Title

BIS(2-METHYLIMIDAZOLIUM) TETRACHLORODIOXOURANIUM (VI), (CH3C3N2H+4)2(UO2Cl4)-2

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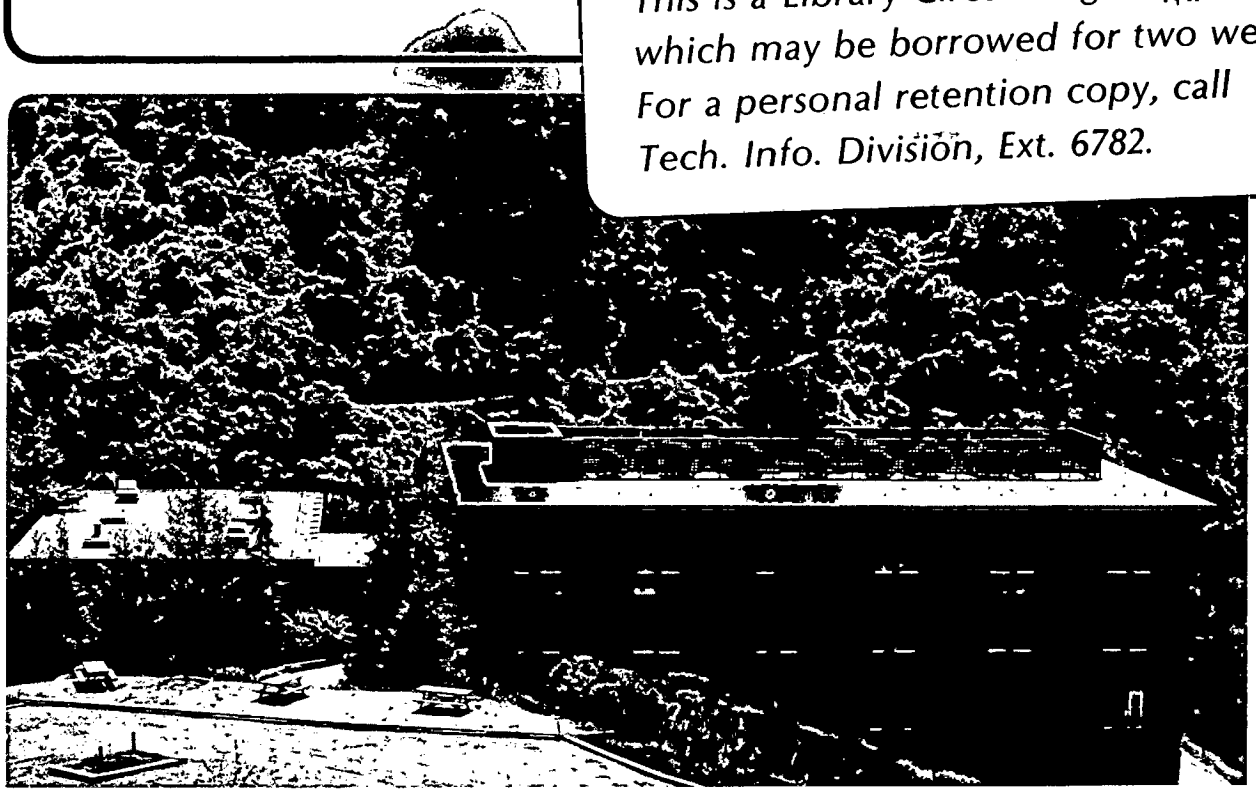
$(CH_3C_3N_2H_4^+)_2(UO_2Cl_4)^{-2}$

Allan Zalkin, Dale Perry, Leon Tsao,
and Zhang Dechun

January 1983



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DISCLAIMER

BIS(2-METHYLIMIDAZOLIUM) TETRACHLORODIOXOURANIUM(VI), $(CH_3C_3N_2H_4^+)_2(UO_2Cl_4)^{-2}$

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January 1983

ABSTRACT

M_r = 578.07, monoclinic, $P2_1/c$, $\underline{a}$ = 7.177(2), $\underline{b}$ = 18.526(4), $\underline{c}$ = 12.600(3) Å, β = 94.08(2)°, U = 1671.1 Å^3, Z = 4, D_x = 2.30 g cm^{-3}, λ(MoKα) = 0.71073 Å, μ(MoKα) = 98.6 cm^{-1}, T = 23°C, R = 0.035 for 1501 observed reflections where $F^2 > \sigma(F^2)$.

INTRODUCTION

Uranyl complexes exhibit a highly characteristic luminescence spectrum both in the solution and solid state. This luminescence will often display considerable vibrational structure, and the spectral details are quite dependent on the overall structure of the complex and the nature of the coordination sphere about the central uranyl ion (Brittain and Perry, 1980; Brittain and Perry, 1981; Perry, 1982). The title compound here is being studied in order to better understand its luminescence properties, which are significantly different from those of the unsubstituted imidazolium tetrachlorodioxouranium(VI) complex (Perry, Freyberg, and Zalkin, 1980).

EXPERIMENTAL

The material was made by combining 2-methylimidazole (2 mmole) and uranyl chloride trihydrate (1 mmole) in water, adjusting the pH to 2 with HCl and evaporating to dryness; crystals were obtained by recrystallization from water. A crystal ca. 0.09 x 0.05 x 0.20 mm was mounted with epoxy to a glass fiber and placed on a modified FACS-I Picker diffractometer. About 40 reflections with $20 < 2\theta < 35^{\circ}$ were used to determine the cell dimensions and their standard deviations. The systematic absences are hol, $l = 2n + 1$ and oko, $k = 2n + 1$. An analytical absorption correction was applied (Templeton and Templeton, 1973) and corrections ranged from 1.52 to 2.68. Intensities were collected to a maximum two-theta value of 45°, and the hkl indices ranged as follows: $-7 \leq h \leq 7$, $0 \leq k \leq 19$, and $-13 \leq l \leq 13$. Three standard reflections ($20\bar{2}$, $\bar{1}1\bar{1}$, 040) were measured at every 200th intensity measurement to an accuracy of better than 1.5 percent; the three standards showed isotropic decay of ~25 percent, and the data were adjusted accordingly. A total of 2,740 intensities were measured and resulted in 2183 unique reflections; 550 reflections were measured twice, and the R_{int} from merging these was 0.028. The number of unobserved reflections, $I < \sigma(I)$, was 603. The atomic positions of uranium and chlorine were derived from a three dimensional Patterson function. An electron density map, calculated from the observed structure factors and using phases based on the heavy atoms, revealed the positions of the carbon, nitrogen and oxygen atoms. The F magnitude was used in the full matrix least squares refinement. The calculated non-methyl type hydrogen atomic positional parameters were included in the least-squares calculations but were not refined. Because of

some large discrepancies in the low angle data, all 73 data where $\sin\theta/\lambda < 0.18$ were excluded from the final refinements. The positional and anisotropic thermal parameters for all of the non-hydrogen atoms were included in the refinement. The final weighted R was 0.027 for 1501 data ($F^2 > \sigma(F^2)$), and the goodness of fit was 1.06. The assigned weights, $w = [\sigma(F)]^{-1}$, were derived from $\sigma(F^2) = [C + (pF^2)^2]^{1/2}$, where C is the variance due to counting statistics and p = 0.02.

After the final refinement, the largest shift/error was less than 0.0004. The maximum and minimum heights in the final difference Fourier were 1.23 and -1.20 e/Å^3, respectively. The F(0,0,0) was 1000.5. An empirical extinction correction of the form $F_{corr} = F_{obs}(1+kI)$, where $k = 3.5 \times 10^{-6}$, was applied to the data. Scattering factors for U, Cl, O, N, and C were taken from International Tables for X-ray Crystallography (1974). Hydrogen scattering factors used were those of Stewart et al. (1965). Anomalous scattering factors were applied (Cromer and Liberman, 1970), and the f" values used for U, Cl, O, N and C were 9.654, 0.159, 0.006, 0.003 and 0.002, respectively. With the exception of ORTEP, all of the computer programs used in this structure determination were written by the authors for a CDC 7600 computer.

DISCUSSION

The atomic coordinates are given in Table I with the numbering scheme as shown in Fig. 1; a list of distances and angles is given in Table 2.* The structure consists of the packing of columns of $UO_2Cl_4^{2-}$ anions and columns of $CH_3C_3N_2H_4^+$ cations that are parallel to the a axis. Figure 1 shows the view down the a axis of one formula unit.

The $UO_2Cl_4^{2-}$ anion is a flattened octahedron with the oxygen atoms occupying the apices and the chlorine atoms the equatorial positions. The anion has been well characterized by other structure determinations, and the distances and angles reported here are in good agreement with those previously determined (Perry, Freyberg and Zalkin, 1980).

The 2-methylimidazolium cation is a planar entity and, with the exception of the methyl group, has the same geometry and dimensions as the unsubstituted imidazolium ion (Perry, Freyberg, Zalkin, 1980). The planes of the two independent 2-methyl imidazolium ions (Fig. 1) are within four degrees of being parallel to each other.

The shortest interatomic distances to the nitrogen atoms are: N(1)-Cl(2), 3.16(1) Å; N(2)-O(1), 3.21(1) Å, N(3)-O(1), 3.12(1) Å; and N(4)-O(2), 3.34(1) Å. These distances are comparable with those in the imidazolium tetrachlorodioxuranium(VI) (Perry, Freyberg and Zalkin, 1980), in which weak hydrogen bonding was suggested.

*Lists of structure factors, anisotropic thermal parameters, and calculated hydrogen positions have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 0000 (11 pp.). Copies may be obtained through the Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

ACKNOWLEDGMENT

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Table 1. Positional parameters and equivalent isotropic thermal parameters ($Å^2$).

$$B_{eq} = \Sigma_i \Sigma_j B_{ij} a_i^* a_j^* \underline{a}_i \cdot \underline{a}_j / 3$$

ATOM	X	Y	Z	B OR BEQ
U	.23303(6)	.12987(2)	.27456(3)	2.82*
CL(1)	-.0720(4)	.12993(16)	.38428(20)	4.10*
CL(2)	.0723(4)	.03771(13)	.13287(21)	3.94*
CL(3)	.5416(4)	.12628(15)	.16763(21)	4.03*
CL(4)	.3920(4)	.22788(14)	.40844(21)	4.15*
O(1)	.1412(11)	.2032(3)	.1970(5)	3.96*
O(2)	.3214(11)	.0564(3)	.3504(6)	4.11*
N(1)	.2030(14)	.8919(5)	.2446(9)	4.08*
N(2)	.2430(14)	.7783(5)	.2461(7)	3.81*
N(3)	.7209(13)	.8607(4)	.2567(6)	3.09*
N(4)	.7125(14)	.9750(4)	.2847(8)	3.49*
C(1)	.2767(17)	.8768(8)	.3436(10)	4.73*
C(2)	.2989(19)	.8036(7)	.3460(11)	4.53*
C(3)	.1836(17)	.8336(7)	.1848(10)	3.51*
C(4)	.1158(21)	.8277(6)	.0711(10)	5.29*
C(5)	.7784(16)	.8711(7)	.3599(9)	3.65*
C(6)	.7767(17)	.9419(7)	.3804(9)	3.96*
C(7)	.6817(16)	.9249(6)	.2111(9)	3.45*
C(8)	.6167(18)	.9370(6)	.0961(9)	4.50*

Table 2. Distances (Å) and Angles (°).

U-Cl(1)	2.671(3)	N(1)-C(1)	1.35(2)	N(3)-C(5)	1.35(2)
U-Cl(2)	2.672(3)	C(1)-C(2)	1.37(2)	C(5)-C(6)	1.34(2)
U-Cl(3)	2.674(3)	C(2)-N(2)	1.38(2)	C(6)-N(4)	1.40(3)
U-Cl(4)	2.678(3)	N(2)-C(3)	1.33(2)	N(4)-C(7)	1.32(2)
U-O(1)	1.773(6)	C(3)-N(1)	1.32(2)	C(7)-N(3)	1.34(2)
U-O(2)	1.756(7)	C(3)-C(4)	1.48(2)	C(7)-C(8)	1.51(2)

Cl(1)-U-Cl(2)	90.9(1)	C(3)-N(1)-C(1)	112(1)
Cl(1)-U-Cl(3)	178.3(1)	N(1)-C(1)-C(2)	105(1)
Cl(1)-U-Cl(4)	90.1(1)	C(1)-C(2)-N(2)	107(1)
Cl(1)-U-O(1)	89.9(3)	C(2)-N(2)-C(3)	109(1)
Cl(1)-U-O(2)	89.8(3)	N(2)-C(3)-N(1)	106(1)
Cl(2)-U-Cl(3)	88.9(1)	N(2)-C(3)-C(4)	125(1)
Cl(2)-U-Cl(4)	176.9(1)	N(1)-C(3)-C(4)	129(1)
Cl(2)-U-O(1)	89.8(3)	C(7)-N(4)-C(6)	109(1)
Cl(2)-U-O(2)	89.4(2)	N(4)-C(6)-C(5)	106(1)
Cl(3)-U-Cl(4)	90.2(1)	C(6)-C(5)-N(3)	109(1)
Cl(3)-U-O(1)	91.7(3)	C(5)-N(3)-C(7)	109(1)
Cl(3)-U-O(2)	88.6(3)	N(3)-C(7)-N(4)	108(1)
Cl(4)-U-O(1)	87.3(2)	N(3)-C(7)-C(8)	126(1)
Cl(4)-U-O(2)	93.6(2)	N(4)-C(7)-C(8)	127(1)
O(1)-U-O(2)	179.1(3)		

FIGURE CAPTION

Fig. 1. An ORTEP (Johnson, 1965) view of the molecule as viewed down the a axis.

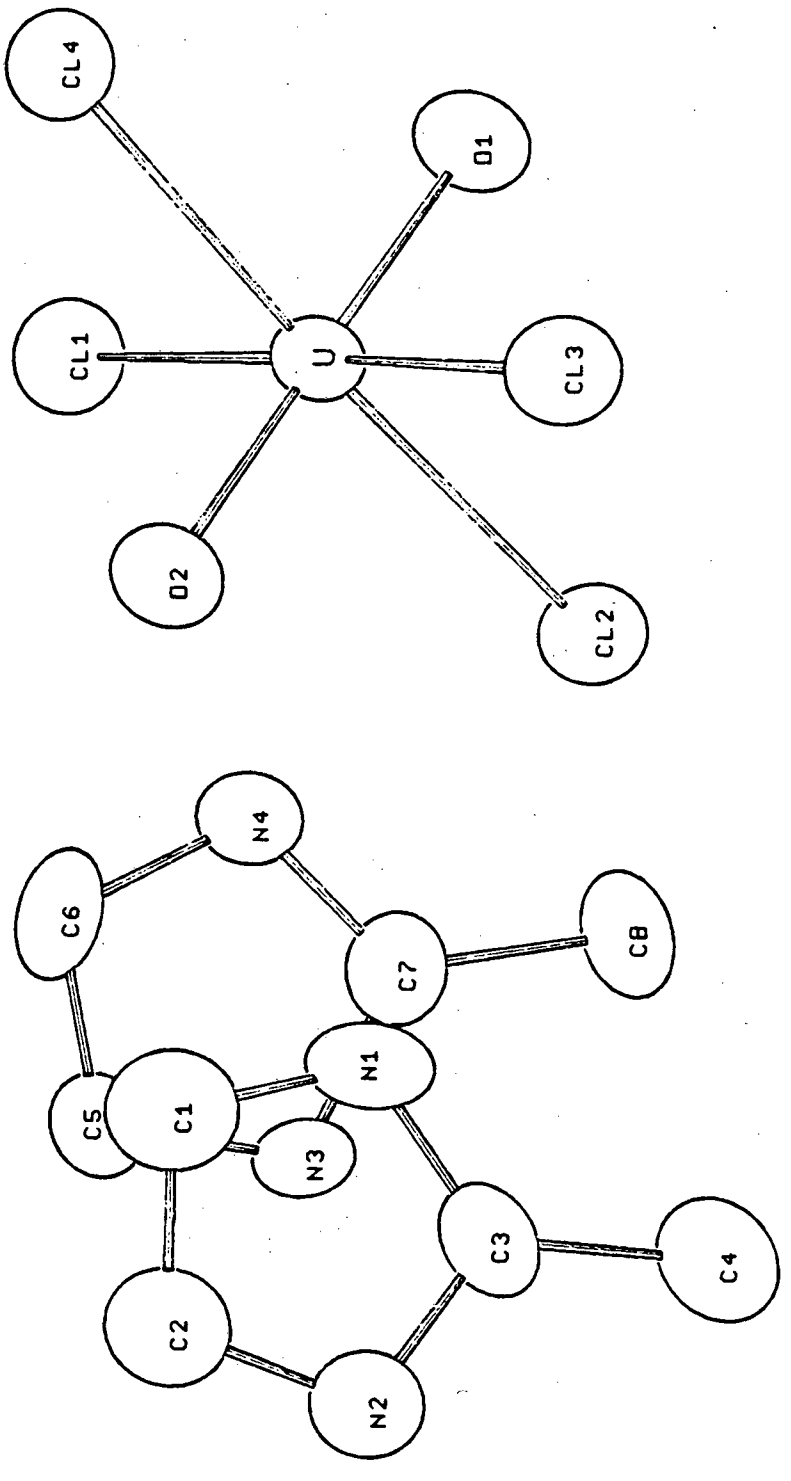

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Fig. 1

SUPPLEMENTARY MATERIALS

BIS(2-METHYLIMIDAZOLIUM) TETRACHLORODIOXOURANIUM(VI), $(CH_3C_3N_2H_4^+)_2(UO_2Cl_4)^{-2}$

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Anisotropic Thermal Parameters*

ATOM	B11	B22	B33	B12	B13	B23
U	3.521(20)	2.221(17)	2.663(18)	.144(23)	-.187(13)	.197(19)
CL(1)	4.35(14)	4.10(13)	3.88(14)	-.31(15)	.47(12)	-.10(13)
CL(2)	4.94(16)	3.18(12)	3.55(14)	-.56(12)	-.64(13)	-.14(10)
CL(3)	4.17(14)	3.74(12)	4.23(14)	-.25(14)	.62(12)	-.01(12)
CL(4)	5.01(17)	3.81(13)	3.53(14)	-.66(12)	-.38(13)	-.11(11)
O(1)	4.6(4)	3.1(3)	4.0(4)	1.0(3)	-.5(4)	.53(26)
O(2)	4.8(4)	3.4(3)	3.9(4)	.3(3)	-.9(3)	.30(27)
N(1)	4.9(7)	2.5(4)	5.0(7)	.0(4)	.9(5)	.2(4)
N(2)	4.0(5)	3.5(4)	4.0(6)	.6(4)	.8(5)	.2(4)
N(3)	4.4(5)	1.9(4)	2.9(5)	.6(4)	.2(4)	-.0(3)
N(4)	4.4(5)	2.6(4)	3.4(5)	-.3(4)	-.0(4)	-.1(4)
C(1)	4.4(6)	4.4(7)	5.4(8)	-1.0(6)	.2(6)	-.2(6)
C(2)	4.4(7)	4.6(7)	4.4(8)	-1.0(6)	-.2(6)	.1(5)
C(3)	3.3(6)	4.2(6)	3.2(7)	.5(5)	1.1(5)	.8(6)
C(4)	6.8(8)	5.0(6)	4.1(7)	.5(6)	.2(7)	.7(5)
C(5)	4.7(6)	3.4(5)	2.9(5)	-1.0(6)	.3(5)	.2(5)
C(6)	4.4(7)	5.4(7)	2.1(6)	-.6(6)	.4(5)	-.8(5)
C(7)	3.1(6)	4.2(6)	3.1(6)	-1.0(5)	1.0(5)	-.1(5)
C(8)	5.7(8)	5.2(6)	2.5(6)	-.7(6)	-.4(6)	.8(4)

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

Table of Calculated Hydrogen Positions

H(1)	0.1698	0.9372	0.2208
H(2)	0.2419	0.731	0.224
H(3)	0.7072	0.8171	0.2233
H(4)	0.6943	1.0234	0.2739
H(5)	0.3085	0.9111	0.4010
H(6)	0.3473	0.7736	0.4065
H(7)	0.8176	0.8333	0.410
H(8)	0.8126	0.9663	0.4473

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 3.0)
BIS(METHYLIMIDAZOLIUM)TETRACHLORODIOXOURANIUM(VI). F(0,0,0) = 3001

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	2	933	0	0*	H,K=		0,	8	H,K=		0,	12	8	63	69	-14*
21	24	0	-360*	3	116	0	10*	0	815	11	-15	0	817	10	-2	H,K=		0,	17
4	201	0	-2*	4	540	7	5	1	187	4	-2	1	225	5	-9	1	60	64	3*
6	461	6	7	5	191	5	-0	2	663	8	-28	2	566	7	-0	2	72	17	-20
8	314	6	3	6	252	5	-3	3	162	4	0	3	0	61	-84*	3	48	66	-15*
10	0	71	-11*	7	61	58	-11	4	458	6	-1	4	221	5	11	4	153	8	-1
12	16	78	-55*	8	188	7	2	5	39	49	22*	5	86	21	-14	5	0	59	-11*
H,K=		0,	1	9	131	10	1	6	331	5	-7	6	178	6	1	6	180	8	2
2	295	0	33*	11	77	19	-8	7	65	28	-6	7	79	14	16	7	0	66	-31*
3	241	0	17*	12	78	36	15	8	169	8	-18	8	199	7	-3	H,K=		0,	18
4	61	0	14*	13	38	68	25*	9	131	10	-10	9	0	74	-28*	0	179	18	3
5	258	5	5	H,K=		0,	5	10	0	64	-26*	10	0	76	-51*	1	285	6	3
6	353	5	13	1	109	0	10*	11	0	78	-11*	H,K=		0,	13	2	180	8	-5
7	335	5	-9	2	183	0	-4*	12	53	75	23*	1	65	23	13	3	222	6	-4
8	539	7	-5	3	235	4	3	H,K=		0,	9	2	147	6	3	4	132	10	10
9	379	6	5	4	279	4	-4	1	197	4	-1	3	11	61	-13*	5	186	8	6
10	310	6	9	5	226	4	2	2	98	6	-5	4	174	6	0	H,K=		0,	19
11	250	7	-10	6	309	5	-3	3	146	5	3	5	154	7	-2	1	69	40	3
12	173	9	9	7	212	5	4	4	192	4	2	6	242	5	-1	2	103	11	19
13	139	12	-16	8	386	6	-5	5	37	37	4*	7	93	25	-38	3	131	10	5
H,K=		0,	2	9	289	6	5	6	334	5	-1	8	337	6	-6	4	42	68	33*
0	85	0	5*	10	418	6	-5	7	233	5	-5	9	111	13	2	H,K=		1,	0
1	911	0	54*	11	254	7	6	8	398	6	-12	10	293	7	6	-12	160	9	6
2	31	0	21*	12	211	9	-7	9	247	6	4	H,K=		0,	14	-10	295	6	-6
3	529	0	34*	13	81	56	-12	10	268	7	-12	0	210	8	-4	-8	572	7	-15
4	149	0	15*	H,K=		0,	6	11	120	13	3	1	508	6	1	-6	543	7	-5
5	228	4	-15	0	100	0	7*	12	135	24	-18	2	194	6	5	-4	402	0	26*
6	143	6	1	1	768	0	38*	H,K=		0,	10	3	390	5	-13	-2	292	0	21*
7	237	5	6	2	157	4	-2	0	329	5	-2	4	160	5	2	0	117	0	8*
8	86	26	-9	3	631	7	-20	1	748	9	-4	5	203	6	-3	2	188	0	22*
9	77	16	2	4	124	5	-2	2	142	5	3	6	105	11	-18	4	376	8	2*
10	62	24	7	5	426	5	-11	3	245	4	1	7	74	48	-26	6	411	5	-2
11	74	51	-9	6	36	56	2*	4	44	46	15*	8	16	72	-4*	8	292	6	1
12	54	72	-25*	7	201	6	-4	5	226	5	-5	9	44	75	-18*	10	278	7	-9
13	70	73	-34*	8	44	57	33*	6	82	20	-0	H,K=		0,	15	12	405	7	2
H,K=		0,	3	9	19	69	-23*	7	218	6	-11	1	105	8	8	H,K=		1,	1
1	235	0	-13*	10	32	65	8*	8	100	12	0	2	31	60	13*	-13	86	18	12
2	29	0	-4*	11	50	71	-12*	9	46	60	32*	3	212	6	-1	-12	96	26	-4
3	314	0	16*	12	0	94	-43*	10	63	63	59*	4	22	64	-31*	-11	0	74	-52*
4	308	0	-1*	H,K=		0,	7	11	81	35	13	5	188	7	2	-10	69	71	-5*
5	76	9	-10	1	65	7	4	H,K=		0,	11	6	118	10	12	-9	62	47	3
6	395	5	2	2	235	4	-6	1	183	5	4	7	180	7	5	-8	151	7	-7
7	264	5	-6	3	263	4	-5	2	119	6	6	8	81	19	-20	-7	81	21	6
8	334	6	1	4	145	5	8	3	223	5	0	H,K=		0,	16	-6	319	5	9
9	448	6	-1	5	389	5	-6	4	4	51	-24*	0	391	7	1	-5	240	4	3
10	287	6	3	6	138	9	-5	5	220	5	7	1	145	8	-12	-4	299	8	23*
11	318	6	3	7	406	5	-3	6	126	8	8	2	327	6	-5	-3	461	0	20*
12	157	10	-13	8	324	6	-3	7	387	6	-12	3	181	7	-4	-2	483	0	29*
13	161	10	-5	9	426	6	-10	8	182	7	-2	4	196	7	-6	-1	580	0	25*
H,K=		0,	4	10	289	6	-11	9	362	6	2	5	118	10	3	0	763	0	102*
0	11	32	0	42*	11	323	7	1	10	155	9	2	6	122	10	8	1	602	0	1*
1	84	0	3*	12	154	10	14	11	209	8	3	7	71	33	45	2	586	0	-17*

STRUCTURE FACTORS CONTINUED FOR
BIS(METHYLIMIDAZOLIUM)TETRACHLORODIOXOURANIUM(VI). PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	518	0	12*	3	813	0	-14*	3	729	9	-4	7	143	7	5	H,K=		1,	10
4	519	6	-12	4	414	5	5	4	714	8	-30	8	28	66	-1*	-11	180	10	-10
5	300	5	-8	5	454	6	0	5	306	4	4	9	65	67	4*	-10	78	35	-2
6	358	5	7	6	275	5	13	6	206	5	2	10	61	61	1*	-9	405	6	-3
7	199	6	2	7	46	65	-12*	7	161	7	4	11	77	28	14	-8	152	9	-20
8	38	59	-34*	8	261	6	6	8	175	7	2	12	84	44	61	-7	507	7	3
9	116	11	-1	9	29	61	6*	9	110	12	-6	H,K=		1,	8	-6	147	7	-3
10	39	72	21*	10	21	74	-15*	10	101	22	-1	-12	167	10	3	-5	369	5	-1
11	65	22	55	11	44	69	9*	11	51	79	37*	-11	0	71	-58*	-4	67	12	16
12	0	78	-43*	12	117	13	9	12	66	73	28*	-10	251	7	0	-3	245	4	-6
13	69	27	-3	13	68	68	-1*	H,K=		1,	6	-8	466	6	-4	-2	0	53	-22*
H,K=		1,	2	H,K=		1,	4	-12	56	79	-2*	-7	246	6	2	-1	138	6	-5
-13	202	9	2	-13	57	68	23*	-11	283	7	3	-6	514	6	-15	0	0	53	-37*
-12	15	52	1*	-12	264	7	0	-10	43	72	-2*	-5	206	5	7	1	41	45	9*
-11	228	7	-11	-11	57	65	38*	-9	320	6	-9	-4	354	5	-3	2	42	53	2*
-10	67	38	22	-10	288	6	-5	-8	23	45	0*	-3	33	48	7*	3	210	5	0
-9	452	6	2	-9	84	26	8	-7	556	7	-14	-2	189	4	-1	4	156	6	-4
-8	44	65	36*	-8	489	6	14	-6	121	7	11	-1	124	5	5	5	341	5	-6
-7	682	8	-2	-7	49	60	-12*	-5	677	8	4	0	37	45	26*	6	155	7	-8
-6	73	28	-17	-6	784	9	-4	-4	6	49	-27*	1	89	6	-2	7	333	5	-15
-5	557	7	-1	-5	39	44	29*	-3	291	4	-8	2	160	4	-4	8	65	69	-13*
-4	130	0	18*	-4	570	7	12	-2	174	4	7	3	228	4	-1	9	261	6	-6
-3	362	0	9*	-3	144	0	4*	-1	32	0	3*	4	274	4	-0	10	56	74	1*
-2	191	0	-13*	-2	114	0	-3*	0	207	0	14*	5	255	5	-0	11	294	7	5
-1	268	0	16*	-1	42	0	8*	1	125	4	6	6	319	5	-0	H,K=		1,	11
0	114	0	-13*	0	130	0	3*	2	99	5	11	7	40	62	-4*	-11	56	76	13*
1	66	0	3*	1	158	0	25*	3	393	5	0	8	290	6	-4	-10	44	72	34*
2	24	0	-13*	2	237	0	8*	4	157	5	-0	9	60	71	17*	-9	43	70	19*
3	375	0	2*	3	225	0	34*	5	342	5	-1	10	304	6	0	-8	48	66	36*
4	209	4	-1	4	522	6	-6	6	29	48	13*	11	108	14	14	-7	163	7	10
5	449	6	-3	5	41	52	14*	7	276	5	4	12	266	8	3	-6	93	12	-4
6	45	51	38*	6	318	5	-1	8	28	68	-13*	H,K=		1,	9	-5	222	6	-5
7	334	5	-6	7	179	6	4	9	397	6	-1	-12	63	70	16*	-4	173	6	1
8	139	7	5	8	337	6	-4	10	110	13	-5	-11	36	69	-25*	-3	341	5	-0
9	357	6	-3	9	47	67	-12*	11	379	7	9	-10	77	49	40	-2	158	5	-0
10	68	70	12*	10	455	7	-6	12	93	16	47	-9	56	25	16	-1	487	6	4
11	434	7	2	11	40	73	28*	H,K=		1,	7	-8	108	10	1	0	187	5	-1
12	29	77	9*	12	327	7	9	-12	0	82	-30*	-7	262	5	-2	1	481	6	-5
13	307	8	-0	13	66	49	39	-11	61	78	-6*	-6	218	5	3	2	266	5	-2
H,K=		1,	3	H,K=		1,	5	-10	63	73	-14*	-5	246	5	-2	3	440	5	-0
-13	89	18	13	-13	78	23	4	-9	44	60	25*	-4	314	5	-1	4	234	5	-1
-12	0	87	-57*	-12	70	58	19	-8	56	23	-5	-3	176	5	-2	5	380	5	-1
-11	128	10	14	-11	56	73	48*	-7	137	7	2	-2	464	6	-1	6	120	9	11
-10	92	27	7	-10	19	64	3*	-6	269	5	-6	-1	313	4	1	7	195	6	-1
-9	37	64	-38*	-9	54	60	22*	-5	364	5	-11	0	615	7	-2	8	43	46	3*
-8	87	13	-5	-8	81	30	0	-4	160	5	-2	1	399	5	-3	9	7	74	-27*
-7	267	5	3	-7	109	3	5	-3	296	4	-6	2	605	7	-8	10	66	39	58
-6	157	6	-3	-6	426	5	5	-2	55	10	-6	3	409	5	-2	11	60	78	38*
-5	461	6	1	-5	350	5	-1	-1	196	4	-4	4	506	6	-5	H,K=		1,	12
-4	357	5	1	-4	645	7	6	0	211	4	-6	5	342	5	-3	-10	186	8	9
-3	380	0	-2*	-3	261	4	4	1	573	7	0	6	359	5	4	-9	135	10	17
-2	488	0	29*	-2	131	0	-8*	2	436	5	-2	7	115	9	-1	-8	368	6	8
-1	738	0	84*	-1	68	0	10*	3	675	8	-9	8	195	7	-8	-7	115	10	15
0	759	0	81*	0	263	0	-12*	4	417	5	-6	9	51	68	40*	-6	384	5	-11
1	928	0	40*	1	553	0	12*	5	321	5	-3	10	34	71	-20*	-5	92	21	-17
2	715	0	-23*	2	1091	0	3*	6	118	7	-5	11	56	77	14*	-4	225	5	-4

STRUCTURE FACTORS CONTINUED FOR
BIS(METHYLIMIDAZOLIUM)TETRACHLORODIOXOURANIUM(VI).

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	182	6	-2	H,K=	1,	15		0	46	56	-12*	-13	179	14	1	-11	110	19	-2
-2	133	7	-8	-8	27	87	-14*	1	35	58	-49*	-12	0	94	-35*	-10	60	81	31*
-1	79	9	15	-7	90	20	21	2	33	78	12*	-11	119	17	4	-9	71	77	17*
0	91	16	-8	-6	56	38	21	3	92	19	-4	-10	63	85	34*	-8	0	82	-53*
1	104	8	-8	-5	269	8	-6	4	138	13	3	-9	45	56	-5*	-7	154	8	12
2	80	10	4	-4	66	25	-4	5	50	62	-51*	-8	128	13	6	-6	292	6	8
3	38	60	-39*	-3	267	7	1	H,K=	1,	19		-7	0	72	-30*	-5	45	61	18*
4	268	5	-1	-2	78	19	13	-3	166	11	9	-6	89	13	7	-4	567	8	-1
5	65	42	19	-1	188	8	-1	-2	28	82	8*	-5	408	6	8	-3	15	53	6*
6	255	6	-2	0	94	16	0	-1	213	9	10	-4	0	60	-25*	-2	694	9	54
7	91	13	-1	1	425	7	-5	0	66	78	33*	-3	726	10	23	-1	89	0	8*
8	164	8	-3	2	133	11	-6	1	253	9	-0	-2	127	0	5*	0	732	0	54*
9	97	25	7	3	491	6	6	2	79	83	21*	-1	368	0	9*	1	122	5	17
10	228	8	11	4	98	14	9	3	257	9	-1	0	89	0	17*	2	702	9	27
H,K=	1,	13		5	185	10	0	H,K=	2,	0		1	243	0	13*	3	113	7	1
-10	38	75	15*	6	86	20	9	-12	144	15	-15	2	59	0	15*	4	534	8	-7
-9	49	69	-15*	7	0	85	-71*	-10	0	80	-28*	3	559	8	-12	5	73	14	17
-8	97	26	5	8	86	90	6*	-8	126	14	-10	4	79	13	-2	6	441	7	-13
-7	26	57	12*	H,K=	1,	16		-6	165	9	-11	5	655	9	-29	7	75	19	16
-6	227	6	-4	-8	213	10	2	-4	734	9	-21	6	92	14	1	8	307	8	-3
-5	97	11	-9	-7	136	13	11	-2	1450	0	-203*	7	373	7	10	9	0	85	-32*
-4	269	5	-3	-6	318	8	3	0	1135	0	140*	8	60	35	13	10	93	22	-8
-3	197	6	3	-5	150	12	-9	2	356	0	-2*	9	39	85	-40*	11	0	89	-16*
-2	372	5	-3	-4	267	8	1	4	774	10	-62	10	132	13	25	12	23	87	6*
-1	179	5	3	-3	44	75	-15*	6	646	9	-12	11	0	89	-10*	H,K=	2,		5
0	498	6	-3	-2	111	14	-1	8	216	9	-5	12	0	91	-36*	-12	210	12	-2
1	230	5	1	-1	45	74	2*	10	113	17	-9	H,K=	2,		3	-11	178	11	4
2	489	6	4	0	0	76	-7*	12	34	82	21*	-13	192	14	-5	-10	177	11	-3
3	191	6	-3	1	59	76	-4*	H,K=	2,		1	-12	201	11	3	-9	138	13	-4
4	366	5	-10	2	115	14	-8	-13	158	14	12	-11	259	9	3	-8	286	7	8
5	65	32	-21	3	17	54	-37*	-12	153	15	-7	-10	194	11	6	-7	266	7	4
6	213	6	2	4	182	9	1	-11	240	10	-13	-9	175	11	-6	-6	495	7	3
7	111	10	2	5	93	18	7	-10	287	8	8	-8	234	7	4	-5	375	6	5
8	88	15	-8	6	144	12	-0	-9	241	9	5	-7	223	7	-1	-4	422	6	1
9	72	46	1	7	114	16	29	-8	273	7	12	-6	364	6	5	-3	289	5	-1
10	68	65	26	H,K=	1,	17		-7	218	8	-4	-5	524	8	-4	-2	208	5	-5
H,K=	1,	14		-7	79	85	4*	-6	276	6	5	-4	303	5	6	-1	151	5	10
-9	201	8	1	-6	227	9	10	-5	401	6	-6	-3	528	7	17	0	133	6	0
-8	89	27	-26	-5	64	37	-12	-4	539	8	8	-2	189	0	8*	1	15	50	-3*
-7	318	6	3	-4	294	8	-7	-3	658	0	19*	-1	135	0	6*	2	25	52	1*
-6	120	14	-8	-3	28	75	-18*	-2	309	0	11*	0	101	0	-3*	3	128	7	-7
-5	305	6	-5	-2	251	8	-1	-1	575	0	48*	1	72	0	16*	4	199	6	-4
-4	159	7	2	-1	101	15	9	0	87	0	15*	2	206	5	-6	5	154	8	1
-3	95	19	-16	0	334	7	-6	1	40	0	12*	3	76	9	22	6	382	6	5
-2	106	9	-4	1	123	13	-6	2	137	0	22*	4	340	5	1	7	181	9	-5
-1	79	25	-7	2	477	8	-0	3	269	5	23	5	257	6	1	8	388	8	-10
0	40	56	-25*	3	156	11	5	4	226	6	2	6	250	6	13	9	196	9	8
1	61	22	11	4	349	8	-1	5	202	7	-17	7	411	7	2	10	251	9	14
2	106	12	19	5	109	17	-12	6	537	8	-1	8	218	9	11	11	131	15	17
3	186	8	-7	6	146	14	-4	7	214	7	17	9	235	9	-13	12	128	17	5
4	77	17	27	H,K=	1,	18		8	290	7	6	10	184	11	1	H,K=	2,		6
5	193	9	-11	-5	215	10	3	9	232	9	-3	11	187	11	9	-12	0	92	-10*
6	118	13	-2	-4	0	86	-60*	10	167	12	-5	12	159	14	-2	-11	157	12	14
7	120	14	-5	-3	168	11	-6	11	243	10	-14	H,K=	2,		4	-10	0	83	-32*
8	157	12	13	-2	0	78	-19*	12	242	10	5	-13	0	96	-67*	-9	0	80	-27*
9	245	9	13	-1	0	87	-45*	H,K=	2,		2	-12	140	16	5	-8	51	83	-40*

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	152	9	-4	-2	548	8	18	6	167	10	-10	-4	360	7	-2	-2	266	7	10
-6	45	65	16*	-1	78	11	-1	7	192	9	4	-3	140	9	5	-1	135	11	7
-5	392	6	11	0	496	7	8	8	42	76	9*	-2	219	7	2	0	288	7	1
-4	120	8	3	1	137	6	8	9	0	55	-34*	-1	194	7	0	1	188	9	5
-3	454	6	3	2	577	8	6	10	0	90	-21*	0	77	18	-2	2	270	7	10
-2	51	16	-3	3	105	10	-6	H,K=		2,	11	1	0	75	-25*	3	151	11	5
-1	481	7	-1	4	653	9	2	-11	247	11	9	2	0	73	-20*	4	218	9	9
0	99	7	5	5	141	9	-3	-10	111	18	4	3	173	8	-1	5	76	80	4*
1	330	8	19	6	488	7	13	-9	292	8	7	4	132	11	-8	6	193	11	-2
2	156	6	-0	7	166	10	8	-8	72	80	-21*	5	91	17	-10	7	39	86	-20*
3	659	8	6	8	223	8	0	-7	230	7	6	6	299	7	1	H,K=		2,	17
4	56	62	-21*	9	0	82	-11*	-6	76	19	-13	7	51	53	20*	-6	265	9	8
5	532	8	-2	10	99	21	-6	-5	355	6	7	8	272	9	6	-5	69	33	-11
6	0	74	-50*	11	51	92	-5*	-4	78	17	-5	9	85	25	5	-4	238	9	9
7	361	7	4	H,K=		2,	9	-3	467	7	4	H,K=		2,	14	-3	97	17	8
8	77	21	14	-11	130	17	3	-2	134	9	4	-9	62	39	17	-2	124	13	-0
9	141	14	-12	-10	258	9	2	-1	169	7	4	-8	77	83	9*	-1	0	76	-7*
10	72	25	66	-9	165	10	19	0	175	7	-1	-7	0	83	-53*	0	71	75	2*
11	0	91	-10*	-8	255	8	1	1	72	14	15	-6	70	25	-1	1	23	53	-9*
12	0	92	-14*	-7	125	12	6	2	70	16	22	-5	295	7	1	2	60	79	52*
H,K=		2,	7	-6	276	7	-9	3	123	10	3	-4	100	15	5	3	39	79	33*
-12	142	17	-5	-5	287	6	11	4	112	11	11	-3	383	7	3	4	124	13	21
-11	277	9	7	-4	351	6	-1	5	296	7	7	-2	167	9	-6	5	36	79	15*
-10	172	10	15	-3	338	6	2	6	123	13	-12	-1	301	7	-9	H,K=		2,	18
-9	246	8	-7	-2	274	5	6	7	246	8	-14	0	202	7	1	-4	138	14	5
-8	148	11	6	-1	20	58	2*	8	115	15	-7	1	314	6	-1	-3	190	10	-4
-7	392	7	7	0	93	10	3	9	175	11	-3	2	169	9	-9	-2	119	15	-6
-6	265	7	-6	1	20	40	6*	10	66	96	-32*	3	331	7	-10	-1	223	9	9
-5	488	7	6	2	88	10	12	H,K=		2,	12	4	132	12	-6	0	149	11	10
-4	348	6	-1	3	111	9	28	-10	0	91	-13*	5	315	7	4	1	199	10	-12
-3	335	5	-1	4	227	6	-9	-9	30	81	19*	6	66	28	-10	2	148	12	-7
-2	126	7	5	5	226	7	9	-8	49	74	30*	7	231	9	7	3	243	9	-1
-1	211	5	2	6	310	7	8	-7	43	52	37*	8	65	87	23*	4	125	16	-2
0	41	54	5*	7	243	8	6	-6	94	16	-15	H,K=		2,	15	H,K=		2,	19
1	53	54	7*	8	228	8	7	-5	60	22	46	-8	0	89	-70*	-2	0	82	-17*
2	48	59	-4*	9	0	85	-54*	-4	397	7	-6	-7	238	8	5	-1	88	22	-3
3	206	6	-1	10	175	12	-3	-3	152	9	18	-6	70	82	-26*	0	0	86	-54*
4	54	23	-13	11	101	21	17	-2	544	8	15	-5	334	7	-6	1	58	81	52*
5	333	6	2	H,K=		2,	10	-1	211	7	6	-4	67	77	-23*	2	0	87	-26*
6	315	6	-5	-11	147	14	17	0	375	6	3	-3	266	7	6	H,K=		3,	0
7	347	7	-2	-10	0	92	-9*	1	115	11	-0	-2	0	80	-91*	-12	239	10	2
8	286	7	8	-9	0	84	-15*	2	312	6	-0	-1	109	12	-3	-10	413	8	7
9	274	8	3	-8	0	80	-14*	3	180	7	13	0	11	75	-53*	-8	312	7	9
10	125	15	6	-7	82	18	-11	4	410	7	-5	1	20	70	12*	-6	287	7	-8
11	177	12	-6	-6	49	70	19*	5	161	9	7	2	63	24	43	-4	539	8	2
H,K=		2,	8	-5	224	7	4	6	369	7	-18	3	95	15	5	-2	472	7	1
-12	301	02	-100*	-4	94	12	0	7	0	84	-29*	4	77	20	10	0	162	5	-7
-11	89	92	22*	-3	552	8	12	8	196	10	6	5	153	11	3	2	52	59	44*
-10	33	85	5*	-2	226	6	-1	9	63	81	35*	6	72	25	15	4	117	11	-5
-9	0	80	-8*	-1	483	7	8	10	0	94	-50*	7	217	10	-9	6	245	8	-7
-8	86	17	6	0	121	8	-3	H,K=		2,	13	H,K=		2,	16	8	329	8	-2
-7	54	74	2*	1	159	7	4	-9	53	60	-27*	-7	71	84	29*	10	387	8	5
-6	204	8	-3	2	36	64	-23*	-8	201	9	2	-6	110	17	3	12	265	10	-5
-5	142	8	-5	3	385	6	-1	-7	109	14	2	-5	108	17	-0	H,K=		3,	1
-4	440	6	-0	4	179	8	-6	-6	290	7	-9	-4	190	10	-4	-12	146	15	-3
-3	188	6	1	5	535	8	9	-5	111	14	-0	-3	44	84	-63*	-11	106	17	24

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
-10	71	87	11*	-6	118	11	-4	0	813	11	35	8	190	9	13	-5	289	6	10
-9	113	15	5	-5	38	69	-33*	1	530	7	-7	9	108	16	28	-4	97	13	7
-8	45	55	4*	-4	226	6	0	2	538	8	13	10	106	20	7	-3	371	6	7
-7	0	79	-13*	-3	420	6	3	3	243	6	-2	11	0	91	-8*	-2	79	14	13
-6	57	70	19*	-2	446	7	-5	4	240	6	3	H,K=		3,	8	-1	260	6	3
-5	219	6	6	-1	753	10	38	5	250	6	6	-11	83	29	9	0	0	65	-26*
-4	232	6	2	0	632	8	11	6	387	7	6	-10	335	9	-1	1	101	11	1
-3	407	6	1	1	549	7	1	7	275	8	-1	-9	122	15	-3	2	62	20	0
-2	486	7	6	2	379	5	-2	8	305	8	3	-8	371	7	-1	3	0	68	-43*
-1	457	6	10	3	324	5	-2	9	115	14	14	-7	130	10	16	4	16	73	-29*
0	450	6	12	4	259	6	3	10	72	86	2*	-6	262	7	1	5	187	8	-1
1	381	6	2	5	223	7	-1	H,K=		3,	6	-5	90	12	13	6	0	52	-48*
2	362	5	-3	6	349	7	4	-12	0	86	-24*	-4	277	6	-2	7	249	8	-4
3	312	6	-7	7	258	8	-1	-11	260	10	12	-3	184	7	-15	8	60	81	-21*
4	363	6	1	8	213	9	-1	-10	62	34	45	-2	318	6	5	9	290	9	2
5	286	6	10	9	228	9	11	-9	401	8	2	-1	156	7	-2	10	124	17	19
6	263	7	10	10	19	85	-20*	-8	78	21	18	0	227	5	6	H,K=		3,	11
7	222	8	11	11	0	88	-40*	-7	436	7	6	1	126	8	-5	-10	75	86	3*
8	175	11	-3	H,K=		3,	4	-6	0	72	-20*	2	97	10	10	-9	58	84	9*
9	108	19	-17	-12	192	13	6	-5	263	6	3	3	115	9	-1	-8	21	55	-13*
10	135	14	18	-11	76	82	43*	-4	68	14	14	4	110	10	10	-7	0	74	-21*
11	30	91	-36*	-10	334	8	4	-3	230	6	1	5	62	24	-11	-6	74	20	19
12	53	91	50*	-9	89	20	12	-2	133	7	-3	6	249	7	2	-5	151	9	0
H,K=		3,	2	-8	487	8	6	-1	309	5	13	7	36	74	22*	-4	115	12	4
-12	54	86	38*	-7	39	77	-36*	0	118	7	10	8	297	8	-2	-3	344	7	0
-11	319	9	-1	-6	380	6	-6	1	123	8	-4	9	128	14	8	-2	141	9	-0
-10	0	89	-11*	-5	96	11	-5	2	127	8	1	10	247	10	-6	-1	392	6	4
-9	454	8	0	-4	276	5	4	3	0	65	-33*	H,K=		3,	9	0	188	7	14
-8	0	78	-6*	-3	20	55	7*	4	61	63	36*	-11	71	87	27*	1	360	6	1
-7	332	8	-13	-2	453	7	1	5	177	7	4	-10	134	14	33	2	185	7	1
-6	52	33	-5	-1	62	12	-4	6	44	50	27*	-9	85	21	7	3	400	7	16
-5	362	6	9	0	339	5	3	7	357	7	-4	-8	0	83	-35*	4	152	9	1
-4	104	9	10	1	204	5	3	8	112	16	-19	-7	0	76	-54*	5	296	7	-9
-3	564	8	8	2	41	56	29*	9	334	8	15	-6	76	17	14	6	126	12	10
-2	33	52	22*	3	53	64	-22*	10	46	88	-26*	-5	56	71	17*	7	160	11	-3
-1	428	6	13	4	89	12	-1	11	183	13	-4	-4	231	6	3	8	106	16	23
0	102	7	-1	5	201	7	-13	H,K=		3,	7	-3	236	6	-2	9	109	19	1
1	83	8	6	6	274	7	-3	-11	156	13	20	-2	446	6	0	H,K=		3,	12
2	198	5	5	7	115	13	25	-10	28	59	-14*	-1	354	6	3	-9	0	94	-96*
3	0	63	-70*	8	452	7	3	-9	24	82	-55*	0	523	8	9	-8	250	8	2
4	0	66	-41*	9	44	82	4*	-8	21	79	-27*	1	279	6	4	-7	79	80	-5*
5	141	10	-14	10	312	9	11	-7	65	77	-6*	2	473	7	4	-6	211	8	4
6	161	9	6	11	0	62	-11*	-6	0	74	-23*	3	237	6	8	-5	152	9	1
7	345	7	8	H,K=		3,	5	-5	124	10	0	4	417	7	-0	-4	291	7	-1
8	0	80	-33*	-12	104	20	19	-4	17	63	-44*	5	178	8	7	-3	142	9	1
9	448	8	-3	-11	86	24	13	-3	210	6	3	6	320	7	-6	-2	316	6	2
10	32	85	23*	-10	99	18	34	-2	342	5	6	7	116	14	-8	-1	0	71	-28*
11	333	9	12	-9	63	38	-19	-1	508	7	5	8	204	10	-2	0	145	9	5
12	56	60	24*	-8	65	27	25	0	378	5	4	9	86	92	-41*	1	66	67	56*
H,K=		3,	3	-7	27	72	15*	1	535	7	-3	10	48	93	-43*	2	0	72	-23*
-12	0	92	-59*	-6	173	8	9	2	239	5	-4	H,K=		3,	10	3	40	70	27*
-11	134	17	-14	-5	75	14	6	3	283	6	-4	-10	100	21	10	4	78	18	8
-10	66	89	-27*	-4	132	8	1	4	135	8	3	-9	319	9	-10	5	0	78	-46*
-9	36	82	29*	-3	110	8	-1	5	251	7	-5	-8	54	80	-10*	6	103	16	-19
-8	62	30	27	-2	357	5	-1	6	116	13	-6	-7	233	8	8	7	28	86	-35*
-7	94	13	25	-1	448	6	3	7	255	8	4	-6	40	73	-9*	8	238	9	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
9	65	83	-11*	-2	164	10	1	5	61	78	10*	-10	58	89	-24*	1	570	8	2
H,K=	3,	13		-1	170	9	12	6	150	12	-1	-9	48	85	2*	2	98	11	2
-9	0	94	-54*	0	100	17	-5	7	135	12	10	-8	62	80	45*	3	510	7	1
-8	0	84	-37*	1	0	83	-71*	8	142	14	0	-7	56	75	34*	4	61	72	-13*
-7	28	55	3*	2	48	79	28*	9	269	9	9	-5	19	68	2*	5	407	7	-2
-6	74	78	4*	3	0	77	-18*	10	253	10	6	-4	151	8	1	6	81	19	2
-5	121	13	3	4	62	34	20	11	233	11	19	-3	7	43	-16*	7	268	8	-1
-4	175	9	-12	5	0	86	-51*	H,K=	4,	2		-2	351	5	6	8	0	57	-34*
-3	105	14	-5	H,K=	3,	17		-12	0	94	-3*	-1	41	59	27*	9	134	15	14
-2	381	7	-7	-5	0	59	-9*	-11	110	21	2	0	598	8	5	10	0	91	-19*
-1	144	10	-4	-4	129	15	-4	-10	74	29	16	1	0	60	-27*	H,K=	4,	7	
0	414	7	2	-3	0	88	-88*	-9	134	13	10	2	552	8	3	-11	109	21	-16
1	159	9	0	-2	281	8	1	-8	76	80	69*	3	0	66	-54*	-10	57	94	-57*
2	303	6	-1	-1	136	13	-0	-7	0	55	-23*	4	403	7	-8	-9	262	9	-1
3	108	11	22	0	392	8	4	-6	11	76	-26*	5	0	72	-28*	-8	220	9	2
4	223	8	-2	1	0	90	-102*	-5	198	7	12	6	330	7	-2	-7	354	7	-7
5	118	12	16	2	276	8	2	-4	100	12	-9	7	70	23	46	-6	211	8	-11
6	210	9	-1	3	98	17	17	-3	121	9	1	8	213	10	5	-5	269	7	2
7	96	19	-4	4	195	9	14	-2	101	9	7	9	0	84	-20*	-4	68	21	-25
8	204	10	13	H,K=	3,	18		-1	216	6	-1	10	89	26	-14	-3	225	6	1
H,K=	3,	14		-3	140	13	6	0	54	58	21*	H,K=	4,	5		-2	92	12	1
-8	123	15	16	-2	107	18	3	1	619	8	26	-11	80	32	-3	-1	234	6	2
-7	218	10	-4	-1	53	89	-42*	2	0	65	-28*	-10	193	11	0	0	191	6	2
-5	162	10	8	0	68	78	38*	3	648	9	-14	-9	219	10	-5	1	102	10	-1
-4	121	12	17	1	61	85	-17*	4	66	70	58*	-8	388	8	-9	2	59	26	-22
-3	220	8	-6	2	88	21	10	5	381	7	-8	-7	283	7	-3	3	65	66	43*
-2	49	73	24*	H,K=	4,	8		6	60	76	56*	-6	311	7	3	4	123	11	4
-1	251	7	2	-12	112	20	2	7	212	9	11	-5	187	8	-5	5	0	80	-94*
0	0	78	-23*	-10	69	35	19	8	67	35	-7	-4	167	7	4	6	59	80	-57*
1	64	71	30*	-8	0	82	-18*	9	178	12	13	-3	158	7	-7	7	149	11	3
2	0	74	-38*	-6	76	85	-49*	11	90	28	3	-2	253	5	3	8	0	86	-69*
3	67	23	18	-4	387	7	10	H,K=	4,	3		-1	160	7	-6	9	163	13	-6
4	57	42	-27	-2	392	6	0	-11	124	18	5	0	243	6	-4	10	136	16	2
5	72	21	31	0	503	7	18	-10	112	18	-5	1	88	10	13	H,K=	4,	8	
6	143	13	-1	4	524	8	-2	-9	231	9	4	2	52	63	15*	-10	0	91	-57*
7	204	10	2	6	223	9	5	-8	256	8	-12	3	59	63	38*	-9	0	84	-43*
H,K=	3,	15		8	297	8	-4	-7	392	7	5	4	92	16	-22	-8	32	78	-13*
-7	63	84	35*	10	226	10	-2	-6	287	7	3	5	20	49	6*	-7	87	18	9
-6	0	82	-31*	H,K=	4,	1		-5	343	6	-2	6	172	9	2	-6	0	71	-56*
-5	90	17	6	-12	62	97	-33*	-4	175	7	6	7	69	28	-10	-5	68	72	-17*
-4	24	78	-26*	-11	124	16	9	-3	203	6	-5	8	184	10	6	-4	140	10	-15
-3	149	11	0	-10	150	14	-19	-2	28	67	-62*	9	131	14	14	-3	10	66	-1*
-2	21	77	-64*	-9	180	11	-4	-1	258	5	2	10	177	13	5	-2	249	6	-1
-1	370	7	10	-8	277	8	7	0	21	41	-4*	H,K=	4,	6		-1	103	11	-1
0	145	11	15	-7	327	7	2	1	202	6	-4	-11	96	23	6	0	479	7	10
1	400	7	14	-6	396	7	-7	2	0	44	-14*	-10	50	89	-26*	1	168	8	2
2	51	82	-32*	-5	425	7	3	3	60	66	-4*	-9	71	86	-5*	2	618	9	12
3	172	10	-2	-4	257	7	1	4	0	72	-39*	-8	41	54	11*	3	119	11	-3
4	70	79	6*	-3	396	6	1	5	176	8	2	-7	0	79	-21*	4	451	7	-9
5	182	10	11	-2	39	41	-3*	6	75	23	-0	-6	38	72	4*	5	68	76	-29*
6	104	17	7	-1	212	5	-2	7	113	15	11	-5	103	12	6	6	254	8	-1
H,K=	3,	16		0	175	6	6	8	169	12	-6	-4	0	68	-7*	7	51	77	38*
-6	216	10	8	1	0	64	-48*	9	161	12	14	-3	196	6	1	8	183	10	-3
-5	124	13	23	2	80	15	-7	10	157	15	-11	-2	46	31	13	9	45	58	32*
-4	172	10	5	3	60	23	4	H,K=	4,	4		-1	441	6	8	H,K=	4,	9	
-3	99	17	-5	4	220	7	15	-11	71	90	55*	0	105	10	-5	-10	145	14	-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
-9	126	15	-4	H,K=	4,	12		0	32	73	10*	-4	42	73	13*	H,K=	5,	5	
-8	262	8	13	-8	0	89	-23*	1	0	77	-51*	-3	391	6	-3	-10	79	29	13
-7	214	9	4	-7	91	17	30	2	0	77	-36*	-2	66	75	-25*	-9	0	88	-64*
-6	322	7	3	-6	65	81	-22*	3	39	79	2*	-1	187	7	-9	-8	0	87	-25*
-5	231	7	3	-5	66	76	36*	4	75	77	32*	0	101	11	1	-7	0	80	-21*
-4	253	7	3	-4	127	11	2	5	80	84	1*	1	117	11	-7	-6	0	84	-24*
-3	58	69	-19*	-3	111	12	1	H,K=	4,	16		2	0	72	-53*	-5	55	71	31*
-2	150	8	5	-2	155	9	-2	-4	77	80	12*	3	67	21	21	-4	136	10	-3
-1	94	13	-3	-1	18	73	-61*	-2	171	10	4	4	82	19	-6	-3	137	10	1
0	110	11	10	0	338	7	-2	-1	113	15	2	5	102	16	4	-2	274	6	0
1	188	7	10	1	140	9	12	0	243	9	-0	6	16	80	-10*	-1	178	7	-3
2	0	73	-41*	2	452	7	3	1	137	11	18	7	196	11	-3	0	213	7	-7
3	60	67	17*	3	156	10	0	2	229	9	9	8	63	42	53	1	119	11	-14
4	31	50	-6*	4	319	7	-9	3	96	18	6	9	199	12	12	2	255	6	10
5	95	16	-14	5	72	23	7	H,K=	4,	17		H,K=	5,	3		3	235	7	-12
6	94	16	-1	6	210	9	16	-1	21	80	6*	-10	69	89	13*	4	430	7	-4
7	49	76	22*	7	0	79	-59*	0	136	13	9	-9	69	82	19*	5	304	7	4
8	167	12	-3	H,K=	4,	13		H,K=	5,	0		-8	0	84	-30*	6	335	7	6
H,K=	4,	10		-8	248	10	6	-10	82	91	-1*	-7	51	76	6*	7	108	18	-21
-9	67	78	21*	-7	132	14	14	-8	195	10	5	-6	0	54	-45*	8	116	15	22
-8	0	80	-24*	-6	309	8	3	-6	472	8	-11	-5	124	12	1	9	69	31	22
-7	0	79	-23*	-5	128	12	3	-4	442	7	-7	-4	121	10	16	H,K=	5,	6	
-6	50	76	21*	-4	209	8	1	-2	208	7	15	-3	235	7	-6	-10	68	87	44*
-5	140	11	-17	-3	133	12	-7	0	143	8	-0	-2	230	7	-4	-9	183	12	4
-4	56	31	-17	-2	150	10	-2	2	97	15	-3	-1	149	8	-12	-8	73	78	44*
-3	172	8	-7	-1	40	74	-8*	4	0	82	-65*	0	217	6	-2	-7	198	10	-15
-2	61	69	-9*	0	175	8	6	6	164	11	11	1	189	7	-3	-6	23	52	11*
-1	134	10	-11	1	99	12	35	8	184	12	8	2	186	8	-16	-5	307	7	-8
0	124	9	19	2	57	73	-14*	H,K=	5,	1		3	320	6	5	-4	96	13	14
1	387	6	-8	3	66	72	54*	-10	55	85	18*	4	302	7	4	-3	357	6	-9
2	189	7	8	4	71	24	-13	-9	0	59	-43*	5	330	8	-4	-2	65	23	-21
3	480	7	-13	5	0	86	-54*	-8	0	89	-49*	6	244	9	-13	-1	227	7	-2
4	145	10	10	6	116	17	-18	-7	65	79	44*	7	238	10	-7	0	0	67	-42*
5	206	8	3	7	18	59	-31*	-6	0	84	-23*	8	82	92	-50*	1	93	14	-3
6	0	77	-39*	H,K=	4,	14		-5	118	13	15	9	107	22	-2	2	46	71	33*
7	112	14	9	-7	87	21	30	-4	127	12	-6	H,K=	5,	4		3	0	72	-11*
8	0	83	-38*	-6	54	78	43*	-3	160	8	2	-10	174	13	10	4	0	51	-8*
H,K=	4,	11		-5	116	14	3	-2	120	9	9	-9	38	83	-3*	5	108	15	4
-9	170	13	-13	-4	116	12	24	-1	172	7	6	-8	199	10	-10	6	81	22	-6
-8	116	16	-10	-3	100	16	-2	0	163	7	3	-7	0	78	-50*	7	137	11	23
-7	283	8	-3	-2	119	14	-11	1	227	6	2	-6	271	8	-22	8	49	87	-15*
-6	148	10	17	-1	204	8	-6	2	309	6	0	-5	0	76	-28*	H,K=	5,	7	
-5	361	7	-2	0	114	13	-7	3	274	8	-3	-4	431	7	0	-9	77	81	41*
-4	132	9	28	1	323	7	2	4	311	7	-3	-3	0	71	-14*	-8	38	80	-9*
-3	221	7	3	2	115	14	6	5	236	9	-12	-2	366	6	-2	-7	64	72	52*
-2	99	14	-17	3	311	7	5	6	244	9	-3	-1	79	15	-1	-6	48	69	20*
-1	0	75	-181*	4	98	17	-2	7	185	12	2	0	150	8	-1	-5	44	51	-13*
0	76	18	-1	5	248	8	5	8	203	11	17	1	32	46	-15*	-4	148	10	-25
1	106	12	11	6	95	20	-3	9	95	27	-33	2	68	68	-9*	-3	180	8	3
2	0	74	-9*	H,K=	4,	15		H,K=	5,	2		3	105	13	-13	-2	124	10	-7
3	34	71	19*	-6	105	18	6	-10	0	93	-11*	4	0	78	-35*	-1	208	7	-9
4	0	74	-6*	-5	205	9	1	-9	168	12	3	5	33	53	-18*	0	72	17	9
5	86	16	20	-4	41	56	-37*	-8	0	85	-10*	6	163	12	-12	1	179	8	-13
6	63	27	14	-3	166	10	-4	-7	294	8	-2	7	7	60	-44*	2	157	8	5
7	76	82	-17*	-2	69	74	23*	-6	40	74	13*	8	143	14	3	3	277	7	-8
8	105	18	5	-1	162	11	9	-5	464	7	-13	9	0	85	-6*	4	201	9	-12

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	307	7	7	7	128	15	7	H,K=	6,	0		2	116	13	-12	H,K=	6,	7	
6	180	11	-1	H,K=	5,	11		-8	97	22	36	3	0	77	-10*	-7	109	17	-1
7	147	13	4	-7	0	81	-2*	-6	33	84	25*	4	0	79	-8*	-6	71	75	13*
8	114	17	17	-6	0	87	-26*	-4	100	16	8	5	0	84	-13*	-5	152	11	-18
H,K=	5,	8		-5	110	15	6	-2	228	7	-8	6	86	92	-15*	-4	107	15	-19
-9	0	89	-54*	-4	44	51	18*	0	343	7	-13	7	54	92	-7*	-3	249	6	-9
-8	165	12	-2	-3	130	12	-19	2	225	8	6	H,K=	6,	4		-2	186	9	-8
-7	64	33	-5	-2	65	23	31	4	162	11	7	-8	0	60	-49*	-1	208	6	0
-6	284	8	1	-1	153	10	-4	6	357	9	14	-7	0	82	-5*	0	104	14	-13
-5	124	12	-2	0	94	15	14	H,K=	6,	1		-6	0	82	-14*	1	115	13	-6
-4	345	7	-5	1	256	7	3	-9	154	16	16	-5	63	51	59	2	58	29	44
-3	135	9	25	2	128	11	-10	-8	144	16	-13	-4	123	11	22	3	19	76	-35*
-2	264	7	-10	3	297	7	4	-7	86	100	-74*	-3	0	74	-44*	4	0	81	-5*
-1	32	47	9*	4	155	11	4	-6	130	14	-10	-2	252	7	-8	5	36	77	2*
0	172	8	-8	5	225	9	4	-5	193	9	-5	-1	30	69	16*	6	0	85	-8*
1	36	69	24*	6	119	16	-1	-4	100	16	-1	0	247	7	-2	H,K=	6,	8	
2	61	25	-0	H,K=	5,	12		-3	247	7	5	1	70	19	15	-7	0	85	-13*
3	124	11	7	-7	90	23	-4	-2	187	8	-1	2	195	8	-4	-6	0	81	-1*
4	0	54	-59*	-6	289	8	6	-1	193	8	-9	3	43	76	-7*	-5	0	78	-21*
5	68	73	49*	-5	117	14	-5	0	179	8	-6	4	255	8	10	-4	98	14	21
6	94	19	-11	-4	300	8	3	1	146	10	5	5	0	81	-24*	-3	61	75	0*
7	100	18	18	-3	66	77	-15*	2	0	78	-18*	6	236	10	-3	-2	190	9	-9
8	123	16	3	-2	167	10	6	3	39	80	-48*	7	36	84	18*	-1	105	14	-4
H,K=	5,	9		-1	94	14	30	4	0	57	-28*	H,K=	6,	5		0	260	6	-13
-8	43	55	5*	0	69	26	-18	5	68	78	43*	-8	116	18	-2	1	57	73	6*
-7	29	77	13*	1	0	80	-42*	6	0	97	-54*	-7	61	40	-12	2	229	6	-9
-6	68	77	52*	2	93	16	23	7	125	18	10	-6	121	12	27	3	55	71	13*
-5	83	19	-3	3	0	78	-3*	H,K=	6,	2		-5	131	12	0	4	205	9	6
-4	110	14	-16	4	61	76	56*	-8	44	85	21*	-4	230	8	-3	5	61	79	19*
-3	111	13	1	5	50	77	34*	-7	0	84	-28*	-3	210	8	-6	H,K=	6,	9	
-2	199	8	-0	H,K=	5,	13		-6	63	33	8	-2	264	7	-6	-6	121	16	-24
-1	57	74	-9*	-6	0	86	-25*	-5	0	73	-18*	-1	160	9	-4	-5	46	82	-35*
0	245	7	-8	-5	0	82	-6*	-4	74	20	18	0	105	14	-25	-4	162	10	2
1	115	12	-19	-4	123	15	-7	-3	128	11	3	1	86	17	-4	-3	140	11	21
2	315	7	-9	-3	58	72	34*	-2	0	72	-29*	2	56	69	6*	-2	195	6	5
3	173	10	-24	-2	164	10	2	-1	269	7	-7	3	33	75	-24*	-1	148	11	-15
4	310	7	-4	-1	43	79	-31*	0	0	73	-17*	4	47	53	36*	0	161	10	-2
5	163	10	-1	0	153	11	-4	1	289	7	-1	5	58	79	50*	1	0	77	-54*
6	237	9	-5	1	0	82	-61*	2	0	76	-58*	6	76	81	10*	2	84	19	5
7	139	13	9	2	194	10	-7	3	241	8	-1	7	88	24	25	3	0	78	-12*
H,K=	5,	10		3	49	57	-28*	4	0	82	-23*	H,K=	6,	6		4	0	82	-11*
-8	0	99	-33*	4	244	9	4	5	256	9	-9	-8	0	86	-4*	5	13	82	-30*
-7	216	10	-10	H,K=	5,	14		6	75	86	46*	-7	66	28	49	H,K=	6,	10	
-6	77	88	-14*	-4	0	83	-61*	7	268	10	9	-6	0	55	-19*	-5	0	82	-39*
-5	351	7	4	-3	259	8	16	H,K=	6,	3		-5	78	19	29	-4	0	80	-20*
-4	54	77	-18*	-2	0	82	-58*	-9	143	16	2	-4	19	73	15*	-3	62	75	-13*
-3	260	7	-0	-1	45	88	-71*	-8	124	17	11	-3	159	10	-10	-2	0	80	-63*
-2	0	72	-14*	0	24	80	-32*	-7	137	14	-1	-2	67	70	12*	-1	188	9	5
-1	172	8	1	1	63	75	18*	-6	60	82	-36*	-1	237	5	-2	0	119	12	27
0	0	74	-24*	2	0	81	-22*	-5	166	11	-12	0	50	72	2*	1	211	9	-10
1	122	12	-4	3	74	84	29*	-4	111	15	-14	1	223	5	-4	2	78	81	19*
2	39	51	-18*	H,K=	5,	15		-3	285	7	5	2	59	73	18*	3	77	86	-46*
3	0	52	-8*	-2	0	83	-55*	-2	124	12	-1	3	256	8	-2	4	0	81	-36*
4	65	26	59	-1	156	12	-6	-1	232	8	-6	4	50	80	-15*	H,K=	6,	11	
5	46	84	-42*	0	70	79	18*	0	130	10	6	5	257	9	-6	-4	32	83	-51*
6	100	16	29	1	116	16	-6	1	64	70	3*	6	0	90	-48*	-3	172	10	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
-2	104	16	3	-5	0	84	-8*												
-1	189	10	-8	-4	174	11	-8												
0	86	19	16	-3	71	75	55*												
1	130	11	18	-2	150	11	1												
2	45	79	4*	-1	0	81	-22*												
3	0	81	-27*	0	169	9	3												
H,K=	6,	12		1	69	25	49												
-3	0	83	-23*	2	118	16	-13												
-2	175	11	-4	3	36	82	34*												
-1	48	78	3*	4	0	85	-24*												
0	226	7	-4	H,K=	7,	5													
1	73	79	-10*	-5	7	83	-2*												
H,K=	7,	0		-4	60	33	18												
-6	193	12	-8	-3	49	53	18*												
-4	79	87	-27*	-2	81	20	0												
-2	162	11	-1	-1	48	79	-13*												
0	188	10	-11	0	157	10	0												
2	83	89	-8*	1	154	10	18												
4	71	82	55*	2	255	6	3												
H,K=	7,	1		3	158	12	-0												
-6	0	90	-23*	H,K=	7,	6													
-5	0	84	-16*	-4	54	81	6*												
-4	31	56	12*	-3	151	11	1												
-3	46	54	-19*	-2	0	80	-12*												
-2	51	53	-0*	-1	148	11	7												
-1	105	14	-6	0	0	78	-11*												
0	161	11	-14	1	65	91	-82*												
1	146	12	-4	2	36	55	21*												
2	182	10	-2	3	79	24	-1												
3	159	12	11	H,K=	7,	7													
4	142	14	0	-4	33	78	22*												
H,K=	7,	2		-3	75	22	28												
-6	8	59	-9*	-2	68	76	54*												
-5	165	12	-1	-1	75	77	-19*												
-4	27	79	-9*	0	114	14	6												
-3	138	12	-6	1	165	11	-2												
-2	0	80	-39*	2	149	11	11												
-1	190	9	-2	H,K=	7,	8													
0	58	75	36*	-2	149	11	-6												
1	172	10	8	-1	53	55	3*												
2	30	80	3*	0	153	11	2												
3	48	83	-24*	1	97	18	13												
4	101	16	63																
H,K=	7,	3																	
-6	58	89	27*																
-5	59	85	42*																
-4	0	80	-42*																
-3	0	80	-15*																
-2	52	78	-37*																
-1	117	12	18																
0	82	22	-23																
1	190	10	-13																
2	159	11	12																
3	182	11	-2																
4	152	13	4																
H,K=	7,	4																	

TECHNICAL INFORMATION DEPARTMENT
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