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CRYSTAL and MOLECULAR STRUCTURES OF THORIUM and URANIUM
TETRAKIS(HEXAFLUOROACETONYLPIRAZOLIDE) COMPLEXES

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Publication Date

1976

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Submitted to Inorganic Chemistry

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CRYSTAL AND MOLECULAR STRUCTURES OF THORIUM AND
URANIUM TETRAKIS(HEXAFLUOROACETONYLPYRAZOLIDE)
COMPLEXES¹

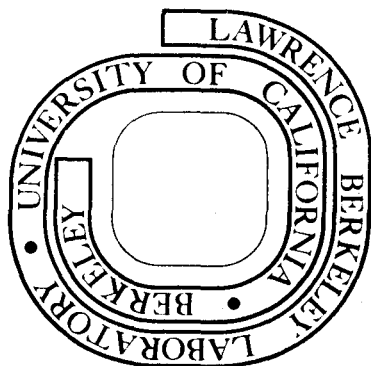
Karl Volz, Allan Zalkin, and David H. Templeton

January 1976

Prepared for the U. S. Energy Research and
Development Administration under Contract W-7405-ENG-48

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Contribution from the Materials and Molecular Research
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 California 94720

Crystal and Molecular Structures of Thorium and Uranium
 Tetrakis(hexafluoroacetylpyrazolide) Complexes¹

KARL VOLZ, ALLAN ZALKIN, and DAVID H. TEMPLETON*

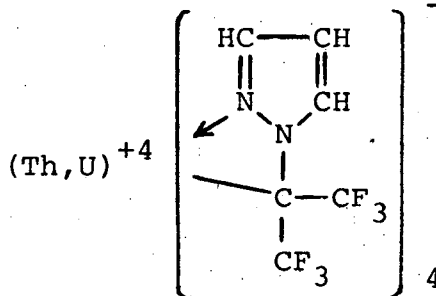
Received

Triclinic crystals of thorium(IV) and uranium(IV) tetrakis-
 (hexafluoroacetylpyrazolide) are isostructural, with space
 group $P\bar{1}$ and $Z = 2$. At 23° for $\text{Th}(\text{C}_6\text{H}_3\text{ON}_2\text{F}_6)_4$: $a =$
 $11.282(5)$, $b = 16.245(7)$, $c = 10.836(5)$ Å, $\alpha = 90.14(5)$,
 $\beta = 108.75(5)$, $\gamma = 107.07(5)^\circ$. For the uranium compound:
 $a = 11.302(5)$, $b = 16.377(8)$, $c = 11.000(5)$ Å, $\alpha = 87.85(5)$,
 $\beta = 111.02(5)$, $\gamma = 109.95(5)^\circ$. X-ray diffraction data were
 measured with a scintillation counter, θ - 2θ scans, and $\text{MoK}\alpha$
 radiation. For thorium the conventional R value is 0.026
 for 2,966 unique data with $I > \sigma(I)$, and for uranium it is
 0.027 for 4,125 unique data with $I > 3\sigma(I)$. The full-matrix
 least-squares refinement of the 598 parameters of each
 structure included anisotropic thermal parameters for the
 61 non-hydrogen atoms and isotropic ones for the 12 hydrogen

atoms. The actinide ion is at the center of an irregular polyhedron of four oxygen and four nitrogen atoms. The average Th-O, Th-N, U-O, and U-N distances are 2.291(4), 2.637(5), 2.237(3) and 2.574(5) Å. The molecules are packed in a manner which resembles cubic closest packing but which is more nearly analogous to the body-centered-tetragonal structure of protactinium metal.

Introduction

Polymeric pyrazolide compounds of the type $M(\text{Pz})_n$ can be formed in the reaction of pyrazole ($\text{HN}_2\text{C}_3\text{H}_3$ or HPz) with ions of transition metals, lanthanides, and actinides. In 1966 Mahler² discovered that hexafluoroacetone (hfa) can react with the pyrazolide compounds to yield metal-pyrazolide-hexafluoroacetone complexes $M(\text{hfaPz})_n$. Several actinide tetrakis(hfaPz) compounds were synthesized by Andruchow and Karraker.³ We studied two of these with X-ray diffraction methods to verify their composition and to establish their molecular structure, which can be represented:



Experimental

Crystalline samples of $\text{Th}(\text{C}_6\text{H}_3\text{ON}_2\text{F}_6)_4$ and $\text{U}(\text{C}_6\text{H}_3\text{ON}_2\text{F}_6)_4$ were kindly provided by D. G. Karraker. The thorium crystals were well-formed colorless prisms which did not require recrystallization. The dark violet uranium crystals after recrystallization from toluene

were fragile hexagonal plates. Crystals of both compounds are air stable and were mounted on glass fibers for x-ray diffraction study. Each exhibited sharp extinction under polarized light. Investigations with oscillation, Weissenberg, and precession photography indicated that the crystals were triclinic. The space group $P\bar{1}$ was assumed and is confirmed by the subsequent refinement of the structure. Unit cell dimensions were obtained in each case by a least-squares analysis of the setting angles for 12 carefully centered reflections with $2\theta > 37^\circ$, using resolved $MoK\alpha_1$ peaks ($\lambda = 0.70926 \text{ \AA}$) with a Picker automated four-circle diffractometer and a graphite monochromator. Intensities were measured for both compounds using a θ - 2θ scan technique. Data for the thorium crystal were collected out to $2\theta = 40^\circ$ at a scan rate of $1^\circ/\text{min}$; data for the uranium crystal were measured to $2\theta = 50^\circ$ at a scan rate of $2^\circ/\text{min}$. For thorium, reflections were scanned from 0.8° below the calculated $K\alpha_1$ position to 0.8° above $K\alpha_2$; for uranium, 0.9° . Background was counted for 4 sec at positions offset 0.9° from each end of the scan. Copper-foil attenuators were inserted when necessary to reduce the maximum counting rate below 10,000 c/sec. All the reflections within the spheres of reciprocal space delineated by the above 2θ limits were measured. Reflections (3 0 0), (0 6 0) and (0 0 3) for the thorium crystal and (5 0 0), (0 10 0) and (0 0 3) for the uranium crystal were measured at intervals of 200 measurements to monitor radiation damage and instrumental stability. Corrections calculated from the average change of the three standards were applied to the data; they ranged from 1.0 to 1.03. The widths at half maximum of the scans increased an average of 0.05° for each crystal during the experiment.

Absorption corrections calculated by an analytical integration⁴ were applied to both data sets and were checked in the following manner. Several test reflections were measured at regular intervals of Ψ , the azimuthal angle corresponding to rotation of the crystal around the direction of the diffraction vector.⁵ These intensities reveal variations in the absorption effect for each reflection, and plots as a function of Ψ before and after correction (Figure 1) indicate the efficacy of the correction and accuracy of the crystal dimensions (Figure 2). The correction factors ranged from 1.294 to 1.447 for the thorium crystal and from 1.213 to 1.594 for uranium. After this correction the agreement of pairs of equivalent reflections is indicated by $R_s = \Sigma |I - I_{ave}| / \Sigma(I) = 0.03$ (0.05) for the thorium (uranium) crystal. Standard deviations were assigned to the average intensities according to counting statistics or the scatter, whichever gave the larger result, and corresponding values of $\sigma(F)$ were derived. These data sets included 3359 (6291) unique reflections for the thorium (uranium) crystal, of which 2,966 with $I < \sigma(I)$ for thorium and 4,125 with $I < 3\sigma(I)$ for uranium were given weight in the final least-squares refinements, $w = (\sigma(F))^{-2}$. The crystal data are listed in Table I.

Determination and Refinement of Structure

The coordinates of the thorium atom were readily obtained from the Patterson function. After least-squares refinement of that one atom, a ΔF Fourier map revealed the locations of the remaining 60 non-hydrogen atoms. Refinement of the 61 atoms with anisotropic thermal parameters for thorium resulted in $R = \Sigma |\Delta F| / \Sigma |F_o| = 0.06$. The 12 hydrogen atoms were introduced at calculated positions, and further refinement of all 73 atoms reduced R to 0.05. Finally, with isotropic thermal parameters for hydrogen and anisotropic parameters for all other atoms

(598 parameters in all) R was reduced to 0.026 for 2,966 reflections with $I > \sigma(I)$. The weighted residual $R_2 = [\sum w(\Delta F)^2 / \sum w F_o^2]^{1/2}$ was 0.013, and R including zero-weight data was 0.037. In the last cycle no parameter of hydrogen shifted more than 0.17σ and for other atoms the largest shift was 0.11σ . The standard deviation of an observation of unit weight was 0.99. In a final ΔF Fourier map the largest peak, $0.66 \text{ e}/\text{\AA}$, was near the thorium atom. The final coordinates are listed in Table II.⁶

The two compounds were known to be nearly isostructural on the basis of similar film data. Refinement of the uranium compound was started with the final parameters for the thorium one and converged with little change. The final refinement reduced R to 0.027 for the 4,125 reflections with $I > 3\sigma(I)$; R_2 was 0.013; R was 0.059 including the zero-weight data. The standard deviation of an observation of unit weight was 1.01. The ten largest peaks in the final ΔF map ranged from 1.40 to $0.76 \text{ e}/\text{\AA}$. Most of them were near uranium or fluorine atoms. The final coordinates are listed in Table III.⁶ In the last cycle none of these changed more than 0.12σ , and no thermal parameter changed more than 0.19σ .⁷

The scattering factors used were those of Doyle and Turner⁸ for neutral carbon, nitrogen, oxygen and fluorine and those of Cromer and Waber⁹ for neutral thorium and uranium, in each case corrected for dispersion according to Cromer and Liberman.¹⁰ Polarized hydrogen scattering factors from Stewart, Davidson and Simpson¹¹ were used with Olson's¹² modified version of our least-squares program, LESQ. Other calculations were done with our unpublished programs MAGPIK, INCOR, ORDER, MORPH, DISMAT, DISTAN, LSPLAN, LIST and LISTAP, L. K. Templeton's absorption correction program ABSOR, and Johnson's¹³ ORTEP.

Discussion

These compounds crystallize as discrete molecular complexes (Figure 3) and are essentially isostructural except for an average difference of 0.06 Å in the actinide-ligand bond lengths as a result of the actinide contraction. Bond lengths and angles are listed in Tables IV to VII. The four ligands are arranged in a roughly tetrahedral fashion with approximately the symmetry of a 2-fold axis in the direction of c^* (Figure 3a). A pair of chelate rings is nearly coplanar (Figure 3b), and the planes of two of these pairs have a dihedral angle of 88°. The molecules in each of these planes are arranged in a trans configuration.

The coordination polyhedron about the actinide atom consists of four oxygen atoms and four nitrogen atoms at average bond distances Th-O = 2.291(4), Th-N = 2.637(5), U-O = 2.237(3) and U-N = 2.574(5) Å. These eight atoms are at the vertices of an irregular dodecahedron (Figure 4) with the bidentate ligands spanning the "m" edges as designated by Hoard and Silverton.¹⁴ The coordinating atoms have a "bite" on the metal atom averaging 2.54 Å with an average O-M-N angle of 61°.

The eight hfaPz molecules of the two complexes have very similar dimensions, and averages for the two crystals are listed in Figure 5. The values for the pyrazole ring are little different from those reported by Berthou, Elguero and Rerat¹⁵ for unsubstituted pyrazole. The atoms of these rings are accurately planar, with a maximum deviation of 0.01 Å, and the carbon and oxygen atoms of the chelate ring in the same ligand come within 0.07 Å of the same plane, on the average, and within 0.12 Å in the extreme case.⁶ The five atoms of each chelate ring are less precisely planar, with the distance of the actinide ion from the mean

plane of the other atoms ranging from 0.00 to 0.27 Å.

As is to be expected, the bonds of the trifluoromethyl groups are nearly trans with respect to the bonds at atom C(1), Figure 5. The torsion angles for rotation around the C-C bonds, for the sixteen examples, range from 0° to 13° with a mean of 4° from exactly trans positions. The fluorine atoms have the largest amplitudes of anisotropic thermal motion in these crystals, and the directions of maximum amplitude correspond to torsional motion of the groups around these C-C bonds. The mean C-F bond length for both structures is 1.32(1) Å (uncorrected) and 1.36(1) Å after correction for thermal motion according to the riding model.¹⁶ These values may be compared with an average of 1.334(4) Å reported for some other polyfluoroparaffins.¹⁷

Figure 6 illustrates the arrangement of the molecules in the unit cell. Each molecule has 12 nearest neighbors for which, in the uranium case, the U-U distances are .8.98, 9.19, 10.45, 11.00 (twice), 11.05, 11.18, 11.24, 11.30 (twice), and 12.63 (twice) Å. The packing resembles the cubic closest packing of spheres, described by a pseudocell given by the matrix $[1 \ 1/2 \ 3/2; 1 \ 1/2 \ -1/2; 1 \ -1/2 \ 1/2]$. The dimensions of this cell, which contains four molecules, are $a = 16.74$, $b = 14.25$, $c = 15.50$ Å, $\alpha = 81.19$, $\beta = 76.89$, $\gamma = 90.08^\circ$. A more precise description of the packing, which considers only the first ten neighbors to be nearest neighbors, is given by the body-centered tetragonal structure described by Zachariasen¹⁸ for protactinium metal. The corresponding pseudocell, containing two molecules and given by the matrix $[1 \ 0 \ 1; 1 \ 1/2 \ -1/2; 0 \ 1/2 \ 1/2]$, has dimensions $a = 12.63$, $b = 14.25$, $c = 10.03$ Å, $\alpha = 96.86$, $\beta = 85.47$, $\gamma = 84.66^\circ$. Neither of these cells is a true cell because the fact that there are two orientations of molecules requires a doubling of

axes for strict periodicity. The molecular packing involves only weak forces which permit the molecules to sublime at 140° under vacuum.³

We thank Dr. D. G. Karraker for providing the compounds, Dr. G. Chapuis and Dr. L. K. Templeton for help with the absorption correction, and Mrs. H. W. Ruben for assistance with the calculations.

Supplementary Material Available. A listing of thermal parameters, deviations of atoms from various least-squares planes, and structure factor amplitudes for each of these crystals will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the supplementary material from this paper only or microfiche (105 × 148 mm, 24× reduction, negatives) containing all of the supplementary material for the papers in this issue may be obtained from the Journals Department, American Chemical Society, 1155 16th St., N. W., Washington, D. C. 20036. Remit check or money order for \$0.00 for photocopy or \$2.50 for microfiche, referring to code number AIC000000.

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- (7) The function minimized is $\sum w |\Delta F|^2$.
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Table I. Crystal Data

	Th(C ₆ H ₃ ON ₂ F ₆) ₄	U(C ₆ H ₃ ON ₂ F ₆) ₄	
F. W.	1,164.4	1,170.4	
Space group	P $\bar{1}$	P $\bar{1}$	
a, Å	11.282(5)	11.302(5) ^a	11.295(5) ^b
b, Å	16.245(7)	16.377(8)	16.393(8)
c, Å	10.836(5)	11.000(5)	10.999(5)
α , °	90.14(5)	87.85(5)	87.98(5)
β , °	108.75(5)	111.02(5)	110.82(5)
γ , °	107.07(5)	109.95(5)	109.79(5)
d _x , g/cm ³ at 23°	2.163	2.186	
d _m , g/cm ³ at 23° ^c	2.16	2.18	
μ , cm ⁻¹ (MoK α)	44.38	44.49	

^aOriginal measurements. ^bMeasurements after data collection was completed, made because setting angle discrepancies had developed.

The change is attributed to radiation damage. ^cMeasured by flotation.

Table II. Atomic Coordinates and Standard Deviations in Thorium

Tetrakis(hexafluoroacetylpyrazolide)

Atom	x	y	z
Th	.00788(3)	.24870(2)	.19733(2)
O(1)	-.1713(4)	.2219(2)	.0104(3)
O(2)	.1484(4)	.2779(2)	.0796(3)
O(3)	-.0710(4)	.3317(2)	.3021(4)
O(4)	.1184(4)	.1637(2)	.3251(4)
N(1)	-.2230(6)	.0724(4)	-.0141(5)
N(2)	-.1048(5)	.0892(3)	.0845(5)
N(3)	.1862(5)	.4263(4)	.0856(5)
N(4)	.0986(5)	.4098(4)	.1513(5)
N(5)	-.2225(5)	.2193(4)	.3549(5)
N(6)	-.1711(5)	.1696(4)	.3016(5)
N(7)	.2773(6)	.2725(4)	.4819(6)
N(8)	.2150(5)	.3242(4)	.4090(5)
C(1)	-.2581(7)	.1499(4)	-.0660(6)
C(2)	-.2512(9)	.1520(5)	-.2041(7)
C(3)	-.3991(7)	.1414(5)	-.0681(8)
C(4)	-.089(1)	.0122(6)	.1088(9)
C(5)	-.193(1)	-.0535(6)	.026(1)
C(6)	-.275(1)	-.0131(6)	-.0510(9)
C(7)	.2125(6)	.3496(4)	.0397(6)
C(8)	.1673(9)	.3421(5)	-.1110(7)
C(9)	.3634(8)	.3650(6)	.0971(9)
C(10)	.0893(9)	.4863(6)	.1780(8)
C(11)	.170(1)	.5516(6)	.1335(9)
C(12)	.2281(9)	.5119(6)	.0745(8)
C(13)	-.1587(7)	.3149(4)	.3646(6)
C(14)	-.2644(8)	.3579(5)	.3044(8)
C(15)	-.0874(8)	.3450(5)	.5123(7)
C(16)	-.2353(8)	.0883(6)	.3131(7)
C(17)	-.3258(8)	.0872(6)	.3750(7)
C(18)	-.3159(8)	.1704(7)	.3989(8)
C(19)	.2215(7)	.1786(4)	.4329(7)
C(20)	.3314(9)	.1506(6)	.4090(9)
C(21)	.1782(8)	.1297(6)	.5418(8)
C(22)	.2782(9)	.4013(5)	.4717(9)
C(23)	.379(1)	.4012(8)	.585(1)
C(24)	.3779(9)	.3175(8)	.5889(9)
F(1)	-.3412(4)	.0847(3)	-.2891(3)
F(2)	-.1342(5)	.1511(3)	-.2040(4)
F(3)	-.2711(5)	.2228(3)	-.2556(4)
F(4)	-.4352(4)	.2070(3)	-.1168(4)
F(5)	-.4044(4)	.1382(3)	.0521(4)
F(6)	-.4884(4)	.0692(3)	-.1383(4)
F(7)	.2290(5)	.4100(3)	-.1580(4)

[Table II continued]

F(8)	.0400(5)	.3359(3)	-.1569(4)
F(9)	.1795(5)	.2730(3)	-.1603(4)
F(10)	.3924(4)	.2966(3)	.0670(5)
F(11)	.4000(4)	.3748(3)	.2274(5)
F(12)	.4368(4)	.4338(3)	.0635(5)
F(13)	-.3576(4)	.3399(3)	.3569(5)
F(14)	-.3208(4)	.3301(3)	.1789(5)
F(15)	-.2132(4)	.4420(3)	.3139(4)
F(16)	-.0137(5)	.4241(3)	.5349(4)
F(17)	-.0085(4)	.2971(3)	.5638(3)
F(18)	-.1682(4)	.3354(3)	.5801(4)
F(19)	.4378(4)	.1628(3)	.5128(5)
F(20)	.3682(4)	.1933(3)	.3180(5)
F(21)	.2891(5)	.0673(3)	.3636(5)
F(22)	.1280(4)	.0456(3)	.5042(4)
F(23)	.0871(5)	.1551(3)	.5646(4)
F(24)	.2752(4)	.1399(3)	.6541(4)
H(1)	-.003(6)	.012(4)	.166(6)
H(2)	-.218(7)	-.113(4)	.018(6)
H(3)	-.358(6)	-.035(4)	-.118(6)
H(4)	.030(5)	.490(4)	.219(5)
H(5)	.166(5)	.612(4)	.135(5)
H(6)	.303(6)	.535(4)	.031(6)
H(7)	-.223(6)	.037(4)	.276(5)
H(8)	-.383(5)	.038(4)	.396(5)
H(9)	-.357(5)	.193(3)	.447(5)
H(10)	.250(4)	.448(3)	.446(4)
H(11)	.454(7)	.451(5)	.639(8)
H(12)	.442(5)	.291(5)	.647(8)

Table III. Atomic Coordinates and Standard Deviations in Uranium

Tetrakis(hexafluoroacetylpyrazolide)

Atom	x	y	z
U	.02415(2)	.24745(1)	.18628(2)
O(1)	-.1596(3)	.2255(2)	.0035(3)
O(2)	.1596(3)	.2721(2)	.0724(3)
O(3)	-.0411(3)	.3329(2)	.2804(3)
O(4)	.1281(3)	.1619(2)	.3109(3)
N(1)	-.2220(4)	.0750(3)	-.0215(4)
N(2)	-.0993(4)	.0920(3)	.0785(4)
N(3)	.2104(4)	.4211(3)	.0737(5)
N(4)	.1233(4)	.4061(3)	.1380(4)
N(5)	-.1927(4)	.2250(3)	.3458(4)
N(6)	-.1517(4)	.1716(3)	.2924(4)
N(7)	.2947(4)	.2681(3)	.4688(4)
N(8)	.2365(4)	.3224(3)	.3925(4)
C(1)	-.2518(5)	.1543(4)	-.0733(5)
C(2)	-.2462(7)	.1577(5)	-.2119(6)
C(3)	-.3940(6)	.1452(4)	-.0789(6)
C(4)	-.0910(6)	.0133(4)	.0996(6)
C(5)	-.2030(7)	-.0534(5)	.0161(7)
C(6)	-.2827(7)	-.0114(4)	-.0595(7)
C(7)	.2311(5)	.3435(4)	.0339(6)
C(8)	.1838(8)	.3358(6)	-.1183(7)
C(9)	.3847(6)	.3579(5)	.0974(8)
C(10)	.1166(6)	.4821(4)	.1596(6)
C(11)	.1998(8)	.5480(5)	.1103(8)
C(12)	.2561(7)	.5075(5)	.0563(7)
C(13)	-.1223(5)	.3194(3)	.3489(5)
C(14)	-.2318(7)	.3601(4)	.2843(7)
C(15)	-.0388(7)	.3555(5)	.4925(6)
C(16)	-.2218(6)	.0918(4)	.3103(6)
C(17)	-.3034(7)	.0936(6)	.3768(7)
C(18)	-.2848(7)	.1781(6)	.3957(7)
C(19)	.2344(5)	.1753(3)	.4233(6)
C(20)	.3431(6)	.1480(5)	.4008(6)
C(21)	.1885(6)	.1252(4)	.5295(6)
C(22)	.3048(6)	.4004(5)	.4582(7)
C(23)	.4089(8)	.3996(6)	.5731(8)
C(24)	.3986(7)	.3151(5)	.5765(7)
F(1)	-.3445(4)	.0920(2)	-.2971(3)
F(2)	-.1303(4)	.1551(3)	-.2084(3)
F(3)	-.2593(4)	.2306(2)	-.2623(3)
F(4)	-.4258(3)	.2132(2)	-.1254(3)
F(5)	-.3965(3)	.1416(2)	.0410(4)
F(6)	-.4919(3)	.0740(2)	-.1486(3)
F(7)	.2579(4)	.4025(3)	-.1629(4)

[Table III continued]

F(8)	.0573(4)	.3352(3)	-.1675(3)
F(9)	.1856(4)	.2638(3)	-.1636(4)
F(10)	.4073(4)	.2892(3)	.0678(4)
F(11)	.4207(3)	.3673(2)	.2266(4)
F(12)	.4632(3)	.4275(3)	.0663(4)
F(13)	-.3190(4)	.3494(3)	.3413(4)
F(14)	-.2999(3)	.3282(2)	.1618(4)
F(15)	-.1734(4)	.4459(3)	.2822(3)
F(16)	.0472(4)	.4352(3)	.5001(4)
F(17)	.0354(3)	.3069(2)	.5484(3)
F(18)	-.1123(4)	.3568(3)	.5613(3)
F(19)	.4531(3)	.1616(3)	.5061(4)
F(20)	.3797(3)	.1894(2)	.3071(4)
F(21)	.2963(4)	.0637(3)	.3626(4)
F(22)	.1260(3)	.0412(2)	.4886(3)
F(23)	.1009(4)	.1531(2)	.5513(3)
F(24)	.2880(3)	.1325(2)	.6411(3)
H(1)	-.009(4)	.004(2)	.182(4)
H(2)	-.211(6)	-.115(4)	.020(6)
H(3)	-.370(4)	-.033(3)	-.127(4)
H(4)	.052(4)	.487(3)	.209(4)
H(5)	.211(5)	.612(4)	.123(5)
H(6)	.338(6)	.530(4)	.025(6)
H(7)	-.202(4)	.043(3)	.279(4)
H(8)	-.367(5)	.047(3)	.395(5)
H(9)	-.321(4)	.213(3)	.438(4)
H(10)	.287(5)	.456(3)	.424(5)
H(11)	.465(6)	.453(4)	.630(6)
H(12)	.447(5)	.277(3)	.637(5)

Table IV. Bond Distances (in Å) and Standard Deviations for the Thorium Compound

	Ligand I	Ligand II	Ligand III	Ligand IV
Th-O(1) ^a	2.286(4)	2.286(4)	2.291(4)	2.300(4)
Th-N(2)	2.623(5)	2.628(5)	2.637(5)	2.661(6)
O(1)-C(1)	1.347(7)	1.333(6)	1.335(6)	1.318(6)
C(1)-C(2)	1.523(9)	1.539(9)	1.525(9)	1.532(9)
C(1)-C(3)	1.548(9)	1.554(9)	1.545(8)	1.552(9)
C(2)-F(1)	1.348(7)	1.320(7)	1.311(8)	1.318(8)
C(2)-F(2)	1.324(8)	1.332(8)	1.316(8)	1.312(8)
C(2)-F(3)	1.327(8)	1.305(8)	1.308(7)	1.329(8)
C(3)-F(4)	1.304(7)	1.314(8)	1.281(7)	1.322(8)
C(3)-F(5)	1.323(8)	1.333(8)	1.342(7)	1.304(8)
C(3)-F(6)	1.333(7)	1.312(8)	1.320(7)	1.320(7)
C(1)-N(1)	1.487(7)	1.482(7)	1.494(7)	1.490(7)
N(1)-C(6)	1.342(8)	1.351(8)	1.343(8)	1.352(9)
N(1)-N(2)	1.365(6)	1.361(6)	1.345(6)	1.349(6)
N(2)-C(4)	1.331(8)	1.317(9)	1.335(8)	1.304(8)
C(4)-C(5)	1.383(11)	1.378(11)	1.387(10)	1.380(11)
C(5)-C(6)	1.355(11)	1.332(11)	1.340(10)	1.357(12)
C(4)-H(1)	0.96(6)	0.93(5)	0.99(5)	0.92(4)
C(5)-H(2)	0.93(6)	1.00(5)	0.95(5)	0.99(7)
C(6)-H(3)	0.95(5)	1.07(6)	0.94(5)	1.00(8)

^aFor each ligand the atoms are numbered as in Fig. 5. For ligand I this corresponds to the numbering in Table II. Similar numbering is used in the following three tables.

Table V. Bond Angles ($^{\circ}$) and Standard Deviations for the Thorium Compound

	Ligand I	Ligand II	Ligand III	Ligand IV
O(1)-Th-N(2)	61.7(2)	62.0(2)	61.6(2)	61.3(2)
Th-O(1)-C(1)	134.7(4)	134.3(4)	134.7(4)	134.8(4)
O(1)-C(1)-N(1)	109.7(5)	110.8(5)	110.0(5)	111.4(5)
C(1)-N(1)-N(2)	115.5(6)	115.8(6)	115.8(6)	115.4(6)
N(1)-N(2)-Th	117.0(4)	117.0(5)	117.3(4)	117.2(4)
N(1)-N(2)-C(4)	105.5(6)	104.3(6)	105.1(6)	104.2(6)
N(2)-C(4)-C(5)	110.9(8)	112.2(9)	110.4(8)	112.7(8)
C(4)-C(5)-C(6)	105.3(8)	105.1(8)	105.6(8)	105.1(9)
C(5)-C(6)-N(1)	108.5(8)	108.3(8)	107.9(8)	106.2(9)
C(6)-N(1)-N(2)	109.8(7)	110.2(7)	110.9(6)	111.9(7)
O(1)-C(1)-C(2)	110.1(6)	110.2(5)	110.2(5)	111.2(6)
O(1)-C(1)-C(3)	110.2(6)	110.0(5)	109.7(6)	109.1(6)
N(1)-C(1)-C(2)	106.9(6)	108.0(5)	109.1(6)	107.3(6)
N(1)-C(1)-C(3)	109.0(6)	107.7(6)	105.9(5)	107.3(6)
C(2)-C(1)-C(3)	110.9(7)	110.1(6)	111.8(6)	110.6(6)
C(1)-C(2)-F(1)	113.8(6)	113.8(6)	113.2(6)	114.8(7)
C(1)-C(2)-F(2)	111.0(7)	108.7(7)	108.9(7)	109.9(7)
C(1)-C(2)-F(3)	111.6(7)	112.1(6)	111.2(7)	111.2(7)
F(1)-C(2)-F(2)	106.8(7)	106.3(6)	107.2(7)	107.2(7)
F(1)-C(2)-F(3)	106.1(6)	108.4(7)	108.7(7)	107.4(7)
F(2)-C(2)-F(3)	107.3(7)	107.2(7)	107.4(6)	105.9(7)
C(1)-C(3)-F(4)	110.9(6)	110.8(7)	112.9(6)	110.2(7)
C(1)-C(3)-F(5)	110.4(6)	108.4(7)	109.2(6)	110.6(6)
C(1)-C(3)-F(6)	112.7(7)	115.4(7)	113.5(6)	113.8(7)
F(4)-C(3)-F(5)	108.6(7)	106.1(7)	106.5(7)	107.4(7)
F(4)-C(3)-F(6)	107.8(6)	109.2(7)	108.1(7)	106.9(6)
F(5)-C(3)-F(6)	106.3(6)	106.5(7)	106.1(6)	107.7(7)

Table VI. Bond Distances (in Å) and Standard Deviations for the Uranium Compound

	Ligand I	Ligand II	Ligand III	Ligand IV
U-O(1)	2.244(3)	2.235(3)	2.222(4)	2.246(3)
U-N(2)	2.539(5)	2.574(5)	2.593(5)	2.589(5)
O(1)-C(1)	1.332(5)	1.328(5)	1.343(5)	1.339(5)
C(1)-C(2)	1.546(8)	1.560(8)	1.542(7)	1.540(7)
C(1)-C(3)	1.542(7)	1.556(8)	1.535(7)	1.543(7)
C(2)-F(1)	1.336(7)	1.329(7)	1.309(7)	1.317(6)
C(2)-F(2)	1.312(7)	1.332(7)	1.310(6)	1.325(6)
C(2)-F(3)	1.330(6)	1.307(8)	1.336(7)	1.321(7)
C(3)-F(4)	1.314(6)	1.311(7)	1.319(7)	1.322(6)
C(3)-F(5)	1.328(6)	1.330(7)	1.327(6)	1.316(6)
C(3)-F(6)	1.323(6)	1.305(6)	1.315(7)	1.309(6)
C(1)-N(1)	1.492(6)	1.476(6)	1.472(6)	1.460(6)
N(1)-C(6)	1.351(7)	1.363(7)	1.345(7)	1.352(7)
N(1)-N(2)	1.370(5)	1.361(5)	1.355(5)	1.370(5)
N(2)-C(4)	1.330(6)	1.307(6)	1.326(6)	1.321(7)
C(4)-C(5)	1.392(8)	1.404(8)	1.376(9)	1.387(8)
C(5)-C(6)	1.348(8)	1.336(9)	1.339(9)	1.348(9)
C(4)-H(1)	1.09(4)	1.08(4)	1.01(4)	1.03(5)
C(5)-H(2)	0.98(6)	1.02(5)	0.93(4)	0.97(6)
C(6)-H(3)	0.95(4)	1.05(6)	1.02(4)	1.03(5)

Table VII. Bond Angles ($^{\circ}$) and Standard Deviations for the Uranium Compound

	Ligand I	Ligand II	Ligand III	Ligand IV
O(1)-U-N(2)	63.5(1)	63.4(1)	62.8(1)	62.7(1)
U-O(1)-C(1)	133.2(2)	133.7(3)	134.7(2)	134.8(2)
O(1)-C(1)-N(1)	110.2(4)	110.7(4)	109.7(4)	109.5(4)
C(1)-N(1)-N(2)	114.6(4)	116.0(4)	116.3(4)	117.1(4)
N(1)-N(2)-U	117.2(2)	116.2(3)	116.0(2)	115.9(2)
N(1)-N(2)-C(4)	103.5(5)	105.8(5)	104.6(5)	104.7(5)
N(2)-C(4)-C(5)	113.1(5)	111.1(6)	111.6(6)	112.5(6)
C(4)-C(5)-C(6)	103.9(6)	105.4(7)	105.2(6)	104.1(7)
C(5)-C(6)-N(1)	108.8(5)	107.9(7)	108.2(6)	109.2(6)
C(6)-N(1)-N(2)	110.6(5)	109.9(6)	110.3(5)	109.5(5)
O(1)-C(1)-C(2)	110.3(4)	110.0(5)	109.6(4)	109.9(4)
O(1)-C(1)-C(3)	110.1(4)	110.2(5)	110.4(4)	110.2(4)
N(1)-C(1)-C(2)	106.4(4)	107.3(5)	107.2(4)	107.7(4)
N(1)-C(1)-C(3)	108.8(4)	108.1(5)	107.8(4)	108.0(4)
C(2)-C(1)-C(3)	110.9(5)	110.5(6)	112.2(5)	111.4(5)
C(1)-C(2)-F(1)	113.3(5)	113.1(5)	115.1(5)	113.7(5)
C(1)-C(2)-F(2)	110.7(5)	108.2(5)	110.3(5)	111.3(5)
C(1)-C(2)-F(3)	111.2(5)	111.6(5)	109.8(5)	111.0(5)
F(1)-C(2)-F(2)	107.4(5)	107.0(5)	107.8(5)	108.0(4)
F(1)-C(2)-F(3)	106.1(4)	108.2(5)	107.4(5)	106.1(4)
F(2)-C(2)-F(3)	108.0(4)	108.4(5)	106.0(4)	106.4(4)
C(1)-C(3)-F(4)	111.2(5)	110.2(5)	110.4(5)	109.9(5)
C(1)-C(3)-F(5)	109.7(4)	108.0(5)	109.0(5)	110.0(5)
C(1)-C(3)-F(6)	114.4(5)	114.5(5)	113.9(5)	113.7(4)
F(4)-C(3)-F(5)	106.8(4)	107.8(5)	106.4(4)	107.1(4)
F(4)-C(3)-F(6)	108.3(4)	109.4(5)	108.6(5)	107.8(4)
F(5)-C(3)-F(6)	106.1(4)	106.7(4)	108.3(4)	108.1(4)

Figure Captions

Figure 1. An example of the azimuthal scan data: plot of intensity before and after absorption correction for the (103) reflection as a function of the azimuthal angle Ψ . For this reflection $\sigma(I)/\langle I \rangle$ was reduced from 9.1% before to 1.9% after the correction.

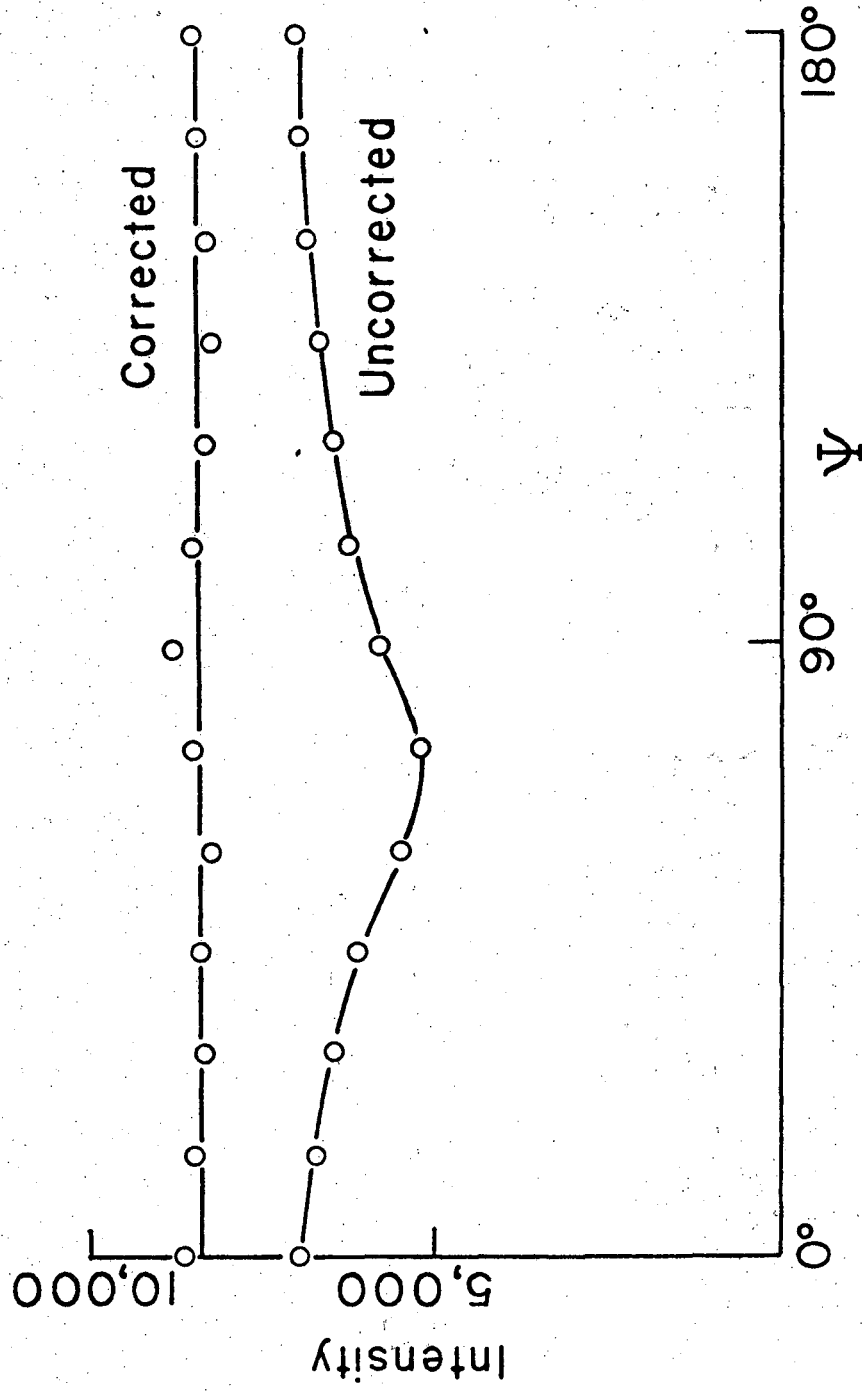
Figure 2. Shapes and dimensions of the crystals used in the measurement of intensities.

Figure 3. Stereoscopic views of the molecular structure of the thorium complex, (a) viewed down the c^* axis and (b) viewed down the b^* axis. The hydrogen atoms are omitted.

Figure 4. Stereoscopic view of the dodecahedral geometry of the eight atoms coordinated to thorium.

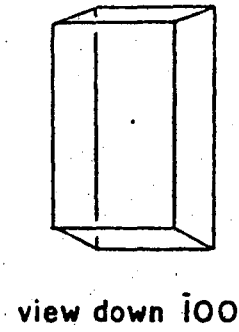
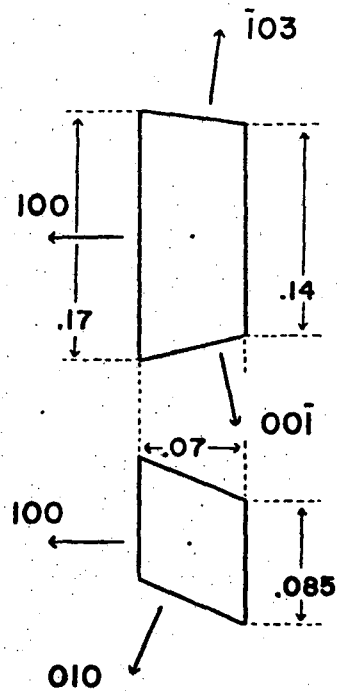
Figure 5. View of Ligand I of the thorium compound. The thermal ellipsoids are scaled to include 30% probability. The size of the hydrogen atoms is arbitrary. In Tables II and III the next larger serial numbers of atoms are assigned in the same sequence to Ligand II, then III, then IV. The distances (in Å) listed by each bond are averages for the four ligands for thorium (upper values) and for uranium (lower values). The standard deviation of the mean in each case is derived from the scatter of the individual values.

Figure 6. Stereoscopic view (for the thorium crystal) showing the unit cell and molecular packing. Hydrogen atoms are omitted.

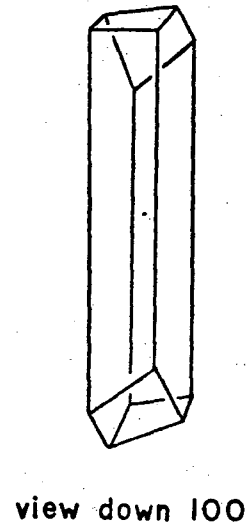
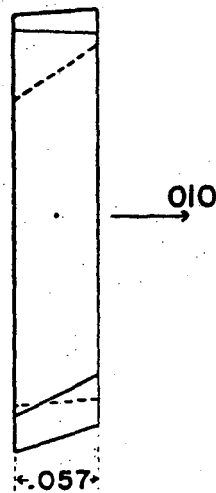
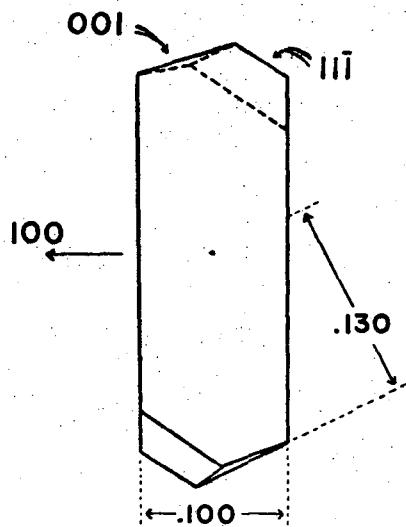


NBL 701 178

Fig. 1

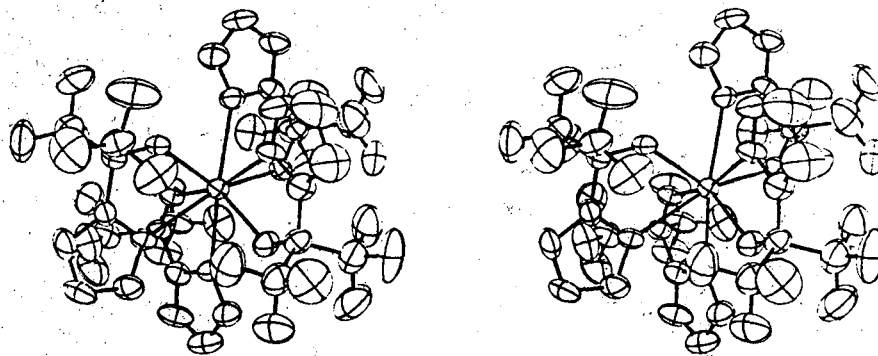


(a)



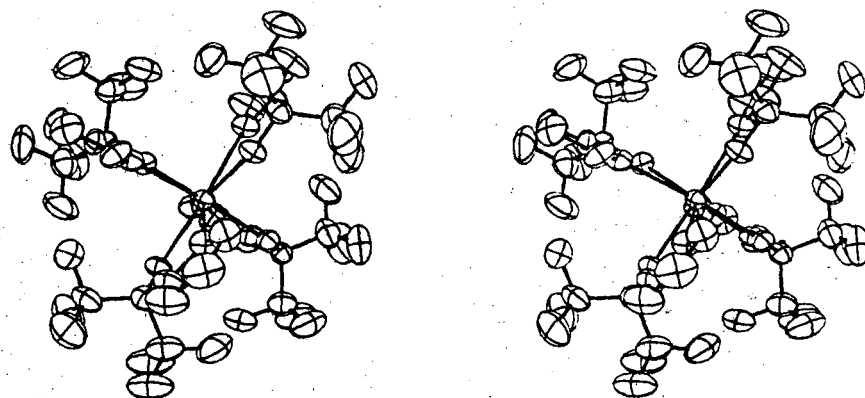
(b)

Fig. 2



XBL 735-1019

Fig. 3(a)



XBL 738-1020

Fig. 3(b)

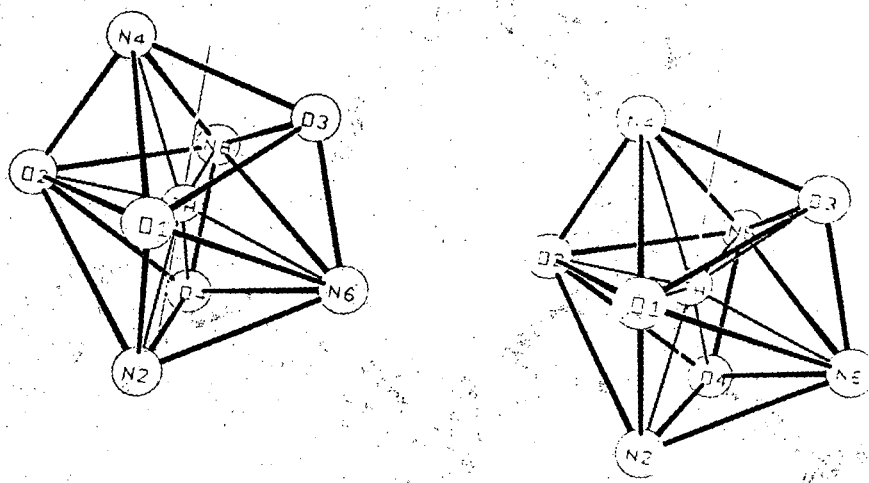


Fig. 4

XBL 738-1021

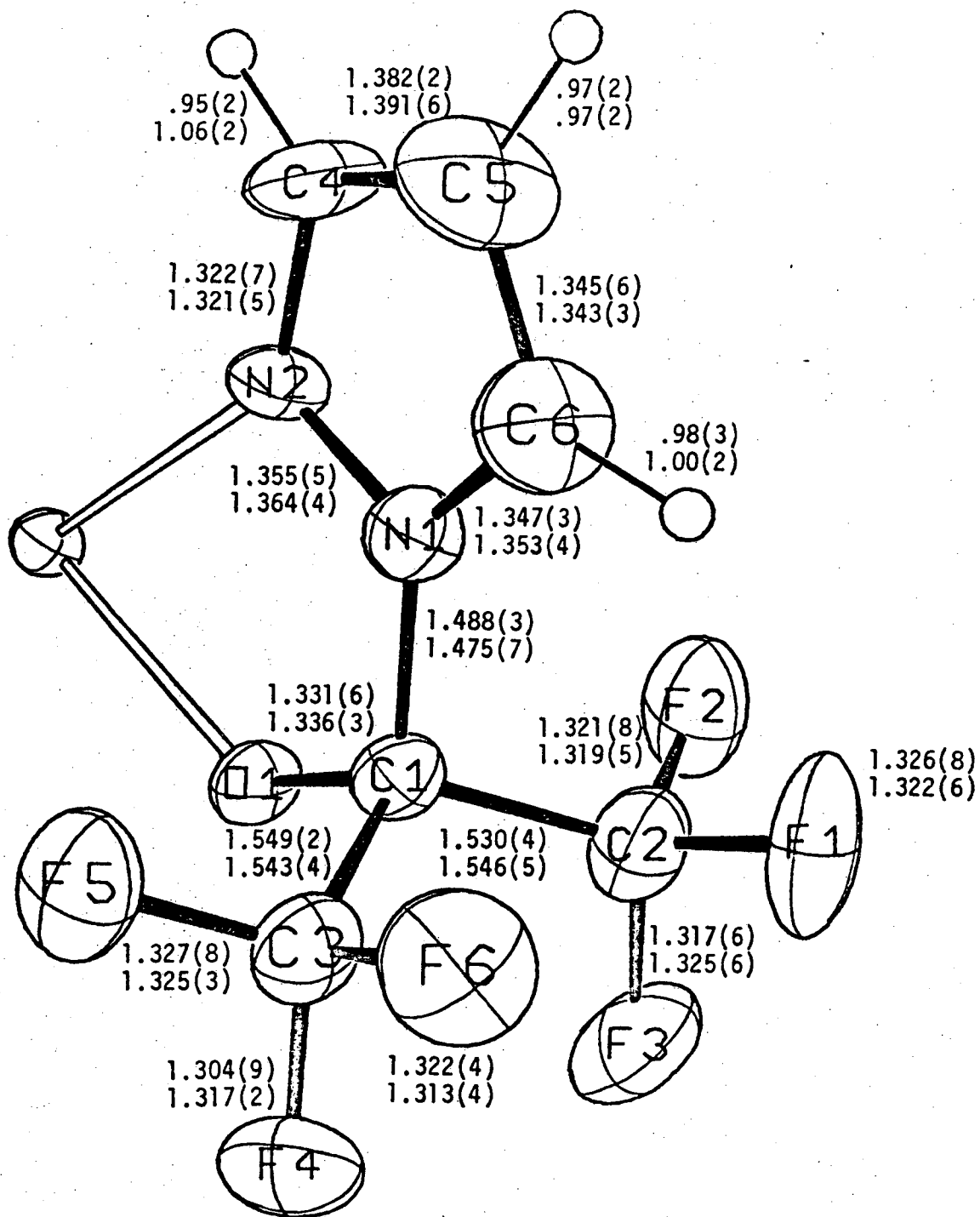
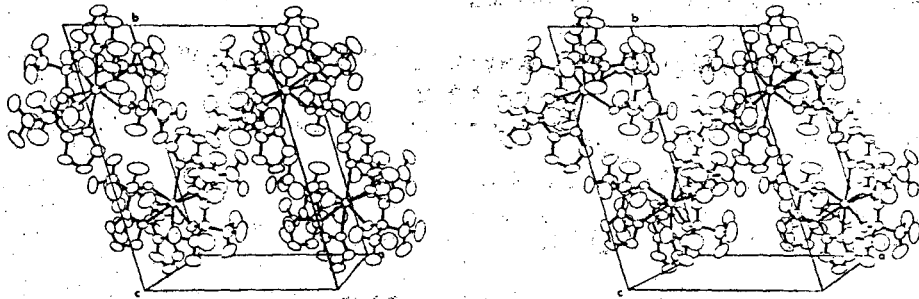


Fig. 5



XBL 733-1018

Fig. 6

Supplementary materials for the paper:

Crystal and Molecular Structures of Thorium and Uranium
Tetrakis(hexafluoroacetylpyrazolide) Complexes

by Karl Volz, Allan Zalkin, and David H. Templeton

The Supplementary Tables which follow contain these data:

Table 1. Thermal parameters for the thorium crystal, isotropic for the hydrogen atoms and anisotropic for the other atoms. The temperature factor is of the form

$$T = \exp(-B\lambda^{-2}\sin^2\theta), \text{ or}$$

$$T = \exp(-0.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \dots)).$$

Table 2. Similar data for the uranium crystal.

Table 3. Deviations of various atoms from least-squares planes fitted to various atoms in the thorium molecule.

Table 4. Similar data for the uranium molecule.

Table 5. Observed structure factors (FOB), their estimated standard deviations (SG), and differences ($DEL = |F_O| - |F_C|$) for the thorium crystal.

Table 6. Similar data for the uranium crystal.

Supplementary
Table 1. Thermal parameters for the thorium crystal

ATOM	B11	B22	B33	B12	B13	B23
TH	2.68(1)	2.71(1)	2.50(1)	.627(8)	.635(8)	.464(8)
O(1)	3.2(2)	2.7(2)	2.9(2)	.0(2)	.3(2)	-.1(2)
O(2)	3.4(2)	3.5(2)	3.2(2)	.9(2)	1.2(2)	.7(2)
O(3)	3.7(2)	2.1(2)	3.5(2)	.6(2)	1.2(2)	.1(2)
O(4)	3.8(2)	3.8(2)	3.3(2)	1.5(2)	.1(2)	.6(2)
N(1)	3.8(3)	3.6(4)	3.3(3)	.3(3)	.5(3)	-.2(3)
N(2)	4.3(3)	2.8(3)	3.8(3)	1.0(3)	1.3(3)	.2(2)
N(3)	4.0(3)	3.5(4)	3.0(3)	.3(3)	1.0(3)	.8(2)
N(4)	4.4(3)	2.9(3)	4.5(3)	1.1(2)	1.8(3)	.6(2)
N(5)	3.0(3)	4.1(4)	4.1(3)	1.0(3)	1.6(2)	.6(3)
N(6)	3.7(3)	2.7(3)	2.9(3)	.8(3)	1.1(2)	1.1(2)
N(7)	4.0(3)	4.2(4)	4.1(3)	1.3(3)	.0(3)	1.4(3)
N(8)	4.0(3)	2.6(3)	3.4(3)	.1(3)	.6(2)	-.0(3)
C(1)	4.2(4)	3.3(4)	3.5(4)	1.2(3)	1.3(3)	1.3(3)
C(2)	7.3(6)	3.8(4)	3.6(5)	.0(4)	1.7(4)	.4(4)
C(3)	3.7(5)	5.2(5)	4.1(5)	.4(4)	-.2(4)	.0(4)
C(4)	5.1(6)	3.8(5)	6.1(5)	1.4(5)	1.5(5)	-.4(4)
C(5)	8.7(7)	3.4(6)	6.3(6)	1.9(6)	2.6(5)	.5(5)
C(6)	7.0(6)	3.5(5)	4.7(5)	-.8(5)	1.0(5)	-.3(4)
C(7)	3.6(4)	3.4(4)	3.5(4)	1.3(3)	1.0(3)	1.0(3)
C(8)	6.0(5)	4.7(5)	4.1(5)	1.4(4)	1.7(4)	1.2(4)
C(9)	4.4(5)	6.6(6)	6.4(5)	2.0(4)	1.9(4)	2.2(5)
C(10)	5.8(5)	4.3(6)	4.4(4)	1.3(5)	1.8(4)	.5(4)
C(11)	8.2(6)	2.5(5)	7.6(5)	1.8(5)	2.8(4)	.9(4)
C(12)	6.4(5)	3.2(5)	6.2(5)	.6(4)	2.9(4)	1.7(4)
C(13)	3.6(4)	3.2(4)	2.8(4)	.7(3)	1.3(3)	.3(3)
C(14)	4.8(5)	4.9(5)	6.1(5)	2.0(4)	1.8(4)	1.3(4)
C(15)	6.3(5)	4.0(4)	4.0(4)	2.0(4)	1.7(4)	.2(4)
C(16)	6.2(5)	3.9(5)	4.2(4)	1.6(4)	2.8(4)	1.4(4)
C(17)	5.4(5)	3.3(5)	5.6(5)	-.1(4)	2.7(4)	1.3(4)
C(18)	4.2(5)	5.7(6)	6.0(5)	.9(4)	3.5(4)	.6(4)
C(19)	4.2(4)	3.8(4)	3.8(4)	1.6(3)	1.0(3)	1.3(3)
C(20)	5.6(5)	7.0(6)	6.1(6)	3.2(5)	2.5(5)	2.1(5)
C(21)	5.2(5)	5.8(5)	5.2(5)	2.7(4)	1.5(4)	2.0(4)
C(22)	7.2(6)	2.8(5)	5.9(6)	1.8(5)	-.8(4)	.1(4)
C(23)	7.5(7)	7.0(7)	5.7(6)	.1(6)	-.2(5)	-.8(5)
C(24)	5.7(6)	7.1(7)	6.1(6)	1.4(5)	-.2(5)	-.2(5)
F(1)	9.6(3)	5.6(2)	3.6(2)	.3(2)	.8(2)	-.6(2)
F(2)	8.3(3)	10.9(4)	5.3(2)	1.9(3)	4.0(2)	.3(2)
F(3)	12.2(3)	5.3(2)	4.1(2)	.9(2)	1.9(2)	1.6(2)
F(4)	5.5(2)	8.6(3)	9.3(3)	3.6(2)	.8(2)	2.7(2)
F(5)	4.8(2)	10.0(3)	5.2(2)	1.5(2)	2.1(2)	.7(2)
F(6)	4.4(2)	8.4(3)	8.3(3)	-1.3(2)	.4(2)	-2.3(2)
F(7)	12.1(4)	7.9(3)	5.2(2)	2.0(3)	4.6(2)	3.1(2)
F(8)	7.1(3)	10.2(3)	3.4(2)	3.4(2)	.4(2)	.7(2)
F(9)	11.6(3)	7.4(3)	5.0(2)	4.0(3)	3.7(2)	.3(2)
F(10)	5.2(2)	8.6(3)	11.2(3)	3.2(2)	3.4(2)	1.6(3)
F(11)	4.6(2)	8.9(3)	6.6(3)	1.2(2)	-.1(2)	1.4(2)
F(12)	5.3(2)	9.0(3)	13.2(4)	-.0(2)	4.5(3)	4.7(3)
F(13)	5.6(3)	10.4(3)	11.0(3)	4.7(2)	4.6(3)	3.7(3)
F(14)	6.9(3)	10.3(3)	5.5(3)	4.6(2)	-.8(2)	.7(2)
F(15)	8.2(3)	4.7(2)	10.9(3)	3.7(2)	2.6(2)	2.3(2)
F(16)	11.6(3)	4.6(2)	5.5(2)	-.6(2)	.7(2)	-1.2(2)
F(17)	8.6(3)	8.1(3)	3.8(2)	4.2(2)	-.2(2)	.2(2)
F(18)	9.0(3)	9.9(3)	4.9(2)	2.0(2)	4.0(2)	-.3(2)
F(19)	5.1(3)	15.2(4)	7.9(3)	5.8(3)	.5(2)	1.8(3)
F(20)	7.0(3)	11.5(4)	8.4(3)	4.3(3)	4.6(2)	4.2(3)
F(21)	10.6(4)	7.4(3)	10.7(3)	5.7(3)	4.7(3)	1.5(3)
F(22)	8.5(3)	5.6(3)	10.1(3)	1.8(2)	3.7(3)	3.6(3)
F(23)	8.2(3)	10.9(3)	7.5(3)	4.8(3)	5.0(2)	3.9(2)

F(24) 7.9(3) 10.8(3) 5.2(2) 3.0(2) .3(2) 4.1(2)

ATOM	B
H(1)	4.2(21)
H(2)	4.6(21)
H(3)	4.7(21)
H(4)	1.4(17)
H(5)	3.1(16)
H(6)	6.5(21)
H(7)	4.0(18)
H(8)	2.9(17)
H(9)	2.8(16)
H(10)	-.3(12)
H(11)	8.7(27)
H(12)	9.9(32)

Supplementary

Table 2. Thermal parameters for the uranium crystal

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ATOM	B11	B22	B33	B12	B13	B23
U(1)	2.282(8)	2.441(9)	2.375(8)	.654(6)	.474(6)	.640(6)
O(1)	2.4(2)	3.2(2)	2.7(2)	.7(1)	-.1(1)	.2(1)
O(2)	2.8(2)	3.7(2)	4.0(2)	.7(1)	1.6(1)	1.8(2)
O(3)	3.6(2)	2.7(2)	3.7(2)	1.0(1)	.9(1)	.4(1)
O(4)	3.3(2)	3.1(2)	3.0(2)	1.4(1)	.5(1)	.9(1)
N(1)	3.3(2)	3.1(2)	3.4(2)	.7(2)	.5(2)	.5(2)
N(2)	3.5(2)	3.2(2)	3.2(2)	1.1(2)	.7(2)	.4(2)
N(3)	3.7(2)	4.0(3)	4.3(3)	.7(2)	1.2(2)	2.1(2)
N(4)	3.6(2)	3.2(3)	4.7(3)	1.3(2)	1.3(2)	.9(2)
N(5)	3.4(2)	3.9(3)	3.5(2)	1.6(2)	1.3(2)	.7(2)
N(6)	3.6(2)	2.3(2)	2.9(2)	1.2(2)	1.4(2)	.8(2)
N(7)	3.0(2)	3.9(3)	3.0(2)	.7(2)	.0(2)	.9(2)
N(8)	3.2(2)	3.0(3)	4.4(3)	.9(2)	.6(2)	1.2(2)
C(1)	3.2(3)	4.0(3)	2.0(3)	1.1(2)	.1(2)	-.2(2)
C(2)	5.5(4)	4.8(4)	3.8(4)	1.3(3)	.2(3)	.2(3)
C(3)	3.3(3)	5.0(4)	4.5(4)	.9(3)	.0(3)	.2(3)
C(4)	4.8(3)	3.5(3)	3.7(3)	1.7(3)	.8(3)	.3(3)
C(5)	6.6(4)	3.5(4)	5.3(4)	1.9(4)	.7(3)	-.7(3)
C(6)	5.0(4)	3.4(4)	5.1(4)	-.2(3)	.3(3)	-.8(3)
C(7)	3.4(3)	4.8(4)	4.1(3)	1.1(3)	1.5(2)	1.9(3)
C(8)	6.5(4)	8.4(6)	3.9(4)	2.9(4)	2.5(3)	2.3(4)
C(9)	3.9(4)	6.1(5)	6.7(5)	.5(3)	2.0(3)	2.9(4)
C(10)	4.8(4)	3.7(4)	5.7(4)	1.7(3)	1.4(3)	1.2(3)
C(11)	7.0(5)	2.5(4)	8.8(5)	1.3(4)	2.2(4)	1.4(4)
C(12)	5.0(4)	4.2(4)	7.1(5)	.3(3)	1.8(3)	3.2(4)
C(13)	4.0(3)	3.0(3)	3.5(3)	2.0(2)	.6(2)	.4(2)
C(14)	5.7(4)	4.6(4)	4.8(4)	3.6(3)	.7(3)	-.2(3)
C(15)	6.4(4)	5.6(4)	4.3(4)	3.6(4)	.3(3)	-.8(3)
C(16)	5.0(4)	3.9(4)	4.6(4)	2.0(3)	2.3(3)	1.6(3)
C(17)	5.5(4)	6.3(5)	7.0(5)	1.9(4)	3.5(4)	3.0(4)
C(18)	5.8(4)	6.5(5)	6.3(4)	3.3(4)	4.0(3)	2.2(4)
C(19)	3.4(3)	2.5(3)	4.2(3)	1.0(2)	.7(2)	.4(2)
C(20)	4.9(4)	6.3(4)	5.3(4)	3.6(3)	1.9(3)	2.4(3)
C(21)	4.1(3)	4.9(4)	4.3(3)	2.0(3)	1.0(3)	1.9(3)
C(22)	5.3(4)	3.3(4)	5.6(4)	.5(3)	.4(3)	.3(3)
C(23)	6.0(4)	5.3(5)	5.4(5)	.5(4)	-1.7(3)	-.5(4)
C(24)	5.3(4)	5.1(4)	4.4(4)	.8(3)	-1.3(3)	.5(3)
F(1)	8.2(2)	6.8(2)	3.1(2)	1.6(2)	.1(2)	-.6(2)
F(2)	7.0(2)	10.1(3)	4.8(2)	2.9(2)	2.9(2)	.9(2)
F(3)	10.1(3)	6.1(2)	4.0(2)	2.6(2)	1.8(2)	2.0(2)
F(4)	4.8(2)	7.5(2)	8.0(2)	3.4(2)	.4(2)	1.8(2)
F(5)	4.0(2)	8.3(3)	5.8(2)	1.5(2)	1.7(2)	.4(2)
F(6)	3.4(2)	7.3(2)	8.2(2)	-.1(2)	-.3(2)	-2.2(2)
F(7)	10.7(3)	9.7(3)	6.5(2)	2.7(2)	5.6(2)	4.7(2)
F(8)	6.9(2)	11.9(3)	4.3(2)	3.4(2)	.9(2)	1.9(2)
F(9)	12.3(3)	8.6(3)	5.6(2)	3.9(2)	4.8(2)	1.2(2)
F(10)	5.1(2)	9.4(3)	11.4(3)	3.1(2)	3.6(2)	2.5(3)
F(11)	3.5(2)	9.1(3)	7.3(2)	1.2(2)	.6(2)	2.2(2)
F(12)	4.5(2)	10.0(3)	12.4(3)	.8(2)	4.0(2)	6.1(2)
F(13)	8.8(3)	14.4(4)	8.5(3)	9.2(3)	4.3(2)	3.0(2)
F(14)	5.6(2)	8.0(3)	5.0(2)	3.8(2)	-.5(2)	.1(2)
F(15)	9.0(2)	5.5(2)	7.2(2)	5.1(2)	-.6(2)	-.5(2)
F(16)	8.1(2)	5.5(2)	7.2(2)	2.6(2)	-.6(2)	-3.0(2)
F(17)	8.3(2)	7.8(2)	3.8(2)	5.3(2)	-.4(2)	-.1(2)
F(18)	10.9(3)	14.3(4)	4.0(2)	8.0(3)	2.4(2)	-.9(2)
F(19)	5.3(2)	15.3(4)	7.1(2)	6.8(2)	.5(2)	1.9(2)
F(20)	6.9(2)	9.9(3)	8.8(3)	4.6(2)	4.9(2)	4.5(2)
F(21)	9.8(3)	7.0(3)	10.4(3)	5.6(2)	5.1(2)	2.1(2)
F(22)	6.6(2)	4.5(2)	7.8(2)	1.4(2)	2.7(2)	2.7(2)
F(23)	8.0(2)	8.1(2)	6.6(2)	4.5(2)	4.3(2)	3.2(2)

F(24) 6.6(2) 10.0(3) 4.8(2) 2.6(2) .6(2) 4.1(2)

ATOM	B
H(1)	2.0(10)
H(2)	9.9(24)
H(3)	3.7(14)
H(4)	2.0(11)
H(5)	6.5(18)
H(6)	7.8(20)
H(7)	1.8(12)
H(8)	3.7(15)
H(9)	3.6(13)
H(10)	5.8(17)
H(11)	8.3(21)
H(12)	6.0(16)

Supplementary

Table 3. Table of Least-Squares Planes and Interplanar Angles
for $\text{Th}(\text{C}_6\text{H}_5\text{CN}_2\text{F}_6)_4$

Atom	Dev A	Atom	Dev A
Planes through the Pyrazole Rings			
Ligand I: N(1), N(2), C(4), C(5), C(6)			
Equation: $-8.241x + 1.119y + 9.504z - 1.775 = 0$			
N(1)	.0097	C(6)	-.0079
N(2)	-.0078	O(1)*	-.0163
C(4)	.0030	C(1)*	-.1074
C(5)	.0029	Th*	.3140
Ligand II: N(3), N(4), C(10), C(11), C(12)			
Equation: $5.630x - 1.916y + 7.065z - 0.835 = 0$			
N(3)	.0014	C(12)	-.0052
N(4)	.0032	O(2)*	.0303
C(10)	-.0064	C(7)*	-.0283
C(11)	.0071	Th*	.1267
Ligand III: N(5), N(6), C(16), C(17), C(18)			
Equation: $5.107x - 2.875y + 7.559z - 0.915 = 0$			
N(5)	.0002	C(18)	-.0031
N(6)	.0029	O(3)*	.0514
C(16)	-.0048	C(13)*	.1246
C(17)	.0048	Th*	-.0987
Ligand IV: N(7), N(8), C(22), C(23), C(24)			
Equation: $9.332x - 0.660y - 8.425z + 1.650 = 0$			
N(7)	-.0017	C(24)	.0057
N(8)	-.0035	O(4)*	-.0917
C(22)	.0072	C(19)*	-.0480
C(23)	-.0078	Th*	-.1034
Planes through the two Trapezoids			
Trapezoid I: O(1), N(2), O(4), N(8)			
Equation: $9.165x - 0.628y - 8.613z + 1.779 = 0$			
O(1)	-.0195	O(4)	-.0381
N(2)	.0344	N(8)	.0232
		Th*	-.0045
Trapezoid II: O(2), N(4), O(3), N(6)			
Equation: $5.998x - 2.614y + 6.785z - 0.648 = 0$			
O(2)	.0567	O(3)	.1115
N(4)	-.1001	N(6)	-.0681
		Th*	.0900

* atoms not contributing to the planes

(continued)

Table 3 (continued).

Atom	Dev A	Atom	Dev A
Planes through the Chelate Rings			
Ligand I: O(1), C(1), N(1), N(2)			
Equation: $-8.519x + 1.301y + 9.309z - 1.820 = 0$			
O(1)	.0240	N(1)	.0419
C(1)	-.0412	N(2)	-.0247
		Th*	.2729
Ligand II: O(2), C(7), N(3), N(4)			
Equation: $5.794x - 1.708y + 6.899z - 0.925 = 0$			
O(2)	.0097	N(3)	.0170
C(7)	-.0168	N(4)	-.0099
		Th*	.0576
Ligand III: O(3), C(13), N(5), N(6)			
Equation: $5.328x - 3.567y + 7.399z - 0.694 = 0$			
O(3)	-.0204	N(5)	-.0358
C(13)	.0351	N(6)	.0212
		Th*	-.0789
Ligand IV: O(4), C(19), N(7), N(8)			
Equation: $9.205x - 1.011y - 8.633z + 1.880 = 0$			
O(4)	-.0011	N(7)	-.0019
C(19)	.0019	N(8)	.0011
		Th*	-.0021

Dihedral Angles between the Plane of the Pyrazole Ring
and the Plane of the Chelate Ring

Ligand I	2.1°	Ligand III	2.6°
Ligand II	1.4°	Ligand IV	2.2°

Dihedral Angle between the two Trapezoids = 88.3°

* atoms not contributing to the planes

Supplementary

Table 4. Table of Least-Squares Planes and Interplaner Angles
for $U(C_6H_3ON_2F_6)_4$

Atom	Dev A	Atom	Dev A
Planes through the Pyrazole Rings			
Ligand I: N(1), N(2), C(4), C(5), C(6)			
Equation: $-8.308x + 1.667y + 9.795z - 1.752 = 0$			
N(1)	.0066	C(6)	-.0058
N(2)	-.0048	O(1)*	.1214
C(4)	.0014	C(1)*	.0169
C(5)	.0026	U*	.2843
Ligand II: N(3), N(4), C(10), C(11), C(12)			
Equation: $5.427x - 1.546y + 6.965z - 1.002 = 0$			
N(3)	.0021	C(12)	-.0039
N(4)	.0005	O(2)*	-.0521
C(10)	-.0028	C(7)*	-.0422
C(11)	.0041	U*	.0444
Ligand III: N(5), N(6), C(16), C(17), C(18)			
Equation: $5.443x - 2.992y + 7.074z - 0.723 = 0$			
N(5)	.0007	C(18)	-.0070
N(6)	.0061	O(3)*	.0398
C(16)	-.0105	C(13)*	.1231
C(17)	.0106	U*	-.0145
Ligand IV: N(7), N(8), C(22), C(23), C(24)			
Equation: $9.568x - 1.448y - 8.536z + 1.565 = 0$			
N(7)	-.0063	C(24)	.0005
N(8)	.0101	O(4)*	-.0178
C(22)	-.0101	C(19)*	-.0596
C(23)	.0058	U*	-.1528

Planes through the two Trapezoids

Trapezoid I: O(1), N(2), O(4), N(8)			
Equation: $9.206x - 1.283y - 8.942z + 1.769 = 0$			
O(1)	-.0197	O(4)	-.0387
N(2)	.0351	N(8)	.0234
		U*	.0086
Trapezoid II: O(2), N(4), O(3), N(6)			
Equation: $5.873x - 2.615y + 6.661z - 0.663 = 0$			
O(2)	.0448	O(3)	.0922
N(4)	-.0820	N(6)	-.0550
		U*	.0725

* atoms not contributing to the planes

(continued)

Table 4. (continued)

Atom	Dev A	Atom	Dev A
Planes through the Chelate Rings			
Ligand I: O(1), C(1), N(1), N(2)			
Equation: $-8.638x + 1.875y + 9.565z - 1.809 = 0$			
O(1)	.0264	N(1)	.0450
C(1)	-.0449	N(2)	-.0265
		U*	.2294
Ligand II: O(2), C(7), N(3), N(4)			
Equation: $5.530x - 1.930y + 6.914z - 0.855 = 0$			
O(2)	.0030	N(3)	.0052
C(7)	-.0052	N(4)	-.0030
		U*	.0891
Ligand III: O(3), C(13), N(5), N(6)			
Equation: $5.687x - 3.657y + 6.883z - 0.500 = 0$			
O(3)	-.0217	N(5)	-.0386
C(13)	.0377	N(6)	.0226
		U*	.0147
Ligand IV: O(4), C(19), N(7), N(8)			
Equation: $9.509x - 1.967y - 8.713z + 1.807 = 0$			
O(4)	-.0019	N(7)	-.0033
C(19)	.0033	N(8)	.0099
		U*	-.0730

Dihedral Angles between the Plane of the Pyrazole
and the Plane of the Chelate Ring

Ligand I	2.6°	Ligand III	2.5°
Ligand II	1.4°	Ligand IV	2.4°

Dihedral Angle between the two Trapezoids = 88.1°

* atoms not contributing to the planes

Supplementary

37.

Table 5.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 4.0) FOR THORIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE) F(C,C,C) = 4339

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	0	-7	251	4	7	6	312	5	-3	3	385	5	2	-6	87	41	4
1	174	27	1	-6	338	3	1	7	183	9	6	4	65	17	0	-5	330	12	3
2	144	8	3	-5	70	8	2	8	218	16	-2	5	277	5	2	-4	110	8	-9
3	473	2	1	-4	437	4	2		H,K= 0,	0	6	6	170	15	4	-3	175	14	10
4	83	4	-1	-3	102	6	-1	-9	78	17	39	7	176	7	-0	-2	230	8	-13
5	314	2	0	-2	234	4	9	-8	116	9	2		H,K= 0,	9	9	-1	70	25	-27
6	215	6	-5	-1	423	2	1	-7	276	8	2	-8	0	84	-30*	0	410	11	-8
7	226	4	-1	0	9	38	-14*	-6	162	10	9	-7	197	6	3	1	0	48	-38*
8	355	8	-3	1	483	3	3	-5	363	3	1	-6	246	5	9	2	225	24	-26
9	52	17	34	2	408	3	5	-4	290	2	2	-5	20	36	11*	3	237	5	-1
	H,K= 0,	1	1	3	361	2	3	-3	400	2	5	-4	435	5	6	4	43	61	-4*
-9	278	3	7	4	590	4	0	-2	211	7	-2	-3	174	7	-10	15	126	8	0
-8	167	11	6	5	0	50	-8*	-1	210	6	-1	-2	190	7	-1		H,K= 0,	13	0
-7	215	13	-13	6	291	11	1	0	312	4	3	-1	369	4	-3	-5	74	32	24
-6	497	2	2	7	341	3	2	1	405	2	1	0	9	48	-23*	-4	260	9	3
-5	100	17	-3	8	87	16	12	2	430	2	1	1	244	47	-32	-3	62	20	-11
-4	102	3	2	9	235	4	-0	3	394	2	-0	2	289	5	8	-2	78	17	0
-3	44	45	-5*		H,K= C,	C,	4	4	41	48	-7*	3	271	5	-2	-1	309	12	-7
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-1	635	10	-10	-8	256	6	6	6	181	9	6	5	12	38	4*	1	251	20	-15
0	124	12	77*	-7	298	3	1	7	135	7	9	6	187	6	-1	2	153	55	-38
1	789	7	-10	-6	219	7	-2	8	164	7	15	7	158	13	8	3	67	69	-77*
2	61	18	16	-5	407	2	2		H,K= 0,	0	7		H,K= 0,	10	10		H,K= 0,	14	0
3	543	1	2	-4	175	5	5	-9	199	12	10	-8	240	6	3	-4	12	82	-22*
4	150	5	-1	-3	420	1	-0	-8	88	12	2	-7	240	11	-0	-3	228	8	-8
5	45	54	-3*	-2	312	5	C	-7	219	7	13	-6	99	24	25	-2	223	4	-2
6	439	2	-0	-1	425	3	3	-6	372	2	-2	-5	310	9	1	-1	49	61	-4*
7	294	3	3	0	70	27	C	-5	100	8	7	-4	109	12	3	0	137	15	-10
8	178	12	0	1	360	4	-5	-4	420	2	2	-3	252	7	3	1	0	55	-37*
9	293	3	2	2	432	1	0	-3	27	53	-12*	-2	336	2	3	2	189	11	1
	H,K= 0,	2	2	3	435	4	0	-2	270	3	3	-1	83	14	-5		H,K= 1,	-15	0
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-8	346	7	-0	5	369	3	2	0	19	33	-13*	1	34	54	-65*	0	54	35	-21
-7	297	8	C	6	70	22	1	1	239	7	-8	2	165	12	-15	1	162	13	-9
-6	192	4	-1	7	182	8	9	2	573	2	4	3	256	8	5	2	0	62	-47*
-5	626	1	1	8	83	17	-23	3	270	2	3	4	100	11	-16		H,K= 1,	-14	0
-4	230	6	2	9	70	37	36	4	446	5	4	5	199	9	-6	-3	165	25	-10
-3	544	2	2		H,K= C,	C,	5	5	69	10	37	6	159	13	4	-2	212	6	-6
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-1	167	7	8	-8	209	9	9	7	107	8	8	-7	137	12	11	0	351	4	2
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1	277	3	-4	-6	410	3	1		H,K= 0,	0	8	-5	29	62	-33*	2	185	6	8
2	747	2	0	-5	24	32	-20*	-8	210	5	15	-4	200	6	7	3	127	11	-16
3	250	2	-1	-4	402	4	4	-7	378	3	4	-3	236	3	-1	4	97	12	4
4	46	8	18	-3	197	5	-0	-6	12	56	-12*	-2	130	9	3		H,K= 1,	-13	0
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6	88	8	10	-1	446	4	1	-4	255	5	-2	0	47	19	-35	-3	55	82	-17*
7	232	6	-2	0	29	46	5*	-3	388	3	2	1	313	7	-2	-2	165	7	-1
8	216	7	-4	1	419	2	2	-2	261	2	0	2	0180	-71*	-1	239	7	2	
9	36	42	-6*	2	386	1	-0	-1	194	4	3	3	109	27	-15	0	0	46	-7*
	H,K= 0,	3	3	3	55	12	1	0	162	6	6	4	228	5	12	1	300	4	10
-9	187	9	7	4	521	2	2	1	312	10	-8	5	125	12	6	2	103	24	15
-8	197	3	7	5	26	50	19*	2	403	2	-1		H,K= 0,	12	12	3	90	54	-17

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	216	18	6	3	188	7	9	5	369	3	-2	2	183	8	-3	-3	589	3	-1
5	72	33	-2	4	231	4	-4	6	207	4	1	3	34	28	-10	-2	100	5	1
	H,K=	1,-12		5	0	41	-38*	7	258	4	0	4	375	2	-4	-1	341	57	-80*
-5	193	20	2	6	347	5	-8	8	165	7	-7	5	187	5	-4	0	804	7	-3
-4	0	47	-14*	7	232	5	1	9	64	20	37	6	397	3	-3	1	0	43	-24*
-3	210	12	-2	8	149	23	7		H,K=	1,-5		7	190	7	-3	2	719	1	0
-2	206	8	-0		H,K=	1,-8		-9	188	11	1	8	238	5	-11	3	694	2	1
-1	283	4	7	-8	174	7	7	-8	50	26	17	9	170	7	6	4	147	5	5
0	398	4	1	-7	102	15	2	-7	250	5	8		H,K=	1,-2		5	146	4	1
1	190	6	-3	-6	227	5	3	-6	264	4	2	-9	47	63	29*	6	196	8	7
2	204	5	-4	-5	335	3	2	-5	23	75	-33*	-8	344	4	-2	7	141	6	18
3	247	4	10	-4	22	38	15*	-4	498	3	-1	-7	221	7	7	8	251	5	2
4	151	12	17	-3	378	5	-5	-3	61	13	19	-6	63	20	-12	9	86	61	-22
5	225	7	9	-2	254	7	-1	-2	416	2	1	-5	617	2	1		H,K=	1,1	1
6	16	46	5*	-1	224	3	3	-1	451	2	1	-4	109	7	3	-10	0	91	-8*
	H,K=	1,-11		0	788	2	3	0	21	56	-5*	-3	469	4	-3	-9	245	5	-0
-6	145	26	-13	1	57	17	5	1	668	3	5	-2	280	8	-4	-8	45	29	-29
-5	72	16	15	2	366	2	1	2	416	3	0	-1	860	3	-3	-7	173	5	-6
-4	188	9	2	3	249	3	1	3	325	2	2	0	868	6	-6	-6	273	3	0
-3	143	19	8	4	101	18	4	4	501	2	2	1	521	2	4	-5	145	4	-1
-2	165	5	-9	5	157	6	-0	5	0	62	-9*	2	658	2	4	-4	91	22	-1
-1	307	5	-1	6	146	6	-2	6	424	3	-3	3	433	4	-3	-3	285	2	2
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2	143	7	-14		H,K=	1,-7		9	315	6	-6	6	126	6	-5	0	202	29	-15
3	242	4	8	-8	137	9	17		H,K=	1,-4		7	180	5	-3	1	473	4	3
4	239	6	-0	-7	243	5	8	-9	35	58	27*	8	196	21	-13	2	451	4	-4
5	20	44	-22*	-6	267	4	4	-8	202	24	-4	9	62	73	31*	3	859	2	1
6	253	5	-2	-5	29	76	-36*	-7	269	4	2		H,K=	1,-1		4	404	2	-1
7	189	19	-4	-4	394	3	-0	-6	84	10	-6	-10	40	61	-9*	5	262	3	2
	H,K=	1,-10		-3	0	46	-35*	-5	407	2	2	-9	306	4	-0	6	353	3	0
-7	181	11	4	-2	401	2	1	-4	152	6	1	-8	178	10	17	7	229	4	4
-6	213	6	-12	-1	281	2	-1	-3	327	3	-0	-7	224	4	-4	8	100	123	-13*
-5	230	13	0	0	0	48	-9*	-2	304	5	-2	-6	362	6	4	9	283	7	3
-4	76	30	26	1	519	2	-1	-1	582	2	1	-5	0	32	-12*		H,K=	1,2	2
-3	276	3	5	2	434	2	-0	0	712	2	0	-4	225	5	-5	-10	216	10	7
-2	285	4	0	3	141	6	5	1	270	6	-5	-3	37	32	3	-9	44	55	-2*
-1	74	15	-14	4	333	3	-2	2	323	3	-3	-2	177	3	3	-8	290	5	6
0	457	3	3	5	31	51	-30*	3	460	2	1	-1	487	16	-8	-7	234	2	-0
1	51	26	33	6	409	4	-2	4	193	3	3	0	97	110	-17*	-6	309	3	0
2	346	6	-5	7	111	11	-8	5	535	2	2	1	362	6	7	-5	655	1	1
3	279	5	1	8	181	5	16	6	90	8	6	2	722	3	2	-4	56	62	25*
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5	299	4	2	-9	37	61	-17*	8	182	16	-3	4	275	2	3	-2	797	2	0
6	69	49	10	-8	190	6	13	9	40	77	25*	5	7	63	-3*	-1	558	2	-2
7	145	38	-13	-7	211	8	5		H,K=	1,-3		6	258	3	-0	0	287	6	7
	H,K=	1,-9		-6	0	66	-42*	-9	192	16	-7	7	95	10	-6	1	155	7	-1
-7	190	8	-4	-5	366	3	-1	-8	53	25	-15	8	220	15	13	2	274	5	1
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0	52	28	-36	2	294	4	1	-1	234	6	4	-6	299	3	-2	9	117	11	9
1	357	3	3	3	407	2	-1	0	176	6	-2	-5	803	2	3		H,K=	1,3	3
2	138	8	6	4	169	10	-1	1	401	2	1	-4	151	5	-2	-10	102	11	12

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	212	7	12	-9	84	17	43	-5	39	55	4*	-2	144	48	3	-5	0	46	-12*
-8	143	15	8	-8	316	3	2	-4	404	3	2	-1	307	4	1	-4	220	4	8
-7	209	5	2	-7	347	8	-16	-3	299	8	6	0	0	48	-32*	-3	133	7	1
-6	396	4	-4	-6	97	11	-8	-2	0278-214*	1	274	4	12	-2	210	6	1		
-5	143	5	8	-5	315	4	1	-1	261	3	-1	2	150	12	-17	-1	176	8	-6
-4	498	2	-1	-4	245	3	1	0	32	40	-0*	3	180	25	9	0	121	21	13
-3	401	6	8	-3	588	2	2	1	206	8	1	H,K=	1, 14	1	263	3	8		
-2	419	3	-0	-2	388	2	-2	2	155	8	-1	-3	162	9	-5	2	129	21	-1
-1	684	2	1	-1	247	6	6	3	114	9	-3	-2	228	6	5	3	153	6	-2
0	117	8	5	0	366	3	-1	4	296	6	-1	-1	0121	-38*	4	276	4	8	
1	708	6	-5	1	227	9	6	5	0	79	-24*	0	126	19	-5	5	80	20	54
2	534	4	0	2	154	4	-9	6	220	15	-2	1	92	16	-7	6	270	5	-3
3	342	2	-0	3	243	3	3	H,K=	1, 10	H,K=	2, -15	7	123	15	-17				
4	475	2	1	4	44	28	5	-8	225	6	11	-2	83	15	10	H,K=	2, -10		
5	210	5	2	5	358	5	-2	-7	136	9	-4	-1	190	7	3	-7	126	12	3
6	337	3	0	6	134	8	7	-6	143	21	-6	0	0	58	-29*	-6	142	21	0
7	227	11	-1	7	224	6	3	-5	256	4	-5	1	178	12	13	-5	249	17	-0
8	202	10	5	8	183	10	2	-4	75	12	19	2	164	17	-19	-4	72	29	0
H,K=	1, 4			H,K=	1, 7			-3	213	5	-4	3	186	7	14	-3	278	8	-1
-9	20	44	-11*	-9	221	7	9	-2	161	88	-46	H,K=	2, -14	-2	252	6	-6		
-8	319	4	-2	-8	56	25	-5	-1	60	16	-3	-4	0	51	-41*	-1	173	7	-4
-7	242	4	5	-7	146	15	-16	0	320	6	1	-3	179	6	14	0	302	3	-1
-6	133	13	8	-6	241	10	-4	1	80	51	-9	-2	119	10	-1	1	56	19	6
-5	511	2	0	-5	55	14	33	2	263	4	2	-1	217	10	-10	2	261	5	2
-4	213	5	4	-4	328	6	-4	3	277	6	16	0	345	4	2	3	187	9	5
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-2	536	2	1	-2	425	3	2	5	226	9	14	2	247	9	6	5	317	3	0
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0	607	2	-1	0	136	5	-1	-7	143	13	5	4	124	18	-1	7	188	7	-5
1	31	36	-13*	1	355	2	0	-6	283	14	9	H,K=	2, -13	H,K=	2, -9				
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3	362	3	-2	3	366	3	2	-4	160	7	-1	-4	164	7	19	-7	217	13	5
4	44	53	15*	4	466	3	4	-3	262	4	-4	-3	0	47	-30*	-6	179	15	5
5	343	3	0	5	0	46	-54*	-2	43	48	-67*	-2	223	5	-2	-5	45	54	-9*
6	177	4	4	6	250	5	11	-1	258	4	-2	-1	258	6	11	-4	308	9	-1
7	186	6	5	7	154	8	4	0	97	11	13	0	24	45	-7*	-3	96	17	-2
8	215	10	-2	H,K=	1, 8			1	339	9	-0	1	317	4	2	-2	138	7	1
H,K=	1, 5			-8	254	8	3	2	205	11	6	2	103	15	-19	-1	434	8	-6
-9	190	6	12	-7	250	6	3	3	162	29	-0	3	196	10	2	0	127	5	-0
-8	108	11	6	-6	94	9	-2	4	237	15	-15	4	212	8	-5	1	514	9	-1
-7	282	3	2	-5	357	5	7	5	87	12	38	5	60	22	1	2	285	10	-4
-6	364	3	-0	-4	89	47	3	H,K=	1, 12	H,K=	2, -12	3	153	9	-7				
-5	56	13	-10	-3	431	2	-1	-6	154	12	14	-6	179	7	-2	4	234	7	-10
-4	527	2	-0	-2	336	23	-11	-5	275	6	4	-5	280	8	12	5	60	34	31
-3	80	7	-2	-1	262	5	4	-4	0	61	-27*	-4	20	65	11*	6	280	7	-6
-2	431	4	4	0	68	12	1	-3	236	11	20	-3	219	8	-1	7	124	7	12
-1	644	2	1	1	255	3	3	-2	309	4	1	-2	176	6	-9	8	242	16	-1
0	112	4	-2	2	374	4	-0	-1	0	51	-34*	-1	198	9	5	H,K=	2, -8		
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2	457	5	8	4	0	58	-12*	1	0	55	-60*	1	24	43	-19*	-7	156	11	8
3	373	2	3	5	371	5	6	2	220	8	4	2	273	4	-1	-6	105	23	-3
4	463	5	0	6	72	43	31	3	225	13	-1	3	196	9	1	-5	445	14	-4
5	7	45	-31*	7	155	13	-6	4	0	54	-7*	4	111	14	7	-4	65	23	-25
6	259	11	4	H,K=	1, 9			H,K=	1, 13	5	236	5	0	-3	265	9	-7		
7	112	10	16	-8	68	18	9	-5	10	48	-6*	6	0	49	-40*	-2	323	5	-5
8	197	6	7	-7	172	7	-10	-4	253	5	2	H,K=	2, -11	-1	176	6	5		
H,K=	1, 6			-6	232	6	-3	-3	120	10	-9	-6	211	6	3	0	498	7	0

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	136	6	1	2	328	3	4	-2	666	13	-2	-7	215	12	-14	-10	211	8	-4
2	210	6	-6	3	441	6	6	-1	497	6	4	-6	478	12	-4	-9	60	72	53*
3	162	10	5	4	420	7	1	0	305	4	0	-5	147	12	-5	-8	367	6	-2
4	54	64	14*	5	43	52	40*	1	413	9	6	-4	333	6	-1	-7	235	12	-13
5	240	5	5	6	363	5	-10	2	473	7	10	-3	745	21	3	-6	77	25	-4
6	146	16	3	7	112	8	8	3	409	10	4	-2	624	9	-4	-5	632	14	5
7	204	5	-1	8	32	47	-7*	4	37	40	-4*	-1	246	5	14	-4	62	24	8
8	189	16	-5	H,K= 2,			-4	5	255	2	1	0	123	10	3	-3	430	9	-3
	H,K= 2,		-7	-9	18	42	12*	6	148	4	1	1	397	4	-2	-2	454	12	6
-8	44	53	5*	-8	289	5	7	7	288	8	-2	2	443	9	-0	-1	17	42	-11*
-7	192	13	-6	-7	222	7	1	8	185	15	-6	3	594	9	9	0	468	6	-4
-6	208	5	-9	-6	278	12	-5	9	91	13	15	4	307	10	-7	1	206	11	-6
-5	12	56	-4*	-5	393	9	-7	H,K= 2,			-1	5	28	58	3*	2	297	5	-1
-4	260	11	-2	-4	11	29	4*-10	42	72	16*	6	438	14	1	3	244	7	-1	
-3	46	12	-16	-3	468	12	-2	-9	231	4	-5	7	163	17	-3	4	60	46	-19
-2	531	10	-0	-2	358	7	3	-8	28	62	-28*	8	197	12	-3	5	252	6	-10
-1	537	16	-11	-1	245	4	1	-7	182	4	5	H,K= 2,			2	6	115	8	-0
0	22	29	-16*	0	701	11	-8	-6	353	8	-7	-10	226	22	-6	7	193	22	-2
1	738	11	4	1	75	20	4	-5	63	10	14	-9	52	62	27*	8	188	12	4
2	105	14	1	2	767	10	10	-4	153	7	-3	-8	308	17	-3	H,K= 2,			5
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4	451	12	7	4	205	3	-2	-2	683	2	3	-6	81	14	21	-8	47	53	25*
5	106	15	-9	5	424	14	-4	-1	269	8	-8	-5	300	8	2	-7	209	8	6
6	302	4	-6	6	183	4	-0	0	89	15	-3	-4	150	3	4	-6	273	5	-4
7	105	11	-15	7	196	5	-0	1	895	5	9	-3	259	5	5	-5	48	23	28
8	148	20	-7	8	228	5	-10	2	468	5	7	-2	193	7	-5	-4	603	8	-2
	H,K= 2,		-6	9	87	32	-5	3	656	8	1	-1	66	17	24	-3	81	15	-6
-9	43	56	30*	H,K= 2,			-3	4	563	4	-0	0	700	7	-3	-2	536	11	-7
-8	290	7	-10	-10	98	47	21	5	45	50	-25*	1	84	14	0	-1	453	5	-5
-7	267	9	-8	-9	264	7	3	6	301	8	5	2	198	4	-1	0	53	28	5
-6	45	61	10*	-8	87	14	-3	7	151	7	-5	3	248	5	-6	1	313	3	-4
-5	465	20	-15	-7	264	6	-5	8	149	13	2	4	208	8	9	2	159	6	-11
-4	21	31	14*	-6	293	14	-5	9	264	6	-9	5	333	11	0	3	336	7	-5
-3	402	5	1	-5	84	11	4	H,K= 2,			0	6	64	56	24	4	310	4	-1
-2	277	9	-3	-4	459	12	-1	-10	214	21	5	7	145	16	1	5	28	51	1*
-1	170	5	8	-3	72	13	-7	-9	36	39	25*	8	245	13	-2	6	215	10	3
0	450	8	-3	-2	121	6	2	-8	275	9	-11	H,K= 2,			3	7	172	11	5
1	338	4	2	-1	373	6	5	-7	201	9	-9	-10	79	33	10	H,K= 2,			6
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3	243	4	5	1	647	4	3	-5	317	11	1	-8	158	9	-1	-8	268	22	-9
4	159	10	-2	2	45	55	8*	-4	157	6	-2	-7	261	9	3	-7	271	16	-7
5	374	6	-1	3	450	2	1	-3	831	13	10	-6	427	4	1	-6	39	47	-6*
6	96	24	23	4	509	14	17	-2	506	7	9	-5	117	5	10	-5	323	5	2
7	191	10	-6	5	65	11	-6	-1	140	8	-2	-4	317	5	2	-4	124	6	0
8	276	14	-4	6	217	5	1	0	109	6	5	-3	380	5	1	-3	317	3	-0
	H,K= 2,		-5	7	114	16	6	1	313	3	-1	-2	690	12	-9	-2	123	6	-16
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-7	242	7	-13	H,K= 2,			-2	4	343	3	-1	1	598	9	-1	1	68	15	-12
-6	315	15	-16	-10	205	15	1	5	360	11	-3	2	208	4	-0	2	380	7	-8
-5	36	41	12*	-9	43	61	40*	6	0	51	-26*	3	433	6	1	3	404	2	-5
-4	586	19	-2	-8	341	23	-9	7	237	7	12	4	400	8	-4	4	67	14	21
-3	70	15	-16	-7	183	9	-0	8	214	5	-2	5	69	14	6	5	367	4	-11
-2	513	14	-7	-6	394	7	-3	H,K= 2,			1	6	212	9	0	6	62	73	7*
-1	643	8	7	-5	619	8	-3	-10	0	60	-11*	7	175	7	6	7	162	6	-7
0	86	12	13	-4	36	11	13	-9	209	7	4	8	185	14	6	H,K= 2,			7
1	405	2	3	-3	434	4	-0	-8	104	7	-7	H,K= 2,			4	-9	204	9	1

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	55	32	18	2	250	12	6	0	64	30	6	-3	39	50	11*	0	353	9	-11
-7	181	9	-2	3	261	9	-16	1	302	11	8	-2	451	7	4	1	275	4	2
-6	336	6	-10	4	65	15	13	2	141	6	-11	-1	448	11	0	2	312	4	-1
-5	61	19	29	5	181	9	5	3	199	8	-10	0	114	5	1	3	460	3	-0
-4	578	12	-7	H,K=	2,	11		4	258	7	0	1	499	4	-5	4	133	4	-2
-3	343	12	-6	-7	198	20	2	5	54	64	-14*	2	91	6	1	5	287	4	-1
-2	167	3	5	-6	242	10	-6	H,K=	3,-12			3	389	12	-5	6	29	49	-13*
-1	397	9	-7	-5	75	17	5	-6	135	18	-9	4	293	16	0	7	223	11	8
0	83	18	-6	-4	214	9	-5	-5	270	6	4	5	37	44	-4*	8	207	14	-9
1	321	7	-4	-3	190	10	-3	-4	38	63	21*	6	247	5	-3	H,K=	3,	-5	
2	163	7	-17	-2	212	9	-4	-3	262	5	-2	7	107	20	8	-9	173	17	3
3	55	66	17*	-1	233	12	-4	-2	182	6	-11	H,K=	3,-8			-8	66	12	15
4	334	12	-4	0	0	74	-21*	-1	93	23	22	-8	229	9	-13	-7	309	10	-8
5	58	69	30*	1	297	6	-4	0	258	7	-5	-7	184	23	-9	-6	304	8	-14
6	229	5	-9	2	199	13	3	1	51	72	15*	-6	96	10	-12	-5	118	4	-4
7	171	15	-3	3	115	31	-19	2	317	5	-1	-5	208	5	-1	-4	479	9	-4
H,K=	2,	8		4	233	5	3	3	98	18	2	-4	90	24	26	-3	324	8	-1
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-7	85	12	3	-6	144	25	-10	5	251	5	9	-2	292	7	-12	-1	192	5	-4
-6	197	5	-2	-5	130	17	-10	6	96	21	8	-1	301	4	2	0	73	5	-3
-5	272	6	8	-4	25	56	-5*	H,K=	3,-11			0	487	6	2	1	347	3	1
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-3	301	8	2	-2	228	16	-19	-6	182	11	-8	2	154	6	-3	3	223	5	-3
-2	366	9	-12	-1	62	72	1*	-5	0	56	-48*	3	275	6	-1	4	359	6	3
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0	305	7	-3	1	84	18	-14	-3	27	54	-23*	5	274	10	-9	6	281	6	-3
1	28	57	13*	2	169	23	-5	-2	176	5	3	6	50	58	22*	7	118	24	-12
2	407	17	-4	3	238	16	-3	-1	275	3	1	7	217	9	4	8	129	17	14
3	190	7	-1	H,K=	2,	13		0	76	24	7	H,K=	3,-7			H,K=	3,-4		
4	0	46	-16*	-4	197	22	-10	1	405	7	-7	-9	157	9	-9	-10	175	6	5
5	392	29	-9	-3	160	18	-22	2	0	37	-31*	-8	34	39	14	-9	55	66	54*
6	15	62	-11*	-2	169	16	-19	3	259	11	-10	-7	235	16	-11	-8	247	3	-5
H,K=	2,	9		-1	213	14	-10	4	298	10	-3	-6	252	9	-18	-7	187	7	3
-8	113	32	-20	0	22	42	-4*	5	45	63	17*	-5	113	19	-7	-6	190	7	3
-7	179	5	-5	1	177	8	-4	6	240	9	-3	-4	262	4	-8	-5	481	8	-5
-6	261	9	-10	H,K=	3,-15			H,K=	3,-10			-3	248	3	-2	-4	38	48	9*
-5	71	17	31	-2	182	12	-13	-7	154	9	-2	-2	588	16	-4	-3	562	3	-1
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-3	221	24	-4	0	8	44	-23*	-5	298	13	-1	0	75	12	-4	-1	198	5	4
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-1	373	10	1	2	156	37	-35	-3	313	8	4	2	167	4	2	1	350	6	4
0	53	18	17	H,K=	3,-14			-2	251	5	-7	3	237	2	1	2	341	7	-1
1	320	5	-13	-4	47	56	13*	-1	200	12	5	4	358	4	2	3	594	6	6
2	162	10	-6	-3	237	5	-2	0	339	9	1	5	20	37	3*	4	300	5	3
3	68	36	5	-2	53	64	-6*	1	163	7	-2	6	263	9	5	5	315	3	-5
4	338	10	-10	-1	176	5	0	2	294	7	-1	7	160	9	-1	6	38	49	-3*
5	27	55	-2*	0	181	10	11	3	111	20	-9	8	137	34	3	7	182	10	-2
H,K=	2,	10		1	185	7	0	4	31	42	-9*	H,K=	3,-6			8	234	14	-7
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-6	164	11	5	3	190	5	3	6	75	38	-16	-8	240	10	5	-10	69	55	-11
-5	219	4	-13	4	96	18	-4	7	223	7	-11	-7	175	10	7	-9	237	6	-3
-4	107	12	-21	H,K=	3,-13			H,K=	3,-9			-6	74	10	-6	-8	134	11	-14
-3	326	9	-1	-5	64	76	5*	-8	66	28	54	-5	326	9	-0	-7	325	5	-5
-2	207	8	-2	-4	216	15	3	-7	168	39	-17	-4	113	6	3	-6	359	10	-6
-1	110	8	-1	-3	37	41	11*	-6	148	14	-1	-3	179	5	-11	-5	104	9	14
0	243	7	-5	-2	204	5	-3	-5	17	43	2*	-2	226	3	4	-4	375	3	0
1	97	17	-5	-1	193	11	-0	-4	333	5	-5	-1	257	2	-0	-3	432	2	1

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	422	3	0	-5	217	6	-3	-8	71	30	7	-6	160	11	10	3	133	16	-0
-1	267	6	-5	-4	139	3	-4	-7	376	3	-0	-5	355	7	-6	4	260	4	-2
0	87	21	7	-3	584	4	-1	-6	212	6	0	-4	129	7	2	H,K=	3,	10	
1	357	4	1	-2	383	6	-3	-5	239	4	-2	-3	286	3	-6	-7	211	15	-4
2	460	7	-2	-1	84	9	-8	-4	275	4	-3	-2	304	4	6	-6	144	6	5
3	267	6	-9	0	395	4	-2	-3	310	3	-2	-1	89	11	5	-5	305	17	-3
4	461	8	2	1	356	3	1	-2	312	2	-1	0	389	2	-5	-4	0	41	-34*
5	177	4	-1	2	625	7	-2	-1	473	6	-3	1	174	6	-2	-3	234	13	1
6	197	8	3	3	175	11	8	0	175	6	-3	2	386	4	-8	-2	252	4	-8
7	95	15	6	4	114	10	2	1	594	10	-3	3	223	11	2	-1	104	14	-8
8	132	8	-2	5	551	10	-7	2	61	13	-6	4	201	7	-2	0	183	11	5
	H,K=	3,	-2	6	69	16	10	3	297	4	2	5	256	7	-7	1	79	13	20
-10	157	17	-8	7	242	8	-8	4	255	5	-4	6	54	58	1*	2	201	10	-10
-9	22	50	2*	8	185	22	8	5	74	77	-23*	H,K=	3,	7	3	266	4	2	
-8	353	15	-13	H,K=	3,	1	1	6	238	10	-13	-9	257	10	-7	4	55	65	-10*
-7	259	15	-12	-10	70	38	25	7	159	9	-2	-8	159	9	-6	H,K=	3,	11	
-6	232	3	4	-9	330	5	-7	H,K=	3,	4	-7	187	7	8	-6	211	7	1	
-5	420	7	-7	-8	111	23	4	-10	211	16	-7	-6	280	15	-9	-5	129	18	11
-4	63	17	-9	-7	235	5	-6	-9	58	69	36*	-5	158	8	-0	-4	323	6	-15
-3	199	7	6	-6	261	7	3	-8	296	4	-3	-4	482	7	-4	-3	106	11	-1
-2	413	10	-7	-5	262	7	-7	-7	155	22	-12	-3	239	16	-7	-2	179	13	-0
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1	449	4	3	-2	307	3	-2	-4	164	6	8	0	36	47	24*	1	226	8	4
2	559	2	-0	-1	507	5	-10	-3	171	3	-1	1	318	3	-2	2	176	13	-14
3	661	8	7	0	210	6	4	-2	382	5	-2	2	251	10	2	3	72	49	1
4	26	44	-15*	1	417	3	-2	-1	111	9	4	3	165	6	-9	H,K=	3,	12	
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6	23	59	-27*	3	423	5	-5	1	62	11	15	5	55	65	7*	-4	12	50	-24*
7	208	18	-7	4	331	9	3	2	422	2	-2	6	202	5	4	-3	294	12	5
8	181	28	-7	5	3	42	-35*	3	356	5	-4	H,K=	3,	8	-2	181	5	9	
	H,K=	3,	-1	6	334	13	-2	4	118	16	-8	-8	165	6	16	-1	11	53	-50*
-10	63	28	-6	7	161	28	-3	5	278	6	1	-7	174	6	-4	0	279	7	-1
-9	220	9	-4	8	139	9	0	6	82	54	20	-6	199	7	1	1	54	66	-22*
-8	76	13	-3	H,K=	3,	2	2	7	231	10	-7	-5	293	6	-10	H,K=	3,	13	
-7	278	3	-3	-10	236	14	-6	H,K=	3,	5	-4	75	20	2	-3	96	40	-14	
-6	465	13	-17	-9	47	66	13*	-9	156	16	-9	-3	365	4	-10	-2	116	32	-13
-5	127	8	2	-8	330	14	-7	-8	52	62	-8*	-2	336	3	-7	-1	198	13	15
-4	569	5	8	-7	190	5	-8	-7	292	5	-7	-1	137	9	-3	H,K=	4,	-15	
-3	330	8	-2	-6	271	3	5	-6	241	6	-6	0	398	4	1	-2	237	5	-3
-2	944	6	-11	-5	212	9	-13	-5	235	6	-4	1	130	12	-16	-1	170	9	0
-1	635	6	-8	-4	452	11	3	-4	416	3	-1	2	225	5	-5	0	71	14	7
0	169	5	1	-3	574	8	-6	-3	380	8	4	3	152	11	-1	1	213	11	-4
1	735	3	-5	-2	197	8	4	-2	357	2	-2	4	114	9	2	2	56	57	-23*
2	335	2	2	-1	68	19	2	-1	389	6	-6	5	215	8	-12	H,K=	4,	-14	
3	117	6	7	0	476	2	-2	0	132	6	2	H,K=	3,	9	-4	24	71	20*	
4	568	12	-6	1	136	9	-3	1	462	6	-5	-8	160	11	-5	-3	267	4	-5
5	20	36	-8*	2	425	3	-2	2	219	6	-5	-7	163	16	-12	-2	40	69	-28*
6	287	7	1	3	331	13	-11	3	99	16	5	-6	272	18	-7	-1	149	24	3
7	138	10	-8	4	33	39	-16*	4	240	6	-1	-5	37	46	22*	0	143	9	-7
8	143	9	-5	5	332	4	-6	5	78	41	-7	-4	292	13	-1	1	34	47	1*
	H,K=	3,	C	6	132	9	-12	6	270	19	-5	-3	45	54	4*	2	231	11	-7
-10	196	5	C	7	197	9	2	7	178	8	12	-2	141	5	-7	3	178	10	-14
-9	56	66	22*	8	127	36	-12	H,K=	3,	6	-1	340	10	3	H,K=	4,	-13		
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-7	182	7	-3	-10	0	65	-36*	-8	134	20	19	1	230	7	-7	-4	301	9	-7
-6	134	17	-5	-9	298	5	-1	-7	159	17	-7	2	136	8	9	-3	21	47	3*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	217	5	-8	-2	434	6	1	2	369	2	-1	3	180	6	-2	3	200	5	-7
-1	141	11	-8	-1	408	5	-1	3	316	6	2	4	383	5	1	4	185	4	-4
0	44	53	-2*	0	178	9	7	4	249	3	2	5	39	42	-3*	5	328	5	-4
1	228	4	1	1	462	7	2	5	318	7	-5	6	267	4	4	6	139	17	3
2	101	21	-12	2	180	9	-3	6	80	85	-15*	7	58	69	33*	7	234	8	6
3	202	17	4	3	164	4	-2	7	293	7	-3	H,K= 4, -2		H,K= 4, 1					
4	218	7	-10	4	310	5	-5	H,K= 4, -5		-10	145	21	6	-10	33	54	-24*		
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-4	364	15	-10	0	578	6	-6	1	338	6	-2	1	50	35	-14	1	564	4	-2
-3	66	27	-3	1	301	6	-2	2	427	11	5	2	239	3	-3	2	297	4	-4

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	202	13	-8	-7	221	5	-4	1	202	18	6	H,K=	5,-10	-1	254	8	4		
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6	278	16	-5	-4	272	9	-1	-2	41	49	-13*	-6	200	10	-7	2	99	11	2
7	177	16	6	-3	116	13	-1	-1	130	40	-22	-5	156	9	-8	3	270	4	-3
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-9	34	43	17*	-1	404	6	-2	-2	181	20	3	-3	290	4	1	5	62	73	3*
-8	216	5	-8	0	28	58	1*	-1	177	8	-7	-2	215	3	-7	6	277	11	2
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
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6	97	13	7	6	403	7	-8	-9	303	8	3	-1	167	7	-3		H,K=	6,-14		
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-10	105	28	-19	-10	154	24	6	-6	268	5	6	2	236	13	2	-2	172	10	5	
-9	182	11	9	-9	73	43	2	-5	218	4	3	3	146	16	-11	-1	176	7	4	
-8	115	13	-6	-8	328	3	5	-4	392	7	6	4	143	7	10	0	229	22	10	
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1	379	2	-3	3	196	4	2	-6	206	7	5		H,K=	5, 11		1	60	36	-11	

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 THURIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUORACETONE)

PAGE 10

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	347	4	-9	-4	21	54	-3*	1	411	4	2	4	65	21	-32	-4	42	67	14*
3	127	15	-21	-3	439	9	-0	2	160	5	-4	5	245	7	3	-3	345	3	-1
4	144	10	-0	-2	41	48	-4*	3	211	5	3	6	25	70	16*	-2	206	6	1
5	227	5	5	-1	193	4	1	4	140	9	2	H,K= 6, 1			-1	112	11	-8	
H,K= 6,			-9	0	322	7	2	5	93	11	28	-9	239	26	-2	0	312	3	1
-8	67	26	27	1	24	34	2*	6	252	8	-4	-8	67	13	41	1	106	10	-4
-7	193	14	4	2	288	5	-1	H,K= 6,			-2	-7	218	14	-3	2	235	4	3
-6	116	17	21	3	189	5	3	-10	227	12	0	-6	358	6	-6	3	148	9	16
-5	156	12	1	4	187	10	-3	-9	10	58	-84*	-5	248	5	9	4	221	4	3
-4	318	3	-5	5	249	5	-1	-8	195	5	-2	-4	306	4	4	H,K= 6,			5
-3	0	65	-11*	6	0	63	-46*	-7	124	17	12	-3	23	34	2*	-8	108	12	11
-2	199	9	-8	H,K= 6,			-5	-6	242	6	6	-2	228	5	-2	-7	188	17	5
-1	261	8	-7	-9	221	10	-4	-5	470	11	-4	-1	204	7	7	-6	204	10	5
0	109	18	4	-8	46	29	38	-4	131	10	8	0	135	8	1	-5	83	9	8
1	335	9	-2	-7	217	8	0	-3	261	3	-4	1	419	8	-10	-4	220	13	-5
2	49	18	-16	-6	254	4	-1	-2	304	7	6	2	124	22	-4	-3	153	14	8
3	242	4	-8	-5	18	34	-3*	-1	387	2	-1	3	254	4	-0	-2	309	3	2
4	164	8	14	-4	345	6	-2	0	520	10	-1	4	274	5	-7	-1	216	9	1
5	134	25	-1	-3	246	5	-0	1	37	37	28*	5	52	35	-15	0	38	68	-8*
H,K= 6,			-8	-2	366	4	-4	2	232	10	8	H,K= 6,			2	1	237	7	4
-8	208	7	-4	-1	192	7	3	3	184	5	2	-9	52	58	42*	2	55	65	9*
-7	92	18	24	0	104	15	9	4	160	12	2	-8	280	8	1	3	230	7	-4
-6	235	8	5	1	359	4	-3	5	285	7	4	-7	105	12	5	4	238	6	7
-5	251	4	1	2	146	15	-10	6	62	82	19*	-6	222	6	3	H,K= 6,			6
-4	65	14	27	3	161	4	4	H,K= 6,			-1	-5	313	7	-4	-8	300	8	0
-3	290	2	0	4	166	9	-3	-10	127	16	3	-4	51	26	46	-7	167	12	4
-2	162	11	-9	5	0	42	-45*	-9	172	14	-9	-3	369	4	3	-6	165	12	10
-1	220	9	-8	6	261	5	0	-8	103	18	11	-2	195	4	-6	-5	174	7	1
0	144	14	-9	H,K= 6,			-4	-7	135	13	9	-1	191	7	4	-4	64	31	18
1	59	15	53	-9	128	27	-8	-6	354	4	-5	0	304	3	-1	-3	316	5	-4
2	348	7	-3	-8	227	8	+6	-5	201	11	-2	1	111	12	-5	-2	187	8	9
3	87	27	-8	-7	115	7	7	-4	347	2	-2	2	302	11	-2	-1	205	11	-3
4	159	13	-1	-6	175	12	4	-3	45	54	17*	3	198	11	-2	0	354	11	4
5	303	4	-7	-5	326	4	1	-2	482	2	3	4	131	18	-3	1	67	69	2*
H,K= 6,			-7	-4	45	56	28*	-1	229	4	-6	5	274	8	13	2	230	6	-1
-9	190	5	6	-3	355	6	1	0	147	9	2	H,K= 6,			3	3	142	9	5
-8	51	67	14*	-2	162	4	-2	1	426	5	-7	-9	218	6	-2	H,K= 6,			7
-7	187	5	7	-1	437	5	0	2	50	59	-4*	-8	0	60	-16*	-7	229	6	0
-6	181	12	0	0	473	2	-1	3	311	5	6	-7	278	3	0	-6	195	5	-3
-5	123	12	-8	1	42	16	25	4	225	5	0	-6	181	6	8	-5	21	51	-7*
-4	341	4	-2	2	268	5	-4	5	125	7	7	-5	117	11	-2	-4	262	11	-6
-3	87	10	4	3	198	6	-1	6	244	22	-5	-4	249	6	-2	-3	86	11	27
-2	223	8	1	4	164	12	-8	H,K= 6,			0	-3	81	34	-8	-2	313	4	-2
-1	187	4	-7	5	252	8	5	-10	217	7	-8	-2	255	4	1	-1	279	11	7
0	139	17	-1	6	102	31	-10	-9	46	49	-3*	-1	338	5	-4	0	48	50	13*
1	316	4	7	H,K= 6,			-3	-8	209	21	-12	0	191	5	7	1	203	10	-7
2	86	21	-7	-10	104	13	-1	-7	120	30	-15	1	379	5	3	2	99	10	21
3	176	8	2	-9	228	6	9	-6	198	5	-9	2	161	5	-7	H,K= 6,			8
4	208	6	3	-8	116	15	24	-5	524	2	3	3	189	6	-9	-7	136	18	22
5	0	74	-14*	-7	192	16	-13	-4	106	7	2	4	241	23	-2	-6	123	26	15
6	253	15	7	-6	159	11	5	-3	341	3	-1	5	81	40	22	-5	166	11	-11
H,K= 6,			-6	-5	44	45	18*	-2	257	5	-3	H,K= 6,			4	-4	99	27	4
-9	34	50	-21*	-4	394	7	-5	-1	79	9	3	-9	72	53	36	-3	264	16	-9
-8	217	16	-6	-3	269	5	-4	0	295	6	-9	-8	288	3	-3	-2	111	10	-3
-7	104	20	-10	-2	551	2	-1	1	44	52	1*	-7	116	17	8	-1	184	9	6
-6	202	7	4	-1	482	2	-1	2	326	6	-1	-6	277	8	-1	0	208	7	-8
-5	296	4	-1	0	79	13	5	3	212	8	-2	-5	222	6	1	1	0	49	-28*

STRUCTURE FACTORS CONTINUED FOR
 THORIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE)

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	6,	9	-8	34	47	11*	5	242	5	4	-2	318	3	-0	-7	158	8	8
-5	5	69	-19*	-7	134	18	-9	H,K=	7,	-5	-1	192	7	-4	-6	197	5	15	
-4	262	6	-0	-6	148	13	3	-9	229	5	-5	0	306	5	-2	-5	308	9	2
-3	93	10	4	-5	155	9	7	-8	37	61	32*	1	49	58	-18*	-4	33	39	-28*
-2	217	11	-16	-4	282	5	-13	-7	189	13	0	2	277	5	1	-3	438	4	4
-1	192	24	-4	-3	0	43	-10*	-6	242	6	5	3	161	11	10	-2	163	13	-3
0	51	61	16*	-2	205	13	6	-5	118	8	-2	4	122	13	0	-1	232	7	9
	H,K=	7,-14		-1	81	18	7	-4	287	3	-2	5	151	7	-2	0	389	4	-3
-3	191	10	9	0	98	8	-10	-3	96	22	-2	H,K=	7,	-1	1	137	11	3	
-2	45	61	-15*	1	320	5	-1	-2	311	6	-7	-9	145	22	-1	2	205	16	5
-1	141	17	8	2	74	13	-1	-1	309	3	1	-8	42	63	35*	3	179	14	-12
0	177	34	-10	3	249	4	5	0	136	10	5	-7	352	6	-8	4	168	12	-2
	H,K=	7,-13		4	250	10	-4	1	378	9	4	-6	198	13	-9	H,K=	7,	3	
-5	86	11	19	H,K=	7,	-8	2	35	42	13*	-5	57	67	23*	-9	166	19	-6	
-4	166	8	1	-8	206	4	-2	3	185	11	11	-4	324	8	0	-8	26	45	-61*
-3	0	48	-42*	-7	64	31	4	4	170	8	4	-3	39	47	1*	-7	171	9	8
-2	178	12	-5	-6	196	13	1	5	108	9	-6	-2	317	6	-1	-6	190	7	-6
-1	145	11	12	-5	279	7	-6	H,K=	7,	-4	-1	133	11	1	-5	158	10	1	
0	76	17	-10	-4	27	60	3*	-9	59	70	-0*	0	106	39	14	-4	288	4	4
1	241	7	7	-3	299	6	-3	-8	228	4	1	1	271	11	-1	-3	35	62	17*
2	61	64	20*	-2	184	7	11	-7	42	47	13*	2	84	84	-4*	-2	376	4	0
	H,K=	7,-12		-1	189	5	-8	-6	254	4	-4	3	237	5	-1	-1	293	5	3
-6	175	5	9	0	288	3	1	-5	256	3	2	4	190	15	-8	0	48	26	18
-5	188	12	-11	1	68	34	2	-4	115	11	6	5	50	59	-3*	1	179	11	1
-4	24	57	-2*	2	265	7	6	-3	345	4	1	H,K=	7,	0	2	82	11	5	
-3	207	5	10	3	65	24	8	-2	174	8	0	-9	97	13	21	3	239	14	0
-2	120	9	-15	4	190	10	1	-1	215	8	3	-8	228	8	4	H,K=	7,	4	
-1	160	19	-5	H,K=	7,	-7	0	371	3	2	-7	268	4	-2	-8	261	6	-6	
0	183	14	12	-8	45	65	37*	1	34	48	8*	-6	122	28	1	-7	160	8	-12
1	0	46	-18*	-7	148	16	-1	2	286	6	5	-5	290	6	-6	-6	92	30	-13
2	209	14	-11	-6	208	13	6	3	130	9	8	-4	65	17	3	-5	213	6	11
3	127	18	-2	-5	105	12	-1	4	175	7	2	-3	354	3	0	-4	44	21	8
	H,K=	7,-11		-4	282	4	5	5	194	8	-2	-2	151	10	-1	-3	325	9	-1
-6	117	12	3	-3	38	49	17*	H,K=	7,	-3	-1	135	7	-11	-2	81	16	-5	
-5	97	27	-24	-2	328	5	5	-9	234	6	-7	0	313	7	9	-1	227	14	2
-4	245	4	-6	-1	326	4	-1	-8	105	35	-13	1	41	44	-11*	0	278	4	-2
-3	45	54	20*	0	52	61	-1*	-7	224	4	-0	2	205	6	0	1	12	59	-22*
-2	244	7	3	1	312	3	-1	-6	109	9	7	3	248	6	11	2	233	5	1
-1	155	6	2	2	37	53	25*	-5	135	6	10	4	163	13	5	3	140	8	-13
0	162	5	14	3	191	7	-4	-4	279	4	-0	H,K=	7,	1	H,K=	7,	5		
1	289	7	-6	4	259	8	-11	-3	15	57	-17*	-9	202	13	3	-8	71	54	33
2	141	6	-0	5	133	17	28	-2	321	3	5	-8	0	74	-28*	-7	204	13	-1
3	182	7	5	H,K=	7,	-6	-1	249	4	-4	-7	226	5	-10	-6	258	7	-2	
	H,K=	7,-10		-9	68	45	-24	0	155	7	-10	-6	253	7	5	-5	111	9	11
-7	97	13	24	-8	255	8	-0	1	271	6	-9	-5	89	31	3	-4	199	5	3
-6	207	5	-7	-7	88	53	16	2	61	71	11*	-4	361	2	-0	-3	54	61	26*
-5	245	8	5	-6	157	7	3	3	263	7	-1	-3	59	16	2	-2	324	7	13
-4	108	7	6	-5	234	6	3	4	183	12	-4	-2	354	8	-3	-1	279	5	2
-3	291	6	2	-4	33	42	2*	5	88	31	8	-1	150	16	5	0	52	29	14
-2	118	11	-0	-3	379	3	-0	H,K=	7,	-2	0	64	77	30*	1	229	6	10	
-1	133	7	-0	-2	82	10	-9	-9	33	42	1*	1	329	12	-8	2	92	11	9
0	231	9	11	-1	295	8	-2	-8	182	11	23	2	186	8	1	H,K=	7,	6	
1	86	25	12	0	383	4	3	-7	87	23	-1	3	255	10	-7	-7	93	24	-12
2	258	4	2	1	102	18	7	-6	234	7	-9	4	197	14	-1	-6	107	22	-10
3	130	10	4	2	243	4	-2	-5	226	8	1	H,K=	7,	2	-5	229	16	3	
4	165	21	-9	3	163	6	10	-4	52	18	-6	-9	50	53	10*	-4	47	54	-12*
	H,K=	7,-9		4	176	11	11	-3	306	8	-2	-8	273	9	-9	-3	195	13	1

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-2	95	20	6	-4	277	7	4	-1	260	5	4	-4	232	4	-1	2	127	29	4	
-1	156	9	4	-3	44	47	-6*	0	188	6	2	-3	56	67	10*	H,K=	8,	4	4	
0	213	6	6	-2	245	4	-8	1	228	7	0	-2	291	3	6	-7	115	14	-2	
1	93	16	-3	-1	234	7	-9	2	93	15	21	-1	190	7	7	-6	166	6	15	
	H,K=	7,	7	0	51	29	21	3	165	25	2	0	167	9	11	-5	287	6	-1	
-6	138	9	6	1	148	10	10	4	178	13	16	1	327	6	2	-4	64	14	28	
-5	43	44	-7*	2	0	65	-24*	H,K=	8,	-4	2	37	56	21*	-3	188	5	12	12	
-4	245	4	8	3	174	15	-3	-9	55	66	29*	3	235	8	-7	-2	119	14	29	
-3	140	9	11	H,K=	8,	-8	-8	224	10	-1	H,K=	8,	0	-1	105	35	5	5	5	
-2	147	19	8	-8	200	9	10	-7	41	48	-6*	-8	308	6	-0	0	133	26	-3	
-1	222	11	2	-7	121	14	-5	-6	138	8	9	-7	186	7	-1	1	86	20	5	
0	167	7	5	-6	115	12	-10	-5	149	8	-4	-6	212	6	-6	H,K=	8,	5	5	
	H,K=	7,	8	-5	220	9	3	-4	46	55	28*	-5	239	11	-2	-6	258	8	6	
-5	141	10	-5	-4	44	63	-11*	-3	326	5	-3	-4	42	52	8*	-5	88	30	4	
-4	66	74	28*	-3	248	8	-2	-2	126	6	11	-3	274	12	7	-4	254	6	3	
-3	183	18	-6	-2	103	19	9	-1	239	7	4	-2	189	6	-4	-3	146	22	24	
-2	181	30	-18	-1	268	7	-0	0	394	5	4	-1	205	7	2	-2	126	18	-2	
-1	109	44	-8	0	210	4	-3	1	82	19	28	0	269	5	1	-1	154	41	6	
	H,K=	8,-13	1	70	18	54	2	186	10	-2	1	35	58	-2*	0	160	22	13	13	
-3	16	72	-0*	2	226	15	-2	3	205	9	10	2	258	5	-2	H,K=	8,	6	6	
-2	138	12	-1	3	135	12	0	4	160	16	1	3	111	15	-6	-5	216	9	6	
-1	12	46	-30*	H,K=	8,	-7	H,K=	8,	-3	H,K=	8,	1	-4	59	59	23*	1	59	59	23*
0	73	87	-26*	-8	27	67	12*	-9	207	6	5	-8	115	14	-6	-3	230	7	1	
	H,K=	8,-12	-7	205	5	-2	-8	60	32	22	-7	250	6	0	-2	145	12	-12	-12	
-5	168	13	5	-6	143	26	-2	-7	247	12	-9	-6	137	20	9	-1	111	38	3	
-4	59	41	10	-5	54	64	14*	-6	185	7	7	-5	135	13	-6	H,K=	9,-12	9,-12	9,-12	
-3	225	16	-3	-4	257	7	3	-5	143	20	9	-4	234	7	-2	-3	223	13	2	
-2	107	40	9	-3	57	20	40	-4	195	4	-8	-3	27	54	17*	-2	57	50	12	
-1	128	24	-7	-2	349	11	5	-3	48	58	5*	-2	297	8	1	-1	161	6	7	
0	199	13	1	-1	314	7	4	-2	352	4	-3	-1	268	6	9	H,K=	9,-11	9,-11	9,-11	
1	53	63	11*	0	143	6	-3	-1	217	7	-0	0	94	28	13	-5	128	16	17	
	H,K=	8,-11	1	198	15	2	0	50	59	-19*	1	207	5	5	-4	183	5	1	1	
-6	99	41	28	2	102	13	-29	1	392	4	7	2	102	11	7	-3	118	8	11	
-5	125	10	-12	3	176	11	9	2	30	72	-8*	3	186	11	2	-2	262	8	6	
-4	208	12	3	4	152	9	-3	3	194	7	1	H,K=	8,	2	-1	190	16	4	4	
-3	51	73	28*	H,K=	8,	-6	4	178	12	0	-8	210	18	4	0	60	71	-7*	-7*	
-2	228	10	4	-8	246	8	2	H,K=	8,	-2	-7	172	5	11	H,K=	9,-10	9,-10	9,-10	9,-10	
-1	160	9	-5	-7	15	49	-1*	-9	15	57	-26*	-6	224	4	1	-6	129	20	0	
0	83	17	-9	-6	189	14	-2	-8	289	10	-12	-5	250	9	13	-5	189	7	6	
1	178	8	-6	-5	145	16	-9	-7	151	6	20	-4	131	7	3	-4	46	80	-12*	
2	63	26	56	-4	47	56	9*	-6	117	7	13	-3	237	8	13	-3	181	10	7	
	H,K=	8,-10	-3	309	7	2	-5	269	7	0	-2	110	30	-5	-2	70	47	28	28	
-7	106	13	-10	-2	140	5	-2	-4	29	60	12*	-1	184	12	-4	-1	164	15	-8	
-6	163	8	2	-1	274	5	-2	-3	250	13	6	0	218	8	0	0	154	12	-9	
-5	182	8	7	0	287	4	13	-2	151	9	2	1	45	30	20	1	100	11	3	
-4	97	14	-7	1	131	22	10	-1	215	10	0	2	277	10	13	H,K=	9,-9	9,-9	9,-9	
-3	256	12	6	2	207	6	-1	0	299	7	4	H,K=	8,	3	-6	122	10	-13	-13	
-2	138	17	0	3	211	10	5	1	49	58	35*	-8	31	91	-16*	-5	74	19	1	
-1	204	5	3	4	152	7	8	2	256	6	2	-7	203	7	18	-4	162	12	-4	
0	203	10	-6	H,K=	8,	-5	3	135	17	1	-6	219	11	10	-3	63	64	18*	18*	
1	59	15	16	-8	88	16	25	4	167	11	11	-5	128	7	4	-2	201	18	-7	
2	172	7	-4	-7	219	5	4	H,K=	8,	-1	-4	237	13	-1	-1	165	13	15	15	
3	80	21	3	-6	196	7	3	-9	170	20	1	-3	56	16	13	0	107	35	-5	
	H,K=	8,-9	-5	119	17	-11	-8	37	73	-1*	-2	195	11	-6	1	262	9	5	5	
-7	157	7	-1	-4	270	6	12	-7	343	4	2	-1	224	4	11	H,K=	9,-8	9,-8	9,-8	
-6	124	7	4	-3	120	19	5	-6	70	60	-1	0	93	14	9	-7	116	14	15	
-5	120	20	5	-2	304	3	-1	-5	77	28	19	1	240	9	5	-6	166	20	-10	

STRUCTURE FACTORS CONTINUED FOR
THORIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE)

PAGE13

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	194	13	6	-6	156	26	9	-4	101	15	13	H,K=	10,	-4					
-4	106	11	-1	-5	127	15	-0	-3	229	7	6	-6	188	26	6				
-3	106	16	8	-4	236	8	8	-2	103	12	15	-5	140	19	2				
-2	74	25	-14	-3	89	20	-2	-1	138	7	10	-4	107	13	2				
-1	192	9	-0	-2	279	4	8	0	176	8	0	-3	209	22	1				
0	136	8	-2	-1	128	11	-3	H,K=	9,	3	-2	89	27	7					
1	54	23	18	0	207	5	-3	-6	175	14	17	-1	131	11	5				
2	270	8	11	1	185	8	6	-5	104	33	7	0	181	12	11				
H,K=	9,	-7	2	0	56	-52*	-4	289	14	8	H,K=	10,	-3						
-7	284	4	-5	H,K=	9,	-2	-3	68	49	-9	-6	141	18	5					
-6	177	8	6	-8	238	6	1	-2	134	8	-0	-5	161	11	-2				
-5	134	19	7	-7	0	69	-51*	-1	129	10	6	-4	187	10	20				
-4	207	8	12	-6	172	12	3	H,K=	9,	4	-3	104	13	24					
-3	73	33	43	-5	248	12	-3	-5	169	12	8	-2	182	26	4				
-2	147	10	11	-4	50	60	4*	-4	57	68	-15*	-1	129	10	2				
-1	147	7	5	-3	347	5	8	-3	188	8	5	0	102	16	-6				
0	132	11	9	-2	161	8	2	-2	103	11	-8	H,K=	10,	-2					
1	289	10	2	-1	166	7	-0	H,K=	10,-	10	-6	174	12	6					
2	76	20	-3	0	184	6	2	-3	175	14	2	-5	206	8	5				
H,K=	9,	-6	1	83	20	-19	-2	88	47	19	-4	44	28	16					
-7	69	33	-0	2	218	14	11	H,K=	10,	-9	-3	165	10	0					
-6	204	9	4	H,K=	9,	-1	-5	79	82	3*	-2	114	23	6					
-5	177	11	7	-8	0	45	-15*	-4	216	8	7	-1	157	7	-4				
-4	69	47	3	-7	146	14	-5	-3	44	47	0*	0	167	13	-1				
-3	150	12	5	-6	164	8	13	-2	164	6	9	H,K=	10,	-1					
-2	159	28	3	-5	122	23	3	-1	114	29	-7	-6	181	12	11				
-1	203	8	2	-4	291	7	8	H,K=	10,	-8	-5	117	23	21					
0	201	5	3	-3	22	60	-24*	-5	127	14	-1	-4	191	14	4				
1	62	74	17*	-2	182	21	-1	-4	69	21	-18	-3	0	53	-47*				
2	247	6	-6	-1	164	16	0	-3	187	11	-5	-2	199	12	-5				
H,K=	9,	-5	0	164	41	33	-2	64	46	-12	-1	149	16	10					
-8	33	86	25*	1	210	6	10	-1	173	13	13	H,K=	10,	0					
-7	236	15	-2	2	71	21	54	0	175	8	2	-6	144	32	13				
-6	134	10	18	H,K=	9,	0	0	H,K=	10,	-7	-5	221	10	4					
-5	147	8	14	-7	72	37	6	-6	126	19	15	-4	59	66	20*				
-4	193	8	3	-6	167	14	1	-5	191	11	-4	-3	236	4	8				
-3	0	40	-46*	-5	275	3	0	-4	241	12	-1	-2	105	22	14				
-2	271	6	2	-4	51	70	-5*	-3	33	49	27*	-1	189	9	10				
-1	231	9	16	-3	250	13	5	-2	173	12	17	H,K=	10,	1					
0	152	10	3	-2	97	19	4	-1	116	10	4	-5	129	14	25				
1	199	14	-1	-1	164	12	4	0	68	74	21*	-4	284	11	3				
2	121	30	31	0	207	13	-1	H,K=	10,	-6	-3	83	15	53					
H,K=	9,	-4	1	88	14	20	-6	190	16	2	-2	247	11	10					
-8	226	5	-1	H,K=	9,	1	-5	180	6	13									
-7	80	15	-21	-7	171	7	-10	-4	173	23	2								
-6	160	7	8	-6	162	9	-10	-3	216	15	6								
-5	164	12	10	-5	113	15	8	-2	78	29	9								
-4	66	21	48	-4	267	6	2	-1	127	10	5								
-3	333	4	6	-3	14	43	0*	0	191	17	4								
-2	163	11	-1	-2	208	12	-1	H,K=	10,	-5									
-1	217	9	-1	-1	189	8	8	-6	111	15	-3								
0	230	11	10	0	69	50	-22	-5	190	10	3								
1	31	46	-6*	1	306	10	10	-4	190	19	10								
2	156	10	-1	H,K=	9,	2	-3	40	48	15*									
H,K=	9,	-3	-7	57	68	-9*	-2	173	17	9									
-8	52	64	26*	-6	165	12	10	-1	136	8	9								
-7	193	25	10	-5	233	9	-8	0	87	41	30								

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 4.0) FOR
URANIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE) F(0,0,0) = 4335

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,		2	742	5	-7	5	365	3	1	9	89	27	-11*	-8	86	34	4*
1	0*	35	-253*	3	357	2	-4	6	176	4	-1	10	70	25	-12*	-7	292	4	3
2	101	5	3	4	145	4	0	7	45	51	23*	11	145	9	4	-6	214	8	9
3	564	1	0	5	378	3	4	8	139	11	11		H,K=	0,	7	-5	120	14	7
4	51	10	6*	6	245	4	1	9	105	9	-0	-11	53	54	-7*	-4	436	6	4
5	191	4	-5	7	39	46	-16*	10	129	12	-2	-10	110	14	-3	-3	164	5	1
6	364	3	3	8	256	6	2	11	182	19	12	-9	211	3	4	-2	201	5	-8
7	69	21	-3*	9	143	10	10		H,K=	0,	5	-8	37	41	4*	-1	374	4	-7
8	360	3	-1	10	151	13	8	-12	168	13	5	-7	367	3	4	0	0	38	-57*
9	168	14	14	11	168	8	10	-11	53	58	21*	-6	392	5	2	1	265	4	-6
10	150	8	9		H,K=	0,	3	-10	184	11	12	-5	21	40	-4*	2	355	6	3
11	201	16	6	-12	154	10	-2	-9	220	13	4	-4	449	1	1	3	149	12	-1
12	77	85	58*	-11	74	21	15*	-8	131	12	2	-3	57	25	3*	4	298	4	-5
	H,K=	0,	1	-10	124	10	12	-7	372	9	6	-2	273	2	4	5	107	11	18
-12	124	34	2*	-9	229	10	1	-6	270	6	-2	-1	282	2	-2	6	103	14	9
-11	70	27	-4*	-8	25	47	-1*	-5	119	4	2	0	0	50	-19*	7	220	7	-1
-10	116	18	-12	-7	359	3	4	-4	501	2	4	1	169	3	-4	8	41	69	14*
-9	230	6	-5	-6	284	4	3	-3	86	10	-11	2	621	2	1	9	124	21	23
-8	36	42	-0*	-5	237	3	0	-2	327	3	4	3	116	4	7	10	108	42	10*
-7	266	7	-6	-4	444	2	4	-1	420	3	1	4	390	4	-3		H,K=	0,	10
-6	382	2	-0	-3	26	31	-5*	0	21	30	0*	5	171	4	4	-10	147	14	5
-5	166	9	-5	-2	280	2	3	1	394	2	-3	6	131	14	1	-9	70	37	-2*
-4	74	10	4	-1	374	2	.2	2	409	3	1	7	163	4	10	-8	224	7	-3
-3	148	5	4	0	0	50	-13*	3	120	12	16	8	90	22	8*	-7	182	7	9
-2	186	4	4	1	443	3	-2	4	558	7	4	9	144	14	-5	-6	137	6	7
-1	695	9	-8	2	432	4	-1	5	71	11	-7	10	122	16	4	-5	298	3	1
1	828	6	-15	3	271	3	3	6	232	8	3		H,K=	0,	8	-4	108	16	1
2	98	9	5	4	572	6	-5	7	275	5	2	-11	182	15	-6	-3	326	3	3
3	431	2	3	5	181	7	2	8	103	19	-4	-10	103	19	-22	-2	320	28	-29
4	116	3	3	6	254	4	2	9	213	9	-3	-9	88	12	18	-1	0	69	-81*
5	185	6	0	7	398	6	-2	10	178	14	6	-8	230	8	3	0	462	5	-1
6	289	6	0	8	35	57	-7*	11	58	81	39*	-7	227	6	7	1	143	5	5
7	364	4	-3	9	197	22	-2		H,K=	0,	6	-6	123	10	3	2	125	13	-4
8	57	57	18*	10	173	12	4	-11	173	11	-1	-5	442	3	-1	3	286	3	5
9	249	10	5	11	25	65	-44*	-10	123	11	-5	-4	150	3	1	4	49	58	4*
10	213	8	4		H,K=	0,	4	-9	104	11	1	-3	337	5	3	5	161	6	1
11	79	41	10*	-12	40	53	19*	-8	146	15	-10	-2	245	2	-3	6	241	10	3
12	152	20	21	-11	201	23	24	-7	171	4	11	-1	100	40	-75*	7	62	31	21*
	H,K=	0,	2	-10	108	25	13*	-6	291	2	3	0	266	3	-4	8	127	25	-1*
-12	60	75	45*	-9	70	30	-4*	-5	379	3	10	1	330	3	4	9	107	38	29*
-11	209	9	-0	-8	335	4	3	-4	90	6	8	2	288	5	-4		H,K=	0,	11
-10	119	17	22	-7	182	10	-12	-3	397	2	3	3	435	2	1	-10	154	11	-9
-9	59	71	21*	-6	362	5	-0	-2	146	3	1	4	80	8	-0	-9	200	17	-1
-8	389	5	3	-5	354	3	-1	-1	221	2	1	5	236	5	-2	-8	49	25	7*
-7	84	8	3	-4	39	12	-4*	0	325	2	-2	6	249	4	8	-7	217	10	-1
-6	334	4	7	-3	436	4	8	1	431	3	-2	7	61	17	-26*	-6	246	12	1
-5	567	9	9	-2	264	4	1	2	350	2	-3	8	230	6	9	-5	24	51	9*
-4	123	7	0	-1	479	3	8	3	393	3	-1	9	93	12	5	-4	257	4	5
-3	582	4	10	0	82	12	5	4	28	44	-38*	10	53	28	0*	-3	186	4	-1
-2	262	1	1	1	451	2	2	5	240	5	-8		H,K=	0,	9	-2	0	101	-157*
-1	290	5	2	2	377	7	1	6	281	9	1	-11	117	21	0	-1	333	11	2
0	954	3	-10	3	485	2	1	7	50	59	12*	-10	101	11	-3	0	0	65	-91*
1	199	5	3	4	40	23	-14*	8	223	7	3	-9	194	22	6	1	290	5	2

STRUCTURE FACTORS CONTINUED FOR
URANIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE)

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	85	12	-18	3	214	6	14	-3	21	55	4*	-7	128	21	-4	10	89	23	12*
3	32	42	-31*	4	9	59	-29*	-2	174	14	5	-6	21	79	-38*	H,K=	1,	-10	
4	199	7	-3	5	149	10	23	-1	65	81	-22*	-5	139	11	-7	-10	47	73	-8*
5	177	7	-7	6	140	9	21	0	53	37	-27*	-4	165	13	4	-9	98	12	-9
6	40	42	-14*	H,K=	0,	15		1	176	18	9	-3	0	45	-19*	-8	189	13	-11
7	184	15	19	-7	131	18	-7	2	0	91	-57*	-2	207	7	-7	-7	34	42	21*
8	42	70	13*	-6	163	24	17	3	116	16	5	-1	136	33	-65*	-6	290	20	2
9	128	19	5	-5	56	63	-6*	4	199	16	10	0	0	60	-97*	-5	179	18	-9
H,K=	0,	12		-4	195	6	-2	5	30	47	30*	1	312	13	-3	-4	72	18	-3*
-9	58	83	--44*	-3	60	71	-66*	H,K=	1,-	16		2	83	13	-27	-3	297	6	4
-8	277	16	4	-2	52	39	-11*	-5	48	58	-28*	3	128	11	-4	-2	150	195	-91*
-7	91	44	8*	-1	179	6	-11	-4	61	67	5*	4	215	9	-3	-1	180	5	-14
-6	121	7	3	0	0	74	-57*	-3	174	12	6	5	0	56	-39*	0	436	13	-5
-5	372	5	7	1	185	36	3*	-2	0	71	-74*	6	186	14	-9	1	38	53	-10*
-4	50	55	-13*	2	159	35	12*	-1	85	36	6*	7	240	11	2	2	344	3	-1
-3	179	13	11	3	54	36	-10*	0	146	28	-15*	8	75	43	-8*	3	317	3	-0
-2	221	18	-17	4	190	8	2	1	0	80	-25*	9	163	13	3	4	185	7	-3
-1	132	7	-19	5	39	48	-36*	2	156	17	-14	H,K=	1,-	12		5	276	10	-6
0	412	3	1	6	73	87	15*	3	135	17	6	-9	91	14	9	6	148	15	-4
1	129	14	0	H,K=	0,	16		4	84	18	0*	-8	116	11	-7	7	61	75	0*
2	212	10	2	-6	105	11	7	5	241	5	14	-7	0	46	-25*	8	199	9	-1
3	265	9	11	-5	224	18	4	6	50	64	-10*	-6	185	21	-5	9	0	77	-11*
4	77	31	-17*	-4	0	67	-40*	7	106	45	-17*	-5	132	14	-13	10	144	22	6
5	65	16	-12*	-3	164	16	3	H,K=	1,-	15		-4	46	55	-19*	H,K=	1,	-9	
6	164	8	10	-2	175	23	2	-6	17	67	-22*	-3	234	6	9	-10	150	18	11
7	0	71	-9*	-1	37	63	28*	-5	109	23	2*	-2	0	112	-127*	-9	90	28	-13*
8	151	30	2*	0	146	18	5	-4	162	8	-9	-1	339	20	-7	-8	36	57	15*
H,K=	0,	13		1	110	46	12*	-3	0	46	-2*	0	341	16	-0	-7	255	14	2
-9	135	19	1	2	62	74	-5*	-2	86	22	-11*	1	110	13	-7	-6	70	26	18*
-8	53	25	37*	3	177	13	21	-1	139	22	-35	2	269	7	3	-5	154	8	-11
-7	206	16	-3	4	64	28	22*	0	73	28	-57*	3	217	8	-0	-4	291	5	-10
-6	151	9	-2	H,K=	0,	17		1	168	6	-3	4	74	27	-21*	-3	2	33	-6*
-5	0	64	-27*	-5	0	48	-31*	2	74	42	-4*	5	245	5	8	-2	227	3	-11
-4	260	8	7	-4	171	11	8	3	123	23	-3*	6	46	49	-12*	-1	391	5	-7
-3	0	136	-60*	-3	107	26	8*	4	145	26	-18	7	192	5	5	0	172	6	-11
-2	30	54	-78*	-2	122	23	8*	5	43	51	27*	8	213	5	-10	1	404	16	12
-1	309	6	-10	-1	164	29	-0	6	207	9	-4	9	0	73	-25*	2	165	8	-7
0	15	87	-82*	0	0	72	-30*	7	127	20	-9	H,K=	1,-	11		3	168	5	-14
1	236	6	1	1	114	21	0*	H,K=	1,-	14		-9	95	21	-6*	4	245	8	-2
2	230	4	1	2	158	25	8	-7	45	53	31*	-8	36	54	4*	5	60	14	9*
3	0	73	-36*	3	0	68	-10*	-6	117	48	-5*	-7	202	21	-6	6	327	10	-7
4	191	10	23	H,K=	0,	18		-5	70	74	-18*	-6	18	42	-16*	7	249	9	-15
5	139	15	4	-3	126	19	-12	-4	86	55	1*	-5	152	20	-4	8	73	13	-8
6	87	104	11*	-2	131	11	-3	-3	183	9	-11	-4	208	6	6	9	215	8	-0
7	146	18	15	-1	6	50	-17*	-2	115	20	-27	-3	24	52	-4*	10	113	18	3
H,K=	0,	14		0	99	30	-9*	-1	184	28	-20	-2	196	15	-42	H,K=	1,	-8	
-8	182	16	13	1	109	34	21*	0	368	19	-12	-1	262	10	-8	-10	31	77	-5*
-7	45	72	-20*	H,K=	1,-	18		1	85	13	8	0	75	12	-20	-9	119	19	13
-6	119	19	-5	-2	29	77	-0*	2	183	15	-4	1	271	5	-2	-8	186	18	-1
-5	263	8	3	-1	101	13	2	3	142	9	1	2	134	15	0	-7	67	32	-6*
-4	13	65	3*	0	117	30	0*	4	64	69	-8*	3	201	8	-5	-6	267	4	-1
-3	187	29	-27	1	0	79	-6*	5	201	7	-0	4	278	9	-4	-5	264	8	-13
-2	214	13	-2	2	143	13	3	6	116	10	-20	5	24	63	13*	-4	161	16	-3
-1	0	69	-35*	3	60	83	-54*	7	148	16	-0	6	252	16	2	-3	398	10	-6
0	202	8	-5	4	80	69	10*	8	157	22	17	7	252	5	-3	-2	97	12	-5
1	41	41	-20*	H,K=	1,-	17		H,K=	1,-	13		8	47	36	-13*	-1	313	3	0
2	167	10	4	-4	135	22	17	-8	72	89	16*	9	160	14	-2	0	765	19	6

STRUCTURE FACTORS CONTINUED FOR
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PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL				
1	0	38	-10*	10	181	14	4	-7	281	8	-7	0	0*20	-22*	7	276	8	10					
2	376	6	-3	11	132	21	-10	-6	369	6	-2	1	399	2	5	8	51	62	7*				
3	254	4	0		H,K=	1,	-5	-5	97	11	-5	2	714	2	1	9	297	11	-5				
4	52	17	13*-11	51	60	21*	-4	427	4	-5	3	264	6	2	10	149	11	-8					
5	168	7	-3	-10	142	23	-17	-3	56	18	-6*	4	354	2	1	11	22	45	-29*				
6	252	10	1	-9	129	17	-1	-2	473	2	-1	5	67	19	-8*		H,K=	1,	2				
7	116	10	-3	-8	112	10	-4	-1	80	7	8	6	207	4	3	-12	46	55	16*				
8	279	17	-15	-7	354	8	-8	0	113	6	-3	7	151	18	-4	-11	227	19	-4				
9	56	36	4*	-6	130	13	4	1	402	2	-1	8	93	20	5*-10		83	46	-3*				
10	170	9	10	-5	204	18	-12	2	172	4	-3	9	186	18	-6	-9	127	11	10				
11	156	10	3	-4	481	5	-8	3	45	13	6*	10	131	17	-11	-8	291	11	-1				
					H,K=	1,	-7	-3	85	9	4	4	400	3	-4	11	85	22	17*	-7	100	17	-5
-11	40	76	14*	-2	454	2	-0	5	48	33	-0*		H,K=	1,	0	-6	455	14	3				
-10	146	27	16*	-1	405	1	-1	6	354	3	0	-12	47	57	32*	-5	620	9	8				
-9	152	14	-3	0	121	4	-3	7	274	3	-0	-11	227	5	4	-4	87	7	-6				
-8	60	35	21*	1	668	7	4	8	163	5	-1	-10	131	9	-2	-3	510	1	1				
-7	280	8	-3	2	411	7	4	9	170	5	4	-9	179	6	-3	-2	759	7	6				
-6	168	17	-14	3	320	3	2	10	97	9	9	-8	355	6	-7	-1	348	7	2				
-5	256	7	-7	4	561	8	-1	11	88	26	3*	-7	81	7	13	0	259	3	2				
-4	327	3	-5	5	71	8	6		H,K=	1,	-2	-6	464	14	6	1	113	6	3				
-3	130	10	13	6	391	4	-1	-12	40	64	23*	-5	640	1	2	2	325	2	0				
-2	443	2	-0	7	227	20	2	-11	183	13	6	-4	183	5	3	3	151	4	-5				
-1	228	3	-1	8	49	26	-10*-10	99	28	-1*	-3	563	2	-0	4	29	43	21*					
0	73	13	-6	9	265	11	-11	-9	191	5	-8	-2	87	4	8	5	285	5	-0				
1	611	9	-5	10	110	8	5	-8	376	11	-11	-1	162	49	-20*	6	265	3	2				
2	444	9	4	11	117	10	23	-7	86	17	14*	0	337708-445*		7	28	35	4*					
3	179	8	-8		H,K=	1,	-4	-6	158	5	-5	1	62	14	5*	8	274	9	-2				
4	373	2	-3	-12	0	55	-39*	-5	586	2	-2	2	679	1	4	9	73	28	19*				
5	55	22	16*-11	160	15	-1	-4	47	16	-3*	3	747	9	2	10	90	21	-15*					
6	328	2	-2	-10	74	56	-2*	-3	552	6	-6	4	116	3	3	11	159	16	17				
7	198	17	-3	-9	94	34	-4*	-2	177	7	-4	5	121	5	4		H,K=	1,	3				
8	113	19	3	-8	192	5	-0	-1	899	2	3	6	261	4	-2	-12	175	6	-1				
9	325	18	-8	-7	68	81	-4*	0	883	5	-1	7	63	28	-22*-11	28	61	5*					
10	141	23	-7	-6	203	6	-5	1	476	3	9	8	261	4	-3	-10	181	10	0				
11	114	14	22	-5	384	8	-5	2	671	1	2	9	46	58	18*	-9	192	8	-16				
					H,K=	1,	-6	-4	85	12	10	3	400	2	1	10	157	10	6	-8	102	8	4
-11	168	21	-0	-3	324	3	1	4	32	22	6*	11	163	32	-6*	-7	296	10	-1				
-10	53	64	-5*	-2	186	4	-5	5	446	11	-4		H,K=	1,	1	-6	305	9	6				
-9	95	22	17*	-1	675	1	1	6	226	10	-12	-12	148	19	-9	-5	130	5	1				
-8	172	5	-1	0	763	8	4	7	94	20	-13*-11	50	30	-8*	-4	500	6	-5					
-7	52	38	-4*	1	213	3	5	8	298	18	-3	-10	172	17	11	-3	275	6	9				
-6	169	7	-9	2	373	7	2	9	63	42	30*	-9	185	17	-15	-2	526	4	-1				
-5	301	5	-3	3	462	5	-2	10	191	9	2	-8	131	12	6	-1	628	6	-5				
-4	121	7	2	4	136	5	1	11	158	17	-1	-7	266	4	-6	0	145	2	-0				
-3	307	2	-2	5	549	9	5		H,K=	1,	-1	-6	85	9	18	1	682	5	-8				
-2	41	15	5*	6	207	4	-4	-12	142	13	3	-5	371	7	-5	2	534	8	-1				
-1	250	4	2	7	294	3	1	-11	74	14	33*	-4	150	15	-10	3	266	3	2				
0	403	3	2	8	225	13	3	-10	195	10	2	-3	149	6	15	4	432	6	-4				
1	49	13	-11*	9	124	7	-1	-9	232	4	2	-2	96	5	-2	5	301	5	1				
2	300	2	-1	10	206	17	-16	-8	83	31	-9*	-1	839	3	-8	6	242	8	-12				
3	430	4	3	11	177	17	2	-7	305	10	-9	0	290	8	-8	7	258	5	-0				
4	104	8	7		H,K=	1,	-3	-6	265	3	6	1	472	4	9	8	63	17	-1*				
5	369	9	-2	-12	163	20	7	-5	315	3	-3	2	473	2	-1	9	261	6	3				
6	318	11	0	-11	45	69	-7*	-4	190	5	-6	3	805	5	4	10	109	14	13				
7	236	8	-0	-10	200	5	3	-3	211	3	-3	4	418	13	-2	11	60	72	4*				
8	194	13	-11	-9	132	11	0	-2	161	5	4	5	287	8	1		H,K=	1,	4				
9	139	27	17*	-8	114	10	-17	-1	460	11	1	6	272	3	4	-12	81	52	31*				

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-11	168	8	-9	-3	526	5	0	8	172	10	1	2	216	6	-5	5	146	16	11
-10	40	48	-28*	-2	341	2	-1	9	45	53	-8*	3	126	14	-5	6	121	19	21
-9	123	10	12	-1	394	3	3	H,K=	1,	9	4	230	5	2	H,K=	1,	15		
-8	334	3	-5	0	309	8	-10	-11	0	70	-67*	5	101	11	1	-7	157	14	0
-7	85	10	18	1	279	5	-3	-10	162	7	-1	6	88	14	13	-6	145	30	-7*
-6	371	8	-8	2	166	10	-6	-9	202	6	3	7	148	14	23	-5	79	15	4*
-5	441	2	0	3	261	3	-8	-8	53	20	-27*	8	57	41	39*	-4	220	23	-11
-4	20	50	-7*	4	0	45	-18*	-7	255	14	12	H,K=	1,	12	-3	106	10	-19	
-3	395	3	0	5	296	10	-6	-6	159	10	7	-10	124	27	1*	-2	120	33	-3*
-2	447	2	-2	6	222	15	-4	-5	133	14	6	-9	87	17	7*	-1	174	9	2
-1	281	4	-3	7	148	6	2	-4	332	5	4	-8	219	6	10	0	0	53	-14*
0	537	3	-4	8	223	15	9	-3	193	6	9	-7	44	72	27*	1	176	10	13
1	62	20	-11*	9	97	26	5*	-2	284	6	0	-6	216	5	1	2	117	13	-1
2	358	6	-2	10	123	14	5	-1	212	5	-10	-5	310	22	-3	3	21	64	-27*
3	396	6	-12	H,K=	1,	7	0	30	40	-15*	-4	0	40	-41*	4	168	15	12	
4	105	4	-5	-11	54	65	28*	1	200	5	-4	-3	238	4	5	5	59	70	13*
5	294	4	-5	-10	122	11	-4	2	194	10	-4	-2	312	8	-1	H,K=	1,	16	
6	259	12	2	-9	169	11	-11	2	133	10	3	-1	0	54	-41*	-6	131	42	4*
7	80	23	-6*	-8	87	10	-6	4	297	7	10	0	296	8	-0	-5	159	13	1
8	257	7	-9	-7	323	6	0	5	90	12	8	1	45	46	-35*	-4	25	63	4*
9	88	22	-2*	-6	192	7	-8	6	188	9	0	2	196	8	-10	-3	168	11	-2
10	147	18	-1	-5	147	19	-9	7	169	12	-5	3	216	7	3	-2	141	30	10*
11	142	10	13	-4	382	5	1	8	73	41	64*	4	87	17	21*	-1	31	48	-28*
H,K=	1,	5	-3	104	17	-0	0	9	137	36	18*	5	116	9	21	0	182	10	21
-12	127	73	-24*	-2	514	5	2	H,K=	1,	10	6	103	13	4	1	76	26	-12*	
-11	63	64	48*	-1	372	4	-6	-10	141	23	6	7	0	67	-30*	2	81	71	-1*
-10	135	14	-5	0	66	12	-4	-9	169	19	14	H,K=	1,	13	3	152	10	0	
-9	160	16	-8	1	393	5	-9	-8	255	13	3	-9	153	10	7	H,K=	1,	17	
-8	89	22	30*	2	129	4	-1	-7	73	32	2*	-8	36	54	20*	-5	61	73	4*
-7	408	9	-12	3	319	6	6	-6	241	5	-1	-7	132	23	-2	-4	164	23	-3
-6	184	4	-2	4	437	18	-7	-5	259	4	-3	-6	137	7	-9	-3	94	38	14*
-5	159	6	-0	5	165	5	-6	-4	30	37	13*	-5	99	50	-4*	-2	140	14	9
-4	605	2	-1	6	190	6	3	-3	278	11	1	-4	230	9	-6	-1	137	13	-3
-3	101	7	5	7	199	15	-4	-2	157	8	-11	-3	37	55	-31*	0	26	46	14*
-2	466	2	3	8	74	19	43*	-1	43	56	-10*	-2	154	11	4	1	127	25	6*
-1	596	6	-0	9	112	21	-18*	0	380	10	5	-1	297	3	-2	2	117	32	13*
0	120	7	-2	10	73	56	-23*	1	54	63	-8*	0	35	53	25*	H,K=	2,-	19	
1	671	10	-18	H,K=	1,	8	2	210	10	-5	1	255	4	-6	0	42	68	-45*	
2	462	2	-2	-11	127	24	-8*	3	290	18	-5	2	201	10	7	1	158	13	14
3	248	2	-2	-10	166	12	13	4	67	71	11*	3	96	16	-20	H,K=	2,-	18	
4	495	7	-6	-9	134	17	17	5	194	5	6	4	197	23	24	-3	147	18	6
5	120	8	5	-8	256	4	-2	6	131	10	-7	5	78	23	11*	-2	0	72	-11*
6	178	6	-7	-7	148	9	-1	7	70	15	16*	6	54	76	-22*	-1	146	23	9
7	185	6	2	-6	163	6	-1	8	149	9	13	H,K=	1,	14	0	176	12	-2	
8	54	58	-24*	-5	411	4	-4	H,K=	1,	11	-8	186	18	1	1	0	65	-29*	
9	177	19	-5	-4	101	21	-3*	-10	154	9	-2	-7	92	16	-1	2	151	7	22
10	132	14	-3	-3	479	5	-3	-9	201	13	1	-6	119	31	13*	3	91	27	4*
H,K=	1,	6	-2	274	8	-8	-8	79	16	14*	-5	197	15	1	4	127	9	33	
-12	76	26	18*	-1	259	6	12	-7	198	16	1	-4	47	54	-13*	H,K=	2,-	17	
-11	138	14	-1	0	79	17	-6*	-6	215	16	0	-3	230	7	13	-5	112	16	6
-10	138	18	7	1	275	3	-1	-5	92	22	10*	-2	222	10	8	-4	122	25	3*
-9	112	25	-2*	2	340	4	4	-4	192	5	6	-1	39	49	-8*	-3	0115	-43*	
-8	289	3	-6	3	337	17	-2	-3	222	6	-1	0	145	6	1	-2	154	21	4
-7	193	11	-9	4	41	51	-32*	-2	120	9	-6	1	100	12	-12	-1	82	14	7
-6	217	5	-7	5	303	4	-5	-1	289	6	-2	2	132	15	-4	0	77	24	-7*
-5	329	5	-3	6	159	7	5	0	34	53	-6*	3	169	10	5	1	168	11	3
-4	98	7	3	7	90	15	-5	1	282	15	-4	4	75	23	69*	2	53	63	26*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	165	24	12	-5	188	12	2	-10	0	53	-34*	2	189	6	-7	H,K=	2,	-5	
4	162	16	15	-4	116	18	2	-9	147	26	8	3	127	6	-4	-12	132	28	-9*
5	45	50	1*	-3	60	26	5*	-8	169	7	-4	4	78	7	4	-11	31	46	20*
6	140	17	-30	-2	274	17	-2	-7	35	46	5*	5	262	3	2	-10	194	7	5
	H,K=	2,-16		-1	180	6	4	-6	214	9	-2	6	155	7	-2	-9	108	54	-8*
-6	142	25	2	0	128	6	-5	-5	201	4	-0	7	187	7	7	-8	140	24	-11
-5	29	52	-52*	1	299	19	-1	-4	86	20	-10*	8	239	6	-1	-7	332	4	-14
-4	77	92	-12*	2	88	29	-5*	-3	273	13	-10	9	39	61	22*	-6	118	9	0
-3	165	29	2	3	251	15	0	-2	182	10	7	10	209	6	-5	-5	276	6	-8
-2	0	54	-33*	4	244	4	4	-1	277	5	-10		H,K=	2,	-7	-4	495	2	1
-1	148	25	-6	5	56	37	15*	0	240	5	-3	-11	20	98	10*	-3	156	8	1
0	170	23	12	6	234	13	6	1	59	61	-17*	-10	157	9	2	-2	516	2	2
1	44	55	30*	7	133	12	1	2	271	6	2	-9	100	19	7*	-1	528	1	-3
2	219	5	5	8	105	15	6	3	157	8	4	-8	177	9	1	0	238	2	1
3	113	18	-17	9	150	25	-21	4	48	21	10*	-7	267	12	-4	1	385	2	2
4	110	22	-18*		H,K=	2,-12		5	322	16	1	-6	204	4	-1	2	270	3	-1
5	190	12	23	-9	98	37	3*	6	179	7	7	-5	244	7	-12	3	423	2	1
6	82	26	45*	-8	98	11	17	7	202	14	4	-4	225	4	-7	4	416	5	2
7	118	16	-1	-7	47	58	16*	8	188	13	-0	-3	65	34	-2*	5	42	50	8*
	H,K=	2,-15		-6	252	8	3	9	34	45	25*	-2	685	14	-3	6	354	10	-2
-7	154	12	2	-5	182	21	-0	10	190	9	18	-1	441	7	1	7	148	8	-2
-6	0	51	-9*	-4	78	79	-7*		H,K=	2,	-9	0	129	5	-8	8	60	43	1*
-5	152	19	-3	-3	268	7	-3	-10	142	10	4	1	761	7	-1	9	242	12	-6
-4	144	10	5	-2	57	24	-8*	-9	95	24	-2*	2	46	47	3*	10	30	44	-14*
-3	40	48	-34*	-1	195	7	-3	-8	111	9	11	3	414	3	-1	11	98	19	12*
-2	144	37	4*	0	191	4	-3	-7	248	6	0	4	464	8	2		H,K=	2,	-4
-1	127	37	-11*	1	104	31	-23*	-6	0	49	-37*	5	148	7	-3	-12	89	106	73*
0	96	11	-8	2	323	9	-5	-5	226	4	-9	6	282	18	7	-11	154	22	-5
1	218	6	-4	3	127	15	0	-4	306	4	-9	7	183	6	-7	-10	75	26	23*
2	184	11	-5	4	102	8	-3	-3	53	21	-0*	8	67	44	2*	-9	183	7	2
3	218	20	3	5	282	5	1	-2	284	12	-7	9	252	7	-1	-8	278	7	-2
4	148	31	7*	6	100	25	11*	-1	413	2	-1	10	85	25	13*	-7	34	55	-8*
5	30	63	-21*	7	204	10	2	0	241	8	-11	11	102	34	1*	-6	407	8	-5
6	224	14	18	8	178	21	3	1	597	13	2		H,K=	2,	-6	-5	295	4	-3
7	103	30	19*	9	0	88	-5*	2	249	7	-4	-11	122	22	-16*	-4	294	8	-0
	H,K=	2,-14			H,K=	2,-11		3	233	8	-3	-10	0	48	-43*	-3	419	4	0
-8	118	23	2*-10	93	49	-15*	4	298	8	6	-9	133	16	-8	-2	335	4	-3	
-7	34	52	28*	-9	69	28	1*	5	25	45	-14*	-8	252	8	-10	-1	384	7	-2
-6	154	8	1	-8	104	18	17	6	276	6	4	-7	59	61	-9*	0	608	2	-1
-5	112	12	2	-7	172	10	2	7	156	12	-7	-6	208	6	-6	1	176	6	-2
-4	125	11	-0	-6	75	23	-29*	8	195	10	-2	-5	378	5	-2	2	762	5	3
-3	134	11	4	-5	138	6	7	9	235	16	-2	-4	260	3	-3	3	281	5	-0
-2	22	42	10*	-4	236	10	7	10	47	56	-37*	-3	451	11	-1	4	167	4	-2
-1	278	12	-13	-3	38	48	10*		H,K=	2,	-8	-2	0	35	-40*	5	443	4	2
0	264	8	-8	-2	248	19	-8	-11	119	33	-12*	-1	335	7	8	6	249	11	-7
1	71	40	-3*	-1	133	6	1	-10	75	35	27*	0	470	2	-4	7	179	4	-3
2	271	9	-10	0	171	15	-0	-9	119	12	5	1	219	5	5	8	238	7	-6
3	177	10	3	1	253	4	-9	-8	176	11	-3	2	414	5	3	9	0	42	-13*
4	140	7	-13	2	87	25	-17*	-7	0	46	-26*	3	244	8	-6	10	238	9	-11
5	209	15	9	3	187	11	-3	-6	180	9	-5	4	147	5	-6	11	142	29	-8*
6	34	67	-20*	4	288	4	0	-5	350	11	-0	5	358	5	4		H,K=	2,	-3
7	142	12	4	5	11	63	8*	-4	80	14	2	6	135	8	-4	-12	108	26	-18*
8	137	10	-2	6	248	8	-6	-3	278	2	1	7	157	8	-6	-11	18	71	-13*
	H,K=	2,-13		7	184	18	-2	-2	184	5	-0	8	296	12	-8	-10	187	11	-2
-8	14	71	-51*	8	166	15	0	-1	350	11	-3	9	44	27	40*	-9	160	11	-20
-7	92	15	-9	9	163	7	7	0	417	2	-1	10	195	6	1	-8	170	16	-8
-6	0	61	-18*		H,K=	2,-10		1	19	38	-25*	11	119	9	10	-7	305	3	-6

STRUCTURE FACTORS CONTINUED FOR
URANIUM(IV) TETRAKIS(PYRAZOLIDE-HEXAFLUOROACETONE)

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	41	46	-7*	1	947	2	4	8	107	7	10	-8	315	12	-0	1	104	11	5
-5	312	4	5	2	471	3	6	9	215	9	7	-7	134	7	10	2	383	8	0
-4	331	5	2	3	668	6	10	10	95	27	-7*	-6	177	9	-3	3	427	4	-3
-3	52	8	19	4	506	3	-4	11	72	36	-12*	-5	523	3	0	4	96	12	1
-2	158	5	-4	5	136	3	0		H,K=	2, 2		-4	293	13	-4	5	344	17	6
-1	237	3	-1	6	308	12	-6	-12	76	36	49*	-3	520	2	-1	6	104	11	-13
0	69	12	-1	7	233	3	-3	-11	200	9	7	-2	260	6	-6	7	94	11	-13
1	704	2	3	8	89	22	-2*	-10	109	13	3	-1	140	6	-14	8	159	10	-16
2	89	9	7	9	282	13	-9	-9	212	9	-3	0	429	4	-3	9	33	48	-28*
3	479	7	2	10	138	10	7	-8	339	8	-6	1	201	15	-8		H,K=	2, 7	
4	548	7	0	11	48	34	-26*	-7	78	18	12*	2	287	3	-2	-12	177	9	6
5	20	36	13*		H,K=	2, 0		-6	259	8	-2	3	214	5	-10	-11	50	76	41*
6	185	4	4	-12	55	30	3*	-5	230	3	1	4	128	15	-9	-10	222	8	7
7	196	11	9	-11	152	28	-7	-4	75	21	15*	5	236	6	-8	-9	135	8	-21
8	0	38	-18*	-10	135	14	-7	-3	475	1	0	6	169	4	1	-8	131	16	-5
9	266	8	-12	-9	155	13	3	-2	12	41	-24*	7	136	9	4	-7	297	6	4
10	106	23	-9*	-8	263	5	-6	-1	186	6	-6	8	223	13	-5	-6	174	14	-18
11	89	53	20*	-7	37	39	24*	0	651	2	-3	9	9	80	0*	-5	154	7	-5
	H,K=	2, -2		-6	498	9	-8	1	58	12	-16*	10	122	10	-15	-4	591	3	-3
-12	0	46	-55*	-5	170	6	-3	2	278	4	1		H,K=	2, 5		-3	219	5	-6
-11	172	12	-1	-4	236	5	-8	3	207	2	-3	-12	122	12	-11	-2	316	8	2
-10	76	20	-5*	-3	914	4	-5	4	171	7	9	-11	71	22	67*	-1	300	4	-5
-9	215	7	-12	-2	218	7	7	5	316	3	0	-10	190	5	-1	0	108	6	12
-8	269	3	-3	-1	58	13	0*	6	102	11	5	-9	161	15	-2	1	364	7	-2
-7	0	35	-23*	0	80	4	0	7	75	12	17	-8	185	8	5	2	103	22	-14*
-6	571	2	-2	1	224	4	-4	8	297	11	-2	-7	344	9	-6	3	0	61	-31*
-5	519	9	4	2	344	4	10	9	39	58	22*	-6	186	6	-6	4	347	3	-7
-4	151	7	6	3	772	6	5	10	142	10	18	-5	221	7	-0	5	62	21	-12*
-3	486	2	2	4	344	9	-0		H,K=	2, 3		-4	558	2	-2	6	193	9	4
-2	460	1	1	5	351	5	-4	-12	149	12	8	-3	198	9	1	7	203	8	1
-1	540	2	2	6	86	8	14	-11	52	62	38*	-2	552	2	-0	8	42	46	25*
0	345	1	-2	7	192	10	-4	-10	195	6	-8	-1	454	2	-4	9	149	9	9
1	324	1	1	8	262	12	-6	-9	206	4	-1	0	115	18	-14		H,K=	2, 8	
2	447	5	5	9	57	23	35*	-8	152	14	5	1	337	3	-11	-11	124	34	-12*
3	373	3	4	10	132	15	6	-7	308	5	2	2	141	6	-2	-10	135	24	-12
4	57	25	15*	11	139	18	1	-6	458	9	2	3	314	2	-2	-9	122	21	-7
5	290	3	-1		H,K=	2, 1		-5	395	7	-7	4	339	2	-3	-8	175	6	-9
6	170	13	-0	-12	149	28	-15*	-4	346	4	-3	5	38	52	-11*	-7	65	24	14*
7	265	5	4	-11	0	56	-35*	-3	189	2	7	6	153	13	-10	-6	298	5	-12
8	240	6	-2	-10	195	19	-3	-2	756	1	-2	7	214	8	-5	-5	239	8	-2
9	29	45	13*	-9	116	46	-6*	-1	561	1	-1	8	0	42	-7*	-4	86	17	6*
10	189	8	5	-8	98	17	-3	0	246	3	-3	9	183	6	-3	-3	392	5	-4
11	148	16	11	-7	315	5	-4	1	585	5	-4	10	82	48	-5*	-2	298	3	-5
	H,K=	2, -1		-6	265	2	2	2	182	4	-6		H,K=	2, 6		-1	256	3	-5
-12	140	10	-3	-5	216	6	-14	3	432	2	1	-12	14	54	-29*	0	256	3	-6
-11	66	73	65*	-4	336	2	1	4	413	2	-3	-11	130	9	-5	1	28	36	14*
-10	171	10	-1	-3	484	2	3	5	79	19	-7*	-10	129	18	18	2	366	2	4
-9	153	10	-2	-2	628	2	1	6	156	5	3	-9	164	6	9	3	232	6	-0
-8	141	10	-14	-1	309	3	-3	7	197	7	-3	-8	257	5	-8	4	0	52	-33*
-7	219	7	-6	0	213	7	-6	8	90	13	5	-7	152	9	-10	5	371	14	-3
-6	74	19	5*	1	386	2	-1	9	186	5	10	-6	207	6	-9	6	93	19	5*
-5	199	3	-0	2	492	4	-2	10	110	28	7*	-5	303	3	-0	7	101	34	16*
-4	102	6	0	3	631	8	6		H,K=	2, 4		-4	138	5	-5	8	160	10	-17
-3	285	6	8	4	326	4	-3	-12	52	62	7*	-3	314	3	0	9	0	48	-43*
-2	852	1	3	5	28	33	15*	-11	203	8	-2	-2	136	15	-9		H,K=	2, 9	
-1	109	8	7	6	425	5	0	-10	72	28	-8*	-1	293	2	-3	-11	28	59	-2*
0	62	17	-3*	7	199	4	0	-9	172	10	-11	0	291	5	-5	-10	152	17	-6

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	167	12	-12	H,K=	2,	12	0	17	44	11*	3	78	40	4*	H,K=	3,-12			
-8	44	53	-2*	-9	97	26	10*	1	163	9	5	4	124	18	2	-9	150	19	7
-7	237	4	-1	-8	195	13	-12	2	110	13	14	5	178	11	8	-8	58	76	-5*
-6	151	17	5	-7	61	68	15*	3	25	50	-27*	6	38	55	30*	-7	12	54	-27*
-5	151	7	1	-6	193	5	0	H,K=	2,	16	H,K=	3,-15	-6	217	12	-2			
-4	429	7	-6	-5	100	27	2*	-6	150	18	23	-7	106	28	-29*	-5	79	15	3*
-3	109	12	-7	-4	61	34	-7*	-5	126	38	-16*	-6	0	64	-21*	-4	136	17	6
-2	212	3	2	-3	283	4	-1	-4	59	68	53*	-5	119	11	-25	-3	283	10	-1
-1	293	10	0	-2	186	6	-15	-3	169	9	-5	-4	129	22	3	-2	41	43	-16*
0	49	21	-1*	-1	133	9	-4	-2	107	10	-8	-3	132	13	-6	-1	189	8	-2
1	328	8	4	0	229	4	1	-1	60	71	3*	-2	227	5	3	0	231	3	1
2	158	10	-7	1	86	31	-15*	0	186	9	5	-1	37	56	-13*	1	48	36	-5*
3	51	17	-12*	2	191	9	-9	1	67	79	25*	0	92	27	-6*	2	342	6	-3
4	340	7	-9	3	219	15	-3	2	102	17	8	1	249	5	-3	3	68	22	8*
5	67	31	17*	4	20	44	-34*	H,K=	2,	17	2	126	27	-8*	4	171	6	9	
6	159	13	-1	5	169	15	15	-3	44	54	-0*	3	246	12	7	5	281	5	1
7	135	15	-13	6	99	60	-3*	-2	113	12	7	4	170	21	-14	6	83	11	-3
8	48	50	20*	H,K=	2,	13	-1	143	12	10	5	18	61	-19*	7	200	16	9	
	H,K=	2,	10	-9	150	34	3*	H,K=	3,-19	6	158	37	-1*	8	141	10	-18		
-10	142	7	17	-8	59	70	47*	-2	144	11	10	7	87	17	14*	9	0	50	-44*
-9	165	7	-1	-7	176	7	-10	-1	55	79	-18*	H,K=	3,-14	H,K=	3,-11				
-8	252	8	-1	-6	69	35	-15*	0	118	13	-1	-8	113	31	9*	-10	121	10	-0
-7	34	56	24*	-5	152	15	-11	1	138	16	8	-7	77	66	19*	-9	61	79	20*
-6	283	7	-9	-4	211	4	2	2	0	53	-1*	-6	185	16	-12	-8	174	13	19
-5	213	9	8	-3	144	6	-1	H,K=	3,-18	-5	93	10	-4	-7	177	11	-3		
-4	41	32	-10*	-2	255	9	-2	-4	91	27	27*	-4	175	5	2	-6	39	54	-26*
-3	380	8	2	-1	188	9	-3	-3	99	13	-14	-3	190	9	-9	-5	169	10	2
-2	117	9	0	0	39	41	9*	-2	11	45	10*	-2	26	79	-38*	-4	246	9	-6
-1	97	23	-13*	1	207	17	-4	-1	162	8	7	-1	214	7	1	-3	125	9	-4
0	297	4	5	2	111	18	7	0	146	8	-8	0	140	9	9	-2	267	7	-5
1	59	14	9*	3	112	22	1*	1	59	70	-31*	1	71	23	-11*	-1	218	11	-5
2	237	15	5	4	156	20	-7	2	163	12	15	2	333	4	1	0	215	4	-4
3	297	5	-7	5	66	69	18*	3	59	68	-11*	3	170	8	0	1	435	8	-7
4	29	43	15*	6	89	15	-12	4	107	34	2*	4	138	9	6	2	96	28	6*
5	167	4	1	H,K=	2,	14	H,K=	3,-17	5	238	5	0	3	319	6	-2			
6	91	12	3	-8	159	21	-12	-5	131	11	3	6	4	67	-33*	4	301	8	-1
7	119	15	6	-7	76	48	23*	-4	96	28	-4*	7	142	20	-10	5	63	65	14*
8	118	13	5	-6	162	8	13	-3	0	47	-40*	8	151	9	-5	6	231	6	-2
	H,K=	2,	11	-5	161	39	3*	-2	165	10	8	H,K=	3,-13	7	129	8	-1		
-10	126	31	12*	-4	0	47	-9*	-1	79	16	5*	-9	54	64	6*	8	108	18	-12
-9	183	17	-1	-3	136	13	-4	0	93108	-11*	-8	130	8	23	9	179	19	-11	
-8	71	23	24*	-2	175	24	4	1	181	15	2	-7	135	20	6	H,K=	3,-10		
-7	249	8	-10	-1	90	25	9*	2	40	47	37*	-6	32	46	3*	-10	36	63	22*
-6	104	11	3	0	155	13	4	3	173	15	-13	-5	183	8	2	-9	189	6	-6
-5	121	17	-6	1	60	68	25*	4	105	11	-5	-4	163	14	-0	-8	106	21	-7*
-4	238	4	-5	2	139	16	-1	5	49	58	-11*	-3	100	8	-11	-7	41	27	29*
-3	89	21	-25*	3	125	10	-3	H,K=	3,-16	-2	238	5	3	-6	193	5	1		
-2	241	7	-6	4	22	50	-13*	-7	47	96	15*	-1	139	10	5	-5	200	7	-5
-1	248	4	-5	5	139	12	10	-6	156	24	-6	0	145	16	9	-4	219	3	0
0	0	44	-53*	H,K=	2,	15	-5	86	87	-16*	1	308	12	8	-3	260	4	-1	
1	298	7	-11	-7	172	14	-2	-4	126	8	18	2	74	37	6*	-2	18	67	-34*
2	211	26	-1	-6	81	15	-23*	-3	180	9	2	3	254	14	-12	-1	372	3	3
3	169	42	41*	-5	72	51	-29*	-2	0	43	-26*	4	259	18	-1	0	298	8	5
4	211	9	3	-4	224	10	10	-1	156	16	11	5	114	12	8	1	81	18	10*
5	30	67	12*	-3	90	35	7*	0	130	20	1	6	227	13	5	2	353	7	1
6	150	16	20	-2	161	14	14	1	0	45	-13*	7	95	25	13*	3	70	23	-2*
7	94	48	-12*	-1	156	29	-1*	2	176	9	-12	8	123	31	-0*	4	61	29	-1*

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL			
5	254	7	-1	-6	156	5	-2	3	351	3	-1	-12	91	35	18*	-3	628	1	0			
6	77	37	-17*	-5	261	9	-5	4	342	6	4	-11	187	9	10	-2	105	6	8			
7	236	5	-0	-4	283	3	-0	5	0	37	-8*	-10	0	40	-46*	-1	221	4	-3			
8	161	12	5	-3	187	4	4	6	302	8	-5	-9	220	7	2	0	288	4	-7			
9	53	27	-20*	-2	628	2	-1	7	153	6	7	-8	254	10	-2	1	464	3	2			
				H,K=	3,	-9	-1	153	6	-4	8	74	12	-9	-7	22	43	9*	2	589	3	5
-11	55	65	29*	0	203	2	-2	9	243	4	6	-6	466	9	-1	3	148	5	4			
-10	164	7	-1	1	346	2	-1	10	38	66	-40*	-5	226	4	-1	4	133	12	10			
-9	47	66	-0*	2	180	6	3				H,K=	3,	-4	-4	258	2	1	5	564	10	-1	
-8	156	15	3	3	242	9	6	-12	39	73	-10*	-3	404	2	2	6	126	7	-0			
-7	216	10	-12	4	342	10	-2	-11	147	9	-3	-2	59	42	-1*	7	198	6	-10			
-6	0	36	-13*	5	34	40	24*	-10	26	46	-0*	-1	707	3	0	8	216	14	-11			
-5	163	21	-4	6	247	4	-2	-9	187	8	8	0	636	1	-2	9	0	47	-33*			
-4	233	9	-12	7	193	6	-5	-8	304	6	-5	1	178	10	16	10	135	13	5			
-3	185	4	5	8	98	16	7	-7	123	10	-7	2	748	8	5				H,K=	3,	1	
-2	570	5	-1	9	203	8	1	-6	354	7	2	3	628	2	2	-12	107	29	-4*			
-1	283	6	-6	10	48	45	-5*	-5	401	3	1	4	93	12	2	-11	0	64	-20*			
0	275	6	-0				H,K=	3,	-6	-4	268	7	-4	5	361	3	-4	-10	223	9	-7	
1	489	3	-1	-12	69	27	16*	-3	595	2	1	6	27	34	-15*	-9	167	6	5			
2	0	34	-20*	-11	121	12	-8	-2	135	5	-0	7	159	14	-4	-8	163	4	-2			
3	412	3	4	-10	44	45	-5*	-1	251	3	1	8	220	4	-1	-7	338	8	-3			
4	265	7	2	-9	154	9	4	C	180	3	-3	9	0	47	-6*	-6	52	20	33*			
5	28	59	-15*	-8	195	6	-8	1	363	3	1	10	130	18	-1	-5	327	3	-4			
6	259	8	1	-7	111	7	12	2	432	3	7				H,K=	3,	-1	-4	882	2	2	
7	152	18	11	-6	289	10	8	3	575	2	3	-12	146	23	10	-3	255	5	2			
8	131	28	7*	-5	175	5	-3	4	346	6	4	-11	71	18	43*	-2	331	3	-1			
9	256	23	-8	-4	119	8	-1	5	332	4	2	-10	206	6	5	-1	527	2	0			
10	60	74	15*	-3	412	2	-4	6	53	26	8*	-9	108	14	9	0	389	3	-1			
				H,K=	3,	-8	-2	20	34	4*	7	215	5	5	-8	186	7	2	1	326	4	-4
-11	82	84	-19*	-1	308	5	4	8	262	16	5	-7	350	5	4	2	66	10	-9			
-10	71	15	34*	0	288	2	-3	9	67	79	11*	-6	245	4	-3	3	496	8	6			
-9	168	7	5	1	419	6	6	10	146	28	-8*	-5	292	3	4	4	344	9	1			
-8	169	18	-4	2	324	2	-1				H,K=	3,	-3	-4	556	3	3	5	76	10	14	
-7	64	11	35	3	488	3	-2	-12	87	38	-9*	-3	0	30	-22*	6	341	14	8			
-6	202	5	1	4	164	15	6	-11	18	65	-42*	-21	049	2	1	7	209	4	-2			
-5	43	51	-14*	5	308	5	-2	-10	181	5	-3	-1	442	2	5	8	86	25	-4*			
-4	211	6	-7	6	90	8	10	-9	150	15	-12	0	380	4	-5	9	162	15	3			
-3	255	4	-4	7	207	9	-3	-8	197	8	-0	1	638	2	0	10	95	38	28*			
-2	38	46	25*	8	252	12	-7	-7	388	3	-4	2	213	2	-0				H,K=	3,	2	
-1	444	9	3	9	47	66	-10*	-6	130	5	0	3	179	3	3	-12	85	54	8*			
0	428	5	5	10	193	10	-2	-5	259	10	-6	4	566	9	-0	-11	194	22	7			
1	195	5	2				H,K=	3,	-5	-4	259	2	2	5	39	24	35*	-10	91	15	8	
2	227	5	-6	-12	111	45	14*	-3	287	3	2	6	238	8	1	-9	282	15	-6			
3	266	4	-1	-11	18	61	-1*	-2	671	8	0	7	191	9	2	-8	331	8	0			
4	211	5	-4	-10	182	7	11	-1	152	4	-2	8	116	8	-6	-7	97	6	4			
5	297	8	1	-9	110	10	1	0	24	40	-16*	9	205	6	8	-6	315	3	-2			
6	69	42	27*	-8	136	5	2	1	592	8	2	10	89	37	16*	-5	88	15	-4			
7	209	8	-2	-7	333	4	-3	2	396	2	3				H,K=	3,	0	-4	211	4	8	
8	165	6	-10	-6	98	15	-12	3	304	2	1	-12	60	71	4*	-3	542	2	-3			
9	34	53	-3*	-5	383	8	-3	4	435	2	4	-11	194	8	-5	-2	98	6	5			
10	185	12	-9	-4	432	7	3	5	194	9	8	-10	43	51	-22*	-1	151	3	-6			
				H,K=	3,	-7	-3	38	9	3*	6	184	9	6	-9	252	6	-13	0	376	1	-1
-11	36	52	16*	-2	376	2	-0	7	134	15	4	-8	266	3	-2	1	219	4	5			
-10	197	22	-6	-1	84	6	-0	8	97	26	7*	-7	44	45	26*	2	442	6	-7			
-9	53	29	-9*	0	142	11	-7	9	256	7	5	-6	292	3	-3	3	323	4	-2			
-8	152	22	3	1	346	2	1	10	84	15	-10	-5	50	18	-8*	4	43	28	4*			
-7	292	13	-2	2	236	4	-0				H,K=	3,	-2	-4	299	5	3	5	354	4	2	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	154	19	-6	-8	132	13	2	3	111	20	-1	-1	125	12	-13	H,K=	3,	14	
7	156	6	4	-7	363	10	-8	4	319	5	-1	0	183	12	4	-7	36	50	3*
8	179	12	0	-6	132	8	-5	5	54	43	-13*	1	0	42	-15*	-6	149	34	10*
9	56	71	40*	-5	389	9	-2	6	171	16	4	2	203	7	7	-5	160	23	-12
10	143	11	6	-4	501	4	0	7	189	10	5	3	289	11	4	-4	40	48	27*
	H,K=	3,	3	-3	156	5	7	8	56	67	21*	4	82	16	18*	-3	202	14	-4
-12	97	32	-14*	-2	337	3	-2	H,K=	3,	8	5	191	9	4	-2	115	32	-4*	
-11	58	69	24*	-1	376	4	2	-11	180	14	3	6	87	34	5*	-1	127	13	15
-10	214	5	-2	0	268	3	1	-10	61	86	-10*	7	97	28	6*	0	217	27	13
-9	179	8	-2	1	385	2	-2	-9	169	11	14	H,K=	3,	11	1	51	60	24*	
-8	258	3	-3	2	185	3	-1	-8	224	6	0	-10	150	9	1	2	145	12	10
-7	359	4	-5	3	132	7	9	-7	48	57	42*	-9	113	35	-14*	3	100	17	7
-6	56	39	6*	4	263	14	-0	-6	328	5	-3	-8	45	82	12*	H,K=	3,	15	
-5	415	11	-10	5	93	15	17	-5	212	4	1	-7	243	5	2	-6	83	91	10*
-4	365	2	-2	6	239	10	-5	-4	245	8	1	-6	25	42	-28*	-5	90	32	15*
-3	115	4	4	7	210	7	6	-3	348	5	-3	-5	234	9	14	-4	168	9	-3
-2	489	4	-5	8	54	44	19*	-2	297	3	-2	-4	327	7	5	-3	19	45	-6*
-1	432	3	2	9	157	15	13	-1	331	7	2	-3	37	42	25*	-2	135	10	-6
0	351	3	1	H,K=	3,	6	0	353	8	-8	-2	267	6	6	-1	167	12	10	
1	565	8	-6	-12	0	50	-31*	1	62	33	-9*	-1	196	10	-1	0	19	66	-25*
2	42	50	14*	-11	189	21	8	2	218	3	2	0	75	41	-3*	1	167	9	6
3	320	4	6	-10	84	61	-6*	3	160	9	-8	1	232	5	2	2	60	66	-19*
4	254	6	-3	-9	138	14	12	4	103	16	-3	2	190	10	-8	H,K=	3,	16	
5	107	10	8	-8	160	10	6	5	212	15	-10	3	99	22	-6*	-4	53	65	14*
6	211	20	1	-7	51	63	21*	6	90	10	5	4	189	5	1	-3	164	8	5
7	186	8	-3	-6	320	9	-10	7	125	11	18	5	58	54	8*	-2	26	80	-55*
8	107	24	9*	-5	239	14	-4	8	149	12	11	6	176	19	19	-1	116	10	10
9	198	10	-6	-4	127	5	-9	H,K=	3,	9	H,K=	3,	12	0	190	14	19		
10	83	19	-1*	-3	316	3	-3	-11	0	64	-14*	-9	85	50	-13*	H,K=	4,	-19	
	H,K=	3,	4	-2	249	5	5	-10	156	7	5	-8	172	6	4	-3	55	65	5*
-12	40	85	-9*	-1	58	10	-4	-9	194	5	8	-7	30	44	22*	-2	151	16	14
-11	149	10	-11	0	274	6	-6	-8	28	68	8*	-6	153	33	-6*	-1	24	47	-18*
-10	95	15	14	1	187	8	6	-7	295	7	-6	-5	77	36	-12*	0	143	8	19
-9	140	11	-4	2	430	5	-4	-6	124	8	-1	-4	49	41	-16*	1	142	16	16
-8	215	15	-2	3	219	9	-3	-5	168	5	-3	-3	313	5	-1	2	47	56	29*
-7	70	50	17*	4	178	16	3	-4	280	8	-0	-2	101	13	-7	H,K=	4,	-18	
-6	276	9	-1	5	255	8	3	-3	80	9	27	-1	112	15	7	-5	41	71	28*
-5	157	3	5	6	75	18	-6*	-2	272	3	0	0	249	9	7	-4	95	22	8*
-4	37	42	9*	7	163	7	15	-1	233	10	2	1	68	28	18*	-3	96	44	-22*
-3	339	3	-2	8	176	8	1	0	82	9	20	2	161	20	18	-2	52	53	33*
-2	74	11	-8	9	60	72	46*	1	269	9	-1	3	151	26	4	-1	134	9	11
-1	223	5	-3	H,K=	3,	7	2	96	20	11*	4	54	33	-19*	0	64	86	-25*	
0	405	2	-0	-12	146	33	4*	3	133	19	10	5	211	26	22	1	83	41	-11*
1	125	7	-8	-11	0	54	-13*	4	254	14	-11	H,K=	3,	13	2	178	18	10	
2	462	6	-4	-10	182	17	-6	5	57	37	44*	-8	49	68	13*	3	61	67	5*
3	336	6	3	-9	197	10	-13	6	129	52	1*	-7	159	7	-3	4	140	20	0
4	129	13	3	-8	63	17	28*	7	130	17	8	-6	38	51	-24*	H,K=	4,	-17	
5	275	11	-3	-7	282	7	5	H,K=	3,	10	-5	161	13	6	-6	0	82	-14*	
6	76	21	-11*	-6	21	56	-39*	-10	58	70	6*	-4	204	8	-4	-5	124	22	0
7	209	7	3	-5	318	7	-0	-9	124	52	-3*	-3	73	74	6*	-4	80	23	-12*
8	228	7	2	-4	475	3	-1	-8	244	4	1	-2	196	10	-13	-3	47	64	-4*
9	20	48	-5*	-3	109	6	7	-7	31	45	4*	-1	143	11	-2	-2	162	10	13
	H,K=	3,	5	-2	247	6	-8	-6	289	8	3	0	0	48	-42*	-1	0	62	-57*
-12	150	18	-8	-1	265	5	-0	-5	227	4	2	1	195	11	20	0	147	28	-1*
-11	0	52	-13*	0	84	19	7*	-4	125	18	15	2	77	30	-0*	1	162	20	12
-10	205	6	15	1	378	11	-3	-3	280	3	-4	3	122	21	8	2	74	22	63*
-9	102	18	-11	2	145	5	1	-2	153	12	-1	4	147	33	-4*	3	171	11	6

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
4	121	25	18*	-5	197	12	17	-10	45	80	36*	3	183	3	-2	-11	28	43	-7*	
5	96	20	5*	-4	219	13	-2	-9	166	29	-12	4	274	4	4	-10	173	14	-3	
H,K= 4,-16				-3	158	6	-10	-8	69	15	-6*	5	233	5	-1	-9	105	20	3*	
-7	45	48	-8*	-2	248	4	6	-7	108	12	6	6	85	15	1	-8	100	24	-1*	
-6	149	19	8	-1	47	56	2*	-6	249	16	9	7	280	6	-7	-7	352	3	3	
-5	64	76	15*	0	114	23	7*	-5	64	35	5*	8	212	6	-2	-6	12	33	-11*	
-4	100	58	-11*	1	227	10	7	-4	176	10	-4	9	30	45	-9*	-5	392	5	-1	
-3	141	10	-6	2	17	52	5*	-3	229	3	-3	H,K= 4,				-7	-4	213	5	-3
-2	73	18	-12*	3	275	7	4	-2	20	32	4*-12	77	84	2*	-3	86	12	-12		
-1	193	14	2	4	182	7	-12	-1	424	4	-1	-11	0	46	-23*	-2	435	3	-2	
0	172	11	-8	5	119	17	-1	0	209	10	1	-10	201	7	11	-1	310	2	-1	
1	76	53	-8*	6	217	9	-5	1	123	9	-7	-9	60	64	-3*	0	448	4	-3	
2	167	28	4	7	52	56	-4*	2	486	4	-6	-8	140	10	10	1	283	2	0	
3	68	25	-30*	8	109	45	-18*	3	179	4	5	-7	293	8	-2	2	76	16	4*	
4	116	13	-4	H,K= 4,-12				4	151	4	5	-6	106	6	3	3	474	8	8	
5	169	35	8*-10	65	41	57*	5	209	10	-2	-5	347	4	-7	4	142	11	-0		
6	65	25	35*	-9	169	8	-5	6	36	73	30*	-4	255	5	-0	5	57	13	12*	
H,K= 4,-15				-8	118	20	-3	7	166	11	-7	-3	119	10	1	6	310	3	-1	
-8	99	23	20*	-7	38	50	-15*	8	152	18	-19	-2	367	2	-1	7	104	16	2	
-7	127	19	1	-6	192	5	5	9	85	24	21*	-1	194	5	1	8	168	10	7	
-6	44	53	11*	-5	80	19	23*	H,K= 4,				-9	0	370	4	1	9	217	19	-8
-5	136	13	20	-4	105	47	-11*-11	62	26	20*	1	483	2	0	10	65	71	49*		
-4	142	9	-13	-3	292	10	6	-10	174	13	6	2	43	10	29*	H,K= 4,				-4
-3	162	8	-19	-2	9	49	-28*	-9	24	51	9*	3	365	4	5	-12	108	22	9*	
-2	239	10	4	-1	228	6	-0	-8	189	5	9	4	253	3	-3	-11	109	20	-0	
-1	46	54	-8*	0	166	5	2	-7	252	4	-1	5	100	8	4	-10	67	83	26*	
0	154	10	1	1	85	20	26*	-6	36	66	33*	6	261	9	9	-9	132	8	5	
1	205	5	9	2	280	8	-6	-5	276	4	-3	7	218	5	-1	-8	348	7	-0	
2	44	49	40*	3	155	22	-1	-4	291	6	-6	8	128	18	13	-7	99	12	-9	
3	158	7	3	4	249	7	-4	-3	99	11	-4	9	180	10	-12	-6	396	6	0	
4	202	8	-8	5	249	12	-7	-2	475	2	2	10	0	54	-19*	-5	229	5	4	
5	33	77	-25*	6	56	68	41*	-1	202	3	-3	H,K= 4,				-6	-4	367	3	0
6	146	9	-12	7	132	13	-9	0	332	5	-1	-12	92	19	3*	-3	302	2	-1	
7	61	73	38*	8	79	36	-22*	1	414	2	1	-11	124	36	7*	-2	110	19	3	
H,K= 4,-14				H,K= 4,-11				2	51	23	26*-10	25	53	8*	-1	308	8	2		
-9	88	31	2*-10	160	16	7	3	220	4	-6	-9	140	8	4	0	172	2	2		
-8	73	27	-12*	-9	37	50	-6*	4	331	5	3	-8	186	9	0	1	262	4	0	
-7	58	54	-15*	-8	167	21	6	5	45	54	11*	-7	200	6	5	2	502	9	2	
-6	115	26	-2*	-7	201	6	-6	6	193	11	5	-6	325	2	-2	3	315	2	-2	
-5	84	27	-6*	-6	9	66	-13*	7	155	9	3	-5	107	6	10	4	335	2	1	
-4	207	12	-9	-5	190	5	2	8	141	9	-7	-4	239	8	-2	5	375	13	-7	
-3	219	12	6	-4	255	6	1	9	201	9	5	-3	385	4	1	6	96	18	-19*	
-2	67	20	10*	-3	73	13	25	H,K= 4,				-8	-2	310	6	7	7	247	6	-3
-1	194	8	3	-2	364	7	-6	-11	135	11	13	-1	414	3	-2	8	186	10	3	
0	86	12	3	-1	153	15	-10	-10	0	62	-11*	0	503	7	-3	9	40	47	17*	
1	100	20	2*	0	230	4	0	-9	212	7	7	1	463	6	4	10	140	19	-15	
2	288	9	4	1	331	2	1	-8	118	8	-4	2	361	3	4	H,K= 4,				-3
3	141	7	-6	2	82	9	31	-7	151	13	4	3	203	3	2	-12	76	30	-3*	
4	106	11	-22	3	249	9	5	-6	219	6	2	4	328	4	6	-11	67	68	-6*	
5	257	6	1	4	227	8	-5	-5	45	48	-6*	5	336	5	-2	-10	165	11	1	
6	21	63	-3*	5	77	12	4	-4	165	15	-5	6	72	20	-0*	-9	158	5	2	
7	193	6	5	6	160	20	3	-3	194	6	2	7	277	3	0	-8	138	22	-4	
H,K= 4,-13				7	102	24	2*	-2	120	9	6	8	184	10	-9	-7	345	5	1	
-9	34	74	-5*	8	136	11	-3	-1	282	4	1	9	56	77	-5*	-6	154	3	4	
-8	120	11	-11	9	167	11	-0	0	244	5	-4	10	154	31	-21*	-5	489	3	4	
-7	155	10	0	H,K= 4,-10				1	404	3	1	H,K= 4,				-5	-4	456	7	-0
-6	55	17	43*-11	119	37	7*	2	565	9	3	-12	37	50	-13*	-3	350	9	2		

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	414	1	-0	5	175	10	11	-11	195	14	-5	0	526	2	-3	-9	200	8	1
-1	128	5	-5	6	315	4	-5	-10	33	48	21*	1	184	9	-1	-8	0	41	-34*
0	186	7	-3	7	151	6	10	-9	199	7	-8	2	316	2	-5	-7	304	4	-6
1	302	3	-2	8	100	21	16*	-8	152	7	-3	3	68	9	-9	-6	24	44	10*
2	330	2	4	9	145	8	-10	-7	72	33	-4*	4	137	6	5	-5	262	7	-8
3	290	5	1	10	0	55	-52*	-6	319	3	0	5	247	4	2	-4	123	15	-8
4	408	4	-6		H,K= 4,	0		-5	315	2	1	6	50	19	16*	-3	74	8	6
5	25	45	11*-13	6	72	72	-1*	-4	155	13	-5	7	150	7	-12	-2	247	11	-5
6	265	5	-1	-12	110	19	3	-3	389	6	-2	8	194	6	10	-1	261	6	-1
7	59	32	15*-11	198	15	-11	-2	211	7	-6	9	49	58	41*	0	112	5	4	
8	136	8	9	-10	36	67	29*	-1	323	2	-2		H,K= 4,	5	1	279	8	4	
9	146	14	18	-9	270	7	-8	0	466	9	-5	-12	161	9	2	2	94	13	0
10	54	67	35*	-8	128	5	-3	1	92	5	13	-11	38	65	13*	3	241	3	7
		H,K= 4,	-2	-7	133	13	7	2	442	6	0	-10	242	7	-21	4	169	8	12
-13	28	64	-9*	-6	310	3	-4	3	259	6	-0	-9	213	6	-3	5	16	55	1*
-12	132	8	24	-5	328	2	-3	4	106	10	11	-8	13	43	-27*	6	157	14	-21
-11	169	11	-5	-4	309	3	-0	5	293	3	-6	-7	252	12	-5	7	137	12	23
-10	38	44	6*	-3	671	4	5	6	21	37	4*	-6	56	29	32*	8	62	72	-13*
-9	247	8	2	-2	321	2	4	7	186	16	-4	-5	303	3	-2		H,K= 4,	8	
-8	229	4	-2	-1	281	2	-2	8	173	10	6	-4	260	3	-1	-11	133	18	-7
-7	113	15	6	0	322	3	-2	9	41	51	30*	-3	37	44	-8*	-10	43	52	19*
-6	359	3	-2	1	34	39	14*		H,K= 4,	3	-2	340	3	-3	-9	171	6	9	
-5	44	13	11*	2	214	5	-4	-12	122	14	-26	-1	360	4	4	-8	236	8	-3
-4	304	5	9	3	164	3	-1	-11	0	46	-45*	0	318	4	-2	-7	45	23	25*
-3	872	2	4	4	206	17	-6	-10	253	10	-10	1	254	7	0	-6	329	6	1
-2	48	21	-2*	5	327	6	-4	-9	98	12	-5	2	57	23	15*	-5	207	9	3
-1	98	3	8	6	121	35	-4*	-8	246	7	-5	3	284	7	-1	-4	190	6	-10
0	80	8	-4	7	251	3	1	-7	294	6	-7	4	166	12	1	-3	212	4	0
1	286	8	0	8	170	10	-2	-6	27	37	6*	5	0	54	-11*	-2	80	14	13
2	504	5	1	9	35	47	23*	-5	416	2	-3	6	291	10	-3	-1	241	4	-1
3	392	3	5	10	119	67	-2*	-4	540	3	4	7	192	6	5	0	227	13	-5
4	394	3	0		H,K= 4,	1	-3	74	7	16	8	74	23	20*	1	28	44	13*	
5	332	3	-6	-13	114	24	9*	-2	629	4	-4		H,K= 4,	6	2	315	11	5	
6	76	11	9	-12	130	24	-6*	-1	321	3	-3	-12	87	24	-16*	3	176	13	-1
7	171	7	-6	-11	74	43	18*	0	325	6	-3	-11	204	8	2	4	126	35	-14*
8	121	10	-5	-10	219	12	-14	1	561	4	-2	-10	48	51	13*	5	186	11	0
9	40	53	32*	-9	140	24	-14	2	184	10	6	-9	168	7	-0	6	80	18	14*
10	155	8	4	-8	222	3	4	3	231	12	-4	-8	243	9	-4	7	137	12	13
		H,K= 4,	-1	-7	336	5	4	4	273	7	2	-7	103	12	-9		H,K= 4,	9	
-13	124	22	11	-6	26	42	12*	5	31	42	22*	-6	267	3	-5	-11	68	61	19*
-12	151	12	7	-5	237	6	1	6	280	6	-0	-5	90	18	-5*	-10	156	11	19
-11	71	60	14*	-4	576	2	4	7	197	13	-3	-4	353	10	6	-9	94	19	-19*
-10	153	7	5	-3	97	6	-6	8	82	44	4*	-3	460	2	-1	-8	116	20	9
-9	224	10	6	-2	328	4	-4	9	148	26	9	-2	225	9	12	-7	291	4	0
-8	131	9	3	-1	287	3	-1		H,K= 4,	4	-1	434	10	2	-6	83	33	-5*	
-7	179	5	-5	0	274	6	-1	-12	0	85	-61*	0	362	3	-8	-5	269	4	-4
-6	74	10	6	1	369	2	-4	-11	172	24	-6	1	39	47	-28*	-4	194	9	-11
-5	465	5	0	2	116	5	3	-10	77	33	58*	2	292	8	8	-3	0	41	-40*
-4	593	3	3	3	271	3	-1	-9	131	27	-17*	3	99	20	-17*	-2	248	10	2
-3	153	8	11	4	296	2	-1	-8	150	5	-8	4	147	12	-3	-1	117	12	-1
-2	357	3	-1	5	39	46	12*	-7	155	4	-1	5	242	13	-2	0	101	10	-4
-1	78	10	-5	6	310	3	3	-6	276	3	-2	6	143	12	-0	1	265	6	-1
0	111	3	-5	7	158	10	6	-5	60	19	16*	7	114	9	-16	2	112	24	-8*
1	255	3	-6	8	72	28	-8*	-4	174	5	3	8	152	8	10	3	173	9	11
2	94	11	-2	9	176	17	2	-3	549	3	-2		H,K= 4,	7	4	201	7	7	
3	285	3	-2		H,K= 4,	2	-2	277	3	-0	-11	56	67	17*	5	0	45	-23*	
4	533	3	3	-12	105	14	3	-1	515	6	-16	-10	197	9	-4	6	147	10	2

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	4,	10	-2	167	9	18	-5	0	65	-7*	1	126	19	5	-2	89	13	1
-10	57	68	24*	-1	124	15	-18	-4	114	19	5	2	37	44	-2*	-1	435	5	-4
-9	99	27	2*	0	59	78	4*	-3	144	7	2	3	253	4	-2	0	133	8	-1
-8	151	18	-8	1	171	25	-5	-2	0	72	-45*	4	170	12	2	1	104	12	-6
-7	28	42	16*	2	30	65	-19*	-1	202	17	-1	5	158	15	16	2	318	3	1
-6	231	11	-2	3	79	26	-4*	0	104	27	-10*	6	201	6	-1	3	105	33	-1*
-5	167	14	11	H,K=	4,	14		1	181	7	-6	7	35	73	-32*	4	209	4	-2
-4	191	9	-8	-7	51	60	24*	2	218	11	16	H,K=	5,-12			5	190	11	-3
-3	268	6	2	-6	140	22	6	3	102	18	3	-10	39	51	4*	6	103	22	11*
-2	130	11	-8	-5	155	19	-5	4	147	8	-9	-9	156	18	15	7	207	7	-1
-1	190	10	7	-4	88	29	32*	5	135	8	4	-8	105	36	-2*	8	85	25	-15*
0	240	4	4	-3	174	14	6	6	50	60	38*	-7	113	18	9	H,K=	5,	-9	
1	28	65	-17*	-2	60	39	7*	H,K=	5,-15			-6	228	10	3	-11	96	27	35*
2	179	8	3	-1	138	15	-8	-8	85	24	-9*	-5	14	39	-38*	-10	130	15	-6
3	133	8	6	0	181	21	14	-7	104	11	4	-4	175	6	5	-9	60	32	-15*
4	86	16	2*	1	43	56	38*	-6	61	44	15*	-3	167	4	0	-8	159	15	6
5	169	9	-10	2	153	12	23	-5	148	17	-4	-2	57	28	4*	-7	185	7	-1
6	79	24	19*	H,K=	4,	15		-4	66	79	-3*	-1	185	8	-9	-6	87	18	11*
	H,K=	4,	11	-5	97	56	1*	-3	136	7	17	0	85	15	3	-5	217	4	-2
-10	167	10	8	-4	143	11	3	-2	223	8	-0	1	125	8	6	-4	228	3	-4
-9	141	10	14	-3	0	62	-1*	-1	40	33	-6*	2	295	5	0	-3	174	12	8
-8	61	68	13*	-2	167	27	5	0	252	11	1	3	105	14	5	-2	341	7	1
-7	182	6	8	-1	120	11	-5	1	135	19	3	4	213	6	-11	-1	127	15	5
-6	49	60	-6*	0	0	64	-57*	2	65	66	-6*	5	198	10	-2	0	269	8	-3
-5	186	9	-5	H,K=	5,-19			3	222	5	6	6	86	16	-17*	1	257	4	-0
-4	249	10	3	-3	112	14	39	4	140	34	-7*	7	179	15	7	2	93	12	-8
-3	102	22	-0*	-2	137	13	-0	5	76	58	3*	8	92	60	5*	3	305	8	-3
-2	207	5	-1	-1	23	69	16*	6	168	8	9	H,K=	5,-11			4	239	5	2
-1	205	11	3	0	138	15	22	H,K=	5,-14	-10	116	16	-8	5	147	11	-4		
0	113	17	12	1	121	23	1*	-9	62	67	-23*	-9	0	52	-34*	6	315	11	0
1	182	14	-1	2	38	82	-6*	-8	78	21	11*	-8	155	6	1	7	95	52	0*
2	119	7	10	H,K=	5,-18			-7	98	19	-0*	-7	183	11	-7	8	111	31	-4*
3	105	44	-16*	-5	26	75	18*	-6	105	61	-13*	-6	97	27	17*	9	100	25	-27*
4	170	7	3	-4	112	21	5*	-5	40	81	-2*	-5	204	9	10	H,K=	5,	-8	
5	11	57	-9*	-3	145	10	18	-4	254	9	2	-4	233	9	-12	-12	80	21	-5*
	H,K=	4,	12	-2	47	39	-4*	-3	195	5	7	-3	155	7	-1	-11	116	30	12*
-9	143	26	21	-1	125	27	8*	-2	0	54	-36*	-2	225	6	-4	-10	0	61	-33*
-8	139	16	-1	0	70	70	5*	-1	234	4	1	-1	90	22	14*	-9	218	10	8
-7	55	71	48*	1	127	31	26*	0	60	76	-3*	0	269	4	2	-8	104	11	10
-6	185	6	13	2	175	6	14	1	189	11	5	1	246	10	-5	-7	150	9	10
-5	149	7	5	3	69	41	48*	2	218	5	12	2	84	12	-0	-6	242	3	1
-4	82	16	-16*	H,K=	5,-17			3	43	51	25*	3	271	6	-2	-5	63	13	-25*
-3	222	9	-4	-6	49	81	12*	4	188	6	-12	4	269	6	-6	-4	304	5	-2
-2	17	54	-2*	-5	131	9	4	5	225	9	3	5	147	19	-8	-3	510	2	-2
-1	213	8	5	-4	91	40	3*	6	49	58	26*	6	180	8	5	-2	104	10	4
0	240	6	-13	-3	126	16	11	7	175	12	9	7	71	19	21*	-1	336	2	-2
1	60	21	42*	-2	164	7	4	H,K=	5,-13			8	155	6	22	0	196	8	-3
2	161	18	16	-1	62	77	22*	-9	30	46	7*	H,K=	5,-10			1	166	5	-3
3	126	31	17*	0	171	6	6	-8	118	30	-5*	-11	87	50	-12*	2	340	6	4
4	72	22	19*	1	114	10	-12	-7	138	17	7	-10	43	58	15*	3	124	7	8
	H,K=	4,	13	2	21	65	12*	-6	55	59	25*	-9	177	8	8	4	299	8	6
-8	87	17	-22*	3	177	17	2	-5	248	12	13	-8	72	14	4*	5	185	8	4
-7	162	34	9*	4	89	22	-4*	-4	133	6	-5	-7	164	7	7	6	73	20	19*
-6	105	38	15*	5	41	65	-14*	-3	114	17	-6	-6	214	10	5	7	267	10	1
-5	116	37	-2*	H,K=	5,-16			-2	184	6	6	-5	0	50	-15*	8	107	20	-2*
-4	187	7	-4	-7	47	61	-26*	-1	26	52	12*	-4	172	8	5	9	49	72	1*
-3	35	57	20*	-6	110	15	-1	0	202	5	-2	-3	322	4	-2	H,K=	5,	-7	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	80	25	5*	-1	77	8	4	9	138	24	-5	-6	399	2	-6	4	132	15	5
-11	86	24	11*	0	313	5	1		H,K=	5,	-2	-5	175	3	6	5	181	11	-9
-10	226	10	7	1	302	2	-0	-13	43	59	15*	-4	89	8	4	6	18	43	12*
-9	100	18	-7	2	127	9	-1	-12	168	25	13	-3	198	7	-11	7	152	7	19
-8	150	13	-3	3	303	3	2	-11	143	11	1	-2	88	18	-4*	8	137	18	15
-7	205	6	-8	4	235	4	-11	-10	50	54	34*	-1	581	4	-3		H,K=	5,	3
-6	111	10	8	5	0	54	-23*	-9	197	5	8	0	325	5	2	-12	129	27	-14*
-5	326	6	4	6	292	4	-3	-8	205	3	2	1	41	44	-2*	-11	79	47	-1*
-4	220	3	-1	7	69	19	-9*	-7	151	13	9	2	390	4	-0	-10	279	12	-5
-3	97	8	8	8	139	29	-4*	-6	303	4	10	3	109	8	16	-9	141	14	1
-2	453	4	-1	9	185	13	5	-5	32	39	1*	4	257	3	2	-8	129	11	-13
-1	109	7	4		H,K=	5,	-4	-4	613	2	1	5	246	7	1	-7	236	4	5
0	218	7	0	-12	133	14	1	-3	460	3	-1	6	97	15	4	-6	43	51	29*
1	399	3	3	-11	145	19	-5	-2	26	32	-22*	7	156	6	-3	-5	340	5	1
2	53	12	-16*	-10	87	19	-4*	-1	611	4	1	8	160	11	14	-4	235	8	4
3	324	4	3	-9	149	11	-1	0	624	2	0	9	58	69	12*	-3	215	7	4
4	136	15	-6	-8	203	7	-3	1	107	16	-4		H,K=	5,	1	-2	404	3	-4
5	73	41	-8*	-7	247	5	3	2	303	2	-3	-13	88	35	-21*	-1	244	5	-0
6	295	5	1	-6	357	4	-0	3	174	5	6	-12	127	20	-6	0	198	3	3
7	96	15	4	-5	206	6	-3	4	229	3	0	-11	128	39	2*	1	312	10	-7
8	118	9	2	-4	611	2	2	5	407	9	-6	-10	237	7	5	2	84	9	2
9	143	11	-9	-3	346	2	-1	6	0	47	-18*	-9	107	24	-1*	3	207	4	-1
	H,K=	5,	-6	-2	292	4	2	7	240	7	-5	-8	216	15	-7	4	188	8	6
-12	122	10	3	-1	518	2	0	8	181	9	-1	-7	393	3	-1	5	186	4	2
-11	136	8	18	0	323	2	1	9	69	23	26*	-6	0	36	-18*	6	208	20	-4
-10	49	59	11*	1	411	5	4		H,K=	5,	-1	-5	365	3	1	7	135	18	12
-9	184	12	-4	2	430	5	9	-13	113	10	2	-4	266	6	5	8	92	33	1*
-8	153	5	-4	3	67	13	-2*	-12	111	10	6	-3	114	16	-1		H,K=	5,	4
-7	159	11	3	4	46	32	-10*	-11	57	20	-12*	-2	427	2	1	-12	118	21	10
-6	278	4	4	5	359	5	-5	-10	166	5	18	-1	286	3	1	-11	197	22	-1
-5	61	40	10*	6	25	40	-24*	-9	148	9	-14	0	463	4	6	-10	11	53	4*
-4	389	3	-3	7	240	5	-2	-8	205	4	6	1	286	3	-2	-9	236	11	-2
-3	488	2	-0	8	180	11	-2	-7	238	4	3	2	97	5	-2	-8	131	14	7
-2	32	14	23*	9	54	56	-13*	-6	113	4	8	3	352	12	-1	-7	86	12	11
-1	358	3	-2		H,K=	5,	-3	-5	395	2	0	4	233	3	-3	-6	298	4	-6
0	437	2	1	-13	155	11	21	-4	197	4	3	5	138	13	12	-5	91	16	-4
1	304	6	-2	-12	59	83	-16*	-3	74	9	2	6	270	11	8	-4	283	4	6
2	417	6	4	-11	86	23	21*	-2	239	5	-10	7	79	26	-8*	-3	414	2	1
3	71	8	1	-10	159	8	12	-1	261	2	1	8	111	11	9	-2	48	48	4*
4	321	4	-9	-9	84	20	-15*	0	270	3	0	9	136	29	-3*	-1	370	5	-2
5	209	3	2	-8	136	5	4	1	412	6	-1		H,K=	5,	2	0	327	2	0
6	92	31	-15*	-7	227	3	-1	2	47	53	13*	-12	111	17	10	1	149	11	-11
7	233	5	-7	-6	55	55	19*	3	410	7	7	-11	184	6	-1	2	337	14	-4
8	134	19	-1	-5	450	4	5	4	64	18	-8*	-10	0	60	-12*	3	118	7	8
9	52	58	-5*	-4	111	16	-11	5	236	5	6	-9	226	5	-4	4	190	8	12
	H,K=	5,	-5	-3	242	5	6	6	405	3	-9	-8	145	15	-3	5	251	7	-2
-12	76	77	26*	-2	186	5	1	7	121	13	5	-7	24	47	-13*	6	104	30	-10*
-11	107	9	12	-1	118	7	3	8	134	8	8	-6	338	4	-5	7	121	19	-14
-10	208	6	1	0	242	3	5	9	163	15	8	-5	79	6	9	8	145	26	17
-9	59	26	15*	1	353	2	-0		H,K=	5,	0	-4	311	3	4		H,K=	5,	5
-8	164	4	5	2	36	43	16*	-13	17	47	-33*	-3	414	5	0	-12	113	30	7*
-7	226	3	-7	3	298	11	1	-12	125	9	-11	-2	33	36	30*	-11	73	66	5*
-6	50	59	18*	4	195	4	-12	-11	139	8	-0	-1	417	2	-2	-10	240	6	3
-5	462	2	-0	5	87	13	14	-10	40	48	-1*	0	318	4	-8	-9	155	11	3
-4	162	6	-2	6	410	8	-11	-9	193	7	-0	1	54	64	-9*	-8	173	8	1
-3	34	41	6*	7	90	29	-7*	-8	207	4	-6	2	370	2	0	-7	180	9	0
-2	548	2	-1	8	151	17	8	-7	124	6	11	3	111	35	-11*	-6	0	43	-27*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	248	7	-0	-9	168	7	8	-3	114	8	2	-4	30	46	-23*	-10	92	17	-0*
-4	224	3	-3	-8	175	16	14	-2	242	7	3	-3	137	9	8	-9	61	72	59*
-3	23	44	4*	-7	45	54	19*	-1	133	25	-6*	-2	126	20	-8	-8	118	20	6
-2	267	2	-4	-6	311	4	7	0	87	22	-13*	-1	43	51	34*	-7	131	28	2*
-1	164	3	-0	-5	162	10	-11	1	191	10	-2	0	196	6	7	-6	64	21	6*
0	182	4	-6	-4	190	10	-1	2	0	48	-36*	1	72	15	-0*	-5	242	12	3
1	328	9	-0	-3	298	5	3	3	137	18	2	2	57	28	5*	-4	60	72	15*
2	83	20	6*	-2	50	60	43*	4	140	18	19	3	169	8	15	-3	89	30	16*
3	250	6	5	-1	225	10	5	H,K=	5, 12	4	94	22	23*	-2	230	9	-1		
4	120	21	-0	0	226	7	2	-8	128	16	9	H,K=	6,-16	-1	0	49	-26*		
5	27	55	13*	1	47	56	32*	-7	0	68	-44*	-7	85	86	13*	0	228	8	2
6	162	11	3	2	289	7	10	-6	222	14	9	-6	134	12	14	1	170	14	7
7	104	21	12*	3	105	10	3	-5	158	25	11	-5	50	60	1*	2	103	18	-3
H,K=	5,	6	4	109	21	14*	-4	84	46	-9*	-4	158	13	10	3	227	7	-1	
-12	132	25	-7*	5	181	16	1	-3	165	7	11	-3	157	24	-10	4	121	28	-4*
-11	168	14	-4	6	54	77	21*	-2	51	72	22*	-2	7	59	-31*	5	161	20	-8
-10	24	55	23*	H,K=	5, 9	-1	153	15	4	-1	210	8	11	6	202	14	5		
-9	167	13	-0	-10	145	13	-10	0	128	36	7*	0	58	24	-4*	7	27	58	-10*
-8	227	5	-4	-9	56	66	-16*	1	9	63	-38*	1	153	7	-1	H,K=	6,-12		
-7	106	21	22*	-8	134	16	18	2	155	18	7	2	183	25	-11	-10	46	59	-9*
-6	345	8	2	-7	189	6	-9	3	105	18	15	3	48	53	27*	-9	132	21	-8
-5	232	5	-6	-6	61	25	-23*	H,K=	5, 13	4	124	13	0	-8	37	47	-28*		
-4	188	8	-1	-5	254	6	-7	-7	146	26	-3	5	150	15	8	-7	146	20	16
-3	266	4	-3	-4	224	8	8	-6	49	52	6*	H,K=	6,-15	-6	227	6	5		
-2	45	48	-7*	-3	80	30	0*	-5	147	15	12	-8	117	25	14*	-5	13	39	-13*
-1	328	4	-0	-2	271	10	7	-4	149	12	16	-7	88	15	6	-4	284	5	-0
0	227	5	3	-1	101	23	11*	-3	42	61	29*	-6	92	17	-21	-3	122	10	1
1	0	48	-15*	0	64	17	-13*	-2	174	12	-0	-5	180	24	12	-2	47	16	9*
2	289	3	-2	1	293	9	-0	-1	64	65	-30*	-4	66	73	16*	-1	295	7	2
3	80	25	17*	2	28	41	6*	0	101	11	10	-3	70	23	20*	0	142	5	-0
4	145	38	13*	3	129	16	3	1	162	18	15	-2	187	5	2	1	184	5	-3
5	254	8	11	4	157	20	2	H,K=	5, 14	-1	0	59	-24*	2	288	12	-1		
6	48	58	4*	5	22	47	-38*	-5	115	13	31	0	222	15	-2	3	75	30	1*
7	149	19	10	H,K=	5, 10	-4	80	26	11*	1	131	10	8	4	190	5	5		
H,K=	5,	7	-10	45	55	19*	-3	144	28	-9*	2	75	28	3*	5	109	25	1*	
-11	61	73	-3*	-9	172	16	-1	-2	8	62	-41*	3	209	5	-3	6	68	18	24*
-10	132	15	-20	-8	156	13	3	-1	116	23	-1*	4	41	45	-5*	7	173	7	0
-9	0	44	-30*	-7	0	57	-23*	0	122	15	-8	5	124	11	6	H,K=	6,-11		
-8	158	19	-1	-6	182	10	9	H,K=	6,-19	6	182	13	-12	-11	57	67	-6*		
-7	243	7	1	-5	138	9	1	-3	94	29	8*	H,K=	6,-14	-10	121	30	3*		
-6	49	29	-23*	-4	203	7	6	-2	138	11	13	-9	110	11	11	-9	68	55	38*
-5	291	8	0	-3	206	18	-3	-1	41	57	20*	-8	69	70	13*	-8	147	7	12
-4	219	4	-1	-2	41	44	-12*	0	153	44	24*	-7	132	11	20	-7	140	10	0
-3	124	10	3	-1	308	7	5	1	73	60	-7*	-6	169	18	5	-6	105	16	10
-2	330	6	5	0	247	8	-3	H,K=	6,-18	-5	0	59	-49*	-5	253	4	-3		
-1	129	8	-20	1	0	60	-27*	-5	0	56	-3*	-4	172	14	13	-4	65	37	3*
0	150	5	-6	2	178	17	2	-4	126	22	13	-3	156	7	15	-3	249	3	-1
1	331	10	6	3	88	14	1	-3	128	10	-3	-2	37	65	14*	-2	210	7	5
2	58	15	5*	4	113	44	11*	-2	77	22	22*	-1	325	4	1	-1	38	47	-20*
3	206	14	-5	5	160	17	13	-1	166	25	11	0	101	16	-6	0	209	5	4
4	187	5	12	H,K=	5, 11	0	63	75	23*	1	135	10	5	1	321	4	-3		
5	17	73	9*	-9	129	21	37	1	137	15	14	2	200	14	13	2	91	29	15*
6	161	12	-14	-8	110	20	18	2	117	28	8*	3	35	41	4*	3	281	5	1
7	90	35	7*	-7	170	12	-4	3	15	68	4*	4	209	9	-1	4	128	24	6*
H,K=	5,	8	-6	36	59	15*	H,K=	6,-17	5	118	10	2	5	233	8	-0			
-11	100	35	-22*	-5	153	12	18	-6	0	56	-42*	6	71	57	28*	6	200	6	2
-10	0	76	-13*	-4	164	12	10	-5	120	9	4	H,K=	6,-13	7	26	44	1*		

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL		
	H,K=	6,-	10	2	303	5	-6	-7	181	4	-6	6	274	5	-1	-6	483	8	-7		
-11	75	83	15*	3	48	42	25*	-6	43	45	30*	7	103	23	-16*	-5	54	65	39*		
-10	49	43	15*	4	240	6	1	-5	261	9	6	8	124	28	-11*	-4	244	4	0		
-9	162	16	11	5	312	5	5	-4	261	4	4				H,K=	6,-	2	-3	230	4	-6
-8	69	28	-1*	6	68	42	9*	-3	87	17	8*	-13	36	61	19*	-2	59	23	2*		
-7	152	5	7	7	186	19	7	-2	330	2	1	-12	145	10	5	-1	244	9	-3		
-6	146	10	-6	8	65	53	-36*	-1	44	16	16*	-11	163	15	-9	0	127	10	1		
-5	34	40	6*				H,K=	6,-	7	0	183	4	0	-10	93	40	27*	1	169	4	-1
-4	368	5	-3	-12	69	82	8*	1	344	7	-3	-9	179	5	-6	2	376	4	5		
-3	150	6	-4	-11	119	16	5	2	32	36	11*	-8	177	6	1	3	96	10	13		
-2	78	13	5	-10	169	12	13	3	246	7	7	-7	71	22	15*	4	178	8	-10		
-1	359	7	-2	-9	50	50	46*	4	45	53	6*	-6	490	4	-2	5	245	9	0		
0	132	18	-6	-8	166	10	2	5	137	14	9	-5	76	16	-9*	6	0	53	-7*		
1	172	4	5	-7	183	5	3	6	292	13	-8	-4	295	5	1	7	142	15	21		
2	376	7	-3	-6	97	17	1	7	41	70	28*	-3	246	2	2	8	124	15	31		
3	50	59	40*	-5	293	2	-0	8	138	20	8	-2	196	4	3				H,K=	6,	1
4	212	8	-7	-4	224	6	-6				H,K=	6,-	-4	-1	396	2	-0	-12	89	21	4*
5	207	5	-2	-3	283	5	3	-12	130	18	-8	0	321	2	1	-11	130	28	-1*		
6	78	52	10*	-2	208	3	3	-11	185	7	11	1	210	7	-4	-10	233	16	-8		
7	178	17	-2	-1	43	22	13*	-10	117	15	16	2	238	5	0	-9	89	17	4*		
8	76	21	-15*	0	226	4	-2	-9	214	7	-1	3	32	46	1*	-8	246	6	-4		
	H,K=	6,-	-9	1	282	4	-2	-8	153	10	-7	4	204	3	1	-7	234	5	-6		
-11	129	8	30	2	56	31	13*	-7	180	8	-4	5	245	8	-2	-6	81	7	25		
-10	141	12	3	3	247	4	6	-6	229	6	-3	6	43	44	17*	-5	353	3	4		
-9	68	68	-24*	4	154	8	1	-5	236	5	9	7	202	8	1	-4	184	6	-6		
-8	177	22	2	5	96	20	10*	-4	356	3	3	8	132	18	-3	-3	237	6	3		
-7	94	25	-17*	6	266	4	2	-3	472	2	2				H,K=	6,-	-1	-2	309	2	0
-6	143	9	5	7	43	60	8*	-2	284	4	7	-13	122	21	5	-1	99	6	12		
-5	279	6	4	8	146	27	-2*	-1	630	3	2	-12	66	76	-5*	0	282	10	0		
-4	132	5	6				H,K=	6,-	-6	0	398	3	2	-11	130	19	11	1	425	6	8
-3	170	4	3	-12	127	19	1	1	196	3	-1	-10	208	8	-9	2	56	24	25*		
-2	276	5	-1	-11	124	28	3*	2	327	8	0	-9	22	48	-1*	3	280	3	1		
-1	36	43	19*	-10	66	14	14*	3	71	18	6*	-8	175	7	-7	4	227	10	-10		
0	221	8	-3	-9	231	6	3	4	185	8	-6	-7	203	7	2	5	155	7	7		
1	310	5	-4	-8	100	20	4*	5	267	5	10	-6	66	13	23*	6	162	6	3		
2	154	5	-4	-7	159	8	9	6	0	55	-35*	-5	549	4	-5	7	62	38	11*		
3	247	7	-7	-6	298	5	3	7	202	10	-7	-4	93	10	-6	8	125	9	-1		
4	101	18	15	-5	130	11	3	8	155	12	7	-3	286	6	-4				H,K=	6,	2
5	222	4	-2	-4	263	2	1				H,K=	6,-	-3	-2	473	2	1	-12	120	9	10
6	218	19	-9	-3	399	2	1	-12	54	64	-16*	-1	108	11	-2	-11	131	18	-1		
7	55	61	12*	-2	262	3	5	-11	99	18	11*	0	378	3	-1	-10	0	46	-9*		
8	141	21	3	-1	287	2	-2	-10	175	7	-13	1	349	2	0	-9	248	4	-3		
	H,K=	6,-	-8	0	322	3	-0	-9	58	69	51*	2	84	7	2	-8	95	55	-11*		
-12	128	43	-1*	1	221	10	3	-8	150	4	-4	3	371	3	3	-7	220	7	-7		
-11	93	23	4*	2	316	3	-1	-7	132	7	-5	4	204	6	-3	-6	294	4	-0		
-10	26	48	16*	3	110	18	1	-6	44	52	18*	5	207	8	8	-5	50	59	-1*		
-9	154	11	-2	4	264	9	-4	-5	428	3	1	6	250	5	5	-4	242	4	-2		
-8	103	31	5*	5	236	14	3	-4	102	13	6	7	109	32	-7*	-3	294	4	-2		
-7	115	8	0	6	65	22	30*	-3	80	7	9	8	147	23	-2	-2	48	34	41*		
-6	279	5	-3	7	245	10	-4	-2	664	2	-0				H,K=	6,-	0	-1	410	2	-3
-5	0	59	-38*	8	136	9	1	-1	105	14	6	-13	0	74	-10*	0	152	5	5		
-4	274	8	2				H,K=	6,-	-5	0	447	6	-4	-12	130	21	6	1	93	11	-4
-3	230	3	-0	-12	44	52	-19*	1	345	4	3	-11	155	9	5	2	324	5	2		
-2	21	31	-17*	-11	115	22	32*	2	41	13	21*	-10	0	48	-18*	3	124	8	9		
-1	269	5	-9	-10	172	13	-2	3	302	8	0	-9	244	5	3	4	245	8	2		
0	33	34	-4*	-9	62	31	7*	4	97	15	2	-8	102	7	-9	5	237	10	0		
1	192	4	4	-8	200	12	4	5	116	19	9	-7	119	7	12	6	0	58	-5*		

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	186	16	9	1	247	3	1	3	76	79	-9*	-4	120	10	7	-8	0	54	-36*
	H,K=	6,	3	2	83	27	18*	4	110	20	4*	-3	45	86	3*	-7	156	7	18
-12	81	40	-2*	3	257	6	-9	5	167	17	16	-2	164	8	11	-6	158	10	-6
-11	51	60	-15*	4	154	15	2		H,K=	6,	9	-1	84	34	14*	-5	28	46	12*
-10	189	13	3	5	44	47	-27*-10	177	8	8		H,K=	7,-19	-4	146	14	10		
-9	51	57	-14*	6	158	7	3	-9	.88	33	25*	-2	103	18	-4	-3	117	16	11
-8	210	8	0		H,K=	6,	6	-8	126	14	17	-1	59	67	29*	-2	89	13	-14
-7	188	4	3	-11	141	43	-2*	-7	168	9	4		H,K=	7,-18	-1	172	6	-8	
-6	158	9	1	-10	46	49	22*	-6	0	45	-16*	-5	56	67	41*	0	45	53	-22*
-5	201	5	-3	-9	209	11	-4	-5	220	6	12	-4	111	10	10	1	183	24	6
-4	171	6	2	-8	184	24	4	-4	161	18	9	-3	80	40	-13*	2	172	12	-3
-3	190	6	7	-7	81	26	-5*	-3	112	9	-13	-2	62	74	-19*	3	49	63	-1*
-2	308	10	1	-6	246	16	4	-2	261	8	1	-1	193	18	10	4	157	26	1
-1	136	11	10	-5	133	8	-4	-1	80	25	-1*	0	0	72	-25*	5	114	16	1
0	319	9	1	-4	226	18	-2	0	117	18	5	1	152	11	16		H,K=	7,-13	
1	394	3	0	-3	276	4	6	1	220	7	2	2	123	13	17	-10	111	41	10*
2	0	58	-4*	-2	93	10	10	2	48	57	45*		H,K=	7,-17	-9	56	39	52*	
3	246	10	-8	-1	347	4	2	3	151	12	9	-6	70	26	14*	-8	143	12	14
4	171	11	-4	0	281	9	1	4	124	20	1	-5	122	17	12	-7	107	25	-18*
5	95	23	-21*	1	54	17	13*		H,K=	6,	10	-4	12	58	-28*	-6	100	21	-2*
6	165	12	-3	2	259	7	4	-9	140	9	-7	-3	120	12	2	-5	169	5	-4
7	69	82	12*	3	85	46	41*	-8	120	12	-8	-2	140	12	11	-4	74	16	11*
	H,K=	6,	4	4	81	71	-20*	-7	93	12	10	-1	0	64	-13*	-3	116	17	-1
-12	137	27	11*	5	167	21	13	-6	216	8	2	0	208	10	7	-2	223	11	-1
-11	149	10	-11	6	0	91	-17*	-5	116	11	24	1	68	43	-4*	-1	25	53	-12*
-10	58	69	13*		H,K=	6,	7	-4	169	21	19	2	96	41	1*	0	192	6	-13
-9	230	6	-10	-11	56	33	-5*	-3	180	7	6	3	118	19	10	1	194	5	-1
-8	176	7	5	-10	156	23	-8	-2	31	85	-1*		H,K=	7,-16	2	102	13	2	
-7	130	10	-0	-9	32	47	15*	-1	180	6	5	-7	91	55	35*	3	214	6	-0
-6	292	3	-5	-8	172	20	3	0	159	16	-6	-6	97	49	-26*	4	32	57	-1*
-5	119	14	-2	-7	233	8	-8	1	56	31	0*	-5	69	82	16*	5	73	32	-26*
-4	180	7	3	-6	57	15	2*	2	181	9	15	-4	163	9	3	6	152	23	-3
-3	338	5	-4	-5	185	4	12	3	104	14	9	-3	98	10	8		H,K=	7,-12	
-2	45	48	37*	-4	234	9	7		H,K=	6,	11	-2	78	19	-9*-10	62	49	12*	
-1	199	3	-0	-3	180	5	-8	-8	99	19	-3*	-1	175	8	-5	-9	100	11	-12
0	237	14	-1	-2	312	3	4	-7	164	15	-10	0	32	49	-15*	-8	70	86	8*
1	65	16	9*	-1	70	48	-7*	-6	68	35	50*	1	137	15	-18	-7	191	5	13
2	238	5	-2	0	148	9	-3	-5	187	16	16	2	146	7	8	-6	172	6	8
3	32	41	11*	1	209	10	-3	-4	106	35	1*	3	67	20	15*	-5	50	60	36*
4	287	6	10	2	57	40	33*	-3	79	34	6*	4	136	18	15	-4	228	9	4
5	207	6	4	3	151	10	-1	-2	209	18	14		H,K=	7,-15	-3	158	6	-8	
6	68	48	51*	4	128	16	0	-1	61	73	-4*	-8	61	69	-8*	-2	88	38	-9*
7	181	10	18	5	63	67	3*	0	131	16	3	-7	53	63	-10*	-1	213	11	-6
	H,K=	6,	5		H,K=	6,	8	1	150	21	-7	-6	110	22	-8*	0	0	51	-40*
-12	87	96	18*-10	37	75	3*	2	68	80	59*	-5	177	7	13	1	161	6	-8	
-11	77	19	-1*	-9	189	15	-7		H,K=	6,	12	-4	58	78	6*	2	224	7	-1
-10	166	8	1	-8	119	9	-16	-7	70	53	15*	-3	167	16	15	3	42	51	18*
-9	23	64	-24*	-7	57	68	-15*	-6	203	8	18	-2	128	19	-2	4	177	12	1
-8	194	7	-5	-6	244	8	8	-5	92	38	28*	-1	28	41	16*	5	125	24	-5*
-7	189	17	-1	-5	102	36	-1*	-4	128	10	14	0	174	9	6	6	0	46	-42*
-6	49	15	16*	-4	191	8	1	-3	185	24	15	1	126	16	-14		H,K=	7,-11	
-5	200	11	-1	-3	250	6	3	-2	39	93	-1*	2	96	48	-8*-11	91	60	24*	
-4	200	3	-3	-2	108	20	18*	-1	122	14	1	3	161	17	8	-10	99	41	-17*
-3	148	9	-4	-1	224	15	1	0	87	71	-13*	4	0	65	-18*	-9	0	63	-19*
-2	358	5	-1	0	188	24	-2	1	84	33	43*	5	164	14	17	-8	142	13	5
-1	100	14	-4	1	128	26	8*		H,K=	6,	13		H,K=	7,-14	-7	114	9	3	
0	200	4	1	2	166	25	1	-5	137	17	8	-9	112	29	3*	-6	164	5	2

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	262	7	-1	-9	199	5	5	6	96	15	-6	-1	20	36	-2*	-7	114	16	5
-4	61	11	36*	-8	54	64	33*	7	202	12	-24	0	325	2	-1	-6	308	10	-8
-3	233	4	-7	-7	111	16	9		H,K= 7,	-5	1	220	8	1	-5	82	19	10*	
-2	251	6	-13	-6	264	7	-4	-12	32	45	-13*	2	209	4	0	-4	294	5	5
-1	27	36	-9*	-5	34	49	17*	-11	110	29	16*	3	304	4	-2	-3	245	4	-1
0	288	8	-4	-4	261	6	0	-10	166	13	8	4	99	38	2*	-2	112	5	-5
1	277	6	-3	-3	210	7	-3	-9	24	53	-1*	5	153	10	3	-1	186	4	2
2	57	21	10*	-2	164	9	-4	-8	194	13	5	6	224	16	-4	0	231	6	-10
3	262	7	4	-1	372	13	-14	-7	74	36	-28*	7	50	62	-2*	1	118	14	1
4	93	28	18*	0	247	8	-1	-6	126	5	9		H,K= 7,	-2	2	289	7	-1	
5	100	31	-34*	1	183	6	3	-5	272	6	-1	-12	112	15	3	3	71	33	-1*
6	164	12	-9	2	205	4	-1	-4	97	9	7	-11	141	9	-13	4	218	5	-2
7	33	54	28*	3	56	39	10*	-3	236	6	3	-10	89	14	28	5	183	12	3
	H,K= 7,	-10	4	310	7	-3	-2	317	4	0	-9	133	6	-7	6	43	53	-0*	
-11	95	23	23*	5	187	19	-4	-1	49	64	13*	-8	81	26	6*	7	170	19	3
-10	56	60	12*	6	83	29	10*	0	372	3	-5	-7	259	18	-4		H,K= 7,	1	
-9	128	8	3	7	214	11	-1	1	255	7	-5	-6	266	7	-5	-12	41	62	-4*
-8	40	48	-18*		H,K= 7,	-7	2	185	5	1	-5	32	38	9*	-11	105	11	-2	
-7	139	7	-1	-12	30	46	-12*	3	269	3	9	-4	264	3	1	-10	165	15	4
-6	199	9	-8	-11	143	16	31	4	79	37	12*	-3	260	4	0	-9	39	47	37*
-5	35	37	21*	-10	127	9	14	5	158	9	-10	-2	76	12	-6	-8	247	10	-5
-4	279	7	-7	-9	95	23	32*	6	220	13	-4	-1	222	4	1	-7	221	7	-4
-3	141	13	1	-8	185	9	-1	7	0	86	-57*	0	158	8	-7	-6	96	12	16
-2	94	27	7*	-7	131	13	-5	8	156	29	12*	1	125	13	13	-5	310	10	-2
-1	135	5	-5	-6	72	16	11*		H,K= 7,	-4	2	248	8	-1	-4	186	7	7	
0	116	11	16	-5	209	7	-7	-12	118	14	-2	3	35	42	19*	-3	309	7	-4
1	122	13	-6	-4	129	8	5	-11	138	9	-16	4	194	8	-9	-2	236	3	-2
2	282	4	6	-3	311	6	-4	-10	82	41	14*	5	153	7	16	-1	45	53	16*
3	58	16	6*	-2	292	5	-9	-9	224	4	6	6	83	21	62*	0	283	15	-2
4	305	12	-9	-1	58	11	13	-8	154	4	-1	7	165	32	4*	1	340	3	-3
5	167	13	3	0	299	4	-7	-7	231	8	-0		H,K= 7,	-1	2	42	48	24*	
6	72	30	12*	1	196	4	3	-6	214	3	-1	-12	61	72	21*	3	314	7	-9
7	188	6	-10	2	123	9	-12	-5	0	34	-5*	-11	121	15	6	4	124	19	11
	H,K= 7,	-9	3	240	5	-3	-4	306	3	0	-10	186	8	-11	5	112	18	5	
-11	96	25	-10*	4	132	11	-1	-3	263	6	7	-9	60	19	29*	6	165	20	10
-10	113	31	-7*	5	200	6	1	-2	95	6	4	-8	207	6	1	7	58	69	25*
-9	44	71	11*	6	176	7	1	-1	340	3	-6	-7	354	4	-10		H,K= 7,	2	
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-7	61	26	-16*		H,K= 7,	-6	1	139	4	2	-5	287	3	1	-11	98	14	-9	
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-5	314	4	0	-11	98	11	-7	3	35	42	-11*	-3	280	4	-1	-9	212	10	-3
-4	85	39	-5*	-10	114	34	25*	4	220	20	-4	-2	264	4	-4	-8	128	17	-9
-3	208	13	-1	-9	219	11	-7	5	148	13	-9	-1	42	50	23*	-7	123	24	1*
-2	244	3	-4	-8	69	29	14*	6	63	28	26*	0	277	2	-3	-6	266	4	1
-1	74	26	-7*	-7	153	13	6	7	143	10	15	1	245	10	-2	-5	25	47	17*
0	233	6	-2	-6	291	12	-10		H,K= 7,	-3	2	49	33	30*	-4	327	3	-5	
1	299	5	-1	-5	37	49	31*	-12	31	48	-4*	3	320	6	-5	-3	286	7	1
2	155	25	-1	-4	300	3	-0	-11	121	24	-3*	4	127	20	3	-2	121	27	-15*
3	261	3	-5	-3	242	8	6	-10	194	23	-22	5	114	17	-4	-1	377	5	-14
4	156	9	10	-2	216	5	-5	-9	0	49	-36*	6	173	10	-5	0	307	4	3
5	229	4	-7	-1	414	3	-5	-8	151	5	4	7	28	45	19*	1	60	14	18*
6	147	18	1	0	192	10	5	-7	112	6	2		H,K= 7,	0	2	253	6	6	
7	62	80	22*	1	341	4	0	-6	111	6	-18	-12	115	26	-1*	3	37	65	1*
	H,K= 7,	-8	2	197	3	7	-5	298	5	1	-11	103	39	-4*	4	246	13	9	
-12	137	14	20	3	62	26	2*	-4	57	12	9*	-10	94	29	13*	5	180	11	8
-11	72	30	-28*	4	246	5	-4	-3	245	9	1	-9	235	4	6	6	71	19	9*
-10	58	53	-0*	5	169	6	-4	-2	456	3	0	-8	103	8	10		H,K= 7,	3	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	45	53	-2*	H,K= 7,	6	-2	232	5	-3	0	0	45	-21*	-4	211	5	-1		
-11	124	11	19	-11	116	12	1	-1	86	26	21*	1	133	17	-2	-3	73	38	-9*
-10	157	12	8	-10	85	18	5*	0	191	14	3	2	118	43	15*	-2	116	22	-4*
-9	47	56	32*	-9	226	13	7	1	139	21	7	3	63	57	-14*	-1	235	4	-3
-8	197	13	-5	-8	83	19	14*	2	0	66	-15*	H,K= 8,-15	0	101	38	-19*			
-7	183	8	-2	-7	183	9	-10	3	133	30	-9*	-8	83	14	1	1	103	36	-5*
-6	94	12	24	-6	170	6	4	H,K= 7, 10	-7	66	23	9*	2	138	8	-10			
-5	215	4	-11	-5	100	10	-20	-8	97	47	1*	-6	105	11	27	3	30	43	-28*
-4	135	11	10	-4	176	6	3	-7	61	72	-14*	-5	143	13	10	4	173	14	-13
-3	330	6	-8	-3	185	8	3	-6	200	7	12	-4	39	74	8*	5	80	29	-27*
-2	351	6	-6	-2	71	85	-20*	-5	44	52	27*	-3	202	16	-10	H,K= 8,-11			
-1	56	13	-2*	-1	278	13	8	-4	127	9	-5	-2	95	20	12*-10	76	28	-6*	
0	207	4	-1	0	47	49	-14*	-3	131	22	-22	-1	33	62	3*	-9	45	33	12*
1	149	8	2	1	195	5	-7	-2	76	74	70*	0	197	28	1	-8	124	9	5
2	73	25	-12*	2	234	8	-6	-1	176	17	9	1	89	25	12*	-7	107	13	-13
3	283	7	7	3	78	29	-6*	0	92	16	-1	2	124	13	6	-6	134	11	-10
4	144	9	12	4	135	28	13*	1	88	19	-11*	3	163	10	10	-5	194	10	-6
5	124	14	3	5	157	22	21	2	176	12	9	4	0	51	-19*	-4	36	62	8*
6	175	17	16	H,K= 7,	7	H,K= 7,	11	H,K= 8,-14	-3	224	7	-4							
H,K= 7,	4	-10	165	15	12	-7	169	8	-4	-9	75	79	-15*	-2	231	6	-2		
-12	125	21	6	-9	24	45	10*	-6	17	80	6*	-8	52	54	47*	-1	92	30	17*
-11	114	21	-7	-8	201	10	8	-5	210	5	20	-7	91	47	-23*	0	193	6	4
-10	59	19	15*	-7	140	7	2	-4	123	21	14	-6	161	14	19	1	126	11	-0
-9	250	5	3	-6	60	23	8*	-3	80	32	9*	-5	38	58	5*	2	148	15	7
-8	175	13	7	-5	184	5	-0	-2	148	11	3	-4	184	6	4	3	181	14	-14
-7	98	23	11*	-4	204	6	3	-1	54	41	19*	-3	76	14	6	4	72	77	33*
-6	200	8	-14	-3	49	28	-29*	0	109	20	-8	-2	111	10	2	5	186	12	6
-5	33	51	26*	-2	217	19	-5	H,K= 7,	12	-1	73	13	-11	6	155	15	-12		
-4	200	5	1	-1	59	19	17*	-5	59	78	19*	0	42	51	2*	H,K= 8,-10			
-3	209	8	-4	0	249	6	1	-4	112	49	-12*	1	177	12	4	-11	85	32	16*
-2	199	15	-10	1	163	11	7	-3	122	12	1	2	136	21	-5	-10	87	24	11*
-1	362	10	-1	2	39	62	14*	-2	43	48	39*	3	58	44	-6*	-9	104	16	3
0	194	6	-4	3	187	15	20	H,K= 8,-18	4	150	22	6	-8	57	69	-27*			
1	146	7	-5	4	106	49	-3*	-4	81	53	-14*	5	113	37	19*	-7	155	9	1
2	242	9	10	H,K= 7,	8	-3	71	77	3*	H,K= 8,-13	-6	129	10	-0					
3	72	15	-17*-10	10	27	59	-16*	-2	76	40	-16*	-9	65	77	33*	-5	73	16	28*
4	185	15	-16	-9	164	16	-2	-1	140	11	11	-8	151	12	8	-4	257	7	-6
5	150	12	5	-8	88	18	-1*	0	76	29	48*	-7	74	18	-26*	-3	91	38	19*
6	26	61	-13*	-7	152	7	-0	1	131	30	1*	-6	111	18	-1	-2	146	5	-4
H,K= 7,	5	-6	175	9	6	H,K= 8,-17	-5	171	5	-1	-1	317	4	-3					
-11	122	10	18	-5	74	34	6*	-6	79	83	4*	-4	10	40	-18*	0	91	12	-5
-10	158	10	-11	-4	167	8	16	-5	96	18	5*	-3	181	9	-3	1	91	9	-18
-9	29	84	12*	-3	209	9	-1	-4	49	50	11*	-2	116	19	-4	2	159	7	1
-8	238	9	1	-2	51	59	39*	-3	140	10	2	-1	80	12	17	3	47	38	10*
-7	223	9	-5	-1	222	12	-1	-2	117	9	2	0	226	12	4	4	269	5	-14
-6	3	52	-34*	0	125	13	6	-1	41	52	-5*	1	173	8	5	5	104	21	-3*
-5	206	4	5	1	116	34	11*	0	187	7	9	2	148	9	2	6	127	18	10
-4	154	7	11	2	131	11	-22	1	117	12	37	3	182	9	-3	H,K= 8,-9			
-3	205	4	3	3	57	23	9*	2	109	22	-2*	4	65	78	29*-11	124	40	24*	
-2	289	3	3	H,K= 7,	9	H,K= 8,-16	5	134	11	9	-10	118	9	-2					
-1	70	74	-3*	-9	0	50	-37*	-7	97	18	3*	H,K= 8,-12	-9	62	32	-2*			
0	180	8	-2	-8	125	12	-15	-6	91	44	-1*-10	81	81	31*	-8	177	6	3	
1	173	5	10	-7	176	22	12	-5	40	47	8*	-9	103	29	9*	-7	114	16	-15
2	40	58	12*	-6	55	76	26*	-4	147	11	-7	-8	58	24	-5*	-6	82	30	9*
3	173	11	5	-5	155	20	6	-3	86	25	9*	-7	146	18	-4	-5	252	9	1
4	157	11	23	-4	83	85	-10*	-2	138	13	10	-6	118	14	5	-4	36	57	2*
5	105	56	8*	-3	112	31	-5*	-1	176	13	14	-5	76	14	3	-3	218	17	5

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	163	18	5	-2	67	67	45*	-3	236	6	2	4	207	6	2	-12	107	15	9
-8	26	54	1*	-1	136	21	17	-2	136	16	4	5	95	20	12**	-11	64	73	25*
-7	151	15	-15		H,K=	9,-18		-1	74	44	29*		H,K=	9,-9	-10	96	34	7*	
-6	179	16	-18	-3	25	82	-1*	C	228	8	7	-11	95	12	11	-9	163	21	-3
-5	41	48	35*	-2	69	82	-30*	1	51	65	-15*-10	61	71	-15*	-8	36	47	20*	
-4	231	14	3		H,K=	9,-17		2	117	19	17	-9	41	56	1*	-7	204	7	0
-3	233	8	8	-5	76	23	-11*	3	141	16	-2	-8	212	9	7	-6	108	14	-1
-2	60	30	38*	-4	0	52	-10*	4	65	75	50*	-7	69	69	-30*	-5	76	37	24*
-1	256	4	11	-3	123	14	-13		H,K=	9,-12		-6	122	19	5	-4	183	10	-10
0	76	12	32	-2	84	16	-0*-10	74	32	3*	-5	196	13	5	-3	130	16	-13	
1	147	9	18	-1	84	40	26*	-9	78	29	-18*	-4	81	67	-7*	-2	163	22	-3
2	164	19	-6	0	116	28	-10*	-8	46	48	44*	-3	95	18	3*	-1	299	9	0
3	52	52	20*	1	93	17	17*	-7	96	17	4	-2	188	9	-3	0	65	33	58*
	H,K=	8,	7		H,K=	9,-16		-6	80	19	-9*	-1	115	14	5	1	128	17	-6
-10	152	24	17	-7	102	44	1*	-5	84	12	12	0	189	13	3	2	213	6	3
-9	50	68	40*	-6	47	53	1*	-4	210	10	-3	1	133	17	-2	3	123	7	-1
-8	150	16	-10	-5	53	64	28*	-3	45	67	12*	2	133	17	-13	4	191	5	-4
-7	113	31	14*	-4	129	21	6	-2	194	5	-0	3	184	11	5	5	92	19	11*
-6	63	52	5*	-3	54	38	-4*	-1	249	9	-2	4	29	48	-13*		H,K=	9,-9	-5
-5	223	8	11	-2	141	13	9	0	70	15	16*	5	143	13	7	-12	0	64	-9*
-4	65	70	-13*	-1	160	20	-10	1	221	6	-3		H,K=	9,-8	-11	122	16	-1	
-3	117	11	13	0	0	94	-28*	2	122	21	-8	-11	46	73	15*-10	115	13	0	
-2	243	4	4	1	107	19	15	3	89	29	22*-10	101	37	12*	-9	40	71	3*	
-1	31	56	11*	2	107	16	-4	4	179	14	-1	-9	148	30	6*	-8	215	13	-2
0	210	8	4		H,K=	9,-15			H,K=	9,-11		-8	45	60	27*	-7	140	11	7
1	133	16	15	-8	135	25	12*-10	66	51	-5*	-7	263	6	2	-6	137	12	16	
2	74	34	12*	-7	32	52	-7*	-9	82	12	28	-6	171	8	-4	-5	174	13	6
3	143	29	-7*	-6	92	48	22*	-8	128	9	6	-5	106	16	0	-4	101	15	13
	H,K=	8,	8	-5	100	36	7*	-7	0	49	-65*	-4	155	17	-9	-3	321	6	-4
-9	170	22	19	-4	54	64	15*	-6	123	20	3	-3	98	21	3*	-2	273	17	-6
-8	9	54	-63*	-3	174	9	-6	-5	188	7	-7	-2	118	23	15*	-1	97	7	1
-7	115	21	6	-2	123	32	-2*	-4	51	57	0*	-1	202	5	1	0	281	9	-9
-6	124	39	-13*	-1	50	69	-36*	-3	213	10	-0	0	0	53	-8*	1	132	6	10
-5	0	64	-10*	0	187	14	11	-2	142	17	-6	1	256	7	-6	2	94	17	-12
-4	160	7	-4	1	15	61	-4*	-1	64	13	5*	2	222	8	3	3	283	4	1
-3	139	9	5	2	99	46	-8*	0	209	9	9	3	66	78	37*	4	52	62	-8*
-2	66	79	28*	3	146	28	6*	1	74	18	16*	4	185	7	-16	5	118	22	-4*
-1	241	4	-0		H,K=	9,-14		2	124	34	-2*	5	91	37	26*		H,K=	9,-9	-4
0	105	17	36	-8	49	58	32*	3	169	6	-0		H,K=	9,-7	-12	114	22	-2*	
1	112	29	5*	-7	85	25	4*	4	47	54	39*-11	100	34	5*-11	17	49	-23*		
2	176	15	28	-6	96	45	-4*	5	135	12	3	-10	84	17	-3*-10	119	12	10	
	H,K=	8,	9	-5	72	43	20*		H,K=	9,-10		-9	37	54	-7*	-9	162	10	-14
-8	150	20	-4	-4	159	6	-0	-11	56	65	23*	-8	209	13	-11	-8	54	64	43*
-7	121	15	-15	-3	42	68	-16*-10	70	47	-10*	-7	86	10	-1	-7	163	11	20	
-6	85	23	29*	-2	112	14	-14	-9	105	40	8*	-6	139	16	0	-6	179	8	7
-5	170	7	2	-1	197	10	3	-8	33	42	-6*	-5	186	6	-0	-5	60	62	39*
-4	80	14	8	0	36	43	8*	-7	200	23	3	-4	34	35	13*	-4	248	5	4
-3	124	30	3*	1	130	20	-5	-6	129	16	-6	-3	128	13	14	-3	216	9	-0
-2	179	7	-1	2	99	26	-22*	-5	26	67	-3*	-2	206	6	-10	-2	173	16	-9
-1	33	51	28*	3	56	66	8*	-4	183	4	5	-1	117	10	13	-1	227	4	4
0	158	12	-6		H,K=	9,-13		-3	0	44	-17*	0	236	9	-2	0	55	33	6*
1	123	10	3	-9	44	70	-25*	-2	161	8	-2	1	198	8	-3	1	171	4	3
	H,K=	8,	10	-8	122	32	14*	-1	188	12	-4	2	133	9	-6	2	214	8	-0
-6	141	19	6	-7	48	69	-21*	0	49	56	24*	3	201	20	10	3	70	17	23*
-5	33	62	23*	-6	97	31	-16*	1	275	6	-6	4	47	55	27*	4	151	13	-5
-4	140	24	-12	-5	152	12	-16	2	117	24	-4*	5	156	7	3	5	98	45	-1*
-3	163	7	16	-4	52	62	37*	3	59	17	14*		H,K=	9,-6		H,K=	9,-9	-3	

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-12	38	72	5*	-11	0	62	-53*	-6	109	20	7	-4	41	49	24*	-5	127	8	22
-11	123	30	15*	-10	86	33	0*	-5	203	7	-5	-3	138	13	12	-4	50	59	30*
-10	120	26	27*	-9	157	19	7	-4	100	55	21*	-2	186	9	0	-3	197	14	-6
-9	63	32	4*	-8	22	41	-12*	-3	101	22	2*	-1	39	66	9*	-2	138	20	16
-8	229	5	-10	-7	188	16	-6	-2	157	14	3	0	125	12	-12	-1	95	23	-17*
-7	75	31	-4*	-6	196	11	-20	-1	43	56	22*	1	95	54	-15*	0	183	9	2
-6	141	8	4	-5	66	36	15*	0	195	10	-9	H,K=	9,	8	1	36	45	-2*	
-5	275	9	-2	-4	234	10	5	1	119	19	2	-7	113	38	2*	2	90	37	-3*
-4	69	10	17	-3	106	20	15*	2	139	11	6	-6	126	30	-1*	3	118	57	1*
-3	280	7	-4	-2	138	13	-2	3	180	22	8	-5	63	46	43*	H,K=	10,	-12	
-2	228	4	3	-1	261	7	1	H,K=	9,	4	-4	175	6	20	-9	54	65	-27*	
-1	109	24	-1*	0	32	55	-1*	-10	90	45	8*	-3	145	24	24	-8	61	24	12*
0	269	5	-0	1	248	9	-2	-9	148	14	-11	-2	80	16	28*	-7	127	13	2
1	12	38	-30*	2	201	5	7	-8	13	63	2*	-1	137	44	-1*	-6	73	34	-2*
2	139	14	-8	3	53	58	46*	-7	179	11	5	H,K=	9,	9	-5	58	61	5*	
3	272	10	-8	4	162	8	0	-6	175	11	-2	-5	156	24	-3	-4	193	22	8
4	79	28	13*	5	113	14	4	-5	75	14	-2*	-4	104	10	37	-3	36	56	-20*
5	104	21	-20*	H,K=	9,	1	-4	263	4	11	-3	106	49	10*	-2	156	18	2	
H,K=	9,	-2	-11	110	32	3*	-3	192	12	5	H,K=	10,-	-17	-1	164	14	-17		
-12	109	11	11	-10	124	18	19	-2	74	55	3*	-4	54	69	-3*	0	69	15	-11*
-11	0	49	-35*	-9	49	32	-12*	-1	204	6	-3	-3	136	8	21	1	155	7	2
-10	129	14	-1	-8	173	15	-1	0	45	53	-3*	-2	45	59	-18*	2	121	13	6
-9	165	9	-19	-7	91	69	-24*	1	152	8	-9	H,K=	10,-	-16	3	43	51	-29*	
-8	44	59	-0*	-6	133	12	-5	2	175	19	9	-6	48	52	-10*	H,K=	10,-	-11	
-7	152	7	0	-5	267	5	2	3	75	45	54*	-5	83	14	19	-10	78	23	24*
-6	200	7	-2	-4	50	57	39*	H,K=	9,	5	-4	116	27	8*	-9	38	47	-40*	
-5	49	25	1*	-3	179	4	7	-10	124	24	3*	-3	41	49	25*	-8	132	22	7
-4	299	9	-5	-2	187	8	7	-9	52	69	42*	-2	103	19	11	-7	17	51	-2*
-3	184	7	-4	-1	10	43	-27*	-8	143	15	-5	-1	89	30	-18*	-6	98	18	-0*
-2	103	11	4	0	212	11	-9	-7	121	15	15	0	0	50	-37*	-5	130	17	10
-1	225	3	1	1	197	9	5	-6	125	14	-11	H,K=	10,-	-15	-4	36	56	30*	
0	10	40	-4*	2	117	17	-5	-5	188	10	3	-7	10	69	-5*	-3	145	32	-8*
1	215	5	1	3	174	6	5	-4	53	74	-9*	-6	86	48	6*	-2	126	7	13
2	193	5	1	4	102	47	6*	-3	124	10	-2	-5	119	31	13*	-1	113	22	0*
3	72	53	44*	H,K=	9,	2	-2	198	11	-1	-4	0	58	-8*	0	185	6	3	
4	167	15	1	-11	45	62	-6*	-1	70	82	43*	-3	149	10	22	1	61	36	40*
5	114	35	-8*	-10	58	69	-14*	0	190	8	1	-2	84	93	-8*	2	163	16	10
H,K=	9,	-1	-9	139	7	1	1	117	28	13*	-1	107	27	12*	3	159	16	4	
-12	45	57	41*	-8	53	23	41*	2	86	50	0*	0	127	29	-2*	4	54	58	47*
-11	127	27	3*	-7	183	9	-7	H,K=	9,	6	1	38	55	25*	H,K=	10,-	-10		
-10	128	19	5	-6	204	6	-1	-9	163	14	12	H,K=	10,-	-14	-10	95	103	3*	
-9	59	21	-0*	-5	39	62	-11*	-8	62	30	15*	-8	54	60	19*	-9	95	44	-3*
-8	210	7	-9	-4	242	9	-5	-7	121	14	9	-7	114	33	21*	-8	13	44	-15*
-7	70	26	-13*	-3	152	12	11	-6	154	8	3	-6	92	26	14*	-7	207	20	10
-6	139	20	-2	-2	98	28	15*	-5	86	12	-2	-5	77	18	27*	-6	94	9	1
-5	277	6	-11	-1	178	8	-3	-4	164	7	-1	-4	139	13	15	-5	49	38	-7*
-4	66	33	36*	0	42	50	19*	-3	126	8	1	-3	51	60	-3*	-4	220	12	-3
-3	231	4	3	1	226	5	4	-2	65	80	-18*	-2	146	10	1	-3	77	16	2*
-2	188	6	-2	2	178	18	7	-1	199	21	1	-1	138	20	-20	-2	141	9	7
-1	47	58	2*	3	63	20	37*	0	74	80	19*	0	79	24	18*	-1	191	9	8
0	236	14	-7	4	159	13	5	1	109	36	-7*	1	134	13	-3	0	27	52	-19*
1	92	12	1	H,K=	9,	3	2	124	25	-5*	2	81	19	8*	1	201	10	2	
2	116	9	-0	-11	94	66	-5*	H,K=	9,	7	H,K=	10,-	-13	2	145	15	10		
3	197	17	7	-10	116	14	5	-8	138	10	-10	-9	53	72	-10*	3	85	29	-5*
4	71	34	2*	-9	59	59	30*	-7	97	28	1*	-8	103	11	3	4	141	14	10
5	98	15	-6	-8	166	9	-2	-6	109	24	19*	-7	50	51	31*	H,K=	10,-	-9	
H,K=	9,	0	-7	128	21	-8	-5	182	6	1	-6	123	15	12	-10	0	68	-61*	

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-9	91	50	28*	-3	65	44	-7*	3	128	11	-7	-6	115	7	22	-2	103	20	0*	
-8	153	11	-15	-2	133	12	-6	4	0	45	-21*	-5	215	8	4	-1	34	53	10*	
-7	74	36	1*	-1	184	9	1		H,K= 10,		-2	-4	46	57	40*	0	156	7	-4	
-6	131	25	2*	0	75	35	35*	-11	60	77	26*	-3	192	12	-14		H,K= 10,		6	
-5	154	24	1	1	218	5	-7	-10	111	20	1	-2	176	7	19	-7	129	15	3	
-4	55	56	16*	2	139	7	9	-9	141	6	4	-1	53	20	4*	-6	119	40	0*	
-3	166	9	19	3	86	47	15*	-8	41	73	30*	0	178	13	-2	-5	67	37	26*	
-2	156	13	9	4	159	13	4	-7	146	16	6	1	66	76	1*	-4	153	14	10	
-1	123	18	10		H,K= 10,		-5	-6	205	15	-1	2	123	10	4	-3	96	19	6*	
0	207	5	-6	-11	128	18	18	-5	73	23	16*	3	141	11	-7	-2	140	24	35	
1	100	29	19*	-10	85	36	-5*	-4	179	5	3		H,K= 10,		2	-1	111	15	-7	
2	143	7	-27	-9	71	13	24*	-3	65	70	-23*	-10	102	13	4		H,K= 10,		7	
3	173	12	-5	-8	159	6	-11	-2	161	8	11	-9	151	9	13	-6	98	42	11*	
4	0	74	-7*	-7	75	17	6*	-1	206	13	7	-8	0	55	-9*	-5	131	12	4	
			H,K= 10,	-8	-6	177	21	-5	0	30	45	11*	-7	164	11	4	-4	46	66	13*
-11	49	50	44*	-5	126	13	-9	1	213	8	10	-6	109	34	-17*	-3	141	14	7	
-10	108	10	13	-4	62	39	38*	2	135	7	-4	-5	94	44	-8*		H,K= 11,-16			
-9	105	21	0*	-3	216	17	2	3	62	78	22*	-4	252	9	5	-3	0	67	-1*	
-8	0	67	-15*	-2	121	18	-1	4	154	15	0	-3	83	25	0*		H,K= 11,-15			
-7	210	9	9	-1	89	8	14		H,K= 10,		-1	-2	149	17	9	-6	112	29	19*	
-6	97	17	-8	0	205	6	-3	-11	130	19	4	-1	177	15	11	-5	95	26	4*	
-5	206	8	7	1	67	28	27*	-10	92	14	5	0	33	48	22*	-4	28	47	-8*	
-4	216	6	2	2	217	5	1	-9	107	44	11*	1	180	10	-9	-3	136	24	22	
-3	70	45	-2*	3	181	14	7	-8	151	18	-4	2	144	8	8	-2	0	57	-32*	
-2	136	13	-7	4	60	77	59*	-7	96	21	14*		H,K= 10,		3	-1	96	18	15*	
-1	164	7	2		H,K= 10,		-4	-6	133	8	18	-10	101	16	-4		H,K= 11,-14			
0	43	47	-7*	-11	20	61	2*	-5	255	7	-7	-9	15	52	-29*	-7	99	23	10*	
1	254	7	-3	-10	65	58	-26*	-4	27	54	17*	-8	142	14	-6	-6	67	26	9*	
2	120	15	9	-9	136	29	-12*	-3	157	26	-14	-7	80	47	1*	-5	108	12	29	
3	85	13	7	-8	69	46	47*	-2	169	14	-0	-6	142	8	8	-4	120	9	-3	
4	179	8	16	-7	158	15	-2	-1	75	19	-8*	-5	193	5	-2	-3	26	50	20*	
			H,K= 10,	-7	-6	135	24	-5	0	226	6	-8	-4	72	56	36*	-2	156	25	3
-11	108	29	17*	-5	126	7	-3	1	115	16	6	-3	163	25	16	-1	124	14	5	
-10	94	42	25*	-4	192	12	1	2	84	22	8*	-2	127	8	12	0	69	22	31*	
-9	69	70	36*	-3	148	12	-2	3	152	9	-0	-1	79	21	34*		H,K= 11,-13			
-8	154	11	5	-2	151	16	-1		H,K= 10,		0	0	182	10	-3	-8	67	48	-16*	
-7	80	47	7*	-1	176	15	4	-11	0	79	-64*	1	106	12	9	-7	0	66	-7*	
-6	213	12	10	0	38	49	-4*	-10	101	13	-5	2	113	13	9	-6	112	12	7	
-5	182	10	-1	1	199	7	-6	-9	108	13	10		H,K= 10,		4	-5	74	28	20*	
-4	88	18	-10*	2	161	20	5	-8	0	49	-23*	-9	145	8	6	-4	24	52	-1*	
-3	176	16	-7	3	13	45	-23*	-7	155	18	6	-8	0	65	-18*	-3	174	27	3	
-2	131	11	-0	4	163	12	1	-6	158	6	-1	-7	157	7	-5	-2	58	62	-7*	
-1	55	49	-2*		H,K= 10,		-3	-5	115	8	31	-6	134	20	11	-1	86	19	-10*	
0	200	9	-14	-11	102	19	-12*	-4	293	11	-8	-5	93	32	16*	0	135	8	-3	
1	102	19	7*	-10	71	81	9*	-3	85	25	-3*	-4	185	17	9	1	0	52	-3*	
2	234	20	5	-9	86	13	-3	-2	181	12	6	-3	72	35	-2*		H,K= 11,-12			
3	196	13	-1	-8	177	13	2	-1	234	11	2	-2	75	35	-11*	-8	80	63	41*	
4	88	45	77*	-7	70	77	8*	0	71	60	38*	-1	159	22	21	-7	113	19	-6	
			H,K= 10,	-6	-6	182	13	4	1	186	11	-2	0	6	47	-24*	-6	31	48	-10*
-11	33	51	21*	-5	197	15	-5	2	139	7	12	1	152	12	8	-5	130	7	15	
-10	119	15	14	-4	31	49	4*	3	49	75	18*		H,K= 10,		5	-4	134	9	2	
-9	117	15	-12	-3	157	5	5		H,K= 10,		1	-8	128	10	8	-3	62	40	24*	
-8	39	64	21*	-2	175	8	6	-11	147	12	52	-7	74	38	14*	-2	148	17	11	
-7	178	24	7	-1	103	12	-2	-10	77	19	-34*	-6	144	13	-14	-1	141	15	15	
-6	98	15	-9	0	187	5	-1	-9	72	60	16*	-5	154	7	-7	0	53	64	-22*	
-5	173	8	-1	1	50	66	-0*	-8	140	14	13	-4	75	60	50*	1	163	24	1	
-4	201	9	1	2	95	21	-29*	-7	95	21	33*	-3	178	19	12	2	73	87	9*	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	11,-11	-10	43	75	-8*	2	75	51	-6*	H,K=	11,	1	-4	140	24	6		
-9	95	12	28	-9	70	46	-5*	3	123	17	24	-9	49	59	1*	-3	45	74	37*
-8	110	16	-5	-8	124	21	4	H,K=	11,	-3	-8	139	19	5	-2	82	33	-8*	
-7	0	48	-27*	-7	16	42	-4*-10	73	19	14*	-7	0	72	-12*	-1	51	72	-1*	
-6	130	24	-2*	-6	146	13	10	-9	108	32	5*	-6	114	10	-24	H,K=	12,-11		
-5	108	21	14*	-5	168	6	-3	-8	116	11	-2	-5	151	18	9	-8	72	51	-10*
-4	61	44	41*	-4	88	19	-5*	-7	0	44	-17*	-4	54	21	42*	-7	36	46	30*
-3	120	46	-0*	-3	188	8	1	-6	167	21	1	-3	137	9	-4	-6	131	9	5
-2	105	13	10	-2	70	32	-23*	-5	173	6	5	-2	101	33	-8*	-5	75	39	-29*
-1	94	23	6*	-1	101	19	2*	-4	63	35	44*	-1	128	11	16	-4	75	39	24*
0	140	8	-1	0	170	14	16	-3	217	23	5	0	167	8	9	-3	137	11	20
1	48	61	38*	1	69	30	17*	-2	85	24	5*	1	17	51	-23*	-2	26	59	15*
2	167	12	13	2	129	12	-6	-1	52	59	-28*	H,K=	11,	2	-1	88	14	-10	
	H,K=	11,-10	3	129	9	-5	0	218	15	-1	-9	102	49	-8*	0	139	11	9	
-9	86	18	-13*	H,K=	11,	-6	1	56	24	35*	-8	0	73	-24*	H,K=	12,-10			
-8	45	79	26*-10	110	28	-6*	2	130	9	4	-7	183	20	6	-8	54	63	5*	
-7	160	8	11	-9	83	26	0*	H,K=	11,	-2	-6	112	17	-1	-7	129	27	2*	
-6	65	77	6*	-8	46	26	31*-10	122	11	26	-5	95	11	28	-6	67	41	12*	
-5	102	16	-7	-7	167	16	17	-9	109	26	-4*	-4	159	17	5	-5	95	57	-13*
-4	170	9	6	-6	93	76	-17*	-8	83	16	30*	-3	74	34	-3*	-4	138	16	-8
-3	50	72	16*	-5	90	15	-0	-7	163	7	13	-2	85	18	12*	-3	36	60	8*
-2	120	29	-1*	-4	186	6	-3	-6	76	22	-28*	-1	120	10	22	-2	67	24	-16*
-1	99	23	-17*	-3	0	43	-36*	-5	111	10	21	0	70	78	49*	-1	108	10	11
0	63	65	12*	-2	127	26	1*	-4	197	11	6	H,K=	11,	3	0	38	49	-18*	
1	216	5	10	-1	134	17	-2	-3	112	20	22	-8	124	10	-6	H,K=	12,-9		
2	85	33	-2*	0	35	59	2*	-2	191	20	5	-7	50	60	25*	-9	58	65	-15*
	H,K=	11,-9	1	212	10	-1	-1	150	8	-8	-6	157	30	10*	-8	74	77	-16*	
-10	51	64	-2*	2	120	17	-13	0	45	36	-1*	-5	152	13	-18	-7	31	61	15*
-9	78	19	10*	3	48	87	-16*	1	164	16	-3	-4	0	66	-6*	-6	130	10	-7
-8	113	17	-4	H,K=	11,-5	2	109	22	19*	-3	136	10	9	-5	133	12	15		
-7	38	50	26*-10	0	60	-43*	H,K=	11,-1	-2	67	67	-23*	-4	92	11	16			
-6	135	27	-9*	-9	119	10	2	-10	90	48	13*	-1	71	85	2*	-3	153	13	12
-5	169	33	-2*	-8	135	26	9*	-9	30	65	-21*	H,K=	11,4	-2	33	52	-0*		
-4	56	61	4*	-7	53	42	22*	-8	130	14	-3	-7	154	13	12	-1	95	51	19*
-3	158	22	-2	-6	169	21	4	-7	17	44	9*	-6	82	15	-7*	0	174	9	6
-2	94	10	3	-5	190	13	-1	-6	135	12	-1	-5	61	41	-11*	1	31	91	31*
-1	115	42	2*	-4	62	16	26*	-5	129	10	-5	-4	181	14	3	H,K=	12,-8		
0	162	8	-6	-3	168	9	-5	-4	0	76	-10*	-3	87	51	56*	-9	63	75	-7*
1	48	57	-4*	-2	61	36	-9*	-3	212	9	-2	-2	114	32	18*	-8	66	66	12*
2	152	17	-3	-1	90	10	-5	-2	142	22	15	H,K=	11,5	-7	133	10	7		
3	120	17	3	0	226	11	-6	-1	111	27	22*	-5	124	30	4*	-6	71	28	15*
	H,K=	11,-8	1	58	36	-6*	0	210	12	18	-4	53	63	24*	-5	101	45	1*	
-10	108	24	1*	2	147	8	21	1	18	71	-8*	H,K=	12,-14	-4	136	23	2		
-9	66	39	-17*	3	139	27	2*	2	103	13	12	-5	99	19	14*	-3	16	48	-4*
-8	61	34	33*	H,K=	11,-4	H,K=	11,0	-4	102	25	-5*	-2	140	40	1*				
-7	156	15	2	-10	113	26	7*-10	104	16	2	-3	36	51	33*	-1	125	39	9*	
-6	72	13	-2*	-9	88	23	-7*	-9	108	22	-1*	H,K=	12,-13	0	27	55	4*		
-5	118	9	4	-8	58	20	14*	-8	81	18	51*	-6	139	48	38*	1	139	19	-3
-4	208	5	-5	-7	148	10	3	-7	159	15	4	-5	75	33	4*	H,K=	12,-7		
-3	61	22	48*	-6	127	10	-5	-6	59	70	7*	-4	51	40	3*	-9	99	29	21*
-2	181	29	1	-5	92	26	17*	-5	118	21	7	-3	147	8	3	-8	112	21	-0
-1	121	11	14	-4	170	21	-8	-4	177	9	-14	-2	41	51	4*	-7	10	59	-5*
0	36	49	26*	-3	68	76	41*	-3	86	22	13*	-1	136	10	16	-6	140	29	18*
1	188	6	1	-2	126	22	9	-2	176	15	5	H,K=	12,-12	-5	112	26	-14*		
2	114	9	23	-1	171	7	12	-1	144	25	-0	-7	113	21	16	-4	52	62	-28*
3	61	73	-1*	0	39	46	1*	0	81	26	17*	-6	48	58	10*	-3	168	27	13
	H,K=	11,-7	1	187	15	-13	1	145	11	-0	-5	87	19	-3*	-2	39	47	-19*	

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