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THE CRYSTAL AND MOLECULAR STRUCTURE OF DI-IODO(BUTANE-1, 4-DIYL)BIS(DIMETHYLPHENYLPHOSPHINE)PLATINUM(IV)

Anthony K. Cheetham, Richard J. Puddephatt, Allan Zalkin, David H. Templeton and Lieselotte K. Templeton

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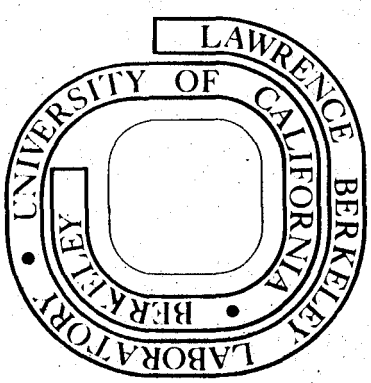

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Contribution from

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The Crystal and Molecular Structure of Di-iodo(butane-1,4-diyl)bis(dimethylphenylphosphine)platinum(IV)[1]

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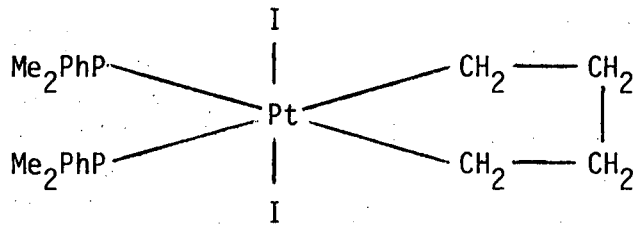
David H. Templeton and Lieselotte K. Templeton

ABSTRACT

The Pt complex $C_{20}H_{30}P_2I_2Pt$ crystallizes in the monoclinic space group C2/c with $\underline{a}$ = 15.286, $\underline{b}$ = 9.709, $\underline{c}$ = 17.036Å, β = 107.49°, $\underline{d}_c$ = 2.15 g/cm^3 for Z = 4. X-ray diffraction intensity data were collected by an automated diffractometer using graphite monochromated Mo Kα radiation. For 1575 reflections with $F^2 > 3\sigma(F^2)$; R_1 = 0.035 and R_2 = 0.044. The six-coordinate Pt atom is at the center of a distorted octahedron; the six neighbors of Pt are two phosphorus atoms at 2.418(3)Å, two iodine atoms at 2.641(1)Å, and two carbon atoms from the butanediyl ligand at 2.15(1)Å. The complex has a crystallographic two-fold axis that passes through the Pt atom.

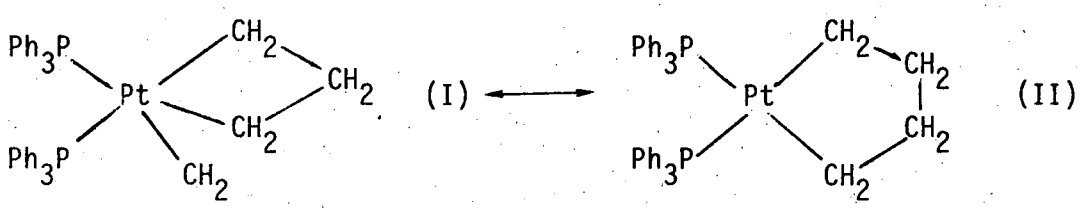
INTRODUCTION

In this paper we report the structure of a cyclic organoplatinum(IV) complex:



Metallocyclic complexes of this general form have been postulated as intermediates in several transition metal complex catalyzed reactions. For example, they may be implicated in the isomerization of strained ring carbocyclic compounds, in olefin metathesis and in cyclo-addition reactions of olefins. There is therefore a need for more information about the chemical properties and structures of these compounds.

It has previously been shown that the similar platinum(II) complex $[Pt(CH_2)_4(PPh_3)_2]$ has high thermal stability and decomposes to give mostly but-1-ene at 120°C in dichloromethane.[4] The structure of the complex[5] is of particular interest in that it shows an unsymmetrical puckering of the $Pt(CH_2)_4$ ring. This puckering was considered to be the result of a contribution to the bonding from the canonical form (I).



The platinum(IV) complex $[PtI_2(CH_2)_4(PMe_2Ph)_2]$ has no vacant stereochemical position and is already an 18-electron complex. Thus a canonical form analogous to (I) can play no part in the bonding, and a symmetrical $Pt(CH_2)_4$ ring is predicted. It was therefore

considered desirable to compare the structures of the Pt(II) and Pt(IV) complexes.

EXPERIMENTAL

The complex was isolated as orange-red crystals by reaction of (butane-1,4-diyl)bis(dimethylphenylphosphine)platinum(II) (prepared from cis-$PtCl_2(PMe_2Ph)_2$ and 1,4-dilithiobutane) with iodine. Suitable crystals were obtained by recrystallization from dichloromethane-methanol, m.p. 214°C (decomp.).

The Pt complex is air stable, and a small crystal was glued with epoxy to a pyrex glass fiber for the x-ray work. Preliminary Weissenberg photography showed the crystal to be monoclinic in space group Cc or C2/c; a successful structure determination was accomplished in C2/c. The crystal was mounted on a Picker FACS-I automated diffractometer equipped with a graphite monochromater and molybdenum tube. The cell dimensions were obtained by a least squares refinement procedure from the angular positions of 12 manually centered reflections for which $K\alpha_1$ peaks were resolved. The space group and cell dimensions are given in Table I with some other details of the experiment. Omega scans at several low angle reflections showed widths at half-peak height of 0.1°. A total of 4676 scans were measured and later averaged to give a set of 2150 unique reflections. Three standard reflections were measured after each 100th scan to monitor for crystal decay, instrumental stability and crystal alignment. After about a week of

irradiation, the standards exhibited about a 38% decay in intensity. A correction was made assuming all the reflections changed in a similar manner.

Absorption corrections were calculated using an analytical integration.[6] The crystal shape was described by eight surface planes. Azimuthal scans of integrated intensities were performed for eight different reflections in as diverse a region of reciprocal space as the instrument would allow, and the dimensions of the crystal were adjusted to fit these scans. The data were processed, averaged, and given estimated standard deviations using formulae presented in the Supplementary Material. The factor $p = 0.05$ was used in the calculation of $\sigma(F^2)$.

The Patterson function revealed the positions of the platinum, iodine and phosphorus atoms. The subsequent electron density Fourier calculated from the phases of the partial structure gave the positions of all the carbon atoms. The structure was refined by full-matrix least squares where the function $\Sigma w(|F_o|-|F_c|)^2$ was minimized. After the application of anisotropic temperature factors to all of the atoms, the central carbon atom of the butane ligand, C(2), was observed to suffer rather severe anisotropy. A ΔF Fourier calculated with only platinum and iodine in the structure showed two peaks that suggested disorder. C(2) was re-introduced into the least-squares calculation as two isotropic atoms, which were given occupancies of 1/3 atom in one position and 2/3 atoms in the second position as suggested by the peak heights in the ΔF Fourier. Least-squares refinements were performed

to convergence; i.e., the largest shift of any parameter was less than 2.4% of its estimated standard deviation. No correction for extinction was indicated, and none was made.

A ΔF Fourier showed 50 peaks that were greater than $0.5e/\mathring{A}^3$; the largest was $2e/\mathring{A}^3$. Although some of these could be interpreted as hydrogen atoms, most could not. No attempt was made to refine the hydrogen atoms.

The final R factors are as follows: $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o| = 0.035$ for the 1575 data were $F^2>3\sigma(F^2)$, and 0.054 for all 2150 data; $R_2 = [\Sigma w||F_o|-|F_c||^2/\Sigma w|F_o|^2]^{1/2} = 0.044$. The goodness of fit was 1.23.

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

Table I. Summary of Crystal Data and Intensity Collection

Compound	$[(CH_3)_2(C_6H_5)P]_2\ I_2\ Pt(CH_2CH_2CH_2CH_2)$
Formula Weight	781.307
a	15.286(6)
b	9.709(4)
c	17.036(6)
β	107.49(5)
V	2412 $Å^3$
Z	4
Density (calc)	2.152 g/cm^3
Space Group	C_{2h}^6 - C2/c
Crystal Shape and Size	Prism with 8 faces; 100, $\bar{1}00$, 110, $\bar{1}\bar{1}0$, $1\bar{1}0$, $\bar{1}10$, $\bar{1}01$, $10\bar{1}$. .06 mm x .11 mm x .14 mm
Crystal volume	0.00124 mm^3
Temperature	23°
Radiation	Mo $K\alpha_1$ (λ 0.70926 Å), monochromated from (002) face of mosaic graphite
Transmission Factors	.42 to .65
μ	81 cm^{-1}
Data Collection Method	θ-2θ scan (1°/min along 2θ)
Scan range	.75° below $K\alpha_1$ to .75 above $K\alpha_2$
Background Counts	4 sec. Background offset from scan limits by 0.5°
2θ Limits	5.0 - 50.0°
Final No. of variables	113
Unique Data Used $F_o^2 > 3\sigma(F_o^2)$	1575

Table II. Atomic Parameters and Standard Deviations[a]

ATOM	B11	B22	B33	B12	B13	B23
Pt	2.70(2)	2.00(2)	2.38(2)	0	.53(2)	0
I	6.39(5)	9.49(6)	5.05(4)	-2.66(4)	3.31(4)	-.22(4)
P	3.0(1)	2.4(1)	4.3(1)	.08(8)	.5(1)	.10(8)
C(1)	6.4(6)	1.8(4)	4.8(5)	-.3(4)	-1.3(5)	.4(3)
C(2)1	4.6(3)					
C(2)2	4.3(6)					
C(3)	6.1(7)	6.1(6)	6.8(8)	-1.2(5)	1.3(6)	3.8(5)
C(4)	5.3(7)	3.8(5)	9.1(9)	1.6(4)	.2(6)	-3.1(5)
C(5)	2.9(4)	2.5(4)	3.5(4)	.5(3)	-.0(3)	.4(3)
C(6)	3.7(5)	3.9(5)	3.9(5)	.2(4)	.7(4)	.2(4)
C(7)	6.1(7)	4.1(5)	4.2(5)	1.0(5)	-.7(5)	-.6(4)
C(8)	3.4(5)	4.5(5)	6.0(7)	-.1(4)	-.1(5)	.5(5)
C(9)	3.6(5)	5.6(6)	5.8(6)	-.2(4)	.8(5)	-.2(5)
C(10)	2.5(4)	4.9(6)	5.8(6)	-.2(3)	1.0(4)	.5(4)

ATOM	X	Y	Z
Pt	0	.02752(5)	.250
I	.10150(6)	.0403(1)	.14920(5)
P	.1045(2)	-.1383(2)	.3350(2)
C(1)	.0824(9)	.1941(9)	.3166(7)
C(2)1	.051(1)	.326(2)	.267(1)
C(2)2	.015(3)	.327(3)	.299(2)
C(3)	.067(1)	-.232(1)	.4118(9)
C(4)	.1424(9)	-.279(1)	.2813(9)
C(5)	.2101(6)	-.0599(8)	.3969(6)
C(6)	.2112(7)	.005(1)	.4702(6)
C(7)	.2920(9)	.077(1)	.5152(7)
C(8)	.3671(8)	.081(1)	.4866(8)
C(9)	.3668(8)	.015(1)	.4152(8)
C(10)	.2869(7)	-.057(1)	.3694(7)

[a]The temperature factor has the form $\exp[-0.25(h^2a^{*2}B_{11} + \ldots + 2hka^*b^*B_{12} + \ldots)]$. C(2)1 and C(2)2 represent the disordered sites of C(2); the site occupancies are 2/3 and 1/3 atoms respectively. The disordered atoms have isotropic thermal parameters.

Table III. Interatomic Distances[a]

Pt	-2	C(1)	2.15(1)
	-2	P	2.418(3)
	-2	I	2.641(1)
P	-	C(3)	1.82(1)
	-	C(4)	1.83(1)
	-	C(5)	1.81(1)
C(1)	-	C(2)1	1.54(2)[b]
	-	C(2)2	1.62(4)[b]
C(2)1	-	C(2)1	1.49(4)[b]
C(2)2	-	C(2)2	1.60(7)[b]
C(5)	-	C(6)	1.40(2)
C(5)	-	C(10)	1.39(2)
C(6)	-	C(7)	1.42(2)
C(7)	-	C(8)	1.38(2)
C(8)	-	C(9)	1.37(2)
C(9)	-	C(10)	1.42(2)

[a]Uncorrected for thermal motion

[b]C(2)1 and C(2)2 represent the two sites of the C(2) atom

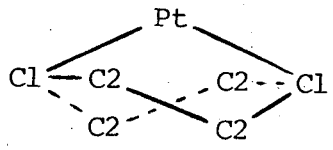
Table IV. Selected Angles

I	-Pt	-I	174.63(5)
I	-Pt	-P	90.55(5)
I	-Pt	-P	93.03(7)
I	-Pt	-C(1)	86.7(4)
I	-Pt	-C(1)	89.3(4)
P	-Pt	-P	96.6(2)
P	-Pt	-C(1)	90.5(3)
P	-Pt	-C(1)	173.0(3)
C(1)	-Pt	-C(1)	82.6(5)
Pt	-P	-C(3)	118.1(5)
Pt	-P	-C(4)	116.6(5)
Pt	-P	-C(5)	112.5(3)
C(3)	-P	-C(4)	101.5(7)
C(3)	-P	-C(5)	102.2(6)
C(4)	-P	-C(5)	104.1(5)
Pt	-C(1)	-C(2)1	107.4(9)
Pt	-C(1)	-C(2)2	105.4(13)
C(1)-C(2)1		-C(2)1	80.6(5)
C(1)-C(2)2		-C(2)2	81.6(9)
P	-C(5)	-C(6)	118.7(8)
P	-C(5)	-C(10)	120.6(8)
C(6)-C(5)		-C(10)	120.6(9)
C(5)-C(6)		-C(7)	118.5(11)
C(6)-C(7)		-C(8)	120.4(11)
C(7)-C(8)		-C(9)	121.2(11)
C(8)-C(9)		-C(10)	119.3(12)
C(9)-C(10)		-C(5)	120.0(11)

DISCUSSION

The neutral molecular complex consists of a Pt atom at the center of a distorted octahedron, as shown in Fig. 1. Platinum, on a two-fold axis, is bonded to two phosphorus, two iodine, and two carbon atoms. The maximum distortion from an ideal octahedron is in the C(1)-Pt-C(1) angle of 82.6°, which is a result of the closed ring made with the butanediyl ligand.

The disorder observed in the butanediyl ligand is a result of the two central carbon atoms alternating between the two forms indicated schematically below:



This puckering of the ring relieves the crowding of the hydrogen atoms on adjacent carbon atoms, and the two conformations are equivalent as far as the immediate neighbors of platinum are concerned. They are not equivalent when one considers the relation to the phenyl rings or the neighboring molecules. The Fourier patterns indicated a predominance of one form over the other of about 2 to 1. Upon refinement of least squares using the indicated occupancy factors, the resulting isotropic thermal parameters are statistically equal. The dominant form is presented in Fig. 1. The anisotropy of the thermal parameters of C(1) are probably more representative of a minor disorder than a large thermal effect. Any disorder in the C(2) would be expected to carry over to C(1) and possibly to other parts of the structure nearby. The disorder does not seriously affect the gross geometrical interpretation, but

does make the bond distances and angles in the region of the disorder less reliable. Interpretation of thermal parameters for the atoms adjacent to the disorder is ambiguous as it is not possible to separate out the disorder effects from the thermal effects. For the puckering of the ring we detect no lack of symmetry with respect to the platinum atom, in contrast to the result reported for the Pt(II) complex.[5] By virtue of the two-fold axis, each configuration is found to be exactly symmetrical, and the Pt-C(2) distances in the two forms, 3.00 and 3.02Å, are equal within the experimental precision. But because of the disorder, one cannot exclude the possibility of a mixture of slightly unsymmetrical configurations.

Acknowledgement: We thank Professor Neil Bartlett for his assistance in the arrangements for this work.

Supplementary Material Available: Data processing formulae (1 page) and a table of observed structure factors (8 pages). Ordering information is given on any current masthead page.

REFERENCES

1. This report was done with support from the United States Energy Research and Development Administration. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the United States Energy Research and Development Administration.
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FIGURES

Figure 1: Stereogram of the molecular structure. Only one form of the disorder in C(2) is shown.

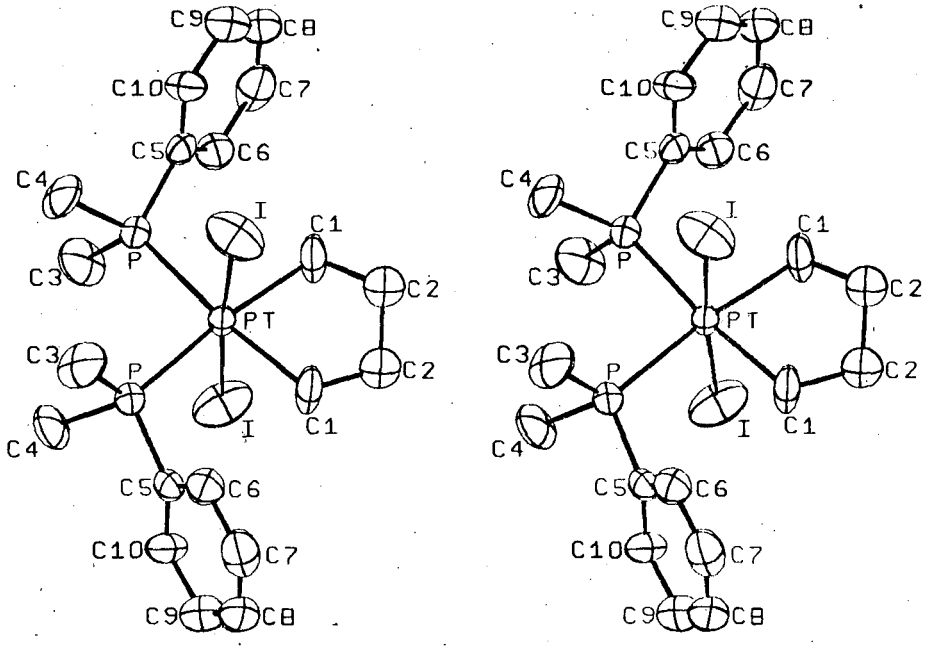

Fig. 1

XBL 764-1138

Supplementary Material for the paper: The Crystal and Molecular Structure of Di-iodo(butane-1,4-diyl)bis(dimethyl-phenylphosphine) platinum(IV) by Anthony K. Cheetham, Richard J. Puddephatt, Allan Zalkin, David H. Templeton and Lieselotte K. Templeton.

The Supplementary Tables which follow contain these data:

1. Data processing formulae
2. Table of observed structure factors (FOB), their estimated standard devisations (SG), and differences (DEL=$|F_o|-|F_c|$).

DATA PROCESSING FORMULAE

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

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

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

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

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

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

$$\sigma(F_a^2) = [\Sigma\sigma^2(F^2)/n]^{\frac{1}{2}}$$ 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 2.0)
C(20)H(30)P(2)I(2)PT F(0,0,0) = 2645

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	1	598	15	-3	-9	186	5	-18	5	63	8	1	-13	130	7	-13
2	913	23	112	2	267	7	5	-8	731	19	16	6	158	4	-3	-12	90	9	-9
4	68	11	-6	3	301	11	10	-7	119	5	-9	7	68	7	7	-11	224	8	1
6	98	10	-15	4	160	6	5	-6	214	6	16	8	263	7	8	-10	82	7	-1
8	621	16	34	5	60	9	19	-5	55	12	-12*	9	197	5	1	-9	324	8	14
10	661	17	-19	6	126	4	6	-4	282	7	5	10	340	9	11	-8	45	27	15*
12	433	11	-24	7	119	4	-2	-3	109	3	-4	11	264	7	-7	-7	312	9	7
14	128	14	-0	8	84	6	6	-2	781	26	60	12	299	8	8	-6	72	9	-4
16	67	13	-4*	9	340	9	0	-1	59	11	13*	13	98	12	-7	-5	185	5	1
18	177	8	-8	10	180	6	3	0	1170	41	-12	14	159	8	-5	-4	183	5	14
H,K=		0,	2	11	333	9	2	1	275	9	15	15	33	2	-15*	-3	218	6	3
0	1169	47	-40	12	123	5	-7	2	929	29	2	16	108	8	-11	-2	171	6	1
1	240	6	8	13	176	5	2	3	449	13	29	17	66	25	2*	-1	403	10	4
2	363	9	-22	14	101	6	-7	4	287	8	8	18	128	10	-3	0	148	6	-5
3	139	4	-3	15	90	8	2	5	59	10	17	H,K=		1,	5	1	505	13	1
4	63	9	5	16	52	11	-15*	6	75	6	-10	-17	128	9	1	2	80	8	-11
5	21	2	-6*	H,K=		0,	8	7	25	2	14*	-16	99	15	-8	3	347	9	10
6	85	4	3	0	41	14	20*	8	292	8	22	-15	105	6	8	4	88	5	1
7	142	5	22	1	282	8	1	9	52	24	-23*	-14	94	10	-15	5	151	5	-2
8	602	15	19	2	53	8	0	10	638	16	-4	-13	129	7	11	6	15	2	-3*
9	227	6	-11	3	221	6	8	11	30	27	-52*	-12	113	8	-7	7	140	5	-2
10	576	15	-11	4	57	10	-4	12	506	13	-1	-11	264	7	0	8	133	5	-3
11	130	7	-15	5	226	6	2	13	0	2	-42*	-10	212	6	0	9	267	7	1
12	305	9	-4	6	47	35	2*	14	196	6	12	-9	384	10	4	10	105	10	3
13	32	2	18*	7	246	7	-3	15	54	11	2*	-8	259	7	-1	11	262	8	-1
14	108	8	-4	8	44	10	34*	16	69	10	8	-7	219	7	5	12	74	11	-3
15	21	2	2*	9	245	7	-5	17	25	2	-13*	-6	223	6	-8	13	187	7	2
16	99	9	-1	10	74	6	17	18	125	6	-8	-5	79	7	11	14	29	2	-14*
17	76	15	-6*	11	210	6	5	H,K=		1,	3	-4	134	5	1	15	96	10	-8
18	187	6	0	12	69	9	8	-19	122	17	-7	-3	63	5	3	H,K=		1,	9
19	80	10	-11	13	144	8	5	-18	197	11	4	-2	164	5	-0	-12	36	2	23*
H,K=		0,	4	H,K=		0,	10	-17	101	15	-13	-1	443	11	-15	-11	165	6	3
0	571	15	-14	0	89	10	-1	-16	142	6	-2	0	322	8	-8	-10	13	2	-3*
1	543	14	-18	1	204	6	-6	-15	8	2	-12*	1	605	15	-11	-9	246	7	-3
2	343	10	-0	2	74	7	14	-14	65	10	-3	2	276	7	-20	-8	45	22	2*
3	225	8	18	3	205	6	8	-13	29	2	12*	3	404	10	3	-7	284	8	-2
4	215	8	12	4	30	2	-4*	-12	104	6	-6	4	319	8	-2	-6	52	11	21*
5	49	4	26	5	217	6	6	-11	157	5	-11	5	106	9	-3	-5	201	7	-2
6	344	9	12	6	24	2	19*	-10	509	13	8	6	103	6	-7	-4	39	19	9*
7	155	5	8	7	208	7	1	-9	423	11	-18	7	67	7	-1	-3	168	6	-1
8	342	9	7	8	53	19	9*	-8	693	18	4	8	189	5	4	-2	30	2	25*
9	384	10	-8	9	168	8	-7	-7	391	10	-2	9	372	10	-3	-1	150	5	-7
10	306	8	5	H,K=		1,	1	-6	409	10	2	10	199	8	5	0	38	20	17*
11	356	9	-5	-19	47	36	-19*	-5	146	4	14	11	402	10	13	1	244	7	-10
12	167	9	-7	-18	218	7	-2	-4	68	10	9	12	205	6	4	2	36	13	25*
13	116	7	3	-17	55	30	-14*	-3	271	7	21	13	177	6	-0	3	277	8	-3
14	105	5	-9	-16	175	6	-1	-2	343	9	26	14	108	8	-20	4	20	2	-13*
15	37	31	6*	-15	18	2	11*	-1	400	10	29	15	72	9	2	5	279	8	2
16	92	8	-12	-14	109	5	3	0	645	17	5	16	105	7	-8	6	16	2	6*
17	72	20	-14*	-13	41	13	-11*	1	554	14	-9	17	66	12	1*	7	183	6	-1
18	169	7	17	-12	204	6	-3	2	726	20	-11	H,K=		1,	7	8	34	2	6*
H,K=		0,	6	-11	12	2	-19*	3	501	13	-5	-15	104	9	-22	9	172	6	-5
0	237	6	8	-10	677	17	11	4	583	16	28	-14	97	8	-6	10	28	2	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
11	146	6	7	3	293	9	-54	-14	97	7	-2	12	38	2	26*	14	252	7	7
H,K=		1,	11	4	672	19	-7	-13	113	6	-1	13	178	7	5	15	45	2	-16*
-6	41	2	30*	5	104	4	-13	-12	111	8	-4	H,K=		2,	10	16	171	9	6
-5	134	6	8	6	140	5	-6	-11	151	5	-3	-10	35	2	14*	17	39	29	32*
-4	26	2	-11*	7	86	6	-18	-10	105	7	-0	-9	197	9	-13	18	79	16	-14*
-3	162	6	-10	8	139	5	-4	-9	315	8	11	-8	44	33	12*	H,K=		3,	3
-2	83	11	-1	9	55	7	5	-8	99	5	-4	-7	208	8	-2	-19	105	8	17
-1	179	10	-5	10	375	10	10	-7	378	10	11	-6	0	2	-9*	-18	179	10	-6
0	111	7	3	11	98	7	-17	-6	199	6	8	-5	203	7	3	-17	140	15	-3
1	162	7	-8	12	439	11	13	-5	273	7	-2	-4	52	2	19*	-16	241	7	2
2	74	8	23	13	188	7	-4	-4	259	7	10	-3	159	12	5	-15	131	6	-3
3	147	6	2	14	239	7	-2	-3	201	6	7	-2	41	23	8*	-14	159	6	3
4	17	2	-1*	15	72	13	-20*	-2	237	6	12	-1	170	7	3	-13	52	9	21
5	153	6	-1	16	99	15	-19	-1	321	9	-3	0	55	17	14*	-12	118	7	-10
H,K=		2,	0	17	41	24	2*	0	240	7	13	1	207	6	-1	-11	0	2	-25*
-18	269	9	3	18	75	35	-24*	1	484	12	-9	2	38	22	12*	-10	255	7	-13
-16	343	10	14	H,K=		2,	4	2	195	5	-0	3	268	8	-5	-9	297	8	-12
-14	153	7	12	-18	164	7	7	3	326	8	11	4	56	11	20*	-8	646	16	5
-12	82	8	-9	-17	160	12	-12	4	135	5	5	5	194	6	7	-7	528	13	-8
-10	440	11	7	-16	160	6	1	5	111	6	10	6	32	2	19*	-6	646	16	-6
-8	771	20	6	-15	107	7	1	6	127	4	2	7	157	8	5	-5	165	5	-6
-6	873	22	58	-14	64	9	-12	7	143	5	-2	8	43	25	19*	-4	180	5	-15
-4	215	6	-10	-13	63	6	16	8	210	7	7	H,K=		3,	1	-3	165	5	-1
-2	487	13	40	-12	87	11	-21	9	254	7	1	-20	90	10	5	-2	63	4	-10
0	714	18	11	-11	130	5	-2	10	122	5	8	-19	22	2	-20*	-1	32	18	13*
21	120	28	-131	-10	311	8	-7	11	269	8	-4	-18	273	10	3	0	347	9	6
4	443	11	-17	-9	357	9	-10	12	124	8	5	-17	0	2	-58*	1	305	8	-15
6	39	33	-4*	-8	504	13	-14	13	219	7	4	-16	395	11	22	2	884	23	21
8	97	6	23	-7	496	13	-4	14	87	8	-3	-15	31	2	7*	3	465	12	-32
10	525	14	9	-6	467	12	5	15	118	9	10	-14	235	8	19	4	669	19	-3
12	552	14	14	-5	130	4	-1	H,K=		2,	8	-13	26	2	-9*	5	329	9	-18
14	237	7	19	-4	72	4	-15	-14	65	14	-4*	-12	30	22	-2*	6	263	7	-7
16	74	16	-1*	-3	85	3	11	-13	122	6	14	-11	30	2	6*	7	39	11	0*
18	104	13	4	-2	46	5	-3	-12	74	29	3*	-10	95	11	-5	8	29	16	-6*
H,K=		2,	2	-1	214	6	-3	-11	172	6	0	-9	162	5	-1	9	60	6	3
-19	85	27	-12*	0	328	8	-2	-10	0	2	-9*	-8	752	20	-1	10	161	5	-2
-18	226	10	-2	1	738	19	13	-9	280	8	1	-7	199	5	-24	11	171	8	-16
-17	88	17	-24*	2	631	16	-2	-8	27	2	4*	-6	1002	26	2	12	304	9	2
-16	257	7	-1	3	441	11	12	-7	319	8	4	-5	151	4	8	13	223	7	-5
-15	0	2	-16*	4	461	12	-10	-6	38	2	10*	-4	435	13	-24	14	262	9	5
-14	84	9	13	5	210	6	7	-5	226	8	1	-3	29	2	8*	15	108	9	-6
-13	62	9	-14	6	171	5	-5	-4	92	5	15	-2	199	5	0	16	160	6	4
-12	78	5	3	7	69	5	9	-3	103	7	3	-1	44	14	6*	17	31	2	-8*
-11	55	7	-7	8	73	14	-17*	-2	106	10	4	0	397	11	37	H,K=		3,	5
-10	471	12	3	9	219	6	-3	-1	209	7	-4	1	395	10	26	-18	105	9	7
-9	340	9	-16	10	152	7	5	0	47	24	-5*	2	855	25	-8	-17	195	10	-4
-8	689	17	-2	11	236	7	-2	1	327	9	-7	3	352	9	-2	-16	132	11	4
-7	470	12	12	12	290	8	14	2	54	9	19	4	831	23	-18	-15	210	8	0
-6	607	15	19	13	213	6	11	3	393	10	-1	5	74	13	-22	-14	113	9	0
-5	32	18	11*	14	196	7	-3	4	41	2	19*	6	275	8	7	-13	82	7	-5
-4	68	9	11	15	80	9	7	5	257	7	1	7	45	13	-18*	-12	114	8	-14
-3	241	6	-27	16	120	8	-14	6	98	5	12	8	151	5	3	-11	18	2	-17*
-2	95	7	15	17	51	24	1*	7	187	6	-5	9	52	12	-4*	-10	111	5	2
-1	107	4	-3	H,K=		2,	6	8	136	6	12	10	298	8	4	-9	206	6	1
0	361	9	-9	-17	176	8	5	9	147	6	0	11	36	2	-32*	-8	265	7	-3
1	610	16	4	-16	103	11	1	10	43	21	21*	12	413	11	7	-7	475	12	-4
21	258	33	-13	-15	162	6	-3	11	195	7	-3	13	116	10	-9	-6	324	8	-6

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	426	11	2	-10	0	2	-19*	-16	339	9	16	3	594	15	-1	-5	268	7	1
-4	187	6	8	-9	235	8	0	-15	126	8	-14	4	462	12	-4	-4	83	7	-12
-3	184	5	8	-8	34	2	23*	-14	324	9	14	5	424	11	-1	-3	241	7	-1
-2	244	6	16	-7	254	8	-5	-13	67	13	14*	6	251	7	5	-2	94	6	4
-1	108	4	4	-6	30	2	9*	-12	117	7	-4	7	127	5	2	-1	199	6	-1
0	184	5	-6	-5	198	6	2	-11	15	2	-2*	8	88	9	-18	0	19	2	9*
1	298	8	-4	-4	24	2	8*	-10	62	5	-8	9	32	2	7*	1	266	7	-11
2	328	8	-16	-3	130	10	1	-9	131	5	5	10	162	6	-8	2	12	2	-18*
3	420	11	-1	-2	92	7	9	-8	472	12	0	11	138	5	-8	3	311	9	-11
4	259	7	-10	-1	170	6	-3	-7	267	7	-5	12	218	7	6	4	55	9	-6
5	375	10	10	0	52	10	30*	-6	780	20	8	13	139	7	-7	5	292	8	6
6	279	8	-6	1	287	8	-8	-5	208	6	-28	14	206	7	-7	6	81	9	-8
7	191	7	-4	2	47	15	12*	-4	727	19	31	15	136	9	3	7	151	8	10
8	63	7	-6	3	326	9	-7	-3	49	8	6	16	128	9	1	8	81	10	19
9	141	6	-5	4	16	2	2*	-2	60	11	0	H,K=	4,	6	9	137	6	-11	
10	169	5	0	5	249	9	4	-1	93	7	14	-17	195	7	3	10	56	28	18*
11	211	6	-7	6	62	11	-1*	0	180	6	30	-16	112	7	14	11	148	7	-4
12	181	7	13	7	147	8	8	1	129	4	0	-15	255	8	6	H,K=	4,	10	
13	209	7	6	8	14	2	11*	2	726	21	37	-14	118	7	-0	-10	12	2	-1*
14	163	9	3	9	120	10	4	3	474	14	4	-13	134	6	7	-9	152	12	-9
15	116	10	3	10	25	2	21*	4	733	20	-14	-12	86	7	-13	-8	48	15	24*
16	95	10	-2	H,K=	3,	11	5	175	5	-4	-11	23	2	-10*	-7	155	9	-2	
H,K=	3,	7	-6	72	12	-10	6	476	14	-4	-10	94	9	2	-6	97	18	18	
-16	95	8	16	-5	161	15	-6	7	22	2	3*	-9	157	5	7	-5	167	6	-1
-15	183	7	0	-4	91	12	8	8	143	5	-3	-8	137	8	-8	-4	58	13	12*
-14	104	8	13	-3	162	9	-5	9	36	18	-13*	-7	410	11	-8	-3	182	7	5
-13	133	9	-2	-2	57	13	-9*	10	136	6	-2	-6	186	6	-18	-2	33	2	28*
-12	98	8	1	-1	156	7	5	11	177	7	-5	-5	539	14	5	-1	187	7	12
-11	122	11	13	0	33	2	-8*	12	199	7	-15	-4	325	8	-6	0	40	2	35*
-10	21	2	-7*	1	143	12	-10	13	158	7	-15	-3	307	8	6	1	230	8	1
-9	236	8	0	2	54	14	4*	14	313	9	3	-2	201	6	3	2	32	2	8*
-8	34	2	-7*	3	153	6	-0	15	92	15	-8	-1	30	14	-4*	3	190	6	-5
-7	392	10	-2	4	72	12	18	16	174	8	-0	0	117	4	10	4	53	20	2*
-6	103	8	-3	H,K=	4,	0	17	24	2	9*	1	89	6	-3	5	167	7	-5	
-5	341	9	9	-20	71	2	1*	H,K=	4,	4	2	91	7	7	6	65	17	11*	
-4	182	5	4	-18	235	11	3	-19	59	15	-6*	3	377	10	-0	7	126	12	-1
-3	234	7	9	-16	442	12	8	-18	116	12	13	4	190	5	-0	H,K=	5,	1	
-2	226	6	15	-14	401	11	25	-17	161	9	-16	5	417	11	7	-20	65	23	10*
-1	219	6	6	-12	57	17	22*	-16	175	6	3	6	182	6	-2	-19	43	39	33*
0	43	9	23*	-10	111	9	-1	-15	254	8	-6	7	263	7	12	-18	116	8	-8
1	290	8	-2	-8	620	16	-3	-14	231	7	3	8	153	5	-6	-17	26	2	-13*
2	28	2	11*	-6	1089	28	-28	-13	123	5	13	9	141	8	-7	-16	347	10	12
3	350	10	5	-4	868	22	-61	-12	170	7	5	10	103	8	1	-15	26	2	-56*
4	34	15	17*	-2	62	2	-20*	-11	37	20	-6*	11	162	7	-3	-14	478	13	24
5	316	9	8	0	237	7	12	-10	148	5	-7	12	61	2	-2*	-13	85	19	-19*
6	210	7	-10	2	436	12	-2	-9	133	7	2	13	173	8	9	-12	207	7	9
7	171	6	0	4	797	20	-45	-8	328	8	3	14	70	31	4*	-11	58	6	8
8	125	6	9	6	638	16	-14	-7	479	12	-9	H,K=	4,	8	-18	98	4	9	
9	127	7	-7	8	205	6	5	-6	294	8	-14	-14	43	23	-0*	-9	0	2	-5*
10	91	8	7	10	179	6	-2	-5	538	14	1	-13	175	6	2	-8	231	7	10
11	199	7	-7	12	208	11	9	-4	328	9	-9	-12	0	2	-19*	-7	66	9	-23
12	25	2	-2*	14	314	9	6	-3	209	6	-5	-11	152	8	3	-6	967	25	16
13	195	7	2	16	197	10	9	-2	181	5	3	-10	0	2	-20*	-5	270	7	0
14	39	2	-2*	H,K=	4,	2	-1	35	12	10*	-9	196	6	-6	-4	1031	28	-13	
H,K=	3,	9	-19	29	2	6*	0	212	6	-3	-8	44	13	24*	-3	146	5	-23	
-12	52	25	20*	-18	167	7	-5	1	129	5	4	-7	265	8	-5	-2	212	6	-8
-11	182	6	-4	-17	59	30	-21*	2	365	9	3	-6	42	26	35*	-1	18	2	-16*

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
0	117	5	-10	-16	98	9	1	9	156	6	3	-17	41	22	17*	4	222	7	8
1	132	4	8	-15	233	8	-3	10	40	2	-3*	-16	201	12	-4	5	336	9	-3
2	214	6	20	-14	181	6	-3	11	121	6	-8	-15	141	8	-20	6	290	8	8
3	38	15	3*	-13	183	6	3	12	43	2	21*	-14	480	13	10	7	255	8	-0
4	767	21	8	-12	175	6	0	H,K=		5,	9	-13	234	7	-9	8	276	8	-5
5	4	2	-26*	-11	40	15	6*	-12	26	2	19*	-12	383	10	1	9	96	6	6
6	771	23	7	-10	158	5	5	-11	182	7	-5	-11	80	9	-5	10	211	6	-8
7	0	2	-12*	-9	70	14	0*	-10	54	14	8*	-10	91	4	-2	11	45	22	18*
8	286	8	12	-8	122	5	0	-9	132	8	-2	-9	139	5	-0	12	139	7	-3
9	45	10	12*	-7	363	10	-10	-8	19	2	8*	-8	48	8	7	13	89	11	-13
10	59	13	-6*	-6	252	7	6	-7	148	9	3	-7	52	15	5*	14	88	22	-13*
11	45	13	5*	-5	625	16	-5	-6	26	2	4*	-6	532	15	17	15	142	8	-7
12	146	6	-20	-4	355	9	-1	-5	199	6	-4	-5	332	9	10	H,K=		6,	6
13	36	2	-36*	-3	328	9	7	-4	0	2	-4*	-4	743	20	11	-17	101	9	-3
14	282	8	-4	-2	275	7	7	-3	232	9	3	-3	387	10	1	-16	56	28	0*
15	36	2	16*	-1	63	6	2	-2	9	2	-17*	-2	625	18	-10	-15	168	7	-5
16	189	14	5	0	217	6	2	-1	262	9	2	-1	153	4	-14	-14	64	15	-11*
H,K=		5,	3	1	69	7	1	0	43	2	-5*	0	187	5	4	-13	221	7	-1
-19	25	2	14*	2	114	4	-3	1	236	8	-2	1	15	2	-20*	-12	142	11	-9
-18	81	17	-5*	3	339	9	-7	2	9	2	6*	2	63	7	12	-11	168	6	6
-17	113	7	-3	4	233	6	13	3	202	7	-7	3	30	2	5*	-10	151	6	4
-16	221	10	-7	5	467	12	1	4	39	22	22*	4	439	11	6	-9	95	7	5
-15	217	7	-6	6	209	6	11	5	156	9	-7	5	160	5	-15	-8	143	5	9
-14	391	10	13	7	289	8	6	6	57	12	15*	6	480	12	-3	-7	232	8	1
-13	203	6	8	8	211	8	-7	7	166	7	-4	7	203	7	-12	-6	155	5	0
-12	284	8	-6	9	126	7	6	8	13	2	-0*	8	347	9	14	-5	429	11	-2
-11	20	2	4*	10	134	6	-8	9	144	9	6	9	135	11	-4	-4	127	8	-7
-10	108	4	-1	11	36	2	-14*	H,K=		5,	11	10	132	11	-0	-3	363	9	10
-9	20	2	4*	12	136	7	11	-4	99	7	23	11	56	12	-14*	-2	170	5	-1
-8	89	4	0	13	116	13	-14	-3	148	7	-13	12	172	7	-14	-1	157	5	15
-7	192	6	-0	14	119	6	15	-2	46	22	8*	13	52	17	-13*	0	142	5	-3
-6	448	11	-5	H,K=		5,	7	-1	153	7	4	14	151	9	-11	1	87	9	-3
-5	403	10	1	-16	0	2	-49*	0	29	2	20*	15	10	2	-45*	2	109	9	-1
-4	634	17	-19	-15	207	14	3	1	137	6	10	H,K=		6,	4	3	242	7	-4
-3	287	8	-4	-14	16	2	-21*	H,K=		6,	0	-19	60	33	21*	4	118	6	10
-2	342	9	-10	-13	184	8	2	-20	85	48	0*	-18	19	2	-19*	5	401	10	2
-1	16	2	-5*	-12	54	11	10*	-18	68	35	6*	-17	77	10	-3	6	159	6	2
0	298	8	15	-11	113	7	-7	-16	232	7	-2	-16	131	6	-3	7	343	9	20
1	122	4	18	-10	103	5	0	-14	523	14	18	-15	200	11	-15	8	118	8	-11
2	285	8	5	-9	138	5	-4	-12	323	9	15	-14	305	8	11	9	140	6	-1
3	317	8	3	-8	61	8	0	-10	50	27	-24*	-13	285	8	-2	10	74	15	-11*
4	427	11	-13	-7	272	8	-3	-8	106	12	-1	-12	293	8	-2	11	67	16	-1*
5	351	9	-9	-6	85	9	-12	-6	718	18	9	-11	132	8	13	12	49	17	7*
6	390	13	0	-5	422	11	-2	-4	842	21	-34	-10	132	5	-6	13	101	11	-13
7	102	6	1	-4	128	5	-3	-2	608	16	-12	-9	43	16	13*	H,K=		6,	8
8	201	6	-5	-3	341	9	11	0	101	9	18	-8	50	8	18	-14	0	2	-22*
9	100	7	-3	-2	65	10	13	2	55	9	9	-7	175	5	10	-13	227	7	0
10	99	6	-19	-1	172	6	11	4	765	20	3	-6	194	5	-2	-12	21	2	-2*
11	65	10	-19	0	78	11	-3	6	644	16	-13	-5	481	12	-2	-11	186	6	0
12	199	7	-0	1	131	7	-9	8	375	10	13	-4	453	13	7	-10	68	12	-12
13	132	7	-13	2	54	24	-3*	10	74	11	5	-3	451	12	-11	-9	119	12	-8
14	220	7	1	3	279	8	-2	12	136	7	-13	-2	570	14	-6	-8	85	8	9
15	86	14	-19	4	123	5	-3	14	162	15	-2	-1	155	5	5	-7	148	5	-4
16	115	17	-12	5	330	9	12	16	204	23	-15	0	263	7	-1	-6	44	2	11*
H,K=		5,	5	6	118	6	-5	H,K=		6,	2	1	27	2	-0*	-5	240	7	-13
-18	61	21	-11*	7	258	7	8	-19	0	2	-25*	2	93	5	-6	-4	43	11	36*
-17	184	10	10	8	127	12	-12	-18	27	2	-20*	3	185	6	4	-3	343	9	7

STRUCTURE FACTORS CONTINUED FOR
C(20)H(30)P(2)I(2)PT

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	18	2	-12*	7	149	6	-9	-6	117	5	5	-3	287	8	-5	7	229	8	-5
-1	292	8	9	8	409	11	11	-5	277	8	-1	-2	37	2	23*	8	362	10	8
0	72	11	2	9	71	12	-1	-4	220	6	-3	-1	276	8	5	9	172	11	8
1	160	5	-4	10	213	8	13	-3	371	10	6	0	40	24	35*	10	266	8	10
2	94	6	12	11	47	23	17*	-2	331	9	1	1	169	10	5	11	29	2	-9*
3	150	8	-8	12	107	7	-2	-1	244	7	13	2	40	19	7*	12	129	7	-4
4	58	11	1*	13	0	2	-6*	0	180	5	-8	3	97	10	-12	13	22	2	11*
5	199	6	-0	14	140	15	-14	1	126	5	1	4	12	2	-8*	14	95	11	-27
6	30	2	-5*	15	32	2	22*	2	136	6	0	5	130	6	-7	H,K=		8,	4
7	210	7	2	H,K=		7,	3	3	164	5	-10	6	60	15	38*	-18	99	7	4
8	43	20	11*	-19	19	2	8*	4	105	8	-2	7	176	8	1	-17	0	2	-13*
9	170	8	-8	-18	25	2	-23*	5	283	8	-6	H,K=		8,	0	-16	90	7	1
10	33	2	11*	-17	14	2	-1*	6	184	6	5	-20	211	12	15	-15	90	9	3
H,K=		6,	10	-16	137	9	-3	7	288	8	2	-18	42	2	-13*	-14	150	6	6
-9	114	13	0	-15	170	7	-11	8	243	7	1	-16	33	2	3*	-13	274	8	2
-8	36	2	-6*	-14	307	8	3	9	122	16	12	-14	193	8	-7	-12	278	8	3
-7	119	7	-1	-13	294	8	3	10	143	10	-12	-12	662	17	2	-11	279	8	5
-6	38	32	-13*	-12	413	11	10	11	84	9	4	-10	537	14	-6	-10	248	7	-5
-5	160	6	-7	-11	182	5	-4	12	99	8	5	-8	88	17	-22*	-9	146	14	11
-4	70	14	13*	-10	208	7	-5	13	107	11	-9	-6	89	7	-13	-8	128	6	-6
-3	217	7	-3	-9	111	8	-6	H,K=		7,	7	-4	519	13	41	-7	46	9	9*
-2	39	25	30*	-8	42	14	-14*	-15	148	8	6	-2	699	18	-8	-6	123	7	-9
-1	230	8	-4	-7	5	2	-27*	-14	0	2	-9*	0	544	14	-20	-5	118	5	1
0	37	2	21*	-6	136	4	1	-13	234	8	5	2	272	9	16	-4	334	9	-3
1	171	8	2	-5	308	8	-1	-12	56	14	-6*	4	139	6	1	-3	349	9	-2
2	44	2	11*	-4	598	15	5	-11	240	8	2	6	312	9	-10	-2	435	11	-2
3	127	6	-7	-3	569	17	-8	-10	133	6	-1	8	314	9	2	-1	386	10	-2
4	60	22	-6*	-2	727	20	-13	-9	161	6	2	10	248	7	23	0	314	8	11
5	122	11	-18	-1	259	7	-14	-8	136	7	3	12	104	12	-18	1	155	6	7
H,K=		7,	1	0	304	8	-10	-7	138	5	2	14	130	11	-23	2	122	7	-11
-20	132	10	7	1	29	2	7*	-6	89	12	1	H,K=		8,	2	3	49	8	16
-19	29	2	24*	2	72	6	-19	-5	254	7	-7	-19	15	2	2*	4	57	10	-16
-18	23	2	-3*	3	38	34	-0*	-4	36	2	19*	-18	73	12	-8	5	125	5	-6
-17	0	2	-5*	4	81	8	-13	-3	362	10	6	-17	35	21	29*	6	235	7	-9
-16	122	9	0	5	188	6	-1	-2	35	2	-18*	-16	42	35	2*	7	183	6	-14
-15	85	19	-8*	6	304	8	5	-1	285	9	18	-15	86	10	6	8	274	8	4
-14	356	10	5	7	275	8	-8	0	148	8	6	-14	203	10	-2	9	171	7	7
-13	152	6	-6	8	362	11	5	1	170	7	8	-13	205	10	-1	10	196	12	2
-12	531	14	8	9	141	10	3	2	195	6	2	-12	542	14	9	11	108	7	8
-11	84	14	6	10	222	9	2	3	158	7	-12	-11	115	10	-17	12	86	22	-3*
-10	313	9	-17	11	84	10	13	4	103	6	2	-10	380	10	13	13	91	12	-4
-9	123	5	-2	12	102	11	-13	5	222	7	-7	-9	38	25	18*	H,K=		8,	6
-8	37	12	-8*	13	42	2	-4*	6	56	19	2*	-8	31	21	-37*	-18	0	2	-43*
-7	0	2	-27*	14	93	12	3	7	236	7	0	-7	56	7	1	-15	73	11	-1
-6	181	7	12	H,K=		7,	5	8	47	17	11*	-6	45	9	7*	-14	28	2	-20*
-5	165	10	5	-18	0	2	-53*	9	171	10	-0	-5	213	8	20	-13	222	9	-13
-4	707	19	27	-17	36	2	11*	10	0	2	-26*	-4	464	12	27	-12	106	8	1
-3	217	8	-3	-16	88	7	9	11	113	9	3	-3	336	9	-6	-11	320	9	1
-2	762	21	-15	-15	134	14	-6	H,K=		7,	9	-2	645	16	-0	-10	168	6	2
-1	65	5	-15	-14	141	6	-9	-11	154	7	-1	-1	266	7	-5	-9	234	8	16
0	239	7	18	-13	285	8	0	-10	0	2	-17*	0	498	13	-3	-8	178	7	-2
1	105	7	8	-12	211	6	-3	-9	111	8	-0	1	30	19	5*	-7	102	6	2
2	182	6	14	-11	264	8	2	-8	38	32	2*	2	135	5	-1	-6	96	8	4
3	130	5	0	-10	203	7	-3	-7	106	13	8	3	85	11	-2	-5	122	8	-6
4	314	8	9	-9	74	11	7	-6	30	2	25*	4	70	13	-6*	-4	43	2	23*
5	0	2	-40*	-8	125	5	6	-5	191	8	-5	5	124	6	-12	-3	275	7	4
6	474	12	-9	-7	125	5	4	-4	49	15	1*	6	357	10	2	-2	100	6	-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
-1	388	10	18	-10	576	17	-7	13	27	2	-4*	H,K=	9,	9		4	178	6	2
0	213	6	-3	-9	11	2	-26*	H,K=	9,	5	-10	21	2	12*		5	110	6	1
1	281	8	12	-8	221	6	-22	-17	38	2	13*	-9	165	9	1		6	132	11	-11
2	187	6	-4	-7	38	26	31*	-16	64	13	-21*	-8	43	20	7*		7	103	10	0
3	153	6	-4	-6	37	15	-19*	-15	14	2	-10*	-7	189	7	5		8	217	7	-16
4	89	9	3	-5	42	11	23*	-14	71	14	8*	-6	0	2	-4*		9	73	18	-8*
5	177	7	-6	-4	153	5	16	-13	180	7	-13	-5	175	6	-4		10	210	8	-2
6	90	11	1	-3	98	5	2	-12	115	8	-2	-4	16	2	15*		11	49	2	17*
7	200	11	8	-2	593	15	5	-11	361	10	10	-3	186	7	-9		12	163	7	7
8	55	14	-8*	-1	105	7	-13	-10	192	6	-8	-2	33	2	6*		H,K=	10,		4
9	152	14	5	0	641	16	-5	-9	292	8	2	-1	177	10	-6		-18	164	11	-4
10	70	12	-11	1	46	13	20*	-8	247	7	-8	0	32	2	25*		-17	70	15	16*
11	122	9	-4	2	345	9	8	-7	28	2	1*	1	158	6	8		-16	108	7	-2
H,K=		8,	8	3	32	2	7*	-6	88	6	3	2	13	2	2*		-15	17	2	-6*
-13	167	6	-3	4	126	5	3	-5	65	12	15*	3	124	7	-2		-14	33	2	-5*
-12	62	13	54*	5	99	10	9	-4	121	5	-1	4	25	2	-5*		-13	77	9	5
-11	194	7	-5	6	152	6	-19	-3	256	8	3	H,K=	10,		0		-12	61	11	-15
-10	69	10	-6	7	110	7	-6	-2	151	7	-3	-18	176	18	-11		-11	316	9	5
-9	159	8	7	8	273	8	-8	-1	469	12	7	-16	30	2	-17*		-10	293	9	2
-8	101	12	-10	9	60	31	-1*	0	233	8	-6	-14	56	43	11*		-9	260	8	-2
-7	121	7	-8	10	286	10	13	1	311	8	13	-12	315	15	14		-8	320	9	3
-6	49	16	8*	11	63	16	56*	2	180	8	-7	-10	627	16	24		-7	58	26	11*
-5	169	7	-6	12	184	7	12	3	122	7	6	-8	392	10	5		-6	226	6	-5
-4	59	23	8*	13	30	2	14*	4	169	6	-9	-6	53	25	8*		-5	47	10	12*
-3	274	8	-5	H,K=		9,	3	5	80	11	-16	-4	49	21	15*		-4	112	5	-12
-2	21	2	13*	-19	85	11	3	6	135	8	-6	-2	395	10	15		-3	220	7	8
-1	262	8	2	-18	147	13	-6	7	140	7	5	0	673	17	-10		-2	105	6	9
0	86	8	-5	-17	8	2	-18*	8	137	9	6	2	413	11	13		-1	286	8	-2
1	185	9	7	-16	48	20	-6*	9	178	9	-5	4	78	12	10		0	213	7	-5
2	124	6	4	-15	0	2	-15*	10	135	8	-3	6	50	18	2*		1	281	9	4
3	121	7	-1	-14	108	15	9	11	171	7	13	8	227	7	-11		2	253	7	-2
4	69	8	28	-13	133	8	-3	H,K=		9,	7	10	266	8	13		3	107	12	8
5	149	8	-6	-12	267	10	9	-15	59	2	-12*	12	211	9	21		4	199	8	-10
6	16	2	9*	-11	267	8	-4	-14	32	2	9*	H,K=	10,		2		5	39	21	8*
7	208	9	0	-10	348	10	11	-13	141	7	-10	-19	103	17	-3		6	137	7	-2
8	58	25	35*	-9	202	6	-10	-12	44	25	-13*	-18	200	9	3		7	74	11	-24
H,K=		8,	10	-8	265	9	-11	-11	254	10	-8	-17	27	2	-14*		8	157	8	-0
-7	141	7	-1	-7	56	15	22*	-10	105	16	3	-16	70	17	-0*		9	164	9	-2
-6	36	2	30*	-6	140	8	-5	-9	258	9	6	-15	32	2	-5*		10	109	19	-1
-5	159	7	-9	-5	65	12	18*	-8	155	6	-3	-14	29	2	-9*		11	116	14	-12
-4	49	39	24*	-4	237	7	-6	-7	122	6	7	-13	0	2	-16*		H,K=	10,		6
-3	178	7	-19	-3	312	8	5	-6	4	2	-26*	-12	191	13	0		-16	84	15	8
-2	45	26	7*	-2	394	10	4	-5	77	18	-9*	-11	190	8	-11		-15	55	25	17*
-1	164	8	-11	-1	329	9	-6	-4	9	2	-12*	-10	471	13	2		-14	53	15	-14*
0	51	18	16*	0	389	10	12	-3	211	6	-4	-9	179	11	-12		-13	125	10	-9
1	146	7	-1	1	96	14	0	-2	42	2	-8*	-8	412	11	-14		-12	57	13	10*
2	24	2	-6*	2	161	5	1	-1	305	9	9	-7	91	8	-13		-11	294	10	-2
H,K=		9,	1	3	39	17	22*	0	151	9	-11	-6	136	6	-12		-10	116	7	-3
-19	46	2	6*	4	114	7	-9	1	252	9	10	-5	37	17	23*		-9	280	8	4
-18	125	12	3	5	76	8	3	2	115	7	-5	-4	68	18	-1*		-8	126	6	-2
-17	12	2	-3*	6	195	6	-0	3	149	6	-1	-3	117	5	2		-7	117	12	14
-16	42	2	-10*	7	152	6	-16	4	73	10	-4	-2	320	8	13		-6	123	6	3
-15	30	2	26*	8	234	7	-6	5	125	10	-2	-1	92	15	-7		-5	42	13	-0*
-14	140	6	-6	9	169	8	1	6	33	2	20*	0	521	13	-4		-4	94	5	6
-13	58	35	9*	10	215	7	3	7	139	13	-2	1	118	9	-7		-3	159	6	-17
-12	479	13	8	11	88	10	10	8	9	2	-4*	2	350	10	9		-2	84	14	-1
-11	61	12	-3*	12	92	10	-14	9	163	8	-1	3	99	10	15		-1	317	8	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
0	136	6	-4	8	149	17	-28	6	109	10	-2	-11	79	11	11	-6	122	7	-9
1	307	8	6	9	26	2	18*	7	80	12	-18	-10	231	10	-4	-5	149	9	10
2	154	9	-5	10	198	8	-2	8	57	17	-13*	-9	241	7	-1	-4	150	11	4
3	156	8	2	11	0	2	-8*	9	154	7	2	-8	439	12	12	-3	104	13	2
4	118	6	-3	H,K=	11,	3		H,K=	11,	7	-7	195	9	-15	-2	95	8	3	
5	57	2	-8*	-18	212	11	6	-13	70	17	-2*	-6	337	9	-3	-1	153	6	-18
6	50	2	10*	-17	91	15	-2	-12	54	35	5*	-5	30	2	9*	0	67	16	3*
7	89	11	-10	-16	135	7	-2	-11	148	9	-4	-4	129	9	2	1	185	7	-8
8	37	2	-22*	-15	32	2	-1*	-10	0	2	-9*	-3	108	6	-0	2	65	25	5*
9	157	9	-6	-14	43	23	22*	-9	205	8	5	-2	136	7	-6	3	158	6	9
H,K=	10,	8	-13	0	2	-12*	-8	44	23	28*	-1	76	8	1	4	94	8	8	
-12	0	2	-19*	-12	50	23	-0*	-7	217	12	14	0	164	6	-5	5	117	8	12
-11	145	12	-8	-11	166	9	5	-6	125	6	-4	1	197	8	-1	6	73	12	-1
-10	38	2	13*	-10	302	9	11	-5	133	12	8	2	342	9	-2	H,K=	12,	8	
-9	224	8	-6	-9	278	8	2	-4	79	14	-1	3	181	7	10	-9	182	8	-3
-8	0	2	-7*	-8	428	11	4	-3	96	7	-4	4	271	9	8	-8	62	30	54*
-7	188	7	9	-7	163	6	-9	-2	65	12	-9	5	60	14	3*	-7	225	7	7
-6	41	2	-3*	-6	289	8	-7	-1	164	9	-17	6	139	6	-0	-6	46	21	-9*
-5	164	7	2	-5	48	26	-3*	0	53	29	12*	7	0	2	-17*	-5	158	7	7
-4	80	8	21	-4	28	2	-8*	1	239	8	-1	8	83	16	-10*	-4	75	14	-7*
-3	131	7	-11	-3	52	14	-1*	2	49	2	-9*	9	45	2	29*	-3	96	8	-1
-2	25	2	8*	-2	85	7	-2	3	186	6	11	10	139	10	-7	-2	39	2	-16*
-1	175	7	-9	-1	122	7	-10	4	0	2	-33*	H,K=	12,	4	-1	103	11	-6	
0	35	2	8*	0	250	8	3	5	108	7	3	-16	151	12	-3	0	61	16	48*
1	201	7	2	1	229	7	-2	6	45	2	6*	-15	55	2	-9*	1	177	7	6
2	37	2	-16*	2	302	9	12	H,K=	11,	9	-14	66	11	-4	H,K=	13,	1		
3	191	7	3	3	174	7	5	-7	225	10	8	-13	0	2	-25*	-17	29	2	-11*
4	53	14	16*	4	248	7	4	-6	50	2	-2*	-12	21	2	-32*	-16	284	9	-1
5	139	7	-4	5	40	31	-3*	-5	137	9	-3	-11	58	15	-4*	-15	53	32	40*
H,K=	11,	1	6	137	14	-13	-4	19	2	-13*	-10	140	7	4	-14	144	8	-6	
-19	67	17	1*	7	65	17	-11*	-3	102	6	6	-9	253	9	7	-13	15	2	-9*
-18	233	9	-9	8	91	10	-24	-2	11	2	0*	-8	298	8	12	-12	40	22	16*
-17	36	2	5*	9	83	10	-11	-1	105	7	4	-7	260	8	1	-11	22	2	-1*
-16	152	7	-6	10	114	13	-2	H,K=	12,	0	-6	245	7	-3	-10	71	24	6*	
-15	42	20	5*	H,K=	11,	5	-18	243	12	-5	-5	102	9	8	-9	111	12	11	
-14	50	12	27*	-16	113	13	-8	-16	248	9	-2	-4	95	11	-12	-8	332	9	4
-13	32	27	3*	-15	52	19	0*	-14	61	28	-5*	-3	0	2	-22*	-7	95	17	8
-12	134	8	5	-14	58	16	-13*	-12	0	2	-26*	-2	31	2	-14*	-6	420	11	-9
-11	53	21	9*	-13	79	15	-1	-10	233	18	10	-1	148	9	-1	-5	39	2	9*
-10	430	11	9	-12	46	23	5*	-8	390	11	21	0	122	9	-10	-4	290	8	6
-9	133	7	-6	-11	179	8	-9	-6	333	15	-9	1	209	7	-3	-3	0	2	-19*
-8	463	12	-6	-10	127	7	-6	-4	155	8	-3	2	274	8	7	-2	47	13	-4*
-7	106	14	0	-9	253	7	-6	-2	195	13	-4	3	142	7	-0	-1	36	18	12*
-6	184	7	-4	-8	199	8	-4	0	197	7	-3	4	237	9	4	0	129	8	-14
-5	26	2	22*	-7	183	7	-2	2	364	10	8	5	51	2	-13*	1	100	7	8
-4	57	14	13*	-6	247	7	-5	4	217	8	8	6	113	13	-6	2	273	8	-9
-3	53	16	-4*	-5	94	13	7	6	155	8	11	7	77	14	-12	3	65	17	-1*
-2	267	7	-6	-4	86	8	-4	8	137	9	-1	8	31	2	-35*	4	232	8	7
-1	45	14	-4*	-3	97	11	-5	10	197	8	2	H,K=	12,	6	5	0	2	-24*	
0	480	12	-14	-2	73	8	-6	H,K=	12,	2	-14	114	8	8	6	183	11	19	
1	102	6	6	-1	275	8	-1	-18	205	14	-4	-13	74	17	15*	7	43	2	7*
2	349	9	13	0	129	10	-7	-17	80	13	-8	-12	58	13	10*	8	136	7	0
3	110	8	2	1	297	8	13	-16	207	12	-8	-11	55	15	-12*	9	0	2	-6*
4	201	7	10	2	233	8	4	-15	17	2	9*	-10	0	2	-13*	H,K=	13,	3	
5	53	26	6*	3	152	8	-1	-14	38	35	-30*	-9	191	8	4	-16	186	9	7
6	95	15	-18	4	174	9	-3	-13	48	2	4*	-8	96	18	0	-15	83	12	11
7	0	2	-8*	5	45	19	0*	-12	0	2	-34*	-7	239	8	0	-14	110	20	-17

STRUCTURE FACTORS CONTINUED FOR
C(20)H(30)P(2)I(2)PT

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-13	36	2	9*	0	3	2	-6*	0	147	7	-4	-1	52	17	7*	-5	137	8	-4
-12	29	2	-35*	1	126	10	-6	1	52	38	-3*	0	121	7	-7	-4	149	10	1
-11	65	10	28	2	48	2	31*	2	118	10	-10	1	24	2	-48*	-3	119	7	10
-10	92	14	-3	H,K=	14,	0		3	149	7	-6	2	75	19	-25*	-2	172	12	-9
-9	178	6	6	-16	263	21	7	4	123	8	-1	3	101	14	1	-1	56	16	-2*
-8	255	9	8	-14	214	9	-2	5	149	10	18	4	134	6	10	0	109	10	-2
-7	211	11	-12	-12	11	2	-15*	H,K=	14,	6		H,K=	15,	5		1	85	12	12
-6	280	9	4	-10	23	2	-17*	-11	4	2	-15*	-12	112	13	-17	H,K=	17,	1	
-5	73	14	6*	-8	241	14	-5	-10	47	25	15*	-11	17	2	-4*	-12	197	13	-2
-4	175	6	10	-6	427	11	6	-9	73	11	-3	-10	83	22	3*	-11	0	2	-9*
-3	8	2	-11*	-4	313	9	8	-8	38	2	16*	-9	53	23	5*	-10	126	10	-4
-2	37	2	-12*	-2	90	16	5	-7	196	7	-3	-8	50	24	21*	-9	0	2	-26*
-1	33	2	-19*	0	127	18	-6	-6	83	11	2	-7	160	9	-3	-8	60	25	-16*
0	142	8	-4	2	118	12	-21	-5	241	8	8	-6	62	21	-2*	-7	40	2	34*
1	175	6	-6	4	242	11	8	-4	133	13	-4	-5	224	7	9	-6	71	15	-27*
2	264	10	-6	6	224	19	21	-3	162	9	15	-4	145	13	4	-5	60	44	-1*
3	144	13	8	H,K=	14,	2		-2	111	22	8*	-3	134	7	22	-4	137	9	-13
4	211	8	4	-16	208	10	-1	-1	55	17	-1*	-2	120	8	-6	-3	85	12	11
5	128	7	12	-15	71	17	-15*	0	33	2	5*	-1	29	2	7*	-2	179	7	14
6	142	7	16	-14	216	8	-6	1	63	22	-5*	0	82	18	-15*	-1	46	28	6*
7	20	2	-16*	-13	38	2	-3*	2	13	2	-15*	1	11	2	-47*	0	133	8	9
8	85	13	9	-12	71	11	-11	H,K=	15,	1	2	54	2	4*	1	0	2	-10*	
H,K=	13,	5	-11	26	2	10*	-15	36	2	-21*	H,K=	16,	0		H,K=	17,	3		
-15	134	11	-16	-10	35	2	-7*	-14	245	8	4	-14	185	12	-12	-13	94	18	-2*
-14	109	9	-14	-9	79	19	4*	-13	21	2	-15*	-12	165	10	-13	-9	43	31	30*
-13	46	26	17*	-8	208	9	2	-12	100	18	-8	-10	76	25	-2*	-8	42	29	-9*
-12	47	23	-44*	-7	90	13	-5	-11	0	2	-3*	-8	90	13	8	-7	49	22	26*
-11	48	26	28*	-6	309	8	12	-10	71	14	22*	-6	201	8	-13	-6	74	15	-2*
-10	31	2	-33*	-5	65	13	-15*	-9	60	15	51*	-4	232	8	-11	-5	79	36	-19*
-9	150	11	-5	-4	238	7	7	-8	125	12	6	-2	155	10	3	-4	142	9	-10
-8	99	11	-7	-3	0	2	-25*	-7	28	2	15*	0	99	17	18	-3	109	19	-6
-7	244	9	-8	-2	100	8	-4	-6	276	9	-4	2	95	15	-20	-2	180	8	-1
-6	161	7	-4	-1	50	28	-10*	-5	35	2	-6*	H,K=	16,	2	-1	97	17	14	
-5	194	9	7	0	138	8	-2	-4	267	9	-6	-13	90	19	-11*	H,K=	18,	0	
-4	163	7	-4	1	90	12	1	-3	0	2	-46*	-12	185	7	-2	-8	73	15	-14*
-3	137	10	11	2	140	11	-10	-2	188	8	15	-11	0	2	-22*	-6	46	22	7*
-2	75	10	-22	3	126	7	4	-1	52	37	19*	-10	58	19	-26*	-4	104	13	-2
-1	91	9	19	4	204	8	2	0	23	2	-33*	-9	38	2	5*				
0	89	14	-1	5	41	2	3*	1	47	25	12*	-8	41	2	7*				
1	103	8	-6	6	162	8	10	2	115	8	-1	-7	26	2	2*				
2	106	13	-20	7	8	2	-2*	3	42	2	12*	-6	130	15	-13				
3	126	8	2	H,K=	14,	4		4	190	7	-6	-5	88	30	-5*				
4	101	19	-8*	-15	151	17	11	5	58	2	49*	-4	208	8	-15				
5	163	11	12	-14	172	12	-2	H,K=	15,	3	-3	122	11	9					
6	94	17	-10	-13	45	2	-1*	-14	205	8	-1	-2	186	7	2				
H,K=	13,	7	-12	136	7	2	-13	98	24	7*	-1	70	12	9					
-11	68	18	15*	-11	0	2	-19*	-12	148	7	1	0	86	26	-13*				
-10	14	2	-3*	-10	53	20	-13*	-11	24	2	13*	1	39	2	3*				
-9	119	9	-9	-9	73	13	-7	-10	79	13	8	2	76	22	-25*				
-8	29	2	21*	-8	82	13	-12	-9	0	2	-14*	3	13	2	3*				
-7	201	7	4	-7	206	6	12	-8	38	2	-13*	H,K=	16,	4					
-6	65	14	-2*	-6	158	9	-2	-7	116	16	1	-11	62	17	12*				
-5	198	7	8	-5	221	9	4	-6	122	9	-13	-10	69	21	-21*				
-4	135	7	4	-4	152	12	-15	-5	168	7	7	-9	21	2	6*				
-3	120	8	-2	-3	101	9	20	-4	223	9	4	-8	0	2	-18*				
-2	91	25	-5*	-2	130	10	-13	-3	57	2	-32*	-7	91	22	3*				
-1	97	11	-13	-1	34	2	10*	-2	211	7	6	-6	74	14	-5				

TECHNICAL INFORMATION DIVISION
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