13	-2
1	934	10	-22	10	52	30	29	3	81	9	17	-3	159	2	2	-5	311	5	-1
2	370	5	16	11	165	6	-4	4	149	5	-7	-2	620	8	-7	-4	121	4	4
3	505	6	1		K _p L=	2,	4	6	133	6	0	-1	34	20	-11	-3	385	7	-8
4	135	3	1	-13	0	47	-10*	8	111	10	-7	0	637	8	5	-1	543	9	2
5	430	6	2	-12	208	6	-2		K _p L=	2,	7	1	197	2	2	1	323	4	2
6	142	4	5	-10	215	5	-2	-11	120	8	1	3	166	2	6	2	62	6	1
7	442	7	-1	-9	0	40	-20*	-10	47	52	7	4	512	9	6	3	388	6	-4
8	95	5	-5	-8	330	6	-1	-9	147	7	10	6	507	8	-2	4	55	10	9
9	257	5	-6	-7	63	12	5	-8	54	14	4	8	443	6	2	5	355	5	1
10	56	13	42	-6	427	7	6	-7	143	6	-2	10	215	4	-4	7	187	4	-5
11	198	6	-5	-5	198	6	-5	-5	208	5	-3	12	239	5	3	9	236	5	8
	K _p L=	2,	2	-4	388	7	1	-4	186	9	19		K _p L=	3,	2		K _p L=	3,	5
-12	201	5	4	-3	100	4	2	-3	162	6	-5	-13	164	7	5	-12	166	7	2
-10	267	5	-10	-2	576	9	7	-2	55	18	4	-12	38	43	8	-10	214	6	7
-8	325	6	2	-1	177	4	3	-1	168	6	-2	-11	308	5	-8	-8	336	6	3
-7	104	5	-1	0	431	6	5	1	191	5	-2	-9	368	6	5	-7	50	18	13
-6	427	7	-7	1	186	3	-2	2	85	12	9	-8	53	8	5	-6	266	4	-3
-4	562	8	-9	2	403	6	-2	3	128	7	0	-7	412	6	-3	-5	41	19	37
-3	0	41	-4*	4	380	6	-8	4	49	38	33	-5	767	11	-8	-4	368	6	1
-2	344	4	3	5	144	4	3	5	116	10	-7	-3	573	8	0	-3	22	35	11

STRUCTURE FACTORS CONTINUED FOR
IMIDAZOLIUM URANYL CHLORIDE

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-2	418	6	-3	4	492	7	3	-12	0	47	-32*	7	148	6	-6	K,L=	5,	1	
-1	75	6	-1	5	114	3	2	-11	209	5	4	8	0	44	-13*	-12	174	6	-14
0	285	5	4	6	288	4	4	-9	215	5	-3	9	116	9	-3	-11	0	41	-15*
1	82	5	6	7	74	9	-5	-8	33	35	-6	K,L=	4,	6	-18	209	4	-5	
2	350	5	-4	8	287	4	3	-7	287	5	0	-12	92	13	-18	-8	293	5	5
4	251	4	1	10	217	4	2	-5	278	5	-2	-11	29	48	-2	-7	101	5	-4
6	168	4	5	12	172	5	6	-3	277	5	-1	-10	146	7	-3	-6	430	6	-5
7	57	16	7	K,L=	4,	1	-2	181	4	-1	-8	150	6	1	-4	416	6	-8	
8	176	6	2	-13	151	8	7	-1	394	6	2	-6	136	8	2	-3	199	3	-1
K,L=	3,	6	-11	198	6	-1	0	79	3	2	-4	186	7	-7	-2	598	8	-19	
-11	112	13	-5	-10	61	13	20	1	323	5	7	-2	176	4	0	-1	146	4	1
-9	197	6	2	-9	346	6	2	3	266	4	6	0	142	6	-2	0	567	9	-3
-7	165	7	2	-8	125	4	0	4	101	4	-2	2	149	5	1	1	47	7	-2
-5	181	5	-8	-7	275	4	-1	5	297	4	-5	3	0	59	-48*	2	593	8	8
-3	249	5	-3	-6	69	6	-4	6	61	7	0	4	113	7	1	3	219	3	0
-2	35	37	8	-5	521	9	2	7	195	5	1	6	121	8	9	6	382	6	-2
-1	128	4	2	-4	63	8	0	8	22	47	21	K,L=	4,	7	8	317	4	4	
1	223	5	-1	-3	784	11	-13	9	163	5	1	-11	116	8	17	9	55	15	-3
3	169	4	-1	-2	270	4	3	18	34	42	18	-9	142	7	6	10	274	5	2
5	94	7	0	-1	562	7	10	11	144	6	-6	-7	128	8	-5	11	0	44	-34*
7	138	7	-5	0	121	3	3	K,L=	4,	4	-6	0	41	-21*	12	168	6	-6	
K,L=	3,	7	1	735	10	-6	-12	161	6	-3	-5	170	5	-4	K,L=	5,	2		
-10	147	6	17	2	36	15	-3	-11	54	57	28	-4	37	41	24	-13	166	6	0
-9	47	37	14	3	602	10	-2	-10	174	5	-3	-3	171	5	-3	-12	34	58	-4
-8	134	8	1	4	60	4	-3	-8	282	5	1	-2	21	46	20	-11	236	7	-1
-6	171	7	1	5	548	8	2	-7	33	36	16	-1	204	6	8	-9	294	6	-4
-4	209	5	1	6	22	38	12	-6	356	8	0	1	202	4	4	-7	394	6	1
-3	67	14	18	7	461	7	-4	-5	52	11	-3	3	138	6	4	-6	140	4	-2
-2	151	6	-9	8	74	6	3	-4	313	6	-4	4	29	43	4	-5	451	7	-11
0	201	5	3	9	277	4	2	-3	124	5	3	5	151	6	7	-4	0	31	-41*
1	23	38	13	11	239	5	-3	-2	495	8	-1	6	0	53	-2*	-3	569	10	-7
2	170	5	-5	12	18	40	12	-1	64	6	-4	K,L=	4,	8	-2	109	4	-9	
3	0	41	-7*	K,L=	4,	2	0	392	6	-1	-9	40	47	36	-1	513	7	1	
4	116	8	1	-12	212	5	-2	1	32	34	22	-8	124	8	-7	0	200	3	5
5	36	56	23	-10	358	5	-2	2	391	6	-4	-6	149	8	2	1	354	5	-1
6	138	7	0	-9	33	36	-2	3	93	4	5	-4	141	6	5	2	51	7	-4
K,L=	3,	8	-8	386	6	-4	4	413	6	-4	-2	133	7	0	3	554	9	0	
-9	111	12	9	-7	35	18	1	6	259	4	3	-1	0	45	-25*	4	177	3	-2
-8	16	45	15	-6	435	7	-12	8	228	6	0	0	154	6	8	5	369	6	1
-7	137	7	2	-5	187	4	1	10	177	5	14	2	101	8	10	6	57	7	0
-6	47	48	25	-3	78	7	-1	K,L=	4,	5	4	89	14	3	7	220	4	-1	
-5	137	6	-13	-2	643	18	4	-12	0	58	-3*	K,L=	4,	9	8	59	12	33	
-3	115	12	-5	-1	73	4	-1	-11	183	6	-14	-7	68	14	-4	9	226	6	-2
-1	155	7	3	0	724	9	-6	-9	261	5	2	-4	0	48	-6*	10	57	14	-16
1	112	8	2	1	69	4	-2	-7	314	7	-13	K,L=	5,	0	11	138	6	-2	
3	84	16	2	2	533	7	7	-6	19	37	-14	1	530	7	0	K,L=	5,	3	
K,L=	3,	9	4	375	5	0	-5	321	6	-2	2	89	3	4	-12	156	8	-1	
-6	77	27	1	5	72	5	-4	-4	62	12	-13	3	431	6	-3	-10	236	5	-14
-5	41	78	34	6	422	6	-6	-3	412	8	-4	4	237	3	0	-9	0	38	-3*
-2	87	18	7	7	186	4	-8	-1	345	6	-5	5	395	6	-3	-8	250	5	-5
0	44	49	-19	8	211	4	4	0	32	27	7	7	315	4	-4	-7	113	7	-2
K,L=	4,	0	9	0	62	-8*	1	253	4	-2	8	55	13	2	-6	243	5	-6	
0	188	4	-2	10	189	4	4	2	54	8	-9	9	235	5	-2	-4	431	8	6
1	229	3	4	11	0	43	-18*	3	302	5	-1	10	92	7	0	-3	52	12	10
2	430	5	-3	K,L=	4,	3	4	51	13	-1	11	231	5	5	-2	417	8	4	
3	45	4	9	-13	125	9	-10	5	173	5	-5	12	65	17	60	0	259	4	1

STRUCTURE FACTORS CONTINUED FOR
IMIDAZOLIUM URANYL CHLORIDE

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
1	143	4	3	1	160	5	4	2	160	3	-1	-3	69	11	-1	-3	53	24	-22
2	302	4	-2	2	0	38	-10*	3	421	7	-7	-2	250	5	0	K,L=	7,	0	
3	84	5	1	3	126	7	2	5	494	8	-2	-1	84	6	-3	1	636	9	2
4	323	5	1	5	131	8	-6	7	185	4	3	0	292	5	-2	2	127	3	-6
5	71	7	10	7	91	10	-5	8	53	13	5	1	29	37	-2	3	517	7	2
6	222	4	0	K,L=	5,	7		9	246	5	2	2	317	5	-4	4	26	30	2
7	84	12	-7	-9	16	48	-7	10	0	41	-10*	4	165	4	-2	5	516	8	-3
8	198	5	5	-8	159	6	10	11	189	5	-1	6	231	6	-2	6	52	11	7
10	130	8	-8	-6	161	6	7	K,L=	6,	2		8	152	6	3	7	347	5	-5
K,L=	5,	4		-5	0	41	-25*	-12	184	6	5	K,L=	6,	5		8	71	7	14
-11	185	6	1	-4	145	7	-4	-10	200	5	-7	-11	168	7	1	9	254	5	-5
-10	64	14	39	-3	74	15	18	-8	367	7	-3	-10	47	48	41	11	230	5	6
-9	271	6	1	-2	180	8	-5	-7	0	42	-26*	-9	166	6	-3	K,L=	7,	1	
-8	24	38	10	-1	38	40	33	-6	284	5	-4	-7	191	5	-4	-12	196	6	6
-7	222	4	3	0	162	5	8	-5	92	5	-4	-6	0	39	-40*	-10	225	5	9
-6	185	6	4	2	138	8	-7	-4	385	7	-8	-5	275	6	-10	-9	0	40	-20*
-5	331	6	-6	4	140	7	10	-3	100	4	5	-3	206	6	-8	-8	250	5	-5
-3	432	8	-12	K,L=	5,	8		-2	662	11	-16	-1	274	4	0	-6	377	6	-8
-2	39	19	-2	-9	98	24	-10	-1	148	4	0	1	247	5	-1	-5	174	3	-1
-1	413	6	0	-7	114	8	-10	0	375	6	10	2	81	6	-1	-4	321	5	-4
0	196	4	0	-5	111	9	-12	1	87	3	-3	3	161	4	0	-3	49	16	8
1	383	6	-2	-3	138	7	-1	2	417	6	-3	4	38	33	-2	-2	433	7	-19
2	25	34	14	-2	52	17	16	3	45	11	-10	5	215	4	2	-1	66	14	9
3	386	4	0	-1	131	9	12	4	465	6	-4	7	124	8	-9	0	385	5	3
4	59	13	13	0	0	57	-5*	5	184	6	3	K,L=	6,	6		1	132	3	0
5	388	5	-4	1	98	9	-4	6	258	4	-2	-10	154	7	7	2	305	5	1
6	89	6	1	3	100	9	5	8	254	4	-8	-8	163	6	-3	4	392	6	4
7	235	5	-6	K,L=	5,	9		9	0	41	-36*	-6	217	5	-6	5	95	5	2
9	145	6	-2	-6	84	40	22	10	184	5	-4	-4	184	6	1	6	216	4	0
K,L=	5,	5		-4	78	27	12	K,L=	6,	3		-2	256	7	0	7	0	37	-9*
-12	138	8	0	K,L=	6,	0		-12	45	51	9	0	231	4	2	8	194	4	0
-10	218	5	0	0	548	9	-5	-11	160	6	2	2	131	5	-1	9	0	50	-17*
-9	74	14	22	2	351	5	-7	-10	52	20	-2	3	0	40	-21*	10	186	5	3
-8	257	5	4	4	505	8	1	-9	303	8	-5	4	192	5	-9	K,L=	7,	2	
-6	260	5	0	5	47	10	3	-7	285	5	-6	5	35	42	14	-12	0	54	-19*
-4	293	5	-6	6	408	7	-1	-5	265	6	-7	6	117	7	-5	-11	155	6	8
-3	96	6	3	7	55	7	0	-3	523	9	-9	K,L=	6,	7		-10	25	41	2
-2	319	6	-3	8	180	5	1	-1	347	5	4	-9	123	13	8	-9	173	5	-1
-1	21	34	19	10	268	5	-1	1	411	6	6	-7	143	6	-3	-8	67	8	1
0	355	6	5	11	48	27	11	2	0	29	-29*	-6	38	30	10	-7	230	4	-5
1	186	4	1	12	161	8	-8	3	413	6	-2	-5	114	7	6	-6	45	27	2
2	228	5	-2	K,L=	6,	1		4	51	11	-2	-3	164	6	3	-5	210	4	-2
3	51	16	8	-12	48	33	20	5	228	4	-1	-1	168	7	-5	-4	55	13	-13
4	202	5	-1	-11	231	6	1	7	285	5	-3	0	55	21	26	-3	328	6	-14
5	33	24	8	-10	27	45	7	8	0	39	-24*	1	93	9	-2	-1	325	5	-2
6	201	7	-7	-9	231	4	-2	9	169	5	1	3	136	6	5	0	0	36	-1*
7	78	25	28	-8	86	6	3	K,L=	6,	4		4	33	54	25	1	226	4	2
8	97	12	-9	-7	344	6	-4	-12	124	9	3	5	82	19	-15	2	162	3	5
K,L=	5,	6		-6	79	7	8	-11	42	58	9	K,L=	6,	8		3	399	6	-3
-11	109	15	-1	-5	386	6	-4	-10	212	5	-2	-8	123	11	18	5	256	4	5
-9	138	8	-10	-4	96	4	-2	-9	45	27	23	-6	92	13	17	7	202	4	-3
-7	186	6	2	-3	469	8	-7	-8	221	5	0	-4	102	10	6	9	224	5	3
-5	144	6	-2	-2	164	3	-1	-7	56	17	9	-2	99	13	-9	10	0	44	-31*
-3	158	5	2	-1	596	11	-22	-6	236	5	4	0	62	24	-19	K,L=	7,	3	
-1	197	5	-1	0	105	4	-3	-5	97	6	-6	2	89	11	-1	-12	146	7	0
0	58	14	1	1	383	4	4	-4	337	6	-10	K,L=	6,	9		-10	227	5	-7

STRUCTURE FACTORS CONTINUED FOR
IMIDAZOLIUM URANYL CHLORIDE

H	F08	SG	DEL	H	F08	SG	DEL	H	F08	SG	DEL	H	F08	SG	DEL	H	F08	SG	DEL
-9	62	15	12	5	165	6	8	-4	315	5	-5	1	174	6	2	10	98	10	-2
-8	384	5	0		K,L=	7,	7	-2	293	6	-8	3	194	5	3		K,L=	9,	2
-7	40	45	22	-9	0	47	-8*	-1	53	9	-7	5	145	6	9	-11	140	7	-5
-6	280	5	-9	-8	134	7	0	0	362	5	7	7	108	9	-10	-10	0	46	-6*
-4	448	8	-5	-7	0	47	-7*	1	40	13	11		K,L=	8,	6	-9	160	7	-10
-3	51	16	49	-6	136	9	6	2	339	5	-3	-10	136	10	-3	-7	146	5	-9
-2	466	9	-10	-4	189	8	-2	3	40	27	-7	-8	164	7	-8	-6	26	42	-17
0	367	6	2	-2	138	6	-7	4	304	4	1	-7	53	25	18	-5	277	5	0
1	18	32	-29	-1	43	48	-1	5	64	9	1	-6	191	5	-3	-4	30	37	-12
2	439	7	-1	0	98	9	-8	6	305	6	2	-4	218	6	-7	-3	202	4	-5
3	69	8	6	2	100	8	1	8	197	6	-3	-2	210	6	-9	-1	273	4	2
4	353	6	3	4	75	17	-10	10	164	6	2	0	205	5	2	0	87	6	-4
5	43	27	25		K,L=	7,	8		K,L=	8,	3	1	70	11	38	1	360	6	4
6	254	5	-2	-7	76	20	-9	-11	175	6	-2	2	209	5	5	2	74	5	-1
8	214	5	-6	-5	81	11	3	-9	218	5	0	3	14	42	-17	3	182	4	3
9	76	10	16	-3	98	11	1	-7	299	6	-7	4	165	6	7	4	83	6	6
10	140	6	4	-1	91	13	12	-5	347	6	-9	5	43	46	27	5	243	4	7
	K,L=	7,	4	0	28	55	17	-3	370	6	-19		K,L=	8,	7	7	229	6	8
-11	173	6	1		K,L=	8,	0	-2	81	8	-3	-7	127	10	16	9	137	6	7
-9	271	6	10	0	418	10	-26	-1	428	7	-7	-5	121	10	-7		K,L=	9,	3
-8	56	20	11	1	158	3	-4	0	83	8	7	-3	95	14	-20	-10	173	7	7
-7	216	5	-1	2	474	9	-12	1	377	6	-1	-1	103	10	1	-8	191	5	-1
-5	305	6	3	3	34	17	9	2	22	32	17	1	97	10	3	-6	308	6	-8
-3	324	6	-11	4	423	6	2	3	310	5	-6	3	66	59	-7	-4	243	5	-1
-1	272	4	3	5	67	10	0	4	93	6	-2		K,L=	8,	8	-2	288	5	-5
1	281	4	-6	6	291	4	2	5	315	5	3	-6	67	22	2	-1	38	32	-7
2	113	4	0	7	73	7	-1	6	54	11	-13	-5	34	40	21	0	401	7	-1
3	197	5	-4	8	280	5	3	7	224	5	5	-4	66	24	0	2	245	4	-3
5	212	5	5	9	30	48	11	8	0	52	-15*	-3	67	22	55	4	286	5	3
6	41	26	19	10	210	6	4	9	144	6	-5	-2	36	42	-34	5	52	16	17
7	156	5	-3		K,L=	8,	1		K,L=	8,	4	-1	41	48	35	6	225	5	9
8	32	37	-3	-11	172	6	-3	-10	154	10	0	0	33	55	-43	8	135	6	2
9	82	12	-5	-9	268	5	6	-8	195	7	-9		K,L=	9,	0		K,L=	9,	4
	K,L=	7,	5	-8	82	7	-6	-7	0	60	-32*	1	379	6	-4	-9	153	7	-6
-11	30	49	22	-7	257	6	3	-6	213	7	-2	2	0	32	-2*	-7	254	5	-5
-10	132	8	-10	-6	23	47	18	-4	195	5	-6	3	483	7	-4	-6	80	13	9
-8	150	6	3	-5	325	5	2	-2	254	5	-3	5	282	4	-3	-5	215	6	-2
-6	163	5	-10	-3	366	6	-3	-1	47	18	-7	7	293	8	-5	-3	222	6	-1
-5	32	44	25	-2	151	6	-5	0	210	5	5	9	230	8	0	-2	37	57	-29
-4	195	6	1	-1	296	5	-3	2	163	4	1		K,L=	9,	1	-1	272	6	-3
-2	191	7	-6	0	20	42	-17	3	62	12	16	-11	38	51	15	0	96	6	-1
-1	96	9	-9	1	356	5	3	4	164	6	1	-10	205	5	-1	1	180	4	7
0	238	5	-9	2	0	42	-2*	5	53	11	14	-9	73	13	19	3	226	5	-2
2	150	6	-4	3	303	5	-4	6	122	6	3	-8	238	4	-2	5	173	5	-3
4	178	5	3	4	66	7	3	8	111	7	12	-7	57	15	-13	6	0	41	-25*
6	184	5	3	5	228	4	-1		K,L=	8,	5	-6	225	5	1	7	80	14	-10
	K,L=	7,	6	6	49	14	18	-10	46	51	31	-4	387	6	-1		K,L=	9,	5
-9	146	7	4	7	205	5	4	-9	116	10	-14	-3	110	4	0	-10	111	12	14
-8	73	16	24	8	45	22	11	-8	28	45	5	-2	298	5	-8	-8	154	7	-5
-7	190	5	-3	9	148	6	-6	-7	159	6	12	-1	52	16	-13	-7	0	39	-11*
-5	180	5	-5		K,L=	8,	2	-6	40	42	1	0	294	5	5	-6	153	6	10
-3	198	5	2	-11	33	39	8	-5	138	6	-2	2	361	5	0	-4	175	5	-3
-1	241	6	-9	-10	179	5	5	-4	0	43	-49*	3	55	12	3	-2	195	7	-10
1	178	5	-3	-9	67	9	5	-3	177	6	-8	4	182	4	5	-1	24	40	10
3	139	7	-17	-8	199	5	-3	-2	0	40	-33*	6	233	4	-5	0	130	5	4
4	0	52	-4*	-6	251	5	-5	-1	183	5	-2	8	212	4	6	1	37	39	3

STRUCTURE FACTORS CONTINUED FOR
IMIDAZOLIUM URANYL CHLORIDE

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
2	185	5	1	6	236	4	0	-3	96	10	1	-1	183	6	-6	-3	168	7	-3
3	58	26	-1	7	77	9	18	8	45	47	7	1	229	5	-1	-2	0	65	-2*
4	157	6	-1	8	142	6	-4		K,L=	11,	0	2	52	19	6	-1	107	9	6
6	96	9	8	9	0	46	-38*	1	229	4	2	3	183	8	-3	1	149	5	-4
	K,L=	9,	6		K,L=	10,	3	2	76	7	2	5	148	6	9	3	162	5	9
-9	131	9	5	-9	133	7	-1	3	175	4	-3	6	59	17	44	4	60	18	56
-7	122	10	5	-7	192	6	-6	4	42	45	-8		K,L=	11,	5	5	63	19	-9
-5	136	7	-17	-5	243	6	-3	5	191	4	-2	-8	131	9	1		K,L=	12,	4
-4	0	46	-11*	-3	195	6	1	7	172	5	1	-6	176	9	-4	-6	116	13	-19
-3	191	6	2	-2	56	15	46	9	130	7	8	-4	173	6	-6	-4	198	9	8
-1	133	9	4	-1	255	6	0		K,L=	11,	1	-3	0	52	-12*	-2	130	8	-5
1	168	6	2	0	62	12	45	-8	198	5	7	-2	146	8	-2	-1	39	45	12
3	124	9	-6	1	219	4	4	-7	44	28	36	0	169	6	2	0	188	8	12
	K,L=	9,	7	2	22	50	16	-6	225	6	-2	2	145	6	-4	1	28	38	11
-6	119	11	15	3	176	4	-1	-5	82	10	-3	3	43	58	18	2	203	5	10
-4	116	8	-3	4	0	48	-41*	-4	224	5	1	4	184	8	-5	4	114	15	-6
-3	0	58	-33*	5	198	4	2	-2	278	6	-14		K,L=	11,	6		K,L=	12,	5
-2	186	13	20	6	38	23	34	0	311	5	8	-5	96	10	-3	-5	174	8	6
0	114	8	0	7	119	7	1	1	55	13	3	-4	48	49	32	-3	126	10	-3
2	90	14	-1		K,L=	10,	4	2	261	4	2	-3	88	11	1	-1	151	9	2
	K,L=	10,	0	-9	38	49	-14	4	262	4	5	-2	61	20	32	1	158	8	9
8	261	6	2	-8	144	9	-9	5	18	40	-20	0	66	26	45		K,L=	13,	0
2	297	5	-2	-7	37	46	-15	6	226	4	-2		K,L=	12,	0	1	198	5	6
4	206	5	-3	-6	187	6	-5	8	171	6	0	0	234	9	-12	2	43	14	21
5	0	47	-14*	-5	45	35	9		K,L=	11,	2	2	133	6	3	3	128	8	0
6	185	4	2	-4	176	5	8	-9	185	6	9	3	44	21	28	5	177	6	10
8	220	5	2	-3	98	8	-4	-8	47	38	41	4	146	6	5	6	39	64	1
10	125	7	7	-2	235	6	0	-7	242	5	10	6	196	5	8	7	125	10	4
	K,L=	10,	1	0	192	5	-5	-6	51	28	11	8	108	9	0		K,L=	13,	1
-10	37	40	-22	2	183	5	8	-5	226	6	-1		K,L=	12,	1	-7	73	28	66
-9	198	6	5	3	35	44	-17	-4	36	42	-8	-7	194	6	1	-6	177	6	-4
-7	209	4	1	4	190	5	4	-3	249	6	-10	-5	185	5	-1	-4	153	8	10
-6	82	8	-13	6	127	7	10	-1	286	6	8	-3	171	5	-5	-2	195	5	-5
-5	251	6	-3		K,L=	10,	5	8	9	35	-2*	-1	292	6	-13	-1	22	44	-32
-4	70	10	8	-9	109	15	-18	1	250	5	0	1	237	5	5	0	221	6	3
-3	284	5	-2	-8	0	48	-8*	2	188	5	7	2	48	19	25	1	51	23	-3
-1	249	5	-8	-7	159	7	-2	3	230	4	7	3	234	5	5	2	172	5	0
0	175	5	-2	-5	144	8	-2	5	186	5	6	4	40	34	26	3	30	41	26
1	390	6	3	-4	41	22	32	7	151	6	0	5	247	5	5	4	205	6	4
3	285	4	-1	-3	198	8	-1	8	70	17	24	6	0	45	-14*	5	48	38	0
5	216	4	2	-1	176	6	4		K,L=	11,	3	7	168	6	3	6	145	6	3
6	86	14	16	0	0	40	-39*	-8	138	7	0		K,L=	12,	2		K,L=	13,	2
7	252	5	3	1	161	5	-3	-6	156	9	5	-8	200	6	7	-7	185	6	8
9	168	7	9	3	163	6	-10	-5	45	40	-2	-7	57	22	37	-5	163	10	5
	K,L=	10,	2	5	104	9	3	-4	150	7	-4	-6	205	6	-3	-3	197	8	2
-10	169	6	-1		K,L=	10,	6	-2	161	6	5	-4	207	6	5	-1	198	6	3
-8	185	6	-6	-8	126	8	13	0	174	5	2	-2	274	6	1	8	43	33	36
-6	275	5	0	-6	117	8	-1	2	175	5	-4	0	207	5	-4	1	158	9	-1
-4	315	6	3	-4	140	7	-1	4	129	6	-2	2	227	5	3	2	63	18	-7
-3	110	6	-6	-2	126	7	10	6	113	7	-2	4	197	7	0	3	208	5	11
-2	228	5	-3	0	116	11	-2		K,L=	11,	4	6	110	7	2	4	55	21	44
0	345	6	1	2	139	14	3	-7	146	10	-8	7	0	54	-14*	5	146	7	16
1	73	18	11	3	56	24	49	-5	198	6	-1		K,L=	12,	3		K,L=	13,	3
2	297	4	0		K,L=	10,	7	-4	16	45	-4	-8	0	47	-11*	-6	114	9	1
3	99	5	-5	-5	125	11	8	-3	179	6	-1	-7	111	9	-15	-4	142	8	-7
4	223	5	1	-4	0	58	-7*	-2	52	31	1	-5	138	7	7	-3	43	48	32

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