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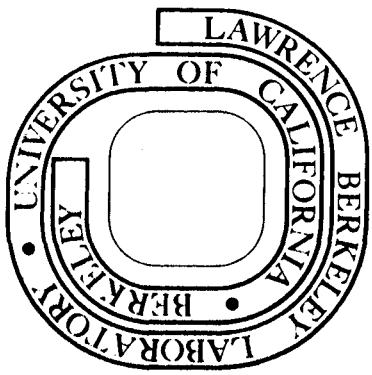

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The Crystal and Molecular Structure of Ferricenium Tetrachlorobismuthate

By N. J. Mammano[1], Allan Zalkin[2], A. Landers and A. L. Rheingold

ABSTRACT

Ferricenium tetrachlorobismuthate, $(C_5H_5)_2FeBiCl_4$, crystallizes in the monoclinic space group $P2_1/c$ with a = 10.998(5)Å, b = 17.449(4)Å, c = 7.569(4)Å, β = 98.46(5)Å. There are four molecules in the unit cell. Reflection intensities were measured by the θ - 2θ scan method with a Picker FACS-1 automated diffractometer, MoKα radiation, and a graphite monochromator. For 1374 data with $F^2 > 3\sigma(F^2)$; R_1 = 0.030, and R_2 = 0.037. The Bi atom is coordinated by 6 chloride ions in an irregular octahedral array; two pairs of Cl^- ions form halogen bridges with neighboring Bi ions resulting in an infinite chain of edge sharing octahedra. There are 6 independent Bi-Cl bond distances: 2.50(1)Å and 2.52(1)Å, to non-bridging chlorines, and 2.70(1)Å, 2.75(1)Å, 2.95(1)Å and 3.10(1)Å to bridging chlorines. The bridging Cl-Bi-Cl bond angles are 80.3° and 83.9°; the ten non-bridging Cl-Bi-Cl bond angles range from 85.9° to 99.3°. The axial Cl-Bi-Cl bond angles are 166.0°, 174.5°, and 175.9°.

The ferricenium cations stack between the polymer chains with cyclopentadiene rings in the eclipsed conformation, unlike the pure ferrocene molecule which shows staggered rings. The average C-C distance in the rings is 1.40(2)Å, the distance between ring centers is 3.40(2)Å and the Fe-ring center distance is 1.70(2)Å.

Introduction

The crystal structure of ferricenium tetrachlorobismuthate, $(C_5H_5)_2FeBiCl_4$, has been determined as part of an investigation of compounds formed between GpV-halides and ferrocene. In addition to the possibility of uncovering a novel derivative of ferrocene, studies of GpV-halide compounds have revealed interesting structural effects, such as halogen bridging[3] and infinite chain structures.[4,5] The distance from the Fe atom to the center of the cyclopentadiene ring is also of some interest, particularly in a non-substituted ferricenium compound where steric influences would be less significant.

Diffraction Data

The cell dimensions and data collection details are given in Table I.

The material was isolated as black crystals by reaction of a 1:1 molar ratio of ferrocene and $BiCl_3$ in acetone. A single crystal was mounted along its needle (c) axis. Weissenberg and precession data revealed systematic extinctions for 0k0 ($k = 2n+1$) and h0ℓ ($\ell = 2n+1$), characteristic of space group $P2_1/c$. The same crystal was placed on a Picker FACS-1 four circle diffractometer; a scintillation counter was used to measure the scanned intensities. Unit cell dimensions were refined by a least-squares program from the diffractometer setting angles of 12 reflections measured manually. A set of three standard reflections ($00\bar{4}$, 600, 800) was checked after every 200th scan in

order to test for instrumental stability and crystal decay; no systematic variation in the intensities was observed.

Standard deviations were assigned to each reflection on the basis of counting statistics where $\sigma(I) = (C + \sigma^2(B))^{1/2}$. The standard deviation of the background count, $\sigma(B)$, was determined as the maximum value of the quantities $\sigma(B) = (t_c/2t_b)(B_1+B_2)^{1/2}$ or $\sigma(B) = (t_c/2t_b)|B_1-B_2|$, where t_c and t_b are the scan counting time and background counting time, respectively, and C is the number of counts recorded during the scan. The weighting parameters, w, used in the least-squares refinement were calculated as $w = 1/\sigma^2$. A "p" factor, of 0.06 was applied to the weighting factors in order to account for instrumental inaccuracies by the equation $\sigma = (\sigma^2(F^2) + pF_o^2)^{1/2}$. A full set of 377t data was averaged to 1893 unique reflections. Lorentz and polarization corrections were made. An absorption correction[6] was applied to the data by assigning 6 faces to the crystal and measuring its dimensions. Azimuthal scans of integrated intensities were performed for five different reflections, and the dimensions of the crystal were adjusted to fit these scans.

Atomic scattering factors for Bi^o, Fe^o, Cl^-, C, and H were used[7] with all appropriately corrected for anomalous dispersion.[8]

Structure Determination

A model was provided by a three dimensional Patterson synthesis which revealed the Bi-Bi, Bi-Fe, and Bi-Cl vectors, from which initial heavy atom coordinates (Bi, Fe, Cl) could be deduced. The carbon atoms

were located by a subsequent difference Fourier. Hydrogen atom coordinates were calculated by assuming them to lie in the plane of the cyclopentadiene rings each at a distance of 0.95Å from the appropriate carbon atom. The coordinates for the Bi, Fe, Cl and C atoms, including anisotropic thermal parameters, were refined by a full matrix least-squares procedure using the 1374 data for which $F^2 > 3\sigma(F^2)$. The calculated hydrogen positions, including assigned isotropic thermal parameters of 8.0Å^2, were not refined but included as fixed parameters in the least-squares minimization. The final R_1 value ($R_1 = \Sigma||Fo|-|Fc||/\Sigma|Fo|$) was 0.03 and the final R_2 ($R_2 = (\Sigma w(|Fo|-|Fc|)^2/\Sigma w|Fo|^2)^{1/2}$ was 0.037. The goodness of fit $\Sigma w(|Fo|-|Fc|)^2/(m-s)$ was 0.96, where m and s are the number of data and number of parameters, respectively. No extinction was indicated by the data and none was applied.

Final positional and thermal parameters are given in Tables II and III, and distances and angles are listed in Tables IV and V.

Discussion

A portion of the crystal structure is shown in Fig. 1; Fig. 2 gives the molecular structure of the ferricenium cation. The view in Fig. 1 (Insert Fig. 1) is a perspective of the bc plane down the a axis. The Bi atoms are surrounded by 6 Cl^- ions in an irregular octahedron; adjacent Bi atoms are connected by halogen bridges resulting in an infinite chain of edge sharing octahedra extending along the c axis. There are six separate Bi-Cl bond distances: four "long" bonds to the bridging chlorines,

Cl(1), Cl(2), Cl(1'), and Cl(2') of 2.75(1)Å, 2.70(1)Å, 2.95(1)Å and 3.10(1)Å, and two "short" bonds to the non-bridging chlorines Cl(3) and Cl(4), of 2.52(1)Å and 2.50(1)Å. The Cl-Bi-Cl bond angles between bridging chlorines, Cl(1)-Bi-Cl(2'), and Cl(2)-Bi-Cl(1') are 80.3(1)° and 83.9(1)°, respectively; the remaining ten interior angles range from 85.9(1)° to 99.3(1)°, resulting in a considerably distorted octahedron.

The "short" non-bridging Bi-Cl bond distances observed in the present instance, 2.50(1)Å and 2.52(1)Å are in good agreement with the "single bond" value observed in an electron diffraction study[9] of $BiCl_3(g)$ which gave Bi-Cl = 2.48 ± 0.02Å. However, the identification of the electron diffraction value as a single bond should be viewed with some reservation in view of a Raman spectral study[10] of $BiCl_3(g)$ which revealed modes that were interpreted as being due to chlorine bridging, suggesting that the material is not monomeric. In solid $BiCl_3$, the identification of a single bond distance is even more ambiguous because the structure has been described[11] as a right trigonal prism with the Bi atom having a total of 8 chloride neighbors, three close at 2.47(1)Å, 2.51(1)Å and 2.52(1)Å and five considerably more distant with values ranging from 3.22(1)Å to 3.45(1)Å. It is clear that the strong tendency to Cl bridging in Bi-Cl compounds precludes the designation of any specific value as a single bond distance. However, the good agreement among the electron diffraction value (2.48Å), the three short values in solid $BiCl_3$ (2.47Å, 2.51Å, 2.52Å) and the short values for non-bridging chlorines measured in the present case (2.50Å, 2.52Å)

suggests that a range of values for a reasonable "single" Bi-Cl bond would be 2.47Å to 2.52Å.

The dihedral angle, α, between planes containing carbon atoms C(1), C(5), C(6) and C(1), C(5), C(10), respectively (Fig. 2) was (Insert Fig. 2) calculated in order to determine the extent to which the cyclopentadiene rings are staggered. The value determined $\alpha \sim 1°$, indicates that the rings are essentially completely eclipsed, unlike pure ferrocene, in which the rings are in a staggered relationship.[12]

The specific mode of octahedral edge sharing observed in this study has been seen in three other GpV-halogen compounds, 2-picolinium tetrabromobismuthate (A),[4] 2-picolinium tetraiodobismuthate (B),[4] and pyridinium tetrachloroantimonate (C).[5] In each of the cases A, B and C, as well as in the present study, the GpV-halogen anion MX_4^-, forms an infinite chain of octahedra through pairs of bridging halogen atoms, with the organic cations, picolinium, pyridinium, or ferricenium packing into the spaces between the chains. In A, B and C, the heterocyclic ring cations stack in channels in the structure, essentially parallel to each other. The dihedral angle between planes formed by the rings is ~12° in A and B, and ~1° in C. The ring-to-ring distance for the parallel pyridinium molecules in C is 3.49Å, while C-C distances for the slightly inclined picolinium rings in A and B are "3.3Å or greater." Non-parallel stacking of molecules in A and B may be due to steric constraints of the methyl group on the picolinium ion. In the present structure, the cyclopentadiene rings of the ferricenium cation are parallel to within ~2°, and the distance between the centers of the

rings is 3.40(2)Å. However, adjacent ferricenium molecules are not parallel (Fig. 1) so that the parallel configuration of the rings occurs pairwise, intramolecularly, rather than in an infinite stack through the crystal as in A, B and C. Nevertheless, the similarity among the structures A, B and C and the present case is evident; even though the picoline and pyridine are discrete single ring compounds, they behave very similarly to the sandwich compound ferrocene from the point of view of crystalline packing. This suggests that the pronounced tendency for halogen bridging in GpV-halogen compounds can manifest itself in infinite anion chains of type $(MX_4)_n^{-n}$ in certain instances, specifically in the presence of planar, ionizable ring compounds such as the single ring heterocyclics, pyridine and picoline, and the double ring sandwich compound ferrocene.

The distance from the Fe atom to the center of the cyclopentadiene ring which we have measured in ferricenium tetrachlorobismuthate (1.70Å) is in very good agreement with value reported for ferricenium picrate,[13] ferricenium triiodide,[14] and 1,1 dimethyl ferricenium triiodide.[15] In the picrate and unsubstituted ferricenium triiodide, the structures were disordered so no detailed conclusions could be drawn, although Fe-ring center distances of 1.68Å and 1.65Å were reported, respectively. In the methyl substituted ferricinium triiodide, the rings were inclined by 6.6°, and the relevant distances to each ring were 1.69Å and 1.70Å. The Fe-ring center distance in pure ferrocene[12] is 1.66Å, which is not significantly different from the values cited above.

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Supplementary Material Available: Table of observed structure factors (8 pages). Ordering information is given on any current masthead page.

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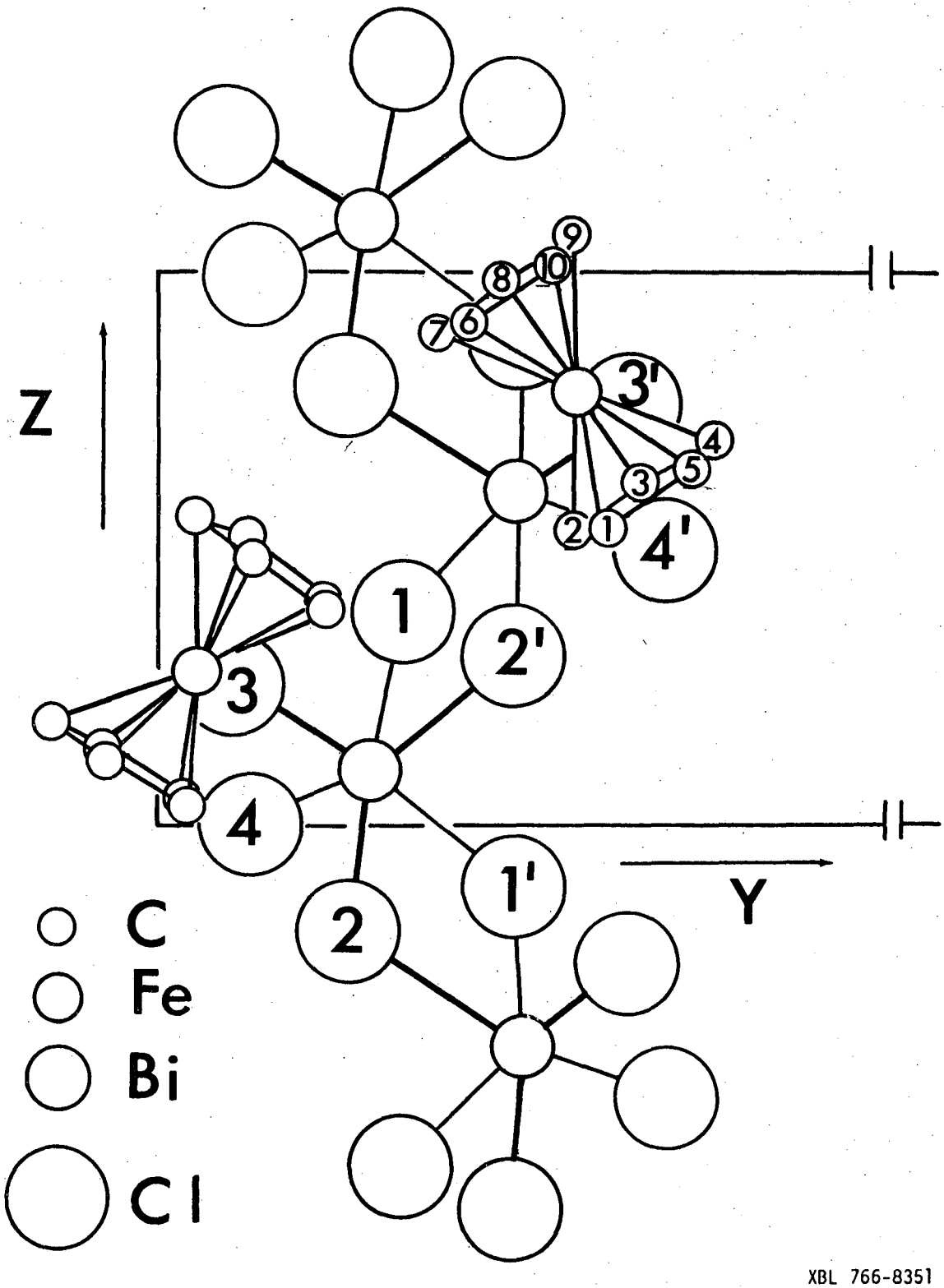
FIGURES

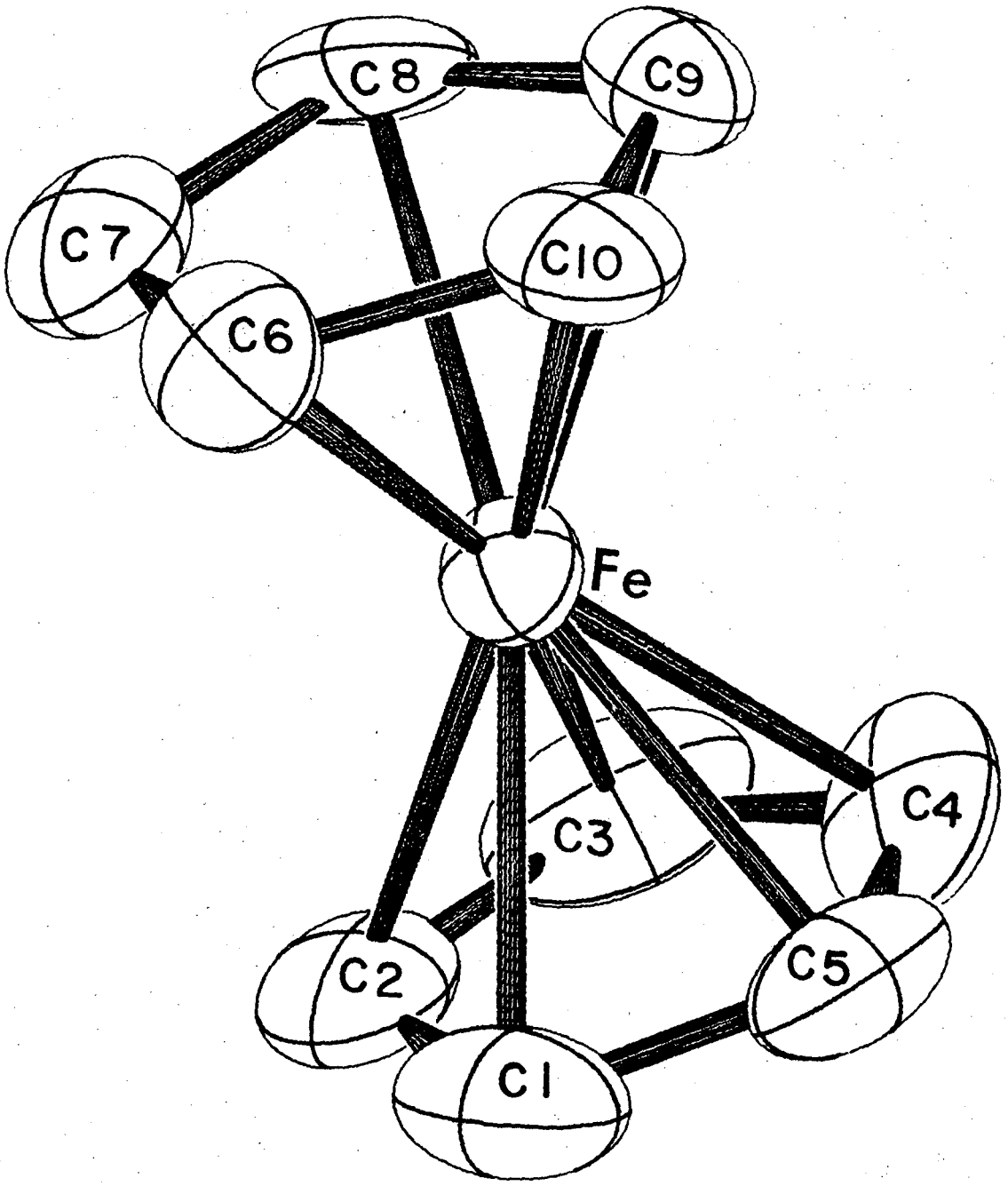
Fig. 1. Schematic projection of the structure on (100). Primed numerals as superscripts refer to equivalent positions x,1/2-y,1/2+z, relative to the reference atom at x,y,z.

Fig. 2. Ortep diagram of the ferricenium cation.



XBL 766-8351

Fig. 1



XBL 766-8352

Fig. 2

Table I. Summary of Crystal Data and Intensity Collection

Compound	$(C_5H_5)_2FeBiCl_4$
Formula Weight	536.8296
a	10.998(5)Å
b	17.449(7)Å
c	7.569(4)Å
β	98.46(5)°
V	1436.7Å^3
Z	4
Density (calc)	2.482 g/cc
Density (obs)	2.59 g/cc
Space Group	C_{2h}^5 - $P2_1/c$
Crystal Shape and Size	Irregular needle with faces 210, $2\bar{1}0$, 010, $0\bar{1}0$, 001, $21\bar{1}$. Dimension ~.15 x ~.08 x ~.06 mm.
Crystal Volume	8.47×10^{-4} mm^3
Temperature	22° - 23° C
Radiation	MoKα (λ = 0.70926Å) graphite monochromatized
Absorption Correction	1.98 to 2.85; average = 2.32
μ	134 cm^{-1}
Receiving Aperture	6 mm x 6 mm, 22 cm from Crystal
Data Collection Method	θ - 2θ scan (2°/min along 2θ)
Scan Range	1.8°
Background Counts	10 sec, offset from scan limits by 1°
2θ Limits	3.0 - 45.0°

Table II. Positional Parameters

Atom	x	y	z
Bi	.26127(4)	.18989(2)	.15136(6)
Fe	.7690(1)	.40136(9)	.9521(2)
Cl(1)	.1092(3)	.2046(2)	.4070(4)
Cl(2)	.4019(3)	.1840(2)	-.1125(4)
Cl(3)	.3942(3)	.0922(2)	.3342(5)
Cl(4)	.1171(3)	.0869(2)	.0215(5)
C(1)	.825(1)	.4032(7)	.703(2)
C(2)	.698(1)	.4189(8)	.686(1)
C(3)	.684(1)	.4858(8)	.785(2)
C(4)	.798(1)	.5132(7)	.860(2)
C(5)	.886(1)	.4618(8)	.809(2)
C(6)	.811(2)	.2951(8)	.064(2)
C(7)	.686(2)	.309(1)	.053(2)
C(8)	.670(1)	.374(1)	.156(2)
C(9)	.791(2)	.3976(9)	.231(2)
C(10)	.873(1)	.349(1)	.168(2)
H(1)	.8627	.3602	.6514
H(2)	.6335	.3887	.6197
H(3)	.605	.509	.7997
H(4)	.8152	.5589	.9335
H(5)	.9738	.4661	.8401
H(6)	.8481	.2539	.0052
H(7)	.621	.2785	-.0135
H(8)	.5924	.398	.1723
H(9)	.8132	.4410	.3109
H(10)	.9621	.3513	.1939

Table III. Thermal Parameters[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Bi	2.40(2)	2.41(2)	2.48(2)	.04(2)	.60(1)	.05(2)
Fe	2.87(2)	2.36(8)	2.93(7)	-.02(6)	.57(6)	.27(6)
Cl(1)	3.2(1)	4.3(2)	4.2(2)	-1.0(1)	1.6(1)	-1.2(1)
Cl(2)	3.9(1)	4.2(2)	4.2(2)	.7(1)	1.8(1)	.4(1)
Cl(3)	3.5(1)	5.2(2)	6.0(2)	.9(1)	.4(1)	2.2(2)
Cl(4)	4.6(2)	3.7(2)	4.4(2)	-1.0(1)	.9(1)	-1.0(1)
C(1)	5.2(7)	2.8(6)	3.0(6)	.4(5)	1.8(5)	-.2(5)
C(2)	5.7(8)	4.9(8)	1.3(5)	-1.1(6)	-.8(5)	-.3(5)
C(3)	4.3(7)	4.5(8)	4.6(7)	.5(6)	1.0(6)	1.4(6)
C(4)	6.0(8)	2.0(6)	5.4(7)	-.4(5)	1.8(6)	.2(5)
C(5)	4.5(7)	4.3(7)	3.2(6)	-.4(5)	1.3(5)	.6(5)
C(6)	6.9(9)	2.7(7)	7.0(9)	.9(6)	2.2(8)	1.8(6)
C(7)	5.7(9)	6.0(10)	5.5(8)	-3.6(8)	-.2(7)	2.8(8)
C(8)	5.2(8)	8.6(12)	4.1(7)	2.3(8)	2.2(6)	3.3(8)
C(9)	7.5(10)	5.4(9)	3.1(6)	-.7(7)	1.5(6)	-.5(6)
C(10)	3.9(7)	5.9(9)	4.3(7)	.3(7)	-.4(6)	2.2(7)
H(1)	8.0					
H(2)	8.0					
H(3)	8.0					
H(4)	8.0					
H(5)	8.0					
H(6)	8.0					
H(7)	8.0					
H(8)	8.0					
H(9)	8.0					
H(10)	8.0					

[a]The form of the temperature factor is exp $[-.025\ (h^2a^{*2}B_{11}+\ldots+2hka^*b^*B_{12}+\ldots)]$ or $(-B\lambda^{-2}\sin^2\theta)$.

Table IV. Interatomic Distances (Å)

Bi-Cl(1)	2.749(3)	C(1) -C(2)	1.41(2)
Bi-Cl(2)	2.702(3)	C(2) -C(3)	1.41(2)
Bi-Cl(3)	2.522(3)	C(3) -C(4)	1.39(2)
Bi-Cl(4)	2.500(3)	C(4) -C(5)	1.39(2)
Bi-Cl(1')	2.949(3)	C(5) -C(1)	1.40(2)
Bi-Cl(2')	3.101(4)	C(6) -C(7)	1.39(2)
Fe-C(1)	2.07(1)	C(7) -C(8)	1.40(2)
Fe-C(2)	2.07(1)	C(8) -C(9)	1.43(2)
Fe-C(3)	2.07(1)	C(9) -C(10)	1.38(2)
Fe-C(4)	2.11(1)	C(10)-C(6)	1.35(2)
Fe-C(5)	2.09(1)	C(1) -C(6)	3.34(2)
Fe-C(6)	2.06(1)	C(2) -C(7)	3.39(2)
Fe-C(7)	2.05(1)	C(3) -C(8)	3.44(2)
Fe-C(8)	2.07(1)	C(4) -C(9)	3.47(2)
Fe-C(9)	2.09(1)	C(5) -C(10)	3.38(2)
Fe-C(10)	2.07(1)		

Table V. Selected Angles (°)

Cl(1) -Bi-Cl(1)'	92.0(1)	C(1) -C(2) -C(3)	107(1)
Cl(1) -Bi-Cl(2)	175.9(1)	C(2) -C(3) -C(4)	110(1)
Cl(1) -Bi-Cl(2)'	80.3(1)	C(3) -C(4) -C(5)	106(1)
Cl(1) -Bi-Cl(3)	92.3(1)	C(4) -C(5) -C(1)	110(1)
Cl(1) -Bi-Cl(4)	85.9(1)	C(5) -C(1) -C(2)	107(1)
Cl(1')-Bi-Cl(2)	83.9(1)	C(6) -C(7) -C(8)	108(1)
Cl(1')-Bi-Cl(2')	96.2(1)	C(7) -C(8) -C(9)	106(1)
Cl(1')-Bi-Cl(3)	174.5(1)	C(8) -C(9) -C(10)	108(1)
Cl(1')-Bi-Cl(4)	86.2(1)	C(9) -C(10)-C(1)	119(1)
Cl(2) -Bi-Cl(2')	99.3(1)	C(10)-C(6) -C(7)	109(1)
Cl(2) -Bi-Cl(3)	91.8(1)		
Cl(2) -Bi-Cl(4)	94.6(1)		
Cl(2')-Bi-Cl(3)	87.9(1)		
Cl(2')-Bi-Cl(4)	166.0(1)		
Cl(3) -Bi-Cl(4)	90.7(1)		

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 1.0)
FERRICINIUM TETRACHLOROBISMUTHATE F(0,0,0) = 973

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	3	0	1	-7*	H,K=		0,	13	3	15	4	-2*	6	24	5	-0*
2	32	4	0	4	143	6	-8	1	27	1	-36*	4	172	8	-19	7	81	3	-2
4	184	6	7	5	126	4	-5	2	0	1	-4*	5	98	3	-12	H,K=		1,	5
6	126	4	6	6	44	2	-1	3	148	5	2	6	99	3	-3	-7	40	3	-0
8	10	1	4*	7	22	7	5*	4	33	3	3	7	10	1	4*	-6	37	4	-1
H,K=		0,	1	H,K=		0,	7	5	0	1	-1*	H,K=		1,	2	-5	79	3	-3
1	25	6	-3*	1	31	20	-12*	H,K=		0,	14	-8	66	3	10	-4	39	2	1
2	148	5	-14	2	178	5	-4	0	111	4	3	-7	81	3	6	-3	166	5	-4
3	38	2	-2	3	101	3	-1	1	46	1	-23*	-6	80	3	6	-2	49	2	-0
4	159	5	-6	4	55	2	-2	2	0	1	-10*	-5	22	3	-1	-1	74	3	1
5	10	1	9*	5	32	4	5	3	12	1	-3*	-4	137	4	-3	0	78	3	6
6	60	2	3	6	35	3	-4	4	48	3	3	-3	126	4	-4	1	294	9	3
7	59	3	6	7	58	3	2	5	89	3	-4	-2	75	3	-5	2	16	3	-0*
8	97	3	11	H,K=		0,	8	H,K=		0,	15	-1	243	8	-6	3	74	3	-2
H,K=		0,	2	0	291	9	20	1	38	20	-20*	0	23	7	0*	4	42	2	-3
0	195	7	14	1	94	6	-2	2	79	3	-2	1	225	7	-11	5	99	3	-3
1	205	7	-9	2	38	2	-2	3	54	3	-1	2	99	3	-8	6	20	6	-1*
2	14	4	1*	3	81	3	-2	4	52	3	-3	3	33	2	-2	7	65	3	0
3	86	3	-6	4	144	5	-3	H,K=		0,	16	4	119	4	-12	H,K=		1,	6
4	157	5	-10	5	12	8	10*	0	70	3	0	5	36	2	-3	-7	96	4	4
5	67	2	-1	6	83	3	1	1	13	1	-16*	6	44	3	-3	-6	60	3	2
6	53	2	0	7	27	5	-3*	2	19	1	-33*	7	50	3	-4	-5	9	1	-2*
7	71	3	1	H,K=		0,	9	3	14	1	11*	H,K=		1,	3	-4	164	5	-6
8	26	5	-1	1	80	40	-30*	4	90	3	1	-8	11	1	6*	-3	193	6	-6
H,K=		0,	3	2	115	4	2	H,K=		0,	17	-7	40	3	4	-2	71	2	-0
1	105	3	-2	3	47	2	-1	1	20	10	-9*	-6	25	5	-4*	-1	46	2	2
2	97	3	-8	4	108	4	-5	2	104	5	-4	-5	129	4	-3	0	44	2	2
3	214	9	-18	5	15	9	-4*	3	20	6	-3*	-4	69	2	-1	1	107	3	2
4	27	2	-1	6	40	4	-1	H,K=		0,	18	-3	80	3	-2	2	153	5	-2
5	9	1	-3*	7	10	1	-6*	0	104	4	-0	-2	7	1	4*	3	132	4	-5
6	13	1	6*	H,K=		0,	10	1	0	1	-14*	-1	212	7	2	4	134	7	-6
7	104	3	3	0	344	11	18	2	0	1	-19*	0	243	7	13	5	13	8	2*
H,K=		0,	4	1	65	1	-27*	H,K=		1,	0	1	309	9	-12	6	63	3	1
0	131	4	10	2	14	6	-1*	-8	113	4	9	2	81	3	-5	7	66	3	4
1	115	4	1	3	6	1	-9*	-6	52	3	4	3	26	2	0	H,K=		1,	7
2	36	2	-1	4	88	3	1	-4	18	3	-1	4	50	2	-5	-7	16	8	0*
3	20	2	2	5	64	3	0	-2	256	8	2	5	162	5	-16	-6	76	3	-2
4	30	2	-4	6	61	3	1	0	0	1	-17*	6	25	3	2	-5	35	4	-5
5	168	5	-8	H,K=		0,	11	2	130	4	3	7	31	3	-4	-4	137	4	-2
6	0	1	-10*	1	43	1	-34*	4	101	3	-7	H,K=		1,	4	-3	49	2	-2
7	7	1	-1*	2	45	3	0	6	18	6	-0*	-7	141	5	5	-2	13	4	-4*
H,K=		0,	5	3	131	4	-2	H,K=		1,	1	-6	25	4	-2	-1	107	3	6
1	147	5	1	4	69	3	-4	-8	38	3	1	-5	16	9	7*	0	303	9	18
2	82	3	-1	5	0	1	-3*	-7	17	5	10*	-4	134	4	-4	1	121	4	7
3	202	6	-8	6	33	4	0	-6	114	4	9	-3	302	9	-19	2	42	2	0
4	58	2	-3	H,K=		0,	12	-5	65	2	1	-2	17	5	2*	3	23	2	2
5	8	1	4*	0	13	9	-1*	-4	185	6	5	-1	93	3	1	4	94	3	-4
6	20	5	1*	1	128	22	-16	-3	9	1	-9*	0	20	3	3	5	90	3	-3
7	89	3	-2	2	20	4	0*	-2	95	3	0	1	163	6	-2	6	54	3	-3
H,K=		0,	6	3	54	2	1	-1	67	3	2	2	50	2	-1	7	5	1	-1*
0	67	3	4	4	36	3	-1	0	231	8	1	3	228	9	-16	H,K=		1,	8
1	172	5	10	5	80	3	-3	1	45	2	-2	4	56	3	-2	-7	16	13	9*
2	93	3	-3	6	20	5	13*	2	71	3	-4	5	10	1	4*	-6	70	3	-0

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	14	7	1*	-6	25	5	-0*	H,K=		1,	17	H,K=		2,	3	0	95	3	4
-4	100	3	-3	-5	17	1	6*	-3	12	1	8*	-8	41	3	6	1	216	7	1
-3	45	2	2	-4	73	3	1	-2	0	1	-13*	-7	124	4	4	2	115	4	-5
-2	162	5	1	-3	118	4	-0	-1	0	1	-3*	-6	26	4	2	3	15	4	-3*
-1	89	3	7	-2	8	1	-1*	0	138	5	1	-5	6	1	3*	4	80	3	-5
0	11	1	-9*	-1	142	4	4	1	19	6	8*	-4	8	1	-5*	5	145	5	-7
1	68	2	3	0	7	1	-8*	2	0	1	-15*	-3	254	10	-7	6	44	3	-3
2	132	4	0	1	132	6	-3	3	7	1	5*	-2	77	3	-1	7	29	6	6*
3	80	3	-3	2	26	3	-1	H,K=		1,	18	-1	83	3	2	H,K=		2,	7
4	125	4	-7	3	91	3	-0	-2	76	3	-0	0	27	4	0	-7	63	3	2
5	32	4	2	4	30	4	-1	-1	13	1	3*	1	120	4	-3	-6	62	3	-1
6	51	3	-2	5	19	6	0*	0	0	1	-3*	2	159	5	-10	-5	10	1	-6*
7	0	1	-3*	6	15	13	7*	1	15	1	7*	3	152	5	-12	-4	16	4	2*
H,K=		1,	9	H,K=		1,	13	2	51	5	-2	4	40	2	-3	-3	174	5	0
-7	15	9	-0*	-5	100	3	0	H,K=		2,	0	5	20	4	-1	-2	213	8	2
-6	92	3	1	-4	29	3	-2	-8	17	8	3*	6	16	6	6*	-1	52	2	2
-5	21	4	5	-3	38	3	-1	-6	101	3	4	7	63	3	-4	0	29	2	2
-4	129	4	-3	-2	57	2	3	-4	137	4	5	H,K=		2,	4	1	32	3	-0
-3	45	2	-4	-1	87	4	2	-2	96	3	3	-7	12	1	3*	2	203	6	-8
-2	86	3	1	0	4	1	-1*	0	423	13	-15	-6	15	1	-3*	3	73	3	-3
-1	33	2	2	1	144	8	-3	2	14	5	-1*	-5	183	6	1	4	45	2	-4
0	227	7	15	2	9	1	3*	4	104	3	3	-4	10	8	3*	5	25	4	-1
1	53	2	-0	3	12	1	-10*	6	120	4	2	-3	71	2	-1	6	8	1	-9*
2	67	2	-0	4	26	5	-9	H,K=		2,	1	-2	16	4	-2*	7	28	5	-2
3	9	1	-0*	5	101	3	0	-8	74	3	7	-1	45	2	-1	H,K=		2,	8
4	133	4	-3	H,K=		1,	14	-7	64	3	1	0	44	2	-0	-7	39	3	3
5	11	1	4*	-5	13	1	6*	-6	122	4	8	1	343	11	-7	-6	85	3	-2
6	97	3	3	-4	6	1	-2*	-5	28	2	4	2	83	3	-5	-5	31	2	0
H,K=		1,	10	-3	137	4	1	-4	105	3	3	3	15	3	3*	-4	123	4	-2
-6	40	3	2	-2	68	3	-2	-3	139	4	0	4	36	2	-3	-3	62	2	-0
-5	32	3	1	-1	21	4	-9*	-2	332	10	5	5	173	5	-11	-2	51	2	-1
-4	12	9	-6*	0	17	1	-9*	-1	10	1	-1*	6	14	7	1*	-1	77	3	4
-3	88	3	-3	1	33	1	-19*	0	62	3	-1	7	27	4	-3	0	190	6	11
-2	170	5	3	2	81	3	0	1	57	2	2	H,K=		2,	5	1	13	5	1*
-1	103	3	4	3	123	4	-3	2	183	7	-3	-7	104	4	1	2	76	3	-1
0	0	1	-5*	4	33	4	-5	3	103	3	-3	-6	25	3	-0	3	11	1	-6*
1	84	3	1	5	14	10	11*	4	162	5	-6	-5	0	1	-4*	4	106	3	-3
2	94	3	0	H,K=		1,	15	5	31	2	-1	-4	16	3	3*	5	13	12	3*
3	56	2	-3	-4	72	3	-3	6	54	4	-5	-3	176	8	-5	6	99	3	-6
4	61	2	2	-3	53	3	-3	7	36	3	4	-2	53	2	0	H,K=		2,	9
5	9	1	8*	-2	24	5	-8*	H,K=		2,	2	-1	123	4	5	-7	14	11	6*
6	11	1	2*	-1	58	3	2	-8	39	3	8	0	47	2	1	-6	82	3	1
H,K=		1,	11	0	102	3	3	-7	53	3	6	1	233	8	0	-5	21	6	3*
-6	49	4	1	1	85	7	-4	-6	102	3	7	2	76	2	-4	-4	73	3	-1
-5	85	3	-2	2	23	16	-14*	-5	33	2	3	3	87	3	-1	-3	25	3	-2
-4	75	3	-2	3	39	6	1	-4	117	4	2	4	40	2	1	-2	225	7	6
-3	8	1	-11*	4	50	3	-4	-3	135	4	2	5	8	1	-3*	-1	66	2	5
-2	15	12	-8*	H,K=		1,	16	-2	22	3	-2	6	17	9	-3*	0	26	2	-2
-1	110	4	5	-4	78	3	-2	-1	190	7	4	7	58	3	2	1	80	3	-1
0	73	3	4	-3	28	5	1*	0	145	4	2	H,K=		2,	6	2	124	4	1
1	98	5	-1	-2	78	3	-0	1	138	4	-6	-7	0	1	-7*	3	16	4	6*
2	63	2	-1	-1	0	1	-6*	2	119	4	-8	-6	100	3	1	4	138	4	-6
3	11	1	7*	0	0	1	-29*	3	43	2	-3	-5	110	4	-4	5	15	1	13*
4	88	3	1	1	0	1	-5*	4	90	3	-6	-4	119	6	-3	6	48	3	-2
5	127	4	-4	2	95	3	-0	5	109	4	-8	-3	28	2	-3	H,K=		2,	10
6	37	3	-5	3	0	1	-8*	6	73	3	-4	-2	38	2	-0	-6	53	3	-4
H,K=		1,	12	4	81	3	-3	7	41	3	-4	-1	60	2	3	-5	59	3	-0

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
-4	72	3	-3	1	136	4	4	3	38	4	-1	-6	40	2	1	4	106	3	-2
-3	57	3	-0	2	21	4	6*	4	109	3	4	-5	113	4	-2	5	13	10	2*
-2	15	1	2*	3	14	8	9*	5	92	3	3	-4	29	3	-0	6	53	3	4
-1	114	4	6	4	16	9	-7*	6	117	4	5	-3	172	7	-1	H,K=		3,	9
0	225	7	13	5	84	3	-1	7	10	1	-6*	-2	7	1	6*	-7	8	1	7*
1	99	3	5	H,K=		2,	15	H,K=		3,	2	-1	178	5	5	-6	78	3	-0
2	18	4	-2*	-4	33	3	4	-8	45	3	4	0	89	3	2	-5	32	3	-2
3	22	5	2*	-3	56	3	2	-7	51	4	2	1	282	9	-2	-4	108	4	-3
4	56	2	-1	-2	81	3	1	-6	104	3	7	2	33	2	2	-3	91	3	0
5	85	3	-3	-1	56	3	2	-5	49	2	2	3	40	2	-1	-2	60	2	-2
6	64	3	-2	0	41	3	1	-4	65	2	2	4	33	2	4	-1	86	3	2
H,K=		2,	11	1	78	3	0	-3	172	5	4	5	103	3	-6	0	51	2	4
-6	50	3	-2	2	98	3	0	-2	203	6	5	6	35	3	-1	1	72	2	1
-5	14	8	3*	3	22	5	-3*	-1	173	5	3	7	86	3	1	2	120	4	-5
-4	61	2	2	4	52	3	0	0	46	2	0	H,K=		3,	6	3	29	3	-2
-3	153	5	-0	H,K=		2,	16	1	117	4	0	-7	88	3	1	4	86	3	-1
-2	84	3	2	-4	85	3	-0	2	195	6	-0	-6	73	3	0	5	17	6	7*
-1	57	2	2	-3	0	1	-5*	3	90	3	-1	-5	23	3	2	6	81	4	2
0	3	1	-3*	-2	36	3	-5	4	83	3	-0	-4	91	3	2	H,K=		3,	10
1	13	8	-6*	-1	8	1	-5*	5	43	2	1	-3	131	6	-2	-6	65	3	1
2	82	3	1	0	86	3	2	6	41	3	-0	-2	106	3	5	-5	15	6	4*
3	129	4	-2	1	23	6	3*	7	42	3	-0	-1	112	4	4	-4	12	1	1*
4	48	3	-1	2	54	3	-6	H,K=		3,	3	0	74	2	3	-3	98	3	-0
5	27	6	0*	3	11	1	-7*	-8	9	1	5*	1	43	2	-1	-2	238	7	9
6	29	5	3*	H,K=		2,	17	-7	14	1	3*	2	138	4	-3	-1	54	2	3
H,K=		2,	12	-3	22	10	8*	-6	63	3	0	3	121	4	-8	0	13	5	8*
-6	22	5	5*	-2	113	4	0	-5	155	5	3	4	59	2	-3	1	18	3	0
-5	67	3	-6	-1	7	1	-8*	-4	33	2	-0	5	27	5	9	2	143	4	-1
-4	16	6	12*	0	0	1	-4*	-3	91	3	1	6	47	3	-3	3	78	3	-2
-3	97	3	-1	1	17	7	-3*	-2	42	2	-1	7	45	3	-2	4	58	3	-1
-2	27	3	2	2	95	3	-3	-1	140	4	5	H,K=		3,	7	5	39	3	-1
-1	124	4	4	H,K=		2,	18	0	220	7	4	-7	15	1	9*	6	13	1	3*
0	11	1	2*	-2	13	1	-9*	1	216	7	-2	-6	99	4	-1	H,K=		3,	11
1	156	5	7	-1	14	1	0*	2	18	4	3*	-5	68	3	-2	-6	56	3	-0
2	54	2	0	0	76	3	0	3	0	1	-8*	-4	104	3	-0	-5	102	4	-3
3	28	3	-3	1	53	3	1	4	14	5	5*	-3	15	4	-4*	-4	39	3	-2
4	30	4	-3	H,K=		3,	0	5	139	4	-4	-2	8	1	4*	-3	47	2	1
5	83	3	-2	-8	83	3	5	6	68	3	1	-1	43	2	2	-2	23	6	-2*
H,K=		2,	13	-6	125	4	5	7	29	4	-1	0	272	8	12	-1	75	3	-0
-5	0	1	-4*	-4	19	5	4*	H,K=		3,	4	1	72	2	1	0	40	2	1
-4	24	4	7	-2	450	14	-4	-7	130	4	8	2	57	2	0	1	111	4	3
-3	129	4	1	0	10	1	-1*	-6	19	7	-2*	3	26	3	-1	2	71	3	-3
-2	17	14	-4*	2	280	9	3	-5	0	1	-5*	4	38	3	-6	3	9	1	6*
-1	82	3	2	4	124	4	7	-4	58	2	-2	5	82	3	-1	4	38	3	-6
0	38	2	2	6	40	3	1	-3	169	7	-0	6	97	3	-2	5	118	4	2
1	59	2	1	H,K=		3,	1	-2	36	2	1	H,K=		3,	8	H,K=		3,	12
2	10	1	5*	-8	38	3	0	-1	143	4	4	-7	13	1	4*	-6	28	5	3
3	112	4	1	-7	25	6	5*	0	20	3	2	-6	105	4	1	-5	23	5	1*
4	69	3	-5	-6	119	4	5	1	104	3	1	-5	38	2	1	-4	9	1	-4*
5	15	10	0*	-5	74	3	1	2	14	4	1*	-4	65	3	0	-3	120	4	2
H,K=		2,	14	-4	128	4	5	3	163	5	-7	-3	61	2	0	-2	4	1	-2*
-5	98	3	-1	-3	18	2	3	4	12	8	2*	-2	224	7	7	-1	139	4	7
-4	48	3	-1	-2	92	3	1	5	32	2	7	-1	87	3	3	0	14	8	9*
-3	19	6	-4*	-1	13	1	-0*	6	25	4	4	0	42	2	0	1	91	3	2
-2	26	3	-1	0	66	2	2	7	64	3	-0	1	85	3	1	2	35	3	7
-1	33	3	-0	1	41	3	-0	H,K=		3,	5	2	164	5	-2	3	97	3	-1
0	96	3	3	2	176	5	1	-7	39	3	-2	3	23	3	1	4	21	4	14*

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	40	3	2	-2	11	8	2*	-4	7	1	2*	H,K=		4,	8	-5	90	3	-2
H,K=		3,	13	0	122	4	1	-3	55	2	1	-7	6	1	-0*	-4	18	5	13*
-5	102	4	-1	2	101	3	2	-2	33	2	0	-6	80	3	3	-3	109	4	-0
-4	22	4	1*	4	30	3	-1	-1	206	8	5	-5	6	1	2*	-2	13	1	3*
-3	52	3	0	6	105	4	5	0	7	1	2*	-4	122	4	-1	-1	106	4	4
-2	41	2	1	H,K=		4,	1	1	220	8	1	-3	27	2	2	0	30	2	4
-1	104	4	8	-7	51	3	4	2	35	2	1	-2	14	7	-2*	1	124	4	4
0	34	2	3	-6	130	4	7	3	11	9	7*	-1	19	3	3	2	14	7	2*
1	165	5	9	-5	9	1	6*	4	30	3	2	0	126	4	4	3	15	11	2*
2	19	5	-4*	-4	108	3	4	5	127	8	-9	1	31	2	2	4	0	1	-8*
3	16	6	4*	-3	102	3	2	6	19	6	4*	2	130	4	-2	5	52	3	-2
4	39	3	-3	-2	243	7	4	7	44	4	-4	3	5	1	-1*	H,K=		4,	13
5	88	3	-2	-1	14	4	4*	H,K=		4,	5	4	73	3	-0	-5	18	7	1*
H,K=		3,	14	0	64	2	-3	-7	58	3	0	5	8	1	-12*	-4	69	3	1
-5	12	1	9*	1	26	2	-1	-6	35	3	-1	6	98	11	-4	-3	80	3	0
-4	12	1	1*	2	220	7	4	-5	56	2	0	H,K=		4,	9	-2	0	1	-4*
-3	79	3	2	3	182	6	4	-4	12	8	6*	-6	105	4	-1	-1	120	4	2
-2	83	3	3	4	121	4	5	-3	72	3	1	-5	0	1	-6*	0	0	1	-5*
-1	64	3	0	5	7	1	5*	-2	74	2	0	-4	89	3	-0	1	35	4	-2
0	17	6	2*	6	67	3	3	-1	278	9	6	-3	10	1	-3*	2	26	3	2
1	45	3	-2	7	24	7	-3*	0	8	1	-3*	-2	190	6	8	3	102	3	2
2	79	3	1	H,K=		4,	2	1	124	4	1	-1	53	2	0	4	34	3	3
3	85	3	-1	-7	8	1	5*	2	25	2	-3	0	70	3	3	H,K=		4,	14
4	17	10	-10*	-6	88	3	3	3	97	3	-3	1	39	2	3	-5	92	3	-1
H,K=		3,	15	-5	113	4	4	4	7	1	-3*	2	158	5	-2	-4	53	3	1
-4	60	3	3	-4	84	3	2	5	64	3	-2	3	11	1	4*	-3	19	11	-4*
-3	52	4	-3	-3	141	4	3	6	9	1	2*	4	107	4	-3	-2	27	4	1
-2	13	1	8*	-2	27	2	0	H,K=		4,	6	5	30	3	0	-1	72	3	0
-1	53	3	-1	-1	123	4	3	-7	12	1	9*	6	51	3	-1	0	84	3	1
0	113	4	5	0	133	4	4	-6	82	3	1	H,K=		4,	10	1	98	3	4
1	71	3	3	1	115	4	-2	-5	148	5	-1	-6	40	3	-4	2	31	3	5
2	46	3	1	2	124	4	2	-4	65	2	-1	-5	81	3	2	3	6	1	2*
3	12	1	-1*	3	15	4	2*	-3	28	3	0	-4	102	7	-0	4	0	1	-11*
4	33	3	2	4	52	2	-0	-2	14	4	-2*	-3	48	2	-1	H,K=		4,	15
H,K=		3,	16	5	57	2	1	-1	95	3	1	-2	0	1	-4*	-4	19	6	-3*
-4	50	3	-3	6	101	3	4	0	110	3	3	-1	81	3	4	-3	32	4	-1
-3	38	3	2	7	52	3	2	1	119	4	4	0	129	4	5	-2	108	4	1
-2	86	3	4	H,K=		4,	3	2	93	3	-5	1	94	3	3	-1	85	3	0
-1	16	8	-6*	-7	99	3	5	3	8	1	-1*	2	59	2	-2	0	23	4	7
0	40	3	-2	-6	23	4	-4*	4	57	2	-2	3	26	3	1	1	50	3	-1
1	13	1	7*	-5	35	3	0	5	90	3	-6	4	23	4	4	2	61	3	-0
2	81	3	-2	-4	87	3	0	6	72	3	-2	5	63	3	-0	3	27	4	-2
3	22	10	-6*	-3	152	5	7	H,K=		4,	7	H,K=		4,	11	H,K=		4,	16
H,K=		3,	17	-2	182	6	6	-7	37	3	-0	-6	41	3	-2	-3	14	11	0*
-3	25	6	-1*	-1	198	6	2	-6	64	3	-5	-5	14	9	4*	-2	5	1	-10*
-2	0	1	-3*	0	20	2	-1	-5	20	4	1*	-4	29	3	-1	-1	0	1	-3*
-1	31	4	2	1	31	2	-1	-4	20	3	5	-3	109	4	3	0	88	3	0
0	110	4	-2	2	80	3	1	-3	97	3	1	-2	89	3	3	1	22	9	9*
1	29	4	-1	3	184	6	-10	-2	247	9	5	-1	55	3	1	2	73	3	1
2	27	4	-2	4	17	4	8*	-1	56	2	2	0	38	2	2	H,K=		4,	17
H,K=		3,	18	5	30	3	2	0	8	1	-1*	1	19	4	3*	-2	113	4	4
-1	0	1	-7*	6	20	7	0*	1	15	4	2*	2	87	3	1	-1	20	6	3*
0	8	1	-5*	7	67	3	4	2	147	5	-3	3	150	5	-5	0	9	1	4*
H,K=		4,	0	H,K=		4,	4	3	116	4	-5	4	41	3	-3	1	10	1	4*
-8	23	5	5*	-7	17	7	4*	4	59	2	-3	5	14	1	5*	H,K=		5,	0
-6	70	3	3	-6	48	3	1	5	10	1	0*	H,K=		4,	12	-6	91	3	-0
-4	165	5	3	-5	200	6	0	6	12	1	7*	-6	26	8	-5*	-4	50	2	2

STRUCTURE FACTORS CONTINUED FOR
FERRICINIUM TETRACHLOROBISMUTHATE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	262	8	3	-1	199	6	1	-3	15	5	2*	3	91	3	-2	1	11	6	4*
0	44	2	1	0	54	2	1	-2	154	5	2	4	28	5	-3	2	98	3	1
2	210	6	3	1	7	1	-1*	-1	37	2	1	H,K=	5,	13		3	100	3	2
4	87	3	3	2	32	2	3	0	70	2	1	-5	87	3	-5	4	111	4	3
6	13	1	8*	3	201	6	-5	1	59	2	-1	-4	8	1	3*	5	0	1	-12*
H,K=	5,	1		4	28	3	4	2	128	4	-2	-3	52	3	-1	6	33	3	7
-7	24	4	0	5	45	3	-0	3	20	4	2	-2	14	8	1*	H,K=	6,	2	
-6	82	3	-2	6	24	4	0*	4	97	3	-1	-1	97	3	5	-7	17	7	15*
-5	104	3	0	H,K=	5,	5		5	8	1	4*	0	0	1	-6*	-6	31	4	1
-4	174	5	1	-7	22	5	2*	H,K=	5,	9		1	92	3	1	-5	98	3	-0
-3	32	2	-0	-6	13	11	0*	-6	68	3	-1	2	69	3	-1	-4	136	4	-1
-2	6	1	3*	-5	112	4	-2	-5	14	13	1*	3	17	10	8*	-3	127	4	-1
-1	15	3	-4*	-4	54	2	2	-4	134	4	-4	4	41	3	5	-2	8	1	-4*
0	169	5	1	-3	127	4	-1	-3	48	2	-1	H,K=	5,	14		-1	107	3	-1
1	111	4	3	-2	36	2	2	-2	8	1	-4*	-4	21	5	10*	0	142	4	2
2	177	5	0	-1	235	7	1	-1	65	2	1	-3	58	3	-0	1	129	4	-2
3	28	3	2	0	77	3	-0	0	101	3	-1	-2	84	3	3	2	87	3	1
4	82	3	3	1	86	3	0	1	12	7	-0*	-1	87	3	-1	3	11	1	8*
5	45	3	2	2	45	2	-1	2	137	4	-5	0	13	1	-4*	4	63	3	1
6	90	3	2	3	16	5	1*	3	15	9	0*	1	13	1	8*	5	36	3	4
H,K=	5,	2		4	26	3	2	4	59	3	-4	2	42	4	-2	6	59	3	-0
-7	35	3	5	5	73	3	-4	5	14	1	1*	3	92	3	-2	H,K=	6,	3	
-6	71	3	-0	6	40	3	-2	H,K=	5,	10		H,K=	5,	15		-7	98	3	2
-5	43	3	7	H,K=	5,	6		-6	38	4	-1	-4	57	3	-2	-6	21	5	2*
-4	33	2	2	-7	73	4	-5	-5	14	11	-4*	-3	51	3	-5	-5	51	3	2
-3	84	3	1	-6	77	3	1	-4	9	1	-5*	-2	26	5	2*	-4	25	3	2
-2	157	5	2	-5	40	3	-1	-3	67	3	1	-1	67	3	4	-3	105	3	2
-1	163	5	2	-4	54	2	1	-2	135	4	1	0	94	3	3	-2	162	5	1
0	71	2	0	-3	72	3	-2	-1	70	3	1	1	32	4	3	-1	187	6	1
1	73	2	1	-2	128	4	2	0	18	4	4*	2	49	3	0	0	19	3	3
2	116	4	1	-1	168	5	4	1	25	3	-1	H,K=	5,	16		1	11	7	1*
3	108	3	1	0	60	2	-1	2	114	4	-2	-3	7	1	-2*	2	20	4	-2*
4	103	3	0	1	33	2	0	3	92	3	-2	-2	85	3	2	3	157	5	-3
5	27	3	1	2	56	2	-0	4	42	3	-2	-1	18	7	-1*	4	83	3	2
6	24	7	-0*	3	163	5	-6	5	24	7	3*	0	35	3	-0	5	38	3	3
H,K=	5,	3		4	73	3	-4	H,K=	5,	11		1	22	5	7*	6	21	5	4*
-7	10	1	10*	5	24	4	-6	-6	36	4	-1	2	54	4	-1	H,K=	6,	4	
-6	4	1	-9*	6	32	4	4	-5	128	4	-7	H,K=	5,	17		-7	0	1	-8*
-5	177	6	-1	H,K=	5,	7		-4	52	3	-3	-1	27	5	1	-6	16	7	-5*
-4	71	3	-3	-7	0	1	-9*	-3	30	3	-1	0	96	3	2	-5	143	5	2
-3	62	2	2	-6	29	4	-2	-2	24	4	-5	H,K=	6,	0		-4	14	5	3*
-2	3	1	-1*	-5	113	4	-4	-1	34	3	1	-6	50	3	2	-3	73	3	-1
-1	125	4	0	-4	119	4	-3	0	65	3	3	-4	217	7	-4	-2	35	2	2
0	145	6	1	-3	15	6	-3*	1	134	4	-0	-2	57	2	-1	-1	120	4	2
1	124	4	-1	-2	16	4	-0*	2	42	4	1	0	260	8	-5	0	27	2	-2
2	57	2	-1	-1	31	3	2	3	27	6	2*	2	68	2	0	1	130	4	2
3	12	6	4*	0	207	6	4	4	29	3	-1	4	44	3	1	2	27	3	1
4	13	8	6*	1	86	3	-0	5	65	3	-0	6	94	3	5	3	26	3	3
5	83	3	2	2	38	2	1	H,K=	5,	12		H,K=	6,	1		4	21	4	-1*
6	58	3	2	3	12	8	-7*	-5	41	3	-1	-7	58	3	1	5	92	3	3
H,K=	5,	4		4	37	2	-3	-4	8	1	-7*	-6	78	3	-1	6	13	1	3*
-7	92	3	1	5	30	3	-2	-3	88	3	-1	-5	5	1	2*	H,K=	6,	5	
-6	16	6	5*	6	90	3	-0	-2	30	3	2	-4	82	3	-0	-7	57	3	2
-5	55	2	1	H,K=	5,	8		-1	148	5	3	-3	9	1	-0*	-6	27	5	2*
-4	8	1	-1*	-6	84	3	-4	0	37	3	2	-2	66	2	0	-5	84	3	1
-3	97	3	2	-5	6	1	4*	1	55	3	-3	-1	34	3	0	-4	25	3	6
-2	14	5	-0*	-4	59	2	-1	2	12	1	7*	0	106	3	2	-3	129	4	-0

STRUCTURE FACTORS CONTINUED FOR
FERRICINIUM TETRACHLOROBISMUTHATE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	67	2	-1	1	41	2	-1	-3	44	3	0	5	83	3	4	-4	32	4	5
-1	235	7	3	2	90	3	-0	-2	93	3	-1	H,K=	7,	4		-3	0	1	-13*
0	15	6	2*	3	15	7	-3*	-1	70	3	-2	-7	116	4	2	-2	104	4	-0
1	54	2	2	4	85	3	1	0	21	6	-2*	-6	15	1	1*	-1	25	3	1
2	12	7	-3*	5	10	1	-1*	1	5	1	-17*	-5	49	2	2	0	89	3	-2
3	132	4	-3	H,K=	6,	10		2	30	4	-3	-4	39	3	-1	1	16	6	1*
4	36	3	2	-6	27	8	3*	H,K=	6,	16		-3	141	4	-1	2	78	3	2
5	74	3	-1	-5	55	3	-0	-1	8	1	6*	-2	24	4	-1	3	46	2	3
6	10	1	9*	-4	134	4	1	0	58	3	-1	-1	107	3	0	4	96	3	-0
H,K=	6,	6		-3	26	3	0	H,K=	7,	0		0	15	5	-9*	H,K=	7,	9	
-7	6	1	0*	-2	31	4	1	-6	58	3	-1	1	0	1	-8*	-5	6	1	1*
-6	36	3	2	-1	30	3	2	-4	0	1	-8*	2	0	1	-9*	-4	122	4	-0
-5	114	4	0	0	159	5	3	-2	159	5	-1	3	163	5	-3	-3	31	3	2
-4	93	3	1	1	76	3	-1	0	78	3	4	4	18	5	-3*	-2	26	4	-4
-3	55	2	-2	2	32	3	-1	2	62	3	2	5	35	3	1	-1	19	4	1*
-2	23	3	6	3	14	1	7*	4	96	3	3	H,K=	7,	5		0	167	5	1
-1	67	2	-0	4	22	5	5*	H,K=	7,	1		-6	0	1	-12*	1	12	10	6*
0	65	3	0	H,K=	6,	11		-7	0	1	-1*	-5	66	3	0	2	90	3	-1
1	106	3	-1	-5	29	4	4	-6	58	3	-2	-4	60	2	-1	3	11	1	-2*
2	84	3	-2	-4	30	7	2*	-5	63	3	1	-3	145	5	-3	4	55	3	2
3	13	7	1*	-3	57	3	1	-4	161	5	-1	-2	0	1	-4*	H,K=	7,	10	
4	64	3	3	-2	32	4	-5	-3	7	1	-2*	-1	91	3	-0	-5	28	4	-2
5	60	3	2	-1	95	3	0	-2	35	2	2	0	45	2	2	-4	14	10	2*
H,K=	6,	7		0	53	3	2	-1	7	1	2*	1	101	3	-2	-3	51	3	1
-6	52	3	-3	1	0	1	-11*	0	211	7	2	2	27	3	1	-2	99	3	-1
-5	0	1	-4*	2	29	4	-1	1	117	4	2	3	33	3	3	-1	88	3	1
-4	12	1	-0*	3	114	4	-2	2	108	4	1	4	20	6	5*	0	32	4	-2
-3	17	4	2*	4	60	3	-0	3	13	1	3*	5	62	3	-1	1	33	3	-0
-2	178	6	-0	H,K=	6,	12		4	70	3	-0	H,K=	7,	6		2	41	3	4
-1	46	3	-2	-5	77	3	-2	5	43	4	2	-6	62	3	-1	3	48	3	-7
0	17	5	-1*	-4	33	4	2	H,K=	7,	2		-5	17	6	-4*	4	56	3	-1
1	8	1	5*	-3	99	3	-0	-7	53	4	-3	-4	46	2	0	H,K=	7,	11	
2	79	3	2	-2	20	6	-1*	-6	64	3	0	-3	92	3	-2	-5	82	3	-5
3	77	3	1	-1	84	3	2	-5	46	2	1	-2	57	3	-2	-4	54	3	-4
4	101	3	-1	0	0	1	-10*	-4	32	3	-4	-1	88	3	2	-3	34	3	-0
5	7	1	2*	1	96	3	-2	-3	72	3	-0	0	69	3	-2	-2	0	1	-3*
H,K=	6,	8		2	3	1	-6*	-2	85	3	1	1	11	1	-2*	-1	26	4	1
-6	53	3	1	3	0	1	-9*	-1	141	4	0	2	52	2	-0	0	68	3	1
-5	12	1	5*	4	13	1	4*	0	78	3	1	3	116	4	-2	1	126	4	1
-4	151	5	2	H,K=	6,	13		1	50	2	0	4	84	3	1	2	39	3	-1
-3	50	2	0	-4	34	3	-7	2	57	2	0	5	24	5	-5*	3	26	4	1
-2	11	1	-3*	-3	81	3	3	3	38	2	-2	H,K=	7,	7		H,K=	7,	12	
-1	53	2	2	-2	12	1	-5*	4	100	3	2	-6	0	1	-8*	-4	18	7	-8*
0	164	5	2	-1	107	4	-1	5	55	3	2	-5	62	3	-1	-3	82	3	0
1	31	2	5	0	4	1	-6*	H,K=	7,	3		-4	149	5	-2	-2	13	12	0*
2	110	4	-0	1	14	11	-2*	-7	18	8	13*	-3	47	2	-2	-1	118	4	-1
3	23	4	-2	2	24	5	3*	-6	28	4	-3	-2	25	3	-1	0	17	6	4*
4	61	3	0	3	98	3	-1	-5	105	3	-0	-1	29	3	2	1	29	4	-2
5	6	1	-7*	H,K=	6,	14		-4	105	3	-1	0	134	4	-0	2	9	1	-2*
H,K=	6,	9		-4	64	3	0	-3	87	3	-2	1	102	3	1	3	57	3	-2
-6	81	3	0	-3	32	4	-2	-2	24	3	2	2	35	3	-3	H,K=	7,	13	
-5	39	3	-2	-2	24	6	-0*	-1	50	2	-1	3	15	1	12*	-4	0	1	-3*
-4	65	3	1	-1	50	3	-4	0	68	2	-1	4	23	5	2*	-3	65	3	-1
-3	43	2	0	0	78	3	3	1	147	5	-2	5	33	4	0	-2	8	1	-1*
-2	68	3	-1	1	67	3	-0	2	8	1	-0*	H,K=	7,	8		-1	33	3	1
-1	70	3	3	2	27	4	-2	3	26	3	0	-6	63	3	-5	0	17	6	-2*
0	99	3	0	H,K=	6,	15		4	9	1	4*	-5	10	1	8*	1	78	3	-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	37	3	4	-6	17	7	6*	H,K=		8,	9	4	29	4	-2	-5	18	7	-5*
H,K=		7,	14	-5	89	3	-2	-5	24	6	-4*	H,K=		9,	2	-4	103	3	-2
-3	62	3	-6	-4	0	1	-4*	-4	18	10	7*	-6	81	3	-1	-3	34	3	-2
-2	69	3	1	-3	112	4	-4	-3	33	3	1	-5	66	3	3	-2	38	3	3
-1	45	3	-3	-2	15	5	5*	-2	84	3	-1	-4	12	1	-0*	-1	15	12	9*
0	16	9	2*	-1	13	6	1*	-1	38	3	3	-3	89	3	-1	0	88	3	-0
1	3	1	-10*	0	26	3	2	0	80	3	-3	-2	94	3	-1	1	53	3	0
H,K=		7,	15	1	180	6	-0	1	26	7	3*	-1	102	3	-1	2	61	3	2
-1	42	4	2	2	49	2	1	2	50	3	4	0	62	3	-2	3	22	4	9*
0	56	3	-1	3	41	3	1	3	14	1	8*	1	16	9	3*	H,K=		9,	8
H,K=		8,	0	4	15	8	-5*	H,K=		8,	10	2	62	3	2	-4	4	1	-0*
-6	25	5	-2*	H,K=		8,	5	-4	90	3	-2	3	32	3	-1	-3	40	3	2
-4	147	5	-0	-6	23	6	0*	-3	51	3	-2	4	55	3	4	-2	120	4	-3
-2	32	2	-0	-5	55	3	-2	-2	27	4	1	H,K=		9,	3	-1	30	3	-2
0	188	6	-0	-4	0	1	-2*	-1	25	5	-3*	-6	8	1	5*	0	70	3	-2
2	38	3	-1	-3	143	5	-4	0	101	3	1	-5	67	4	1	1	18	6	7*
4	30	4	2	-2	43	2	1	1	61	3	-1	-4	63	3	0	2	58	3	1
H,K=		8,	1	-1	108	4	-1	2	17	11	-5*	-3	99	3	-0	3	21	6	1*
-6	91	3	-4	0	34	3	-1	3	19	6	3*	-2	38	2	1	H,K=		9,	9
-5	15	6	3*	1	46	2	3	H,K=		8,	11	-1	12	1	1*	-4	68	3	-1
-4	22	4	2	2	38	2	4	-4	25	6	-2*	0	51	3	0	-3	45	3	-1
-3	17	4	2*	3	75	3	2	-3	49	3	0	1	137	4	2	-2	31	7	-2*
-2	102	3	-1	4	43	3	-2	-2	34	3	0	2	42	2	5	-1	26	7	-4*
-1	55	2	1	H,K=		8,	6	-1	87	3	2	3	31	3	0	0	75	3	-3
0	107	3	0	-6	48	3	2	0	38	3	3	4	12	1	6*	1	14	11	-10*
1	16	8	0*	-5	59	3	1	1	0	1	-2*	H,K=		9,	4	2	78	3	0
2	56	2	1	-4	84	3	-1	2	21	5	4*	-5	30	5	-3	H,K=		9,	10
3	43	2	4	-3	89	3	1	H,K=		8,	12	-4	24	4	1	-3	38	4	0
4	104	4	2	-2	10	1	3*	-3	102	4	0	-3	85	3	-1	-2	128	4	-2
5	11	1	0*	-1	10	1	3*	-2	11	1	-1*	-2	32	3	-2	-1	55	3	-3
H,K=		8,	2	0	44	2	0	-1	57	3	-4	-1	81	3	1	0	19	7	-6*
-6	31	4	-3	1	144	5	-1	0	11	1	8*	0	15	8	0*	1	0	1	-4*
-5	21	5	-0*	2	96	3	2	1	87	3	2	1	0	1	-10*	2	22	6	-4*
-4	107	4	-2	3	25	5	3*	2	43	3	0	2	21	4	2*	H,K=		9,	11
-3	121	4	-1	4	40	3	2	H,K=		8,	13	3	93	3	0	-3	55	3	-1
-2	30	3	2	H,K=		8,	7	-2	0	1	-5*	4	9	1	2*	-2	25	5	-3*
-1	85	3	-4	-5	16	8	0*	-1	69	3	-2	H,K=		9,	5	-1	19	6	0*
0	89	3	-3	-4	0	1	-4*	0	41	4	0	-5	61	3	-3	0	34	3	4
1	84	3	-2	-3	28	3	-2	1	14	1	13*	-4	38	3	4	1	86	3	-1
2	99	3	-2	-2	127	4	-2	H,K=		9,	0	-3	125	4	-4	H,K=		9,	12
3	0	1	-6*	-1	50	2	-0	-6	93	3	-0	-2	17	5	15*	-2	8	1	5*
4	41	3	4	0	46	2	1	-4	42	3	3	-1	38	3	-0	-1	77	3	-2
5	58	4	10	1	14	7	12*	-2	206	6	-1	0	22	4	-2*	0	12	1	8*
H,K=		8,	3	2	58	3	-1	0	36	3	-3	1	136	4	-0	H,K=		10,	0
-6	33	4	-0	3	28	3	1	2	50	3	0	2	15	8	-3*	-4	94	3	-1
-5	39	3	-0	4	78	3	1	4	93	3	5	3	43	3	4	-2	40	3	1
-4	23	3	3	H,K=		8,	8	H,K=		9,	1	H,K=		9,	6	0	48	3	3
-3	103	3	-0	-5	24	4	0*	-6	50	3	2	-5	15	11	-11*	2	72	3	1
-2	88	3	-0	-4	109	4	-1	-5	34	3	0	-4	8	1	-7*	H,K=		10,	1
-1	98	3	-1	-3	47	3	-1	-4	76	3	1	-3	63	3	-1	-5	11	1	1*
0	11	1	-2*	-2	20	4	-1*	-3	33	3	0	-2	31	3	3	-4	18	1	17*
1	13	10	-0*	-1	52	3	-3	-2	37	3	-0	-1	57	3	1	-3	35	3	2
2	35	3	1	0	123	4	1	-1	7	1	5*	0	64	3	-1	-2	129	4	-0
3	90	3	2	1	10	1	6*	0	84	3	1	1	20	5	17*	-1	41	3	-3
4	44	3	-1	2	84	3	1	1	64	3	-1	2	56	3	-2	0	77	3	-0
5	39	3	-1	3	16	10	4*	2	99	3	5	3	64	3	1	1	15	1	-0*
H,K=		8,	4	4	40	3	3	3	13	1	-2*	H,K=		9,	7	2	68	3	2

STRUCTURE FACTORS CONTINUED FOR
FERRICINIUM TETRACHLOROBISMUTHATE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	47	3	-2	-1	16	13	0*												
H,K=	10,	2		0	55	3	-0												
-5	29	5	1	1	25	6	2*												
-4	53	3	-1	H,K=	10,	9													
-3	83	3	-2	-3	8	1	-2*												
-2	36	4	-1	-2	97	3	-0												
-1	46	3	-3	-1	14	1	0*												
0	51	3	-1	0	54	3	1												
1	38	3	3	H,K=	10,	10													
2	89	3	1	-1	27	4	1												
3	32	4	5	H,K=	11,	0													
H,K=	10,	3		-4	24	5	4*												
-5	45	4	-3	-2	129	4	-4												
-4	22	4	4*	0	32	3	2												
-3	44	3	-3	H,K=	11,	1													
-2	63	3	-1	-4	65	3	-1												
-1	88	3	-0	-3	26	4	4												
0	7	1	1*	-2	45	3	1												
1	7	1	3*	-1	19	8	2*												
2	26	4	6	0	37	3	-2												
3	72	3	1	1	43	3	2												
H,K=	10,	4		H,K=	11,	2													
-5	93	3	2	-4	25	4	16												
-4	18	7	-1*	-3	49	3	-2												
-3	77	3	-4	-2	78	3	2												
-2	10	1	3*	-1	66	3	-5												
-1	16	10	7*	0	58	3	-1												
0	3	1	2*	1	14	10	11*												
1	143	5	3	H,K=	11,	3													
2	23	4	2	-3	63	3	-1												
H,K=	10,	5		-2	19	9	7*												
-4	10	1	3*	-1	10	1	1*												
-3	58	3	-2	0	39	3	-3												
-2	26	5	-5*	1	75	3	-1												
-1	110	4	-1	H,K=	11,	4													
0	19	7	-5*	-3	16	1	1*												
1	16	10	6*	-2	19	6	4*												
2	22	5	-0*	-1	116	4	-1												
H,K=	10,	6		0	30	4	1												
-4	33	4	-2	1	21	6	-4*												
-3	59	3	-1	H,K=	11,	5													
-2	37	4	-0	-3	74	3	0												
-1	7	1	4*	-2	14	1	-4*												
0	50	3	0	-1	54	3	-0												
1	92	3	1	0	23	6	-0*												
2	76	3	0	1	60	3	-2												
H,K=	10,	7		H,K=	11,	6													
-4	18	9	2*	-2	35	4	-2												
-3	33	4	0	-1	76	3	-5												
-2	116	4	2	0	53	3	2												
-1	56	3	-0	H,K=	11,	7													
0	36	6	-3	-1	13	1	8*												
1	0	1	-4*																
2	27	5	-7																
H,K=	10,	8																	
-3	13	1	-7*																
-2	40	3	3																

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