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CHLORO-, METHYL-, AND TETRAHYDROBORATO-TRIS (HEXAMETHYLDISILYLAMIDO) -THORIUM (IV) AND URANIUM (IV) . CRYSTAL STRUCTURE OF TETRAHYDROBORATO TRIS (HEXAMETHYLDISILYLAMIDO) -THORIUM (IV)

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CHLORO-, METHYL-, AND TETRAHYDROBORATO- TRIS (HEXAMETHYLDISILYLAMIDO)-THORIUM(IV) AND URANIUM(IV). CRYSTAL STRUCTURE OF TETRAHYDROBORATO TRIS (HEXAMETHYLDISILYLAMIDO)-THORIUM(IV).

Howard W. Turner, Richard A. Andersen,
Allan Zalkin and David H. Templeton

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Contribution from the
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Chloro-, Methyl-, and Tetrahydroborato- Tris(hexamethyldisilylamido)-Thorium(IV) and Uranium(IV). Crystal Structure of Tetrahydroborato Tris(hexamethyldisilylamido)-Thorium(IV).

By Howard W. Turner, Richard A. Andersen*, Allan Zalkin* and David H. Templeton*

ABSTRACT

Reaction of sodium hexamethyldisilylamide with thorium tetrachloride or uranium tetrachloride yields chlorotris(hexamethyldisilylamido)-thorium(IV) or - uranium(IV), respectively. The chloroamides of thorium or uranium react with dimethylmagnesium or methyllithium yielding the methyl derivatives, $MeTh[N(SiMe_3)_2]_3$ or $MeU[N(SiMe_3)_2]_3$, respectively. The chloro compounds yield $BH_4M[N(SiMe_3)_2]_3$ upon reaction with lithium tetrahydroborate, where M is thorium or uranium. Infrared spectra of the tetrahydroborate derivatives suggest that BH_4^- is bonded in a tridentate fashion in both compounds, the metal atoms being six coordinate. Single crystal x-ray analysis of the thorium borohydride confirms the infrared result. The white $BH_4Th[N(Si(CH_3))_2]_3$ crystals are rhombohedral with cell dimensions a_r = 11.137 Å and α_r = 113.61°; the triply primitive hexagonal cell is a_h = 18.640(3) Å, c_h =

8.604(1) Å, V = 2489 $Å^3$, Z = 3, and D_x = 1.40 g/cm^3, space group R3m. The structure was refined by full-matrix least squares to a conventional R factor of 0.031 for 1014 data. The Th atom is on a three fold axis 2.32 Å from three nitrogen atoms and 2.61 Å from the boron atom, a distance which represents a triple bridge bond between Th and B. The three dimethylsilylamide ligands are disordered by a mirror plane parallel to the 3-fold axis. $CH_3Th[N(Si(CH_3)_3)_2]_3$ is isomorphous with $BH_4Th[N(Si(CH_3)_3)_2]_3$ with cell dimensions a_h = 18.68(1) Å and c_h = 8.537(6) Å. The diffraction data yielded f'' = 12.16 ± 0.33 e for the imaginary scattering term for Th with CuKα radiation.

INTRODUCTION

Tris(hexamethyldisilylamido) metal compounds have been described for a large group of p-, d-, and 4f- block metal atoms.[1,2,3] In contrast, only four silylamido compounds have been described for the 5f- block series, $ClTh[N(SiMe_3)_2]_3$,[4] $O_2U[N(SiMe_3)_2]_2(thf)_2$, $OU[N(SiMe_3)_2]_3$, and $U[N(SiMe_3)_2]_3$.[5] This paper describes the series, $X\,M[N(SiMe_3)_2]_3$, where M is thorium or uranium and X is chloro, methyl, or tetrahydroborate. The crystal structure of one of these compounds, $(BH_4)Th[N(SiMe_3)_2]_3$, is also described.

RESULTS AND DISCUSSION

Sodium hexamethyldisilylamide reacts with thorium or uranium tetrachloride affording chlorotris(hexamethyldisilylamido)-thorium or -uranium, respectively. The air- and moisture-sensitive, monomeric (by mass spectrometry) amides are readily soluble in pentane from which they may be crystallized. Physical properties of the compounds are shown in Table I.

The chloro-silylamide of uranium reacts with methyllithium yielding the monomethyl derivative, $MeU[N(SiMe_3)_2]_3$. In contrast methyllithium displaces a hexamethyldisilylamide group from the coordination sphere of $ClTh[N(SiMe_3)_2]_3$, lithium hexamethyldisilylamide being the only product isolated. The monomethylthorium compound, however, can be isolated by using dimethylmagnesium as alkylating agent. The four-coordinate monomethyl derivatives are soluble in

hydrocarbon solvents and are rather air- and moisture-sensitive. This sensitivity is to be contrasted with that of the air- and moisture-stability of the zirconium and hafnium analogues.[5] This is doubtless a kinetic effect and must be related to the larger ionic radii of the 5f-block metal atoms.

The ^{1}H NMR spectra of the alkyl derivatives are temperature independent to -65°C. Again, this is to be contrasted with those of the hafnium analogue which are temperature dependent. The hafnium analogue shows two-equal area resonances due to trimethyl silyl groups, the coalescence temperature being ca. -25°C. This latter observation has been previously described.[5] The diamagnetic thorium compounds have been further characterized by $^{13}C\{^{1}H\}$NMR spectroscopy. The $ClTh[N(SiMe_3)_2]_3$ shows a single resonance at δ 3.98 due to the carbon atoms of the Me_3Si group, and $MeTh[N(SiMe_3)_2]_3$ shows two single absorptions at δ 4.17 and δ 1.28 due to the carbon atoms of the Me_3Si and Me groups, respectively.

The chloro-amides of thorium or uranium yield hydrocarbon soluble tetrahydroborate derivatives upon reaction with lithium tetrahydroborate. The infrared spectra, which are essentially identical, strongly suggest that the tetrahydroborate is bonded in a tridentate fashion, one absorption in the terminal and two absorptions in the bridging B-H stretching frequency region.[6] This has been confirmed by a single crystal x-ray analysis (see below).

The ^{1}H NMR spectrum of $(BH_4)Th[N(SiMe_3)_2]_3$ shows a 1:1:1:1 quartet at δ 4.34, $J_{^{1}H-^{11}B}$ = 81 Hz and a singlet at δ 0.58 in an area ratio of

4:54. The paramagnetic (f^2) uranium analogue shows a 1:1:1:1 quartet centered at δ-101, $J_{^1H-^{11}B}$ = 79 Hz and a singlet at δ-1.87 in an area ratio of 4:54. Lowering the temperature to -80°C only results in slight line broadening. Thus these are fluxional molecules even at this temperature.

The crystal structure has disorder consisting of two possible orientations of the molecule. A picture of the ordered molecule is shown in Fig. 1. Atomic parameters, distances, and angles for BH_4-$Th[N(SiMe_3)_2]_3$ are listed in Tables II-IV.

The thorium atom is on a 3-fold axis and lies 0.47 Å below the plane of the three nitrogen atoms. The shape and dimensions of the tris[bis(trimethylsilyl)amido]thorium part of this structure are similar to the geometry found in the molecule $M[N(Si(CH_3)_3)_2]_3$ where M = Eu,[8] Yb,[9] Sc,[8] and Nd;[10] in all these compounds the metal atom is out of the plane of the nitrogen atoms.

All of the atoms with the exception of thorium, boron, and the terminal hydrogen atom on the borom atom are disordered. The nature of disorder is such that the atoms are on one side or the other of a mirror plane that runs parallel to the z axis. It is not possible with these data to distinguish a random disorder from twinning; our description is that of a random disorder.

From an analogy with the distances in the $U(BH_4)_4$[11] structure one can deduce how the borohydride group is bonded to the thorium atom. In $U(BH_4)_4$, the borohydride is bonded to the uranium atom by triple hydrogen bridge bonds and by double hydrogen bridge bonds with resulting U-B distances of 2.5 Å and 2.9 Å respectively. In this structure

the Th-B distance is 2.6 Å and represents a triply bridged hydrogen bond. The terminal hydrogen atom was found in the Fourier maps and refined, but the three bridging hydrogen bonds are disordered and were not found. Thorium is hexacoordinate being bonded to three nitrogen and three hydrogen atoms.

EXPERIMENTAL

Analyses were by the microanalytical laboratory of this department. Solution magnetic susceptibilities were measured on a Varian T-60 machine operating at 25°C by Evans' method.[7] The ^{1}H NMR spectra were measured on a modified Bruker WH 1180 machine operating at 180 MHz in toluene-d_8. The $^{13}C\{^{1}H\}$NMR spectra were recorded on a Nicolet TT-23 instrument operating at 25.14 MHz in benzene-d_6. All operations were performed under nitrogen.

Chlorotris(hexamethyldisilylamido)thorium (IV). This compound was previously described in a note without experimental details.[4] Sodium hexamethyldisilylamide (10.0 g, 0.0545 mol) in tetrahydrofuran (100 mL) was added to thorium tetrachloride (6.80 g, 0.0182 mol) in tetrahydrofuran (200 mL). The mixture was stirred for 72 h. The tetrahydrofuran was filtered and the filtrate was evaporated to ca. 60 mL in vacuum. Pentane (200 mL) was added and the solution was cooled (-10°C). The white needles were collected and dried in vacuum, mp, 210-212°C. Yield was 10.2g (75%).

Chlorotris(hexamethyldisilylamido)uranium (IV). Sodium hexamethyldisilylamide (14g, 0.076 mol) in tetrahydrofuran (100 mL) was added to uranium tetrachloride (9.7g, 0.026 mol) in tetrahydrofuran (200 mL). The mixture was stirred for 24 h and was filtered. The residue was extracted with tetrahydrofuran (150 mL) and the combined extracts were concentrated to ca. 100 mL. Pentane (200 mL) was added and the solution was cooled (-10°C). The tan needles were collected and dried in vacuum, mp 178-180°C. Yield was 13g (70%). Anal. Calcd. for $C_{18}H_{54}ClN_3Si_6U$: C, 28.7; H, 7.17, Cl, 4.70; N, 5.57. Found: C, 28.5; H, 6.93; Cl, 4.50; N, 5.54.

Methyltris(hexamethyldisilylamido)thorium (IV). Dimethylmagnesium (1.3 ml of a 1.0 M diethyl ether solution, 0.0013 mol) was added to a solution of chlorotris(hexamethyldisilylamido)thorium (2.0g, 0.0027 mol) in diethyl ether (50 mL) at 0°C. The mixture was stirred for 20 h (0°C). The diethyl ether was removed in vacuum and residue was extracted with pentane (50 mL). The pentane extract was filtered and concentrated to ca. 30 mL. Cooling (-78°C) afforded white needles, mp, 133-135°C. Yield was 1.5g (78%). Anal. Calcd. for $C_{19}H_{57}N_3Si_6Th$: C, 31.4; H, 7.84; N, 5.78. Found: C, 31.0; H, 7.88; N, 5.80.

Methyltris(hexamethyldisilylamido)uranium (IV). Methyllithium (2.3 ml of a 0.88 M diethyl ether solution, 0.0020 mol) was added to chlorotris(hexamethyldisilylamido)uranium (1.5g, 0.0020 mol) in diethyl

ether (50 mL) at 0°C. The mixture was stirred for 15 h at 0°C. The diethyl ether was removed in vacuum and residue was extracted with pentane (50 mL). The extract was concentrated to ca. 30 mL and cooled (-10°C).. The light brown needles were collected and dried in vacuum, mp 130-132°C. Yield was 1.2g (80%). Anal. Calcd. for $C_{19}H_{57}N_3Si_6U$: C, 31.1; H, 7.72; N, 5.70. Found: C, 30.6; H, 7.69; N, 5.68.

Tetrahydroboratotris(hexamethyldisilylamido)thorium (IV). Lithium tetrahydroborate (0.055g, 0.0025 mol) in diethyl ether (20 mL was added to chlorotris(hexamethyldisilylamido)thorium (1.9g, 0.0025 mol) in tetrahydrofuran (30 mL) at 0°C. The mixture was stirred for 20 h at 0°C. The volatile material was removed in vacuum and residue was extracted with pentane (50 mL). Concentration in vacuum of the extract to ca. 25 mL and cooling (-10°C) afforded white needles, mp 168-171°C. Yield was 1.5g (82%). Anal. Calcd. for $C_{18}H_{58}BN_3Si_6Th$: C, 29.7; H, 7.98; N, 5.78. Found: C, 29.0; H, 7.63; N, 5.55.

Tetrahydroboratotris(hexamethyldisilylamido)uranium (IV). Lithium tetrahydroborate (0.058g, 0.0027 mol) in diethyl ether (20 mL) was added to chlorotris(hexamethyldisilylamido)uranium (2.0g, 0.0027 mol) in diethyl ether (50 mL) at 0°C. The mixture was stirred at 0°C for 15 h. Diethyl ether was removed in vacuum and residue was extracted with pentane (50 mL). The extract was concentrated in vacuum to ca. 20 mL. Cooling afforded light brown needles, mp 150-155°C in 65%

yield (1.3g). Anal. Calcd. for $C_{18}H_{58}BN_3Si_6U$: C, 29.5; H, 7.91; N, 5.73. Found: C, 29.0; H, 7.53; N, 5.64.

X-ray Diffraction. A colorless hexagonal needle shaped crystal with approximate dimensions .06 × .09 × .23 mm was sealed inside a quartz capillary in an argon filled dry box. Weissenberg photography showed the crystal to be rhombohedral, and rough cell dimensions were obtained. The crystal was examined on a Picker FACS-I automatic diffractometer equipped with a graphite monochromator and a Cu X-ray tube ($\lambda(K\alpha_1)$ 1.54056 Å). ω scans of several low-angle reflections showed peaks with half-widths of 0.12 - 0.14°. The setting angles of 12 manually centered reflections ($94° < 2\theta < 119°$) were used to determine by least-squares the dimensions of the triply primitive hexagonal cell, a_h = 18.640(3) Å, c_h = 8.604(1) Å, and V = 2589 Å^3. For Z = 3 and a molecular weight of 728.05 the calculated density is 1.40 g/cm^{-3}. The rhombohedral cell parameters are a_r = 11.137 Å and α_r = 113.61°. The structure was solved in the space group R3m, using hexagonal coordinates.

Intensity data were collected using the θ-2θ scan technique with a scan speed of 2°/min on 2θ. Each peak was scanned from 0.75° before the $K\alpha_1$ peak to 0.75° after the $K\alpha_2$ peak, and backgrounds were counted for 10 s at each end of the scan range, offset by 0.25°. The temperature during data collection was 22 ± 1°C. Three standard reflections, (003, 600, and $\bar{4}80$), were measured after every 200th scan. The intensity of the 003 reflection decayed about 10%, whereas the two other reflections decayed by 4%; a linear decay correction of 5% was applied uniformly to the data.

The data were corrected for absorption by an analytical method[12] using an estimated absorption coefficient of 161 cm^{-1}; absorption corrections varied from 2.3 to 5.1. A total of 5462 scans, not including standards, resulted in 1014 unique reflections (Friedel pairs not averaged).

Because there were no observed space group extinctions, all five point groups in the two trigonal Laue groups were considered. A careful perusal of the intensity variation of the Friedel pairs as well as certain classes of reflections, did in fact strongly indicate R3m as the space group. The 3-dimensional Patterson function was calculated but it was not consistent with an ordered structure in R3m. An attempt to solve the structure in space group R3 indicated a disorder with a symmetry describable in R3m. Once the disorder was adopted a series of least-squares refinements in space group R3m, in which the function $\Sigma w(|F_o|-|F_c|)^2/\Sigma wF_o^2$ was minimized, converged rapidly to the final structure. The expressions that were used in processing the data and to estimate weights are given in the supplementary material; the "ignorance factor", p, was set to 0.05 and q was set to 250. Scattering factors and anomalous dispersion corrections from the International Tables[13] were used; for Th, f' = -5.091 e and f" = 12.330 e. Anisotropic thermal parameters were included only for thorium. An empirical extinction correction was applied for $F_{corr} = F_o(1 + kI)$ and $k = 4.2 \times 10^{-7}$, where I is the raw intensity, F_o is the observed structure factor and F_{corr} is the modified observed structure factor. The discrepancy

indices for all 1014 data (Friedel pairs not averaged) are

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

$$R_w = [\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2} = 0.037.$$

The error in an observation of unit weight is 1.40. In the last cycle no parameter changed more than 0.004 σ.

A least-squares refinement with f'' of thorium as an adjustable parameter[14] confirmed that the correct absolute orientation of the structure had been chosen. The result was f'' = 12.16 ± 0.33 e, in excellent agreement with the value 12.330 e calculated by Cromer and Liberman[15] for $CuK\alpha_1$ radiation. This agreement also indicates that the specimen was substantially free of inversion twinning.

A single crystal of $Th[N(Si(CH_3)_3)_2]_3CH_3$ was examined by x-ray diffraction method and found to be isomorphous with the $Th[N(Si(CH_3)_3)_2]_3BH_4$ reported here. The methyl derivative has cell dimensions a = 18.68(1) Å and 8.537(6) Å. Weissenberg patterns of the two isomorphs showed intensities that were visually the same. The crystals of the methyl derivative were too poor in quality to be used for collecting a suitable set of intensity data.

ACKNOWLEDGEMENT

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SUPPLEMENTARY MATERIALS AVAILABLE

Data processing formulas, and the listing of structure factor amplitudes (6 pages). Ordering information is given on any current masthead.

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Table I. Physical Properties of the Series $XM[N(SiMe_3)_2]_3$

		^1H NMR[b]		Infrared[c]		
Compound	μ_B[a]	M-Me	M-N(SiMe$_3$)$_2$	M-N	M-Cl	M-BH$_4$
$ClTh[N(SiMe_3)_2]_3$	diamagnetic	--	0.50	385 s	270 m	--
$ClU[N(SiMe_3)_2]_3$	2.8	--	-2.22	385 s	272 m	--
$MeTh[N(SiMe_3)_2]_3$	diamagnetic	0.85	0.57	385 s	--	--
$MeU[N(SiMe_3)_2]_3$	2.7	-224	-1.49	385 s	--	--
$BH_4Th(N(SiMe_3)_2]_3$	diamagnetic	--	0.58	385 s	--	2500 s, 2345 w, 2240 s, 2180 m
$BH_4U[N(SiMe_3)_2]_3$	2.6	--	-1.87	390 s	--	2500 s, 2335 w, 2240 s, 2170 m

(a) Benzene solution at 25°C, by Evans' method,[7] expressed in Bohr magnetons.

(b) Benzene solution at 25°C, expressed in δ units (positive value, high frequency), relative to Me_4Si.

(c) Nujol mulls, cm^{-1}.

Table II. Positional and Thermal Parameters with Estimated Standard Deviations[a]

Atom	x	y	z	B(Å^2)
Th	0.0	0.0	0.0	[b]
B	0.0	0.0	-0.303(3)	4.4(4)
H	0.0	0.0	-0.43(2)	4.4[c]
N[d]	0.1014(7)	0.1351(7)	0.055(1)	3.3(2)
Si(1)	0.0886(4)	0.1915(2)	0.2023(4)	3.4(1)
Si(2)	0.1901(3)	0.1790(3)	-0.0605(5)	3.9(1)
C(1)	-0.015(1)	0.129(1)	0.293(2)	5.5(4)
C(2)	0.165(1)	0.219(1)	0.366(2)	5.7(4)
C(3)	0.100(1)	0.289(1)	0.128(2)	6.0(4)
C(4)	0.210(1)	0.096(2)	-0.138(2)	4.9(4)
C(5)	0.286(1)	0.255(1)	0.045(2)	5.9(4)
C(6)	0.180(1)	0.236(1)	-0.230(2)	6.0(4)

[a] Here and in the following tables the number in parenthesis is the estimated standard deviation in the least significant digit.

[b] The anisotropic temperature factor for thorium has the form $\exp(-.25(B_{11}h^2a^{*2} + 2B_{12}hka^*b^* + \ldots))$, where $B_{11} = 2.98(2)$, $B_{22} = 2.98$, $B_{33} = 3.30(2)$, $B_{12} = 1.49$, $B_{13} = B_{23} = 0$.

[c] The thermal parameter for hydrogen was restrained to equal that for boron.

[d] The N, Si and C atoms are all disordered.

Table III. Selected Interatomic Distances (Å)

Th	- B	2.61(3)
	- 3N	2.32(2)
N	- Si(1)	1.74(2)
	- Si(2)	1.74(2)
Si(1)	- C(1)	1.86(2)
	- C(2)	1.88(2)
	- C(3)	1.84(2)
Si(2)	- C(4)	1.89(2)
	- C(5)	1.87(2)
	- C(6)	1.87(2)
B	- H	1.1(2)

Table IV. Selected Angles (deg.)

N - Th - N	115.9(2)
Si(1) - N - Th	122(1)
Si(2) - N - Th	117(1)
Si(1) - N - Si(2)	121(1)
C(1) - Si(1) - N	110(1)
C(2) - Si(1) - N	113(1)
C(3) - Si(1) - N	111(1)
C(1) - Si(1) - C(2)	105(1)
C(1) - Si(1) - C(3)	110(1)
C(2) - Si(1) - C(3)	107(1)
C(4) - Si(2) - N	110(1)
C(5) - Si(2) - N	114(1)
C(6) - Si(2) - N	112(1)
C(4) - Si(2) - C(5)	106(1)
C(4) - Si(2) - C(6)	108(1)
C(5) - Si(2) - C(6)	106(1)

FIGURE CAPTION

Fig. 1. View of the $Th[N(Si(CH_3)_2)]_3BH_4$ molecule as viewed down, but slightly off of the c axis.

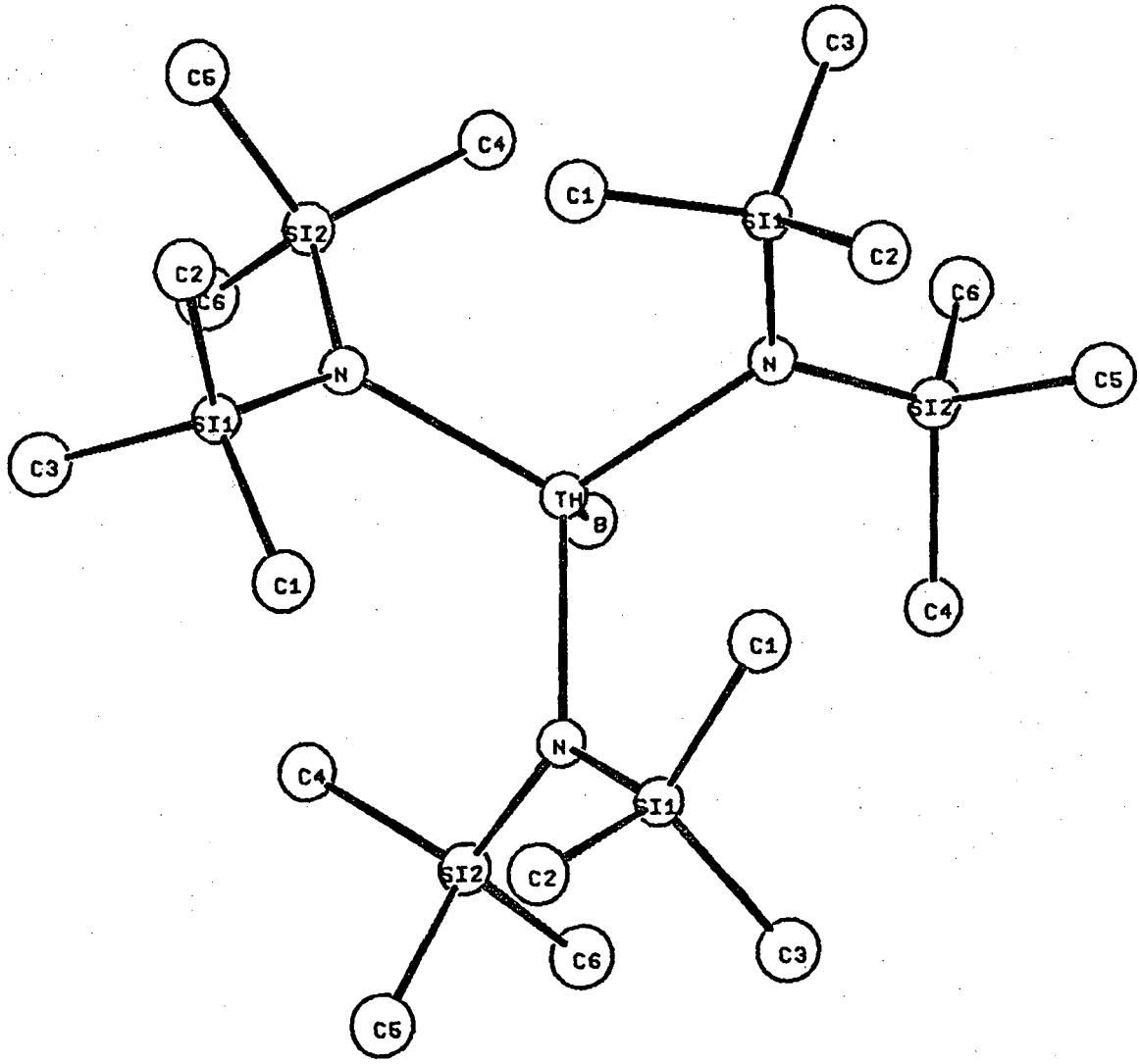
C6
C4
SI2
C2
C6
N
SI1
C3
C1
TH
B
C3
C1
SI1
C2
C6
N
SI2
C5
C4
C1
N
C4
SI1
SI2
C2
C6
C3
C5

Fig. 1

Supplementary Materials for the Paper:

Chloro-, Methyl-, and Tetrahydroborato- Tris(hexamethyldisilylamido)-Thorium(IV) and Uranium(IV). Crystal Structure of Tetrahydroborato Tris(Hexamtheyldisilylamido)-Thorium(IV).

by Howard W. Turner, Richard A. Andersen*, Allan Zalkin* and David H. Templeton*

DATA PROCESSING FORMULAE

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

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

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

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

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

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

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

When $S(F_a^2) > 4\sigma(F_a^2)$, $\sigma(F_a^2)$ is replaced by $S(F_a^2)$.

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

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

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

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

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

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

C = counts recorded during a scan

I = individual raw intensity, background removed.

t_c = scan count time

t_b = background count time

B_1 = individual background count

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

F = structure factor

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

A = absorption correction

Lp = Lorentz and polarization corrections

θ_m = monochromater angle

θ = crystal diffraction angle

S = scatter

a = average

q = additional uncertainty that affects the weak intensities

p = estimate of non-statistical errors

wtg = weighting factors in least squares

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
TH(N(SI(CH3)3)2)3+BH4- F(0,0,0) = 2755

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

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
K,L=	0,		-6	1	189	7	6	13	278	7	8	2	393	8	8	4	210	7	19
0	280	9	-8	4	253	7	15	16	198	7	0	5	712	15	15	7	223	7	5
K,L=	0,		-3	7	325	8	10	K,L=	1,		4	8	469	10	2	K,L=	2,		9
0	619	13	-4	10	159	8	12	2	586	12	11	11	293	7	2	2	221	7	15
K,L=	0,		0	13	154	7	0	5	412	9	-1	14	304	7	7	5	154	8	5
3	551	11	8	K,L=	0,		8	8	373	8	16	17	141	8	-2	K,L=	3,		-8
6	682	14	-2	2	242	8	12	11	288	7	0	K,L=	2,		1	-2	236	7	-6
9	535	11	-12	5	194	7	11	14	235	7	11	0	827	19	-23	K,L=	3,		-7
12	394	9	5	8	214	7	14	K,L=	1,		5	3	474	10	-2	-1	345	8	-5
15	246	7	10	11	79	14	-3	0	462	10	7	6	539	11	15	K,L=	3,		-6
18	153	8	7	K,L=	0,		9	3	414	9	7	9	412	9	11	-3	464	10	0
K,L=	0,		1	0	146	11	18	6	283	7	11	12	277	7	6	0	253	7	-3
11	126	24	-31	3	236	7	9	9	330	8	8	15	268	7	9	K,L=	3,		-5
4	451	10	25	6	83	16	-19	12	217	7	8	K,L=	2,		2	-2	345	8	-7
7	785	17	13	K,L=	1,		-8	15	156	7	5	1	843	17	-4	K,L=	3,		-4
10	613	13	15	-1	143	10	-1	K,L=	1,		6	4	384	8	-7	-1	543	11	-6
13	126	9	9	K,L=	1,		-7	1	372	8	8	7	407	9	11	K,L=	3,		-3
16	286	7	15	0	164	8	-1	4	225	7	16	10	438	9	8	-3	787	16	31
K,L=	0,		2	K,L=	1,		-5	7	324	8	10	13	254	7	12	0	573	12	-29
2	449	9	-24	-1	460	10	-6	10	235	7	11	16	219	6	5	K,L=	3,		-2
5	669	14	-17	K,L=	1,		-4	13	143	8	2	K,L=	2,		3	-2	790	16	-3
8	557	11	-24	0	586	13	2	K,L=	1,		7	2	517	11	-19	K,L=	3,		-1
11	323	8	2	K,L=	1,		-2	2	350	8	18	5	438	9	-10	-1	353	8	4
14	182	7	7	-1	589	12	-28	5	233	7	12	8	471	10	5	K,L=	3,		0
17	239	7	8	K,L=	1,		-1	8	281	7	17	11	326	7	4	0	408	9	-7
K,L=	0,		3	01131		27	12	11	123	9	-4	14	226	6	9	3	760	16	-10
0	648	13	41	K,L=	1,		0	K,L=	1,		8	K,L=	2,		4	6	467	10	-4
3	602	12	-15	1	876	18	-22	0	133	10	8	0	508	11	25	9	312	7	6
6	573	12	0	4	740	15	-4	3	298	7	15	3	447	9	12	12	321	7	5
9	318	7	0	7	463	10	2	6	180	7	5	6	426	9	8	15	240	7	12
12	255	7	16	10	617	13	17	9	149	8	2	9	370	8	1	K,L=	3,		1
15	262	7	-1	13	240	7	6	K,L=	1,		9	12	236	7	8	1	833	17	14
K,L=	0,		4	16	240	7	14	1	178	7	9	15	200	7	3	4	646	14	5
1	579	12	13	K,L=	1,		1	4	184	7	4	K,L=	2,		5	7	247	6	13
4	604	12	2	2	303	7	-7	7	127	9	5	1	356	8	7	10	388	8	6
7	233	7	-7	5	689	14	-15	K,L=	2,		-8	4	421	9	12	13	302	7	10
10	377	8	9	8	407	9	4	0	230	7	-3	7	341	8	8	16	168	7	4
13	264	7	14	11	451	9	-1	K,L=	2,		-7	10	287	7	10	K,L=	3,		2
16	188	7	5	14	196	7	14	-2	315	8	3	13	193	7	5	2	512	11	-15
K,L=	0,		5	17	214	7	10	K,L=	2,		-6	K,L=	2,		6	5	472	10	12
2	509	11	8	K,L=	1,		2	-1	337	8	-13	2	399	9	18	8	390	8	14
5	289	7	9	0	563	12	-46	K,L=	2,		-5	5	374	8	14	11	432	9	13
8	284	7	6	3	510	11	1	0	450	10	-12	8	267	7	12	14	194	7	2
11	287	7	8	6	706	14	13	K,L=	2,		-4	11	220	7	4	K,L=	3,		3
14	159	7	7	9	335	7	7	-2	491	10	15	K,L=	2,		7	0	831	17	32
K,L=	0,		6	12	250	7	4	K,L=	2,		-3	0	358	8	27	3	290	7	-12
0	332	8	3	15	243	7	10	-1	632	13	1	3	288	7	17	6	584	12	-1
3	271	7	19	K,L=	1,		3	K,L=	2,		-2	6	294	7	12	9	403	9	4
6	311	8	5	1	623	13	8	0	502	10	-13	9	184	7	5	12	285	7	5
9	308	7	13	4	624	13	14	K,L=	2,		-1	12	181	7	1	15	165	7	4
12	169	7	0	7	468	10	-11	-2	849	17	-1	K,L=	2,		8	K,L=	3,		4
K,L=	0,		7	10	299	7	2	K,L=	2,		0	1	262	7	10	1	386	8	3

STRUCTURE FACTORS CONTINUED FOR
TH(N(SI(CH3)3)2)3+BH4-

H	FOB	SG	DEL
4	484	10	9
7	513	11	-1
10	242	7	5
13	220	7	5
K,L=		3,	5
2	461	10	8
5	449	9	13
8	320	7	9
11	212	7	11
14	227	6	10
K,L=		3,	6
0	478	10	19
3	448	9	9
6	299	7	21
9	262	7	8
12	207	6	9
K,L=		3,	7
1	399	9	6
4	264	7	16
7	219	7	5
10	235	7	8
K,L=		3,	8
2	251	7	12
5	202	7	17
8	208	7	4
K,L=		3,	9
0	156	8	8
3	216	7	12
K,L=		4,	-8
-4	178	8	-12
-1	279	7	-13
K,L=		4,	-7
-3	363	8	-11
0	294	8	0
K,L=		4,	-6
-2	377	8	-7
K,L=		4,	-5
-4	463	10	-6
-1	357	8	-4
K,L=		4,	-4
-3	386	8	-9
0	563	12	-11
K,L=		4,	-3
-2	465	10	-29
K,L=		4,	-2
-4	931	19	-1
-1	494	10	-20
K,L=		4,	-1
-3	870	18	17
0	528	11	27
K,L=		4,	0
1	732	15	5
4	617	13	-5
7	469	10	8
10	263	7	12
13	329	7	10
16	160	7	-2
K,L=		4,	1
2	610	12	-9
5	476	10	-1
8	301	7	6
11	383	8	21
14	221	7	9
K,L=		4,	2
0	938	19	-2
3	406	9	12
6	530	11	10
9	404	9	12
12	283	7	12
15	158	7	-2
K,L=		4,	3
1	577	12	16
4	347	8	7
7	546	11	13
10	327	7	5
13	189	7	6
K,L=		4,	4
2	447	9	7
5	487	10	16
8	315	7	6
11	214	7	7
14	165	7	-1
K,L=		4,	5
0	411	9	10
3	558	12	13
6	311	7	17
9	244	7	15
12	198	7	10
K,L=		4,	6
1	398	9	12
4	408	9	21
7	184	7	2
10	257	7	12
K,L=		4,	7
2	259	7	10
5	230	7	16
8	216	7	7
K,L=		4,	8
0	222	7	-3
3	188	7	14
6	194	7	8
K,L=		4,	9
1	142	8	1
4	186	7	10
K,L=		5,	-8
-3	231	7	-7
0	189	8	0
K,L=		5,	-7
-5	237	7	-6
-2	279	7	-8
K,L=		5,	-6
-4	390	8	-10
-1	236	7	1
K,L=		5,	-5
-3	462	10	-9
0	342	8	-2
K,L=		5,	-4
-5	480	10	-10
-2	442	9	-1
K,L=		5,	-3
-4	572	12	6
-1	623	13	1
K,L=		5,	-2
-3	519	11	-6
0	728	15	-13
K,L=		5,	-1
-5	724	15	-46
-2	493	10	13
K,L=		5,	0
2	710	14	14
5	498	10	3
8	363	8	3
11	342	8	9
14	208	7	9
K,L=		5,	1
0	648	13	-56
3	584	12	23
6	504	10	9
9	345	8	14
12	278	7	8
15	159	7	3
K,L=		5,	2
1	625	13	-2
4	518	11	5
7	377	8	10
10	362	8	21
13	179	7	9
K,L=		5,	3
2	417	9	-9
5	508	11	14
8	253	7	8
11	303	7	8
14	145	8	5
K,L=		5,	4
0	450	10	2
3	378	8	14
6	376	8	8
9	227	7	12
12	217	7	4
K,L=		5,	5
1	370	8	12
4	327	7	17
7	249	7	8
10	188	7	13
13	160	7	2
K,L=		5,	6
2	317	7	9
5	227	7	14
8	250	7	10
11	140	8	6
K,L=		5,	7
0	239	7	13
3	257	7	16
6	172	7	5
9	215	7	11
K,L=		5,	8
1	185	7	12
4	171	7	11
7	155	7	3
K,L=		5,	9
2	180	7	4
K,L=		6,	-9
-6	113	11	-14
0	69	21	-18
K,L=		6,	-8
-5	171	7	-4
-2	214	7	-3
K,L=		6,	-7
-4	238	7	-3
-1	228	7	-5
K,L=		6,	-6
-6	232	7	-19
-3	383	8	-14
0	333	8	-19
K,L=		6,	-5
-5	371	8	-10
-2	410	9	-5
K,L=		6,	-4
-4	474	10	-5
-1	452	9	-15
K,L=		6,	-3
-6	751	18	-23
-3	319	7	-19
0	589	12	-15
K,L=		6,	-2
-5	684	14	-7
-2	341	8	-18
K,L=		6,	-1
-4	667	14	10
-1	677	14	-24
K,L=		6,	0
0	664	14	-20
3	468	10	-6
6	535	11	33
9	361	8	10
12	256	7	10
K,L=		6,	1
1	419	9	-6
4	606	12	10
7	370	8	18
10	307	7	15
13	193	7	6
K,L=		6,	2
2	450	9	-4
5	601	12	20
8	199	7	7
11	280	7	13
14	175	7	8
K,L=		6,	3
0	751	15	-1
3	381	8	4
6	344	8	6
9	274	7	10
12	215	7	0
K,L=		6,	4
1	545	11	-9
4	237	7	15
7	296	7	10
10	266	7	12
13	132	8	-2
K,L=		6,	5
2	335	8	14
5	237	7	6
8	281	7	18
11	161	7	7
K,L=		6,	6
0	196	7	1
3	291	7	20
6	226	7	4
9	201	7	14
K,L=		6,	7
1	247	7	12
4	234	7	9
7	182	7	11
K,L=		6,	8
2	225	7	7
5	132	8	4
K,L=		6,	9
0	144	8	-4
K,L=		7,	-9
-5	162	8	-13
-2	141	9	-23
K,L=		7,	-8
-7	213	7	-19
-4	190	7	-1
-1	141	8	-5
K,L=		7,	-7
-6	255	7	-9
-3	221	7	-2
0	292	7	-8
K,L=		7,	-6
-5	276	7	-9
-2	342	8	-9
K,L=		7,	-5
-7	236	7	-13
-4	501	10	-11
-1	307	7	-17
K,L=		7,	-4
-6	516	11	-20
-3	492	10	-4

STRUCTURE FACTORS CONTINUED FOR
TH(N(SI(CH3)3)2)3+BH4-

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
0	211	7	-18	0	228	7	7	K,L=		8,	3	K,L=		9,	-1	-2	233	7	-6
K,L=		7,	-3	3	205	7	10	2	435	9	10	-7	451	9	-11	K,L=		10,	-5
-5	431	9	-20	K,L=		7,	9	5	302	7	-1	-4	486	10	-4	-10	340	8	-14
-2	440	9	-15	1	167	7	1	8	266	7	13	-1	435	9	-3	-7	264	7	-11
K,L=		7,	-2	K,L=		8,	-9	11	204	7	1	K,L=		9,	0	-4	292	7	4
-7	492	10	7	-7	140	9	-19	K,L=		8,	4	0	585	12	-8	-1	311	7	-5
-4	368	8	1	-4	172	7	-16	0	559	12	-2	3	299	7	7	K,L=		10,	-4
-1	680	14	6	-1	110	10	-7	3	253	7	9	6	384	8	9	-9	317	7	-13
K,L=		7,	-1	K,L=		8,	-8	6	352	8	18	9	199	7	12	-6	260	7	-4
-6	426	9	-12	-6	202	7	-9	9	231	7	5	12	189	7	2	-3	459	10	-20
-3	594	12	3	-3	197	7	-6	K,L=		8,	5	K,L=		9,	1	0	410	9	-16
0	789	16	7	0	154	8	-15	1	326	7	0	1	522	11	-2	K,L=		10,	-3
K,L=		7,	0	K,L=		8,	-7	4	256	7	14	4	260	7	5	-8	380	8	-1
1	476	10	1	-8	270	7	-9	7	271	7	6	7	315	7	17	-5	507	11	-2
4	432	9	0	-5	226	7	2	10	185	7	2	10	194	7	4	-2	448	9	-8
7	446	9	8	-2	269	7	-11	K,L=		8,	6	K,L=		9,	2	K,L=		10,	-2
10	270	7	11	K,L=		8,	-6	2	301	7	11	2	391	8	5	-10	371	8	-15
13	140	8	-3	-7	262	7	-2	5	263	7	14	5	314	7	10	-7	532	11	4
K,L=		7,	1	-4	346	8	-1	8	176	7	-1	8	272	7	8	-4	559	11	-1
2	454	9	1	-1	312	7	-9	K,L=		8,	7	11	169	7	0	-1	320	7	-6
5	508	11	12	K,L=		8,	-5	0	285	8	15	K,L=		9,	3	K,L=		10,	-1
8	295	7	12	-6	300	7	1	3	243	7	7	0	363	8	21	-9	494	10	-17
11	192	7	4	-3	409	9	-14	6	159	7	-4	3	344	8	0	-6	614	13	0
14	184	7	7	0	241	7	-7	K,L=		8,	8	6	325	7	19	-3	263	7	-3
K,L=		7,	2	K,L=		8,	-4	1	190	7	2	9	218	7	3	0	580	12	-4
0	484	10	13	-8	505	11	-19	4	169	7	7	K,L=		9,	4	K,L=		10,	0
3	569	12	17	-5	372	8	-5	K,L=		9,	-8	1	309	7	0	1	619	13	15
6	275	7	11	-2	382	8	-11	-8	180	7	-15	4	330	8	5	4	298	7	11
9	265	7	15	K,L=		8,	-3	-5	152	8	-1	7	188	7	5	7	242	7	11
12	200	7	1	-7	611	12	-20	-2	198	7	-17	10	191	7	2	10	245	7	7
K,L=		7,	3	-4	339	8	-11	K,L=		9,	-7	K,L=		9,	5	K,L=		10,	1
1	630	13	-2	-1	402	9	-25	-7	254	7	-16	2	295	7	6	2	293	7	8
4	410	9	10	K,L=		8,	-2	-4	219	7	-6	5	274	7	16	5	325	7	10
7	204	7	3	-6	422	9	-17	-1	240	7	-12	8	132	8	-4	8	242	7	11
10	308	7	16	-3	394	8	-3	K,L=		9,	-6	K,L=		9,	6	11	208	6	8
13	157	7	-1	0	540	11	-34	-9	286	8	7	0	309	8	21	K,L=		10,	2
K,L=		7,	4	K,L=		8,	-1	-6	278	7	4	3	231	7	6	0	390	8	-2
2	367	8	0	-8	315	7	-23	-3	282	7	-4	6	180	7	-1	3	224	7	2
5	289	7	2	-5	555	11	14	0	264	7	-5	K,L=		9,	7	6	377	8	19
8	275	7	13	-2	515	11	13	K,L=		9,	-5	1	186	7	7	9	168	7	2
11	240	7	8	K,L=		8,	0	-8	294	7	-9	4	198	7	5	K,L=		10,	3
K,L=		7,	5	2	435	9	-4	-5	319	7	0	K,L=		9,	8	1	281	7	2
0	304	7	7	5	386	8	7	-2	301	7	-12	2	147	8	5	4	355	8	12
3	242	7	8	8	301	7	12	K,L=		9,	-4	K,L=		10,	-8	7	236	7	3
6	341	8	14	11	211	7	11	-7	320	7	-15	-10	107	10	-13	10	128	8	-2
9	206	7	7	K,L=		8,	1	-4	473	10	-2	-7	163	8	-8	K,L=		10,	4
K,L=		7,	6	0	384	8	-17	-1	328	7	-5	-4	184	7	-13	2	323	7	10
1	272	7	13	3	457	10	3	K,L=		9,	-3	-1	142	8	-15	5	283	7	13
4	277	7	9	6	374	8	10	-9	374	8	13	K,L=		10,	-7	8	134	8	3
7	271	7	14	9	214	7	7	-6	324	7	-5	-9	170	7	-9	K,L=		10,	5
10	109	10	-5	12	195	7	6	-3	548	11	-15	-6	213	7	-5	0	352	8	7
K,L=		7,	7	K,L=		8,	2	0	338	8	-11	-3	224	7	-15	3	243	7	14
2	286	7	8	1	415	9	18	K,L=		9,	-2	0	136	9	-3	6	152	7	4
5	220	7	9	4	414	9	3	-8	390	8	8	K,L=		10,	-6	K,L=		10,	6
8	145	8	4	7	244	7	15	-5	478	10	-4	-8	277	7	-7	1	240	7	5
K,L=		7,	8	10	226	7	1	-2	403	9	8	-5	239	7	2	4	137	8	3

STRUCTURE FACTORS CONTINUED FOR
TH(N(SI(CH3)3)2)3+BH4-

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
7	158	7	-4	4	318	7	19	K,L=	12,	-1		0	231	7	-8	-6	250	7	-5
K,L=	10,	7		7	264	7	8	-10	304	7	-3	K,L=	13,	-3		-3	213	7	-9
2	165	7	4	10	130	8	2	-7	494	10	-3	-11	335	8	-16	0	114	10	-2
K,L=	10,	8		K,L=	11,	3		-4	317	7	0	-8	285	7	-11	K,L=	14,	-4	
0	93	12	0	2	341	8	3	-1	422	9	-18	-5	245	7	-8	-14	180	7	-13
K,L=	11,	-8		5	283	7	8	K,L=	12,	0		-2	278	7	-11	-11	270	7	-11
-9	130	8	-12	8	155	7	1	0	389	9	5	K,L=	13,	-2		-8	335	8	-7
-6	109	10	-9	K,L=	11,	4		3	315	7	4	-13	364	8	-11	-5	219	7	-2
-3	184	7	-22	0	362	8	6	6	255	7	14	-10	240	7	-6	-2	200	7	-5
0	100	11	-11	3	316	7	12	9	193	7	-1	-7	240	7	-3	K,L=	14,	-3	
K,L=	11,	-7		6	142	8	-3	K,L=	12,	1		-4	379	8	-4	-13	283	7	-10
-11	112	10	-7	K,L=	11,	5		1	310	7	-1	-1	250	7	-3	-10	341	8	-7
-8	214	7	-14	1	286	7	7	4	306	7	11	K,L=	13,	-1		-7	212	7	-9
-5	179	7	-13	4	185	7	10	7	187	7	9	-12	314	7	-11	-4	278	7	-16
-2	176	7	-5	7	120	9	0	K,L=	12,	2		-9	219	7	-6	-1	255	7	-8
K,L=	11,	-6		K,L=	11,	6		2	281	7	7	-6	353	8	5	K,L=	14,	-2	
-10	210	7	-12	2	192	7	6	5	284	7	7	-3	396	9	-3	-12	277	7	-8
-7	265	7	-19	5	134	8	4	8	134	8	-1	0	154	8	-7	-9	282	7	-6
-4	178	7	-12	K,L=	11,	7		K,L=	12,	3		K,L=	13,	0		-6	168	7	-7
-1	215	7	1	0	123	9	3	0	352	8	7	1	226	7	4	-3	388	8	-5
K,L=	11,	-5		3	159	7	-2	3	273	7	15	4	332	8	11	0	208	7	-10
-9	286	7	-6	K,L=	12,	-8		6	219	7	0	7	170	7	8	K,L=	14,	-1	
-6	261	7	-9	-8	149	8	-14	K,L=	12,	4		K,L=	13,	1		-14	316	8	-1
-3	282	7	-11	-5	139	8	-18	1	282	7	6	2	292	7	9	-11	231	7	-1
0	297	8	-5	K,L=	12,	-7		4	207	7	2	5	278	7	14	-8	316	7	-5
K,L=	11,	-4		-10	150	8	-11	7	162	7	2	8	115	9	-1	-5	353	8	6
-11	400	9	-15	-7	206	7	-10	K,L=	12,	5		K,L=	13,	2		-2	271	7	-4
-8	218	7	-7	-4	200	7	-13	2	203	7	7	0	399	9	12	K,L=	14,	0	
-5	376	8	-4	-1	124	9	-15	5	185	7	4	3	213	7	11	2	292	7	7
-2	358	8	-18	K,L=	12,	-6		K,L=	12,	6		6	217	7	7	5	219	7	7
K,L=	11,	-3		-12	205	7	-12	0	219	7	4	K,L=	13,	3		K,L=	14,	1	
-10	309	7	-13	-9	210	7	-12	3	158	7	8	1	330	7	14	0	330	8	16
-7	355	8	-9	-6	215	7	-7	K,L=	12,	7		4	172	7	-3	3	264	7	15
-4	536	11	-3	-3	241	7	-9	1	188	7	5	7	192	7	1	6	145	8	0
-1	333	8	-12	0	160	8	-16	K,L=	13,	-7		K,L=	13,	4		K,L=	14,	2	
K,L=	11,	-2		K,L=	12,	-5		-12	161	7	-18	2	212	7	8	1	311	7	14
-9	370	8	-10	-11	280	7	-13	-9	201	7	-11	5	208	7	2	4	193	7	11
-6	589	12	4	-8	245	7	-8	-6	149	8	-9	K,L=	13,	5		K,L=	14,	3	
-3	411	9	-3	-5	223	7	-5	-3	211	7	-12	0	221	7	0	2	189	7	8
0	288	7	-2	-2	276	7	-11	0	143	8	-24	3	198	7	8	5	208	6	5
K,L=	11,	-1		K,L=	12,	-4		K,L=	13,	-6		K,L=	13,	6		K,L=	14,	4	
-11	501	11	-14	-10	315	7	-12	-11	171	7	-8	1	242	7	9	0	207	7	7
-8	468	10	-9	-7	297	7	-16	-8	244	7	-8	K,L=	14,	-7		3	196	7	8
-5	530	11	-3	-4	294	7	-6	-5	216	7	-7	-11	150	8	-19	K,L=	14,	5	
-2	385	8	0	-1	302	7	-19	-2	213	7	-14	-8	146	8	-19	1	204	7	14
K,L=	11,	0		K,L=	12,	-3		K,L=	13,	-5		-5	179	7	-7	K,L=	15,	-7	
2	288	7	2	-12	345	8	-12	-13	224	7	-17	-2	168	7	-18	-7	116	9	-17
5	350	8	13	-9	308	7	-11	-10	195	7	-5	K,L=	14,	-6		K,L=	15,	-6	
8	173	7	1	-6	362	8	-13	-7	315	7	-9	-13	223	7	-17	-12	128	8	-12
K,L=	11,	1		-3	375	8	-13	-4	235	7	-3	-10	139	8	-4	-9	169	7	-13
0	518	11	7	0	269	7	-3	-1	200	7	-8	-7	227	7	-6	-6	176	7	-4
3	205	7	11	K,L=	12,	-2		K,L=	13,	-4		-4	243	7	-8	-3	187	7	-13
6	339	8	10	-11	349	8	-11	-12	266	7	-12	-1	122	9	-18	K,L=	15,	-5	
9	174	7	4	-8	364	8	-8	-9	292	7	-8	K,L=	14,	-5		-14	196	7	-4
K,L=	11,	2		-5	397	9	0	-6	296	7	-10	-12	178	7	-7	-11	152	7	0
1	345	8	1	-2	399	9	-13	-3	226	7	-12	-9	233	7	-5	-8	253	7	-15

STRUCTURE FACTORS CONTINUED FOR
TH(N(SI(CH3)3)2)3+BH4-

H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL	H	FOB	SG	DEL
-5	184	7	-7	-12	202	7	-11	-10	207	7	-12	0	183	7	5				
-2	164	7	-10	-9	190	7	-11	-7	292	7	-10	K,L=	18,	1					
K,L=	15,	-4		-6	242	7	-10	-4	186	7	-7	1	129	8	1				
-13	185	7	-9	-3	206	7	-12	-1	191	7	-12	K,L=	19,	-4					
-10	265	7	-3	0	189	8	-13	K,L=	17,	-2		-12	131	8	-17				
-7	262	7	-5	K,L=	16,	-3		-15	149	8	-11	-9	173	7	-17				
-4	204	7	-6	-14	174	7	-9	-12	253	7	-17	-6	110	10	-18				
-1	202	7	-9	-11	276	7	-7	-9	251	7	-8	K,L=	19,	-3					
K,L=	15,	-3		-8	252	7	1	-6	284	7	-1	-14	176	7	-17				
-15	218	7	-6	-5	293	7	-10	-3	173	7	-5	-11	136	8	-9				
-12	255	7	-5	-2	213	7	-13	0	229	7	-8	-8	184	7	-17				
-9	305	7	0	K,L=	16,	-2		K,L=	17,	-1		-5	116	9	-11				
-6	264	7	-5	-16	215	7	-8	-17	140	8	-11	K,L=	19,	-2					
-3	238	7	-15	-13	190	7	-1	-14	227	7	-3	-16	137	8	-16				
0	264	7	-16	-10	352	8	-5	-11	333	8	-13	-13	181	7	-14				
K,L=	15,	-2		-7	266	7	-3	-8	211	7	-5	-10	156	8	-9				
-14	280	7	-5	-4	272	7	0	-5	269	7	-5	-7	174	7	-15				
-11	326	7	-3	-1	234	7	-8	-2	240	7	-8	-4	134	8	-12				
-8	205	7	-1	K,L=	16,	-1		K,L=	17,	0		K,L=	19,	-1					
-5	336	8	-3	-15	242	7	-6	2	151	8	4	-18	111	10	-13				
-2	237	7	0	-12	298	7	-5	K,L=	17,	1		-15	173	7	-9				
K,L=	15,	-1		-9	291	7	2	0	147	8	3	-12	177	7	-14				
-13	282	7	-3	-6	306	7	-2	K,L=	17,	2		-9	173	7	-13				
-10	318	7	-3	-3	271	7	-8	1	165	7	5	-6	177	7	-13				
-7	262	7	-2	0	284	7	-3	K,L=	17,	4		-3	146	8	-13				
-4	380	8	4	K,L=	16,	0		0	171	7	3	K,L=	20,	-3					
-1	184	7	1	1	252	7	13	K,L=	18,	-5		-13	166	8	-21				
K,L=	15,	0		4	154	7	1	-11	121	9	-18	-10	128	9	-14				
0	245	7	13	K,L=	16,	1		-8	154	8	-14	-7	128	9	-16				
3	229	7	9	2	183	7	7	-5	132	8	-14	K,L=	20,	-2					
K,L=	15,	1		K,L=	16,	2		K,L=	18,	-4		-15	157	8	-18				
1	249	7	10	0	216	7	8	-13	182	7	-22	-12	135	8	-12				
4	202	7	9	3	157	7	-1	-10	106	10	-14	-9	141	8	-15				
K,L=	15,	2		K,L=	16,	3		-7	217	7	-11	-6	155	7	-8				
2	173	7	5	1	197	7	6	-4	155	7	-17	K,L=	20,	-1					
5	177	7	3	K,L=	16,	5		K,L=	18,	-3		-14	122	9	-16				
K,L=	15,	3		0	127	9	1	-15	146	8	-11	-11	158	8	-15				
0	243	7	13	K,L=	17,	-6		-12	180	7	-18	-8	174	7	-11				
3	151	7	6	-10	156	7	-16	-9	193	7	-12	-5	155	8	-11				
K,L=	15,	4		-7	110	10	-20	-6	200	7	-16	K,L=	21,	-2					
1	191	7	10	K,L=	17,	-5		-3	142	8	-14	-11	118	9	-13				
K,L=	15,	5		-15	129	9	-14	K,L=	18,	-2		K,L=	21,	-1					
2	153	7	3	-12	174	7	-16	-17	161	7	-13	-13	103	10	-14				
K,L=	16,	-6		-9	136	8	-13	-14	143	8	-10	-10	175	7	-12				
-11	133	8	-7	-6	136	8	-8	-11	245	7	-4	-7	176	7	-12				
-8	159	7	-18	-3	196	7	-14	-8	219	7	-13								
-5	136	8	-9	K,L=	17,	-4		-5	155	8	-8								
K,L=	16,	-5		-17	148	8	-19	-2	191	7	-12								
-16	120	9	-19	-14	184	7	-18	K,L=	18,	-1									
-13	167	7	-11	-11	151	8	-13	-16	162	7	-12								
-10	167	7	-11	-8	202	7	-17	-13	240	7	-5								
-7	182	7	-12	-5	204	7	-13	-10	253	7	-6								
-4	187	7	-7	-2	195	7	-15	-7	175	7	-13								
-1	148	8	-10	K,L=	17,	-3		-4	184	7	-11								
K,L=	16,	-4		-16	187	7	-13	-1	213	7	-10								
-15	184	7	-8	-13	157	7	-19	K,L=	18,	0									

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