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LBL 5131

Contribution from

Materials and Molecular Research Division Lawrence Berkeley Laboratory

and

Department of Chemistry University of California Berkeley, California 94720

The Crystal and Molecular Structure of

Di-iodo(butane-1,4-diyl)bis(dimethylphenylphosphine)platinum(IV)¹

Anthony K. Cheetham,² Richard J. Puddephatt,³ Allan Zalkin,^{*} 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 <u>a</u> = 15.286, <u>b</u> = 9.709, <u>c</u> = 17.036Å, β = 107.49°, <u>d</u>_c = 2.15 g/cm³ for Z = 4. X-ray diffraction intensity data were collected by an automated diffractometer using graphite monochromated Mo K α radiation. For 1575 reflections with $F^2>3\sigma(F^2)$; R₁ = 0.035 and R₂ = 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-l-ene at 120°C in dichloromethane.⁴ The structure of the complex⁵ is of particular interest in that it shows an unsymmetrical puckering of the Pt(CH₂)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(CH₂)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 <u>cis</u>-PtCl₂(PMe₂Ph)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 α_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:

-3-

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 $\Sigma w (|F_0| - |F_c|)^2$ 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/Å³; the largest was 2e/Å³. 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: $R_1 = \Sigma ||F_0| - |F_c||/\Sigma |F_0| = 0.035$ for the 1575 data were $F^2 > 3\sigma(F^2)$, and 0.054 for all 2150 data; $R_2 = [\Sigma w ||F_0| - |F_c||^2 / \Sigma w |F_0|^2]^{1/2} = 0.044$. 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

-5-

 $[(CH_3)_2(C_6H_5)P]_2 I_2 Pt(CH_2CH_2CH_2CH_2)$ Compound Formula Weight 781.307 15.286(6)a 9.709(4)b 17.036(6)С 107.49(5)β 2412 Å³ ۷ Ζ 4 2.152 g/cm³ Density (calc) $C_{2h}^{6} - C_{2/c}$ Space Group Crystal Shape and Size .06 mm x .11 mm x .14 mm 0.00124 mm^3 Crystal volume 23° Temperature Mo Kal (λ 0.70926 Å), monochromated from Radiation (002) face of mosaic graphite **Transmission Factors** .42 to .65 81 cm⁻¹ μ θ -2 θ scan (1°/min along 2 θ) Data Collection Method .75° below $K\alpha_1$ to .75 above $K\alpha_2$ Scan range **Background Counts** 4 sec. Background offset from scan limits by 0.5° 20 Limits $5.0 - 50.0^{\circ}$ Final No. of variables 113 Unique Data Used 1575 $F_{0}^{2} > 3\sigma(F_{0}^{2})$

Atomic Parameters and Standard Deviations^a

	¢					
ATOM	B11	B22	B 3 3	B12	B13	B23
Pt	2.70(2)	2.00(2)	2.38(2)	0	.53(2)	Ô.
I	6.39(5)	9.49(6)	5.05(4)	-2.66(4)	3.31(4)	22(4)
Ρ	3.0(1)	2.4(1)	4.3(1)	.08(8)	.5(1)	.10(8)
C(1)	6.4(6)	1-8(4)	48(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	Ŷ	Z
Pt		.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 (i)	.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)

^aThe temperature factor has the form $exp[-0.25(h^2a^{*2}B_{11} + ... + 2hka^{*}b^{*}B_{12} + ...)]$. 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.

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Table III. Interatomic Distances^a

Pt	-2	C(1)	2.15(1)
	-2	Р	2.418(3)
•	-2	I	2.641(1)
Р	-	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	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)

^aUncorrected for thermal motion

 $^{\rm b}$ C(2)1 and C(2)2 represent the two sites of the C(2) atom

Selected Angles

		. · · ·
I -Pt	-1	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)
and the second		

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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.

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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.

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- This report was done with support from the United States Energy 1. 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.



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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 $(DEL=|F_0|-|F_c|)$.

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DATA PROCESSING FORMULAE

$$\begin{split} \mathbf{I} &= \mathbb{C} - \left(\mathbf{t}_{c}/2\mathbf{t}_{b}\right)(\mathbf{B}_{1}+\mathbf{B}_{2}\right) \\ \mathbf{o}(\mathbf{B}) &= \operatorname{Max}\left[\left(\mathbf{t}_{c}/2\mathbf{t}_{b}\right)(\mathbf{B}_{1}+\mathbf{B}_{2}\right)^{\frac{1}{2}}, \left(\mathbf{t}_{c}/2\mathbf{t}_{b}\right)|\mathbf{B}_{1}-\mathbf{B}_{2}|\right] \\ \mathbf{o}(\mathbf{I}) &= \left[\mathbf{0} + \sigma^{2}(\mathbf{B})\right]^{\frac{1}{2}} \\ \mathbf{F}^{2} &= \left[\mathbf{D}\cdot\mathbf{A}/\mathbf{Lp}\right)\mathbf{I} \\ \mathbf{o}(\mathbf{F}^{2}) &= \left[\mathbf{D}\cdot\mathbf{A}/\mathbf{Lp}\right)\mathbf{o}(\mathbf{I}\right] \\ \mathbf{F}_{a}^{2} &= \mathbf{\Sigma}\mathbf{F}^{2}/n \\ \mathbf{o}(\mathbf{F}_{a}^{2}) &= \left[\mathbf{\Sigma}\mathbf{C}^{2}(\mathbf{F}^{2})/n\right]^{\frac{1}{2}} \\ \mathbf{When S}(\mathbf{F}_{a}^{2}) > 4\mathbf{o}(\mathbf{F}_{a}^{2}), \mathbf{c}(\mathbf{F}_{a}^{2}) \text{ is replaced by S}(\mathbf{F}_{a}^{2}) \\ \mathbf{S}(\mathbf{r}_{a}^{2}) &= \left[\mathbf{\Sigma}\mathbf{C}^{2}(\mathbf{F}^{2})/n\right]^{\frac{1}{2}} \\ \mathbf{When S}(\mathbf{F}_{a}^{2}) > 4\mathbf{o}(\mathbf{F}_{a}^{2}), \mathbf{c}(\mathbf{F}_{a}^{2}) \text{ is replaced by S}(\mathbf{F}_{a}^{2}) \\ \mathbf{S}(\mathbf{r}_{a}^{2}) &= \left[\mathbf{\Sigma}\mathbf{C}^{2}(\mathbf{F}_{a}^{2}) + (\mathbf{p}\mathbf{F}_{a}^{2})^{2} + \mathbf{q}^{2}\right]^{\frac{1}{2}} \\ \mathbf{F}_{o} &= (\mathbf{r}_{a}^{2})^{\frac{1}{2}} \\ \mathbf{O}(\mathbf{F}) &= \mathbf{F}_{o} - \left[\mathbf{F}_{a}^{2} - \mathbf{o}(\mathbf{F}_{o}^{2})\right]^{\frac{1}{2}} \text{ when } \mathbf{o}(\mathbf{F}_{o}^{2})\mathbf{S}\mathbf{F}_{a}^{2} \text{ or } \left[\mathbf{c}(\mathbf{F}_{a}^{2})^{\frac{1}{2}} + \mathrm{when } \mathbf{c}(\mathbf{F}_{a}^{2}) > \mathbf{F}_{a}^{2} \\ \mathbf{L}\mathbf{p} &= \left[\cos^{2}\mathbf{2}\mathbf{\theta}_{m} + \cos^{2}\mathbf{2}\mathbf{\theta}\right]/\left[\sin\mathbf{2}\mathbf{\theta} + \cos^{2}\mathbf{2}\mathbf{\theta}_{m}\right]. \\ \mathbf{wtg} &= t/\sigma^{2}(\mathbf{F}) \\ \mathbf{C} &= \text{ counts recorded during a scan } \qquad \mathbf{\theta}_{m} = \text{ monochromater angle} \\ \mathbf{I} &= \text{ individual raw intensity}, \qquad \mathbf{\theta} = \text{ crystal diffraction angle} \\ \mathbf{b} \text{ background count time} \\ \mathbf{q} &= \text{ additional uncertainty that} \\ \mathbf{a}_{1} = \text{ individual background count } \\ \mathbf{r} &= \mathbf{stimated standard dev} \\ \text{ istion of the total back-} \\ \text{ ground count} \\ \mathbf{F} &= \text{ structure factor } \\ \mathbf{D} &= \text{ decay correction; an empir-ically applied correction} \\ \mathbf{o} \text{ obtained rfore the fluctuations} \\ \mathbf{o} \text{ of the standard reflections.} \\ \mathbf{A} &= \text{ absorption correction} \\ \mathbf{I}_{a} &= \text{ Loreats and nolarisation} \end{aligned}$$

corrections

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 FCB. DEL = /FOB/ - /FCA/. * INDICATES ZERO WEIGHTED DATA.

L	F08	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	HγK¤	. 01	, 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	-18	82	7	-1
8	621	16	34	5	60	ģ	19	-5	55	12	-12#	q	197	5	•	- Q	124	Â	4 4
10	661	17	-19	6	126	Ĺ	6	- 6	282	7	5	10	740	á	44	- A	45	27	458
12	477	4.4	-24	7	149	L.	-2	- 7	4 0 0	, 7	-4	44	264	7	-7	-7	74.2	~ 'a	7
44	128	4 4	-0	Ŕ	84	Å	· 2 6		784	25	68	4.2	204	, 0		-6	312		-4
16	67	4 2	4	ă	748	ä		- 4	50	44	474	17	233	4.2	-7	-5	195	Ē	
48	477	L J A	- 8	40	480	ś	7	1	23	1. A	13.	13	4 50	12	-7		103	5	1
To		0	-0	10	100	0	3	01		41	-12	14	122	0	-9		103	2	. 14
•	19K2	1.7		11	333	7	_ 4	1	212	20	17	17	33	2	-17	3	210	0	. .
0	1103	41	-40	12	123	2	-/	. 2	929	29	2	10	100	0	-11	- Z-	1/1	0	1
1	240	0	0	13	1/0		2	· 3	449	13	29	11	66	25	2.	1	403	10	· •
2	303		-22	14	101	b	-7	4	287	8	8	18	128	10	-3	0	148	6	-5
3	1 39	- :4	-3	15	90	8	2	5	59	10	17	_	1,K=	1	, 5	1	505	13	1
K.	63	9	5	16	52	11	-15	* 6	75	6	-10	-17	128	9	1	2	80	8	-11
5	21	2	-6*	1	H, K=	.0 1	8	7	25	2	14*	-16	99	15	- 8	3	347	9	10
6	85	4	3	0	41	14	201	F 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	1 30	7	-15	5	226	6	2	13	0	2	-42*	-10	212	6	0	ġ	267	7	1
12	305	9	-4	6	47	35	21	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	344	16	69	18	A	-7	24 9	7	5	12	74	11	-3
		-		•	– – – ,	T.A.		T.A.			•	· •	617					-	
15	21	2	2*	9	245	7	-5	17	25	2	-13*	-6	223	6	-8	13	187	7	2
15 16	21 99	2	2* -1	9 10	245 74	7	-5. 17	17	25	2	-13* -8	-6 -5	223 79	6 7	-8	13	187	7	2 -14*
15 16 17	21 99 76	2 9 15	2* -1 -6*	9 10 11	245 74 210	7	-5 17 5	17 18	25 125 1•K=	2 6	-13* -8 3	-6 -5 -4	223 79 134	6 7 5	-8 11 1	13 14 15	187 29 96	7 2 10	2 -14# -8
15 16 17 13	21 99 76 187	2 9 15 6	2* -1 -6*	9 10 11 12	245 74 210 69	7 6 6 9	-5 17 5	17 18 -19	25 125 1,K= 122	2 6 11	-13* -8 3 -7	-6 -5 -4 -3	223 79 134 63	6 7 5 5	-8 11 1 3	13 14 15	187 29 96	7 2 10	2 -14* -8 9
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15 16 17 18 9 0 12 34 56 7 8 90 112	219767 1881743355945246667	291560 15610 154088495908997	2* -1-6* -114-18 -148-182-18 126-287-5-7-	9 10 112 1 1 12 3 4 5 6 7 8 9 9 9 8 1 7	245 210 14K 94 2074 2094 2074 2075 2174 208 368 2168 2168 208 2168 208 2168 208 2168 208 208 208 208 208 208 208 208 208 20	7 6 9 8 0 10 6 7 6 2 6 2 7 19 8 1 9 8 19 36 7	-5 17 5 8 5 10 -1 -6 14 8 -4 6 19 1 9 -7 1 -19	17 18 -18 -18 -116543210987654	255 = 271 1 1 2 27 1 1 2 27 1 2 2 1 2 2 2 2	2 6 11 17 11 15 6 2 10 2 6 5 13 11 18 10 4 0	$ \begin{array}{c} -13^{+} \\ -8 \\ 3 \\ -7 \\ -13 \\ -12^{+} \\ -12^{+} \\ -18 \\ -18 \\ -18 \\ -2 \\ 14 \\ 9 \\ -14 \\ 9 \\ -14 \\ -2 \\ -14 \\ -2 \\ -2 \\ -14 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2$		223 79 134 163 164 325 276 310 103 19 279 103 19 205 19 205 19 205 19 205 19 205 10 205 205 205 205 205 205 205 205 205 20	6755511815710896751081060	$\begin{array}{c} -8 \\ 11 \\ 1 \\ -8 \\ -15 \\ -8 \\ -11 \\ -20 \\ 3 \\ -2 \\ -3 \\ -7 \\ -1 \\ 4 \\ -3 \\ 5 \\ 13 \\ 4 \\ \end{array}$		187 29 96 165 165 165 245 284 2019 168 30 150 38 46 37 38 46 37	7 2 10 1 26 27 20 1 7 2 8 7 20 1 7 2 10 2 117 19 20 7 13 2	2 -14* -8 9 23* -3 -3 -3 -3 -3 -3 -3 -3 -3 -3 -3 -3 -3
15 16 17 18 19 0 12 34 56 7 8 9 0 11 12 34	21967 18817433559452466676	295600540884959089975	2^{*} -1 -6 -11 -14 -14 -18 -18 -18 -18 -18 -18 -18 -18 -16 -11 -14 -18 -18 -16 -11 -14 -18 -16 -11 -12 -16 -17 -17 -17 -17 -17 -17 -17 -17 -17 -17	9 10 112 3 10 1 2 3 4 5 6 7 8 9 9 9 9 8 7 1 9 10 1 2 3 4 5 6 7 8 9 9 19 8 7 1	2454 21094 14 89445 2070 2014 2056 14 89445 2056 2056 2056 2056 2056 2056 2056 205	7 6 9 8 9 10 6 7 6 9 10 6 7 6 7 6 7 6 7 6 7 8 19 8 36 7 30	-5 17 5 8 5 10 -1 -6 14 8 -4 6 19 -7 1 -19 -12 -14	17 18 -18 -1165432109876543	255 = 27 1, K = 27 1	2 6 11 17 11 15 6 2 10 2 6 5 13 1 18 10 4 10 7 7	$ \begin{array}{c} -13^{*} \\ -8 \\ 3 \\ -7 \\ -13 \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -11 \\ 8 \\ -18 \\ -2 \\ 14 \\ 9 \\ 21 \\ \end{array} $	-654321012345678901123 1123	223 79 134 63 164 322 605 276 409 103 679 379 4025 177	6755518570896751081066	$\begin{array}{c} -8 \\ 11 \\ 3 \\ -15 \\ -15 \\ -11 \\ -20 \\ 3 \\ -2 \\ -3 \\ -7 \\ -14 \\ -3 \\ 5 \\ 13 \\ -0 \end{array}$	1345 1211 -111 	187 96 165 165 245 284 284 201 30 150 246 201 30 150 246 277	7 2 10 1 26 27 28 1 79 2 27 1 28 1 79 2 27 1 17 1 20 7 38 2 138 3	2 -14* -8 9 23* -3* -3* -3* -2* -21* -2 9* -25* -7* -10 25* -3
15 16 17 18 19 0 1 2 3 4 5 6 7 8 9 0 112 13 14	299670±1335594524666765	291560 1560 1540 8849590 89975	2^{*} -1 -6 [*] -11 -14 -14 -18 -18 -126 -11 -14 -18 -126 -12 -12 -12 -12 -12 -12 -12 -12 -12 -12	9 10 11 12 1 0 12 3 4 5 6 7 8 9 19 8 - 18 - 18 - - - - - - - - - - - - -	245 245 269 14K=9 270 207 207 207 207 207 207 205 307 205 205 205 205 205 205 205 205 205 205	7 6 9 8 0 10 6 7 6 2 7 9 8 1 9 8 1 9 8 1 9 8 1 9 8 1 9 8 7 6 2 7 9 8 10 6 7 6 2 7 9 8 0 9 8 9 8	-5 17 5 8 5 10 -1 -6 14 8 -4 19 -7 -19 -19 -14 -1	17 18 -118 -117 -117 -117 -117 -1109 -165 -109 -165 -17 -17 -1109 -17 -17 -17 -17 -17 -17 -17 -17	255 = 27 1, K = 271, K = 27 1, K = 27 1, K = 271, K =	2 6 11 17 11 15 6 2 10 2 6 5 13 118 10 4 10 7 9	$ \begin{array}{c} -13^{*} \\ -8 \\ 3 \\ -7 \\ -13 \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -18 \\ -18 \\ -2 \\ 14 \\ 9 \\ 21 \\ 26 \\ \end{array} $		223 79 134 63 164 322 605 276 409 106 276 409 106 372 199 205 178 108	6755518570896750810668	$\begin{array}{c} -8 \\ 11 \\ 1 \\ -8 \\ -15 \\ -8 \\ -11 \\ -20 \\ -2 \\ -3 \\ -7 \\ -4 \\ -3 \\ 5 \\ 13 \\ -0 \\ -20 \end{array}$	1345 21298765432101234	187 96 165 165 245 285 201 30 150 245 201 30 150 245 201 30 245 201 20 277 20	7 2 10 1 26 2 7 2 8 1 7 2 8 1 7 2 8 2 13 2	$\begin{array}{c} 2 \\ -14^{*} \\ -8 \\ 9 \\ 23^{*} \\ -3 \\ -3 \\ -3 \\ 24 \\ -2 \\ 21^{*} \\ -2 \\ 9^{*} \\ -1 \\ 25^{*} \\ -7 \\ 17^{*} \\ -10 \\ 25^{*} \\ -3 \\ -13^{*} \end{array}$
156789 1234567890 112345 112345	29788K744214454805611030	291560 1560 1540 8849590 899751 31	2^{*} -1 -6 [*] -11 -14 -14 -18 -18 -18 -18 -18 -18 -18 -18 -18 -18	9 0 1 1 2 3 4 5 6 7 8 9 9 8 7 6 5 	245 245 210 14K 20 20 217 20 217 20 217 20 217 20 217 20 217 20 217 20 217 20 217 20 217 20 217 20 20 217 20 20 20 20 20 20 20 20 20 20 20 20 20	7 6 9 8 9 10 6 7 6 9 10 6 7 6 9 10 6 7 6 9 10 6 7 6 7 6 7 6 7 6 7 6 7 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 <	-5 17 5 8 5 10 -1 -6 14 8 -4 6 19 -7 19 -7 19 -7 19 -12 -14 -11	17 18 -18 -18 -18 -116 -15 -132 -109 87 65 -4 	255 = 2711 1, 127 1, 127	2 6 11 17 11 15 6 2 10 2 6 5 13 1 18 10 4 10 7 9 10	$ \begin{array}{c} -13^{*} \\ -8 \\ 3 \\ -7 \\ 4 \\ -13 \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -12^{*} \\ -2 \\ 14 \\ 9 \\ 21 \\ 26 \\ 29 \\ \end{array} $		213 223 79 134 63 164 322 605 276 409 103 103 193 103 193 103 193 103 193 103	675551815708967508106689	$\begin{array}{c} -8 \\ 11 \\ 3 \\ -15 \\ -15 \\ -8 \\ -11 \\ -20 \\ 3 \\ -7 \\ -14 \\ -35 \\ 13 \\ -0 \\ -20 \\ 2 \\ \end{array}$	1345 2110987654321012345	187 96 365 165 245 284 201 39 150 245 201 30 30 30 279 279	7 2 1 1 2 2 1 1 2 2 1 1 1 2 2 1	2 -14* -8 9 23* -3 -3 -3 -3 -3 -3 -2 21* -2 -2 -2 -7 17* -25* -7 17* -10 -15* -13* -13* -13*
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STRUCTURE FACTORS CONTINUED FOR C(20)H(30)P(2)I(2)PT

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-5	1 34	6	8	6	140	5	-6	-11	151	5	-3	-10	35	2	144	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	1 39	5	-4	-9	315	8	11	8	44	33	12		H,K=	3	3
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-1	179	10	-5	10	375	10	10	-7	378	10	11	-6	0	2	-9,4	-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	194	-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	84	-14	159	6	3
4	17	2	-1-	15	72	13	-201	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	144	-12	110	7	-10
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-18	269	9	3	18	75	35	-241	<mark>۲</mark> 1	484	12	-9	2	38	22	12*	-10	255	7	-13
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-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
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-6	607	15	19	13	213	6	11	3	393	10	-1	5	74	13	-22	-14	113	9	0
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-3	241	6	-27	16	120	8	-14	6	98	5	12	8	151	5	3	-11	18	2	-17*
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.0	361	9	-9	-17	176	8	. 5	9	147	6	0	11	36	2	- 32*	- 8	265	7	-3
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24	258	33	-13	-15	162	6	-3	11	195	7	-3	13	116	10	-9	-6	324	8	-6

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

L	FOB	SG	DEL	L	FOB	SG	DEL	1 .	FOB	SG	DEL	L	FOR	SG	DEL	L	FOR	SĠ	DEL
-5	426	14		-10		2	-194-	46	779	ā	4.6		604	16	-4		26.8	7	4
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-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	144	6	251	7	5	-2	94	6	- 4
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2	320	8	-10	-3	1 30	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	- Â	52	10	30*	-6	780	20	8	13	1 39	7	-7	5	292	8	6
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10	169	- 5	· 0	. 5	249	9	4	-1	93	7	14	-17	195	7	3	10	56	28	18*
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15	116	10	3	10	25	2	21*	- 4	733	20	-14	-12	86	7	-13	- 8	48	15	24*
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-1	219	6	6	-12	57	17	22*-	16	175	6	3	6	182	6	-2	-19	43	-39	- 33*
0	43	9	234	-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*
5	28		444		4 8 8 9	28	-28 -	4 2	4 2 7	ŝ	4 2	ā	464	Â	-7		767	40	4.2
<u>د</u>	7 64	4 0	E .		82.9	27	-64 -	13	476	7	1.2 1.2	40	147			E	571	70	164
3	370	10		· • • •	000	22	-01 -	12	1/0		2	10	103		. 1	-13	20	2	
4	34	12	10	· •2	02	2	+20+-	11	37	20	-6-	11	102	ſ	-3	-14	4/8	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	<u> </u>	797	20	-45	- 8	328	8	3	14	70	31	64	-11	58	- 6	. 8
- A	4.25	· 6	ā	6	678		- 4 h	- 7	170	4.2	_0	· • •	4.K-	Ţ.		-48	96	i.	ā
· · · ·	197	7	.7		2020	10	-14		717	10	-7	!	1984		, O	-16	70		7
7	121	(-/	0	207	0	2	-0	274	Ö	-14	-14	45	25	-0-	- 7	IJ	2	-7*
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	1 52	-8	3	-6	967	25	16
13	195	7	2	16	197	10	q	- 2	181	5	ź	-10		2	- 24		27.0	~ 7	۰ ۵
4 6	20	 	 		H . K -			<u>ج</u>	75	42	تى 4 م #	C	404	۲ ۲	~~~~		6074		
	37 1. M-	5	- 27				2 C	-1	37	12	10"		130	0			1031	20	-13
		51) 7	-17	29	Ž	0-	- 0	212	Ø	-3	-0	44	13	24ª	-3	140	2	-Z3
-12	>2	25	20*	-18	167	7	-5	1	129	5.	4	-7	265	8	-5	-2	212	6	- 8
	-	·					F	-		~	_			- 1	- 6 -			-	

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

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L	FOB	SG	DEL	L	F 08	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	. L	FOB	Se.	DEL
0	117	5	-10	-16	98	9	1	9	156	6	3	-17	41	22	17.4	· 4	222	7	8 -
1	1 32	- 4	8	-15	233	8	-,3	10	40	2		-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	I	H,K=	5	9	-13	234	7	-9	8	276	8	-5
5	4.	2	-26*	-11	40	15	64	*-12	26	2	194	-12	383	10	1	9	96	6	6
6	771	23	7	-10	1 58	5	5	-11	182	7	-5	-11	80	- ĝ	-5	10	211	6	-8
7	Ō	2	-12*	-9	70	14	0.4	-10	54	14	84	-10	91	4	-2	11	45	22	18*
. 8	286	8	12	- 8	1 2 2	5	n	-9	1 32	Â	-2	-9	+ 39	5	- 0	12	1 79	7	-7
ğ	45	10	12*	-7.	363	10	-10	- 8	19	2	. 81	× -8	48	á	7	13	89	11	-13
10	59	13	- 6+	-6	252	7	6	-7	148	5	3	-7	52	15	54	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	Ĩġ	-1	-5	199	6	-4	-5	332	Ťģ	10	I	I.Ka	6	. 6
13	36	2	-36+	-3	328	Ξģ	7	-4	î.	2	-4	* -4	743	20	11	-17	101	ğ	
44	282	- R	-4	-2	275	7	7	- 7	222	ā	7	- 7	787	4.0	4.	- 1 6	56	28	
46	76	2	4 6 #	-4	67	6		- 3	232	2	-474	-3	501	10		-16	468	20	-5
10	1 9 0	<u>د</u>	10-	- 1 - 1	03	6		- 2	750	2	-11	-2	457	19	-14	-12	100		
10	107	14.		U	211	7	2	-1	202	. 9	2	-1	173	4	-14	-14	04	17	-11
	1, 5	21). <u>5</u>	-1	69		1	0	. 43	2		- 0	107	2	4	-13	221		-1
-19	27	2	14*	2	114	4	-3	1	236	8	-2	. 1	12	2	-20-	-12	142	11	. - y
-10	01	11	- >-	- 3	339	y ,	- 1	2	9	2	. 51	- 2	63	ſ	.12	-11	160	, p	· D
-1/	113	(- 3	- 4	233	6	13	3	202	7	-7	3	30	2	51	-19	151	6	4
-16	221	10	-7	5	467	12	1	4	39	22	22'	- 4	439	11	· 6	-9	95	7	5
-15	21/		-6	b.	209	6	11	5	156	.9	-7	. 5	160	5	-15	- 8	143	- 5	9
-14	391	10	13	. (289	8	6	6	57	12	15'	. 6	480	12	-3	-7	232	8	1
-13	203	6	8	8	211	8	-7		100	(-4	. /	203		-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	1 34	6	- 8	9	144	9	6	9	135	11	-4	-4	127	8	-7
-10	108	4	-1	11	36	2	-14	r 1	H,K=	5	11	10	1 32	11	-0	- 3	-363	9	10
-9	20	2	4*	12	1 36	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	84	^r 13	52	17	-13	6	142	5	-3
-6	448	11	-5	ł	l,K≡	5	, 7	-1	153	7	- 4	-14	151	9	-11	1	87	9	-3
-5	403	10	1	-16	0	2	-49	۰ ۲	29	.2	201	15	10	2	-454	⁺ 2	109	9	1
-4	634	17	-19	-15	207	14	3	1	137	6	10	1	H,Km	6	, 4	3	242	7	-4
-3	287	8	-4	-14	16	2	-214	н <u></u> ј	H,K#	.6	, 0	-19	60	33	21	- 4	118	.6	10
-2	342	9	-10	-13	184	8	2	-20	85	48	Ö.	¹ -18	19	2	-194	5	401	10	2
-1	16	2	- 5*	-12	54	11	10'	-18.	68	35	. 64	-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	۵	-14	523	14	18	-15	200	11	-15	8	118	8	-11
2	285	8	5	-9	1 38	5	-4	-12	323	-9	15	-14	305		11	9	140	6	-1
3	317	8	3	- 8	61	8	n	-10	50	27	-24	-13	285	8	2	10	74	15	-114
L.	427	11	-13	-7	272	A	-7	-8	106	12	-1	012	297	A		11	67	16	-14
5	254	Å,	-9	-6	85	ā	-12	-6	748	4.8	à	. 16	1 7 2	R	4 7	12	49	17	- -
ś	391	+ 7	Ó	-5	432	44	-2	- 4	840	24	-74	- 1 1	1 72	័ត		4 7		4.4	-13
7	462	5	4	-4	4 28	- <u></u>	7	- 2	6092	46	- 12	0	132		4 7 8	1.J.			. A
.r A	204	6	-5		120	2		- 2	404	10	-12		40	1.0	1.3	- + +	19 5. .0	2	a ∪ 4
0	100	7	-7	- 3	341	10	11	' U 2	101	2	10	7	20	0. E	10	-14	227	7	~22
10	99	6	-+9	ے 1 – 1	172	10	1.5	<u>د</u>	765	20	· 7	-6	194	5	-2	-13	21	2	-24
11	65	1 0	-19	n	7.8	4.4	- 7	Ā	644	46	-17	-5	484	12		-11	186	6	. 2.
12	199	7	-0		4 74	7	-9	. U	275	10	17	- 4	457	4 2	7	-+	6.8	+2	-12
47	1.50	. 7		* 2	191	24	ر د د ــــــ	F 4 A	372	4 A	· 13	۳۳ ۳. ـــ	7/3	13		0	4 4 0	4 3	- <u>0</u>
4 J.	195	7	- T 2	2	24	24	-3	· 10	74	11	2	- 3	471	12	-11	- 3	112	12	-0
14	220	ſ	1	5	213	5	- 2	12	130	1	-13	-2	2/0	14	b	- 8	05	ō	9
15	00	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*
•	1 • K.#	51	5	6	118	6	-5	1	1. K=	61	2	1	-27	2	÷0*	- 5	240	7	-13
-18	61	21	-11*	7	258	7	8	-19	1. Ö	2	-251	2	- 93	· 5	-6	-4	43	11	36*
-17	184	10	10	· 8	127	12	-12	-18	27	2	-20	<mark>۲</mark> 3	185	6	4	- 3	343	- 9	. 7

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

L -2	F08	SG	DEL	L 7	F08	SG		L -6	FOB	SG	DEL	L.	FOB	SG	DEL	Ļ	F08	SG	DEL
- 1	292	2 8	9	Ŕ	419	4.4		-0	277	8	-1	2	201	2		. 'A	263	4.0	J
ō	72	11	2	ğ	71	12	-1	-4	220	6	-3	-1	.276	8	5	ğ	172	11	B
1	160	-5	-4	10	213	8	13	-3	371	10	6	ō	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 _y K=	8	• 4
ſ	210	1	2	0	1, K≇ ⊿Ω:	1	• 3	.3	164	5	-10	5	60	15	38-	-18	- 99	7	. b
0 0	470	20	11	-17	- 17	2	-27	- 4	107	0	-2		110	0	1	-1/		27	-13-
10	33	2	114	-17	14	2	-23	н <u>Б</u>	184	6	-0	-20	79 ∿ ₽ 211	12	15	-10	90 90	ģ	. 1
	1. Ks	6	10	-16	1 37	9	-3	7	288	8	2	⊂18	42	2	-13*	-15	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	Ē	-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	-18	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		1, 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	Z30	8	-4	-1	5	2	-27	-14	0	2	-91		544	14	-20	-5	11 4	5	1
U	474	2	21*	-0	130	4	1	-13	234	8	5	<u>ک</u>	2/2	9	16	-4	334	9	-3
. <u>.</u>		- 3			500	45	-1	-12	260	. 17	-0-		137	0	1	-3	377	7	-2
2 7	127	6	-7	-7	569	17		-11	477	6	-1	U A	312	2	-18		437	11	72
4	60	22	-6*	-2	727	20	-13	-9	161	6	2	10	- 317. - 248	7	23	- T	304	A	- 2
5	122	11	-18	-1	259	7	-14	-8	136	7	3	12	184	12	-18	. 1	155	ଁଁ	7
ł	I.Ks	. 7	1	Ō	304	8	-10	-7	138	5	. 2	14	130	11	-23	2	122	7	-11
-20	1.32	10	- 7	1	29	2	71	-6	89	12	1	I	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	- 34	3	38	34	-0,	* =4	36	2	19'	-18	73	12	-8	5	125	5	-6
-1/	0	2	-5+	4	81	8	-13	-3	362	10	6	-17	35	21	29*	· 6	235	7	-9
-10	122	9	U 	· 7	100	0	-1	-2	35	2	-18	-10	42	35	2-	1	183	0	-14
~17 -16	256	19	- 0+ 5	7	504	O A		-1	207	7 8	10	-17	202	18	-3	0	274	7	- 44 · 7
+13	152	- 6	-6	8	262	11	5	4	170	7		- 1 T	203	10		- 4 0	196	42	2
-12	534	14	. 8	ğ	141	10		2	195	6	2	-12	542	14	9	11	108	7	E . R
-11	84	14	. 6	10	222	1 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	18	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*	-16	0	2	-43*
-7	D	2	-27*	14	93	12	3	7.	236	7	0	-7	56	- 7	1	-15	73	11	-1
-6	181	7	12	+	1, K=	71	, 5	8	47	17	11	-6.	45	. 9	7+	-14	28	2	-20+
>	105	10	5	-18	0	2	-53	• 9	1/1	10	-0	-5	213	8	20	-13	222	9	-13
-4	<u>(U/</u>	19	27	-11	30	2	11	- 10	0	2	-26	-	404	12	21	-12	100	8	· 1
-3	21/	24	-15	-10	4 74	44	ب کست	11	113	9	<u> </u>	-3	330	45		-11	320	y 6	1
- C - 4	65	<u> </u>	-15	-12	1.37	6			454	7	-1	- 2	266	10	-5	-1u -0	274	, D	46
ñ	239	7	18	-13	285	Å		-10	T 24	2	-171	- T	200	12	-7	- 9	178	7	
- 1	105	7	-8 -	-12	211	6	-3	-9	111	8	-0	1	30	19		-7	102	6	2
ź	182	6	14 -	-11	264	.8	2	-8	38	32	24	2	135	ົ້ງ	-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	251	F 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	1ª	- 6	357	10	2	-2	100	6	-12

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

L	F 08	ŚG	DEL	Ľ	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	E	FOB	SG	DEL
-1	388	10	18 .	-10	576	17	-7	13	27	2	-4*	⊦	I∎K≡	ં 9 ₁	9	- 4	178	6	2
0	213	6	-3	-9	11	2	-264	۴ ۴	1 , K=	91	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	314	-16	64	13	-21*	-8	43	20	7*	7	103	10	0
3	153	6	-4	-6	37	15	-194	-15	14	2	-10*	-7	189	7	5	8	217	7	-16
4	89	9	3	-5	42	11	234	-14	71	14	-8*	-6	0	2		- 9	73	18	-8*
5	177	7	-6	-4	153	- <u>-</u>	16	-13	180	7	-13	-5	175	6	-4	10	210		-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	Ō	641	16	-5	-9	292	8	2	-1	177	10	-6	-18	164	11	-4
10	70	12	-11	1	46	13	204	- 8	247	7	-8	Ō	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	74	-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	. 1	1.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	-14	۳ <u>آ</u>	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	564	۲Ž	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	F 4	169	6	-9	-6	53	25	8*	-5	47	10	12*
- 3	274	8	-5	1	1 , K #	91	3	5	80	11	-16	-4	49	21	15*	-4	112	5	-12
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STRUCTURE FACTORS CONTINUED FOR C(20)H(30)P(2)I(2)PT

L	F 08	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	.L	FOB	SG	DEL	L	FOB	SG	DEL
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. 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
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5 e	57	2	- 8-	-18	212	11	6	-13	70	17	-2*	-6	337	. 9	-3	-1	153	6	-18
7	20	2	10-	-11	91	17	-2.	-12	24	32	5*	-7	30	2	9 -		0/	10	3*
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-7	188	7	g.	-7	163	-6	- 9	-2	65	12	-9	5	60	14	34	-7	225	7	7
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-5	164	7	2	-5	48	26	-3*	ō	53	29	12*	7		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	- <u>-</u> 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*	ł	1.K=	12	, 4	-1	103	11	-6
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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	1	1, K#	11	, 9	-14	66	11	-4	1	i,Ke	13	• 1
3	191	7	3	3	174	7	. 5 .	-7	225	10	8	-13	0	2	-25*	-17	29	2	~11 *
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-12	134	8	5	-14	58	16	-13*	-12	0	2	-26*	-2	31	2	-14	-6	421	11	-9
-11	53	21	9#	-13	79	15	-1	-10	233	18	10	-1	148	ģ	-1	-5	39	2	g.
-10	430	11	9	-12	46	23	5+	-8	390	11	21	Ō	122	ġ	-10	-4	290	8	6
-9	133	-7	-6	-11	179	8	-9	-6	333	15	-9	1	209	7	-3	-3		2	-19*
~8	463	12	-6	-10	127	7	-6	-	155	8	-3	2	274	8	7	-2	47	13	-4*
-7	106	14	0	-9	253	7	-6	•2	195	13	-4	<u> </u>	142	. 7	-0	-1	36	18	12*
~B	184	7	-4	- 8-	199	8	-4	0	197	7	-3	<u> </u>	237	9	4	0	129	8	-14
-5	26	2	22*	-7	183	7	-2	-2	364	10	8	5	- 51	2	-13*	1 d.	100	7	8
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STRUCTURE FACTORS CONTINUED FOR C(20)H(30)P(2)I(2)PT

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- 12 3	20	2	-75+	4	4 26	40	-6	1	52	7 A .	-74	n	1 2 1	7	-7	- 4	110	10	
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-9 17	8	6	6	-16	263	21	1	4	123	8	-1	- 3	101	14	· 1 ·	-1	56	16	* 2 *
-8 2	55	9	8 ·	-14	214	9	-2	5	149	10	18	4	134	6	10	0	109	10	-2
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-5 7	73 1	14	- 6*	-8	241	14	-5	-10	47	25	15*	•11	17	2	-4*	-12	197	13	-2
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-3	8	2	-11*	-4	313	9	8	- 8	38	2	16*	-9	-53	23	5*	-10	126	10	-4
-2 3	37	2	-12*	-2	90	16	5	-7	196	- 7	-3	-8	50	24	21*	-9	0	- 2	=26*
-1 3	33	2	-19*	0	127	18	-6	-6	83	11	2	-7	160	9	-3	- 8	60	25	-16*
0 14	2	8	-4	2	118	12	-21	-5	241	8	8	-6	62	21	-2*	-7	40	2	34*
1 17	15	6	-6	4	242	11	8	-4	133	13	-4	-5	224	7	9	-6	71	15	-27*
2 28	54	1.0	-6	6	224	19	21	- 3	162	- 9	15	-4	145	13	4	-5	60	44	1+
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-10 3	31	2	-33*	- 5	65	13	-15*	-9	60	15	- 51 *	-4	232	8	-11	- 5	79	36	-19*
-9 15	50 1	L1	-5	-4	238	7	7	- 8	125	12	6	-2	155	10	3	-4	142	9	-10
-8 9	99 g	11	-7	-3	. 0	2	-25*	-7	28	2	15*	0	99	17	18	-3	109	19	-6
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