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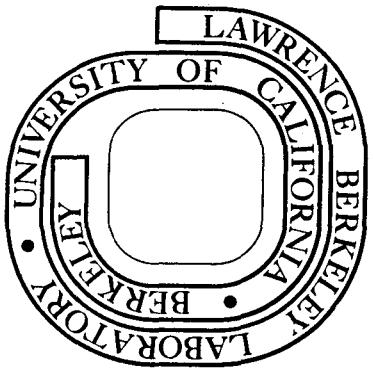

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CESIUM HYDROGEN TARTRATE AND ANOMALOUS DISPERSION OF CESIUM

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ABSTRACT

Cesium hydrogen (+)-tartrate is orthorhombic, $P2_12_12_1$, a = 8.076(3), b = 11.621(5), c = 7.692(3) Å, Z = 4, D_x = 2.594 g cm^{-3}, at 22°C. Its structure, nearly the same as that of ammonium hydrogen tartarte, was refined to R = 0.016 for 2442 reflections ($F^2 > 3\sigma$) out to d = 0.66 Å. Our least-squares program was modifed to treat anomalous dispersion terms as independent adjustable parameters, and f" for cesium was determined as 2.22(6) electrons for MoKα radiation. In the determination of absolute configuration or polarity, refinement of f" for a heavy atom has the advantage that one can detect inversion twinning, as well as save on computational time.

INTRODUCTION

Anomalous scattering of x-rays and its use in diffraction analysis is receiving wide attention (Ramaseshan and Abrahams, 1975), but there remains a need for more detailed and accurate knowledge of these dispersion effects, especially for the heavier atoms and near the L edges. The availability of synchrotron radiation (Phillips, Wlodawer, Goodfellow, Watenpaugh, Sieker, Jensen, and Hodgson, 1977, and references therein) as a sharply tunable and intense source permits diffraction experiments at arbitrary wavelengths and gives a new opportunity for experimental measurement of the dispersion corrections.

There is strong correlation between scattering factors, thermal parameters, and scale factors, and relatively few reflections can be observed at long wavelengths. These facts require one to have independent information of some of the parameters if accurate scattering factors are to be obtained from the diffraction intensities. In anticipation of experiments with cesium in the neighborhood of the L edges, we have determined the crystal structure of cesium hydrogen (+)-tartrate using MoKα radiation, for which the dispersion corrections are relatively small, and incidentally derived a value for f" for Cs at this wavelength.

Cell dimensions, slightly smaller than our values, were reported by Hémon (1931), but there appears to have been no further x-ray study of this cesium salt. The full structure was determined for the isomorphous ammonium hydrogen tartrate by van Bommel and Bijvoet (1958).

ANOMALOUS DISPERSION IN LEAST SQUARES

The method of least squares requires the derivatives:

$$\frac{\partial|F|}{\partial u} = \frac{A}{|F|}\frac{\partial A}{\partial u} + \frac{B}{|F|}\frac{\partial B}{\partial u} \qquad (1)$$

where u is a parameter and $F = A + iB$. If $f = f_o + f' + if''$ for a particular element, the derivatives with respect to f' and f'' have the simple forms:

$$\frac{\partial A}{\partial f'} = \sum T \cos Q \qquad (2a)$$

$$\frac{\partial B}{\partial f'} = \sum T \sin Q \qquad (2b)$$

$$\frac{\partial A}{\partial f''} = \sum -T \sin Q \qquad (2c)$$

$$\frac{\partial B}{\partial f''} = \sum T \cos Q \qquad (2d)$$

where $Q = 2\pi(hx + ky + lz)$ and T is the temperature factor. The sums include all the atoms of the particular element in the unit cell, whether they are related by symmetry or not.

In the calculation of f' or f'' by a series expansion (Hönl, 1933) the largest angle-dependent terms go as $\cos 2\theta = 1 - 2\sin^2\theta$. As a first step in looking for such effects in our experiments, we have expressed the dispersion corrections as:

$$f' = f_1' + f_2' \lambda^{-2}\sin^2\theta \qquad (3a)$$

$$f'' = f_1'' + f_2'' \lambda^{-2}\sin^2\theta \qquad (3b)$$

because of the custom of listing form factors as a function of $\lambda^{-1}\sin\theta$. Then the derivatives with respect to the angle-independent parts f_1' and

f_1'' are the same as given above for f' and f", and the derivatives with respect to f_2' and f_2'' differ only by the factor $\lambda^{-2}\sin^2\theta$:

$$\frac{\partial A}{\partial f_2'} = \lambda^{-2}\sin^2\theta \frac{\partial A}{\partial f_1'}, \text{ etc.} \qquad (4)$$

Similar relations occur if $\lambda^{-2}\sin^2\theta$ is replaced by some other function of θ.

Because of the simplicity of these relations, there is no difficulty in modifying a crystallographic least-squares program to include the anomalous dispersion parameters as independent variables, apart from the bookkeeping details of the various arrays. We have made such changes in our local program, Zalkin's LESQ. However, the rate of convergence and the reliability of the result are contingent on avoidance of excessive correlation.

With a chiral crystal which is known to be a pure enantiomer, f" for a heavy atom is determined by the magnitudes of differences in structure factors for Bijvoet pairs, and is little correlated with other variables, assuming that f" is known or negligible for other atoms in the structure. Thus one can expect f" to be well determined by data for a single x-ray wavelength. On the other hand, f' is strongly correlated with thermal parameters and is very subject to errors which are systematic with respect to scattering angle. We expect that its determination will be much improved by combination of data from more than one wavelength.

In this work enantiomeric purity is crucial, and one of our reasons for choosing a tartrate salt is the ready availability of pure (+)-tartrate. It is commonplace that questions of absolute

configuration are discussed as binary choices of right- or left-handed structure, without any consideration of mixtures related by inversion twinning. This is an appropriate procedure when the molecules themselves are a pure enantiomer, but not when the chirality exists only in the crystal structure or when one has racemic starting material. The refinement of f" for a heavy atom is a direct test for inversion twinning. Such twinning results in a magnitude for f" less than the correct value. The results described below are an example of good agreement with theory for a pure enantiomer. In a recent study of $U(BH_4)_4 \cdot O(C_2H_5)_2$ by Rietz, Zalkin, Templeton, Edelstein and Templeton (1977), an example of the second kind, this test revealed a 70-30 ratio of enantiomers. Since the addition of one parameter has an insignificant effect on the cost of refinement, this method is also more economical than the more common procedure of refining twice, once with each handedness. If one tests the wrong structure, f" simply refines to a negative value. The factor by which f" exceeds it standard deviation can be used as an index of the decisiveness of the determination of configuration. Similar statements apply to the question of absolute orientation of polar but achiral structures, except that then twinning is always possible.

EXPERIMENTAL

Cesium hydrogen (+)-tartrate was prepared from CsCl (Fisher, "purified") and (+)-tartaric acid (Matheson Coleman and Bell, "reagent"). Analysis by x-ray fluorescence showed 0.12% rubidium, and atomic absorption spectroscopy showed 0.03% potassium in the CsCl (0.24 mole % Rb and 0.13 mole % K relative to Cs). The best crystals were obtained by using a slight excess of CsCl; 2.9 g (19.3 mmol) tartaric acid and 3.30 g (19.6 mmol) CsCl were each dissolved in 6 ml water. The solutions were mixed and heated for 10 min, then let stand at room temperature. After several days numerous small crystals had formed in the sirup; some were needles and others were nearly equal in their dimensions. Weissenberg photographs of a needle showed it to be the same structure as the more nearly square habit.

A crystal about 0.14 x 0.14 x 0.25 mm in size was used for measurements with a Picker FACS-I diffractometer equipped with a graphite monochromator and Mo radiation (λ = 0.70926 Å for $K\alpha_1$). Cell dimensions were derived by least squares from the setting angles of 12 reflections ($40° < 2\theta < 50°$). Diffraction intensities were measured by θ-2θ scan technique at 2°/min for 2θ for all reflections in the full sphere ($\pm h, \pm k, \pm l$) up to $2\theta = 55°$, and for the half sphere ($\pm h, \pm k, +l$) up to $2\theta = 65°$ or d = 0.66 Å. The scan width was 1° in 2θ (up to 55°) or 1.2° (55° to 65°) plus the α_1-α_2 splitting. Background was counted for 4 sec (or 10 sec above 55°) at each end of the scan. Three strong reflections

(600, 060, 006) checked at intervals of 200 measurements indicated no decay within the accuracy of the experiment.

Absorption corrections calculated by an analytical integration (Templeton and Templeton, 1973) with the shape defined by 10 plane faces ranged from 1.539 to 1.907, with $\mu = 50.67$ cm^{-1}.

Measurements of 8963 reflections not excluded by the space group were averaged to give 2632 unique reflections (point group 222) for 2442 of which $F^2 > 3\sigma$.

CRYSTAL DATA

$CsHC_4H_4O_6$, space group $P2_12_12_1$; at 22 ± 1°C: a = 8.076(3), b = 11.621(5), c = 7.692(3) Å, Z = 4, V = 721.90 Å^3, D_x = 2.594 g cm^{-3}.

STRUCTURE REFINEMENT

Cesium hydrogen tartrate is isomorphous with ammonium hydrogen tartrate, and refinement starting with parameters for that salt (van Bommel and Bijvoet, 1958) converged with little change. Since our axes are chosen according to the convention of Donnay (1943), with a and c interchanged from the setting of van Bommel and Bijvoet, the coordinates must be transformed as 1/4 + z, 1/4 - y, 1/4 + x to retain right-handed axes and the standard choice of origin for $P2_12_12_1$. Scattering factors for Cs^+ and neutral C and O were taken

from Doyle and Turner (1968) and for H from Stewart, Davidson and Simpson (1965). Dispersion corrections were from Cromer and Liberman (1970).

With isotropic thermal parameters for hydrogen, anisotropic parameters for all other atoms, and with f" for Cs as an adjustable parameter, least-squares refinement reduced $R = \Sigma|\Delta F|/\Sigma|F_o|$ to 0.016 for 2442 reflections with $F^2 > 3\sigma$ and to 0.019 for all 2632 reflections. The weighted $R_w = [\Sigma w(\Delta F)^2/\Sigma wF_o^2]^{1/2}$, the quantity minimized, was 0.016. Zero weight was assigned to reflections weaker than 3σ; for others $w = (\sigma(F))^{-2}$; $\sigma(F)$ was derived from $\sigma(F^2) = [S^2 + (0.015\ F^2)^2]^{1/2}$ where S^2 is the variance due to counting statistics. An empirical extinction correction was applied which increased F for the strongest reflection by 6% and changed only 7 other structure factors by as much as 2%. In the last cycle no parameter changed as much as 0.03 σ. Final coordinates and thermal parameters are listed in Tables 1 and 2.*

RESULTS AND DISCUSSION

The value of f" for Cs refined to 2.22(6) electrons, in good agreement with 2.119 calculated by Cromer and Liberman (1970). Another refinement, with f" defined as in eq. (3b), yielded $f'' = 2.1(1) + [0.3(5)]\lambda^{-2}\sin^2\theta$, with insignificant changes in the other

*A listing of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No.

parameters and agreement indices. Thus the precision of this data set is not great enough to reveal any angular dependence of f".

The structure is nearly the same as that of ammonium hydrogen tartrate (van Bommel and Bijvoet, 1958). Bond distances (Fig. 1) and angles (Table 3) of the bitartrate ion are identical within about 5 times the estimated standard deviations. The cesium ion has nine oxygen neighbors (Table 4), eight of them approximately at the corners of a square antiprism, with the ninth, O(6), at a slightly greater distance capping one square face (Fig. 2). A similar arrangement occurs in the ammonium salt, but with shorter distances from nitrogen to its oxygen neighbors. Hydrogen bonds from O(1) to O(6), O(3) to O(6), and O(4) to O(5) are the same in the two salts, with O-O distances 2.58, 2.76, and 2.84 Å in the Cs salt and 2.55, 2.74, and 2.80 Å in the ammonium salt, respectively.

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Table 1. Parameters for Heavy Atoms. The form of the temperature factor is $\exp[-0.25(h^2a^{*2}B_{11} + 2hka^*b^*B_{12} + \ldots)]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cs	.33234(2)	.03245(1)	1.15984(1)	1.972(5)	1.876(4)	1.753(4)	-.021(4)	-.194(4)	-.075(4)
O(1)	.6303(2)	-.1364(1)	1.0462(2)	3.52(9)	2.28(6)	1.37(5)	.86(6)	-.40(5)	-.36(5)
O(2)	.7043(2)	-.3202(1)	1.0193(2)	3.77(9)	2.36(6)	1.79(6)	1.08(6)	-.36(6)	.24(5)
O(3)	.5722(2)	-.3332(1)	.6945(2)	2.02(6)	1.85(6)	2.07(6)	-.11(5)	-.22(5)	-.31(5)
O(4)	.8606(2)	-.1787(2)	.6841(2)	1.32(6)	3.00(7)	2.01(6)	-.20(5)	-.26(5)	-.11(5)
O(5)	.4830(2)	-.1129(1)	.4607(2)	1.91(6)	3.04(7)	1.83(6)	.52(6)	-.14(5)	.28(5)
O(6)	.7354(2)	-.1544(2)	.3611(2)	2.13(6)	4.11(8)	1.28(6)	.62(6)	.20(5)	-.26(6)
C(1)	.6455(3)	-.2330(2)	.9595(2)	1.59(8)	2.04(7)	1.22(6)	.21(6)	.10(6)	.11(5)
C(2)	.5805(3)	-.2230(2)	.7743(3)	1.44(8)	1.80(8)	1.20(6)	.23(6)	.04(6)	-.01(6)
C(3)	.6952(2)	-.1444(2)	.6700(3)	1.53(7)	1.64(6)	1.37(6)	-.04(5)	-.06(6)	-.19(6)
C(4)	.6323(3)	-.1366(2)	.4819(3)	1.89(8)	1.61(7)	1.40(7)	.07(6)	-.10(6)	.06(6)

Table 2. Parameters for Hydrogen Atoms. The form of the temperature factor is $\exp(-B\lambda^{-2}\sin^2\theta)$.

	x	y	z	B
H(1)	.468(3)	-.186(2)	.774(3)	1.0(4)
H(2)	.689(3)	-.076(2)	.714(3)	1.9(5)
H(3)	.474(5)	-.344(3)	.652(4)	4.8(8)
H(4)	.876(4)	-.237(3)	.638(4)	3.5(8)
H(5)	.648(5)	-.139(3)	1.158(5)	5.5(9)

Table 3. Bond Angles (Deg.) in Bitartrate Ion.

O(1)-C(1)-O(2)	124.1(2)	O(5)-C(4)-O(6)	125.2(2)
O(1)-C(1)-C(2)	112.2(2)	O(5)-C(4)-C(3)	117.1(2)
O(2)-C(1)-C(2)	123.7(2)	O(6)-C(4)-C(3)	117.7(2)
C(1)-C(2)-C(3)	109.2(2)	C(2)-C(3)-C(4)	109.2(2)
C(1)-C(2)-O(3)	110.5(2)	C(2)-C(3)-O(4)	111.6(2)
C(3)-C(2)-O(3)	109.9(2)	C(4)-C(3)-O(4)	113.9(2)
C(1)-C(2)-H(1)	110(1)	C(2)-C(3)-H(2)	108(2)
C(3)-C(2)-H(1)	107(1)	C(4)-C(3)-H(2)	107(2)
O(3)-C(2)-H(1)	110(1)	O(4)-C(3)-H(2)	107(2)
C(1)-O(1)-H(5)	117(2)	C(3)-O(4)-H(4)	112(2)
	C(2)-O(3)-H(3)	110(2)	

Table 4. Cesium-Oxygen Distances (Å).

Cs-O(1)	3.226(2)	Cs-O(4)^{iv}	3.012(2)
-O(2)^{i}	3.008(2)	-O(5)^{v}	3.113(2)
-O(2)^{ii}	3.019(2)	-O(5)^{vi}	3.116(2)
-O(3)^{i}	3.321(2)	-O(6)^{iii}	3.684(2)
-O(3)^{iii}	3.234(2)		

Symmetry Code:

i =	-1/2 + x, -1/2 - y, 2 - z	iv =	3/2 - x, -y, 1/2 + z
ii =	1 - x, 1/2 + y, 5/2 - z	v =	x, y, 1 + z
iii =	1 - x, 1/2 + y, 3/2 - z	vi =	1/2 - x, -y, 1/2 + z

FIGURE CAPTIONS

Fig. 1. View of the bitartrate ion with 50% probability ellipsoids, drawn with Johnson's ORTEP, showing molecular conformation, absolute configuration, and bond distances (in Å). The size of the hydrogen atoms is arbitrary. Standard deviations are about 0.03 Å for bonds to hydrogen and 0.003 Å or less for other bonds.

Fig. 2. Coordination polyhedron for oxygen neighbors of the cesium atom. The numbers and symmetry code are the same as in Table 4.

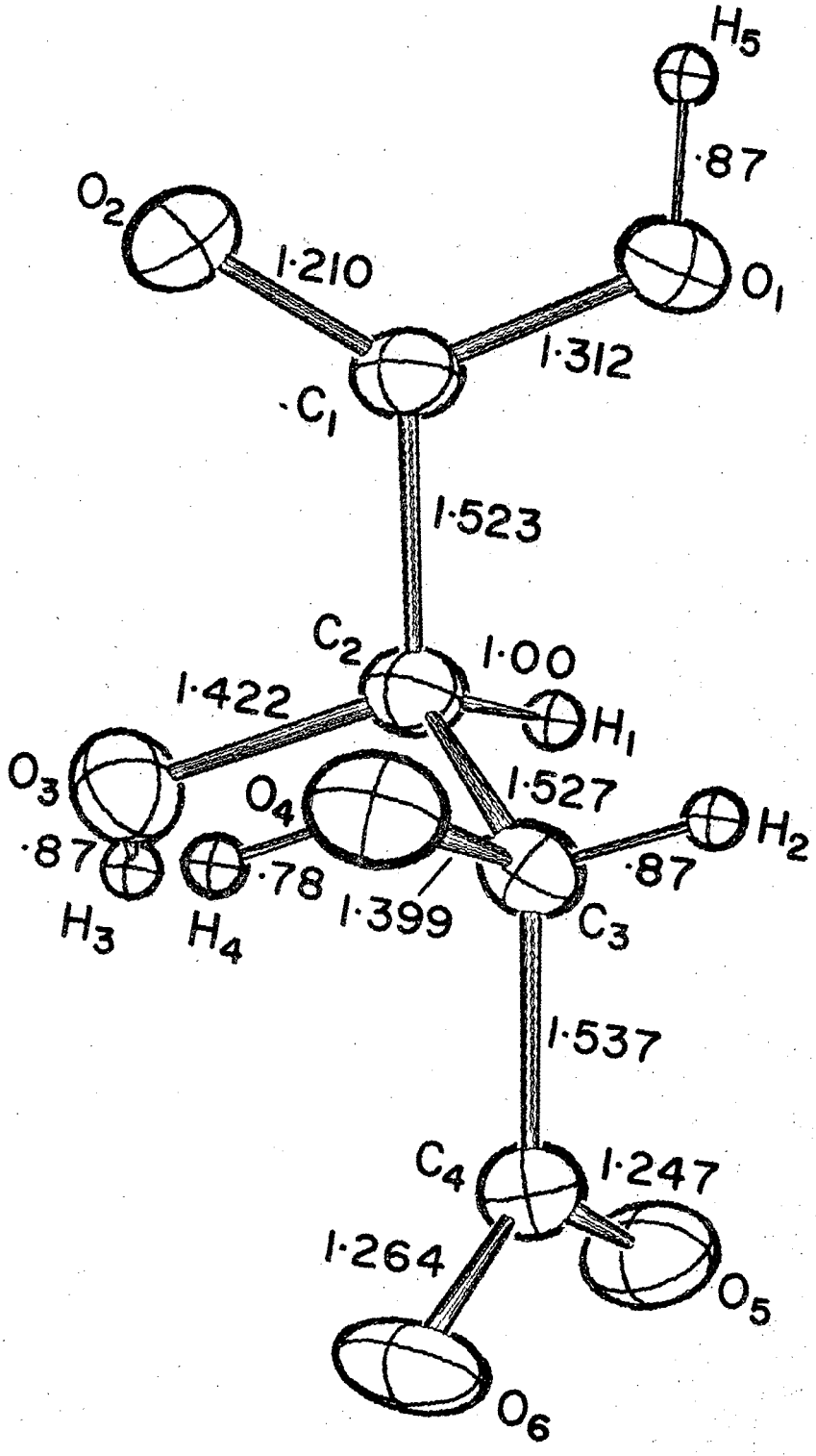

Fig. 1

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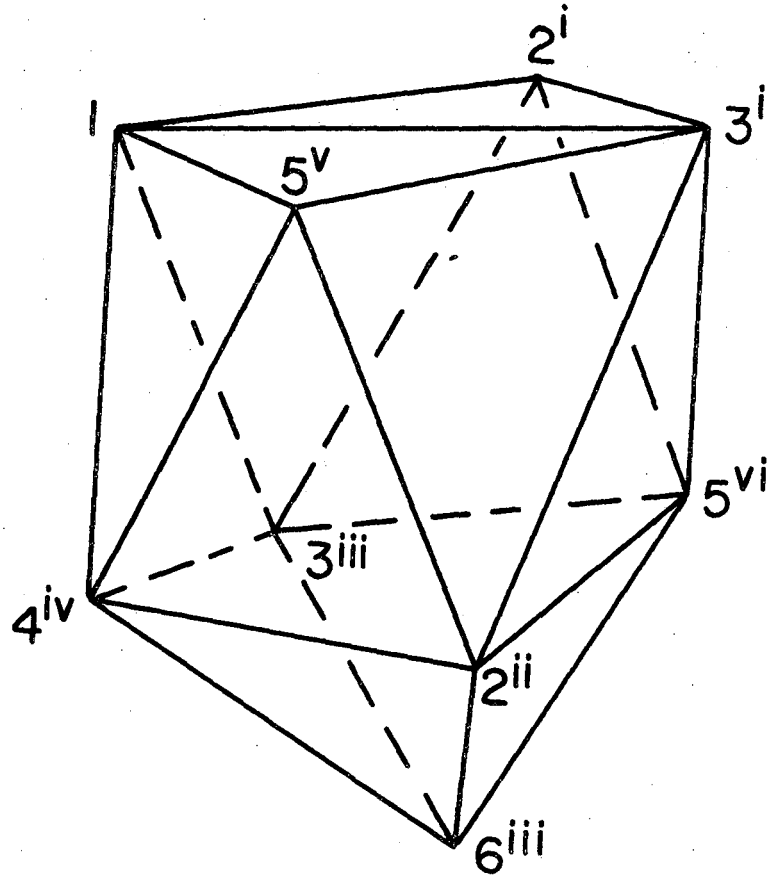

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Fig. 2

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 6.0)
CESIUM HYDROGEN TARTRATE F(0,0,0) = 3130

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		9	78	5	-1	3	589	5	-6	5	0	23	-17*	9	174	4	-0
2	311	2	-3	10	123	6	1	4	67	3	3	6	196	4	-3	10	167	5	0
4	323	3	-13	11	152	5	-4	5	156	3	3	7	61	6	3	11	26	22	3*
6	756	7	-17	H,K=	0,	5		6	28	11	8*	H,K=	0,	15		H,K=	1,	2	
8	128	3	-1	1	257	2	0	7	289	4	2	1	16	21	-4*	-11	95	4	-1
10	266	3	0	2	377	3	3	8	76	4	1	2	188	5	-6	-10	158	4	-0
H,K=	0,	1		3	419	4	-3	9	183	4	2	3	17	24	-0*	-9	129	4	-3
1	190	2	6	4	280	3	2	10	20	23	2*	4	167	6	-1	-8	324	4	-1
2	885	7	-28	5	57	3	9	H,K=	0,	10		5	32	10	18*	-7	142	2	-1
3	627	5	-4	6	89	2	-4	0	335	3	-5	6	80	5	0	-6	166	2	-0
4	660	5	-20	7	260	3	-1	1	425	4	-2	H,K=	0,	16		-5	246	3	-1
5	91	2	-3	8	199	2	2	2	101	2	1	0	222	6	-7	-4	566	5	-11
6	169	2	-0	9	232	3	5	3	17	19	4*	1	28	11	12*	-3	181	2	-4
7	127	2	-6	10	108	4	2	4	152	3	-0	2	133	6	1	-2	882	7	2
8	374	4	-7	11	21	27	12*	5	366	4	3	3	35	9	8*	-1	549	4	10
9	94	4	0	H,K=	0,	6		6	176	3	-3	4	127	6	-4	0	35	3	19
10	213	6	2	0	633	5	15	7	136	3	0	H,K=	0,	17		1	569	4	11
11	55	9	0	1	819	6	8	8	25	19	-1*	1	42	8	4	2	855	7	0
H,K=	0,	2		2	186	2	3	9	48	7	4	2	172	5	-9	3	187	2	-4
0	421	3	8	3	192	2	-0	H,K=	0,	11		3	61	8	3	4	576	5	-8
1	318	2	4	4	165	2	-1	1	199	3	1	H,K=	1,	8		5	236	2	-2
2	367	3	2	5	355	3	3	2	257	3	-4	1	378	3	6	6	162	2	-0
3	184	2	2	6	280	3	-1	3	236	3	4	2	742	6	2	7	159	2	1
4	556	5	-10	7	346	4	3	4	164	3	-1	3	338	3	10	8	322	4	-2
5	347	3	-7	8	36	9	-11*	5	66	3	3	4	475	4	-8	9	131	2	-0
6	450	4	-13	9	177	3	6	6	57	6	-4	5	252	2	-4	10	152	4	2
7	94	2	1	10	42	7	5	7	138	3	-7	6	251	2	-1	11	96	4	6
8	50	4	0	H,K=	0,	7		8	156	5	-1	7	239	2	-3	H,K=	1,	3	
9	0	20	-7*	1	371	3	3	9	146	5	2	8	333	3	-1	-11	100	5	7
10	188	3	-7	2	108	2	9	H,K=	0,	12		9	111	2	-2	-10	193	4	-1
11	109	5	2	3	846	7	-1	0	295	4	-2	10	85	4	2	-9	145	3	0
H,K=	0,	3		4	41	3	5	1	210	3	1	11	104	5	6	-8	155	3	-1
1	612	5	15	5	182	2	-1	2	84	3	6	H,K=	1,	1		-7	285	3	-3
2	854	7	14	6	59	3	4	3	54	4	4	-11	18	23	-4*	-6	438	4	-3
3	427	3	1	7	237	3	-0	4	150	3	3	-10	153	4	-6	-5	263	3	-4
4	457	4	1	8	44	8	-3	5	189	3	1	-9	186	3	3	-4	472	4	2
5	200	2	2	9	259	6	-2	6	182	3	5	-8	72	3	-3	-3	198	2	1
6	90	2	-2	10	42	9	8*	7	105	6	-5	-7	146	3	0	-2	451	4	10
7	207	3	-3	H,K=	0,	8		8	10	25	-2*	-6	451	4	-5	-1	580	5	9
8	338	4	-2	0	19	10	6*	H,K=	0,	13		-5	134	2	-4	01111		11	-7
9	165	3	1	1	457	4	-3	1	82	4	2	-4	383	3	-3	1	584	5	8
10	31	27	-8*	2	138	2	2	2	290	4	4	-3	641	5	-3	2	440	3	7
11	36	9	7*	3	76	3	0	3	193	4	-4	-2	383	3	2	3	180	2	-0
H,K=	0,	4		4	49	5	-1	4	219	4	-2	-1	239	2	1	4	483	4	3
0	188	2	-11	5	489	5	-2	5	53	5	5	0	723	8	-5	5	257	3	-3
1	578	5	8	6	43	4	2	6	48	9	-1	1	221	2	-2	6	438	4	-4
2	446	4	15	7	246	3	-1	7	30	14	7*	2	387	3	3	7	280	3	-3
3	103	2	2	8	23	14	14*	H,K=	0,	14		3	630	5	-1	8	157	2	1
4	332	3	2	9	76	6	7	0	284	6	-1	4	389	3	-1	9	140	3	-0
5	514	4	-3	10	43	9	8*	1	71	4	-2	5	141	2	-1	10	196	5	0
6	251	3	-1	H,K=	0,	9		2	108	3	-4	6	447	4	-4	11	94	5	-0
7	176	3	2	1	335	3	1	3	34	7	10*	7	143	2	-1	H,K=	1,	4	
8	30	13	4*	2	147	2	6	4	153	4	-3	8	80	3	4	-11	86	6	-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
-10	148	4	2	0	544	4	4	-8	133	4	0	9	50	11	-3*	-1	79	4	-3
-9	183	3	4	1	362	3	4	-7	185	4	1	H,K=	1,	12		0	253	3	2
-8	236	3	0	2	142	2	-3	-6	87	4	-2	-8	126	4	4	1	80	4	-4
-7	294	3	-1	3	632	5	-3	-5	340	4	3	-7	149	6	1	2	77	5	-5
-6	143	2	0	4	210	2	1	-4	152	2	5	-6	102	3	6	3	138	4	3
-5	401	4	-3	5	152	2	-3	-3	115	2	-3	-5	97	3	-1	4	114	4	1
-4	363	4	3	6	302	3	-1	-2	228	2	3	-4	197	3	-2	5	55	6	-2
-3	549	5	0	7	272	3	-3	-1	436	5	-0	-3	242	4	-4	6	171	4	3
-2	581	5	11	8	93	3	3	0	170	2	-2	-2	241	4	-2	H,K=	1,	16	
-1	567	4	11	9	213	3	6	1	442	4	2	-1	174	3	-1	-4	117	5	-3
0	236	2	-0	10	104	4	-3	2	221	3	3	0	200	3	2	-3	39	9	0*
1	555	4	12	H,K=	1,	7		3	115	2	-2	1	166	3	-4	-2	170	4	-8
2	586	5	10	-10	80	7	-4	4	159	2	1	2	242	4	-0	-1	81	5	8
3	563	5	2	-9	136	4	0	5	336	4	3	3	245	3	-3	0	42	5	6
4	359	3	-2	-8	134	3	-4	6	90	3	2	4	205	4	1	1	74	5	5
5	398	4	-3	-7	209	4	-3	7	184	3	0	5	101	3	2	2	179	6	2
6	124	2	-2	-6	121	2	-0	8	125	4	-7	6	97	4	-3	3	39	10	-0*
7	283	3	-1	-5	386	4	-1	9	80	5	-7	7	148	5	2	4	122	7	1
8	236	3	-4	-4	259	3	2	H,K=	1,	10		8	124	5	-0	H,K=	1,	17	
9	188	3	-1	-3	153	2	6	-9	160	4	7	H,K=	1,	13		-2	76	5	0
10	145	6	-2	-2	282	3	2	-8	101	7	-11	-7	96	5	-1	-1	60	6	4
11	93	4	4	-1	493	4	-3	-7	146	4	-5	-6	189	4	0	0	142	3	6
H,K=	1,	5		0	41	2	7	-6	130	4	-0	-5	109	3	-7	1	60	6	4
-11	167	6	1	1	498	4	-1	-5	140	3	-4	-4	141	4	-4	2	75	6	-0
-10	98	5	2	2	268	3	-3	-4	216	3	1	-3	148	3	-6	H,K=	2,	0	
-9	66	6	1	3	145	2	1	-3	330	5	3	-2	116	4	-1	0	699	5	2
-8	140	3	-1	4	251	3	-1	-2	209	2	-1	-1	126	3	-0	1	257	2	2
-7	216	3	1	5	382	4	-1	-1	295	3	0	0	328	5	-4	2	163	1	5
-6	257	3	-2	6	130	4	0	0	55	5	-1	1	119	4	-3	3	884	7	-4
-5	525	5	1	7	218	3	4	1	302	4	1	2	117	3	2	4	356	3	3
-4	285	3	4	8	134	3	-3	2	210	2	-2	3	151	3	-2	5	139	2	-0
-3	251	2	6	9	134	6	-2	3	333	3	5	4	142	4	-1	6	375	3	-4
-2	403	3	5	10	80	5	-1	4	204	3	-3	5	118	4	-1	7	356	3	-12
-1	608	5	3	H,K=	1,	8		5	140	2	-1	6	191	4	3	8	16	13	12*
0	467	4	8	-10	82	7	8	6	125	3	-2	7	107	4	5	9	231	3	-0
1	594	5	3	-9	203	4	5	7	157	3	2	H,K=	1,	14		10	112	5	-8
2	418	3	6	-8	33	9	-2*	8	107	4	-0	-7	53	9	-5	11	61	6	1
3	265	2	5	-7	180	3	2	9	147	5	-7	-6	69	7	-2	H,K=	2,	1	
4	276	3	1	-6	205	3	2	H,K=	1,	11		-5	119	5	2	-11	190	5	0
5	531	5	-1	-5	106	3	1	-9	57	7	2	-4	161	4	-0	-10	116	4	0
6	249	3	-2	-4	125	3	1	-8	85	6	-1	-3	60	5	2	-9	113	3	0
7	217	3	-2	-3	473	5	-3	-7	151	4	-6	-2	215	5	-3	-8	199	3	1
8	141	3	-2	-2	185	2	4	-6	125	3	3	-1	144	3	1	-7	234	3	-6
9	84	4	3	-1	214	2	-1	-5	215	3	2	0	60	5	0	-6	117	2	-2
10	93	4	-3	0	438	4	1	-4	219	3	-6	1	148	3	3	-5	559	5	-5
11	171	4	6	1	215	2	-0	-3	89	3	3	2	217	4	-0	-4	324	3	-4
H,K=	1,	6		2	187	2	2	-2	250	3	2	3	63	4	7	-3	341	3	7
-10	106	4	3	3	467	4	-2	-1	289	3	-1	4	159	5	-3	-2	499	4	-0
-9	213	3	1	4	126	2	5	0	121	2	-3	5	114	5	0	-1	667	5	-1
-8	92	3	-4	5	112	2	-2	1	290	3	-1	6	65	8	-6	0	675	5	7
-7	275	3	-1	6	200	3	3	2	255	3	2	7	52	8	-4	1	681	5	-0
-6	292	4	-0	7	183	3	-0	3	89	3	4	H,K=	1,	15		2	517	4	1
-5	151	2	1	8	32	9	-4*	4	220	4	-2	-6	169	5	0	3	351	3	9
-4	211	2	2	9	192	4	-3	5	212	3	-4	-5	59	6	1	4	310	3	-1
-3	636	5	-2	10	82	5	4	6	129	3	2	-4	115	5	3	5	555	5	-2
-2	127	2	-1	H,K=	1,	9		7	154	5	2	-3	132	4	-2	6	189	2	0
-1	364	3	5	-9	85	5	-5	8	83	5	-3	-2	74	5	-6	7	235	3	-1

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	199	3	2	-7	191	2	-2	3	238	2	5	-5	135	2	1	-5	79	5	-7
9	113	3	1	-6	155	3	2	4	388	4	-1	-4	234	3	1	-4	150	3	2
10	120	4	2	-5	240	3	2	5	282	3	-2	-3	262	3	-6	-3	287	2	2
11	187	4	-1	-4	437	4	-2	6	214	3	-0	-2	155	2	-1	-2	186	3	0
H,K=		2,	2	-3	398	3	-3	7	143	3	0	-1	186	3	-0	-1	188	3	1
-11	52	7	13	-2	623	5	1	8	250	4	2	0	602	6	-5	0	136	3	-1
-10	108	5	-3	-1	379	3	2	9	84	5	-2	1	198	2	-1	1	184	3	-3
-9	233	3	-0	0	292	3	3	10	109	7	-3	2	160	2	2	2	189	3	-2
-8	150	3	-4	1	382	3	3	H,K=		2,	7	3	267	3	-5	3	285	3	-3
-7	291	4	-1	2	638	5	3	-10	148	4	7	4	240	3	-2	4	141	4	-4
-6	217	3	-6	3	392	3	-6	-9	148	4	3	5	132	2	-1	5	88	3	4
-5	203	2	-1	4	424	4	-4	-8	38	12	-7*	6	323	4	2	6	109	6	6
-4	214	2	-1	5	230	2	1	-7	143	2	6	7	142	3	-1	7	153	4	3
-3	647	5	-1	6	143	2	2	-6	363	4	2	8	67	7	-0	8	100	5	0
-2	443	3	8	7	183	2	-3	-5	168	3	2	9	116	6	2	H,K=		2,	13
-1	655	5	-0	8	236	4	-4	-4	317	4	-1	H,K=		2,	10	-7	94	5	-1
0	408	3	-2	9	200	3	2	-3	304	3	-3	-9	57	8	-9	-6	89	4	0
1	658	5	1	10	90	5	-1	-2	236	3	3	-8	195	5	-2	-5	191	4	1
2	429	4	8	11	87	9	3	-1	221	2	5	-7	135	4	2	-4	116	3	0
3	644	5	-2	H,K=		2,	5	0	568	5	0	-6	107	3	2	-3	73	6	-6
4	230	2	0	-11	68	9	-5	1	208	2	1	-5	189	3	4	-2	152	3	-2
5	217	3	1	-10	157	4	-2	2	237	2	4	-4	288	5	-2	-1	203	3	5
6	229	3	-1	-9	137	3	1	3	310	3	-1	-3	217	3	0	0	93	3	1
7	305	4	-2	-8	56	4	2	4	319	3	1	-2	384	4	-0	1	193	4	0
8	150	3	-3	-7	148	2	2	5	154	2	-3	-1	199	2	1	2	150	3	-5
9	239	3	2	-6	299	3	3	6	351	4	-4	0	170	2	-2	3	78	3	-3
10	103	4	-3	-5	196	2	1	7	133	3	3	1	202	3	1	4	111	4	2
11	44	7	11	-4	417	4	3	8	42	8	-7*	2	381	5	-2	5	191	4	-5
H,K=		2,	3	-3	239	2	0	9	149	5	-2	3	217	3	-3	6	86	5	-1
-11	126	4	-2	-2	380	3	5	10	132	5	-3	4	286	4	-2	7	92	5	-2
-10	99	4	4	-1	338	3	5	H,K=		2,	8	5	177	4	-2	H,K=		2,	14
-9	114	3	3	0	472	4	1	-10	85	7	-3	6	112	4	4	-6	89	5	-5
-8	182	4	-3	1	332	3	4	-9	36	8	6*	7	135	3	-1	-5	40	8	-3*
-7	312	3	2	2	369	3	2	-8	247	4	6	8	187	4	-9	-4	81	4	5
-6	314	3	-6	3	229	2	0	-7	137	3	2	9	54	8	-14	-3	229	3	6
-5	439	4	-1	4	406	4	1	-6	78	3	4	H,K=		2,	11	-2	60	5	-1
-4	308	3	-3	5	210	2	2	-5	217	3	0	-8	74	6	1	-1	117	4	3
-3	304	3	-2	6	305	4	3	-4	291	3	1	-7	107	4	6	0	124	4	-4
-2	371	3	1	7	151	3	-2	-3	45	3	7	-6	177	4	2	1	113	3	-0
-1	770	6	-3	8	51	4	3	-2	481	4	2	-5	211	3	1	2	66	5	2
0	525	4	6	9	129	3	2	-1	310	3	3	-4	185	2	1	3	223	3	2
1	776	6	-3	10	162	5	5	0	64	3	-0	-3	165	4	-3	4	82	5	3
2	371	3	2	11	72	6	-3	1	307	3	0	-2	178	2	-0	5	43	8	-3
3	307	3	-1	H,K=		2,	6	2	471	4	2	-1	267	3	-3	6	85	7	-2
4	320	3	-2	-10	120	5	10	3	43	4	8	0	255	3	2	H,K=		2,	15
5	435	4	-3	-9	81	6	-6	4	296	3	-0	1	258	3	-5	-5	115	5	-4
6	324	4	-4	-8	241	4	-1	5	224	3	2	2	179	3	0	-4	100	4	6
7	309	4	0	-7	143	3	3	6	75	3	1	3	163	3	3	-3	56	7	2
8	183	3	-2	-6	214	3	0	7	130	3	1	4	183	3	-1	-2	110	5	-5
9	117	3	2	-5	284	3	2	8	244	4	5	5	218	3	-0	-1	180	3	4
10	96	6	-4	-4	388	4	-1	9	33	10	10*	6	176	4	-0	0	60	5	2
11	122	6	-9	-3	239	2	6	10	85	5	-3	7	102	5	3	1	184	4	2
H,K=		2,	4	-2	419	4	-4	H,K=		2,	9	8	74	7	3	2	111	4	-7
-11	81	5	-4	-1	318	3	6	-9	114	5	2	H,K=		2,	12	3	54	7	-1
-10	88	4	-1	0	281	3	5	-8	68	5	5	-8	104	5	8	4	91	5	-3
-9	196	3	-4	1	314	3	5	-7	140	3	2	-7	149	4	1	5	114	6	1
-8	242	4	-2	2	430	4	-2	-6	321	4	-1	-6	98	4	-4	H,K=		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
-4	77	6	2	-6	202	2	3	4	327	4	-2	-5	48	3	4	-9	46	13	-8*
-3	176	4	-2	-5	516	5	-7	5	422	4	-3	-4	438	4	-0	-8	41	10	9*
-2	52	6	1	-4	140	2	-0	6	329	4	-3	-3	58	4	2	-7	76	6	-1
-1	110	4	3	-3	142	2	5	7	169	4	-0	-2	604	6	-7	-6	228	3	-0
0	96	4	-5	-2	135	2	0	8	45	6	1	-1	85	2	1	-5	121	3	-2
1	102	4	-5	-1	642	5	-10	9	39	8	-4*	0	102	2	4	-4	260	3	3
2	52	6	7	0	347	3	3	10	164	6	-1	1	87	2	-2	-3	55	3	4
3	176	5	1	1	670	5	-6	H,K=		3,	5	2	615	6	-7	-2	222	3	1
4	75	5	-2	2	127	2	-1	-10	110	6	3	3	58	4	-0	-1	167	3	-1
H,K=		2,	17	3	136	2	4	-9	133	4	-3	4	434	5	-2	0	335	4	1
-2	96	5	-1	4	149	2	0	-8	320	4	-0	5	43	6	3	1	166	2	-3
-1	135	4	-2	5	511	5	-6	-7	151	3	4	6	93	4	3	2	215	3	-3
0	53	8	2	6	195	2	1	-6	55	3	1	7	47	6	1	3	59	4	6
1	138	4	-0	7	267	4	-1	-5	123	2	4	8	279	3	-1	4	255	3	-3
2	93	5	2	8	27	9	1*	-4	307	3	-3	9	29	14	-10*	5	123	3	2
H,K=		3,	0	9	114	4	4	-3	453	4	1	10	132	5	6	6	229	3	1
1	907	7	-27	10	71	5	-0	-2	605	5	1	H,K=		3,	8	7	79	6	-3
2	205	2	4	11	199	6	5	-1	149	2	0	-9	26	14	8*	8	37	10	5*
3	77	1	-2	H,K=		3,	3	0	83	2	2	-8	34	9	-9*	9	66	8	11
4	90	1	-0	-11	28	31	-3*	1	137	2	-2	-7	57	4	3	H,K=		3,	11
5	616	5	-2	-10	77	5	-3	2	603	6	-3	-6	349	4	4	-8	146	5	3
6	19	9	9*	-9	197	3	4	3	450	4	-1	-5	41	4	5	-7	103	5	5
7	321	3	-0	-8	162	3	2	4	297	3	-5	-4	302	4	4	-6	76	4	1
8	22	8	1*	-7	318	3	-2	5	125	2	-4	-3	57	4	7	-5	44	5	-1
9	116	2	0	-6	155	2	-2	6	59	4	6	-2	239	3	-2	-4	231	3	-2
10	32	13	-8*	-5	184	2	0	7	149	3	1	-1	99	2	1	-3	176	3	1
11	181	5	5	-4	377	4	3	8	320	4	-2	0	534	5	-8	-2	262	3	-1
H,K=		3,	1	-3	616	5	-0	9	136	3	2	1	180	2	4	-1	166	2	2
-11	25	30	5*	-2	374	3	-4	10	111	4	4	2	233	3	-6	0	40	5	-0
-10	38	12	8*	-1	404	3	3	H,K=		3,	6	3	58	3	7	1	166	3	-1
-9	304	4	-1	0	23	4	5*	-10	154	5	1	4	309	4	1	2	264	3	-0
-8	52	6	-8	1	394	3	2	-9	83	4	7	5	47	4	12	3	177	3	2
-7	285	3	1	2	351	3	-5	-8	59	4	5	6	347	5	1	4	237	4	-1
-6	53	4	5	3	616	6	3	-7	159	4	1	7	62	4	8	5	48	5	8
-5	176	2	-2	4	393	4	6	-6	443	5	2	8	48	7	2	6	70	5	-2
-4	226	3	3	5	180	2	2	-5	108	3	2	9	33	11	12*	7	105	4	6
-3	726	6	-10	6	156	3	0	-4	351	4	-1	H,K=		3,	9	8	138	5	-5
-2	205	2	2	7	316	4	-2	-3	96	2	2	-9	31	12	-6*	H,K=		3,	12
-1	620	5	10	8	155	3	-3	-2	301	3	-1	-8	241	5	2	-8	52	10	5*
0	24	5	11*	9	198	3	3	-1	299	3	1	-7	57	5	-2	-7	113	4	3
1	643	5	12	10	77	5	-3	0	762	7	-8	-6	85	4	2	-6	188	5	-2
2	213	2	1	11	43	13	12*	1	298	3	1	-5	32	9	8*	-5	193	3	5
3	730	6	-12	H,K=		3,	4	2	309	3	-5	-4	283	3	-1	-4	105	3	2
4	221	2	3	-10	170	4	1	3	95	2	0	-3	181	3	-3	-3	70	4	-1
5	173	3	-1	-9	50	5	4	4	340	3	-1	-2	415	4	-6	-2	56	4	2
6	51	4	1	-8	41	6	-3	5	186	2	7	-1	31	5	14	-1	221	3	5
7	288	4	1	-7	170	2	1	6	438	5	-0	0	72	3	-1	0	349	4	-1
8	62	4	2	-6	325	4	-1	7	158	3	1	1	20	10	1*	1	217	4	-1
9	304	4	1	-5	419	5	-8	8	52	5	1	2	407	5	-3	2	59	4	-2
10	20	24	-9*	-4	329	3	0	9	81	6	3	3	180	3	-4	3	67	4	0
11	16	27	-6*	-3	55	2	7	10	154	8	0	4	282	3	-2	4	95	3	2
H,K=		3,	2	-2	239	2	1	H,K=		3,	7	5	16	20	-12*	5	192	3	5
-11	192	5	4	-1	492	4	2	-10	128	5	2	6	80	4	-4	6	186	5	-3
-10	71	5	6	0	600	5	1	-9	30	12	-8*	7	67	4	2	7	109	4	4
-9	106	3	-8	1	477	4	1	-8	279	4	-1	8	237	6	-1	8	52	7	5
-8	28	19	1*	2	223	2	-0	-7	45	5	4	9	44	8	9	H,K=		3,	13
-7	268	3	1	3	54	3	0	-6	92	3	4	H,K=		3,	10	-7	136	5	-1

STRUCTURE FACTORS CONTINUED FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	41	8	6*	4	120	2	1	-6	241	3	1	7	207	3	-0	1	212	2	-2
-5	74	6	-1	5	103	2	-2	-5	363	4	0	8	103	3	1	2	426	5	-3
-4	126	3	-2	6	229	2	-1	-4	253	3	1	9	120	4	-6	3	27	6	7*
-3	278	4	0	7	272	3	-2	-3	191	2	1	10	109	4	-7	4	321	4	-6
-2	160	3	3	8	73	2	-0	-2	236	2	1	H,K=		4,	6	5	266	4	1
-1	161	3	-3	9	239	3	1	-1	423	4	-6	-10	79	8	0	6	57	5	0
0	24	11	8*	10	88	4	6	0	491	5	2	-9	115	4	2	7	61	4	12
1	155	3	-4	11	27	20	22*	1	419	4	-3	-8	205	3	0	8	226	6	-6
2	160	3	2	H,K=		4,	1	2	255	3	1	-7	159	4	-1	9	49	7	14
3	276	4	-4	-10	88	5	5	3	194	2	3	-6	107	3	-2	H,K=		4,	9
4	126	3	1	-9	67	5	1	4	254	3	0	-5	158	3	-1	-9	48	7	-3
5	66	5	-9	-8	190	4	-5	5	362	4	-0	-4	325	3	0	-8	76	5	9
6	33	20	-4*	-7	269	3	-1	6	235	3	-4	-3	169	2	-2	-7	128	3	5
7	132	4	1	-6	145	3	3	7	177	2	4	-2	433	5	-6	-6	287	3	5
H,K=		3,	14	-5	483	5	-8	8	102	3	-1	-1	287	3	2	-5	60	4	-1
-6	65	7	6	-4	204	3	-0	9	98	4	1	0	128	2	-1	-4	246	3	5
-5	222	5	-3	-3	130	2	2	10	97	4	-3	1	283	3	4	-3	174	3	-2
-4	47	7	-4	-2	486	4	-0	H,K=		4,	4	2	433	4	-7	-2	197	3	-3
-3	27	14	2*	-1	650	5	-5	-10	119	4	6	3	169	2	-1	-1	159	3	-1
-2	41	6	4	0	232	2	8	-9	116	4	-3	4	330	4	0	0	446	4	-4
-1	242	4	-5	1	635	5	-8	-8	240	3	4	5	167	3	-2	1	169	2	-2
0	73	5	4	2	468	4	8	-7	160	3	3	6	111	3	2	2	199	4	-4
1	241	3	-5	3	125	2	4	-6	161	3	3	7	164	3	4	3	179	3	-2
2	32	12	-3*	4	202	3	-8	-5	171	2	-1	8	214	4	1	4	238	3	2
3	30	16	0*	5	474	5	-9	-4	283	3	2	9	118	4	7	5	68	3	4
4	52	8	-4	6	148	2	1	-3	403	4	-3	10	86	6	5	6	282	5	-1
5	225	5	-4	7	271	3	-1	-2	412	4	-3	H,K=		4,	7	7	125	4	0
6	63	6	3	8	188	4	-4	-1	223	3	-5	-9	120	4	-2	8	72	5	8
H,K=		3,	15	9	70	5	-2	0	299	3	5	-8	33	22	-1*	9	59	6	9
-5	75	5	8	10	80	5	0	1	228	2	-5	-7	101	5	-0	H,K=		4,	10
-4	21	24	7*	H,K=		4,	2	2	414	4	-3	-6	310	3	3	-8	164	5	5
-3	209	5	-5	-10	104	5	-5	3	407	4	-2	-5	134	2	3	-7	113	5	2
-2	32	9	18*	-9	231	4	0	4	271	3	-0	-4	260	3	2	-6	78	4	2
-1	142	4	-2	-8	92	3	-1	5	166	3	2	-3	235	3	3	-5	115	5	1
0	19	22	6*	-7	242	3	-3	6	155	3	-0	-2	205	3	0	-4	232	3	2
1	139	4	-4	-6	198	3	-3	7	152	2	-0	-1	277	3	-1	-3	173	3	1
2	5	23	-11*	-5	252	3	2	8	234	3	-0	0	477	5	-6	-2	292	3	-3
3	213	5	2	-4	356	4	-3	9	124	5	1	1	276	3	-0	-1	178	3	-2
4	19	29	6*	-3	522	5	-1	10	105	4	-3	2	195	3	-1	0	138	3	-2
5	63	8	-4	-2	293	3	1	H,K=		4,	5	3	222	3	-1	1	177	3	-0
H,K=		3,	16	-1	486	4	4	-10	112	8	-0	4	253	3	-1	2	307	4	1
-3	40	7	19	0	235	2	-3	-9	130	4	6	5	130	2	1	3	174	3	0
-2	21	26	16*	1	478	4	1	-8	95	3	-2	6	302	4	-6	4	221	3	-1
-1	155	4	-8	2	291	3	1	-7	211	4	1	7	101	3	0	5	117	3	1
0	58	6	-7	3	523	5	-0	-6	301	3	3	8	18	29	-9*	6	76	4	-0
1	177	3	12	4	359	4	-4	-5	173	2	2	9	120	5	2	7	100	6	-7
2	17	24	10*	5	255	3	1	-4	319	4	-1	H,K=		4,	8	8	154	6	-2
3	15	29	-9*	6	198	3	-4	-3	282	3	1	-9	38	12	3*	H,K=		4,	11
H,K=		3,	17	7	248	4	1	-2	291	3	-1	-8	236	6	1	-8	68	6	3
-1	81	5	6	8	87	4	0	-1	305	3	-4	-7	47	6	-3	-7	122	4	3
0	23	12	17*	9	234	4	4	0	447	4	-11	-6	57	5	-1	-6	170	4	-3
1	76	6	-5	10	117	4	3	1	307	3	-5	-5	274	3	4	-5	190	3	4
H,K=		4,	0	H,K=		4,	3	2	292	4	-3	-4	318	3	-2	-4	135	3	-0
0	540	5	3	-10	107	4	6	3	290	3	4	-3	24	9	3*	-3	148	3	2
1	341	3	3	-9	91	4	-8	4	329	3	1	-2	439	5	-1	-2	138	3	-3
2	170	2	3	-8	100	4	-1	5	182	3	-1	-1	206	3	-0	-1	182	3	2
3	684	6	-8	-7	171	3	0	6	293	3	1	0	16	18	6*	0	275	4	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
1	177	3	-3	2	85	5	-5	2	492	5	-3	-7	108	3	-1	9	75	5	2
2	135	3	-4	3	30	14	1*	3	190	2	-1	-6	151	2	-0	H,K=		5,	8
3	141	3	-3	4	81	5	-5	4	389	4	-1	-5	391	5	-7	-9	143	5	6
4	137	3	-0	H,K=		4,	16	5	259	3	-0	-4	225	3	-1	-8	16	24	-10*
5	182	4	-1	-3	150	4	-5	6	126	2	0	-3	125	2	2	-7	182	3	3
6	175	4	-4	-2	39	9	-8*	7	187	3	1	-2	216	3	-2	-6	153	3	1
7	114	8	-3	-1	105	4	5	8	214	4	-1	-1	396	4	-4	-5	55	4	5
8	66	6	5	0	90	3	2	9	94	4	6	0	251	3	-5	-4	102	3	2
H,K=		4,	12	1	92	8	-6	10	96	4	0	1	392	4	-5	-3	369	4	-3
-7	104	6	-3	2	37	10	-4*	H,K=		5,	3	2	210	3	-2	-2	8	18	-0*
-6	92	6	4	3	161	4	1	-10	107	5	3	3	116	2	-1	-1	205	3	2
-5	108	4	-2	H,K=		5,	0	-9	150	5	-1	4	231	3	2	0	217	2	-2
-4	115	3	1	1	366	3	1	-8	123	3	-1	5	402	5	-2	1	285	3	0
-3	216	3	-1	2	444	4	-6	-7	204	3	-3	6	147	3	-1	2	23	10	4*
-2	140	4	-2	3	35	3	3	-6	321	5	-3	7	111	3	-3	3	372	5	1
-1	179	3	1	4	288	3	-1	-5	225	4	-3	8	146	3	3	4	100	3	3
0	129	3	-2	5	190	2	-1	-4	183	3	-0	9	95	5	-7	5	52	5	5
1	179	3	3	6	54	3	3	-3	321	4	-3	10	110	7	-0	6	158	3	3
2	142	3	-3	7	138	2	-4	-2	267	3	-3	H,K=		5,	6	7	189	3	6
3	211	4	-5	8	282	3	2	-1	414	4	-0	-9	153	5	-2	8	23	25	1*
4	118	3	3	9	63	6	-2	0	646	6	-6	-8	56	5	7	9	127	5	-8
5	112	6	-3	10	80	6	-4	1	427	4	0	-7	212	4	5	H,K=		5,	9
6	87	6	-4	H,K=		5,	1	2	261	3	-3	-6	182	3	-1	-8	102	4	5
7	105	5	-8	-10	157	5	1	3	326	4	-5	-5	138	3	2	-7	159	4	5
H,K=		4,	13	-9	104	7	0	4	183	3	-1	-4	176	3	3	-6	61	4	2
-6	63	11	-6	-8	41	6	6	5	215	3	1	-3	321	4	-4	-5	225	3	3
-5	161	4	-2	-7	139	3	1	6	329	4	-2	-2	149	3	-5	-4	132	3	1
-4	78	5	-2	-6	328	4	1	7	200	3	-1	-1	279	3	3	-3	61	3	5
-3	87	4	-2	-5	64	3	8	8	129	3	-2	0	346	4	-3	-2	190	3	2
-2	129	3	4	-4	378	5	-5	9	153	4	0	1	277	3	-1	-1	304	4	-3
-1	187	4	-1	-3	305	4	-3	10	97	8	-3	2	158	3	-4	0	93	3	0
0	102	4	-2	-2	285	3	-2	H,K=		5,	4	3	322	4	-2	1	307	4	-2
1	183	3	-3	-1	103	2	0	-10	86	9	-1	4	179	2	3	2	196	3	-5
2	132	3	3	0	468	4	-7	-9	135	5	2	5	138	3	1	3	57	3	5
3	92	4	-1	1	94	2	-2	-8	209	4	0	6	179	3	-6	4	136	3	2
4	80	5	2	2	288	3	-8	-7	164	3	1	7	214	3	5	5	221	3	2
5	158	7	-7	3	302	3	-3	-6	190	4	-2	8	57	7	3	6	56	5	-1
6	62	6	1	4	372	4	-6	-5	212	3	0	9	155	6	-0	7	153	5	-6
H,K=		4,	14	5	49	4	2	-4	289	4	-4	H,K=		5,	7	8	94	5	-7
-5	19	27	-1*	6	324	3	-0	-3	424	5	-3	-9	65	6	1	H,K=		5,	10
-4	122	4	-2	7	142	2	2	-2	425	5	-4	-8	99	4	3	-8	71	7	-1
-3	177	4	-0	8	28	10	-1*	-1	304	3	0	-7	154	4	2	-7	111	7	-1
-2	110	4	-1	9	102	5	-2	0	229	3	-3	-6	74	3	1	-6	116	3	5
-1	88	4	-6	10	152	5	-5	1	298	3	-2	-5	302	4	-1	-5	118	3	-1
0	91	4	0	H,K=		5,	2	2	432	5	-6	-4	240	3	-2	-4	135	3	5
1	93	4	-5	-10	94	5	1	3	417	4	-6	-3	50	3	2	-3	286	3	-0
2	111	4	4	-9	94	4	3	4	281	3	-1	-2	230	3	-0	-2	175	3	-2
3	171	4	-2	-8	224	4	3	5	203	3	-1	-1	332	4	-5	-1	193	3	2
4	124	5	-1	-7	187	3	2	6	194	3	2	0	20	12	-3*	0	209	3	2
5	29	13	9*	-6	133	3	0	7	161	3	2	1	338	4	-2	1	187	3	-1
H,K=		4,	15	-5	245	4	-3	8	214	3	2	2	232	3	0	2	170	3	-0
-4	78	7	-4	-4	378	4	-3	9	134	5	2	3	55	5	1	3	287	4	-2
-3	37	9	5*	-3	189	3	2	10	81	5	-8	4	234	3	-3	4	127	3	-1
-2	92	7	-1	-2	506	5	-1	H,K=		5,	5	5	298	4	-4	5	119	3	0
-1	165	4	2	-1	268	3	-3	-10	114	5	4	6	73	4	2	6	111	4	3
0	18	21	11*	0	75	3	6	-9	103	4	-3	7	151	3	1	7	107	6	-1
1	167	5	2	1	267	3	-4	-8	154	4	7	8	89	6	-4	8	77	6	7

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
H,K=		5,	11	5	83	5	5	1	287	3	-1	-3	447	5	-2	-5	306	4	3
-7	126	5	6	H,K=		5,	15	2	275	3	-1	-2	280	4	-3	-4	57	5	-6
-6	113	5	-5	-3	95	6	-7	3	37	4	1	-1	235	3	-3	-3	36	6	-2
-5	166	5	-2	-2	63	5	12	4	286	3	1	0	35	5	5	-2	52	4	5
-4	142	3	-1	-1	47	8	1	5	242	3	-4	1	233	3	-5	-1	429	5	-2
-3	85	4	-4	0	176	4	-2	6	320	5	-2	2	274	3	-1	0	15	20	1*
-2	193	4	-3	1	51	9	2	7	99	3	1	3	444	5	-1	1	428	5	-4
-1	210	3	-4	2	57	8	7	8	40	8	8*	4	214	3	3	2	54	4	9
0	179	3	3	3	104	7	8	9	31	11	7*	5	113	3	5	3	44	5	1
1	210	3	-3	H,K=		5,	16	10	132	7	-4	6	33	6	9*	4	61	5	-0
2	189	3	1	0	9	21	1*	H,K=		6,	3	7	187	3	5	5	303	5	-2
3	85	4	3	H,K=		6,	0	-9	148	6	-1	8	110	4	-2	6	21	23	15*
4	150	3	3	0	638	6	0	-8	224	5	-2	9	134	5	2	7	170	4	-1
5	162	6	-8	1	35	3	3	-7	150	3	1	H,K=		6,	6	8	15	30	1*
6	118	6	1	2	116	2	-2	-6	80	4	4	-9	86	5	2	H,K=		6,	9
7	117	4	0	3	183	2	1	-5	83	3	4	-8	28	23	12*	-8	72	5	-3
H,K=		5,	12	4	276	3	1	-4	196	4	3	-7	212	5	1	-7	151	4	-0
-7	91	4	5	5	23	8	-9*	-3	247	4	-1	-6	93	4	-5	-6	21	26	11*
-6	93	8	-12	6	394	4	-2	-2	323	4	1	-5	291	4	2	-5	87	3	3
-5	99	4	5	7	35	5	-8	-1	221	3	0	-4	73	4	0	-4	84	3	4
-4	139	5	1	8	86	3	1	0	38	5	-0	-3	148	3	1	-3	326	4	-2
-3	142	3	-1	9	77	6	4	1	229	2	2	-2	90	3	-2	-2	155	3	-1
-2	181	4	-3	10	174	4	3	2	330	3	1	-1	362	4	2	-1	180	4	-0
-1	116	3	1	H,K=		6,	1	3	245	3	4	0	123	3	-3	0	54	7	1
0	81	4	-6	-10	121	7	7	4	187	3	1	1	359	4	-1	1	181	2	1
1	116	4	-2	-9	33	11	4*	5	86	4	1	2	93	2	1	2	151	3	0
2	178	3	-4	-8	260	3	2	6	72	4	-3	3	140	3	-2	3	326	5	-2
3	141	3	-3	-7	84	4	-2	7	161	4	0	4	74	4	0	4	85	3	-0
4	139	4	-3	-6	118	3	-3	8	223	6	-4	5	286	4	-2	5	84	3	-1
5	95	10	-0	-5	62	3	2	9	149	8	1	6	97	3	-1	6	25	20	15*
6	105	6	-1	-4	443	6	-6	H,K=		6,	4	7	208	3	-1	7	146	5	-8
7	85	6	2	-3	98	2	-1	-9	64	7	0	8	27	17	8*	8	79	6	2
H,K=		5,	13	-2	561	7	-6	-8	6	25	-25*	9	80	5	-1	H,K=		6,	10
-6	117	5	-12	-1	81	2	2	-7	98	3	-2	H,K=		6,	7	-7	111	4	0
-5	111	4	2	0	57	3	-8	-6	242	3	2	-9	179	5	4	-6	107	4	3
-4	134	5	-1	1	77	2	3	-5	260	3	2	-8	65	6	-2	-5	233	4	-0
-3	142	4	-5	2	575	6	-6	-4	248	3	-3	-7	197	5	-5	-4	80	4	6
-2	93	5	-4	3	105	3	-8	-3	82	3	0	-6	67	5	5	-3	55	5	-3
-1	106	3	1	4	437	5	-6	-2	172	2	2	-5	99	3	2	-2	59	4	3
0	190	3	0	5	54	4	-3	-1	263	3	-4	-4	68	3	3	-1	209	4	1
1	110	3	5	6	122	4	-5	0	336	5	-8	-3	384	5	-5	0	135	4	-4
2	100	4	0	7	77	4	-2	1	267	3	-4	-2	99	3	1	1	201	4	-0
3	143	4	-7	8	259	4	1	2	170	2	-2	-1	216	3	-1	2	63	4	4
4	134	5	3	9	40	8	9*	3	88	2	-2	0	141	3	-7	3	68	3	8
5	104	6	-5	10	124	4	5	4	245	3	-1	1	215	3	1	4	80	3	2
6	129	6	2	H,K=		6,	2	5	258	4	2	2	94	3	-0	5	226	8	-9
H,K=		5,	14	-10	137	4	3	6	244	3	5	3	391	6	-5	6	113	5	11
-5	72	5	-7	-9	0	24	-18*	7	103	3	1	4	64	4	-5	7	115	6	3
-4	114	6	-6	-8	32	10	-5*	8	22	25	-8*	5	84	3	-6	H,K=		6,	11
-3	61	9	7	-7	99	3	3	9	57	7	-11	6	62	4	0	-7	102	5	3
-2	179	5	3	-6	317	5	-2	H,K=		6,	5	7	192	6	-1	-6	48	9	5
-1	120	4	-1	-5	239	4	-5	-9	138	5	2	8	52	12	-14*	-5	71	5	-2
0	30	9	4*	-4	279	4	8	-8	116	5	2	9	185	7	7	-4	128	4	1
1	119	4	-0	-3	36	5	4	-7	179	3	-2	H,K=		6,	8	-3	218	3	1
2	175	5	-1	-2	277	4	-2	-6	41	7	10	-8	0	31	-13*	-2	163	3	-2
3	34	12	-14*	-1	289	3	-1	-5	104	3	-0	-7	173	6	2	-1	154	4	-3
4	119	6	-0	0	577	7	-11	-4	289	3	3	-6	18	22	15*	0	29	11	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
1	152	4	-7	8	181	5	-5	5	190	3	2	5	103	3	6	-4	87	4	-1
2	170	3	3	9	23	25	1*	6	228	5	3	6	100	3	3	-3	184	3	3
3	218	4	2	H,K=	7,	1		7	100	3	1	7	160	4	-0	-2	126	3	1
4	129	4	2	-9	92	5	-1	8	57	7	-10	8	47	11	2*	-1	152	4	1
5	71	8	-3	-8	79	6	3	9	31	17	-6*	H,K=	7,	7		0	102	3	-1
6	35	23	-11*	-7	125	3	2	H,K=	7,	4		-8	66	6	-1	1	150	3	-1
7	95	6	-6	-6	292	4	-8	-9	122	5	4	-7	155	5	-4	2	131	3	-2
H,K=	6,	12		-5	68	3	6	-8	164	5	-2	-6	47	14	5*	3	183	3	3
-6	143	6	0	-4	218	4	1	-7	122	4	3	-5	228	5	5	4	85	5	-0
-5	124	5	2	-3	231	4	-3	-6	99	4	-4	-4	170	3	-2	5	78	8	-4
-4	128	4	7	-2	169	3	-2	-5	174	4	-5	-3	82	4	-1	6	68	6	-2
-3	19	26	6*	-1	146	2	-1	-4	201	3	4	-2	178	3	2	H,K=	7,	11	
-2	81	4	0	0	500	6	-5	-3	249	4	-2	-1	287	4	-1	-6	99	4	2
-1	146	3	-1	1	142	3	-1	-2	279	4	-3	0	72	4	-1	-5	146	5	2
0	227	5	3	2	181	2	-0	-1	196	2	1	1	291	5	2	-4	82	4	2
1	154	3	5	3	237	3	-3	0	153	2	6	2	179	3	-4	-3	78	4	9
2	72	4	-7	4	217	3	2	1	192	3	2	3	87	3	2	-2	93	4	3
3	2	23	-12*	5	63	4	1	2	291	3	1	4	165	3	-5	-1	171	4	-3
4	124	4	3	6	281	4	-1	3	261	3	1	5	223	3	2	0	152	3	-0
5	117	4	-3	7	121	3	3	4	193	3	2	6	36	9	-3*	1	173	3	-0
6	141	6	-3	8	77	5	-5	5	174	3	-3	7	157	5	-3	2	89	4	-1
H,K=	6,	13		9	95	9	-2	6	109	3	6	8	74	8	4	3	70	6	2
-5	11	25	-5*	H,K=	7,	2		7	104	5	-0	H,K=	7,	8		4	79	5	3
-4	117	4	-1	-9	94	5	-5	8	162	9	-5	-7	132	4	-1	5	150	5	3
-3	95	4	2	-8	183	7	-0	9	122	5	1	-6	116	4	-4	6	92	5	-2
-2	168	5	2	-7	122	3	-1	H,K=	7,	5		-5	75	5	1	H,K=	7,	12	
-1	55	5	4	-6	88	3	7	-8	102	5	0	-4	135	3	2	-5	70	5	7
0	42	6	-6	-5	137	3	1	-7	171	4	3	-3	299	5	-5	-4	116	5	6
1	56	7	5	-4	300	4	-2	-6	153	4	4	-2	45	6	-8	-3	128	4	-6
2	168	6	-3	-3	183	4	-2	-5	242	4	-3	-1	155	3	3	-2	141	6	1
3	84	6	-6	-2	399	5	-1	-4	111	3	2	0	163	4	-2	-1	94	4	-2
4	113	7	0	-1	170	3	0	-3	87	3	3	1	154	4	4	0	69	3	3
5	17	25	-2*	0	40	5	8	-2	179	3	-1	2	51	4	4	1	97	5	-1
H,K=	6,	14		1	165	2	4	-1	353	5	1	3	295	5	-4	2	128	6	-8
-4	103	6	4	2	384	5	-1	0	204	3	-2	4	134	3	1	3	135	4	-2
-3	25	20	-2*	3	176	3	1	1	347	4	1	5	85	4	5	4	108	6	-3
-2	79	5	-2	4	311	4	-1	2	174	3	-0	6	113	11	-8	5	66	5	7
-1	62	6	0	5	134	3	-1	3	76	3	-1	7	132	6	-3	H,K=	7,	13	
0	211	4	-3	6	85	3	4	4	126	3	5	H,K=	7,	9		-4	96	7	2
1	71	5	6	7	120	4	-1	5	249	3	2	-7	98	5	2	-3	96	5	10
2	86	5	5	8	186	5	3	6	158	3	4	-6	76	5	9	-2	94	6	4
3	17	25	-9*	9	91	5	-2	7	164	8	-1	-5	197	5	-1	-1	92	6	2
4	103	5	1	H,K=	7,	3		8	107	7	3	-4	101	3	1	0	165	4	-2
H,K=	6,	15		-9	30	32	-9*	H,K=	7,	6		-3	44	7	-2	1	88	5	1
-2	166	4	4	-8	69	6	-3	-8	49	10	3*	-2	126	5	0	2	89	5	1
-1	18	24	9*	-7	96	4	-0	-7	154	4	3	-1	204	3	-0	3	89	5	1
0	28	9	20*	-6	223	4	-3	-6	102	3	2	0	77	3	3	4	101	4	5
1	22	24	15*	-5	188	3	-1	-5	105	3	6	1	205	4	-4	H,K=	7,	14	
2	158	5	-2	-4	220	4	0	-4	97	3	-2	2	126	3	2	-2	142	5	-1
H,K=	7,	0		-3	140	3	1	-3	328	4	-2	3	45	5	2	-1	78	4	11
1	318	3	-6	-2	219	3	-1	-2	107	3	0	4	98	4	-0	0	27	9	-7*
2	335	4	-2	-1	178	2	0	-1	194	3	3	5	190	7	-6	1	71	6	6
3	21	8	10*	0	282	3	3	0	235	4	2	6	72	5	6	2	138	8	-5
4	278	3	-1	1	183	3	1	1	199	3	0	7	106	5	7	H,K=	8,	0	
5	153	2	-1	2	212	3	-4	2	106	3	8	H,K=	7,	10		0	178	3	-3
6	72	3	-2	3	140	3	-0	3	329	5	-2	-6	66	6	-1	1	136	2	3
7	130	3	1	4	216	3	-2	4	98	3	3	-5	93	4	11	2	192	2	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
3	283	4	1	6	112	5	-1	-6	145	5	-2	-4	130	7	8	4	77	4	-3
4	114	2	4	7	118	5	2	-5	69	5	3	-3	87	5	3	5	227	4	3
5	57	3	0	8	58	7	-3	-4	161	3	0	-2	120	4	-1	6	95	7	-2
6	142	3	-1	H,K=	8,	4		-3	156	4	-2	-1	102	4	4	7	136	6	5
7	143	5	-7	-8	120	7	-4	-2	110	4	-1	0	152	5	-1	H,K=	9,	3	
8	44	8	3	-7	129	6	4	-1	99	3	1	1	95	6	-2	-7	112	5	3
H,K=	8,	1		-6	88	5	-6	0	227	5	5	2	116	4	-4	-6	54	6	2
-8	124	6	0	-5	138	3	8	1	101	3	-1	3	92	7	5	-5	38	15	-3*
-7	128	4	4	-4	146	3	-3	2	119	4	6	4	126	5	3	-4	134	4	1
-6	41	6	1	-3	239	4	3	3	158	3	-3	H,K=	8,	12		-3	230	4	-1
-5	248	4	-2	-2	202	3	-2	4	157	3	2	-3	137	5	-1	-2	158	4	-0
-4	149	4	2	-1	203	4	-1	5	66	7	-0	-2	113	4	2	-1	112	3	-1
-3	84	3	2	0	182	2	-4	6	149	6	-2	-1	78	5	5	0	58	4	5
-2	200	3	0	1	207	4	3	7	52	10	-0	0	62	4	-2	1	114	3	1
-1	287	4	-0	2	205	4	-4	H,K=	8,	8		1	78	10	-1	2	156	3	0
0	16	18	-1*	3	238	3	-2	-7	95	4	6	2	109	4	-4	3	232	5	-5
1	293	4	2	4	145	3	-1	-6	66	6	1	3	132	5	-7	4	133	3	-2
2	209	3	1	5	131	3	-1	-5	126	4	2	H,K=	8,	13		5	19	25	-23*
3	78	4	-4	6	96	4	3	-4	145	5	-1	-1	115	5	5	6	54	7	-3
4	143	3	-4	7	125	8	-3	-3	52	5	-0	0	51	6	-7	7	102	4	-1
5	247	4	-2	8	124	5	-3	-2	230	4	-3	1	112	5	4	H,K=	9,	4	
6	45	6	0	H,K=	8,	5		-1	134	3	-0	H,K=	9,	0		-7	95	5	-5
7	130	4	2	-8	54	8	-1	0	52	4	5	1	245	3	-4	-6	147	4	0
8	129	4	4	-7	124	4	7	1	141	4	2	2	11	17	4*	-5	159	5	-0
H,K=	8,	2		-6	200	6	1	2	224	4	-1	3	25	8	7*	-4	139	3	1
-8	88	5	3	-5	143	4	3	3	54	5	-1	4	25	8	-0*	-3	58	7	3
-7	156	6	-4	-4	170	3	4	4	148	8	-4	5	271	4	5	-2	69	5	-4
-6	154	3	8	-3	126	3	2	5	120	4	-3	6	25	18	-8*	-1	196	3	0
-5	70	4	-1	-2	116	3	2	6	65	8	1	7	115	4	5	0	218	5	-2
-4	136	3	3	-1	164	3	-1	7	88	9	-2	H,K=	9,	1		1	197	4	0
-3	309	5	-6	0	318	4	-12	H,K=	8,	9		-7	153	5	0	2	79	5	2
-2	160	3	5	1	155	3	-5	-6	157	6	-1	-6	27	29	-5*	3	57	4	7
-1	205	4	-7	2	112	3	2	-5	86	4	9	-5	89	4	-1	4	127	3	-1
0	211	3	3	3	119	4	-0	-4	113	4	7	-4	24	13	-4*	5	152	6	-3
1	211	3	-3	4	171	3	-0	-3	150	4	3	-3	304	5	-4	6	149	8	-1
2	157	4	-2	5	139	3	1	-2	71	4	1	-2	40	6	-2	7	97	5	-0
3	306	4	-0	6	204	5	0	-1	109	4	2	-1	212	4	0	H,K=	9,	5	
4	138	4	1	7	116	5	2	0	243	4	-2	0	47	6	-3	-7	81	6	0
5	76	4	2	8	56	7	6	1	104	3	-2	1	201	4	-5	-6	58	9	1
6	149	3	4	H,K=	8,	6		2	67	5	-4	2	44	5	0	-5	49	7	0
7	163	7	-0	-7	67	6	4	3	143	6	-1	3	305	4	2	-4	176	5	0
8	73	6	-11	-6	86	4	2	4	111	7	3	4	29	11	2*	-3	153	4	-4
H,K=	8,	3		-5	131	4	3	5	77	5	-0	5	92	4	-1	-2	246	4	1
-8	62	7	3	-4	196	3	8	6	155	6	3	6	37	11	8*	-1	93	4	1
-7	113	5	0	-3	21	22	-4*	H,K=	8,	10		7	161	5	4	0	43	6	-2
-6	120	4	-1	-2	228	4	-1	-5	82	5	-1	H,K=	9,	2		1	100	3	5
-5	193	3	-3	-1	140	3	3	-4	131	4	-4	-7	133	4	1	2	250	4	4
-4	177	4	1	0	79	3	5	-3	72	5	2	-6	100	4	2	3	151	3	-1
-3	157	2	4	1	130	3	-4	-2	170	4	-0	-5	222	3	1	4	177	7	0
-2	195	3	0	2	228	4	-3	-1	147	5	-5	-4	78	4	5	5	57	6	9
-1	244	4	-1	3	40	8	1*	0	72	4	5	-3	65	5	-2	6	64	5	12
0	190	3	3	4	191	3	-2	1	144	7	-4	-2	58	4	5	7	86	5	0
1	243	4	-5	5	126	4	-1	2	168	7	-7	-1	279	5	-1	H,K=	9,	6	
2	191	4	0	6	91	5	8	3	71	5	4	0	186	3	-3	-6	173	5	3
3	159	3	1	7	53	7	-2	4	139	4	4	1	281	5	-0	-5	67	9	4
4	173	4	0	H,K=	8,	7		5	90	4	5	2	57	4	3	-4	158	6	-2
5	196	3	-2	-7	61	6	5	H,K=	8,	11		3	66	5	-5	-3	47	6	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
-2	134	4	-1	H,K=	9,	11		6	109	5	5	3	9	29	-18*	0	92	5	1
-1	72	4	4	-3	112	5	7	H,K=	10,	4		4	132	6	0	1	93	6	0
0	238	4	6	-2	141	7	-3	-6	49	12	-7*	H,K=	10,	9		2	112	5	-5
1	66	4	-0	-1	73	5	9	-5	63	6	-4	-3	63	8	-10	3	122	7	7
2	134	3	2	0	9	20	8*	-4	123	4	-2	-2	81	6	-1	4	97	5	7
3	44	6	-3	1	54	8	-7	-3	135	4	3	-1	49	11	6*	H,K=	11,	5	
4	160	7	-3	2	128	5	-6	-2	146	4	9	0	139	5	-2	-3	56	6	4
5	72	5	4	3	111	5	6	-1	109	4	6	1	50	10	7*	-2	112	6	2
6	178	5	8	H,K=	10,	8		0	85	4	-7	2	75	6	-7	-1	104	4	-5
H,K=	9,	7		0	142	3	-4	1	104	4	1	3	56	9	-11	0	89	5	6
-6	55	10	14	1	161	3	3	2	137	5	2	H,K=	10,	10		1	112	5	2
-5	27	28	5*	2	40	5	2	3	127	5	-6	-1	59	6	8	2	111	7	2
-4	159	4	2	3	233	3	2	4	117	5	-9	0	45	6	3	3	59	6	8
-3	59	5	1	4	81	4	3	5	66	9	-3	1	55	8	4	H,K=	11,	6	
-2	227	4	4	5	83	5	-1	6	52	12	-6*	H,K=	11,	0		-3	123	5	2
-1	28	11	-1*	6	78	8	-4	H,K=	10,	5		1	42	9	-10*	-2	67	5	7
0	31	9	1*	H,K=	10,	1		-5	81	6	5	2	194	5	6	-1	100	5	5
1	21	22	-8*	-6	34	16	-4*	-4	102	7	-5	3	41	9	17*	0	69	5	-6
2	223	5	1	-5	188	5	2	-3	102	5	2	4	102	4	8	1	112	6	12
3	55	8	-4	-4	61	10	0	-2	81	5	-6	5	68	6	3	2	60	8	0
4	150	5	-1	-3	45	8	-6	-1	120	4	-0	H,K=	11,	1		3	120	5	3
5	20	23	-1*	-2	127	4	3	0	195	3	1	-5	62	11	1	H,K=	11,	7	
6	50	7	8	-1	217	4	-0	1	109	5	-6	-4	107	6	-4	-2	69	6	5
H,K=	9,	8		0	75	5	-5	2	81	7	-4	-3	105	7	-1	-1	112	5	3
-5	18	24	-0*	1	215	5	-1	3	97	8	-1	-2	79	5	-5	0	39	12	-10*
-4	133	4	-2	2	138	3	6	4	115	5	2	-1	64	6	5	1	113	6	1
-3	28	15	17*	3	44	9	-5*	5	84	7	6	0	174	4	-2	2	74	8	7
-2	106	4	-3	4	60	8	-3	H,K=	10,	6		1	65	5	4	H,K=	12,	0	
-1	20	23	-6*	5	189	8	5	-5	104	5	6	2	94	5	4	0	167	8	-4
0	280	6	-2	6	32	17	-8*	-4	111	5	-3	3	108	5	-1	1	20	25	17*
1	45	6	18	H,K=	10,	2		-3	91	5	-7	4	114	4	6	2	100	5	4
2	106	4	-1	-6	85	5	3	-2	179	5	3	5	66	6	1	H,K=	12,	1	
3	9	24	-4*	-5	68	6	9	-1	106	6	3	H,K=	11,	2		-2	135	7	1
4	141	5	1	-4	107	4	0	0	44	5	4	-4	118	9	4	-1	52	8	9
5	33	11	18*	-3	198	6	-3	1	98	6	-3	-3	87	6	3	0	29	9	9*
H,K=	9,	9		-2	99	4	-2	2	179	8	0	-2	142	6	-1	1	30	16	-11*
-5	27	14	10*	-1	118	4	5	3	99	4	1	-1	133	5	2	2	146	4	6
-4	136	4	-4	0	88	4	-2	4	112	4	0	0	51	5	1	H,K=	12,	2	
-3	82	5	3	1	115	4	-1	5	100	6	5	1	132	4	3	-1	48	7	5
-2	195	5	3	2	105	3	3	H,K=	10,	7		2	136	5	-1	0	156	5	1
-1	40	9	10*	3	201	5	0	-4	109	5	2	3	85	5	4	1	41	13	1*
0	47	8	-6	4	105	6	-4	-3	88	4	5	4	110	6	-5	H,K=	12,	3	
1	45	7	9	5	48	8	-9	-2	98	5	2	H,K=	11,	3		-1	50	13	-8*
2	198	6	0	6	76	8	-0	-1	94	4	6	-4	79	6	-3	0	17	28	9*
3	74	5	-5	H,K=	10,	3		0	284	4	2	-3	102	5	-0	1	65	6	0
4	136	7	-7	-6	106	7	-1	1	89	6	-1	-2	74	5	-1				
5	20	26	5*	-5	133	4	1	2	104	6	5	-1	126	4	7				
H,K=	9,	10		-4	99	5	-0	3	91	5	2	0	148	3	1				
-4	102	6	4	-3	49	8	3	4	99	8	-4	1	117	4	-0				
-3	19	25	5*	-2	104	3	-1	H,K=	10,	8		2	71	5	-1				
-2	59	9	-2	-1	147	3	-1	-4	133	5	5	3	109	6	6				
-1	69	8	-4	0	126	3	-1	-3	24	26	0*	4	79	5	1				
0	176	4	-1	1	143	4	-7	-2	169	6	-4	H,K=	11,	4					
1	73	7	4	2	92	4	-9	-1	66	8	3	-4	94	8	5				
2	67	6	-2	3	38	9	-8*	0	12	24	10*	-3	114	6	2				
3	0	25	-17*	4	104	4	6	1	63	7	-1	-2	112	4	1				
4	100	4	5	5	132	5	-2	2	165	6	-1	-1	96	4	-1				

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