

A Redetermination of the Crystal and Molecular Structure of Zeise's Salt, $\text{KPtCl}_3 \cdot \text{C}_2\text{H}_4 \cdot \text{H}_2\text{O}$

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The space group of Zeise's salt, $\text{KPtCl}_3 \cdot \text{C}_2\text{H}_4 \cdot \text{H}_2\text{O}$, has been found to be $P2_1/c$, $a = 11.212$ (3), $b = 8.424$ (6), $c = 9.696$ (6) Å, $\beta = 107.52$ (4)°, with four molecules in the unit cell. The structure has been redetermined with counter diffractometer data, and refinement using 860 significant reflexions led to a final R value of 0.041. The ethylene molecule forms an approximately symmetrical π -type bond with the platinum atom. The C=C bond length [1.37 (3) Å] is slightly longer than in free ethylene, consistent with a small decrease in bond-order on complexing. The Pt-Cl bond *trans* to ethylene [2.327 (5) Å] is slightly longer than the two *cis*-Pt-Cl bonds [average 2.305 (7) Å], suggesting a small static weakening of the *trans*-bond by ethylene. These two differences however, are significant only at the 2σ level. The molecules are linked into infinite two-dimensional layers by weak O-H...Cl hydrogen bonds (O...Cl = 3.28 Å) parallel to c , ionic ...O...K+...O... chains (O...K+ = 2.77 Å) parallel to b , and ionic forces between the potassium and chlorine atoms (K+...Cl = 3.24–3.76 Å). Each potassium atom is coordinated to six chlorine atoms at the corners of a distorted trigonal prism. Each prism is linked to four others by sharing the four edges of one prism face. The K+...O bonds emerge from two of the three prism faces. The ethylene groups form the two surfaces of each layer.

The new structure differs very little from the old in its nearest-neighbour distances and coordination; the principal difference is in the method of linking of the potassium coordination polyhedra.

In our recent study of Zeise's salt (Black, Mais & Owston, 1969) we used the space group $P2_1$, originally reported by Mellor & Wunderlich (1954, 1955), and Bokii & Kukina (1965), which we verified only cursorily. The same space-group was used by Hamilton, Klanderman & Spratley (1969) in their neutron diffraction analysis. We have since attempted to re-refine our data, making corrections for both the real and imaginary components of anomalous dispersion, which should have important effects in this polar space group, but without success. We therefore re-examined the crystals and found, from well-exposed photographs of the zones $\{h1l\}$ etc., that the c axis is doubled, and the true space-group is $P2_1/c$ (Jarvis, Kilbourn & Owston, 1970). We have therefore re-measured the reflexion intensities and re-determined the structure.

Results and discussion

(i) Unit cell

The relationships between the old ($P2_1$) and new ($P2_1/c$) unit-cell parameters and indices (distinguished by primed and unprimed symbols respectively) are (see Fig. 1):

$$\begin{array}{ll} a' = 10.750 \text{ (6) \AA} & a = 11.212 \text{ (3) \AA} \\ b' = 8.405 \text{ (3)} & b = 8.424 \text{ (6)} \\ c' = 4.836 \text{ (2)} & c = 9.696 \text{ (6)} \\ b' = 97.73 \text{ (6)^\circ} & \beta = 107.52 \text{ (4)^\circ} \end{array}$$

$$\begin{array}{l} h = -h' - l' \\ k = k' \\ l = 2l' \end{array}$$

It can be seen that the indices of the zone $\{0k'l'\}$ transform to $\{-lk2l'\}$; the corresponding Weissenberg photograph thus gives no indication of the doubling of the c axis, since only reflexions with l even can appear, and this has helped to mislead previous workers. Only photographs of zones like $\{h1l'\}$ allow this error to be avoided.

The additional reflexions characteristic of the new space-group (*i.e.* those with l odd) are few in number [86 out of a total of 860 reflexions with $l \geq 3\sigma(I)$], and are relatively weak. The correct structure is thus a kind of super-structure based on the one reported previously. The relationships of the atoms with their nearest neighbours are only slightly (though significantly) different. There are important differences in longer-range structure as required by the higher symmetry of the 'super-cell'.

It will be noted that the new unit-cell dimensions do not correspond exactly with the old when transformed by the vector relationships $\mathbf{a} = -(\mathbf{a}' + \mathbf{c}')$; $\mathbf{b} = \mathbf{b}'$; $\mathbf{c} = 2\mathbf{c}'$. The new values are calculated from careful measurements in which each plane was observed at four different values of χ , to minimize centring errors, and are more accurate than the old.

(ii) Coordination round platinum

Our previous results gave the average structure of the two molecules that are related by the glide plane, and the large and highly anisotropic values for some of the thermal parameters were a result of this averaging. In particular, the Cl(2)-Pt-Cl(3) axes are now the chlorine atoms corresponding to root-mean-square

found to be inclined at + and -7° to the b axis, whereas they were formerly deduced to be approximately parallel to b , with very high U_{33} parameters for

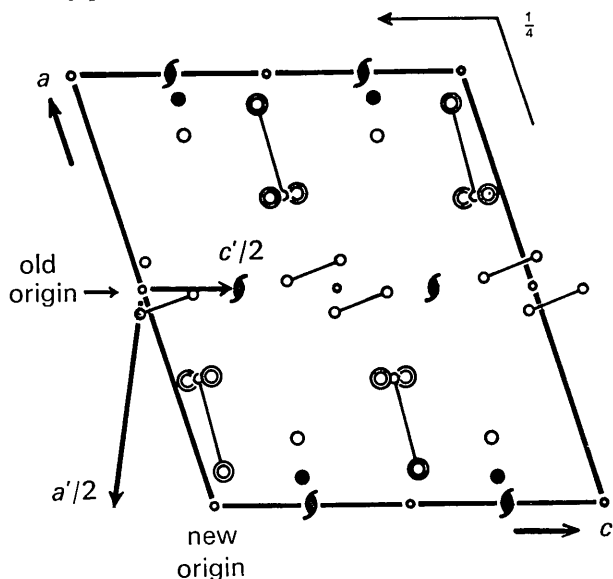


Fig. 1. Structure of Zeise's salt projected down the b axis. The relation of the old axes to the new cell and its symmetry elements is shown. Cl atoms are represented by double circles, K atoms by solid circles; O atoms by large open circles, and C atoms by smaller open circles.

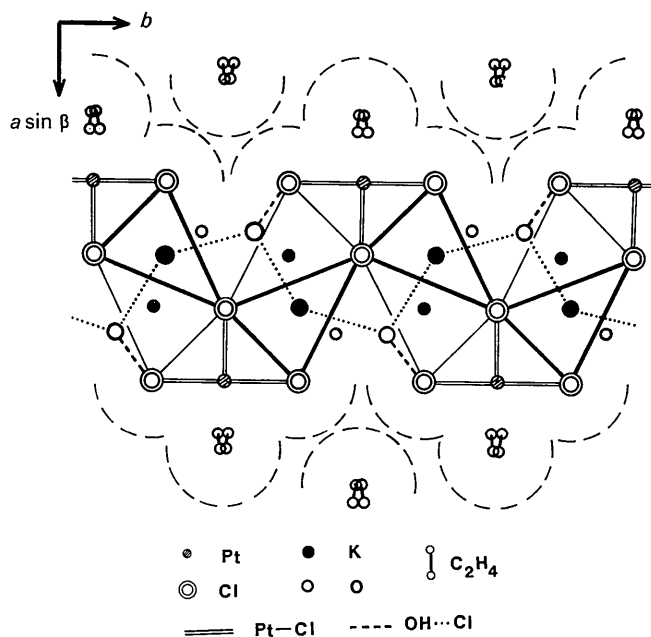


Fig. 2. Structure of Zeise's salt projected down the c axis, showing a cross-section of a layer, bounded on either side by ethylene molecules. For the atoms in the upper half of the unit cell, the distorted trigonal prismatic coordination polyhedra of the K^+ ions are shown as thick continuous lines, and the $Cl \cdots O \cdots Cl$ hydrogen bonds and $O \cdots K^+ \cdots O$ interactions are also shown. For the atoms in the lower half of the unit cell only the K^+ coordination polyhedra are indicated (by light continuous lines).

vibration amplitudes of approximately 0.4 \AA . Similar high values for the apparent amplitudes of thermal vibration were deduced from neutron diffraction data (Hamilton, Klanderma & Spratley, 1969).

The revised molecular parameters (Fig. 2 and Table 1) are slightly different from our earlier results. The C=C bond remains nearly perpendicular to and symmetrical about the platinum coordination plane. As usual in this type of complex, the structure departs slightly from ideal symmetry; the bond is here inclined at $84.2(12)^\circ$ to the coordination plane, and its centre is $0.20(3) \text{ \AA}$ above the plane.

The Pt-C distances [$2.13(2) \text{ \AA}$] are longer than the radius sum for Pt-C(sp^2), 2.06 \AA , and are longer, though less significantly so, than that for Pt-C(sp^3), 2.09 \AA . As is usual in π -type complexes the C=C bond, $1.37(3) \text{ \AA}$, is longer than a double bond, 1.335 \AA , though the difference of less than two standard deviations is not unequivocal. Hamilton, Klanderma & Spratley (1969) derived a similar value, $1.354(15) \text{ \AA}$, from their neutron diffraction study; they also showed that the ethylene molecule is not planar in this complex, and that the hybridization of the carbon atoms, though nearly sp^2 , tends slightly towards sp^3 .

All these facts are consistent with the views on the structures of π -type complexes put forward by Chatt & Duncanson (1953).

Because the positions of the chlorine atoms are no longer the average of the positions in two different molecules, the Pt-Cl bond-lengths are more accurately determined, and corrections for 'thermal motion' have not been considered necessary. The two Pt-Cl bond-lengths *cis* to ethylene differ by about 2σ ; their average, $2.305(7) \text{ \AA}$, is equal to the Pt-Cl bond-lengths in K_2PtCl_4 (Mais, Owston & Wood, unpublished results). The environments of these two *cis*-chlorine atoms are so similar (see below) that no significance can be attached to the difference between these two Pt-Cl distances. The bond *trans* to ethylene is longer than Pt-Cl(2) by 2σ , which is of doubtful significance, but is appreciably longer than Pt-Cl(3). There may therefore be a small lengthening of the Pt-Cl bond *trans* to ethylene, which could be the result of a small static *trans* weakening by the ethylene ligand, or of the difference in environment of the *cis* and *trans* chlorine atoms (see below). It seems to be scarcely sufficient to explain the high chemical lability of the *trans* chlorine atom, which is presumably to be attributed to the dynamic π -bond effects discussed by Chatt, Duncanson & Venanzi (1955).

(iii) Crystal structure

The structure consists of layers parallel to the b and c axes, with a central ionic core, and surfaces covered by ethylene molecules (Fig. 2). The core itself consists of pairs of sheets of $[PtCl_3C_2H_4]^-$ ions, and of K^+ ions and H_2O molecules, which alternate along the c axis. These pairs of sheets are of two kinds: the first, comprising the lower layers of Figs. 2 and 3, is effec-

tively identical with that shown before (Black, Mais & Owston, 1969): the second is related to it by the c -glide plane. Because this glide plane $y = \frac{1}{4}$ is also nearly a mirror plane through the $[\text{PtCl}_3\text{C}_2\text{H}_4]^-$ ion, the glide operation is nearly equivalent to a simple translation of $c/2$, so far as the atoms of the complex ion are concerned; refinement in the space group $P2_1/c$ therefore places these atoms in nearly the same relative positions as refinement in $P2_1$. The potassium and oxygen atoms however, now appear in quite different positions in this second layer, and are coordinated to different chlorine atoms. The coordination round potassium is nevertheless effectively the same as before: six chlorine atoms are at the corners of a distorted trigonal prism round the potassium atom, which in turn has bonds to two water molecules passing through two of the prism faces. Five of the $\text{K}^+\cdots\text{Cl}$ distances are within the range 3.20–3.40 Å, which is normal; the sixth, $\text{K}^+\cdots\text{Cl}(1)$, is so long (3.76 Å) that the interaction must be quite weak. The $\text{K}^+\cdots\text{O}$ distances (average 2.77 Å) are close to the sum of ionic radii, 2.73 Å.

The coordination polyhedra of the potassium ions were previously thought to be linked along c by sharing the terminal triangular faces, but are now seen to be linked by sharing only one edge of each terminal face (Fig. 3).

A further correction is that the environments of the $\text{Cl}(2)$ and $\text{Cl}(3)$ atoms are now seen to be effectively equivalent, each interacting with one water molecule and one K^+ ion. The *trans*-chlorine atom $\text{Cl}(1)$ interacts, as before, with four K^+ ions. The difference in length between the two types of $\text{Pt}-\text{Cl}$ bond may be attributed partly to this difference in environment.

The chain of hydrogen bonds linking the molecules in the c direction contains the atoms $-\text{Cl}(2)\cdots\text{O}\cdots\text{Cl}(3)-\text{Pt}-\text{Cl}(2)\cdots\text{O}\cdots\text{Cl}(3)-\text{Pt}$ -*etc.*, rather than a continuous chain $\text{Cl}\cdots\text{O}\cdots\text{Cl}\cdots\text{O}\cdots$. The coordination

round the water molecule is approximately tetrahedral with bonds to two K^+ ions and two chlorine atoms ($\text{O}\cdots\text{Cl} = 3.34$ and 3.23 Å). The $\text{O}\cdots\text{Cl}$ distances are so long that the hydrogen bonds must be relatively weak.

Experimental

Crystal data

Yellow prisms or needles, $\text{C}_2\text{H}_4\text{KPtCl}_3 \cdot \text{H}_2\text{O}$,
 $M = 386.8$; monoclinic,
 $a = 11.212$ (3), $b = 8.424$ (6), $c = 9.696$ (6) Å,
 $\beta = 107.52$ (4)°;
 $U = 873.4$ Å³;
 $D_m(\text{floatation}) = 2.94$ g.cm⁻³, $Z = 4$, $D_c = 2.95$ g.cm⁻³.
 $F(000) = 696$; space group $P2_1/c$ (No. 14, C_{2h}^5);
 $\mu(\text{Mo } K\alpha) = 197.1$ cm⁻¹.

Intensities were measured on a Picker 4-circle diffractometer with a crystal of approximate dimensions $0.05 \times 0.07 \times 0.10$ mm. The $\theta-2\theta$ scan method was used, scanning from 0.8° below α_1 to 0.50 above α_2 at 2° 2θ .minute⁻¹, with a 20 sec background count at each end of the scan. About every two hours the 500 and 040 reflexions were measured; over 4 days these intensities decreased by 3%. To correct for this deterioration each intensity was scaled according to the moving average of the standard reflexions intensities.

A total of 2200 reflexions with $\sin \theta/\lambda < 0.7$ was measured and corrected for Lorentz-polarization factors. Reflexions with $I \geq 3\sigma(I)$, the standard deviations of the intensities, $\sigma(I)$, being evaluated from the background and integrated reflexion intensities in the usual way, were corrected for absorption by the method of Busing & Levy (1957) modified to give a more even sample-point distribution; 297 sample points were used. After averaging values from equivalent reflexions the structure amplitudes of 860 independent reflexions were obtained and used in the analysis.

Table 1. *Interatomic distances and angles with e.s.d.'s in parentheses*

Pt—Cl(1)	2.327 (5) Å		
Pt—Cl(2)	2.314 (7)		
Pt—Cl(3)	2.296 (7)		
Pt—C(1)	2.121 (19)		
Pt—C(2)	2.134 (19)		
C(1)—C(2)	1.37 (3)		
$\text{K}^+\cdots\text{Cl}(1)$	3.238 (9)		
	3.255 (10)		
	3.764 (10)		
	3.396 (10)		
$\text{K}^+\cdots\text{Cl}(2)$	3.287 (9)		
$\text{K}^+\cdots\text{Cl}(3)$	3.196 (10)		
$\text{K}^+\cdots\text{O}$	2.712 (19)		
	2.834 (20)		
$\text{O}\cdots\text{Cl}(3)$	3.335 (19)		
$\text{O}\cdots\text{Cl}(2)$	3.227 (20)		
$\text{Cl}(1)-\text{Pt}-\text{Cl}(2)$	90.1 (3)°	$\text{Cl}(2)\cdots\text{O}\cdots\text{Cl}(3)$	111.3 (5)°
$\text{Cl}(1)-\text{Pt}-\text{Cl}(3)$	90.2 (3)	$\text{K}^+\cdots\text{O}\cdots\text{K}^+$	106.1 (6)
$\text{Cl}(2)-\text{Pt}-\text{Cl}(3)$	177.5 (3)	$\text{Cl}(2)\cdots\text{O}\cdots\text{K}^+$	116.8 (6)
			90.2 (5)
$\text{Cl}(1)-\text{Pt}-\text{C}(1)$	156.3 (6)	$\text{Cl}(3)\cdots\text{O}\cdots\text{K}^+$	119.2 (6)
$\text{Cl}(1)-\text{Pt}-\text{C}(2)$	166.2 (6)		108.7 (6)

Structure determination

The good agreement between F_{obs} and F_{calc} obtained when the structure was described in terms of the space group $P2_1$ means that a very similar relative spatial arrangement of atoms must also be present in the new cell. The problem was to find the position of this arrangement relative to the new symmetry elements so as to account for the weak reflexions with odd values of l .

The Pt atoms must now lie almost exactly on the glide-planes at $y = \frac{1}{4}, \frac{3}{4}$. In the original structure, all $[\text{PtCl}_3]$ groups at different y levels were related by 2_1 axes, whereas in the new space group half of the 2_1

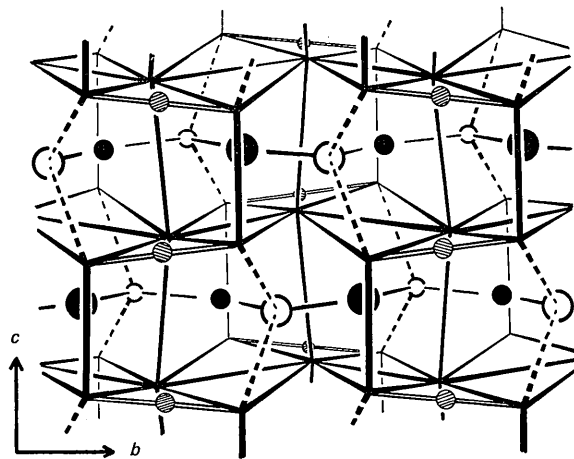


Fig. 3. Orthorhombic projection of the structure, approximately on the bc plane, showing a side view of the same portion of a layer as was shown in cross-section in Fig. 2. The K^+ coordination polyhedra are indicated by tapered lines, the $\text{O}\cdots\text{Cl}\cdots\text{O}$ bonds by broken lines, the $\text{O}\cdots\text{K}^+\cdots\text{O}$ interactions by thin continuous lines running approximately horizontally, and the $\text{Pt}-\text{Cl}$ bonds by double lines. The ethylene molecules have been omitted and the symbols for the chlorine atoms which are at the corners of the coordination polyhedra, are also omitted; the symbols used for the other atoms are the same as in Fig. 2.

axes must be replaced by symmetry centres in rows along the a axis. The difficulty was to decide which half, because the existence in the $\text{Pt}-\text{Cl}_3$ group of a pseudo-mirror plane perpendicular to the b axis means that any two groups related by a screw-axis also have a pseudo-centre of symmetry midway between them.

Structure factors and observed electron density maps were calculated for both possibilities, based on the Pt and Cl atoms, with the chlorine atoms $\text{Cl}(2)$ and $\text{Cl}(3)$ displaced by $\pm 0.2 \text{ \AA}$ along c to ensure that the $\text{Cl}-\text{Pt}-\text{Cl}$ line was no longer exactly parallel to the b axis. In both maps a peak presumed to be K^+ appeared, but in one of them this peak was so close to a symmetry-centre that an impossibly close $\text{K}^+\cdots\text{K}^+$ separation ($\sim 1.3 \text{ \AA}$) resulted. The other model structure, which also had a slightly better R value, was therefore assumed to be correct. After inclusion of structure factor contributions for K^+ , a difference map showed the positions of the light atoms.

Three cycles of least-squares refinement with isotropic temperature factors converged to an R value of 0.06. An electron-density difference map showed evidence of anisotropic vibrations of the heavy atoms. Six more cycles of least-squares refinement, with anisotropic thermal parameters for all atoms, converged with $R=0.041$. In the last two cycles, the shifts in the positional parameters were all less than a quarter of the estimated standard deviations; the shift in U_{33} for $\text{C}(2)$ was ~ 0.5 e.s.d., and all other shifts in the thermal parameters were less than 0.3 e.s.d. The positional and vibration parameters are given in Table 2. All positional parameters were refined in one matrix block, with separate 6×6 matrix blocks for the thermal parameters of each atom. Unit weights were used for reflexions with amplitudes less than $160e$; $(160/F)^2$ for amplitudes greater than $160e$. The atomic form factors (Cromer & Waber, 1965) of Pt, Cl, K^+ were corrected for the real part of anomalous dispersion. The observed and calculated structure factors are listed in Table 3 and compared in Table 4.

Table 2. Atomic positional parameters and mean square atomic vibrations (\AA^2)

	x/a	y/b	z/c
Pt	0.28574 (7)	0.25020 (21)	0.05933 (8)
Cl(1)	0.0769 (5)	0.2365 (10)	0.0532 (6)
Cl(2)	0.2841 (6)	0.5221 (9)	0.0930 (7)
Cl(3)	0.2911 (7)	-0.0208 (8)	0.0369 (8)
K^+	-0.0609 (6)	0.0462 (8)	0.2524 (7)
O	-0.1479 (17)	0.3485 (21)	0.2293 (20)
C(1)	0.4378 (19)	0.2667 (35)	-0.0275 (23)
C(2)	0.4851 (18)	0.2573 (44)	0.1197 (25)

	U_{11}	$2U_{12}$	$2U_{13}$	U_{22}	$2U_{23}$	U_{33}
Pt	0.0415 (3)	0.0062 (21)	0.0337 (5)	0.0411 (3)	0.0060 (17)	0.0372 (3)
Cl(1)	0.052 (3)	0.018 (8)	0.053 (5)	0.045 (3)	0.015 (9)	0.082 (4)
Cl(2)	0.068 (4)	-0.012 (7)	0.049 (7)	0.055 (4)	-0.012 (6)	0.066 (4)
Cl(3)	0.082 (4)	0.009 (7)	0.080 (8)	0.045 (4)	0.003 (7)	0.082 (5)
K^+	0.075 (4)	0.010 (7)	0.063 (7)	0.052 (3)	0.032 (7)	0.074 (4)
O	0.078 (12)	0.013 (19)	0.064 (19)	0.054 (11)	-0.009 (18)	0.071 (12)
C(1)	0.055 (11)	0.013 (30)	0.051 (20)	0.044 (14)	0.001 (30)	0.064 (12)
C(2)	0.044 (10)	-0.002 (46)	0.062 (21)	0.066 (14)	-0.029 (46)	0.087 (15)

Table 3. Observed and calculated structure factors

h	k	l	F _o	F _c	h	k	l	F _o	F _c	h	k	l	F _o	F _c										
2	233	293	11	23	26	-1	0	0	0	-8	86	85	-11	0	0	-5	0	0	-11	0	0	-3	0	0
4	78	74	-3	271	255	-1	0	0	0	-4	38	40	-10	83	83	-3	59	60	-10	66	62	-2	242	244
6	152	152	-2	271	255	1	0	0	0	-5	0	0	-7	0	0	-2	130	123	-7	0	0	-1	58	56
8	108	108	3	0	0	2	78	75	0	-7	81	83	-1	0	0	0	67	64	-1	0	0	0	125	123
10	69	67	0	282	279	4	8	0	0	-3	30	30	-7	0	0	-2	20	20	-7	0	0	2	47	49
12	0	0	1	228	203	5	0	0	0	-2	208	206	-5	0	0	-2	0	0	-5	38	33	3	35	36
0	0	1	3	0	0	6	37	37	-1	0	0	0	-4	162	159	-2	0	0	-2	0	0	-4	172	177
1	0	0	4	88	87	7	0	0	0	1	0	0	-2	150	155	-3	58	61	-3	28	31	5	0	0
2	242	222	5	0	0	8	0	0	0	2	83	86	-1	0	0	5	0	0	-2	208	210	7	0	0
3	21	21	7	0	0	9	0	0	0	3	27	25	0	137	139	-1	0	0	4	58	58	1	0	0
4	242	232	8	10	0	10	0	0	0	4	61	58	-1	35	33	7	0	0	0	126	135	8	38	39
5	29	33	9	0	0	11	0	0	0	5	0	0	-3	28	28	3	28	23	3	2	2	42	40	
6	135	134	10	44	46	12	0	0	0	6	87	88	4	97	99	5	39	33	4	119	121	5	0	0
7	0	0	11	0	0	13	0	0	0	7	0	0	-2	62	62	8	63	69	8	0	0	12	0	0
8	0	0	12	0	0	14	0	0	0	8	0	0	9	0	0	10	30	20	9	0	0	11	0	0
10	34	40	13	0	0	15	0	0	0	9	0	0	10	0	0	11	0	0	10	0	0	12	0	0
11	0	0	14	40	46	16	0	0	0	10	25	25	-1	0	0	12	0	0	11	0	0	13	0	0
0	0	2	15	0	0	17	0	0	0	11	0	0	13	0	0	14	0	0	12	0	0	14	0	0
0	231	212	16	0	0	18	0	0	0	12	0	0	14	0	0	15	0	0	13	0	0	15	0	0
2	228	216	17	0	0	19	0	0	0	13	45	66	-11	0	0	16	0	0	14	0	0	16	0	0
3	0	0	18	0	0	20	0	0	0	14	0	0	15	0	0	17	0	0	15	0	0	17	0	0
4	0	0	19	138	141	21	0	0	0	15	141	141	-12	0	0	18	0	0	16	0	0	18	0	0
5	0	0	20	0	0	22	0	0	0	16	0	0	19	0	0	19	0	0	17	0	0	19	0	0
6	7	69	21	149	146	23	0	0	0	17	0	0	20	0	0	20	0	0	18	0	0	20	0	0
7	0	0	22	0	0	24	0	0	0	18	0	0	21	0	0	21	0	0	19	0	0	21	0	0
8	114	114	23	0	0	25	0	0	0	19	0	0	22	0	0	22	0	0	20	0	0	22	0	0
9	0	0	24	0	0	26	0	0	0	20	0	0	23	0	0	23	0	0	21	0	0	23	0	0
10	59	59	25	0	0	27	0	0	0	21	0	0	24	0	0	24	0	0	22	0	0	24	0	0
11	0	0	26	0	0	28	0	0	0	22	0	0	25	0	0	25	0	0	23	0	0	25	0	0
0	0	3	27	0	0	29	0	0	0	23	0	0	26	0	0	26	0	0	24	0	0	26	0	0
1	0	0	28	0	0	30	0	0	0	24	0	0	27	0	0	27	0	0	25	0	0	27	0	0
2	212	205	29	0	0	31	0	0	0	25	0	0	28	0	0	28	0	0	26	0	0	28	0	0
3	233	221	30	0	0	32	0	0	0	26	0	0	29	0	0	29	0	0	27	0	0	29	0	0
4	34	31	31	0	0	33	0	0	0	27	0	0	30	0	0	30	0	0	28	0	0	30	0	0
5	129	121	32	0	0	34	0	0	0	28	0	0	31	0	0	31	0	0	29	0	0	31	0	0
6	0	0	33	0	0	35	0	0	0	29	0	0	32	0	0	32	0	0	30	0	0	32	0	0
7	0	0	34	0	0	36	0	0	0	30	0	0	33	0	0	33	0	0	31	0	0	33	0	0
8	0	0	35	0	0	37	0	0	0	31	0	0	34	0	0	34	0	0	32	0	0	34	0	0
10	39	40	36	0	0	38	0	0	0	32	0	0	35	0	0	35	0	0	33	0	0	35	0	0
11	0	0	37	0	0	39	0	0	0	33	0	0	36	0	0	36	0	0	34	0	0	36	0	0
0	0	4	38	0	0	40	0	0	0	34	0	0	37	0	0	37	0	0	35	0	0	37	0	0
1	344	324	39	0	0	41	0	0	0	35	0	0	38	0	0	38	0	0	36	0	0	38	0	0
2	52	53	40	0	0	42	0	0	0	36	0	0	39	0	0	39	0	0	37	0	0	39	0	0
3	214	204	41	0	0	43	0	0	0	37	0	0	40	0	0	40	0	0	38	0	0	40	0	0
4	34	35	42	0	0	44	0	0	0	38	0	0	41	0	0	41	0	0	39	0	0	41	0	0
5	27	18	43	0	0	45	0	0	0	39	0	0	42	0	0	42	0	0	40	0	0	42	0	0
6	92	94	44	0	0	46	0	0	0	40	0	0	43	0	0	43	0	0	41	0	0	43	0	0
7	30	31	45	0	0	47	0	0	0	41	0	0	44	0	0	44	0	0	42	0	0	44	0	0
8	92	89	46	0	0	48	0	0	0	42	0	0	45	0	0	45	0	0	43	0	0	45	0	0
9	0	0	47	0	0	49	0	0	0	43	0	0	46	0	0	46	0	0	44	0	0	46	0	0
10	40	41	48	0	0	50	0	0	0	44	0	0	47	0	0	47	0	0	45	0	0	47	0	0
11	0	0	49	0	0	51	0	0	0	45	0	0	48	0	0	48	0	0	46	0	0	48	0	0
0	0	5	50	0	0	52	0	0	0	46	0	0	49	0	0	49	0	0	47	0	0	49	0	0
1	0	0	51	0	0	53	0	0	0	47	0	0	50	0	0	50	0	0	48	0	0	50	0	0
2	106	104	52	0	0	54	0	0	0	48	0	0	51	0	0	51	0	0	49	0	0	51	0	0
3	24	21	53	0	0	55	0	0	0	49	0	0	52	0	0	52	0	0	50	0	0	52	0	0
4	144	139	54	0	0	56	0	0	0	50	0	0	53	0	0	53	0	0	51	0	0	53	0	0
5	0	0	55	0	0	57	0	0	0	51	0	0	54	0	0	54	0	0	52	0	0	54	0	0
6	83	79	56	0	0	58	0	0	0	52	0	0	55	0	0	55	0	0	53	0	0	55	0	0
7	0	0	57	0	0	59	0	0	0	53	0	0	56	0	0	56	0	0	54	0	0	56	0	0
8	0	0	58	0	0	60	0	0	0	54	0	0	57	0	0	57	0	0	55	0	0	57	0	0
9	0	0	59	0	0	61	0	0	0	55	0	0	58	0	0	58	0	0	56	0	0	58	0	0
10	0	0	60	0	0	62	0	0	0	56	0	0	59	0	0	59	0	0	57	0	0	59	0	0
0	162	137	61	0	0	63	0	0	0	57	0	0	60	0	0	60	0	0	58	0	0	60	0	0
1	36	33	62	0	0	64	0	0	0	58	0	0	61	0	0	61	0	0	59	0	0	61	0	0
2	106	101	63	0	0	65	0	0	0	59	0	0	62	0	0	62	0	0	60	0	0	62	0	0
3	0	0	64	0	0	66	0	0	0	60	0	0	63	0	0	63	0	0	61	0	0	63	0	0
4	0	0	65	0	0	67	0	0	0	61	0	0	64	0	0	64	0	0	62	0	0	64	0	0
5	0	0	66	0	0	68	0	0	0	62	0	0	65	0	0	65	0	0	63	0	0	65	0	0
6	52	55	67	0	0	69	0	0	0	63	0	0	66	0	0	66	0	0	64	0	0	66	0	0
7	0	0	68	0	0	70	0	0	0	64	0	0	67	0	0	67	0	0	65	0	0	67	0	0
8	06	06	69	0	0	71	0	0	0	65	0	0	68	0	0	68	0	0	66	0	0	68	0	0
9	0	0	70	0	0	72	0	0	0	66	0	0	69	0	0	69	0	0	67	0	0	69	0	0
10	37	39	71	0	0	73	0	0	0	67	0													

Table 3 (cont.)

L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC	L	FO	FC
H=5 K=7	H=6 K=5	H=7 K=3	H=8 K=1	H=9 K=1	H=10 K=1	H=11 K=2	H=12 K=4	H=5 K=7	H=6 K=5	H=7 K=3	H=8 K=1	H=9 K=1	H=10 K=1	H=11 K=2	H=12 K=4	H=5 K=7	H=6 K=5	H=7 K=3	H=8 K=1	
5 0 0 +	-11 0 0 +	-11 0 0 +	4 0 0 +	-4 106 100 -	4 0 0 0 +	-10 0 0 0 +	-3 0 0 0 +	-8 50 49 +	-10 49 42 -	-10 37 41 -	5 0 0 0 +	-3 0 0 0 +	4 0 0 0 +	-10 0 0 0 +	-3 0 0 0 +	6 55 54 -	-11 0 0 0 +	-11 0 0 0 +	5 0 0 0 +	
0 0 0 0 +	-10 0 0 0 +	-10 0 0 0 +	5 0 0 0 +	-3 0 0 0 +	5 0 0 0 +	-10 0 0 0 +	-2 0 0 0 +	-7 0 0 0 +	-9 0 42 -	-9 0 42 -	6 44 42 -	-2 0 0 0 +	-2 0 0 0 +	-10 0 0 0 +	-2 0 0 0 +	0 0 0 0 +	-8 70 70 -	-8 0 0 0 +	6 0 0 0 +	
0 0 0 0 +	-8 0 0 0 +	-8 0 0 0 +	7 0 0 0 +	-1 0 0 0 +	7 0 0 0 +	-1 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	-8 0 0 0 +	-8 0 0 0 +	0 60 61 -	-1 0 0 0 +	-1 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	0 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	8 0 0 0 +	1 0 0 0 +	8 0 0 0 +	1 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	1 0 0 0 +	1 0 0 0 +	1 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	0 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	9 0 0 0 +	2 0 0 0 +	9 0 0 0 +	2 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	-5 24 23 -	-5 24 23 -	2 96 92 +	-11 0 0 0 +	-11 0 0 0 +	-4 66 61 -	-4 66 61 -	0 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-5 0 0 0 +	-5 0 0 0 +	10 0 0 0 +	3 0 0 0 +	10 0 0 0 +	3 0 0 0 +	-5 0 0 0 +	-5 0 0 0 +	-4 126 124 -	-4 126 124 -	3 0 0 0 +	-10 0 0 0 +	-10 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	0 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	11 0 0 0 +	4 0 0 0 +	11 0 0 0 +	4 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	-3 84 86 -	-3 84 86 -	4 69 67 +	-5 0 0 0 +	-5 0 0 0 +	-2 0 0 0 +	-2 0 0 0 +	0 0 0 0 +	-2 0 0 0 +	-2 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	12 0 0 0 +	5 0 0 0 +	12 0 0 0 +	5 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	-2 100 98 -	-2 100 98 -	5 0 0 0 +	-8 59 59 +	-8 59 59 +	-1 0 0 0 +	-1 0 0 0 +	0 0 0 0 +	-1 0 0 0 +	-1 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-2 0 0 0 +	-2 0 0 0 +	13 0 0 0 +	6 0 0 0 +	13 0 0 0 +	6 0 0 0 +	-2 0 0 0 +	-2 0 0 0 +	-1 50 50 -	-1 50 50 -	6 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	0 44 43 +	0 44 43 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	-1 0 0 0 +	-1 0 0 0 +	14 0 0 0 +	7 0 0 0 +	14 0 0 0 +	7 0 0 0 +	-1 0 0 0 +	-1 0 0 0 +	0 0 0 0 +	0 0 0 0 +	7 0 0 0 +	-9 98 103 -	-9 98 103 -	1 0 0 0 +	1 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	15 0 0 0 +	8 0 0 0 +	15 0 0 0 +	8 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-1 60 83 -	-1 60 83 -	8 0 0 0 +	-5 0 0 0 +	-5 0 0 0 +	2 48 53 +	2 48 53 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	16 0 0 0 +	9 0 0 0 +	16 0 0 0 +	9 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-2 95 100 -	-2 95 100 -	9 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	3 0 0 0 +	3 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	17 0 0 0 +	10 0 0 0 +	17 0 0 0 +	10 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	10 0 0 0 +	-3 0 0 0 +	-3 0 0 0 +	4 0 0 0 +	4 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	18 0 0 0 +	11 0 0 0 +	18 0 0 0 +	11 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	11 0 0 0 +	-4 0 0 0 +	-4 0 0 0 +	5 0 0 0 +	5 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	19 0 0 0 +	12 0 0 0 +	19 0 0 0 +	12 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-5 0 0 0 +	-5 0 0 0 +	12 0 0 0 +	-5 0 0 0 +	-5 0 0 0 +	6 0 0 0 +	6 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	20 0 0 0 +	13 0 0 0 +	20 0 0 0 +	13 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	13 0 0 0 +	-6 0 0 0 +	-6 0 0 0 +	7 0 0 0 +	7 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	21 0 0 0 +	14 0 0 0 +	21 0 0 0 +	14 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	14 0 0 0 +	-7 0 0 0 +	-7 0 0 0 +	8 0 0 0 +	8 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	22 0 0 0 +	15 0 0 0 +	22 0 0 0 +	15 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-8 0 0 0 +	-8 0 0 0 +	15 0 0 0 +	-8 0 0 0 +	-8 0 0 0 +	9 0 0 0 +	9 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	23 0 0 0 +	16 0 0 0 +	23 0 0 0 +	16 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-9 0 0 0 +	-9 0 0 0 +	16 0 0 0 +	-9 0 0 0 +	-9 0 0 0 +	10 0 0 0 +	10 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	24 0 0 0 +	17 0 0 0 +	24 0 0 0 +	17 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-10 0 0 0 +	-10 0 0 0 +	17 0 0 0 +	-10 0 0 0 +	-10 0 0 0 +	11 0 0 0 +	11 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	25 0 0 0 +	18 0 0 0 +	25 0 0 0 +	18 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-11 0 0 0 +	-11 0 0 0 +	18 0 0 0 +	-11 0 0 0 +	-11 0 0 0 +	12 0 0 0 +	12 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	26 0 0 0 +	19 0 0 0 +	26 0 0 0 +	19 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-12 0 0 0 +	-12 0 0 0 +	19 0 0 0 +	-12 0 0 0 +	-12 0 0 0 +	13 0 0 0 +	13 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	27 0 0 0 +	20 0 0 0 +	27 0 0 0 +	20 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-13 0 0 0 +	-13 0 0 0 +	20 0 0 0 +	-13 0 0 0 +	-13 0 0 0 +	14 0 0 0 +	14 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	28 0 0 0 +	21 0 0 0 +	28 0 0 0 +	21 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-14 0 0 0 +	-14 0 0 0 +	21 0 0 0 +	-14 0 0 0 +	-14 0 0 0 +	15 0 0 0 +	15 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	29 0 0 0 +	22 0 0 0 +	29 0 0 0 +	22 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-15 0 0 0 +	-15 0 0 0 +	22 0 0 0 +	-15 0 0 0 +	-15 0 0 0 +	16 0 0 0 +	16 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	30 0 0 0 +	23 0 0 0 +	30 0 0 0 +	23 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-16 0 0 0 +	-16 0 0 0 +	23 0 0 0 +	-16 0 0 0 +	-16 0 0 0 +	17 0 0 0 +	17 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	31 0 0 0 +	24 0 0 0 +	31 0 0 0 +	24 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-17 0 0 0 +	-17 0 0 0 +	24 0 0 0 +	-17 0 0 0 +	-17 0 0 0 +	18 0 0 0 +	18 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	32 0 0 0 +	25 0 0 0 +	32 0 0 0 +	25 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-18 0 0 0 +	-18 0 0 0 +	25 0 0 0 +	-18 0 0 0 +	-18 0 0 0 +	19 0 0 0 +	19 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	33 0 0 0 +	26 0 0 0 +	33 0 0 0 +	26 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-19 0 0 0 +	-19 0 0 0 +	26 0 0 0 +	-19 0 0 0 +	-19 0 0 0 +	20 0 0 0 +	20 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	34 0 0 0 +	27 0 0 0 +	34 0 0 0 +	27 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-20 0 0 0 +	-20 0 0 0 +	27 0 0 0 +	-20 0 0 0 +	-20 0 0 0 +	21 0 0 0 +	21 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	35 0 0 0 +	28 0 0 0 +	35 0 0 0 +	28 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-21 0 0 0 +	-21 0 0 0 +	28 0 0 0 +	-21 0 0 0 +	-21 0 0 0 +	22 0 0 0 +	22 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	36 0 0 0 +	29 0 0 0 +	36 0 0 0 +	29 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-22 0 0 0 +	-22 0 0 0 +	29 0 0 0 +	-22 0 0 0 +	-22 0 0 0 +	23 0 0 0 +	23 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	37 0 0 0 +	30 0 0 0 +	37 0 0 0 +	30 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-23 0 0 0 +	-23 0 0 0 +	30 0 0 0 +	-23 0 0 0 +	-23 0 0 0 +	24 0 0 0 +	24 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	38 0 0 0 +	31 0 0 0 +	38 0 0 0 +	31 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-24 0 0 0 +	-24 0 0 0 +	31 0 0 0 +	-24 0 0 0 +	-24 0 0 0 +	25 0 0 0 +	25 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	39 0 0 0 +	32 0 0 0 +	39 0 0 0 +	32 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-25 0 0 0 +	-25 0 0 0 +	32 0 0 0 +	-25 0 0 0 +	-25 0 0 0 +	26 0 0 0 +	26 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	40 0 0 0 +	33 0 0 0 +	40 0 0 0 +	33 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-26 0 0 0 +	-26 0 0 0 +	33 0 0 0 +	-26 0 0 0 +	-26 0 0 0 +	27 0 0 0 +	27 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	41 0 0 0 +	34 0 0 0 +	41 0 0 0 +	34 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-27 0 0 0 +	-27 0 0 0 +	34 0 0 0 +	-27 0 0 0 +	-27 0 0 0 +	28 0 0 0 +	28 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	42 0 0 0 +	35 0 0 0 +	42 0 0 0 +	35 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-28 0 0 0 +	-28 0 0 0 +	35 0 0 0 +	-28 0 0 0 +	-28 0 0 0 +	29 0 0 0 +	29 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	43 0 0 0 +	36 0 0 0 +	43 0 0 0 +	36 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-29 0 0 0 +	-29 0 0 0 +	36 0 0 0 +	-29 0 0 0 +	-29 0 0 0 +	30 0 0 0 +	30 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	44 0 0 0 +	37 0 0 0 +	44 0 0 0 +	37 0 0 0 +	0 0 0 0 +	0 0 0 0 +	-30 0 0 0 +	-30 0 0 0 +	37 0 0 0 +	-30 0 0 0 +	-30 0 0 0 +	31 0 0 0 +	31 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	
0 0 0 0 +	0 0 0 0 +	0 0 0 0 +	4																	

Table 4. Comparison of observed and calculated structure factors

Range $ F_{\text{obs}} $	No. in range	$\sum F_{\text{obs}} $	$\sum F_{\text{calc}} $	$\sum \Delta F$	Average $w \Delta F ^2$	R
13—26	38	875	829	103	13.4	0.118
26—38	159	5245	5150	540	18.9	0.103
38—51	142	6448	6359	408	13.9	0.063
51—64	139	7952	7976	342	11.4	0.043
64—73	79	5526	5498	211	11.0	0.038
77—89	75	6204	6214	184	8.8	0.030
89—102	53	5064	5070	129	9.11	0.025
102—115	44	4774	4764	138	12.7	0.029
115—128	26	3147	3162	71	16.7	0.023
128—153	40	5633	5651	130	16.1	0.023
153—230	48	9052	9070	227	23.5	0.025
230—383	17	4761	4630	178	53.6	0.037
Total	860	64681	64393	2661		
sin θ/λ						
0—0.1	3	561	561	9	8.0	0.016
0.1—0.2	39	5431	5312	249	37.2	0.046
0.2—0.3	102	11206	11190	327	13.1	0.029
0.3—0.4	162	14512	14566	458	12.3	0.032
0.4—0.5	214	15959	15918	534	10.7	0.033
0.5—0.6	244	12820	12797	748	15.9	0.058
0.6—0.7	96	4191	4051	335	19.3	0.080
l						
0	103	9423	9519	379	19.8	0.040
1	28	942	920	65	7.7	0.069
2	180	17260	17140	681	19.5	0.039
3	30	1006	960	71	10.0	0.071
4	162	13847	13684	492	14.1	0.036
5	19	632	619	45	13.7	0.071
6	138	10400	10390	346	10.8	0.033
7	8	245	235	17	8.0	0.069
8	110	6787	6789	289	11.1	0.043
9	1	30	26	4	17.2	0.136
10	68	3504	3513	218	15.3	0.062
11	—	—	—	—	—	—
12	13	605	593	54	28.3	0.089

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