

# **Lawrence Berkeley National Laboratory**

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**Title**

STRUCTURE OF PENTAKIS (UREA) DIOXOURANIUM(VI)NITRATE LUO<sub>2</sub> (OC (NH<sub>2</sub>)<sub>2</sub>)<sub>5</sub> (NO<sub>3</sub>) 2

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 $[UO_2(O\bar{C}(NH_2)_2)_5](NO_3)_2$

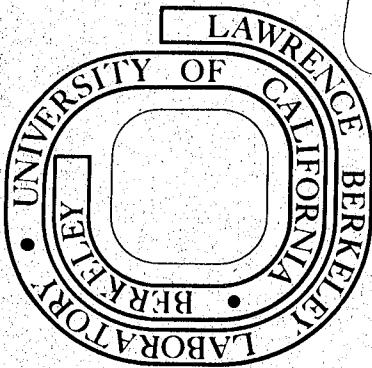
Allan Zalkin, Helena Ruben and David H. Templeton

August 1978

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STRUCTURE OF PENTAKIS(UREA)DIOXOURANIUM(VI)NITRATE,  
 $[UO_2(OC(NH_2)_2)_5](NO_3)_2$

by Allan Zalkin\*, Helena Ruben and David H. Templeton

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and

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AUGUST 1978

In our ongoing studies of uranium complexes we have determined the crystal structure of  $UO_2(\text{urea})_5(NO_3)_2$  by X-ray diffraction. Gentile and Campisi<sup>1</sup> reported the preparation of this compound and concluded, on the basis of infrared spectra, that the nitrate groups are not coordinated to uranium, a fact which we confirm. The uranyl ion is coordinated by oxygen atoms of the five urea molecules in a complex which is monomeric, not a polymer as suggested earlier.<sup>1</sup>

From an aqueous solution of uranyl nitrate and urea which was allowed to evaporate slowly overnight, small fluorescent lime-green crystals precipitated. The crystals were stable in air and showed no decomposition during the two weeks the X-ray experiments were being conducted. Weissenberg photography showed the crystal to be monoclinic, and rough cell dimensions were obtained.

A crystal of dimensions  $.08 \times .11 \times .21$  mm was glued to a glass fiber and examined with a Picker FACS-I automatic diffractometer equipped with a graphite monochromator and a Mo x-ray tube ( $\lambda K\alpha_1$  0.70930 Å).  $\omega$  scans of the 800, 040, and 006 reflections showed peaks with half-widths of  $0.16^\circ$ ,  $0.15^\circ$  and  $0.11^\circ$  respectively. The setting angles of 8 manually centered reflections ( $16^\circ < 2\theta < 25^\circ$ ) using MoK $\beta$  ( $\lambda$  0.632288 Å) and 3 reflections ( $40^\circ < 2\theta < 43^\circ$ ) using MoK $\alpha_1$  were used to determine the cell parameters  $a = 15.944(8)$  Å,  $b = 8.952(4)$  Å,  $c = 15394(6)$  Å,  $\beta = 106.31(3)^\circ$ , and  $V = 2108.8$  Å $^3$ . The observed extinctions are unique to space group P2 $_1/n$ . For Z=4 and a molecular weight of 694.32 the calculated density is  $2.19$  g cm $^{-3}$ .

Intensity data were collected with a scan speed of  $2^\circ/\text{min}$  on  $2\theta$ . Each reflection was scanned from  $0.7^\circ$  before the  $K\alpha_1$  peak to  $0.7^\circ$  after the  $K\alpha_2$  peak, and backgrounds were counted for 4 s at each end of the scan range. The temperature during data collection was  $21 \pm 1^\circ\text{C}$ . Three standard reflections were measured after every 200th scan. The 10,524 scans, not including standards, resulted in 4869 unique intensities, 2954 of which were greater than  $3\sigma$ . An absorption correction was applied,  $^2\mu = 73$  cm $^{-1}$ , and the maximum and minimum corrections were 2.24 and 1.77 respectively. The intensities of all three standards decayed about 3% during the data collection period, and the data were corrected accordingly.

The trial coordinates of the uranium atom position was derived from a three dimensional Patterson function. The Fourier map,

calculated with the phases of the uranium atom alone, revealed eleven of the light atoms. A least-squares refinement and the subsequent Fourier calculation, phased by the twelve atoms, revealed the locations of the remaining atoms. A series of 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 the weights are given in the supplementary material; the "ignorance factor",  $p$ , was set to 0.03. Scattering factors from Doyle and Turner<sup>3</sup> were used, and anomalous dispersion corrections<sup>4</sup> (for  $U f' = -10.673$ ,  $f'' = 9.654$ ) were applied. Hydrogen atoms could not be identified in the final difference maps and were not included in the least-squares refinement. The largest peak in the last difference Fourier map was 1.2 e. Anisotropic thermal parameters were included for all atoms refined. The discrepancy indices for 2954 data where  $I > 3\sigma$  are

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.031$$

$$R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w |F_o|^2]^{1/2} = 0.032.$$

R for all 4869 data is 0.073. The error in an observation of unit weight is 1.09. In the last cycle no parameter changed more than  $0.11\sigma$ .

A powder pattern, calculated from this structure and listed in the supplementary material, is consistent with the pattern published by Gentile and Campisi.<sup>1</sup>

## RESULTS AND DISCUSSION

Atomic parameters, distances, and angles are listed in Tables I-III. The molecular structure (Figure 1) consists of a uranium atom at the center of a pentagonal bipyramid of two uranyl oxygen atoms at each apex and of five urea oxygen atoms on the equator. The average U-O(urea) distance is 2.38 Å (corrected for thermal motion). The uranium atom and the equatorial atoms are all within 0.09 Å of their least-squares plane which is nearly perpendicular to the O-U-O axis. The geometry and bond distances and angles are in very close agreement with those found by a neutron diffraction study<sup>5</sup> in  $\text{UO}_2(\text{H}_2\text{O})(\text{urea})_4(\text{NO}_3)_2$ , in which water occupies one of the coordination sites. In both structures the nitrate and urea groups are planar, and the nitrate ions have no close contacts to uranium.

Hydrogen bonding in the structure is mostly rather weak. There are only five N(urea) to O(nitrate or urea) distances that are less than 3 Å and only one of these is less than 2.9 Å; see Table II. As in the tetrakis(urea) compound there are numerous other N-O contacts in the range 3.0-3.3 Å which may be very weak hydrogen bonds, but there is no satisfactory way to assign all the hydrogen atoms to them. There are no N(urea) - O(uranyl) short distances.

SUPPLEMENTARY MATERIAL AVAILABLE: Data processing formulas, a table of anisotropic thermal parameters, calculated powder pattern, and the listing of structure factor amplitudes (22 pages). Ordering information is given on any current masthead page.

ACKNOWLEDGEMENT

This work was supported by the Division of Nuclear Sciences, Office of Basic Energy Sciences, U. S. Department of Energy.

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Table I. Postional Parameters with Estimated Standard Deviations<sup>a</sup>  
for  $[UO_2(OC(NH_2)_2)_5][NO_3]_2$

ATOM	X	Y	Z
U	.10526(2)	.23262(3)	.35415(2)
O(1)	.2351(3)	.2567(6)	.4749(3)
O(2)	.2221(3)	.1642(7)	.2981(4)
O(3)	.0470(3)	.1537(6)	.2019(3)
O(4)	-.0473(3)	.2691(7)	.3158(4)
O(5)	.0692(3)	.3429(6)	.4807(3)
O(6)	.0933(3)	.0518(6)	.3944(4)
O(7)	.1176(4)	.4166(6)	.3192(4)
O(8)	.6173(4)	.0050(7)	.4578(4)
O(9)	.7213(5)	.1643(8)	.4926(5)
O(10)	.7080(5)	.0237(8)	.3782(5)
O(11)	.0014(4)	.2446(8)	.7611(4)
O(12)	.0511(4)	.1518(7)	.8930(4)
O(13)	.1235(4)	.1202(7)	.7956(4)
N(1)	.2544(5)	.5006(8)	.5172(5)
N(2)	.3484(5)	.3197(9)	.5930(5)
N(3)	.3676(5)	.1744(9)	.3638(5)
N(4)	.3080(5)	.2755(9)	.2204(6)
N(5)	.0893(8)	.078(1)	.0839(6)
N(6)	.0677(7)	.322(1)	.1021(7)
N(7)	.8104(5)	.306(1)	.2907(6)
N(8)	.8867(5)	.175(1)	.4180(6)

Table I. Continued

N(9)	.0250(5)	.3883(8)	.6045(4)
N(10)	.1122(5)	.1836(8)	.6007(5)
N(11)	.6821(5)	.0652(8)	.4426(6)
N(12)	.0592(5)	.1723(8)	.8174(5)
C(1)	.2775(5)	.359(1)	.5269(5)
C(2)	.2976(5)	.205(1)	.2940(6)
C(3)	.0671(5)	.184(1)	.1312(5)
C(4)	.8860(5)	.243(1)	.3415(6)
C(5)	.0691(5)	.3060(9)	.5612(5)

<sup>a</sup>Here and in the following tables the numbers in parentheses are the estimated standard deviations in the least significant digit.

Table II. Interatomic Distances ( $\text{\AA}$ )

<u>Uranium neighbors</u>		<u>Corr.<sup>a</sup></u>
U	- O(6)	1.76(1) 1.78
	- O(7)	1.76(1) 1.78
	- O(1)	2.37(1) 2.38
	- O(2)	2.34(1) 2.36
	- O(3)	2.37(1) 2.38
	- O(4)	2.36(1) 2.38
	- O(5)	2.39(1) 2.40
<u>Urea</u>		
C(1)	- O(1)	1.28(1) 1.28
C(2)	- O(2)	1.28(1) 1.29
C(3)	- O(3)	1.25(1) 1.25
C(4)	- O(4)	1.26(1) 1.26
C(5)	- O(5)	1.28(1) 1.28
C(1)	- N(1)	1.32(1) 1.35
	- N(2)	1.34(1) 1.37
C(2)	- N(3)	1.34(1) 1.36
	- N(4)	1.35(1) 1.37
C(3)	- N(5)	1.30(1) 1.39
	- N(6)	1.32(1) 1.39

Table II. Continued

C(4)	- N(7)	1.36(1)	1.36
	- N(8)	1.32(1)	1.41
C(5)	- N(9)	1.32(1)	1.35
	- N(10)	1.34(1)	1.37

Nitrate

N(11)	- O(8)	1.25(1)	1.26
	- O(9)	1.22(1)	1.26
	- O(10)	1.23(1)	1.27
N(12)	- O(11)	1.25(1)	1.30
	- O(12)	1.22(1)	1.25
	- O(13)	1.25(1)	1.28

Possible H bonds (under 3 Å)

N(4)	- O(11)	2.98(1)
N(5)	- O(12)	2.91(1)
N(6)	- O(8)	2.99(1)
N(9)	- O(5)	2.94(1)
N(9)	- O(11)	2.85(1)

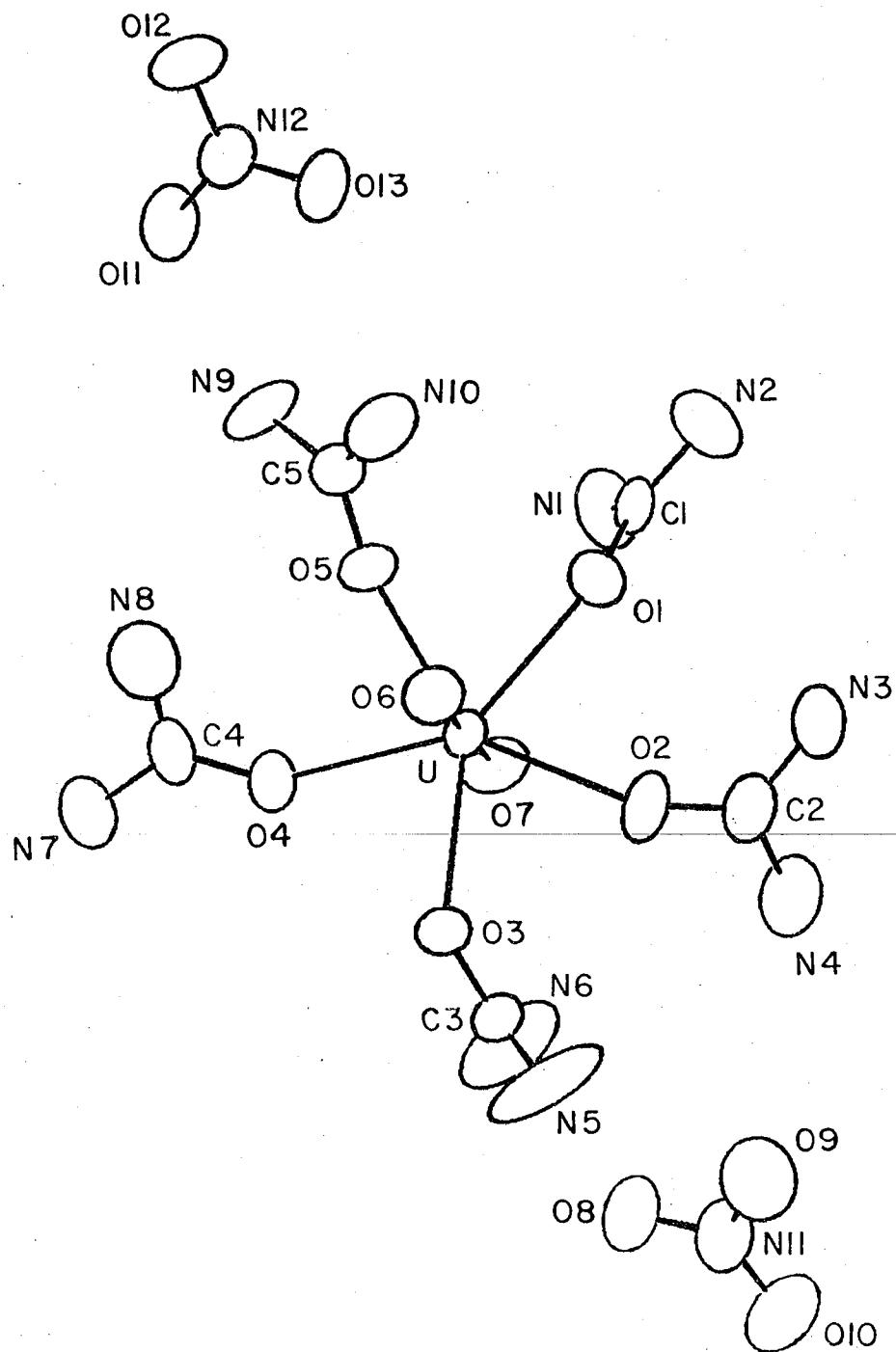
<sup>a</sup>Corrected for thermal motion assuming the "riding" model.

Table III. Selected Angles (deg.)

O(6)	-U	-O(7)	177.3(3)	N(1)	-C(1)	-N(2)	119.0(8)
O(1)	-U	-O(2)	72.8(2)	N(3)	-C(2)	-N(4)	119.6(8)
O(2)	-U	-O(3)	71.9(2)	N(5)	-C(3)	-N(6)	117.9(9)
O(3)	-U	-O(4)	72.8(2)	N(7)	-C(4)	-N(8)	119.0(9)
O(4)	-U	-O(5)	71.3(2)	N(9)	-C(5)	-N(10)	119.9(8)
O(5)	-U	-O(1)	71.4(2)	O(1)	-C(1)	-N(1)	122.4(8)
O(6)	-U	-O(1)	88.1(2)	O(10)	-C(1)	-N(2)	118.6(8)
O(6)	-U	-O(2)	93.7(2)	O(2)	-C(2)	-N(3)	119.0(9)
O(6)	-U	-O(3)	91.3(2)	O(2)	-C(2)	-N(4)	121.4(9)
O(6)	-U	-O(4)	90.5(2)	O(3)	-C(3)	-N(5)	120.6(10)
O(6)	-U	-O(5)	91.1(2)	O(3)	-C(3)	-N(6)	121.6(9)
O(7)	-U	-O(1)	90.4(2)	O(4)	-C(4)	-N(7)	116.0(10)
O(7)	-U	-O(2)	88.0(3)	O(4)	-C(4)	-N(8)	124.7(8)
O(7)	-U	-O(3)	91.3(2)	O(5)	-C(5)	-N(9)	119.4(8)
O(7)	-U	-O(4)	89.4(3)	O(5)	-C(5)	-N(10)	120.7(8)
O(7)	-U	-O(5)	86.3(2)	O(8)	-N(11)-O(9)		120.0(8)
C(1)	-O(1)	-U	138.6(6)	O(8)	-N(11)-O(10)		120.2(9)
C(2)	-O(2)	-U	143.1(6)	O(9)	-N(11)-O(10)		119.8(8)
C(3)	-O(3)	-U	132.3(6)	O(11)	-N(12)-O(12)		118.9(7)
C(4)	-O(4)	-U	143.3(6)	O(11)	-N(12)-O(13)		120.3(7)
C(5)	-O(5)	-U	138.1(6)	O(12)	-N(12)-O(13)		120.8(7)

FIGURE CAPTION

Fig. 1. ORTEP view of  $[\text{UO}_2(\text{OC}(\text{NH}_2)_2)_5][\text{NO}_3]_2$  showing the numbering scheme.



XBL 784-8191

Fig. 1

Supplemental materials for the paper:

STRUCTURE OF PENTAKIS(UREA)DIOXOURANIUM(VI)NITRATE,  
 $[\text{UO}_2(\text{OC}(\text{NH}_2)_2)_5](\text{NO}_3)_2$

by Allan Zalkin, Helena Ruben and David H. Templeton

The Supplementary Tables which follow contain these data:

1. Data Processing Formulas
2. Table of Anisotropic Thermal Parameters
3. Calculated Powder Pattern
4. Observed Structure Factors

DATA PROCESSING FORMULAE

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

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

$$\sigma(I) = [0 + \sigma^2(B)]^{\frac{1}{2}}$$

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

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

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

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

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

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

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

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

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

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

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 dev-  
iation of the total back-  
ground count

p = estimate of non-statistical  
errors

F = structure factor

wtg = weighting factors in least  
squares

D = decay correction; an empir-  
ically applied correction  
obtained from the fluctuations  
of the standard reflections.

A = absorption correction

Lp = Lorentz and polarization  
corrections

Table of Anisotropic Thermal Parameters<sup>a</sup>

ATOM	B11	B22	B33	B12	B13	B23
U	2.11(1)	3.07(1)	2.38(1)	-0.13(1)	.900(7)	-0.33(1)
O(1)	3.0(2)	4.1(3)	3.5(2)	-0.1(2)	.5(2)	-1.1(2)
O(2)	3.1(3)	6.3(4)	5.7(3)	-0.8(2)	2.5(3)	-2.2(3)
O(3)	3.2(2)	5.8(3)	2.4(2)	-0.9(2)	.8(2)	-0.5(2)
O(4)	2.4(2)	7.9(4)	4.1(3)	.6(3)	1.0(2)	-0.8(3)
O(5)	3.9(3)	4.1(3)	2.4(2)	.6(2)	1.1(2)	.1(2)
O(6)	4.0(3)	3.6(3)	3.5(3)	-0.3(2)	1.2(2)	.2(2)
O(7)	5.1(3)	4.3(3)	3.4(3)	-0.4(2)	1.7(2)	.0(2)
O(8)	4.3(3)	5.0(3)	6.5(4)	-0.6(3)	2.7(3)	.1(3)
O(9)	6.3(4)	4.6(4)	8.1(5)	-1.1(3)	1.8(4)	-1.9(3)
O(10)	7.5(5)	7.7(5)	6.9(4)	-1.7(4)	4.2(4)	-1.1(4)
O(11)	3.8(3)	5.5(5)	5.5(3)	2.3(3)	1.8(2)	4.4(3)
O(12)	6.8(4)	6.3(4)	2.8(3)	.3(3)	2.0(3)	1.3(3)
O(13)	3.4(3)	7.4(4)	5.2(3)	1.8(3)	2.1(3)	1.5(3)
N(1)	3.8(4)	3.1(3)	7.2(5)	-0.2(3)	.9(3)	-0.9(3)
N(2)	4.2(4)	5.0(4)	5.1(4)	-1.0(3)	-0.5(3)	-1.0(3)
N(3)	3.0(3)	7.0(5)	5.6(4)	.1(3)	1.5(3)	.4(4)
N(4)	4.6(4)	5.9(5)	6.9(5)	1.2(3)	2.4(3)	2.2(4)
N(5)	16.9(10)	7.4(6)	6.4(5)	2.0(6)	8.4(6)	-0.0(4)
N(6)	13.2(9)	6.3(6)	8.1(6)	.4(5)	7.5(6)	2.0(5)
N(7)	3.1(3)	16.8(9)	5.5(5)	2.0(5)	.5(3)	.1(6)
N(8)	5.2(5)	6.7(5)	6.3(5)	-1.1(4)	1.4(4)	1.5(4)
N(9)	6.8(5)	5.4(4)	3.6(3)	2.7(3)	3.3(3)	.5(3)
N(10)	6.1(5)	4.7(4)	4.6(4)	1.9(3)	2.7(4)	1.1(3)
N(11)	3.9(4)	3.7(4)	5.7(4)	.4(3)	1.7(4)	.7(3)
N(12)	3.6(3)	4.2(3)	3.9(3)	-0.1(3)	1.6(3)	1.1(3)
C(1)	2.0(3)	4.8(5)	3.7(4)	-1.1(3)	1.6(3)	-1.4(3)
C(2)	3.4(4)	4.4(5)	5.3(5)	.0(3)	2.0(4)	-1.7(4)
C(3)	2.8(4)	6.6(5)	2.3(3)	-0.5(3)	1.0(3)	-0.0(3)
C(4)	2.2(3)	7.1(6)	5.2(4)	.4(4)	.7(3)	-2.6(5)
C(5)	3.3(4)	4.0(4)	2.8(4)	-0.7(3)	.9(3)	.1(3)

<sup>a</sup>The anisotropic temperature factor has the form  $\exp(-0.25(B_{11}h^2a^*{}^2 + 2B_{12}hka^*b^* + \dots))$ .

CALCULATED POWDER PATTERN FOR UO<sub>2</sub>(NH<sub>2</sub>CONH<sub>2</sub>)<sub>5</sub>(NO<sub>3</sub>)<sub>2</sub>  
X-RAY WAVE LENGTH = 1.54180 ANGSTROMS.

A = 15.944 B = 8.952 C = 15.394  
ALPHA = 90.00 BETA = 106.31 GAMMA = 90.00

H	K	L	D	I	2 THETA	SINSQ
1		-1	12.532	2.	7.05	.00378
1	0	1	9.392	607.	9.42	.00674
1	1	0	7.727	16.	11.45	.00995
0	1	1	7.656	3.	11.56	.01014
2	0	0	7.651	36.	11.57	.01015
0	1	2	7.387	14.	11.98	.01089
1	1	-1	7.284	1000.	12.15	.01120
1	2	1	6.480	28.	13.66	.01415
2	1	-2	6.266	418.	14.13	.01514
2	2	-1	5.855	21.	15.13	.01734
2	1	0	5.816	731.	15.23	.01757
1	2	-2	5.763	17.	15.37	.01789
0	2	2	5.698	689.	15.55	.01831
3	1	-1	5.303	81.	16.72	.02113
2	1	-2	5.133	1.	17.27	.02255
1	1	-3	5.127	56.	17.30	.02261
2	1	1	5.057	3.	17.54	.02324
1	1	2	4.997	7.	17.75	.02380
2	1	2	4.696	60.	18.90	.02695
3	1	-1	4.562	2.	19.46	.02855
0	2	0	4.476	332.	19.83	.02966
3	1	1	4.451	42.	19.95	.02999
1	1	-3	4.449	1.	19.96	.03003
3	1	0	4.432	2.	20.03	.03026
1	1	3	4.346	66.	20.44	.03147
0	1	3	4.315	0.	20.58	.03192
1	-1	0	4.296	3.	20.68	.03220
3	1	-2	4.290	4.	20.70	.03229
0	2	1	4.284	15.	20.73	.03239
2	1	-3	4.230	0.	21.00	.03321
1	1	-1	4.215	0.	21.08	.03345
3	1	-3	4.177	2.	21.27	.03406
2	1	2	4.159	12.	21.37	.03436
1	1	1	4.041	262.	22.00	.03640
3	1	1	3.986	131.	22.30	.03741
1	1	3	3.909	127.	22.75	.03889
2	1	-1	3.875	0.	22.95	.03958
4	0	-2	3.870	2.	22.98	.03969
2	0	0	3.863	28.	23.02	.03981
1	1	-2	3.848	10.	23.11	.04014
0	1	2	3.828	61.	23.24	.04055
4	0	0	3.826	87.	23.25	.04061
3	1	-3	3.785	108.	23.50	.04147
2	0	-4	3.766	2.	23.62	.04190
0	1	4	3.694	72.	24.09	.04356
2	1	-2	3.642	60.	24.44	.04480
4	1	-1	3.641	9.	24.45	.04484
2	1	1	3.614	0.	24.63	.04549
1	1	2	3.593	59.	24.78	.04604
4	1	-2	3.552	182.	25.07	.04710

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)  
URANYL UREA NITRATE  
 $F(0,0,0) = 3596$

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
H,K= 0, 0	2 648	10	10	15	45 49	-5*		H,K= 0, 0	9 -19	157	16	19			
2 15 3	3 -11	3 141	4 -4	16 129	11 7		1 108	10 4	-18	47	57	46*			
4 79 1	12 21	4 358	6 7	17 106	15 15		2 135	9 -16	-17	107	14	1			
6 49 0	8 -8	5 39 12	9*	H,K= 0,	6 -8		3 200	8 6	-16	41	55	3*			
8 26 5	5 -9	6 351	6 -8	0 227	6 -3		4 62 23	15*-15	290	7	-8				
10 27 4	5 2	7 221	5 -7	1 254	6 -7		5 30 51	12*-14	0 44	-24*					
12 5 1	20 -9*	8 481	8 2	2 190	5 2		6 94 17	-5 -13	55	24	44*				
14 26 2	6 -10	9 34 43	4*	3 173	7 -7		7 169 11	4 -12	19	38	14*				
16 13 4	22 1	10 116	8 -3	4 298	6 5		8 97 19	1*-11	412	8	-7				
18 14 3	11 -11	11 119	7 6	5 243	5 -9		9 24 54	-34*-10	12 42	-4*					
H,K= 0, 1	12 344	7 0		6 220	9 -4		10 39 55	21*-9	240	5 3					
1 3 4	11 -14*	13 146	10 2	7 38	32 36*		11 123 13	2 -8	68	6 9					
21 0 6	1 28	14 106	15 -10	8 110	9 2		12 60 73	-19*	-7 658	10 5					
3 4 2	5 14	15 18 47	-31*	9 188	9 -6		H,K= 0,	10 -6	61	6 5					
4 7 4	7 11	14 196	8 -7	10 275	6 -9		0 116 15	16 -5	780	12 6					
5 2 1	9 4	0 17 82	19 17*	11 88	12 7		1 137 10	2 -4	23	15 14*					
6 2 6	9 5	-9 18 143	14 17	12 51	26 17*		2 0 60	-23*	-3 39	6 -10					
7 9 7	5 -3	H,K= 0,	4	13 146	8 17		3 51 55	-14*	-2 166	3 0					
8 6 2	9 10	0 585	12 -1	14 154	9 4		4 74 19	8*	-1100	3 17 -1					
9 3 1	32 5*	1 208	4 2	15 124	17 23		5 165 9	-6	0 115	3 -4					
10 1 4	6 5	-1 2 144	5 -1	16 81	21 2*		6 70 22	-3*	1 191	3 3					
11 1 0	3 15	-5 3 32	18 14*	H,K= 0,	7 7		7 33 53	21*	2 120	3 1					
12 3 4	9 7	-1 4 396	7 -5	1 193	5 -3		8 53 70	23*	3 699	11 16					
13 4 2	30 0*	5 276	5 -2	2 262	5 3		9 135 12	13 4	287	5 2					
14 9 3	13 -11	6 351	7 -4	3 223	6 -4		H,K= 0,	11 5	533	8 -28					
15 3 3	44 19*	7 101	6 7	4 137	8 -6		1 71 25	-18*	6 75	5 11					
16 2 2	8 8	8 240	5 7	5 18 54	-9*		2 41 55	-24*	7 243	4 4					
17 2 7	5 0	11*	9 169	8 1	6 149	7 -2		3 134 13	1 0	39 -22*					
18 1 4	3 18	19 10 430	7 -15	7 202	6 -7		4 73 34	52*	9 484	8 0					
19 4 9	5 58	40*	11 105	16 4	8 201	6 0		5 29 54	9*	10 64	10 -5				
H,K= 0,	2 2	12 44	48 28*	9 51	22 34*		6 73 23	50*	11 31	36 -1*					
0 1 3 6	5 21	15 13 158	8 4	10 0	52 -26*		H,K= 1,	0 12	0 38	-13*					
1 2 0	9 4	-1 14 229	7 -5	11 148	10 -1		-19 135 12	2 13	307	6 0					
2 5 2	4 10	40 15 128	9 24	12 170	10 -1		-17 203 9	-5 14	60	17 18*					
3 3 4	4 5	19 16 112	13 6	13 78	29 -18*-15		118 11	-7 15	183	8 2					
4 5 5	1 9	4 17 36	60 -8*	14 31	53 -20*-13		400 7	-4 16	58	23 50*					
5 9 7	4 4	18 91	21 -2*	15 85	19 33*-11		65 14	-12*	17 191	9 4					
6 4 9	9 0	3 H,K= 0,	5	H,K= 0,	8 -9		576 9	20 18	0 53	-32*					
7 4 7	15 -4*	1 245	7 -4	0 184	8 11		-7 524 8	-8 H,K= 1,	2						
8 2 5	2 5	-8 2 552	11 4	1 149	10 -10		-5 561 8	13 -19	124	22 2					
9 1 0	5 7	-1 3 345	8 5	2 68	21 19*		-3 479 7	-2 -18	60	29 5*					
10 4 0	5 7	-5 4 186	5 -4	3 112	15 0		-1 0 217	-39*-17	207	7 2					
11 5 1	15 -7*	5 73	8 8	4 114	8 11		1 819 12	-36 -16	0 48	-11*					
12 0	3 0	-5* 6 287	6 5	5 215	8 0		3 628 10	6 -15	85	15 0					
13 1 1	0 8	-4 7 199	16 5	6 167	7 -8		5 607 9	-11 -14	0 48	-60*					
14 3 0	4 6	-3 8 322	6 1	7 0	45 -3*		7 613 9	7 -13	404	7 2					
15 5 6	6 2	-14* 9 36	38 25*	8 91	15 5		9 105 7	3 -12	108	7 0					
16 1 3	4 12	-4 10 72	12 -3	9 182	8 11		11 349 6	-7 -11	172	6 -4					
17 4 0	6 9	29* 11 147	7 -1	10 138	14 -6		13 96 9	-2 -18	0 41	-8*					
18 1 4	1 14	-5 12 252	6 -2	11 84	20 15		227 8	1 -9	647	10 -3					
H,K= 0,	3 13	7 8 18 -20*	12 0	62 -12*	17 114		12 -13	-8 29	37 9*						
1 0	2 25	-33* 14 57	26 -12* 13 87	26 3*	H,K= 1,	1 -7	345 6	4							

STRUCTURE FACTORS CONTINUED FOR  
URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-6	157	4	5	12	107	12	3	-6	198	5	4	15	132	11	10	7	159	10	-6
-5	330	6	8	13	292	6	-5	-5	446	9	6	16	89	20	-14*	8	74	20	16*
-4	170	3	-1	14	52	24	8*	-4	101	6	-7	H,K*	1,	7	9	34	46	24*	
-3	629	10	1	15	115	10	3	-3	52	11	9*-15	93	18	-10*	10	135	13	-11	
-2	191	3	-4	16	5	49	-18*	-2	306	8	9	-14	65	27	-20*	11	109	19	-14
-1	2323	6*	17	126	12	-7	-1	512	10	-1	-13	0	53	-19*	12	117	17	10	
0	98	4	7	18	89	17	19*	0	227	7	-7	-12	118	10	14	13	43	57	0*
1	939	15	-4	H,K*	1,	4	1	161	5	-2	-11	197	7	1	H,K*	1,	9		
2	505	11	0	-16	108	14	42	2	86	7	-21	-10	213	7	15	-12	66	71	-7*
3	285	5	11	-17	158	10	11	3	415	9	-4	-9	67	32	-10*	-11	77	22	-21*
4	202	4	8	-16	35	64	-18*	4	371	9	1	-8	57	21	-7*	-10	165	9	2
5	320	5	-3	-15	58	27	-5*	5	400	9	3	-7	246	6	-5	-9	50	39	13*
6	229	4	3	-14	83	18	0*	6	62	11	10	-6	231	6	1	-8	38	48	35*
7	541	9	0	-13	256	6	0	7	216	6	7	-5	212	6	-8	-7	93	14	-21
8	3436	25*	-12	169	8	-14	8	198	9	-1	-4	81	11	-8	-6	170	8	-9	
9	151	5	4	-11	94	10	10	9	237	5	-8	-3	73	19	29*	-5	81	28	-16*
10	2735	9*	-10	125	11	-8	10	113	8	12	-2	151	6	-1	-4	66	18	8*	
11	358	6	-9	-9	366	6	8	11	47	24	14*	-1	290	9	-1	-3	37	51	25*
12	053	-13*	-8	173	7	4	12	82	13	-7	0	197	7	-4	-2	148	10	-5	
13	8014	10	-7	320	6	-9	13	174	7	-6	1	67	12	19	-1	144	13	2	
14	4926	-3*	-6	49	16	11*	14	69	20	-13*	2	138	6	3	0	130	12	-7	
15	24510	-2	-5	253	5	4	15	59	72	-18*	3	186	6	5	1	34	49	2*	
16	051	-14*	-4	238	5	6	16	34	57	5*	4	255	6	0	2	77	26	-6*	
17	12717	-9	-3	650	12	-4	17	55	65	-17*	5	204	8	-13	3	67	19	-16*	
18	3457	27*	-2	44	15	19*	H,K*	1,	6	6	24	40	14*	4	160	9	-8		
	H,K*	1,	3	-1	26	28	5*-16	82	18	25*	7	65	16	-24*	5	88	28	-5*	
-18	4153	18*	0	211	5	-12	-15	72	22	15*	8	210	8	4	6	61	24	20*	
-17	11512	-4	1	561	11	0	-14	89	17	-7*	9	185	7	-4	7	23	53	-18*	
-16	6122	4*	2	404	8	3	-13	131	9	12	10	93	16	-8	8	166	8	2	
-15	2548	-3	3	432	9	-7	-12	140	9	0	11	36	56	-5*	9	99	18	-9*	
-14	7417	-15*	4	142	5	4	-11	0	45	-40*	12	99	13	-3	10	68	26	-21*	
-13	4723	40*	5	269	6	-4	-10	33	45	-16*	13	124	13	-4	11	36	52	27*	
-12	4821	-3*	6	249	5	-3	-9	241	6	-8	14	105	18	3	H,K*	1,	10		
-11	396	7	-1	7	352	6	-2	-8	262	6	-4	15	54	57	-6*	-10	20	60	-17*
-10	1177	-4	8	116	6	-11	-7	199	7	-12	H,K*	1,	8	-9	66	28	-7*		
-9	2395	-1	9	101	10	9	-6	26	42	9*-14	116	13	22	-8	140	13	4		
-8	034	-2*	10	83	11	22	-5	152	7	6	-13	129	11	21	-7	21	55	-31*	
-7	4147	1	11	285	6	1	-4	212	5	-4	-12	128	12	4	-6	16	63	-15*	
-6	818	-12	12	96	10	12	-3	519	10	0	-11	34	49	27*	-5	37	53	-8*	
-5	64811	0	13	60	19	-2*	-2	146	5	-2	-10	43	47	5*	-4	142	10	-2	
-4	3412	-8*	14	70	24	5*	-1	7	35	-15*	-9	137	17	-4	-3	69	24	-21*	
-3	2630	-7*	15	206	7	-3	0	155	6	-7	-8	218	7	-5	-2	115	16	-3	
-2	4858	9	16	107	11	54	1	423	9	-10	-7	117	13	-7	-1	27	56	26*	
-1	78413	6	17	125	17	-3	2	227	7	5	-6	36	43	7*	0	110	22	2*	
0	3416	3	H,K*	1,	5	3	213	7	-4	-5	60	19	-23*	1	83	16	-8*		
1	744	-6	-17	115	17	19	4	71	10	1	-4	173	9	-4	2	150	10	-5	
2	1784	4	4	-16	91	16	4	5	171	9	1	-3	217	6	-1	3	14	54	-16*
3	5118	-3	-15	147	24	-6*	6	253	8	-1	-2	171	7	7	4	2	50	-26*	
4	3606	7	7	-14	88	13	16	7	288	6	1	-1	15	41	6*	5	48	50	6*
5	4648	0	-13	44	50	16*	8	51	19	-11*	0	147	9	-1	6	159	10	4	
6	2830	-4*	-12	117	9	8	9	37	46	-17*	1	177	6	2	7	97	24	14*	
7	2134	-2	-11	264	6	2	10	120	9	0	2	163	7	-6	8	22	59	-28*	
8	787	9	-10	141	7	-4	11	179	10	5	3	105	9	4	9	40	53	28*	
9	4087	-7	-9	140	6	0	12	129	9	9	4	46	29	2*	H,K*	1,	11		
10	5916	13*	-8	34	46	-6*	13	78	16	22*	5	104	18	0	-6	107	30	-15*	
11	2338	-14*	-7	299	6	5	14	44	58	-10*	6	203	10	2	-5	52	64	17*	

STRUCTURE FACTORS CONTINUED FOR  
URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL					
-4	86	18	36*	5	17	28	-8*-17	33	50	-18*	2	425	8	9	-12	237	6	-1		
-3	52	57	40*	6	627	10	8	-16	95	12	9	3	230	5	-4	-11	149	8	5	
-2	11	6	14	5	7	6	31	-11*-15	84	15	-1	4	238	6	-8	-16	109	11	5	
-1	48	58	-14*	8	126	5	-10	-14	299	7	-3	5	40	15	16*	-9	52	25	4*	
0	13	6	11	19	9	59	11	6*-13	178	11	-2	6	265	5	-1	-8	164	6	-4	
1	0	53	-25*	10	378	6	-3	-12	108	8	1	7	162	6	-2	-7	230	5	0	
2	69	38	10*	11	17	41	-29*-11	52	16	7*	8	338	6	-4	-6	297	7	-4		
3	75	21	30*	12	63	14	2*-10	481	8	-8	9	99	9	-1	-5	123	7	4		
4	13	7	12	6	13	43	31	11*-9	213	5	-1	10	43	24	15*	-4	137	8	-8	
5	49	55	9*	14	210	7	5	-8	365	8	2	11	12	42	-25*	-3	233	5	2	
6	42	55	32*	15	23	49	17*	-7	23	29	3*	12	255	6	-3	-2	404	8	0	
H,K=	2,	8	16	132	10	13	-6	287	5	-4	13	158	9	8	-1	252	7	1		
-18	78	20	-35*	17	71	19	58*	-5	47	8	13	14	120	13	8	0	110	6	11	
-16	22	6	8	18	118	13	18	-4	645	11	-3	15	53	30	41*	1	184	5	-2	
-14	77	11	10	H,K=	2,	2	-3	216	5	19	16	148	13	17	2	326	7	8		
-12	38	5	7	-4	-19	40	53	33*	-2	167	3	6	17	91	17	12*	3	296	8	-4
-10	29	6	6	9	-18	98	15	-8	-1	151	3	-3	H,K=	2,	5	4	247	5	3	
-8	54	0	9	-14	-17	31	49	-22*	0	310	6	-17	-17	66	26	5*	5	20	39	0*
-6	27	2	5	-4	-16	231	7	5	1	143	3	15	-16	62	27	-1*	6	159	6	4
-4	13	4	3	4	-15	32	46	8*	2	289	5	5	-15	103	14	13	7	191	6	1
-21	00	9	16	-61	-14	47	27	-12*	3	224	4	18	-14	197	7	4	8	249	7	-3
0	26	0	4	3	-13	0	41	-10*	4	322	7	-4	-13	159	8	4	9	83	12	-3
2	52	7	8	-19	-12	405	7	-9	5	381	7	7	-12	54	22	-8*	10	24	43	9*
4	82	7	13	24	-11	151	5	10	6	475	8	0	-11	63	28	8*	11	101	11	3
6	33	1	6	0	-10	283	6	9	7	93	6	1	-10	330	7	-4	12	182	7	2
8	55	7	9	-11	-9	39	16	19*	8	220	5	-4	-9	220	5	-3	13	72	21	-24*
10	62	11	-3*	-8	380	6	-10	9	88	8	0	-8	195	5	8	14	88	17	19*	
12	26	7	6	-3	-7	88	5	5	10	396	7	-2	-7	11	35	-25*	15	47	52	29*
14	13	0	8	-3	-6	554	9	-3	11	149	7	-6	-6	159	8	-2	H,K=	2,	7	
16	17	8	0	6	-5	218	4	3	12	98	11	-9	-5	171	5	-1	-15	120	13	30
18	14	8	13	5	-4	133	3	9	13	92	20	14*	-4	599	12	-8	-14	114	13	-15
H,K=	2,	1	-3	6	22	-12*	14	235	6	-2	-3	25	35	-9*	-13	111	21	6*		
-19	69	53	30*	-2	478	7	-27	15	29	48	-19*	-2	76	7	9	-12	83	14	36	
-18	15	7	12	-6	-1	28	10	-7*	16	126	11	-1	-1	185	6	2	-11	87	13	26
-17	51	33	40*	0	314	5	-9	17	41	51	32*	0	422	10	-12	-18	161	12	-21	
-16	93	12	1	1	10	25	-33*	H,K=	2,	4	1	290	7	-2	-9	189	8	12		
-15	0	47	-35*	2	372	6	2	-18	115	17	20	2	187	4	10	-8	113	9	-6	
-14	35	7	7	0	3	32	12	-2*-17	92	15	18	3	26	36	13*	-7	42	36	-26*	
-13	9	3	9	-7	4	583	9	3	-16	176	8	-4	4	244	6	-4	-6	132	7	-10
-12	11	0	7	-5	5	85	6	-4	-15	55	25	1*	5	276	7	3	-5	186	6	-10
-11	16	39	5*	6	305	5	-10	-14	42	43	38*	6	270	5	0	-4	272	6	-3	
-10	40	1	7	-7	7	194	5	-1	-13	38	47	19*	7	132	6	-1	-3	210	5	-3
-9	12	5	5	8	486	8	-14	-12	359	7	-6	8	141	7	-5	-2	55	15	43*	
-8	47	2	8	0	9	28	34	9*-11	149	6	5	9	178	6	-2	-1	180	6	1	
-7	11	3	5	13	10	30	36	17*-10	250	6	-11	10	291	6	5	0	233	7	7	
-6	32	3	5	8	11	28	38	-15*	-9	0	36	-28*	11	104	10	-3	1	243	5	-3
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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6	202	7	-11	-5	88	10	2	-5	54	55	27*	-6	53	7	-12	-14	360	7	
7	280	6	-1	-4	165	6	0	-4	174	7	8	-41	296	20	-9	-13	129	7	
8	138	8	-2	-3	328	6	-4	-3	134	9	-5	-2	125	3	18	-12	170	6	
9	5429	9*	-2	212	5	0	-2	155	8	11	0	860	13	44	-11	62	16		
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13	048	-20*	-1	136	6	-6	-6	82	27	11*	2	66	23	-3*	-3	77	4	-3	
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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3	608	10	15	-17	47	37	40*	3	606	13	2	-11	197	6	9	13	78	22	1*
4	250	5	-6	-16	95	20	-1*	4	136	5	-11	-10	0	42	-32*	H, K=	5,	8	
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6	71	19	2*	-14	111	12	4	6	97	7	-7	-8	171	7	1	-13	130	11	10
7	97	6	19	-13	190	6	-11	7	377	7	-5	-7	280	9	-8	-12	175	14	3
8	36	41	-13*	-12	59	14	22*	8	98	16	-3	-6	153	6	-5	-11	104	13	3
9	428	8	4	-11	302	8	-2	9	83	11	-16	-5	26	42	-18*	-10	46	47	-12*
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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-1	38	50	-22*	-3	206	5	11	16	7	61	-53*	-1	258	6	-5	-13	13	52	1*
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
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8	81	20	2*	-9	49	59	-3*	-6	26	31	-14*	13	93	24	-12*
9	70	20	-3*	-8	10	54	-6*	-5	24	28	3*	14	81	19	31*
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3	55	28	5*-14	0	41	-2*	5	420	7	2	-10	231	5	0	12
4	22	60	-12*-13	252	5	3	6	53	15	-11*	-9	361	7	8	13
5	127	11	4	-12	81	9	11	7	110	7	-16	-8	100	7	10
6	78	27	-11*-11	304	6	4	8	96	9	-11	-7	57	12	0*	H,K#
7	101	21	-8*-10	63	10	1	9	339	7	0	-6	141	8	18	-17

## STRUCTURE FACTORS CONTINUED FOR URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-16	27	53	-13*	10	22	66	-14*	-5	18	57	-51*	7	58	15	-8*	-9	104	8	-4
-15	15	9	-2	11	71	28	-3*	-4	148	15	19	8	357	7	1	-8	39	22	-14*
-14	16	5	10	14	12	112	15	9	-3	23	73	-30*	9	8	51	-19*	-7	152	5
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-12	4	2	44	28*	-14	143	12	11	-1	66	28	7*	11	40	45	31*	-5	164	4
-11	11	5	10	-5	-13	60	46	2*	0	138	14	-6	12	164	8	2	-4	339	8
-10	16	8	7	-1	-12	0	69	-23*	1	47	55	-29*	13	39	52	17*	-3	130	6
-9	21	6	8	-11	81	18	-1*	2	43	54	-1*	14	178	12	5	-2	371	7	4
-8	14	7	7	-1	-10	124	11	-14	3	25	62	6*	15	0	55	-3*	-1	277	7
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11	9	9	14	0	9	74	23	-11*	12	200	8	-2	-2	357	7	7	-16	57	59
12	5	9	30	47*	10	116	19	2	14	67	39	14*	-1	101	5	4	-15	0	47
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8	13	7	10	0	-7	82	21	73*	5	30	37	-10*	-11	145	7	0	11	88	15
9	5	3	38	-16*	-6	124	12	29	6	111	7	-4	-10	447	8	-10	12	169	8

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	
13	0	65	-25*	5	158	7	1	5	136	18	1	13	161	10	-1	
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	H, Ks	8,	5	7	150	8	-1	7	105	16	-12	-19	170	10	-28	
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-16	16	211	-2	9	57	59	27*	9	0	55	-25*-17	116	10	17	4 124 6 -5	
-15	14	411	19	10	79	19	-17*	H, Ks	8,	9	-16	66	19	25*	5 73 11 -6	
-14	88	13	21	11	98	16	-10	-11	139	12	-7	-15	209	6	-5	
-13	60	20	19*	12	109	17	3	-10	107	15	18	-14	0	48	-46*	
-12	10	911	-1	H, Ks	8,	7	-9	84	22	7*-13	300	6	5	8 57 20 13*		
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-10	27	49	-7	-14	38	68	-35*	-7	110	12	0	-11	197	6	4	
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	
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-8	140	8	9	-14	37	48	15*	-11	130	15	3	-8	104	6	3	-11	33	45	-25*	
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1	297	6	-3	-1	119	12	1	-6	131	14	5	9	42	45	15*	-3	179	5	1	
2	122	8	2	0	197	7	-12	-5	24	56	-11*	10	100	26	-11*	-2	417	8	4	
3	61	43	27*	1	182	9	8	-4	62	51	22*	11	44	48	29*	-1	82	14	-10	
4	115	9	-12	2	98	14	-14	-3	52	54	-8*	12	209	9	1	0	130	7	-1	
5	307	6	0	3	0	54	-9*	-2	157	11	21	13	0	55	-7*	1	135	9	-1	
6	88	13	-5	4	133	10	0	-1	71	25	5*	14	54	54	42*	2	334	6	4	
7	127	9	-2	5	182	14	0	0	56	61	14*	H,K8	10,	2	3	177	5	-2		
8	29	47	-21*	6	72	23	-30*	1	27	55	0*	-19	0	58	-61*	4	111	9	2	
9	143	10	-4	7	107	11	21	2	81	25	-37*-18	75	21	-9*	5	47	50	-4*		
10	118	15	5	8	45	52	3*	H,K8	10,	0	-17	0	49	-19*	6	290	6	2		

## STRUCTURE FACTORS CONTINUED FOR URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
7	53	25	-15*	-1	101	8	-5	0	79	15	-13*	0	65	65	-2*	-16	23	53	20*
8	158	10	1	0	110	8	4	1	135	8	4	H,K=	11,	0	-19	125	9	-1	
9	0	47	-2*	1	229	6	0	2	162	8	5	-19	196	9	0	-14	72	16	-18*
10	134	11	10	2	293	6	0	3	142	11	-4	-17	180	8	-1	-13	365	7	-6
11	51	56	4*	3	164	7	0	4	43	50	-3*	-15	136	9	-12	-12	51	21	-2*
12	179	10	-3	4	20	50	-42*	5	116	10	22	-13	329	9	2	-11	30	40	2*
13	55	61	20*	5	61	37	6*	6	117	21	-8	-11	80	12	-2	-10	38	38	18*
	H,K=	10,	4	6	239	11	-5	7	130	12	15	-9	292	5	-1	-9	393	6	-6
-18	36	57	-22*	7	139	15	0	8	103	24	4*	-7	206	5	2	-8	124	9	-3
-17	22	51	9*	8	128	13	7	9	34	60	24*	-5	383	7	-13	-7	185	5	-6
-16	149	14	-5	9	0	54	-9*	H,K=	10,	8	-3	375	6	4	-6	4	35	-22*	
-15	105	12	-2	10	83	20	-17*	-13	55	40	4*	-1	67	10	-24	-5	311	6	-6
-14	199	7	3	11	75	29	-1*	-12	0	59	-42*	1	528	9	9	-4	35	33	-13*
-13	64	17	10*	H,K=	18,	6	-11	123	15	-5	3	143	6	-8	-3	384	6	-6	
-12	71	15	8*-16	90	19	-35*	-10	149	10	-1	5	354	7	-3	-2	34	38	-3*	
-11	102	14	3	-15	135	19	10	-9	108	13	-7	7	209	7	-1	-1	171	5	-7
-10	357	9	-1	-14	124	11	4	-8	48	55	40*	9	160	8	11	0	87	9	-4
-9	33	11	-29	-13	64	21	-1*	-7	98	12	26	11	218	12	3	1	428	8	-8
-8	72	11	8	-12	48	61	-15*	-6	117	14	7	13	42	55	22*	2	64	27	8*
-7	117	8	-5	-11	125	9	10	-5	197	7	0	H,K=	11,	1	3	95	9	-3	
-6	326	6	-8	-10	198	7	0	-4	119	12	0	-19	92	17	15*	4	50	22	15*
-5	146	7	0	-9	132	9	-6	-3	42	59	34*	-18	0	54	-12*	5	303	6	-10
-4	353	8	-4	-8	45	31	12*	-2	96	13	-7	-17	189	8	-3	6	67	16	-5*
-3	57	14	28*	-7	68	17	-11*	-1	145	9	4	-16	62	23	3*	7	178	10	2
-2	276	6	-7	-6	248	6	9	0	132	10	6	-15	240	6	5	8	3	46	-13*
-1	229	5	-2	-5	210	7	-4	1	95	25	-5*	-14	18	51	12*	9	112	13	1
0	410	7	4	-4	154	10	-1	2	46	57	45*	-13	49	25	-16*	10	52	34	5*
1	52	19	28*	-3	45	23	28*	3	99	14	-12	-12	72	17	0*	11	194	9	-5
2	45	21	14*	-2	164	6	6	4	127	11	10	-11	389	7	-2	12	48	54	41*
3	77	11	-4	-1	204	7	2	5	81	20	-20*	-10	47	21	-23*	H,K=	11,	3	
4	267	8	0	0	284	7	-7	6	67	31	6*	-9	108	7	-2	-10	43	59	42*
5	140	8	-7	1	130	8	13	7	55	46	34*	-8	65	11	4	-17	171	12	0
6	87	15	-14	2	50	50	31*	H,K=	10,	9	-7	392	7	6	-16	83	16	-8*	
7	42	51	31*	3	125	13	-21	-10	44	67	23*	-6	6	35	-27*	-15	223	7	2
8	197	7	9	4	225	8	9	-9	89	31	-1*	-5	434	8	-11	-14	54	26	-18*
9	74	20	-25*	5	131	9	1	-8	78	23	-14*	-4	34	47	21*	-13	64	22	-12*
10	139	11	-14	6	80	30	-10*	-7	151	11	-5	-3	316	6	3	-12	134	8	14
11	38	60	23*	7	0	50	-16*	-6	71	22	15*	-2	0	35	-13*	-11	375	7	-5
12	26	54	-21*	8	85	25	-29*	-5	67	22	22*	-1	373	6	-2	-10	233	7	-17
	H,K=	10,	5	9	98	16	-6	-4	31	52	-52*	0	22	35	16*	-9	102	10	7
-17	112	14	7	10	116	14	4	-3	167	10	3	1	52	17	-3*	-8	71	14	2*
-16	98	14	19	H,K=	10,	7	-2	80	18	-5*	2	39	26	14*	-7	398	8	-8	
-15	44	47	22*-14	60	66	-25*	-1	63	24	22*	3	491	9	-7	-6	112	8	12	
-14	112	19	-5	-13	119	12	-8	0	0	56	-31*	4	83	12	-10	-9	299	6	1
-13	109	10	0	-12	165	8	16	1	136	12	21	5	192	6	5	-4	16	36	-10*
-12	221	8	-7	-11	116	11	10	2	99	16	17	6	31	56	8*	-3	216	5	-11
-11	100	15	0	-10	22	57	0*	3	101	16	25	7	277	6	-1	-2	110	6	6
-10	56	19	30*	-9	103	12	-10	4	51	66	22*	8	38	47	-10*	-1	321	7	1
-9	85	11	0	-8	195	7	0	5	44	60	-6*	9	223	7	13	0	26	37	12*
-8	338	6	8	-7	169	8	-3	H,K=	10,	10	10	10	53	46	49*	1	48	45	-9*
-7	108	8	4	-6	97	11	2	-6	71	36	8*	11	78	18	17*	2	130	7	2
-6	154	6	-3	-5	46	31	7*	-5	134	13	0	12	53	60	41*	3	350	6	-6
-5	53	26	-3*	-4	179	7	-3	-4	42	55	-6*	13	166	10	7	4	113	10	-1
-4	224	5	4	-3	166	11	-13	-3	47	53	33*	H,K=	11,	2	5	5	145	9	4
-3	188	5	-1	-2	163	8	-2	-2	60	61	38*-18	69	27	23*	6	26	44	19*	
-2	342	8	-1	-1	63	19	-12*	-1	131	12	5	-17	163	9	14	7	193	8	6

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
8	110	14	-21	3	241	6	4	6	51	51	20 <sup>a</sup> -17	40	50	21 <sup>a</sup>	7	30	37	-22 <sup>a</sup>	
9	173	8	-2	4	141	8	-10	7	86	23	2 <sup>a</sup> -16	169	9	7	8	215	7	2	
10	0	55	-6 <sup>a</sup>	5	111	11	-2	8	110	17	7	-15	0	47	-35 <sup>a</sup>	9	0	60	-5 <sup>a</sup>
11	62	29	10 <sup>a</sup>	6	25	51	-14 <sup>a</sup>	H, K <sub>8</sub>	11,	8	-14	292	7	-2	10	0	53	-45 <sup>a</sup>	
12	30	65	-3 <sup>a</sup>	7	158	9	10	-12	63	32	-17 <sup>a</sup> -13	34	43	5 <sup>a</sup>	11	0	71	-41 <sup>a</sup>	
	H, K <sub>8</sub>	11,	4	8	116	13	-7	-11	13	52	3 <sup>a</sup> -12	20	43	-32 <sup>a</sup>	12	170	11	-4	
-17	113	19	5	9	132	16	5	-10	107	19	3	-11	47	23	15 <sup>a</sup>	H, K <sub>8</sub>	12,	3	
-16	0	52	-28 <sup>a</sup>	10	26	64	6 <sup>a</sup>	-9	137	11	1	-10	382	7	2	-18	119	13	6
-15	139	10	-3	11	0	56	-37 <sup>a</sup>	-8	143	9	3	-9	60	16	-9 <sup>a</sup> -17	68	30	62 <sup>a</sup>	
-14	106	13	19	H, K <sub>8</sub>	11,	6	-7	40	58	-23 <sup>a</sup>	-8	209	8	-4	-16	127	11	12	
-13	254	6	0	-15	99	15	16	-6	44	48	13 <sup>a</sup>	-7	48	17	3 <sup>a</sup> -15	86	27	-4 <sup>a</sup>	
-12	92	12	-6	-14	104	20	8 <sup>a</sup>	-5	106	13	-10	-6	320	6	2	-14	258	7	-2
-11	57	19	43 <sup>a</sup> -13	168	9	0	-4	187	7	15	-5	0	38	-29 <sup>a</sup> -13	0	45	-26 <sup>a</sup>		
-10	82	13	14	-12	83	24	10 <sup>a</sup>	-3	126	12	18	-4	389	7	0	-12	58	22	23 <sup>a</sup>
-9	327	7	-7	-11	27	48	21 <sup>a</sup>	-2	30	49	-18 <sup>a</sup>	-3	124	7	-4	-11	56	20	3 <sup>a</sup>
-8	160	7	-8	-10	78	15	-8 <sup>a</sup>	-1	58	29	36 <sup>a</sup>	-2	199	5	-10	-10	320	6	-8
-7	167	9	-2	-9	234	10	-1	0	137	19	0	-1	72	10	-11	-9	140	7	6
-6	51	17	25 <sup>a</sup>	-8	147	9	3	1	134	9	16	0	350	6	2	-8	156	6	1
-5	218	5	1	-7	99	13	-1	2	122	11	15	1	31	39	8 <sup>a</sup>	-7	44	26	10 <sup>a</sup>
-4	132	6	-10	-6	10	43	-3 <sup>a</sup>	3	0	62	-24 <sup>a</sup>	2	11	44	-3 <sup>a</sup>	-6	314	6	-2
-3	294	6	-2	-5	165	8	-1	4	31	53	-34 <sup>a</sup>	3	40	38	22 <sup>a</sup>	-5	183	7	1
-2	52	18	-15 <sup>a</sup>	-4	205	6	4	5	75	25	-12 <sup>a</sup>	4	397	7	-2	-4	345	7	1
-1	174	5	12	-3	220	7	-3	6	99	18	-14	5	50	27	39 <sup>a</sup>	-3	0	44	-24 <sup>a</sup>
0	172	6	-9	-2	62	18	-13 <sup>a</sup>	H, K <sub>8</sub>	11,	9	6	178	8	11	-2	162	6	-9	
1	302	6	-4	-1	134	9	3	-9	0	54	-2 <sup>a</sup>	7	56	23	33 <sup>a</sup>	-1	107	9	-9
2	107	11	5	0	158	9	-5	-8	77	24	24 <sup>a</sup>	8	148	9	-3	0	302	6	4
3	73	13	2	1	175	7	-1	-7	75	42	3 <sup>a</sup>	9	46	56	8 <sup>a</sup>	1	73	24	-15 <sup>a</sup>
4	86	12	-9	2	133	19	4	-6	128	13	-19	10	224	9	4	2	39	42	-24 <sup>a</sup>
5	269	6	5	3	61	27	19 <sup>a</sup>	-5	78	21	2 <sup>a</sup>	11	45	70	37 <sup>a</sup>	3	45	28	-4 <sup>a</sup>
6	80	26	-27 <sup>a</sup>	4	118	9	29	-4	31	51	23 <sup>a</sup>	12	0	55	-6 <sup>a</sup>	4	281	6	0
7	161	13	8	5	191	13	14	-3	82	30	40 <sup>a</sup>	H, K <sub>8</sub>	12,	2	5	58	24	-1 <sup>a</sup>	
8	0	50	-26 <sup>a</sup>	6	128	10	-2	-2	147	13	-10	-18	142	13	-9	6	178	7	12
9	120	11	26	7	108	22	-2 <sup>a</sup>	-1	62	32	-22 <sup>a</sup> -17	50	51	6 <sup>a</sup>	7	0	49	-11 <sup>a</sup>	
10	87	10	16 <sup>a</sup>	8	21	53	19 <sup>a</sup>	0	71	23	-8 <sup>a</sup> -16	198	7	5	8	114	12	-13	
11	146	14	4	9	83	28	12 <sup>a</sup>	1	64	26	61 <sup>a</sup> -15	49	31	26 <sup>a</sup>	9	63	26	-11 <sup>a</sup>	
	H, K <sub>8</sub>	11,	5	H, K <sub>8</sub>	11,	7	2	75	29	-12 <sup>a</sup> -14	79	15	-23 <sup>a</sup>	10	178	16	3		
-17	146	14	15	-14	70	25	32 <sup>a</sup>	3	63	78	-8 <sup>a</sup> -13	73	15	12 <sup>a</sup>	11	48	54	36 <sup>a</sup>	
-16	117	13	6	-13	43	65	0 <sup>a</sup>	H, K <sub>8</sub>	12,	0	-12	369	7	1	H, K <sub>8</sub>	12,	4		
-15	160	12	-8	-12	112	14	1	-18	169	15	12	-11	104	9	-4	-17	81	29	-3 <sup>a</sup>
-14	62	23	8 <sup>a</sup> -11	156	10	-2	-16	211	7	5	-10	114	9	-1	-16	149	10	-2	
-13	86	18	-15 <sup>a</sup> -10	116	19	9	-14	64	20	18 <sup>a</sup>	-9	96	9	4	-15	49	55	19 <sup>a</sup>	
-12	119	10	4	-9	75	15	69 <sup>a</sup> -12	509	9	-6	-8	331	6	4	-14	92	14	2	
-11	220	6	5	-8	75	24	8 <sup>a</sup> -10	128	7	8	-7	97	9	2	-13	93	12	4	
-10	150	7	-2	-7	157	8	-5	-8	331	6	3	-6	297	6	4	-12	237	6	1
-9	26	59	10 <sup>a</sup>	-6	174	11	-3	-6	284	6	11	-5	52	14	21 <sup>a</sup>	-11	121	11	10
-8	55	20	-16 <sup>a</sup>	-5	125	10	-7	-4	312	7	-4	-4	296	5	3	-18	26	60	-3 <sup>a</sup>
-7	241	6	-3	-4	0	46	-5 <sup>a</sup>	-2	333	6	1	-3	95	8	0	-9	50	24	-17 <sup>a</sup>
-6	190	6	0	-3	74	20	-15 <sup>a</sup>	0	147	6	-6	-2	339	6	-4	-8	276	6	7
-5	205	6	-1	-2	187	7	-5	2	463	9	-1	-1	68	15	-2 <sup>a</sup>	-7	158	8	2
-4	70	12	7	-1	169	7	-2	4	149	7	9	0	82	20	3 <sup>a</sup>	-6	203	6	-3
-3	141	8	2	0	117	13	-1	6	299	8	-4	1	80	10	7	-5	44	23	37 <sup>a</sup>
-2	136	9	-3	1	61	22	43 <sup>a</sup>	8	250	7	-1	2	354	6	0	-4	209	7	-6
-1	266	7	2	2	82	19	-15 <sup>a</sup>	10	55	63	14 <sup>a</sup>	3	88	11	-3	-3	166	7	-1
0	98	10	-5	3	145	11	11	12	193	9	6	4	139	8	-6	-2	349	7	-9
1	853	-17 <sup>a</sup>	4	120	11	3	H, K <sub>8</sub>	12,	1	5	30	43	11 <sup>a</sup>	-1	59	31	8 <sup>a</sup>		
2	114	16	15	5	0	51	-59 <sup>a</sup> -18	128	12	-8	6	259	8	-7	0	27	40	22 <sup>a</sup>	

STRUCTURE FACTORS CONTINUED FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	133	7	-1	2	214	9	-5	0	64	32	-19*	-12	71	18	-4*-14
2	305	6	-3	3	145	8	13	1	62	35	-19*	-11	377	7	-2*-13
3	152	8	15	4	87	15	2	H, K#	13,	0	-10	129	8	0*-12	
4	93	11	4	5	63	23	14*	-17	121	12	0	-9	143	9	-4*-11
5	2645	10*	6	115	12	7	-15	197	7	-2	-8	0	43	-11*-10	
6	176	9	5	7	113	22	1*-13	100	11	0	-7	345	6	2*-9	
7	118	19	-2	8	100	32	-4*-11	329	9	3	-6	102	9	-13*-8	
8	154	10	-6	H, K#	12,	7	-9	168	6	-2	-5	321	6	-2*-7	
9	4454	29*-13	67	27	-12*	-7	364	8	5	-4	44	24	-15*	-6	
10	7821	23*-12	20	52	1*	-5	394	7	-2	-3	182	6	-3*-5		
	H, K#	12,	5	-11	116	18	7	-3	188	5	-6	-2	42	14*	
-16	8220	-7*-10	117	12	-12	-1	406	7	-10	-1	397	7	-1*-3		
-15	13012	26	-9	130	11	-3	1	71	12	11	0	35	39	16*	
-14	1738	-1	-8	66	19	12*	3	380	7	-1	1	49	34	16*	
-13	7040	-7*	-7	11	48	4*	5	191	6	9	2	73	14	-12*	
-12	5733	39*	-6	147	9	9	7	162	8	6	3	339	6	4	
-11	10311	-1	-5	165	10	-7	9	185	16	-4	4	36	46	18*	
-10	2096	1	-4	141	11	10	11	0	78	-4*	5	147	8	-12	
-9	1649	1	-3	50	38	18*	H, K#	13,	1	6	48	50	23*	4	
-8	7014	7*	-2	88	13	28	-18	34	55	18*	7	119	10	15	
-7	043	-46*	-1	140	10	8	-17	165	14	-15	8	54	35	-15*	
-6	2006	-5	0	183	11	2	-16	48	58	41*	9	179	16	-4	
-5	1736	5	1	136	9	11	-15	88	14	5	10	77	32	70*	
-4	2247	2	2	74	17	26*-14	43	65	-7*	11	0	67	-9*	9	
-3	5817	38*	3	61	26	-15*-13	296	9	3	H, K#	13,	3	H, K#	13,	
-2	10110	11	4	122	12	0	-12	0	44	-6*-17	155	12	-7*-16		
-1	2036	-7	5	121	13	2	-11	53	21	-11*-16	26	54	-2*-15		
0	3126	1	6	65	31	-30*-10	47	26	11*-15	87	14	12	-14		
1	7814	2	7	62	33	54*	-9	318	6	3	-14	82	15	6*-13	
2	8312	9	H, K#	12,	8	-8	82	11	16	-13	278	7	-4	-12	
3	7117	13*-11	122	12	19	-7	259	6	0	-12	84	17	-14*-11		
4	2179	1	-10	7	53	2*	-6	44	31	-2*-11	0	47	-30*-10		
5	11711	-5	-9	56	56	-18*	-5	275	5	7	-10	47	27	1*	
6	14615	0	-8	115	12	19	-4	40	25	13*	-9	345	7	-4	
7	4950	47*	-7	171	9	0	-3	394	7	2	-8	139	8	-7	
8	8439	-9*	-6	101	16	14	-2	39	30	24*	-7	241	6	1	
9	7524	-7*	-5	32	50	23*	-1	65	12	23	-6	25	47	-9*	
10	12614	1	-4	104	13	2	0	29	41	20*	-5	233	6	2	
	H, K#	12,	6	-3	141	10	2	1	397	7	0	-4	107	8	
-15	4061	3*	-2	103	14	-7	2	55	18	10*	-3	338	7	6	
-14	8517	23*	-1	73	20	-8*	3	201	6	-7	-2	47	23	-12*	
-13	10630	0*	0	0	50	-1*	4	45	30	32*	-1	69	13	9*	
-12	13812	-1	1	97	15	7	5	236	10	-7	0	117	12	3	
-11	11611	-1	2	99	16	-7	6	0	47	-38*	1	345	7	-9	
-10	4753	26*	3	92	29	-4*	7	218	8	-3	2	41	47	20*	
-9	8322	4*	4	53	57	-2*	8	0	50	-3*	3	111	10	-3	
-8	1727	-10	5	17	55	-18*	9	51	45	-6*	4	32	44	13*	
-7	1799	-5	H, K#	12,	9	10	45	54	20*	5	186	7	7		
-6	10510	3	-8	28	54	-8*	11	187	11	5	6	108	11	-2	
-5	2446	2*	-7	27	56	7*	H, K#	13,	2	7	188	8	-4		
-4	1507	0	-6	65	29	-16*-18	0	53	-14*	8	23	59	8*	9	
-3	14710	1	-5	144	11	12	-17	117	15	3	9	67	25	21*	
-2	2436	7	-4	103	17	22	-16	53	39	-24*	10	26	56	-29*-14	
-1	12610	14	-3	58	62	12*-15	208	8	-7	H, K#	13,	4	-13		
0	048	-6*	-2	52	76	28*-14	37	51	28*-16	95	15	9	-12		
1	1538	9	-1	120	21	-3	-13	32	46	-25*-15	207	12	15	-11	

STRUCTURE FACTORS CONTINUED FOR  
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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL				
-10	90	16	-12	-4	123	14	-3	-9	39	59	-16*	-9	102	22	-20*	0	214	7	1
-9	69	20	0*	-3	112	14	26	-8	243	6	2	-8	167	9	2	1	93	16	-9
-8	59	22	28*	-2	71	27	5*	-7	24	41	13*	-7	0	44	-8*	2	71	41	5*
-7	142	12	-6	H, K=	14,	0	-6	265	6	-5	-6	202	8	-13	3	0	61	-33*	
-6	180	7	8	-16	50	55	-22*	-5	123	7	7	-5	170	6	10	4	109	32	-11*
-5	145	9	-10	-14	256	7	-12	-4	392	9	-7	-4	278	6	3	5	123	12	2
-4	70	16	3*	-12	31	45	4*	-3	82	15	-11	-3	30	45	-24*	6	85	38	-39*
-3	117	11	16	-10	299	7	3	-2	31	41	18*	-2	37	43	6*	H, K=	14,	7	
-2	108	11	-10	-8	188	7	-10	-1	52	19	29*	-1	46	30	-3*	-12	111	15	-10
-1	203	7	-4	-6	237	6	-7	0	293	6	4	0	290	7	-3	-11	115	14	-6
0	119	11	8	-4	419	8	9	1	92	10	10	1	82	23	-17*	-10	78	19	22*
1	1360	-40*	-2	36	39	26*	2	188	9	-1	2	65	21	-31*	-9	36	51	11*	
2	90	16	25	0	357	6	-3	3	45	50	34*	3	25	50	17*	-8	118	13	-8
3	187	8	8	2	181	6	-7	4	217	7	0	4	149	9	1	-7	146	10	-2
4	110	16	-22	4	232	7	0	5	59	22	28*	5	99	14	0	-6	132	12	15
5	118	13	-12	6	206	9	3	6	177	8	-7	6	176	9	-6	-5	46	49	-2*
6	0	54	-28*	8	0	58	-54*	7	0	51	-2*	7	17	59	2*	-4	64	24	-12*
7	36	60	-28*	10	195	11	18	8	46	53	-6*	8	94	32	46*	-3	139	9	20
	H, K=	13,	7	H, K=	14,	1	9	63	31	16*	H, K=	14,	5	-2	151	16	6		
-13	103	23	-16*-17	33	52	4*	10	166	11	6	-15	14	68	-52*	-1	85	17	-17*	
-12	110	14	10	-16	221	7	-4	H, K=	14,	3	-14	58	30	28*	0	66	23	25*	
-11	57	24	44*-15	0	52	-6*-17	32	55	-25*-13	70	43	-3*	1	75	24	8*			
-10	88	16	5*-14	35	46	28*-16	188	9	-5	-12	165	9	-15	2	105	15	-15		
-9	165	8	19	-13	17	59	-32*-15	13	50	-17*-11	126	10	4	3	113	16	-3		
-8	146	9	0	-12	326	7	-1	-14	59	23	40*-10	54	27	-1*	4	117	18	21	
-7	94	14	-8	-11	0	49	-38*-13	80	29	13*	-9	28	51	-7*	H, K=	14,	8		
-6	0	49	-27*-10	131	8	12	-12	239	8	0	-8	211	7	2	-9	140	12	8	
-5	132	10	9	-9	77	13	-3	-11	76	15	2*	-7	131	8	-3	-8	93	17	4*
-4	150	9	-1	-8	310	7	-9	-10	125	9	15	-6	185	7	1	-7	0	64	-21*
-3	150	9	-2	-7	43	29	31*	-9	30	43	5*	-5	81	20	4*	-6	65	66	-23*
-2	101	12	8	-6	340	7	-11	-8	288	6	-9	-4	115	9	2	-5	135	15	0
-1	1648	3*	-5	70	17	-3*	-7	140	8	-12	-3	130	12	-4	-4	126	12	15	
0	113	11	14	-4	129	9	7	-6	315	6	-20	-2	263	9	-3	-3	42	57	-34*
1	161	9	0	-3	34	39	25*	-5	42	47	-27*	-1	89	13	-14	-2	0	59	-10*
2	118	16	12	-2	418	8	-6	-4	156	7	-1	0	92	14	5	-1	97	16	-3
3	4764	-10*	-1	66	20	-7*	-3	54	19	-8*	1	76	28	-8*	0	112	22	0*	
4	5923	38*	0	102	9	8	-2	361	8	-2	2	189	8	-10	1	90	22	5*	
5	9517	7	1	29	42	14*	-1	129	9	0	3	115	13	-2	H, K=	15,	0		
6	8025	-35*	2	303	6	-9	0	112	9	-2	4	125	12	-2	-17	209	11	7	
	H, K=	13,	8	3	32	44	23*	1	25	45	-41*	5	37	51	11*	-15	60	26	28*
-10	115	14	-5	4	140	14	-15	2	249	6	6	6	63	42	-12*-13	247	7	-1	
-9	72	22	29*	5	9	46	4*	3	49	32	-15*	7	66	29	-22*-11	120	9	-5	
-8	67	28	30*	6	146	21	6	4	119	11	-18	H, K=	14,	6	-9	280	7	8	
-7	112	13	12	7	43	59	9*	5	0	68	-17*-13	115	12	21	-7	326	6	-3	
-6	126	13	-29	8	203	10	-5	6	123	12	11	-12	51	47	32*	-5	100	10	-17
-5	8730	-7*	9	53	53	46*	7	84	17	8*	-11	70	41	10*	-3	415	8	-11	
-4	5141	16*	10	9	64	5*	8	176	10	10	-10	166	9	8	-1	123	9	-1	
-3	5861	13*	H, K=	14,	2	9	27	63	1*	-9	129	12	-12	1	262	7	-8		
-2	147	9	15	-17	43	51	22*	H, K=	14,	4	-8	127	10	-7	3	231	6	1	
-1	112	23	-2*-16	80	19	6*-16	90	17	8*	-7	40	51	33*	5	150	12	4		
0	100	14	10	-15	0	49	-27*-15	51	59	-9*	-6	127	10	-9	7	199	9	8	
1	2853	-3*-14	254	9	1	-14	213	8	0	-5	116	11	-7	9	24	56	-5*		
2	4559	-8*-13	40	45	29*-13	33	54	-29*	-4	191	7	2	H, K=	15,	1				
3	9417	11	-12	36	45	5*-12	19	47	3*	-3	79	16	-5*-17	95	18	39*			
	H, K=	13,	9	-11	42	44	-9*-11	54	28	6*	-2	46	47	32*-16	51	57	15*		
-5	6927	11*-10	278	6	-9	-10	241	7	-14	-1	73	19	-22*-15	236	9	0			

## STRUCTURE FACTORS CONTINUED FOR URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	
-14	7	52	-7*-11	268	7	3	-3	0	52	-18*	2	234	7	0	-13	70	36	0*		
-13	50	29	19*-10	73	17	-9*	-2	98	13	8	4	182	14	-1	-12	106	16	5		
-12	21	53	5*	-9	220	6	1	-1	229	7	11	6	58	38	-28*-11	0	47	-5*		
-11	29	6	7	2	-8	57	23	32*	0	121	11	3	H,K=	16,	1	-18	184	9	-8	
-10	43	44	7*	-7	185	9	2	1	111	11	29	-16	25	53	-7*	-9	90	13	-3	
-9	19	8	6	3	-6	99	10	6	2	44	63	10*-15	42	60	37*	-8	243	7	-7	
-8	49	24	29*	-5	283	6	-4	3	147	10	8	-14	238	9	6	-7	37	46	22*	
-7	28	5	8	-2	-4	0	45	-35*	4	111	17	2	-13	21	54	-9*	-6	112	19	3
-6	63	20	3*	-3	42	59	32*	5	134	16	3	-12	157	17	0	-5	136	9	0	
-5	35	8	7	-7	-2	44	38	-6*	6	0	56	-16*-11	57	24	29*	-4	259	6	0	
-4	25	50	21*	-1	313	7	3	H,K=	15,	6	-10	210	6	-2	-3	59	65	9*		
-3	0	46	-8*	0	81	22	-13*-12	100	22	4*	-9	29	46	19*	-2	84	19	16*		
-2	0	55	-17*	1	121	10	1	-11	19	54	-51*	-8	252	6	10	-1	51	65	-3*	
-1	34	2	7	0	2	0	47	-28*-10	58	38	47*	-7	25	44	11*	0	218	7	-5	
0	71	22	13*	3	156	8	2	-9	132	13	4	-6	97	12	4	1	79	28	-11*	
1	23	7	7	19	4	86	18	8*	-8	121	13	1	-5	47	50	2*	2	124	14	-5
2	41	47	35*	5	154	9	4	-7	164	8	17	-4	300	6	-1	3	31	49	9*	
3	16	0	9	-8	6	34	51	26*	-6	29	56	-12*	-3	68	15	27*	4	99	18	-11
4	73	31	31*	7	75	22	25*	-5	76	20	9*	-2	0	45	-19*	5	21	54	-31*	
5	17	2	8	12	8	59	67	11*	-4	150	9	12	-1	34	45	23*	6	152	11	4
6	29	53	27*	H,K=	15,	4	-3	142	9	-6	0	281	8	0	H,K=	16,	4			
7	64	31	-18*-15	53	43	15*	-2	97	16	-2	1	19	64	-19*-14	20	64	-7*			
8	0	71	-24*-14	29	53	-3*	-1	0	50	-44*	2	130	11	-23	-13	69	22	29*		
9	15	8	12	3	-13	221	11	-14	0	63	24	10*	3	40	49	22*-12	177	9	-16	
H,K=	15,	2	-12	102	13	-5	1	155	10	2	4	133	10	-1	-11	104	16	16		
-16	58	32	31*-11	91	14	-11	2	119	18	-2	5	98	12	89	-10	139	9	-5		
-15	59	28	26*-10	50	29	31*	3	76	34	-1*	6	185	10	-8	-9	0	48	-8*		
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-13	28	1	7	5	-8	106	11	-14	H,K=	15,	7	H,K=	16,	2	-7	144	8	5		
-12	54	27	-19*	-7	270	6	3	-10	116	14	-6	-16	220	9	8	-6	211	7	2	
-11	11	2	10	-15	-6	47	52	16*	-9	108	22	11*-15	58	31	15*	-5	21	58	-5*	
-10	25	57	-26*	-5	112	13	4	-8	62	47	60*-14	63	26	18*	-4	10	58	-11*		
-9	28	7	6	3	-4	120	9	-10	-7	53	55	-23*-13	37	73	-22*	-3	121	11	4	
-8	90	11	4	-3	241	6	14	-6	119	12	7	-12	242	7	2	-2	234	7	-1	
-7	28	4	7	-5	-2	101	12	8	-5	115	20	-5	-11	35	48	15*	-1	120	10	16
-6	45	47	4*	-1	50	58	-18*	-4	60	29	-5*	-10	219	6	11	0	68	21	-5*	
-5	96	10	3	0	104	11	1	-3	0	54	-14*	-9	45	51	22*	1	56	60	27*	
-4	60	17	3*	1	216	7	-2	-2	71	24	-27*	-8	196	8	-3	2	139	13	4	
-3	37	5	8	4	2	85	17	-3*	-1	117	18	-13	-7	113	10	14	3	64	35	-22*
-2	68	20	3*	3	118	15	-6	0	110	16	12	-6	315	6	-8	4	140	11	-2	
-1	88	12	1	4	41	49	39*	1	61	63	12*	-5	0	45	-19*	5	39	59	35*	
0	57	18	-5*	5	97	16	4	2	0	64	-22*	-4	74	14	31*	H,K=	16,	5		
1	25	3	8	-9	6	61	32	-20*	H,K=	15,	8	-3	44	44	-8*	-13	109	18	18	
2	74	16	2*	7	144	14	3	-5	48	56	11*	-2	247	7	-4	-12	18	56	-31*	
3	15	1	9	-4	H,K=	15,	5	-4	92	28	-25*	-1	99	11	-4	-11	33	51	24*	
4	49	61	38*-14	100	16	14	-3	93	18	-7*	0	99	13	13	-10	136	11	-8		
5	79	20	-14*-13	17	52	-9*	H,K=	16,	0	1	0	48	-4*	-9	110	12	3			
6	59	29	-7*-12	41	56	18*-16	236	8	3	2	204	8	-3	-8	175	8	3			
7	18	4	15	-2	-11	155	9	-8	-14	52	53	15*	3	16	49	-16*	-7	34	49	
8	23	55	8*-10	97	21	-8*-12	274	9	6	4	151	10	-5	-6	91	13	24			
H,K=	15,	3	-9	181	10	4	-10	180	7	-6	5	47	51	46*	-5	181	13	-12		
-16	51	53	3*	-8	0	66	-9*	-8	188	7	-8	6	96	33	31*	-4	190	7	11	
-15	20	16	-4	-7	99	15	-3	-6	287	6	2	7	70	25	33*	-3	95	13	29	
-14	87	16	10	-6	118	10	-6	-4	43	36	30*	H,K=	16,	3	-2	42	49	-25*		
-13	53	63	9*	-5	201	7	11	-2	297	6	1	-15	60	30	34*	-1	43	61	-17*	
-12	34	47	-11*	-4	47	48	-8*	0	73	16	13*-14	209	9	1	0	176	12	8		

## STRUCTURE FACTORS CONTINUED FOR URANYL UREA NITRATE

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L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
1	107	17	-11	0	14	48	5*	-8	2	60	-16*	-9	29	51	24*	-7	71	22	17*
2	101	15	4	1	184	12	-11	-7	60	26	-24*	-8	68	23	-11*	-6	99	59	36*
3	31	53	19*	2	69	32	29*	-6	63	17	6*	-7	65	59	22*	-5	82	17	28*
4	84	31	7*	3	176	9	2	-5	200	7	0	-6	228	8	-18	-4	222	8	-1
H,K	16,	6	4	50	52	47*	-4	86	17	26*	-5	39	48	1*	-3	40	53	-26*	
-11	124	21	7	5	73	29	-7*	-3	0	58	-45*	-4	50	63	25*	-2	81	19	9*
-10	105	24	8*	6	78	22	51*	-2	88	15	4	-3	0	69	-10*	-1	31	53	16*
-9	54	69	51*	H,K	17,	2	-1	184	9	1	-2	256	7	0	0	153	10	23	
-8	79	20	-3*	-15	196	10	2	0	74	30	-14*	-1	21	50	-13*	1	110	18	6
-7	106	13	16	-14	57	70	13*	1	77	22	-22*	0	119	11	0	2	130	13	-6
-6	163	9	15	-13	130	14	17	2	10	53	-4*	1	0	58	-5*	H,K	18,	5	
-5	76	18	15*	-12	0	63	-18*	3	114	15	-8	2	129	25	6*	-9	0	55	-33*
-4	0	52	-5*	-11	191	8	-15	4	56	50	-1*	3	32	59	23*	-8	99	15	29
-3	101	17	-6	-10	59	34	33*	H,K	17,	5	4	174	11	-13	-7	113	15	29	
-2	137	16	-5	-9	191	7	-4	-11	105	15	1	H,K	18,	2	-6	172	9	14	
-1	77	26	-22*	-8	40	46	31*	-10	20	59	-26*	-13	75	22	21*	-5	46	54	-30*
0	32	54	-33*	-7	100	14	9	-9	77	22	-20*	-12	146	16	4	-4	43	69	11*
1	22	63	-11*	-6	58	23	24*	-8	107	25	0*	-11	46	57	33*	-3	46	53	4*
2	122	21	13	-5	270	6	9	-7	146	10	-17	-10	153	9	7	-2	146	11	-6
H,K	16,	7	-4	27	51	1*	-6	81	23	21*	-9	62	23	7*	-1	75	24	-17*	
-8	109	15	-9	-3	58	33	17*	-5	41	51	19*	-8	245	7	-1	H,K	19,	0	
-7	43	54	-7*	-2	0	48	-42*	-4	100	15	-3	-7	5	53	-17*	-11	191	8	10
-6	58	37	13*	-1	268	7	6	-3	170	11	-4	-6	50	51	18*	-9	114	13	-2
-5	98	16	-5	0	66	19	13*	-2	79	33	2*	-5	23	48	4*	-7	252	10	-12
-4	130	13	10	1	93	23	-10*	-1	62	31	-9*	-4	239	7	7	-5	60	43	35*
-3	101	21	15*	2	0	50	-4*	0	59	32	25*	-3	73	18	25*	-3	222	8	2
-2	55	48	32*	3	110	13	5	1	143	16	16	-2	84	17	-16*	-1	130	18	-11
-1	55	50	-5*	4	67	25	25*	2	102	16	6	-1	0	60	-5*	1	115	17	5
H,K	17,	0	5	163	11	-2	H,K	17,	6	0	185	9	-10	H,K	19,	1			
-15	224	8	8	H,K	17,	3	-9	127	14	4	1	44	72	-21*	-12	57	34	56*	
-13	106	13	-7	-14	54	56	27*	-8	71	24	46*	2	165	10	3	-11	146	13	9
-11	209	8	9	-13	211	8	-3	-7	63	23	25*	3	56	58	41*	-10	0	58	-19*
-9	174	8	-1	-12	61	28	-5*	-6	87	26	-9*	4	72	27	-5*	-9	208	8	-1
-7	134	13	6	-11	167	9	10	-5	141	11	7	H,K	18,	3	-8	34	54	17*	
-5	269	6	-5	-10	54	29	25*	-4	78	21	8*-13	12	55	-10*	-7	62	32	38*	
-3	30	45	15*	-9	130	10	0	-3	12	58	-31*-12	183	9	13	-6	57	29	52*	
-1	257	0	-2	-8	54	34	-40*	-2	83	31	26*-11	33	53	-23*	-5	237	7	6	
1	161	17	0	-7	225	7	6	-1	132	15	0	-10	178	11	-6	-4	20	51	7*
3	122	14	4	-6	38	50	-1*	0	95	26	-14*	-9	39	51	8*	-3	126	15	17
5	172	10	1	-5	36	47	10*	H,K	18,	0	-8	90	16	-16	-2	0	53	-3*	
H,K	17,	1	-6	54	29	-8*-14	172	11	-2	-7	74	19	-10*	-1	167	9	-2		
-15	42	52	29*	-3	251	7	-1	-12	157	14	-14	-6	219	8	-4	0	63	27	28*
-14	31	71	9*	-2	16	56	-35*	-10	152	11	3	-5	47	51	-19*	1	166	10	5
-13	227	9	5	-1	77	17	3*	-8	220	7	7	-4	18	53	-11*	2	0	55	-10*
-12	0	49	-26*	0	57	33	10*	-6	73	18	91*	-3	56	66	-1*	H,K	19,	2	
-11	206	7	6	1	166	9	3	-4	246	7	12	-2	211	8	-4	-12	41	54	-23*
-10	10	55	-18*	2	112	12	36	-2	85	29	-13*	-1	56	67	2*	-11	191	9	18
-9	162	8	1	3	156	11	12	0	240	7	12	0	114	13	1	-10	42	66	22*
-8	25	47	-30*	4	49	55	44*	2	180	9	0	1	57	34	51*	-9	98	18	1*
-7	235	7	5	5	15	57	-47*	4	77	29	-4*	2	120	18	10	-8	48	53	-4*
-6	33	40	23*	H,K	17,	4	H,K	18,	1	3	47	64	-7*	-7	241	8	-2		
-5	0	46	-54*	-13	46	55	-17*	-14	115	13	29	H,K	18,	4	-6	46	58	0*	
-4	43	50	28*	-12	50	54	38*	-13	0	54	-21*	-11	33	54	8*	-5	66	26	22*
-3	291	6	0	-11	129	13	-23	-12	195	9	7	-10	151	10	6	-4	0	54	-35*
-2	29	46	18*	-10	77	22	13*	-11	42	54	34*	-9	110	16	11	-3	236	7	9
-1	08	14	-6	-9	214	8	1	-10	190	8	1	-8	185	9	2	-2	71	29	42*

## STRUCTURE FACTORS CONTINUED FOR URANYL UREA NITRATE

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