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### Title

A STRUCTURE OF DI-Y-AQUO-BIS(DIOXODI-NITRATOURANIUM(VI) DIIMIDAZOLE,  
(UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>·H<sub>2</sub>O·C<sub>3</sub>H<sub>4</sub>N<sub>2</sub>)<sub>2</sub>. A WATER BRIDGED DIMER OF URANYL NITRATE

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## Materials & Molecular Research Division

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A STRUCTURE OF DI- $\mu$ -AQUO-BIS(DIOXODIIMIDAZOLE)NITRATOURANIUM(VI)  
DIIMIDAZOLE,  $[\text{UO}_2(\text{NO}_3)_2 \cdot \text{H}_2\text{O} \cdot \text{C}_3\text{H}_4\text{N}_2]_2$ ,  
A WATER BRIDGED DIMER OF URANYL NITRATE

Dale L. Perry, Helena Ruben, David H. Templeton, BERKELEY LABORATORY  
and Allan Zalkin

October 1979

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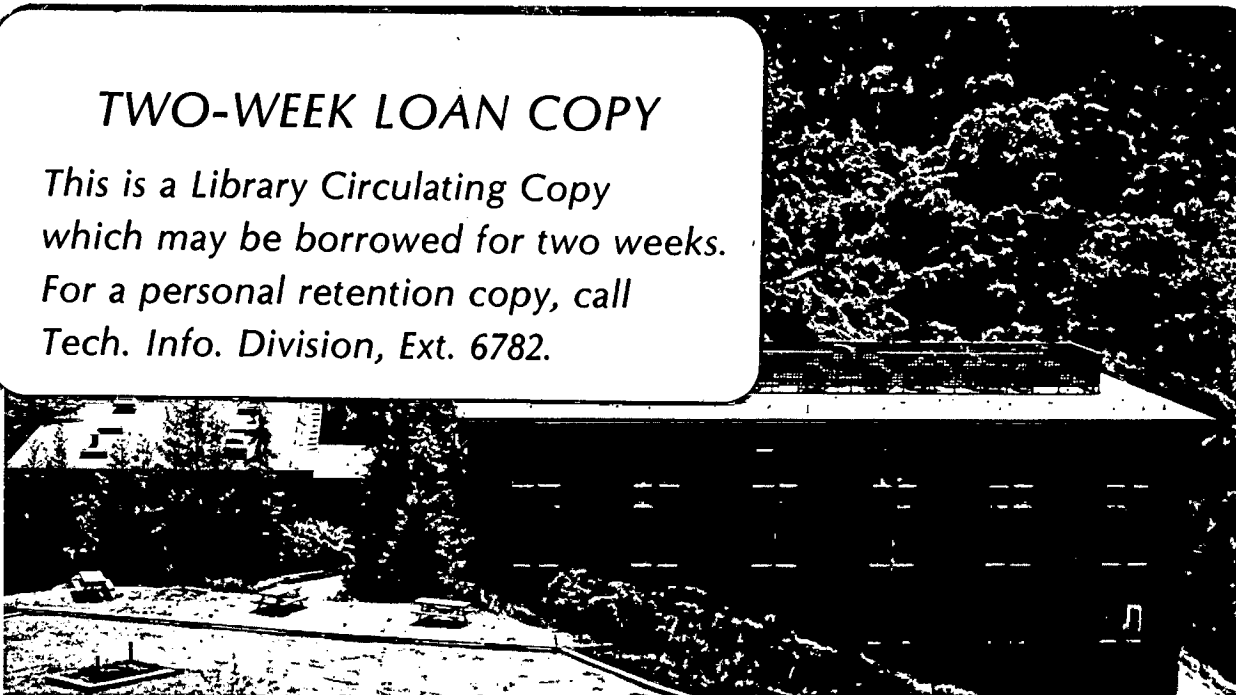
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A STRUCTURE OF DI- $\mu$ -AQUO-BIS(DIOXODINITRATOURANIUM(VI))  
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 A WATER BRIDGED DIMER OF URANYL NITRATE

by Dale L. Perry\*,<sup>1</sup> Helena Ruben, David H. Templeton\*  
 and Allan Zalkin\*

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and

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 University of California  
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ABSTRACT

Crystals of  $\text{UO}_2(\text{NO}_3)_2 \cdot \text{H}_2\text{O} \cdot \text{C}_3\text{H}_4\text{N}_2$  are monoclinic: space group  $P2_1/c$ ,  $a = 9.314(4) \text{ \AA}$ ,  $b = 16.230(16) \text{ \AA}$ ,  $c = 7.053(3) \text{ \AA}$ ,  $\beta = 100.72(4)^\circ$ ,  $Z = 4$ , and  $D_x = 3.04 \text{ gm cm}^{-3}$ . With anisotropic temperature factors for all of the non-hydrogen atoms  $R = 0.042$  for 2009 data where  $F^2 > 3\sigma$ . The structure is a dimer of two formula units in which two water molecules bridge two  $\text{UO}_2(\text{NO}_3)_2$  groups. The water molecule is hydrogen bonded to the imidazole molecule, and to a nitrate oxygen of an adjacent dimer, forming an infinite chain of dimers. Uranium is octacoordinate at the center of a distorted hexagonal bipyramid of oxygen atoms with average distances: U-O (uranyl)  $1.77 \pm 0.01 \text{ \AA}$ , U-O (water)  $2.36 \pm 0.01 \text{ \AA}$  and U-O (nitrate)  $2.55 \pm 0.04 \text{ \AA}$ . The bridging angles U-O-U and O-U-O are  $112.3(3)^\circ$  and  $67.7(3)^\circ$  respectively.

STRUCTURE OF DI- $\mu$ -AQUO-BIS(DIOXODINITRATOURANIUM(VI))  
DIIMIDAZOLE,  $[\text{UO}_2(\text{NO}_3)_2 \cdot \text{H}_2\text{O} \cdot \text{C}_3\text{H}_4\text{N}_2]_2$ ,  
A WATER BRIDGED DIMER OF URANYL NITRATE

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OCTOBER 1979

While a large number of uranium complexes have been postulated as dimers, trimers, or polymers, relatively few of them have been corroborated by x-ray crystallography. Several of these compounds are connected by oxygen-containing bridging units such as carboxylates or hydroxy groups; uranyl acetate dihydrate, for example, is a dimer with both bridging and terminal acetate groups.<sup>2</sup> Uranyl oxalate trihydrate<sup>3</sup> contains bridging, coordinated oxalate groups (with both coordinated and uncoordinated hydrogen bonded water molecules) that contribute to the formation of a pentagonal bipyramidal structure. Hydrogen bonding also plays a role in the dimerization of uranyl complexes involving thiocarboxylic-like donor centers.<sup>4,5</sup> Dimeric, trimeric, and tetrameric complexes of uranium(IV) have recently been reported.<sup>6-9</sup>

Imidazole and its related derivatives play an important role in the coordination chemistry of transition metal ions in biological systems. Biomolecular species such as proteins, nucleotides, and phospholipids possess a large number of potential coordinating groups which can combine with metals, imidazole being one of the principal heterocyclic donor systems.<sup>10</sup> Presumably, for example, three of the four ligands of cobalt(II) in carbonic anhydrase are nitrogen donors, most likely imidazole nitrogen of histidine residues.<sup>11</sup> Important systems containing imidazole as a ligand include hemoglobin which has  $\text{Fe}^{2+}$  attached octahedrally with the four nitrogen of heme, a histidine molecule, and either a water or oxygen molecule also coordinated;<sup>12</sup> myoglobin,<sup>12b</sup> histidine deaminase,<sup>13</sup> cytochrome c,<sup>14</sup> and cytochrome oxidase<sup>15</sup> are other examples.

In forming chemical systems with metal ions, imidazole, which is somewhat more basic than pyridine and slightly more acidic than pyrrole, can exist in several forms.<sup>10</sup> First, the pyridine-like nitrogen (N-3) possesses a pair of electrons for coordination with metal ions, thus effectively acting as a monodentate ligand. Second, the N-3 nitrogen can be protonated in acidic solutions to form the imidazolium cation which forms salts with metal ions such as the uranyl ion.<sup>16</sup> Third, the neutral imidazole can undergo deprotonization in strongly basic solutions to form the imidazolate anion which possesses two equivalent nitrogen coordination sites and is thus a potential bridging ligand.<sup>10</sup>

Imidazole, however, also participates in the formation of hydrogen bonds in a number of systems,<sup>10</sup> and it this property which is utilized in still another mode of bonding in the compound  $\text{UO}_2(\text{NO}_3)_2 \cdot \text{H}_2\text{O} \cdot \text{C}_3\text{H}_4\text{N}_2$  which is reported here. The molecules of imidazole act as secondary ligands in the complex, since they are not directly bonded to the uranium species but are hydrogen bonded to the bridging water molecules.

#### EXPERIMENTAL

All solvents were reagent grade and used as received. Commercially obtained reagent grade imidazole (Aldrich Chemicals) and uranyl nitrate hexahydrate (Alfa Ventron) were also used without further purification.

Infrared spectra were obtained in the  $400\text{-}4000\text{ cm}^{-1}$  region on a Perkin-Elmer Model 283 infrared spectrometer. The samples were prepared as Nujol mulls between KBr plates.

The title compound was prepared by very slowly evaporating (in one or two weeks) a 1:1 millimole ratio of uranyl nitrate

hexahydrate and imidazole in 500 ml of water. The complex, which appeared as greenish yellow crystals, was then washed with diethyl ether and air dried for several hours. The rate of evaporation seems to be quite critical, with other products and mixtures of other products sometimes being formed. The infrared spectrum of the complex in the 2500-3500  $\text{cm}^{-1}$  region, however, is quite distinctive (see discussion below) and provides a good "fingerprint" identification.

A small green yellow-fluorescent crystal, approximately 0.11 x 0.10 x 0.06 mm in size, was glued to a glass fiber and examined with a Picker FACS-I automated diffractometer equipped with a graphite monochromator and a Mo X-ray tube ( $\lambda(\text{K}\alpha_1)$  0.70930 Å). Omega scans of several low angle reflections showed peaks with half-widths of  $\sim 0.15^\circ$ . The space group is  $\text{P}2_1/\text{c}$ . The setting angles of twelve manually centered reflections ( $40 < 2\theta < 48^\circ$ ) were used to determine by least-squares the following cell parameters:  $a = 9.314(4)$  Å,  $b = 16.230(16)$  Å,  $c = 7.053(3)$  Å,  $\beta = 100.72(4)^\circ$  and  $V = 1047.6$  Å<sup>3</sup>. For  $Z=4$  and a molecular weight of 480.13, the calculated density is 3.04  $\text{g}/\text{cm}^3$ .

Intensity data were collected using a  $\theta$ - $2\theta$  scan technique with a scan speed of  $2^\circ/\text{min}$  on  $2\theta$ . Each peak was scanned  $0.6^\circ$  before the  $\text{K}\alpha_1$  peak to  $0.6^\circ$  after the  $\text{K}\alpha_2$  peak, and backgrounds were counted for 4s at each end of the scan range offset by  $0.3^\circ$ . The temperature during the data collection was  $22 \pm 1^\circ\text{C}$ . Three standard reflections were measured every 250th scan. A total of 6418 scans ( $4^\circ < 2\theta < 60^\circ$ ) yielded 3064 unique reflections of which 2012 had  $F^2 > 3\sigma$ . An absorption



correction ( $\mu = 147 \text{ cm}^{-1}$ ) was applied<sup>17</sup> which ranged from 2.4 to 3.1. The variation of the three standard reflections was about 1% from the mean values, and no correction for decay was indicated.

A three-dimensional Patterson calculation showed the uranium atom and three oxygen atom positions, and subsequent least-squares refinements and Fourier calculations revealed all of the non-hydrogen atoms in the structure. After several least-squares refinements of the structure, in which the atoms were given anisotropic thermal parameters, a difference Fourier map was calculated. Positive peaks were observed in regions where hydrogen atoms were expected to be, but were scattered among a larger number of "noise" peaks of comparable size. Isotropic hydrogen atoms at calculated positions, 0.95 Å from the atoms to which they are bonded, were included in the final least-squares refinements but not refined. The least-squares function used minimizes the function  $\sum w(|F_o| - |F_c|)^2 / \sum w F_o^2$ . 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 0.06. Scattering factors from Doyle and Turner<sup>18</sup> were used, and anomalous dispersion corrections<sup>19</sup> were applied.

The discrepancy indices for 2009 data where  $F^2 > 3\sigma$  are

$$R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} = 0.042$$

$$R_w = \left[ \frac{\sum w(|F_o| - |F_c|)^2}{\sum |F_o|^2} \right]^{1/2} = 0.049$$

R for all 3063 data is 0.073. The error in an observation of unit weight is 1.16. In the last cycle, no parameter changed more than

0.02 $\sigma$ . The three largest peaks in the final difference Fourier were 2.5 to 3.9 e/ $\text{\AA}$  and are associated with ripples near the uranium atom.

## RESULTS AND DISCUSSION

Positional parameters, distances and angles are listed in Tables I-III. Figure 1 shows an ORTEP view of two formula units that form the water-bridged dimer.

The structure is a dimer of two formula units related to each other by a center of symmetry. Two  $\text{UO}_2(\text{NO}_3)_2$  units are bridge bonded via the oxygen atoms of two water molecules. The water molecule is hydrogen bonded to the non-protonated nitrogen atom (N3) of the imidazole, and to a nitrate oxygen (O5) of an adjacent dimer. The nitrate to water bond links the dimers together into an infinite chain.

Uranium is eight-coordinate at the center of a distorted hexagonal bipyramid which has the uranyl oxygen atoms at the apices. The O-U-O axis is more or less perpendicular to the distorted equatorial plane; the largest deviation from orthogonality of the O-U-O axis to any U-O bond in the equatorial plane is 6°. A slight twist of the nitrate groups out of the equatorial plane indicates some crowding in the coordination environment about  $\text{UO}_2^{2+}$ . The geometry and bond distances of the water bridged uranyl dimer in this structure are remarkably similar to the hydroxy bridged uranyl dimer found in  $[(\text{NO}_3)_2\text{UO}_2(\text{OH})_2\text{UO}_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$ ,<sup>20</sup> in which hydroxide instead of  $\text{H}_2\text{O}$

is the bridging group, and three waters occupy one end of the dimer rather than two nitrate groups. Another similar type uranyl dimer is found in the  $\text{Cl}(\text{H}_2\text{O})_3\text{UO}_2(\text{OH})_2\text{UO}_2(\text{H}_2\text{O})_3\text{Cl}$  structure,<sup>21</sup> which has heptacoordinate rather than octacoordinate uranium. The U-U distances in the title compound is 3.927 Å and compares to 3.939 Å<sup>20</sup> and 3.944 Å<sup>21</sup> in the two other compounds mentioned above. The bridging U-O (water) distances are about 0.2 Å shorter than the U-O (nitrate) distances, and this is consistent with what is observed in the other compounds.<sup>20,21</sup> The double oxygen bridging of the uranyl ion is somewhat rare, but several examples exist for thorium in which the Th-Th distances vary from 3.97 to 4.09 Å in a series of double hydroxo-bridged thorium(IV) complexes.<sup>22</sup>

The imidazole molecules are associated by hydrogen bonds to the bridging water molecules and are not directly bonded to the uranyl cations. The bond distances and angles of the imidazole molecules are in agreement with previous structural studies.<sup>23,24</sup>

The infrared spectrum of the complex is quite distinctive in the O-H and N-H stretching region and is shown in Fig. 2. Rather than the broad band in the 3500  $\text{cm}^{-1}$  region which is customarily seen for metal ion complexes involving water, a single, considerably sharpened peak is found at 3500  $\text{cm}^{-1}$ . An N-H stretching band, similar in contour to the O-H band, is found at 3328  $\text{cm}^{-1}$ , while a second, sharper N-H frequency lies at 3132  $\text{cm}^{-1}$ . These values compare quite favorably with those of transition metal-imidazole complexes.<sup>25</sup>

ACKNOWLEDGEMENT

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Supplementary Material Available: Data processing formulas, the table of anisotropic thermal parameters, calculated powder pattern, and the listing of structure factor amplitudes (15 pages). Ordering information is given on any current masthead page.

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Table 1. Positional Parameters with Estimated Deviations<sup>a</sup>

Atom	x	y	z
U	.12027(4)	.06380(2)	.20731(5)
O(1)	.2646(8)	.0649(5)	.075(1)
O(2)	-.0243(8)	.0640(5)	.337(1)
O(3)	.0481(8)	-.0685(4)	.090(1)
O(4)	.2137(9)	.2052(5)	.331(1)
O(5)	.127(1)	.3233(5)	.227(1)
O(6)	.0270(9)	.2098(5)	.102(1)
O(7)	.303(1)	.0706(5)	.522(1)
O(8)	.2552(9)	-.0503(5)	.408(1)
O(9)	.407(1)	-.0330(6)	.679(1)
N(1)	.121(1)	.2485(5)	.220(2)
N(2)	.325(1)	-.0051(6)	.544(1)
N(3)	.295(1)	-.1653(6)	.059(2)
N(4)	.524(1)	-.1888(7)	.090(2)
C(1)	.426(1)	-.1310(8)	.087(2)
C(2)	.313(1)	-.2483(8)	.049(2)
C(3)	.454(1)	-.2634(8)	.069(2)
H(1)	.6259	-.1805	.1034
H(2)	.4450	-.0735	.1017
H(3)	.2366	-.2885	.0302
H(4)	.4994	-.3162	.0699
H(5)	-.0099	-.1043	.1506
H(6)	.1313	-.1010	.0796

<sup>a</sup>Here and in the following tables the number in parentheses is the estimated standard deviation for the least significant figures.



Table II. Distances (Å)

U	-U	3.927(2)	N(2)-O(7)	1.25(2)
	-O(1)	1.78(1)	-O(8)	1.28(2)
	-O(2)	1.76(1)	-O(9)	1.19(2)
	-O(3)	2.35(1)	O(3)-O(3) <sup>a</sup>	2.63(2)
	-O(3) <sup>a</sup>	2.37(1)	-O(5)	2.87(2)
	-O(4)	2.55(1)	-N(3)	2.83(2)
	-O(6)	2.59(1)	C(1)-N(3)	1.32(2)
	-O(7)	2.54(1)	-N(4)	1.31(2)
	-O(8)	2.52(1)	C(2)-N(3)	1.36(2)
	N(1)-O(4)	1.26(2)	C(3)-N(4)	1.37(2)
	-O(5)	1.22(2)	C(2)-C(3)	1.32(2)
	-O(6)	1.26(2)		

<sup>a</sup>At position -x, -y, -z

Table III. Selected Angles (deg.)

O(1)-U-O(2)	179.1(4)	O(7)-U -O(8)	49.9(3)
O(1)-U-O(3)	91.0(3)	U -O(3)-U	112.3(3)
O(1)-U-O(3) <sup>a</sup>	88.6(3)	O(5)-O(3)-N(3)	103.6(4)
O(1)-U-O(4)	85.9(3)	O(5)-N(1)-O(4)	121(1)
O(1)-U-O(6)	95.0(3)	O(5)-N(1)-O(6)	123(1)
O(1)-U-O(7)	90.5(4)	O(4)-N(1)-O(6)	116(1)
O(1)-U-O(8)	87.5(3)	O(7)-N(2)-O(8)	115(1)
O(2)-U-O(3)	89.3(4)	O(7)-N(2)-O(9)	123(1)
O(2)-U-O(3) <sup>a</sup>	90.8(3)	O(8)-N(2)-O(9)	123(1)
O(2)-U-O(4)	93.8(4)	C(1)-N(3)-C(2)	108(1)
O(2)-U-O(6)	84.2(4)	N(3)-C(2)-C(3)	108(1)
O(2)-U-O(7)	90.1(4)	C(2)-C(3)-N(4)	107(1)
O(2)-U-O(8)	93.3(4)	C(3)-N(4)-C(1)	109(1)
O(3)-U-O(3)	67.7(3)	N(3)-C(1)-N(4)	109(1)
O(4)-U-O(6)	49.3(3)		

<sup>a</sup>At position -x, -y, -z.

FIGURE CAPTION

Fig. 1. An ORTEP drawing of two formula units in the dimer configuration.

Fig. 2. Infrared spectrum of the title compound taken as a Nujol mull.

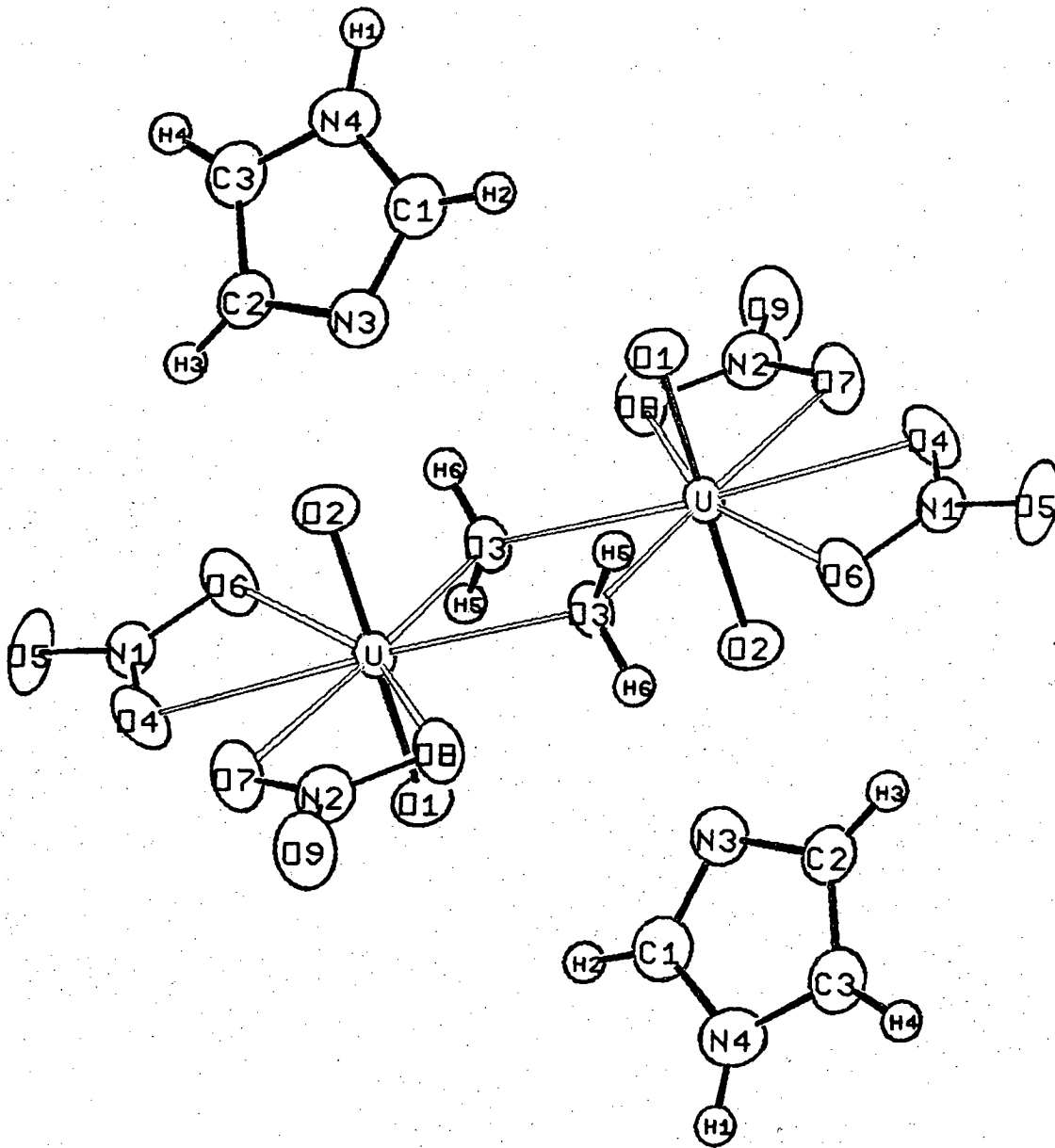
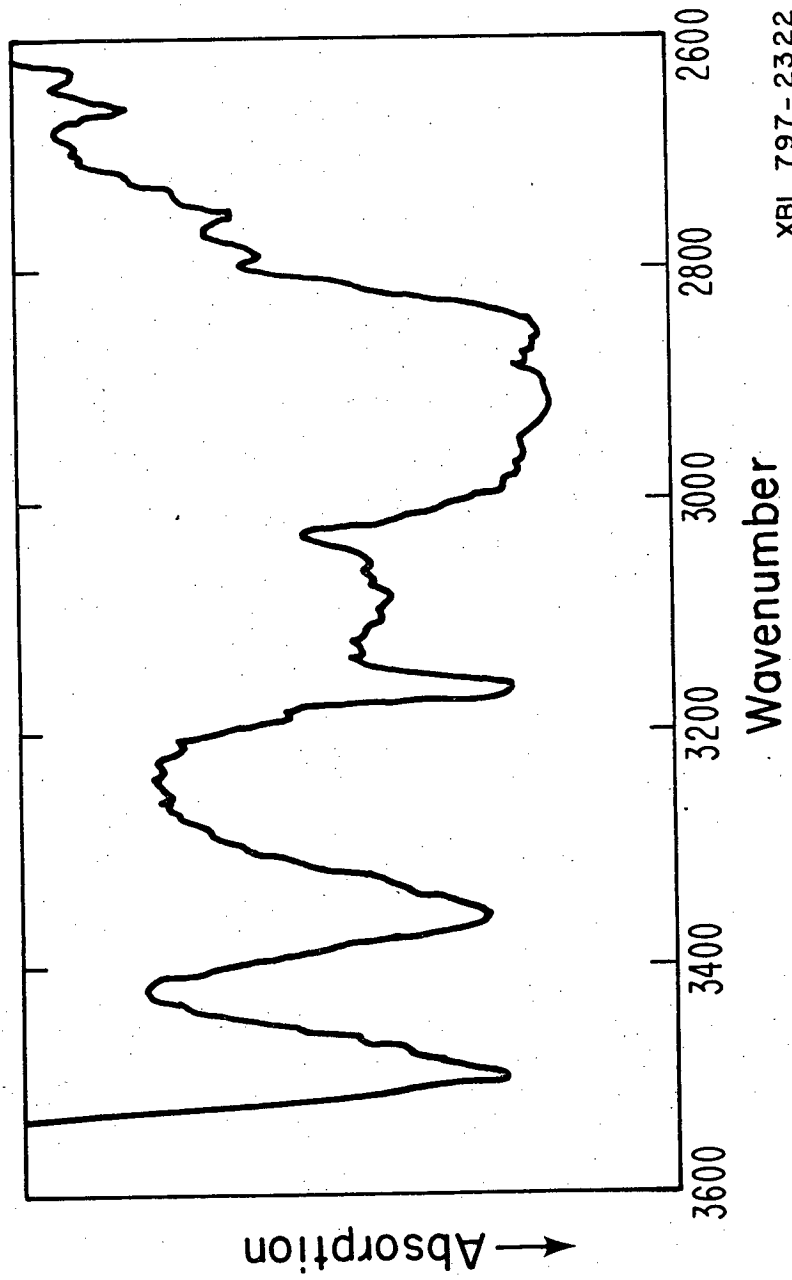


Fig. 1

XBL 7810-11953



XBL 797-2322

Fig. 2

Supplementary Materials for the paper:

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DATA PROCESSING FORMULAE

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

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

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

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

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

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

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

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

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

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

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

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

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

C = counts recorded during a scan

$\theta_m$  = monochromater angle

I = individual raw intensity,  
background removed.

$\theta$  = 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

Lp = Lorentz and polarization corrections

Anisotropic Thermal Parameters for  $\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O}) \cdot \text{C}_3\text{H}_4\text{N}_2^{\text{a}}$

ATOM	B11	B22	B33	B12	B13	B23
U	1.59(1)	1.0(4)(1)	2.07(1)	-0.05(1)	.032(9)	-0.06(2)
O(1)	2.2(3)	2.6(3)	3.0(3)	.1(3)	.9(2)	.2(3)
O(2)	2.2(3)	3.4(4)	3.1(3)	.0(3)	1.0(3)	-0.1(3)
O(3)	2.2(3)	1.1(3)	2.8(3)	-0.1(2)	.0(2)	-0.0(3)
O(4)	2.8(3)	2.0(3)	4.2(4)	-0.7(3)	-0.7(3)	-0.1(3)
O(5)	6.7(6)	.5(2)	4.4(5)	-0.4(3)	2.6(4)	-0.3(3)
O(6)	3.1(4)	2.2(4)	3.3(4)	-0.3(3)	-0.8(3)	-0.1(3)
O(7)	3.7(4)	2.3(4)	3.2(4)	.2(3)	-0.8(3)	-0.6(3)
O(8)	3.0(3)	1.9(3)	2.9(3)	-0.1(3)	-0.2(3)	-0.3(3)
O(9)	4.3(4)	3.2(4)	2.9(4)	.6(4)	-0.8(3)	-0.1(3)
N(1)	2.7(4)	1.2(3)	3.7(5)	-0.3(3)	1.1(3)	-0.4(4)
N(2)	2.8(4)	1.8(4)	2.9(4)	.3(3)	.4(3)	.4(3)
N(3)	2.5(4)	2.7(4)	3.0(4)	.3(3)	-0.1(3)	-0.2(4)
N(4)	2.4(4)	3.2(5)	4.0(5)	.3(4)	.4(4)	.4(4)
C(1)	3.4(6)	2.4(5)	3.2(6)	.4(4)	.1(4)	-0.1(4)
C(2)	2.7(5)	2.7(5)	4.4(7)	-0.1(4)	.5(4)	-1.2(5)
C(3)	3.5(6)	2.3(5)	4.1(7)	1.1(4)	.3(5)	-0.3(5)

<sup>a</sup>The temperature factor has the form  $\exp(-0.25(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hka + 2B_{13}hkl + 2B_{23}kbl + \dots))$ .



CALCULATED POWDER PATTERN FOR URANYL NITRATE IMIDAZOLE  
X-RAY WAVE LENGTH = 1.54180 ANGSTROMS.

A = 9.314 B = 16.230 C = 7.053  
ALPHA = 90.00 BETA = 100.72 GAMMA = 90.00

H	K	L	D	I	2 THETA	SINSQ
1	0	0	9.151	956.	9.66	.00710
1	1	0	7.972	331.	11.10	.00935
0	1	1	6.373	58.	13.89	.01463
1	2	0	6.072	326.	14.59	.01612
1	1	-1	5.708	1000.	15.52	.01824
0	2	1	5.270	430.	16.82	.02140
1	2	-1	4.875	196.	18.20	.02501
1	1	1	4.855	140.	18.27	.02521
1	3	0	4.657	261.	19.06	.02740
2	0	0	4.576	1.	19.40	.02838
2	1	0	4.404	334.	20.16	.03064
1	2	1	4.311	246.	20.60	.03198
0	3	1	4.264	28.	20.83	.03268
2	1	-1	4.061	679.	21.89	.03604
0	4	0	4.058	16.	21.90	.03610
1	3	-1	4.047	89.	21.96	.03629
2	2	0	3.985	3.	22.30	.03741
2	2	-1	3.726	14.	23.88	.04281
1	4	0	3.709	1.	23.99	.04319
1	3	1	3.705	0.	24.01	.04326
0	4	1	3.501	434.	25.44	.04847
2	3	0	3.494	180.	25.50	.04869
0	0	2	3.465	75.	25.71	.04950
1	0	-2	3.461	18.	25.74	.04962
2	1	1	3.448	226.	25.84	.04999
0	1	2	3.389	0.	26.30	.05176
1	1	-2	3.385	218.	26.33	.05188
1	4	-1	3.378	37.	26.38	.05208
2	3	-1	3.315	72.	26.90	.05409
2	2	1	3.236	21.	27.56	.05676
0	2	2	3.187	70.	28.00	.05852
1	2	-2	3.183	0.	28.03	.05865
1	4	1	3.172	280.	28.13	.05905
1	5	0	3.059	108.	29.19	.06350
1	0	2	3.058	265.	29.21	.06357
3	0	0	3.050	24.	29.28	.06386
2	0	-2	3.049	7.	29.29	.06394
2	4	0	3.036	0.	29.42	.06448
1	1	2	3.005	2.	29.73	.06582
3	1	0	2.998	24.	29.80	.06612
2	1	-2	2.996	41.	29.82	.06620
2	3	1	2.955	57.	30.24	.06804
3	1	-1	2.955	19.	30.24	.06804
0	5	1	2.940	7.	30.41	.06878
0	3	2	2.918	47.	30.64	.06980
2	4	-1	2.916	2.	30.66	.06988
1	3	-2	2.915	45.	30.67	.06993
1	5	-1	2.865	29.	31.22	.07239
1	2	2	2.861	80.	31.26	.07259
3	2	0	2.855	5.	31.33	.07289

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)  
 URANYL NITRATE IMIDAZOLE UO<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>·(C<sub>3</sub>N<sub>2</sub>H<sub>4</sub>)H<sub>2</sub>O F(0,0,0) = 2468

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

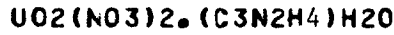
L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	0,	0	6	366	12	19	6	22	45	4*	3	48	19	15*	-7	189	8	3
2	508	16	-17	7	143	8	4	7	71	19	8*	4	154	10	-11	-6	129	9	20
4	215	7	4	8	211	9	6	8	90	13	7	5	31	43	29*	-5	418	13	17
6	52	16	-2*	9	48	33	8*		H,K=	0,	11	6	56	25	35*	-4	205	7	11
8	164	9	-11		H,K=	0,	6	1	21	31	-9*		H,K=	0,	17	-3	496	15	-6
	H,K=	0,	1	0	775	24	56	2	282	9	11	1	104	11	27	-2	649	20	-1
1	189	6	16	1	690	21	58	3	68	10	-7	2	60	36	-5*	-1	763	25	-42
2	24	24	0*	2	418	13	29	4	424	13	13	3	224	10	1	0	299	9	-15
3	423	25	8	3	302	9	25	5	143	7	13	4	172	8	3	1	354	14	-2
4	268	19	6	4	182	7	13	6	332	11	8	5	226	9	-4	2	56	5	-7
5	329	27	-10	5	44	15	14*	7	60	62	-13*	6	136	11	6	3	117	5	4
6	152	6	-1	6	0	37	-8*	8	165	9	7		H,K=	0,	18	4	31	14	14*
7	297	11	-15	7	87	13	6		H,K=	0,	12	0	224	10	-5	5	227	8	-11
8	87	11	-13	8	105	10	9	0	107	8	9	1	249	9	-2	6	151	7	2
9	125	9	-3	9	100	13	5	1	574	18	24	2	151	12	-12	7	217	8	-16
	H,K=	0,	2		H,K=	0,	7	2	0	33	-16*	3	174	8	-3	8	109	12	2
1	631	19	58	1	189	7	0	3	355	11	7	4	92	16	11	9	188	9	-5
2	429	13	37	2	98	5	5	4	74	10	-13	5	61	27	18*		H,K=	1,	2
3	475	18	35	3	413	13	27	5	63	31	-19*	6	22	48	12*	-9	139	11	1
4	177	6	4	4	84	6	0	6	30	46	24*		H,K=	0,	19	-8	152	13	-1
5	22	32	8*	5	369	12	19	7	55	63	-9*	1	53	21	43*	-7	221	9	13
6	46	13	6*	6	104	8	-9	8	10	49	-9*	2	140	9	-19	-6	196	7	5
7	103	8	9	7	298	10	12		H,K=	0,	13	3	36	44	-9*	-5	160	6	4
8	109	14	7	8	103	9	26	1	42	49	-18*	4	215	9	-22	-4	186	6	11
9	83	17	-16*	9	134	12	16	2	236	8	0	5	69	18	5*	-3	111	4	11
	H,K=	0,	3		H,K=	0,	8	3	202	7	7		H,K=	0,	20	-2	18	21	-4*
1	197	6	13	0	1009	31	60	4	223	8	1	0	41	52	-14*	-1	449	15	30
2	388	12	32	1	137	5	16	5	137	8	-16	1	295	10	-19	0	441	17	18
3	224	7	23	2	583	18	44	6	259	9	6	2	16	50	-29*	1	540	21	6
4	387	15	20	3	48	9	14*	7	118	10	5	3	188	9	-2	2	479	23	8
5	224	7	10	4	177	6	-3	8	137	13	5	4	21	47	0*	3	451	22	3
6	401	13	9	5	53	11	32*		H,K=	0,	14		H,K=	0,	21	4	361	18	-5
7	87	10	-11	6	29	39	26*	0	430	14	17	1	67	19	-3*	5	231	15	-9
8	189	8	7	7	19	46	7*	1	305	10	15	2	119	10	-4	6	199	7	-5
9	56	23	2*	8	124	10	4	2	241	8	8	3	109	12	10	7	95	8	-6
	H,K=	0,	4	9	60	72	43*	3	214	8	0		H,K=	0,	22	8	27	44	19*
0	225	7	17		H,K=	0,	9	4	114	8	13	0	238	13	-19	9	0	61	-11*
1	938	29	55	1	197	7	14	5	0	46	-32*	1	141	10	-20		H,K=	1,	3
2	0	22	-12*	2	163	6	13	6	22	43	7*	2	163	10	-13	-9	15	48	6*
3	604	19	45	3	313	10	8	7	40	47	-12*		H,K=	1,	0	-8	69	25	26*
4	32	16	30*	4	154	7	5		H,K=	0,	15	-8	235	9	11	-7	124	8	10
5	124	6	9	5	354	11	23	1	137	7	5	-6	394	12	25	-6	263	9	11
6	7	35	5*	6	178	8	4	2	68	13	5*	-4	67	6	-3	-5	182	7	16
7	110	12	-7	7	270	9	18	3	299	10	1	-2	238	7	-19	-4	683	21	48
8	16	48	9*	8	74	16	3*	4	92	10	-10	0	545	19	-143	-3	329	10	19
9	151	9	10		H,K=	0,	10	5	246	9	0	2	992	30	-138	-2	369	11	23
	H,K=	0,	5	0	539	17	38	6	84	24	3*	4	404	13	-31	-1	371	13	27
1	144	5	5	1	377	12	25	7	209	13	-7	6	313	10	-18	0	533	21	25
2	388	12	29	2	323	10	15		H,K=	0,	16	8	67	12	10*	1	26	9	7*
3	262	8	13	3	316	10	15	0	531	17	2		H,K=	1,	1	2	176	6	3
4	368	12	27	4	159	7	9	1	90	9	-2	-9	42	43	20*	3	20	24	2*
5	235	8	21	5	54	13	22*	2	314	10	-4	-8	45	25	-14*	4	164	6	-1

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	106	7	4	1	579	18	46	-2	166	6	5	0	59	12	6*	6	62	21	6*
6	269	18	-6	2	575	18	40	-1	469	15	26	1	514	16	12	7	173	9	0
7	101	12	19	3	421	13	34	0	393	12	30	2	177	7	-1	H,K=	1,	16	
8	212	8	0	4	348	11	31	1	328	10	21	3	551	17	21	-7	53	32	25*
9	75	22	7*	5	188	8	2	2	66	7	0	4	25	38	4*	-6	202	9	4
	H,K=	1,	4	6	191	8	10	3	101	6	1	5	270	9	11	-5	19	43	-9*
-9	186	9	24	7	130	8	16	4	69	13	7*	6	36	42	-8*	-4	36	42	-23*
-8	49	23	22*	8	33	44	9*	5	164	7	3	7	99	12	-2	-3	14	40	6*
-7	345	11	20	9	39	48	37*	6	101	10	1	8	0	49	-5*	-2	124	8	-3
-6	15	35	13*		H,K=	1,	7	7	209	9	3		H,K=	1,	13	-1	78	11	6
-5	247	8	12	-9	45	46	43*	8	93	15	-13	-8	19	49	-13*	0	318	10	-3
-4	29	20	26*	-8	35	43	11*		H,K=	1,	10	-7	56	25	-14*	1	42	26	-17*
-3	57	7	10	-7	158	8	-1	-8	121	11	-5	-6	145	8	6	2	436	14	-15
-2	29	10	10*	-6	96	8	10	-7	209	11	4	-5	119	8	5	3	48	21	14*
-1	286	9	18	-5	337	11	28	-6	177	8	6	-4	315	12	3	4	296	11	-1
0	45	5	4	-4	214	7	15	-5	142	7	-8	-3	208	7	3	5	24	45	-11*
1	832	28	42	-3	530	16	38	-4	81	8	-1	-2	332	11	12	6	164	9	1
2	0	23	-4*	-2	257	8	14	-3	0	31	-11*	-1	256	8	2		H,K=	1,	17
3	923	36	48	-1	791	24	47	-2	82	6	-1	0	343	11	8	-6	75	24	-14*
4	42	10	14*	0	172	6	18	-1	297	10	21	1	86	8	13	-5	203	10	10
5	374	18	9	1	340	11	16	0	309	10	19	2	80	8	3	-4	149	9	-6
6	53	12	20*	2	25	26	-6*	1	379	12	20	3	34	35	8*	-3	258	9	0
7	135	8	-3	3	52	8	8	2	448	14	28	4	100	14	13	-2	188	7	8
8	14	42	9*	4	62	11	7	3	448	14	29	5	71	16	1*	-1	262	9	-9
9	26	46	15*	5	188	7	11	4	327	11	17	6	178	8	2	0	159	8	-12
	H,K=	1,	5	6	93	8	9	5	215	8	14	7	106	12	-2	1	143	8	0
-9	37	47	34*	7	259	12	1	6	167	8	11		H,K=	1,	14	2	54	18	11*
-8	63	16	16*	8	68	17	0*	7	61	18	6*	-7	128	15	0	3	0	43	-5*
-7	59	18	-15*	9	189	13	4	8	20	51	-3*	-6	138	10	-6	4	57	40	9*
-6	278	9	18		H,K=	1,	8		H,K=	1,	11	-5	75	24	-7*	5	112	14	-4
-5	228	9	17	-9	40	47	30*	-8	65	19	17*	-4	68	13	-10	6	81	19	-12*
-4	595	18	44	-8	237	9	11	-7	72	15	12*	-3	34	36	24*		H,K=	1,	18
-3	254	8	21	-7	54	21	16*	-6	236	9	9	-2	58	19	-8*	-6	113	16	19
-2	572	18	36	-6	256	9	17	-5	127	12	4	-1	170	7	2	-5	128	14	12
-1	301	9	18	-5	12	36	-4*	-4	481	15	21	0	327	11	10	-4	59	25	14*
0	543	17	34	-4	169	7	13	-3	152	6	4	1	327	10	13	-3	0	53	-10*
1	220	7	17	-3	47	10	-3*	-2	454	14	22	2	341	11	11	-2	49	49	-8*
2	163	5	8	-2	201	7	9	-1	217	7	9	3	231	8	10	-1	146	8	7
3	0	27	-15*	-1	124	5	3	0	410	13	18	4	178	9	0	0	170	10	-9
4	150	6	4	0	677	21	44	1	104	6	-5	5	140	9	-12	1	236	9	0
5	87	7	7	1	79	6	5	2	190	7	6	6	125	10	-4	2	197	8	-2
6	276	10	6	2	623	19	43	3	26	40	-19*	7	74	18	3*	3	278	10	0
7	113	18	4	3	38	13	11*	4	119	7	8		H,K=	1,	15	4	145	12	-2
8	216	8	8	4	460	14	31	5	29	37	-1*	-7	109	12	-4	5	149	12	-3
9	91	16	6	5	23	34	8*	6	245	10	2	-6	68	20	0*		H,K=	1,	19
	H,K=	1,	6	6	240	8	3	7	74	14	9*	-5	228	9	-3	-5	64	23	23*
-9	136	9	20	7	15	41	3*	8	187	9	10	-4	123	8	4	-4	245	10	-19
-8	183	8	3	8	54	23	23*		H,K=	1,	12	-3	358	11	-3	-3	67	16	-1*
-7	215	8	23		H,K=	1,	9	-8	0	65	-21*	-2	148	7	-3	-2	257	9	-18
-6	212	8	18	-9	29	48	19*	-7	241	9	-1	-1	407	13	-1	-1	87	12	-11
-5	132	6	7	-8	23	45	8*	-6	50	50	-2*	0	90	11	12	0	230	9	-7
-4	156	6	13	-7	128	9	5	-5	171	7	-3	1	229	8	-2	1	21	44	-35*
-3	21	28	7*	-6	86	9	6	-4	51	14	27*	2	54	18	5*	2	65	19	-18*
-2	128	5	8	-5	367	12	14	-3	0	34	-28*	3	0	39	-7*	3	22	50	20*
-1	197	6	6	-4	203	7	7	-2	13	41	10*	4	32	40	26*	4	74	31	-9*
0	579	18	30	-3	387	12	24	-1	321	10	15	5	165	8	-5	5	43	47	26*

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE



L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	1,	20	-8	155	9	4	8	0	44	-13*	4	77	7	7	4	302	10	12
-4	35	49	22*	-7	226	8	-4	9	124	11	4	5	104	9	12	5	308	10	4
-3	0	46	-17*	-6	302	10	-5		H,K=	2,	5	6	23	38	-8*	6	179	8	11
-2	23	49	12*	-5	330	11	-5	-9	57	23	8*	7	66	21	-18*	7	142	9	-1
-1	154	9	-20	-4	288	9	-4	-8	130	9	16	8	77	15	40*	8	96	14	-8
0	26	44	-18*	-3	246	8	-4	-7	50	17	27*		H,K=	2,	8		H,K=	2,	11
1	274	10	-8	-2	56	5	-4	-6	26	34	6*	-9	27	50	23*	-8	85	15	-14
2	68	24	2*	-1	147	5	-4	-5	81	8	-5	-8	196	9	2	-7	0	54	-7*
3	254	11	-18	0	62	6	0	-4	334	11	14	-7	39	52	32*	-6	22	47	-6*
4	0	53	-40*	1	217	7	3	-3	200	7	6	-6	377	12	17	-5	29	38	12*
	H,K=	1,	21	2	391	14	-10	-2	483	17	15	-5	51	22	-1*	-4	266	9	3
-3	124	10	-5	3	300	16	-17	-1	226	7	16	-4	407	13	13	-3	161	7	-2
-2	212	9	-10	4	302	14	-19	0	715	30	6	-3	62	8	20	-2	400	12	14
-1	123	16	-23	5	301	11	-18	1	338	13	17	-2	340	11	20	-1	199	7	3
0	159	12	-15	6	177	7	-7	2	753	27	32	-1	57	7	-1	0	530	17	18
1	0	62	-63*	7	172	8	-10	3	282	9	9	0	70	39	48*	1	210	7	9
2	19	62	-54*	8	110	12	-16	4	171	6	12	1	18	27	-10*	2	545	17	20
3	43	49	20*	9	94	12	6	5	47	12	21*	2	437	14	12	3	125	7	-4
	H,K=	1,	22		H,K=	2,	3	6	54	13	21*	3	57	9	6	4	180	7	1
-2	47	58	5*	-9	43	56	-7*	7	35	40	-2*	4	374	12	8	5	53	16	13*
-1	80	15	10	-8	127	9	7	8	128	9	4	5	53	22	-6*	6	39	41	18*
0	165	10	-26	-7	28	45	-3*	9	84	29	28*	6	338	11	17	7	41	59	16*
1	157	10	-5	-6	47	14	37*		H,K=	2,	6	7	30	47	13*	8	109	12	3
2	202	12	-11	-5	103	6	4	-9	108	16	17	8	186	10	5		H,K=	2,	12
	H,K=	2,	0	-4	301	9	0	-8	163	9	5		H,K=	2,	9	-8	27	59	0*
-8	242	9	2	-3	84	5	-1	-7	185	10	13	-9	79	31	-15*	-7	245	10	3
-6	342	11	-30	-2	384	12	2	-6	293	10	12	-8	63	18	25*	-6	50	20	12*
-4	602	19	-64	-1	392	14	10	-5	312	10	14	-7	73	12	18	-5	374	12	6
-2	163	5	-17	0	567	25	-4	-4	375	12	18	-6	44	20	26*	-4	108	8	-2
0	35	11	3*	1	381	17	-3	-3	274	9	13	-5	68	10	-2	-3	339	12	11
2	446	14	-29	2	828	33	-15	-2	242	8	6	-4	152	7	6	-2	0	34	-5*
4	433	13	-37	3	259	8	5	-1	27	17	11*	-3	323	10	8	-1	122	6	12
6	333	11	-25	4	149	6	-5	0	67	5	11	-2	280	9	13	0	22	36	-1*
8	200	9	-26	5	62	10	0	1	132	5	3	-1	487	15	27	1	219	7	13
	H,K=	2,	1	6	35	35	-11*	2	359	11	15	0	175	6	11	2	98	8	8
-9	106	14	-2	7	66	12	6*	3	231	8	11	1	536	17	31	3	345	11	9
-8	49	57	-19*	8	128	10	2	4	341	11	11	2	269	9	22	4	79	10	2
-7	85	9	1	9	37	50	-11*	5	284	9	5	3	345	11	12	5	356	11	1
-6	41	25	9*		H,K=	2,	4	6	267	9	5	4	48	17	5*	6	19	52	0*
-5	85	9	-7	-9	133	14	3	7	173	8	-1	5	53	25	-2*	7	207	11	7
-4	194	6	-7	-8	44	51	33*	8	110	20	-17	6	51	36	39*		H,K=	2,	13
-3	339	11	-23	-7	328	11	13	9	78	17	1*	7	81	18	4*	-8	60	42	-16*
-2	301	9	-19	-6	27	34	-2*		H,K=	2,	7	8	63	20	12*	-7	26	52	-8*
-1	846	26	-99	-5	573	18	23	-9	120	12	7		H,K=	2,	10	-6	41	42	26*
0	542	19	-66	-4	0	33	-9*	-8	36	63	-6*	-8	129	13	8	-5	78	13	-10
1	593	21	-56	-3	396	12	8	-7	74	12	20	-7	202	8	2	-4	187	7	0
2	327	10	-17	-2	53	5	-4	-6	44	22	39*	-6	261	9	8	-3	118	8	2
3	387	17	-25	-1	84	4	4	-5	108	7	3	-5	325	11	10	-2	317	10	6
4	76	6	0	0	33	7	3*	-4	107	6	-4	-4	270	9	9	-1	215	7	5
5	103	7	-9	1	311	13	12	-3	388	12	16	-3	216	8	1	0	387	13	18
6	5	42	2*	2	34	13	-4*	-2	206	7	12	-2	111	6	10	1	247	9	0
7	119	8	-8	3	539	21	13	-1	816	27	44	-1	130	6	10	2	364	11	18
8	44	31	-10*	4	10	30	-5*	0	270	8	13	0	39	12	25*	3	134	9	0
9	128	10	-18	5	428	20	3	1	604	21	23	1	151	7	8	4	73	18	3*
	H,K=	2,	2	6	22	35	-2*	2	281	9	18	2	263	9	15	5	42	30	17*
-9	95	13	11	7	244	9	3	3	314	14	13	3	328	11	8	6	11	43	0*

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	47	51	17*	2	185	9	-5	-2	964	31	-127	0	330	13	-13	-2	509	19	17
	H,K=	2,	14	3	192	8	11	0	311	10	-29	1	351	11	-3	-1	381	14	13
-7	137	10	5	4	66	17	15*	2	98	4	-3	2	711	29	-25	0	245	8	-4
-6	166	11	-11	5	32	47	-21*	4	230	8	-14	3	241	8	-8	1	132	5	7
-5	209	8	10	6	0	62	-12*	6	244	8	-24	4	450	19	-10	2	40	10	5*
-4	260	9	1		H,K=	2,	18	8	214	9	-24	5	164	6	2	3	77	7	1
-3	157	9	-2	-6	129	15	-7		H,K=	3,	1	6	147	7	-17	4	105	6	5
-2	157	7	4	-5	198	12	-15	-9	152	9	-4	7	58	15	22*	5	193	7	7
-1	81	11	1	-4	131	13	-14	-8	68	15	-11*	8	30	44	-5*	6	178	7	-9
0	34	35	11*	-3	134	15	-7	-7	189	7	-24	9	43	44	36*	7	166	8	0
1	99	7	13	-2	70	14	-9*	-6	107	9	-6		H,K=	3,	4	8	180	8	6
2	198	7	-2	-1	72	12	11	-5	210	7	-12	-9	40	44	37*		H,K=	3,	7
3	203	8	0	0	0	41	-13*	-4	42	17	3*	-8	22	49	21*	-9	165	9	12
4	219	8	-4	1	62	17	-15*	-3	68	5	-2	-7	162	10	-2	-8	77	14	15
5	185	8	10	2	120	12	-9	-2	168	5	-14	-6	43	19	41*	-7	204	8	-2
6	194	10	-8	3	234	9	7	-1	204	7	-16	-5	545	17	-3	-6	29	40	-15*
7	152	10	20	4	154	11	-5	0	233	7	-14	-4	19	27	3*	-5	208	8	-3
	H,K=	2,	15	5	194	9	-1	1	528	16	-62	-3	606	22	-2	-4	59	11	9*
-7	48	61	4*		H,K=	2,	19	2	226	7	-19	-2	96	4	5	-3	70	7	2
-6	30	43	7*	-5	47	51	25*	3	511	16	-39	-1	457	14	-1	-2	13	27	-5*
-5	80	13	-10	-4	151	9	5	4	223	7	-19	0	26	24	-8*	-1	360	11	10
-4	88	11	-7	-3	66	67	-1*	5	340	11	-32	1	457	17	2	0	202	7	14
-3	251	9	-5	-2	239	11	-17	6	119	7	-9	2	32	12	26*	1	485	15	9
-2	55	33	-28*	-1	81	14	-18	7	99	8	0	3	110	5	10	2	133	6	5
-1	480	15	-6	0	293	11	-17	8	48	28	35*	4	38	15	23*	3	524	16	14
0	154	7	1	1	75	19	4*	9	61	19	41*	5	302	10	-5	4	140	6	3
1	348	11	5	2	255	11	-21		H,K=	3,	2	6	3	36	-2*	5	342	18	8
2	156	8	-4	3	0	56	-42*	-9	0	45	-4*	7	197	9	-6	6	121	7	11
3	237	8	4	4	96	15	-11	-8	79	14	25	8	0	44	-9*	7	79	24	-3*
4	56	57	6*		H,K=	2,	20	-7	71	15	-9*		H,K=	3,	5	8	31	46	19*
5	55	24	-15*	-4	55	61	9*	-6	169	7	-15	-9	71	18	-13*		H,K=	3,	8
6	28	56	26*	-3	171	9	-17	-5	349	11	-24	-8	193	8	8	-9	18	51	8*
	H,K=	2,	16	-2	41	45	12*	-4	331	10	-26	-7	106	9	6	-8	72	25	11*
-7	0	54	-29*	-1	77	16	12*	-3	427	13	-27	-6	214	8	8	-7	54	17	52*
-6	242	9	2	0	67	23	37*	-2	450	14	-26	-5	96	12	-7	-6	233	8	-6
-5	76	19	23*	1	105	15	10	-1	353	13	-17	-4	130	5	4	-5	29	50	18*
-4	309	10	-11	2	55	25	22*	0	118	4	-4	-3	26	30	-7*	-4	540	17	14
-3	40	46	30*	3	190	10	-15	1	194	6	-10	-2	201	7	6	-3	81	6	8
-2	180	8	5	4	68	27	46*	2	26	15	-9*	-1	239	11	4	-2	608	19	15
-1	58	14	14*		H,K=	2,	21	3	74	7	-9	0	384	15	-1	-1	85	6	6
0	6	37	-13*	-3	94	23	1*	4	136	6	-11	1	398	16	12	0	378	12	16
1	50	16	45*	-2	198	9	-5	5	199	7	-20	2	621	26	6	1	31	18	24*
2	250	10	9	-1	146	9	-4	6	156	7	-19	3	276	14	11	2	82	7	3
3	77	11	4	0	232	9	-8	7	170	7	-11	4	451	22	2	3	27	31	3*
4	300	10	-2	1	134	10	-6	8	131	9	-17	5	153	7	1	4	183	7	6
5	47	31	18*	2	169	9	-9	9	120	10	8	6	203	8	3	5	24	48	15*
6	217	10	-11	3	65	43	-20*		H,K=	3,	3	7	22	47	0*	6	241	9	8
	H,K=	2,	17		H,K=	2,	22	-9	72	23	21*	8	48	28	8*	7	32	46	4*
-6	41	48	39*	-2	106	12	6	-8	208	8	0		H,K=	3,	6	8	204	10	3
-5	48	51	-25*	-1	35	48	11*	-7	95	9	-8	-9	40	57	39*		H,K=	3,	9
-4	125	9	16	0	60	22	45*	-6	217	8	-7	-8	47	30	-1*	-9	143	12	3
-3	182	8	5	1	67	25	31*	-5	81	7	2	-7	86	10	-1	-8	89	13	-6
-2	151	9	-1		H,K=	3,	0	-4	124	5	0	-6	201	7	6	-7	193	8	10
-1	275	10	-8	-8	102	10	-6	-3	47	7	6	-5	304	10	6	-6	84	18	-2*
0	196	8	-1	-6	271	9	-22	-2	138	5	-7	-4	373	12	7	-5	178	7	-3
1	297	10	1	-4	595	19	-77	-1	50	5	10	-3	476	15	10	-4	59	11	-10*

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE



L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	20	31	-10*	0	0	33	-6*	-7	59	27	52*	0	34	68	4*	2	326	10	-16
-2	143	6	3	1	264	9	1	-6	178	11	-5	1	110	12	-22	3	154	6	-16
-1	244	8	6	2	122	7	11	-5	11	44	-24*	2	0	47	-5*	4	141	7	-7
0	188	7	9	3	48	17	-1*	-4	304	10	-10	3	32	49	3*	5	53	11	4*
1	436	14	12	4	31	45	-15*	-3	83	11	-5		H,K=	3,	21	6	66	11	6
2	223	7	9	5	199	8	7	-2	377	13	-9	-3	0	51	-6*	7	75	18	-1*
3	516	16	11	6	8	47	-10*	-1	63	18	13*	-2	75	17	9*	8	93	12	-3
4	178	7	-4	7	189	10	1	0	250	10	5	-1	72	19	-30*		H,K=	4,	3
5	263	10	7		H,K=	3,	13	1	27	44	2*	0	171	9	-12	-9	71	20	4*
6	32	52	-37*	-8	145	12	6	2	74	13	-7	1	133	9	9	-8	166	8	-10
7	67	22	6*	-7	84	14	5	3	35	50	30*	2	204	9	-12	-7	106	10	0
8	30	46	23*	-6	134	9	-15	4	104	11	-5		H,K=	3,	22	-6	311	10	-14
	H,K=	3,	10	-5	186	12	1	5	14	54	-30*	-1	126	10	3	-5	161	7	-11
-8	80	14	20	-4	73	12	-15	6	153	14	-8	0	105	18	-12	-4	374	12	-13
-7	80	14	-5	-3	25	43	6*		H,K=	3,	17	1	51	43	-22*	-3	95	5	3
-6	160	9	1	-2	153	7	-2	-6	92	14	-1		H,K=	4,	0	-2	209	7	-4
-5	285	10	14	-1	170	6	7	-5	112	10	0	-8	99	11	-2	-1	65	6	3
-4	312	10	16	0	257	9	10	-4	8	58	-11*	-6	43	18	11*	0	115	6	0
-3	307	10	13	1	245	9	10	-3	31	49	5*	-4	331	11	-25	1	134	5	2
-2	378	12	20	2	355	11	9	-2	78	14	-3*	-2	854	26	-89	2	260	8	-15
-1	318	10	14	3	183	7	-4	-1	150	9	-9	0	474	15	-62	3	198	7	-2
0	214	7	10	4	300	10	6	0	113	12	0	2	473	15	-28	4	443	14	-25
1	178	6	7	5	137	8	7	1	286	10	-6	4	315	10	-17	5	77	9	-3
2	45	12	5*	6	127	9	9	2	207	8	-5	6	93	10	-10	6	244	8	-13
3	47	16	-4*	7	41	57	18*	3	294	11	-1	8	121	9	-1	7	97	10	0
4	73	10	-8		H,K=	3,	14	4	139	10	-16		H,K=	4,	1	8	144	8	4
5	169	7	15	-7	64	30	8*	5	152	12	-5	-9	146	8	6		H,K=	4,	4
6	147	8	9	-6	112	13	0		H,K=	3,	18	-8	66	20	-13*	-9	111	12	-16
7	160	10	0	-5	191	8	-1	-6	58	30	-22*	-7	211	8	-14	-8	17	42	15*
8	128	11	1	-4	247	9	2	-5	186	9	4	-6	151	7	-15	-7	38	27	6*
	H,K=	3,	11	-3	277	9	-2	-4	155	9	-6	-5	365	11	-27	-6	23	34	20*
-8	203	9	12	-2	334	11	4	-3	204	8	-7	-4	196	7	-20	-5	141	7	0
-7	77	14	26*	-1	181	8	-1	-2	176	9	-10	-3	367	11	-26	-4	20	29	17*
-6	209	9	1	0	158	7	15	-1	183	8	-18	-2	157	5	-6	-3	456	18	-10
-5	65	12	16*	1	139	7	-3	0	100	10	-7	-1	38	7	-13*	-2	39	9	-7*
-4	73	10	5	2	29	48	-22*	1	119	9	3	0	18	23	8*	-1	696	24	-13
-3	28	33	22*	3	20	38	1*	2	71	14	24*	1	224	7	-15	0	37	9	22*
-2	160	6	8	4	88	10	-2	3	45	34	14*	2	164	6	-6	1	689	28	-18
-1	128	6	2	5	138	13	6	4	62	24	20*	3	371	12	-35	2	23	30	14*
0	396	12	-1	6	144	10	-9	5	110	13	-7	4	200	7	-15	3	341	11	-7
1	109	6	6		H,K=	3,	15		H,K=	3,	19	5	339	11	-27	4	32	35	-14*
2	618	19	20	-7	154	10	-11	-5	50	36	25*	6	148	11	-8	5	58	11	8*
3	177	7	4	-6	40	55	3*	-4	59	64	16*	7	220	9	-10	6	10	37	1*
4	382	12	12	-5	100	28	-27*	-3	40	45	12*	8	77	19	8*	7	108	10	-1
5	89	20	-12*	-4	54	29	26*	-2	103	12	0		H,K=	4,	2	8	66	15	64*
6	141	9	-2	-3	0	40	-25*	-1	76	17	32*	-9	80	14	-9		H,K=	4,	5
7	45	41	7*	-2	37	38	-3*	0	219	8	-4	-8	86	11	8	-9	86	12	31
	H,K=	3,	12	-1	223	8	-3	1	47	29	-12*	-7	10	37	-33*	-8	185	8	9
-8	42	48	25*	0	124	7	-6	2	301	11	-20	-6	0	35	-9*	-7	122	8	-9
-7	117	10	-1	1	410	13	-4	3	90	12	18	-5	99	7	-9	-6	316	10	0
-6	12	49	-23*	2	122	11	-8	4	224	9	-6	-4	136	6	-6	-5	169	7	1
-5	382	12	8	3	302	10	2		H,K=	3,	20	-3	337	10	-26	-4	394	12	2
-4	72	13	12*	4	109	10	8	-4	61	28	20*	-2	336	10	-25	-3	138	5	-6
-3	419	13	11	5	241	10	0	-3	261	11	-6	-1	382	12	-22	-2	202	7	2
-2	57	11	6*	6	64	21	10*	-2	44	45	2*	0	430	13	-25	-1	104	5	0
-1	403	13	9		H,K=	3,	16	-1	222	9	-17	1	432	13	-20	0	92	6	3

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	127	5	-5	0	430	16	6	3	96	8	4	-5	291	10	3	1	40	47	27*
2	262	8	-1	1	0	35	-24*	4	384	12	10	-4	86	11	6	2	169	13	0
3	204	7	-1	2	380	12	6	5	81	11	-5	-3	236	9	4	3	54	54	-1*
4	439	19	-12	3	0	35	-10*	6	242	9	10	-2	59	18	14*	H,K=	4,	20	
5	146	8	-3	4	214	8	4	7	54	27	-7*	-1	60	20	-10*	-4	32	50	16*
6	269	11	-6	5	37	39	34*	H,K=	4,	12	0	13	38	11*	-3	190	14	-16	
7	108	9	12	6	56	22	-2*	-8	27	48	20*	1	116	8	0	-2	44	55	4*
8	150	9	17	7	35	43	24*	-7	48	28	14*	2	63	14	-9*	-1	258	12	-15
	H,K=	4,	6	8	134	12	12	-6	49	26	15*	3	289	11	-1	0	50	32	-8*
-9	73	17	-10*	H,K=	4,	9	-5	117	9	-3	4	57	22	-25*	1	217	10	-23	
-8	74	14	9*	-9	109	13	-3	-4	25	47	12*	5	264	10	-2	2	0	48	-43*
-7	43	27	5*	-8	80	14	11	-3	380	12	-5	6	69	28	8*	3	138	10	-5
-6	35	38	29*	-7	210	8	7	-2	109	7	10	H,K=	4,	16	H,K=	4,	21		
-5	113	12	0	-6	135	11	-5	-1	447	14	6	-6	56	24	24*	-3	68	37	-21*
-4	236	8	0	-5	276	9	-3	0	100	9	-1	-5	26	49	9*	-2	58	27	-24*
-3	299	10	0	-4	141	6	2	1	459	14	7	-4	185	9	0	-1	29	54	24*
-2	451	17	4	-3	326	11	8	2	9	35	-20*	-3	60	23	-4*	0	0	49	-6*
-1	371	11	-5	-2	176	6	2	3	234	8	4	-2	364	12	-10	1	74	16	27*
0	384	15	-4	-1	56	14	7*	4	27	44	-13*	-1	57	16	-3*	H,K=	5,	0	
1	395	12	7	0	28	36	18*	5	63	18	21*	0	359	12	-1	-8	203	8	-8
2	333	10	1	1	218	7	4	6	26	44	6*	1	39	40	24*	-6	173	12	-17
3	173	8	0	2	137	6	7	7	83	16	4*	2	272	10	0	-4	21	29	-3*
4	120	6	2	3	305	10	7	H,K=	4,	13	3	36	50	5*	-2	185	6	-7	
5	35	36	-3*	4	223	9	2	-8	135	11	18	4	130	13	-3	0	553	17	-36
6	51	18	14*	5	312	10	2	-7	75	16	-11*	5	41	46	36*	2	385	12	-27
7	66	16	11*	6	108	11	-10	-6	199	9	2	H,K=	4,	17	4	470	15	-28	
8	93	23	0*	7	180	11	-1	-5	151	8	0	-6	108	12	-2	6	221	9	3
	H,K=	4,	7	H,K=	4,	10	-4	272	10	3	-5	181	9	-9	8	19	45	14*	
-9	134	10	12	-8	79	14	29	-3	153	7	5	-4	115	12	-2	H,K=	5,	1	
-8	78	13	20	-7	37	43	-2*	-2	161	7	-1	-3	166	9	-12	-9	54	21	38*
-7	229	8	19	-6	51	23	38*	-1	39	40	18*	-2	115	9	20	-8	20	44	-12*
-6	121	7	-4	-5	111	9	-1	0	75	14	11*	-1	54	22	12*	-7	122	8	-8
-5	361	12	2	-4	160	7	-1	1	84	8	11	0	43	35	25*	-6	120	7	-6
-4	124	7	7	-3	267	9	8	2	148	7	2	1	122	8	9	-5	280	9	-18
-3	425	13	5	-2	335	11	7	3	144	8	1	2	130	8	5	-4	285	9	-15
-2	31	34	-9*	-1	308	10	6	4	311	10	-1	3	207	8	4	-3	646	20	-43
-1	71	9	2	0	352	11	8	5	155	10	2	4	140	11	-3	-2	240	8	-22
0	37	11	12*	1	416	13	19	6	221	9	1	5	194	9	0	-1	373	12	-31
1	221	8	3	2	327	10	8	H,K=	4,	14	H,K=	4,	18	0	188	6	-2		
2	114	5	1	3	134	8	-2	-7	54	59	45*	-5	71	18	9*	1	158	6	-4
3	317	11	-7	4	106	8	-4	-6	35	55	22*	-4	74	23	-17*	2	27	26	-9*
4	134	7	-4	5	22	39	10*	-5	85	11	18	-3	172	9	-2	3	62	8	3
5	399	13	-7	6	67	14	28*	-4	148	8	10	-2	176	10	-4	4	113	6	-7
6	79	18	0*	7	63	19	5*	-3	184	8	0	-1	221	9	-4	5	255	9	-11
7	219	9	-8	H,K=	4,	11	-2	291	10	-1	0	161	8	-14	6	96	9	-1	
8	67	44	19*	-8	166	9	8	-1	290	11	7	1	250	9	-3	7	223	9	-11
	H,K=	4,	8	-7	79	15	-17*	0	266	9	4	2	129	10	-7	8	48	52	-26*
-9	0	48	-9*	-6	313	10	15	1	198	8	-8	3	124	12	-4	H,K=	5,	2	
-8	67	17	0*	-5	84	9	7	2	170	7	1	4	44	48	-26*	-9	129	10	2
-7	28	54	26*	-4	309	10	2	3	111	16	-9	H,K=	4,	19	-8	128	8	-4	
-6	20	36	11*	-3	89	9	-3	4	99	12	11	-5	49	51	-1*	-7	131	8	-11
-5	27	45	5*	-2	210	7	5	5	53	23	19*	-4	184	9	-14	-6	128	7	-14
-4	290	9	5	-1	60	10	0	6	82	15	46	-3	0	46	-52*	-5	115	7	-2
-3	114	6	-5	0	18	33	-11*	H,K=	4,	15	-2	106	15	-14	-4	11	29	-2*	
-2	655	20	12	1	85	8	0	-7	152	11	-4	-1	27	43	2*	-3	69	6	-9
-1	11	28	2*	2	299	10	7	-6	72	29	-5*	0	41	53	12*	-2	125	5	0

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	230	7	-15	-2	536	17	-11	-1	38	39	-3*	4	147	8	1	-2	103	15	-1
0	308	10	-18	-1	183	6	-7	0	428	13	7	5	68	15	-5*	-1	230	9	-6
1	290	9	-15	0	374	12	-14	1	18	30	-8*	6	188	10	5	0	89	10	-6
2	303	10	-23	1	120	6	-9	2	429	13	4	7	40	49	-22*	1	138	7	12
3	341	11	-23	2	14	29	5*	3	43	21	-13*	H,K=	5,	12	2	51	23	30*	
4	221	8	-13	3	0	32	-8*	4	363	12	2	-8	46	47	20*	3	61	15	25*
5	195	7	-10	4	189	7	-8	5	29	49	4*	-7	160	9	-1	4	56	22	26*
6	107	13	-8	5	89	10	-4	6	169	10	9	-6	0	44	-24*	5	141	11	-25
7	61	20	-11*	6	230	8	-1	7	22	46	15*	-5	103	9	-11	H,K=	5,	16	
8	41	45	21*	7	106	12	-1	H,K=	5,	9	-4	19	39	17*	-6	116	13	-17	
H,K=	5,	3		8	157	11	-7	-8	63	26	46*	-3	56	13	8*	-5	20	49	13*
-9	26	45	9*	H,K=	5,	6		-7	96	15	-20	-2	39	39	26*	-4	23	45	-12*
-8	53	20	-14*	-9	103	15	-2	-6	115	11	18	-1	303	10	2	-3	0	43	-2*
-7	68	11	10	-8	130	11	-7	-5	237	8	2	0	155	7	3	-2	127	9	-4
-6	232	8	-12	-7	125	8	4	-4	194	7	8	1	397	12	-1	-1	0	42	-10*
-5	120	6	-2	-6	142	8	-6	-3	426	18	-2	2	29	44	0*	0	316	12	-12
-4	321	10	-15	-5	105	8	-9	-2	205	7	3	3	367	12	-2	1	43	51	-23*
-3	292	9	-16	-4	53	11	-10*	-1	378	12	6	4	49	22	16*	2	303	10	-10
-2	556	17	-23	-3	91	6	10	0	94	9	0	5	219	8	12	3	39	46	1*
-1	158	5	-5	-2	218	7	-3	1	113	6	3	6	27	54	12*	4	248	9	-3
0	414	13	-15	-1	230	8	4	2	0	41	-21*	H,K=	5,	13	5	0	53	-22*	
1	140	6	-1	0	345	11	-6	3	51	36	10*	-7	81	14	23	H,K=	5,	17	
2	34	14	-6*	1	186	6	-4	4	60	13	11*	-6	166	9	-4	-6	60	26	-22*
3	39	13	12*	2	316	10	-5	5	181	8	0	-5	115	10	4	-5	147	15	-9
4	172	7	-6	3	319	10	-5	6	113	16	-8	-4	242	10	6	-4	138	9	1
5	104	11	-2	4	316	11	-3	7	202	9	0	-3	197	7	0	-3	235	10	-12
6	228	8	-6	5	228	8	0	H,K=	5,	10	-2	329	11	0	-2	155	8	-11	
7	80	22	-1*	6	120	10	12	-8	134	10	11	-1	143	8	-2	-1	202	8	-9
8	171	9	-5	7	57	21	7*	-7	137	12	-2	0	217	8	2	0	83	13	-20
H,K=	5,	4		H,K=	5,	7		-6	107	14	10	1	76	17	-15*	1	98	11	-5
-9	188	11	1	-9	18	49	1*	-5	110	8	0	2	42	23	23*	2	59	28	46*
-8	34	40	31*	-8	32	45	11*	-4	15	36	-23*	3	29	42	10*	3	38	47	16*
-7	208	8	-2	-7	117	9	-6	-3	58	14	0*	4	111	12	11	4	25	49	-33*
-6	25	36	13*	-6	85	12	3	-2	140	8	5	5	76	26	-8*	H,K=	5,	18	
-5	113	7	-6	-5	324	11	4	-1	218	7	-2	6	168	9	0	-5	19	48	-38*
-4	30	30	-5*	-4	175	7	2	0	295	10	-1	H,K=	5,	14	-4	43	51	27*	
-3	45	10	-7*	-3	546	21	1	1	333	11	0	-7	92	14	-3	-3	34	51	16*
-2	43	12	-11*	-2	192	7	3	2	281	9	11	-6	122	10	-9	-2	58	20	-8*
-1	411	13	-11	-1	398	12	0	3	314	10	-2	-5	47	59	-17*	-1	145	10	-9
0	27	38	18*	0	109	6	0	4	226	8	7	-4	42	35	5*	0	148	9	-1
1	559	17	-13	1	144	6	-6	5	145	12	3	-3	58	21	31*	1	248	9	2
2	27	28	7*	2	41	43	23*	6	99	17	5	-2	129	10	-6	2	160	9	-5
3	430	14	-7	3	61	24	-11*	7	58	24	7*	-1	148	7	-3	3	177	9	-18
4	17	38	11*	4	71	10	-7	H,K=	5,	11	0	213	8	-3	4	122	14	1	
5	267	9	-7	5	215	8	4	-8	56	27	-11*	1	207	8	3	H,K=	5,	19	
6	0	39	-23*	6	93	16	13	-7	34	57	8*	2	222	9	-2	-4	199	9	-10
7	104	9	7	7	223	10	0	-6	222	9	14	3	214	8	8	-3	69	22	-13*
8	0	50	-4*	H,K=	5,	8		-5	121	10	-8	4	240	9	6	-2	249	10	-4
H,K=	5,	5		-9	68	41	52*	-4	341	11	4	5	147	9	4	-1	39	50	-9*
-9	30	50	12*	-8	185	9	-2	-3	158	7	-1	6	70	21	-14*	0	188	8	8
-8	47	29	-16*	-7	36	49	18*	-2	418	13	9	H,K=	5,	15	1	13	46	-6*	
-7	50	43	-8*	-6	166	7	9	-1	117	7	0	-7	101	18	3	2	46	42	22*
-6	230	8	-14	-5	23	42	14*	0	338	11	2	-6	77	16	13*	3	46	48	31*
-5	125	7	-12	-4	68	9	2	1	60	13	2*	-5	213	9	-2	H,K=	5,	20	
-4	403	21	-1	-3	51	12	51*	2	19	42	-21*	-4	84	12	-10	-3	56	26	15*
-3	248	8	0	-2	182	7	-6	3	14	37	4*	-3	383	12	-6	-2	38	60	-9*

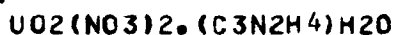


STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE



L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	135	20	-14	-6	31	37	5*	-4	230	9	4	0	241	8	1	-6	55	20	33*
0	0	56	-34*	-5	48	13	13*	-3	181	7	4	1	384	17	-4	-5	63	34	22*
1	227	9	-13	-4	197	7	-12	-2	141	6	-2	2	80	9	-1	-4	163	8	-7
2	52	51	32*	-3	136	6	-6	-1	30	34	-15*	3	168	7	4	-3	149	8	-3
	H,K=	5,	21	-2	420	13	-17	0	95	8	5	4	43	45	8*	-2	254	9	2
-1	36	55	-60*	-1	281	9	-13	1	168	7	-2	5	31	41	24*	-1	224	10	-2
0	88	36	-26*	0	603	19	-31	2	193	8	-5	6	68	17	54*	0	329	11	0
	H,K=	6,	0	1	194	7	-6	3	247	8	2		H,K=	6,	10	1	131	8	2
-8	187	9	-11	2	267	9	-11	4	253	9	1	-8	125	12	6	2	191	8	-4
-6	327	11	-22	3	118	6	-2	5	197	9	-5	-7	147	11	-9	3	80	16	-4*
-4	354	11	-6	4	102	9	4	6	214	9	-4	-6	166	9	7	4	51	29	-23*
-2	172	6	-7	5	0	38	-13*	7	125	13	0	-5	167	7	6	5	61	28	56*
0	111	5	-3	6	39	41	-11*		H,K=	6,	7	-4	155	8	-4		H,K=	6,	14
2	350	11	-11	7	38	44	8*	-9	81	16	-5*	-3	202	8	-2	-7	128	11	8
4	335	11	-10		H,K=	6,	4	-8	33	52	16*	-2	122	7	-6	-6	160	8	15
6	318	11	-9	-9	145	9	11	-7	19	44	-25*	-1	0	49	-24*	-5	148	10	7
	H,K=	6,	1	-8	28	45	19*	-6	0	40	-14*	0	105	7	7	-4	181	8	-1
-9	77	16	-25*	-7	279	10	-6	-5	122	10	-6	1	145	7	3	-3	114	8	5
-8	43	43	20*	-6	42	27	22*	-4	56	24	9*	2	161	7	4	-2	86	9	4
-7	36	39	-1*	-5	289	9	-2	-3	396	12	0	3	223	9	3	-1	17	40	-21*
-6	0	37	-30*	-4	0	32	-3*	-2	157	7	1	4	155	8	1	0	61	14	17*
-5	118	7	-1	-3	247	9	-2	-1	429	14	2	5	204	8	3	1	85	16	-6*
-4	129	10	0	-2	25	30	-13*	0	184	7	-3	6	184	10	9	2	154	13	2
-3	336	11	-12	-1	67	7	-11	1	398	13	-1		H,K=	6,	11	3	174	9	8
-2	258	8	-12	0	36	16	6*	2	93	7	1	-8	39	50	-18*	4	209	9	1
-1	545	17	-22	1	229	8	2	3	254	9	1	-7	39	45	35*	5	143	10	-4
0	205	7	-2	2	47	11	14*	4	65	19	0*	-6	28	42	-8*		H,K=	6,	15
1	484	13	-22	3	352	12	-5	5	6	46	-8*	-5	52	18	15*	-6	18	49	5*
2	174	7	-8	4	13	35	7*	6	0	49	-4*	-4	191	8	-3	-5	90	12	3
3	270	9	-8	5	278	9	-11	7	89	14	-1	-3	112	7	1	-4	0	45	-41*
4	84	8	0	6	0	41	-13*		H,K=	6,	8	-2	426	13	0	-3	251	10	-6
5	0	38	-5*	7	209	9	-1	-8	170	12	-2	-1	130	8	1	-2	140	8	6
6	40	43	7*		H,K=	6,	5	-7	0	44	-25*	0	478	16	5	-1	347	11	-4
7	108	13	5	-9	75	15	33*	-6	262	10	-4	1	154	8	3	0	135	8	15
	H,K=	6,	2	-8	80	17	9*	-5	0	56	-14*	2	259	9	0	1	243	10	-3
-9	94	13	3	-7	26	45	20*	-4	311	10	1	3	57	17	-9*	2	81	17	12*
-8	114	10	-20	-6	41	23	2*	-3	36	23	-12*	4	93	10	13	3	171	9	-3
-7	188	8	-8	-5	37	27	-2*	-2	142	6	-3	5	8	54	-5*	4	52	35	13*
-6	156	7	-12	-4	200	7	-1	-1	39	15	13*	6	34	47	-19*	5	28	48	25*
-5	198	7	-8	-3	176	6	-1	0	115	6	6		H,K=	6,	12		H,K=	6,	16
-4	223	8	-9	-2	460	19	-15	1	18	44	-5*	-7	216	9	-4	-6	201	9	4
-3	191	7	-11	-1	324	10	-5	2	214	8	-5	-6	60	17	10*	-5	49	32	10*
-2	86	6	-3	0	526	16	-19	3	50	22	21*	-5	232	9	5	-4	204	9	-8
-1	35	13	8*	1	201	7	-7	4	349	11	2	-4	47	19	35*	-3	0	45	-33*
0	127	6	0	2	284	9	-8	5	33	50	-4*	-3	205	8	-6	-2	111	10	4
1	145	6	-3	3	75	8	14	6	255	9	-2	-2	20	39	5*	-1	16	43	13*
2	168	6	-10	4	131	8	-18	7	0	64	-22*	-1	43	21	-19*	0	45	29	-4*
3	278	9	-20	5	17	38	15*		H,K=	6,	9	0	51	15	18*	1	47	59	19*
4	200	7	-4	6	47	49	-4*	-8	61	28	28*	1	149	7	2	2	188	8	-2
5	227	8	0	7	12	57	-31*	-7	43	48	0*	2	55	24	-11*	3	44	46	-2*
6	180	10	-14		H,K=	6,	6	-6	29	47	2*	3	274	10	-11	4	225	10	4
7	125	12	-11	-9	63	23	-26*	-5	105	8	-2	4	49	21	40*		H,K=	6,	17
	H,K=	6,	3	-8	137	9	-3	-4	99	8	-10	5	255	10	3	-5	56	45	-5*
-9	35	53	-8*	-7	180	8	0	-3	276	10	0	6	0	54	-34*	-4	85	14	10
-8	80	14	-3	-6	193	8	-4	-2	149	6	3		H,K=	6,	13	-3	173	9	-15
-7	0	40	-3*	-5	187	7	2	-1	428	14	-3	-7	57	61	48*	-2	133	10	-5

STRUCTURE FACTORS CONTINUED FOR  
URANYL NITRATE IMIDAZOLE



L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-1	271	10	-5	-6	133	7	-5	-3	47	14	-7*	4	118	15	-2	-1	316	10	-3
0	186	8	-2	-5	194	9	-8	-2	151	6	5	5	43	54	33*	0	45	39	7*
1	222	9	1	-4	228	8	-12	-1	158	6	-7	6	205	9	-4	1	89	11	1
2	91	13	-8	-3	268	9	-9	0	388	12	-9		H,K=	7,	9	2	37	40	31*
3	107	12	-12	-2	273	9	-16	1	173	7	-8	-8	43	51	-30*	3	65	17	11*
	H,K=	6,	18	-1	282	9	-5	2	393	13	-12	-7	150	8	6	4	10	58	-6*
-4	103	24	4*	0	200	7	-5	3	157	9	-3	-6	68	14	-5*	5	152	9	3
-3	118	13	-2	1	63	11	-7	4	233	8	-5	-5	92	12	-6		H,K=	7,	13
-2	62	20	-3*	2	23	37	-9*	5	55	18	-12*	-4	0	37	-11*	-7	88	15	6
-1	50	56	17*	3	44	17	-2*	6	133	9	4	-3	54	15	-13*	-6	114	11	-3
0	40	45	15*	4	127	8	2	7	0	50	-25*	-2	63	11	2	-5	51	39	16*
1	105	11	-7	5	156	8	-1		H,K=	7,	6	-1	268	9	-2	-4	38	47	19*
2	46	71	-41*	6	168	8	0	-8	18	58	-33*	0	141	7	2	-3	39	42	3*
3	139	15	-17	7	150	9	10	-7	121	15	11	1	338	11	0	-2	121	8	5
	H,K=	6,	19		H,K=	7,	3	-6	170	8	3	2	233	8	1	-1	127	8	7
-3	53	27	15*	-9	77	17	23*	-5	194	8	-9	3	271	10	1	0	222	9	-1
-2	212	9	-16	-8	149	9	-16	-4	275	9	0	4	77	13	-15	1	155	9	-2
-1	53	29	-6*	-7	90	20	16*	-3	216	8	-11	5	148	9	-9	2	301	11	-3
0	265	10	-9	-6	149	8	-6	-2	248	8	-3	6	15	47	-29*	3	124	10	-13
1	73	37	8*	-5	16	35	-9*	-1	247	8	-8		H,K=	7,	10	4	185	9	1
2	141	18	-30	-4	0	37	-25*	0	203	7	-5	-8	34	48	-3*	5	78	21	4*
	H,K=	6,	20	-3	17	33	-8*	1	96	7	1	-7	124	9	15		H,K=	7,	14
-2	23	50	7*	-2	199	7	-5	2	38	23	6*	-6	142	11	4	-6	109	15	-9
-1	41	59	17*	-1	162	6	-9	3	71	12	-5	-5	171	8	6	-5	134	10	1
0	34	61	15*	0	374	12	-12	4	124	11	2	-4	222	8	0	-4	182	10	-5
	H,K=	7,	0	1	138	6	-3	5	130	8	3	-3	218	8	-1	-3	157	9	-12
-8	59	21	-28*	2	391	13	-8	6	154	10	-9	-2	206	8	1	-2	176	8	-1
-6	246	9	-13	3	101	7	0		H,K=	7,	7	-1	255	10	-2	-1	151	8	-6
-4	444	14	-22	4	214	8	-6	-8	37	49	-17*	0	203	10	4	0	123	9	0
-2	346	11	-12	5	93	10	1	-7	149	10	-14	1	66	14	10*	1	53	21	5*
0	350	11	-11	6	125	18	-7	-6	65	17	6*	2	0	39	-24*	2	0	44	-11*
2	53	19	2*	7	0	48	-19*	-5	119	12	7	3	55	16	9*	3	19	44	-11*
4	212	8	0		H,K=	7,	4	-4	0	36	-14*	4	111	9	8	4	89	15	-4
6	210	8	5	-9	38	58	9*	-3	53	19	-2*	5	122	10	-4		H,K=	7,	15
	H,K=	7,	1	-8	19	43	13*	-2	61	14	6*	6	124	12	4	-6	58	24	23*
-9	142	14	10	-7	160	8	-9	-1	311	10	-8		H,K=	7,	11	-5	53	29	-15*
-8	86	12	-2	-6	39	49	25*	0	65	10	-11	-7	14	60	-24*	-4	18	54	14*
-7	181	8	-9	-5	267	9	-7	1	367	12	-5	-6	101	11	-13	-3	53	26	12*
-6	45	53	-16*	-4	9	39	-31*	2	145	7	-3	-5	25	40	1*	-2	62	24	17*
-5	89	10	8	-3	403	13	-11	3	351	11	-12	-4	52	16	18*	-1	208	9	-2
-4	26	33	16*	-2	39	14	18*	4	85	11	-8	-3	25	42	8*	0	69	15	-12*
-3	51	10	1*	-1	482	15	-11	5	189	8	-7	-2	159	7	-1	1	287	10	-1
-2	70	7	-7	0	27	30	13*	6	51	26	22*	-1	48	20	-26*	2	77	15	-5*
-1	319	10	-9	1	101	10	-6		H,K=	7,	8	0	376	12	-5	3	258	10	-4
0	191	7	-2	2	61	9	25	-8	56	27	-10*	1	102	14	-6	4	78	16	12*
1	414	13	-20	3	91	8	1	-7	31	43	18*	2	329	11	-1		H,K=	7,	16
2	193	7	-10	4	59	13	33*	-6	220	8	1	3	100	10	6	-5	54	37	17*
3	316	11	-9	5	179	8	0	-5	56	15	4*	4	385	99	97*	-4	234	11	-16
4	155	10	-5	6	19	45	11*	-4	325	11	1	5	45	46	-10*	-3	0	53	-38*
5	212	8	8	7	207	12	-9	-3	0	35	-13*		H,K=	7,	12	-2	243	9	-5
6	65	15	18*		H,K=	7,	5	-2	354	11	2	-7	137	14	4	-1	29	44	6*
7	63	18	10*	-8	154	15	-18	-1	16	34	10*	-6	0	54	-5*	0	177	8	8
	H,K=	7,	2	-7	96	10	10	0	233	8	3	-5	224	9	-8	1	53	22	43*
-9	66	17	54*	-6	146	7	5	1	17	34	-5*	-4	62	18	-4*	2	20	46	-8*
-8	48	50	0*	-5	73	12	21	2	40	21	22*	-3	299	10	-3	3	0	50	-16*
-7	120	11	0	-4	0	40	-6*	3	25	37	8*	-2	52	16	16*		H,K=	7,	17

STRUCTURE FACTORS CONTINUED FC#  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	51	32	43*	3	130	8	-2	-5	70	14	-10*	5	220	9	7	-4	126	13	7
-3	30	45	2*	4	44	26	-9*	-4	157	7	-1	H,K#	8,	10	-3	112	11	-18	
-2	49	31	-5*	5	41	36	23*	-3	181	7	4	-7	0	47	-15*	-2	177	16	-5
-1	180	11	5	6	28	46	-3*	-2	274	9	-7	-6	61	23	38*	-1	175	8	3
0	150	9	-3	H,K#	8,	3	-1	228	8	-11	-5	97	10	10	0	197	8	3	
1	227	9	-1	-8	141	10	-21	0	288	9	-6	-4	133	8	2	1	172	9	-1
2	142	10	4	-7	84	14	0	1	235	8	-10	-3	178	7	3	2	164	11	1
H,K#	7,	18	-6	212	8	-9	2	207	8	1	-2	236	8	6	3	89	14	4	
-4	114	12	-8	-5	121	9	9	3	164	8	6	-1	291	10	2	H,K#	8,	15	
-3	167	12	6	-4	219	8	-10	4	44	53	-7*	0	236	8	1	-5	192	11	0
-2	104	14	-11	-3	88	8	10	5	30	43	27*	1	227	9	6	-4	46	46	-6*
-1	161	9	-1	-2	117	8	-3	6	25	47	-17*	2	166	8	8	-3	104	18	-1
0	105	17	12	-1	28	35	25*	H,K#	8,	7	3	80	13	-5	-2	25	47	-8*	
1	76	24	13*	0	117	6	-4	-8	71	18	13*	4	50	34	7*	-1	65	16	49*
2	27	51	8*	1	92	8	-8	-7	213	9	1	5	35	46	31*	0	11	51	-11*
H,K#	7,	19	2	264	10	-1	-6	61	19	-12*	H,K#	8,	11	1	128	10	-6		
-2	89	16	-8	3	82	10	8	-5	254	9	6	-7	51	33	-12*	2	59	21	17*
-1	49	34	24*	4	235	9	-5	-4	90	11	2	-6	195	10	-12	3	190	9	-8
0	214	9	-1	5	106	10	1	-3	137	7	-10	-5	74	14	0*	H,K#	8,	16	
H,K#	8,	0	6	208	9	16	-2	56	12	15*	-4	187	8	3	-4	160	9	9	
-8	55	23	0*	H,K#	8,	4	-1	39	22	24*	-3	68	12	10	-3	0	53	-13*	
-6	67	17	1*	-8	23	46	14*	0	70	9	3	-2	118	8	4	-2	238	10	-15
-4	238	8	1	-7	38	49	18*	1	187	8	-4	-1	41	32	28*	-1	58	21	28*
-2	370	12	-2	-6	24	40	7*	2	86	12	9	0	83	13	4	0	257	11	-1
0	407	13	-8	-5	150	7	4	3	276	10	0	1	51	19	18*	1	10	48	-32*
2	404	13	-9	-4	0	37	-37*	4	77	13	2	2	224	8	3	2	203	9	9
4	81	10	12	-3	297	10	-5	5	228	9	1	3	89	13	14	H,K#	8,	17	
6	10	49	-47*	-2	0	35	-13*	6	54	69	-5*	4	215	9	6	-3	88	15	4
H,K#	8,	1	-1	417	13	-11	H,K#	8,	8	5	71	21	3*	-2	0	50	-34*		
-8	70	17	-13*	0	0	39	-9*	-8	57	68	-3*	H,K#	8,	12	-1	35	55	16*	
-7	194	8	-17	1	381	13	-8	-7	15	45	14*	-6	30	55	25*	0	38	48	0*
-6	126	8	-2	2	36	27	31*	-6	36	44	-14*	-5	119	10	1	1	75	18	-12*
-5	296	10	-8	3	171	7	0	-5	46	23	30*	-4	44	27	13*	H,K#	8,	18	
-4	82	9	-13	4	35	39	15*	-4	220	9	8	-3	223	9	-5	-2	125	12	2
-3	124	7	5	5	16	46	15*	-3	28	50	9*	-2	84	15	-4	-1	209	13	-1
-2	80	13	1	6	43	45	38*	-2	260	9	-9	-1	332	12	-4	H,K#	9,	0	
-1	9	32	2*	H,K#	8,	5	-1	17	48	-1*	0	29	53	15*	-8	120	12	-17	
0	55	14	-17*	-8	154	9	3	0	394	12	-7	1	295	10	5	-6	127	9	-3
1	193	7	-1	-7	84	13	-3	1	43	44	6*	2	0	43	-31*	-4	38	28	15*
2	153	7	-4	-6	245	9	-5	2	279	9	-2	3	122	10	-5	-2	205	7	4
3	291	10	-10	-5	124	7	10	3	44	24	37*	4	52	27	45*	0	347	11	10
4	95	9	0	-4	205	8	-3	4	89	13	42	H,K#	8,	13	2	358	11	3	
5	238	9	-3	-3	90	8	-9	5	48	38	34*	-6	137	17	-16	4	275	10	8
6	93	12	9	-2	105	8	3	H,K#	8,	9	-5	89	14	-17	H,K#	9,	1		
H,K#	8,	2	-1	22	33	8*	-7	162	9	-3	-4	160	8	7	-8	40	49	7*	
-8	48	31	2*	0	75	9	-10	-6	72	17	-17*	-3	53	21	-3*	-7	124	10	11
-7	18	51	11*	1	59	14	-8*	-5	218	9	-5	-2	71	14	-6*	-6	111	9	4
-6	50	19	17*	2	293	10	-8	-4	119	8	5	-1	0	42	-26*	-5	264	10	-3
-5	90	9	-3	3	88	15	-5	-3	130	8	-6	0	73	15	7*	-4	133	7	2
-4	126	8	2	4	244	9	4	-2	0	37	-31*	1	69	25	-6*	-3	288	9	-1
-3	171	7	-1	5	122	12	-10	-1	30	52	12*	2	183	9	-4	-2	110	8	4
-2	248	9	-8	6	174	12	2	0	65	18	16*	3	96	12	-12	-1	220	8	4
-1	320	10	-6	H,K#	8,	6	1	118	9	-12	4	191	12	8	0	112	7	3	
0	279	9	-11	-8	66	19	25*	2	96	9	3	H,K#	8,	14	1	112	9	-4	
1	257	9	-8	-7	47	27	36*	3	224	10	-5	-6	0	56	-24*	2	10	39	3*
2	177	7	0	-6	50	20	12*	4	119	10	-3	-5	45	48	-15*	3	102	9	0

STRUCTURE FACTORS CONTINUED FCF  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	66	15	4*	0	135	8	4	1	58	27	-12*	1	171	9	5	1	93	13	10
5	153	14	-4	1	14	38	-6*	2	27	41	18*	2	216	13	9	2	177	8	10
	H,K=	9,	2	2	42	25	26*	3	70	20	-1*		H,K=	9,	15	3	46	58	-14*
-8	99	12	13	3	32	41	-10*	4	27	47	-23*	-4	58	46	-16*	4	32	46	-23*
-7	104	11	-3	4	129	9	1		H,K=	9,	10	-3	186	9	-4		H,K=	10,	4
-6	98	12	4	5	58	24	-12*	-6	87	16	20*	-2	70	17	5*	-7	150	10	-1
-5	69	13	26*		H,K=	9,	6	-5	71	15	13*	-1	159	12	8	-6	0	45	-11*
-4	38	28	27*	-7	44	57	-43*	-4	46	39	42*	0	32	47	-8*	-5	211	10	0
-3	52	14	5*	-6	99	10	5	-3	49	35	0*	1	55	33	-11*	-4	0	42	-11*
-2	122	7	10	-5	57	16	18*	-2	114	9	4		H,K=	9,	16	-3	180	9	0
-1	139	7	-8	-4	53	25	44*	-1	151	8	-4	-3	33	48	24*	-2	15	46	14*
0	186	9	2	-3	27	38	-2*	0	162	9	6	-2	124	10	8	-1	0	51	-21*
1	306	10	-3	-2	118	10	13	1	231	9	-6	-1	0	63	-33*	0	0	49	-3*
2	214	8	-3	-1	148	8	-1	2	184	8	3	0	184	11	-20	1	187	11	16
3	200	8	0	0	216	8	-4	3	177	9	2		H,K=	10,	0	2	25	43	14*
4	161	12	0	1	260	9	-4	4	133	10	-8	-6	228	10	2	3	235	10	5
5	92	15	-10	2	272	10	-2		H,K=	9,	11	-4	187	8	15	4	40	56	26*
	H,K=	9,	3	3	178	8	-1	-6	155	14	-8	-2	117	8	13		H,K=	10,	5
-8	50	33	-7*	4	176	8	14	-5	74	15	3*	0	102	10	5	-7	0	52	-11*
-7	62	17	14*	5	69	28	-22*	-4	257	10	1	2	259	10	4	-6	37	47	-19*
-6	184	9	5		H,K=	9,	7	-3	73	14	-1*	4	250	10	12	-5	68	16	-1*
-5	117	12	-5	-7	116	17	-3	-2	259	10	7		H,K=	10,	1	-4	166	8	2
-4	269	9	-13	-6	52	24	-13*	-1	98	10	11	-7	7	45	-1*	-3	137	8	11
-3	112	7	7	-5	260	9	-1	0	129	8	6	-6	17	59	1*	-2	269	9	1
-2	289	10	-9	-4	93	11	13	1	28	43	3*	-5	118	10	11	-1	107	9	6
-1	118	9	-1	-3	244	9	4	2	13	44	2*	-4	92	11	0	0	264	11	3
0	140	7	11	-2	89	14	-8	3	19	46	-4*	-3	240	9	-3	1	91	11	-14
1	61	14	4*	-1	221	9	9	4	118	12	11	-2	125	8	-6	2	181	9	4
2	11	44	9*	0	72	17	8*		H,K=	9,	12	-1	275	9	8	3	7	54	-33*
3	78	12	12	1	92	10	-5	-6	33	58	25*	0	135	7	9	4	61	23	8*
4	137	9	5	2	8	41	3*	-5	72	21	5*	1	257	9	13		H,K=	10,	6
5	48	57	-5*	3	95	11	4	-4	47	44	41*	2	105	10	2	-7	106	12	8
	H,K=	9,	4	4	33	58	2*	-3	58	20	2*	3	129	9	11	-6	160	9	9
-8	60	27	53*	5	152	9	9	-2	0	44	-21*	4	10	54	-10*	-5	129	11	-9
-7	139	11	12		H,K=	9,	8	-1	181	11	-4		H,K=	10,	2	-4	135	12	-1
-6	0	48	-12*	-7	0	48	-4*	0	29	52	-3*	-7	78	20	-23*	-3	103	9	6
-5	82	12	-9	-6	140	9	5	1	287	10	-3	-6	157	8	12	-2	60	15	21*
-4	30	37	21*	-5	41	41	23*	2	51	24	26*	-5	172	8	4	-1	49	18	33*
-3	83	9	-3	-4	36	40	30*	3	219	9	-5	-4	137	8	5	0	43	31	-6*
-2	34	35	12*	-3	0	44	-2*		H,K=	9,	13	-3	94	10	-11	1	125	9	7
-1	253	9	1	-2	169	7	0	-5	115	17	6	-2	33	47	-8*	2	167	8	9
0	0	36	-21*	-1	27	42	3*	-4	177	10	-5	-1	38	44	11*	3	151	11	2
1	328	11	-2	0	240	9	1	-3	119	10	4	0	40	29	-2*	4	197	9	12
2	0	47	-11*	1	29	41	-13*	-2	186	9	4	1	129	9	14		H,K=	10,	7
3	282	11	2	2	332	11	-4	-1	53	42	-16*	2	161	8	6	-6	0	47	-12*
4	26	49	22*	3	47	26	20*	0	82	13	-11	3	184	9	9	-5	129	9	15
5	163	10	-5	4	204	9	-7	1	32	60	-13*	4	178	10	-2	-4	83	12	19
	H,K=	9,	5		H,K=	9,	9	2	31	46	26*		H,K=	10,	3	-3	226	9	2
-8	70	25	2*	-7	112	11	13	3	0	49	-45*	-7	17	46	15*	-2	62	23	-6*
-7	65	26	6*	-6	92	19	6*		H,K=	9,	14	-6	45	33	1*	-1	255	9	-1
-6	172	10	7	-5	201	9	-12	-5	37	52	2*	-5	0	43	-43*	0	106	10	20
-5	131	8	7	-4	109	11	22	-4	23	50	22*	-4	190	8	6	1	259	12	8
-4	289	11	-12	-3	236	10	-2	-3	0	50	-34*	-3	124	9	-3	2	82	13	8
-3	131	8	5	-2	122	10	4	-2	95	12	21	-2	272	9	9	3	107	12	8
-2	276	9	-1	-1	189	9	-4	-1	108	10	9	-1	85	11	6	4	46	59	33*
-1	130	7	9	0	53	35	1*	0	173	9	5	0	243	9	-3		H,K=	10,	8

STRUCTURE FACTORS CONTINUED FCB  
URANYL NITRATE IMIDAZOLE

UO2(NO3)2.(C3N2H4)H2O

L	FOB	SG	DEL	L	FCB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	172	12	-1	1	98	15	13	H,K= 11,	5	H,K= 11,	11	0	83	15	3				
-5	25	45	19*	H,K= 10,	14			-6	64	22	-1*	-4	0	52	-6*	1	41	47	-1*
-4	170	10	-1	-3	90	14	16	-5	46	34	25*	-3	0	48	-27*	H,K= 12,	6		
-3	19	42	8*	-2	56	42	19*	-4	0	46	-5*	-2	131	13	3	-4	126	11	15
-2	60	19	-1*	-1	42	52	21*	-3	41	51	2*	-1	33	50	-1*	-3	147	9	18
-1	0	50	-3*	0	71	18	25*	-2	144	8	5	0	184	10	13	-2	176	9	17
0	93	13	22	H,K= 11,	0			-1	48	34	-16*	H,K= 11,	12			-1	171	9	10
1	27	42	16*	-6	168	9	11	0	237	10	19	-3	215	10	1	0	183	9	21
2	186	11	-7	-4	264	10	13	1	92	13	-5	-2	0	49	-15*	1	108	12	0
3	65	17	49*	-2	243	10	7	2	203	9	6	-1	131	10	7	H,K= 12,	7		
H,K= 10,	9			0	165	11	13	3	114	12	11	H,K= 12,	0			-4	25	49	-16*
-6	0	50	-16*	2	39	44	12*	H,K= 11,	6			-4	165	9	9	-3	117	10	28
-5	105	14	7	H,K= 11,	1			-6	124	10	17	-2	263	10	16	-2	40	56	35*
-4	77	27	7*	-6	42	48	16*	-5	124	10	5	0	257	10	21	-1	72	16	52*
-3	210	8	4	-5	31	45	2*	-4	174	13	5	2	129	10	6	0	44	47	31*
-2	116	9	1	-4	0	45	-7*	-3	154	9	-9	H,K= 12,	1			H,K= 12,	8		
-1	230	9	7	-3	91	11	11	-2	173	9	4	-5	136	9	23	-3	0	52	-13*
0	112	14	-8	-2	60	39	-14*	-1	115	10	-2	-4	61	24	5*	-2	221	11	15
1	195	13	3	-1	193	8	11	0	82	13	0	-3	85	14	-10	-1	57	24	29*
2	69	23	6*	0	129	10	11	1	38	45	-7*	-2	10	41	-1*	0	219	9	15
3	92	14	-5	1	231	11	11	2	52	28	28*	-1	0	42	-10*	H,K= 12,	9		
H,K= 10,	10			2	86	14	-8	3	58	60	13*	0	34	68	0*	-2	56	26	50*
-6	92	16	-21	3	210	10	2	H,K= 11,	7			1	139	10	7	-1	45	59	40*
-5	134	10	-1	H,K= 11,	2			-5	52	27	11*	2	68	19	17*	H,K= 13,	0		
-4	132	8	18	-6	86	15	-4	-4	45	54	43*	H,K= 12,	2			-2	134	12	12
-3	99	14	4	-5	128	10	0	-3	84	23	3*	-5	78	16	18*	H,K= 13,	1		
-2	36	44	-5*	-4	173	9	7	-2	54	27	10*	-4	99	13	-2	-3	150	11	6
-1	33	42	19*	-3	193	8	-4	-1	175	8	9	-3	152	11	5	-2	94	13	14
0	0	45	-41*	-2	158	8	5	0	63	19	-10*	-2	161	10	12	-1	126	12	-4
1	95	16	-3	-1	134	8	10	1	235	9	8	-1	188	8	11	H,K= 13,	2		
2	120	12	4	0	68	24	-17*	2	47	47	-16*	0	120	17	-5	-2	79	17	8*
3	141	11	-13	1	55	20	18*	H,K= 11,	8			1	115	14	-4	-1	128	16	-3
H,K= 10,	11			2	18	49	-5*	-5	0	60	-4*	2	77	26	-22*	H,K= 13,	3		
-5	0	68	-34*	3	47	45	-9*	-4	212	10	11	H,K= 12,	3			-2	152	10	22
-4	160	9	-11	H,K= 11,	3			-3	42	44	22*	-5	7	48	-41*				
-3	76	22	18*	-6	61	22	-10*	-2	220	10	8	-4	131	12	9				
-2	245	9	2	-5	37	44	24*	-1	32	46	18*	-3	47	49	12*				
-1	81	20	-3*	-4	22	46	18*	0	105	25	1*	-2	44	44	13*				
0	235	9	8	-3	32	42	6*	1	42	46	30*	-1	47	30	46*				
1	81	14	19	-2	138	9	1	2	62	19	44*	0	84	13	16				
2	150	9	7	-1	80	12	7	H,K= 11,	9			1	37	52	-11*				
H,K= 10,	12			0	222	10	12	-5	0	49	-32*	2	155	19	9				
-5	176	10	8	1	54	29	-21*	-4	0	47	-2*	H,K= 12,	4						
-4	0	47	-20*	2	205	12	10	-3	89	12	20	-5	97	24	11*				
-3	135	10	11	3	110	10	23	-2	61	19	9*	-4	31	52	29*				
-2	41	46	29*	H,K= 11,	4			-1	154	9	14	-3	215	10	18				
-1	0	44	-9*	-6	24	59	16*	0	113	11	11	-2	31	48	29*				
0	0	48	-16*	-5	214	10	9	1	188	9	4	-1	251	9	15				
1	130	10	6	-4	22	44	20*	2	107	11	22	0	28	45	24*				
2	41	50	34*	-3	264	10	-2	H,K= 11,	10			1	177	9	20				
H,K= 10,	13			-2	32	41	31*	-4	140	10	11	H,K= 12,	5						
-4	110	15	-3	-1	159	8	-3	-3	166	9	-2	-5	90	17	32*				
-3	104	14	-2	0	0	43	-16*	-2	128	13	-17	-4	129	12	8				
-2	187	9	4	1	69	18	17*	-1	112	10	12	-3	38	46	0*				
-1	98	22	-1*	2	13	45	11*	0	91	17	27*	-2	48	30	15*				
0	191	9	0	3	67	22	-6*	1	25	48	-2*	-1	64	17	52*				

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