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The crystal structure of meyerhofferite, $CaB_3O_3(OH)_5 \cdot H_2O$ *

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With 2 figures

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Auszug

Meyerhofferit, $CaB_3O_3(OH)_5 \cdot H_2O$ ist triklin, in der Raumgruppe $P\bar{1}$ mit $a = 6{,}63$, $b = 8{,}35$, $c = 6{,}46$ Å (sämtlich $\pm$ 0,015 Å), $\alpha = 90°46'$, $\beta = 101°59'$, $\gamma = 86°55'$ (sämtlich $\pm$ 5'), $Z = 2$; Dichte: berechnet 2,125, gemessen 2,120. Die mit Hilfe der statistischen Methode von Hauptman und Karle aus 4193 Interferenzen berechneten Strukturfaktorvorzeichen ließen die Aufstellung einer Struktur zu, deren Parameter anschließend durch mehrfache Elektronendichte-Projektionen und mittels der Methode der kleinsten Quadrate verfeinert wurden. Für die endgültige Struktur ist der restliche Diskrepanzfaktor 0,14 aus 2678 Interferenzen mit $|F_{hkl}| > 0$.

Meyerhofferit enthält Polyionen $[B_3O_3(OH)_5]$ aus zwei B—O-Tetraedern und einem B—O-Dreieck, die durch gemeinsame Sauerstoffionen ringförmig verbunden sind. Die Polyion-Inseln sind miteinander durch Ca—O-Bindungen zu Zickzackstreifen parallel [001] verknüpft. Diese Streifen wechseln mit Wassermolekülen ab, mit denen sie über ein Netzwerk von Wasserstoffbindungen zusammenhängen. Die Struktur ist im Einklang mit der beobachteten Spaltbarkeit.

Abstract

Meyerhofferite, $CaB_3O_3(OH)_5 \cdot H_2O$, is triclinic $P\bar{1}$, $a = 6.63$, $b = 8.35$, $c = 6.46$ Å (all $\pm$ 0.015 Å), $\alpha = 90°46'$, $\beta = 101°59'$, $\gamma = 86°55'$ (all $\pm$ 05'), $Z = 2$, density (g. cm^{-3}): calc. 2.125, obs. 2.120. Signs for the observed reflections, calculated by the statistical method of Hauptman and Karle, using 4193 three-dimensional data, permitted the establishment of a trial structure which was refined by successive electron-density projections and least-squares analysis. For the final structure, the residual factor is 0.14 for 2678 terms with $|F_{hkl}| > 0$. Meyerhofferite contains the polyion $[B_3O_3(OH)_5]^{-2}$ consisting of two boron-oxygen tetrahedra and a boron-oxygen triangle linked at corners to form

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a ring. The insular polyions are linked together by calcium-oxygen bonds to form zigzag strings along [001]; the strings and the water molecule are in turn linked by a network of hydrogen bonds. The structure is in good accord with the observed cleavage.

Introduction

In the series $2CaO \cdot 3B_2O_3 \cdot xH_2O$, meyerhofferite has $x = 7$; other known members of the series are colemanite, with $x = 5$; a synthetic compound, with $x = 9$; and inyoite, with $x = 13$. As part of a systematic investigation of the crystal structures of borate minerals, the crystal structure of each of the members of this series has been determined. Colemanite was described by CHRIST, CLARK, and EVANS (1958), a preliminary note has appeared on meyerhofferite (CHRIST and CLARK, 1956), the synthetic compound was described by CLARK and CHRIST (1959), and inyoite was reported by CLARK (1959). The present paper presents the detailed results of the structure investigation of meyerhofferite; the phase determination which led to the solution of the crystal structure is described in detail in an accompanying paper (CLARK and CHRIST, 1960).

Experimental work

Crystal description, space group, and unit-cell dimensions

The crystals of meyerhofferite used in this study are synthetic and were grown by W. T. SCHALLER, U.S. Geological Survey, on ulexite fragments placed in water and held at 70–80 °C for approximately six months (CHRIST, 1953). X-ray powder data and a description of the morphology, together with the cell constants originally obtained by SWITZER (PALACHE, 1938) are given by CHRIST (1953). Subsequently, x-ray precession patterns were taken with Zr-filtered Mo radiation on a quartz-calibrated precession camera. Film measurements were corrected for both horizontal and vertical film shrinkage to obtain the crystallographic data given in CHRIST and CLARK (1956). These data are repeated here in Table 1, together with the reciprocal cell elements, the projection elements, and the direct and reciprocal Cartesian matrices.

Intensity measurements

For the intensity measurements multiple-film Weissenberg patterns were prepared using chiefly Zr-filtered Mo radiation; some small-angle reflections were obtained with Ni-filtered Cu radiation. For the Mo

Table 1. *Crystallographic data for meyerhofferite*

Triclinic, space group $P\bar{1} - C_i^1$, $Z = 2$ [$CaB_3O_3(OH)_5 \cdot H_2O$]

Direct-cell elements:

$a = 6.63_0$ Å	$\alpha = 90°46'$
$b = 8.35_2$	$\beta = 101°59'$
$c = 6.46_2$	$\gamma = 86°55'$
(all ± 0.015 Å)	(all ± 05′)

$a:b:c = 0.794:1:0.774$

($\lambda_{MoK\alpha} = 0.7107$ Å; $\lambda_{CuK\alpha} = 1.5418$ Å)

Volume = 349.5 Å³ Density (g.cm⁻³), calc. 2.125, obs. [Schaller (1916) for the mineral] 2.120

Reciprocal-cell elements:

$a^* = 0.1544$ Å^{-1}	$\alpha^* = 89°52'$
$b^* = 0.1199$	$\beta^* = 78°02'$
$c^* = 0.1582$	$\gamma^* = 92°59'$

$p_0:q_0:r_0 = 0.976:0.758:1$

Projection elements:

$x_o' = 0.2124$	$p_o' = 0.9977$
$y_o' = 0.0024$	$q_o' = 0.7748$

$\nu = 92°59'$

Cartesian matrices*:

$v_1 = 0.0521_4$ $v_2 = 0.9985_5$

$$\text{Direct matrix:} \quad \begin{Vmatrix} 6.485 & 0.435 & 0 \\ 0 & 8.340 & 0 \\ -1.377 & -0.112 & 6.462 \end{Vmatrix} \quad (\text{in Å})$$

$$\text{Reciprocal matrix:} \quad \begin{Vmatrix} 0.1542 & 0 & 0.0329 \\ -0.0080 & 0.1199 & 0.0004 \\ 0 & 0 & 0.1548 \end{Vmatrix} \quad (\text{in Å}^{-1})$$

* Values calculated from direct- and reciprocal-cell elements using equations given by Evans (1948).

patterns three films interleaved with 0.0005 in. Ni foil were used for each exposure. Patterns about [001] were taken for each level up to *hk*9, and the 0*kl*, *h*0*l* and *h*1*l* levels were also recorded. Exposure times were approximately 70 hours at 50 kV and 20 ma for each level, and, as necessary, short exposures of the order of 2–4 hours were also made in order to bring the stronger reflections into the range of measurement. Intensities were estimated visually by comparison with a standard spot strip of intensities, prepared from the same meyerhofferite crystal used for the other patterns. Controlled exposures on the standard strip were made so that the intensity of the nth spot is given by $I_n = I_0(2)^{n/2}$, where I_0 corresponds to a barely perceptible blackening of the film. In the reciprocal sphere of radius $s = (\sin\theta)/\lambda = 0.9$ Å^{-1} there are 4342 independent reflections; 2678 of these had observable intensities, 1515 had intensities below the threshold of observation and were assigned the value zero, and 149 reflections, all with $s > 0.8$ Å^{-1}, were not recorded and were omitted from the compilation of data.

The equi-inclination Weissenberg instrument used for this study covered a 200° traverse at one setting, so that two settings were required for each upper level in order to record the entire 360° range. Weissenberg-instrument geometry for upper-level films is such that distortion occurs in the recording of reflections, some being contracted and some, extended. Systematic differences in intensity readings are therefore inevitable. In order to eliminate the systematic errors, comparison was made of different readings for the same reflection which had registered on a given level with each type of distortion. The comparison was carried out for as many reflections as possible on each level, and an average linear scale factor relating readings for contracted and extended reflections was found. This scale factor was then multiplied into readings for the extended reflections in order to place all readings on approximately the same scale.

The estimated intensities were corrected for Lorentz and polarization factors to obtain the F^2_{hkl}'s. For this correction the $1/Lp$ factor was calculated for each reciprocal lattice point, as a function of its cylindrical coordinates, by punched-card methods. Small and nearly equant crystals, about 0.2 mm on edge, were used to minimize absorption effects, but no absorption corrections were made. The F^2_{hkl}'s from various films were all put on the same relative scale by the use of appropriate film factors. Through the use of the triple-film technique, together with short and long exposures, a range of intensities from 1 to 8000 and of F^2_{hkl} from 1 to about 800 was obtained*.

* The ranges of 1 to 10,000 and 1 to 3,000 referred to as ranges of F^2_{hkl} in previous publications by the authors on colemanite, inyoite and $CaB_3O_3(OH)_5 \cdot 2H_2O$ are actually ranges of intensities.

Other considerations

In preparation for application of the Hauptman-Karle phase-determination procedures to the meyerhofferite data, a $K(s)$ curve (KARLE and HAUPTMAN, 1953) was prepared for meyerhofferite (CLARK and CHRIST, 1960). Initially the factor $[K(0)]^{1/2}$ was used to place the data on an approximate absolute scale. At all later stages of the study, observed and calculated structure factors were related by use of the scaling constant k, where $k\Sigma|F_o| = \Sigma|F_c|$.

Refinement of the projection data was carried out with an average isotropic temperature factor, determined by the method of WILSON (1942). Maxima on the electron-density projections were located by the method of BOOTH (1948). Refinement of the three-dimensional data was carried out using one-fifth of the 2678 data that have $|F_o| > 0$, selected by arranging the terms in order of increasing s and taking every fifth one. This portion of the data was given eleven cycles of least-squares refinement on a Burroughs 205 digital computer with a program developed by D. E. APPLEMAN and E. MONASTERSKI, U.S. Geological Survey. Non-diagonal terms were neglected in the solution of the normal equations, except for those terms involving both the temperature and scale factors. Atomic scattering curves were used as follows: for boron, the B^0 curve of IBERS (1957), for all oxygen atoms, the O^0 curve of BERGHUIS *et al.* (1955), and for calcium, a curve constructed by plotting the BERGHUIS *et al.* values for Ca^0 for $(\sin\theta)/\lambda \geq 0.3$ Å^{-1} and smoothing in to $f = 18$ at $(\sin\theta)/\lambda = 0$.

Determination and refinement of the structure

The structural problem consists in determining the coordinates for one calcium, three boron, and nine oxygen atoms (including OH^- and H_2O) in the positions $2(i)$ of space group $P\bar{1}$ (Internat. Tables, 1952). Direct determination of the signs of 2303 of the 2678 terms with $|F_o| > 0$ was made with Hauptman-Karle statistical procedures (CLARK and CHRIST, 1960). The projection data with known signs (F_{hk0}, F_{h0l}, F_{0kl}) were then used to calculate the three electron-density projections, each taken on a plane normal to a principal crystallographic axis. One of these, $\varrho_y(x, z)$, was shown in the preliminary note (Fig. 1, CHRIST and CLARK, 1956). The three maps considered together with a ball model were readily interpreted, and from positions of peak maxima, atomic coordinates were assigned to all thirteen atoms in the asymmetric unit (Table 2, column 1). From structure factors based on these coordinates signs were obtained for over $90^0/_0$ of the

Table 2. *Atomic positional parameters and temperature coefficients for meyerhofferite*

Atom	Parameter[2]	Stage of refinement[1]			
		(1)	(2)	(3)	(4)
Ca	x	0.014	0.010	0.010	0.010
	y	0.377	0.377	0.377	0.377
	z	0.243	0.243	0.244	0.244
	B				0.75
O_1	x	0.410	0.407	0.406	0.406
	y	0.732	0.734	0.733	0.732
	z	0.313	0.327	0.331	0.331
	B				0.99
O_2(OH)	x	0.419	0.422	0.423	0.423
	y	0.890	0.889	0.887	0.888
	z	0.660	0.651	0.643	0.643
	B				1.36
O_3	x	0.118	0.115	0.116	0.116
	y	0.782	0.776	0.776	0.776
	z	0.500	0.502	0.495	0.493
	B				1.09
O_4(OH)	x	0.340	0.339	0.336	0.335
	y	0.461	0.461	0.461	0.461
	z	0.206	0.211	0.203	0.201
	B				1.15
O_5	x	0.058	0.058	0.062	0.063
	y	0.644	0.642	0.650	0.652
	z	0.148	0.145	0.150	0.151
	B				0.70
O_6(OH)	x	0.173	0.165	0.167	0.167
	y	0.370	0.374	0.378	0.378
	z	0.615	0.615	0.617	0.617
	B				1.02
$O_7(H_2O)$	x	0.157	0.132	0.148	0.151
	y	0.108	0.104	0.109	0.109
	z	0.202	0.211	0.216	0.217
	B				1.55
O_8(OH)	x	0.146	0.145	0.151	0.151
	y	0.117	0.126	0.123	0.123
	z	0.792	0.797	0.800	0.800
	B				1.19
O_9(OH)	x	0.329	0.334	0.330	0.330
	y	0.672	0.673	0.668	0.668
	z	0.955	0.955	0.956	0.957
	B				1.08

Table 2 (*continued*)

Atom	Parameter[2]	Stage of refinement[1] (1)	(2)	(3)	(4)
B_1	x	0.312	0.318	0.322	0.321
	y	0.798	0.792	0.798	0.798
	z	0.489	0.497	0.487	0.485
	B				0.86
B_2	x	0.308	0.308	0.290	0.285
	y	0.642	0.642	0.634	0.634
	z	0.183	0.183	0.173	0.167
	B				0.74
B_3	x	0.050	0.030	0.034	0.037
	y	0.233	0.278	0.269	0.267
	z	0.710	0.683	0.695	0.698
	B				0.78
Residual, R					
	$hk0$	0.19	0.18	—	—
	$h0l$	0.19	0.16	—	—
	$0kl$	0.21	0.16	—	—
	hkl	—	—	0.147[3]	0.145[4]
Scale factor, k					
	$hk0$	2.5	2.5	—	—
	$h0l$	2.4	2.4	—	—
	$0kl$	2.6	2.7	—	—
	hkl	—	—	2.9[3]	2.7_3[4]
Average isotropic B					
	$hk0$	0.66	0.66	—	
	$h0l$	1.00	1.00	—	
	$0kl$	0.94	0.94	—	
	hkl	—	—	0.87[3]	

[1] Stages of refinement: (1) from peak positions on electron-density projections calculated with signs determined by Hauptman-Karle procedures; (2) from peak positions of second set of electron-density projections; (3) at end of 5 cycles of least-squares refinement for one-fifth of three-dimensional data, average isotropic B; (4) final parameters at end of 11 cycles of least-squares refinement for one-fifth of three-dimensional data, individual isotropic B's.

[2] x, y, z in cycles; B in $Å^2$; standard errors in B: $\varepsilon_{Ca} = 0.03$, $\varepsilon_O = 0.17$ $\varepsilon_B = 0.17$ $Å^2$.

[3] For 535 terms with $|F_{hkl}| > 0$.

[4] For 2678 terms with $|F_{hkl}| > 0$.

Table 3. *Comparison of observed and calculated structure factors for hkl data of meyerhofferite.* Calculated F_{hkl} are based on the atomic parameters of Table 2, column 4

h k l	F_c	$\vert F_o \vert$
11 6 0	- 3	
5	11	15
4	-10	10
3	3	
2	9	11
1	- 7	6
0	- 1	
- 1	- 3	
- 2	- 2	
- 3	6	
- 4	- 4	
11 5 1	- 0	
4	7	8
3	- 4	
2	6	6
1	- 4	6
0	- 3	6
- 1	10	12
- 2	- 9	10
- 3	- 5	8
11 3 2	- 6	
2	- 4	
1	7	6
0	- 2	
- 1	- 1	
10 8 0	3	
7	- 3	
6	- 4	
5	10	11
4	- 2	
3	- 0	
2	6	6
1	- 5	
0	3	5
- 1	- 4	
- 2	-10	12
- 3	9	9
- 4	- 1	
- 5	5	7
- 6	1	
- 7	- 5	
10 8 1	- 1	
7	8	10
6	- 9	9
5	3	
4	4	5
3	- 5	6
2	5	7
1	- 5	5
0	- 6	8
- 1	12	13
- 2	- 6	
- 3	5	
- 4	- 1	
- 5	- 9	11
- 6	10	10
10 7 2	- 1	
6	8	9
5	- 5	
4	1	
3	1	
2	- 9	10
1	10	10
0	- 0	
- 1	- 4	
- 2	5	
- 3	- 5	
- 4	5	
- 5	- 1	
10 5 3	-10	11
4	- 2	
3	9	9
2	- 8	8
1	4	
0	6	
- 1	- 8	6
- 2	11	8
- 3	- 5	
- 4	- 7	6
10 3 4	- 2	
2	2	
1	- 5	
0	7	
- 1	- 6	
9 10 0	6	7
9	- 4	
8	0	
7	2	
6	- 0	
5	11	11
4	- 3	
3	- 5	8
2	4	6
1	-17	22
0	5	5
- 1	7	8
- 2	- 2	
- 3	4	5
- 4	1	
- 5	2	
- 6	1	
- 7	-11	11
- 8	- 1	
- 9	4	
9 9 1	-11	13
8	0	6
7	10	13
6	- 7	11
5	3	8
4	5	6
3	- 7	7
2	13	14
1	-12	14
0	- 3	
- 1	10	11
- 2	-16	20
- 3	11	12
- 4	7	9
- 5	-13	13
- 6	8	6
- 7	1	

h k l	F_c	$\vert F_o \vert$
9 $\bar{8}$ 1	- 4	
9 9 2	12	13
8	1	
7	-10	14
6	2	
5	- 4	
4	3	
3	- 2	
2	- 5	7
1	13	16
0	0	
- 1	3	
- 2	- 3	
- 3	- 6	5
- 4	0	
- 5	- 5	
- 6	2	
- 7	9	10
- 8	- 8	
9 8 3	2	
7	- 6	
6	11	13
5	- 4	
4	-15	15
3	13	10
2	- 2	
1	0	
0	2	
- 1	- 5	5
- 2	7	6
- 3	- 0	
- 4	- 6	6
- 5	5	
- 6	- 2	
- 7	- 2	
9 6 4	- 3	
5	7	8
4	- 4	
3	9	9
2	- 4	
1	-11	14
0	13	13
- 1	- 6	
- 2	- 4	
- 3	5	
- 4	- 3	
- 5	7	7
9 4 5	5	8
3	-10	6
2	6	
1	1	
0	- 6	
- 1	2	
- 2	- 1	
- 3	3	
8 11 0	- 3	
10	2	
9	- 7	7
8	8	9
7	4	
6	-11	14
5	14	17
4	- 5	
3	- 2	
2	3	5
1	-11	11
0	2	
- 1	5	6
- 2	- 1	
- 3	6	5
- 4	- 3	
- 5	0	
- 6	1	
- 7	- 7	10
- 8	7	7
- 9	- 5	6
-10	2	
8 11 1	- 2	
10	7	8
9	- 3	4
8	- 3	
7	12	10
6	- 9	7
5	6	6
4	- 2	
3	-16	15
2	15	15
1	- 3	
0	- 4	
- 1	13	13
- 2	- 7	6
- 3	- 4	4
- 4	8	8
- 5	-12	14
- 6	5	
- 7	0	
- 8	- 2	
- 9	5	
-10	- 2	
8 10 2	- 6	10
9	6	6
8	- 3	
7	2	
6	- 1	
5	- 9	7
4	15	14
3	- 6	5
2	1	
1	6	5
0	-12	11
- 1	6	6
- 2	- 0	
- 3	-12	12
- 4	16	12
- 5	- 6	5
- 6	- 2	
- 7	13	16
- 8	-11	10
- 9	4	
8 10 3	- 1	
9	- 2	

h k l	F_c	$\vert F_o \vert$
8 8 3	3	
7	-14	12
6	5	
5	2	
4	- 5	5
3	7	6
2	2	
1	4	
0	2	
- 1	-11	9
- 2	1	
- 3	0	
- 4	- 7	6
- 5	9	9
- 6	- 2	
- 7	4	
- 8	1	
8 9 4	- 6	
8	10	9
7	- 3	
6	- 1	
5	5	
4	-11	11
3	8	7
2	- 2	
1	- 9	8
0	9	10
- 1	- 1	
- 2	1	
- 3	8	8
- 4	-12	14
- 5	8	8
- 6	- 3	
- 7	-11	10
8 7 5	11	10
6	- 4	
5	4	
4	5	
3	-10	8
2	- 1	
1	- 1	
0	- 4	
- 1	6	5
- 2	- 3	
- 3	5	
- 4	4	
- 5	- 6	
- 6	3	
8 5 6	- 6	
4	9	11
3	- 4	
2	- 2	
1	10	9
0	- 8	9
- 1	- 1	
- 2	7	7
- 3	-10	9
- 4	4	
7 12 0	-10	11
11	- 1	
10	12	12
9	-14	15
8	13	16
7	7	11
6	- 7	8
5	0	
4	-15	15
3	- 1	
2	3	
1	-11	13
0	20	20
- 1	10	12
- 2	- 6	5
- 3	7	7
- 4	-18	19
- 5	9	10
- 6	- 7	6
- 7	-14	19
- 8	18	20
- 9	1	
-10	- 2	
-11	8	9
7 12 1	1	
11	- 7	9
10	5	
9	- 3	
8	0	
7	11	11
6	-11	8
5	5	6
4	8	8
3	-11	11
2	- 2	4
1	5	5
0	- 7	8
- 1	5	5
- 2	- 6	6
- 3	9	7
- 4	4	6
- 5	-10	8
- 6	5	
- 7	1	
- 8	- 1	
- 9	- 3	
-10	- 4	
-11	5	
7 11 2	- 3	
10	- 3	5
9	10	9
8	-15	13
7	2	
6	0	
5	- 6	6
4	13	13
3	- 3	5
2	1	
1	16	17
0	-20	18
- 1	0	
- 2	2	
- 3	-15	13

h k l	F_c	$\vert F_o \vert$
7 $\bar{4}$ 2	13	12
- 5	- 2	
- 6	7	9
- 7	5	6
- 8	-12	13
- 9	6	
-10	2	
7 11 3	8	6
10	- 4	
9	2	
8	- 1	
7	- 7	6
6	11	9
5	- 5	5
4	- 5	6
3	15	12
2	- 8	5
1	- 4	
0	7	6
- 1	-12	10
- 2	12	10
- 3	- 4	
- 4	- 3	
- 5	8	8
- 6	- 7	6
- 7	1	
- 8	4	
- 9	- 4	
-10	1	
7 10 4	- 2	
9	- 7	
8	7	8
7	- 2	
6	0	
5	3	
4	- 2	
3	4	5
2	- 4	6
1	- 9	10
0	16	14
- 1	- 8	7
- 2	- 4	5
- 3	11	12
- 4	- 8	8
- 5	4	
- 6	0	
- 7	- 7	9
- 8	4	
- 9	1	
7 9 5	1	
8	- 1	
7	5	
6	- 6	6
5	2	
4	- 1	
3	-11	12
2	10	10
1	- 1	
0	0	
- 1	7	7
- 2	- 8	10
- 3	11	7
- 4	- 9	10
- 5	- 9	9
- 6	11	9
- 7	- 5	
- 8	1	
7 7 6	5	7
6	6	6
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4	3	
3	1	
2	- 8	10
1	7	
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- 1	5	
- 2	3	
- 3	- 7	7
- 4	4	
- 5	2	
- 6	- 2	
7 5 7	- 4	
4	3	6
3	9	5
2	- 8	6
1	6	4
0	- 2	
- 1	-10	11
- 2	5	5
- 3	- 4	
- 4	4	
6 13 0	10	13
12	- 8	10
11	0	
10	8	8
9	- 6	8
8	8	7
7	- 4	
6	- 7	8
5	8	9
4	-14	13
3	8	10
2	13	13
1	-21	25
0	22	22
- 1	- 6	7
- 2	- 2	
- 3	3	4
- 4	-21	24
- 5	11	8
- 6	11	11
- 7	-11	8
- 8	7	7
- 9	- 2	
-10	- 1	
-11	6	9
-12	-11	13
6 13 1	- 0	
12	2	
11	- 4	
10	12	12

h k l	F_c	$\vert F_o \vert$
6 9 1	- 3	
8	- 3	5
7	8	7
6	-10	9
5	- 5	7
4	5	3
3	-13	12
2	21	19
1	- 1	
0	- 0	
- 1	12	12
- 2	-23	19
- 3	6	3
- 4	9	8
- 5	-14	11
- 6	4	
- 7	3	
- 8	- 1	
- 9	11	8
-10	-12	9
-11	1	
-12	4	
6 12 2	7	8
11	- 4	6
10	- 6	8
9	5	6
8	- 0	
7	1	5
6	2	
5	- 1	
4	12	11
3	- 7	7
2	- 8	9
1	- 1	
0	-14	12
- 1	15	15
- 2	- 2	
- 3	3	
- 4	10	10
- 5	- 8	8
- 6	3	
- 7	5	6
- 8	-20	18
- 9	3	
-10	6	
-11	- 2	
6 12 3	- 2	6
11	8	6
10	-13	9
9	2	
8	- 0	
7	-17	13
6	21	17
5	7	7
4	-13	12
3	19	16
2	-12	11
1	2	
0	- 3	4
- 1	-18	16
- 2	11	9
- 3	2	
- 4	2	
- 5	10	10
- 6	- 9	8
- 7	2	
- 8	1	
- 9	- 7	6
-10	8	7
-11	-11	
6 11 4	5	7
10	- 1	
9	- 2	
8	6	6
7	- 2	
6	- 5	5
5	1	
4	-11	9
3	12	13
2	2	
1	-13	13
0	18	15
- 1	3	4
- 2	- 6	5
- 3	- 2	
- 4	- 9	10
- 5	- 0	
- 6	6	6
- 7	- 4	
- 8	8	9
- 9	- 1	
-10	0	6
6 10 5	4	
9	0	
8	1	
7	7	6
6	- 9	6
5	5	5
4	- 2	
3	-16	11
2	12	8
1	- 2	
0	7	7
- 1	3	5
- 2	-11	11
- 3	11	10
- 4	2	
- 5	-14	16
- 6	6	
- 7	- 3	
- 8	2	
- 9	6	11
6 9 6	8	7
8	- 7	7
7	- 0	
6	4	
5	- 9	8
4	10	9
3	- 4	
2	2	
1	5	7

h k l	F_c	$\vert F_o \vert$
6 0 6	-15	15
- 1	7	6
- 2	5	5
- 3	-11	10
- 4	5	
- 5	1	
- 6	2	
- 7	8	9
- 8	-13	11
6 7 7	- 3	
6	6	6
5	- 3	
4	- 1	
3	5	
2	- 5	6
1	3	
0	- 2	
- 1	- 2	
- 2	1	
- 3	- 3	
- 4	6	
- 5	6	8
- 6	-12	10
6 5 8	11	10
4	- 5	
3	5	7
2	- 3	6
1	- 8	11
0	6	6
- 1	- 3	6
- 2	1	
- 3	7	8
- 4	- 5	
5 14 0	- 4	
13	2	
12	- 3	
11	10	12
10	4	
9	- 9	8
8	10	10
7	- 1	
6	-19	18
5	- 3	
4	-14	17
3	30	32
2	9	11
1	- 1	
0	13	16
- 1	-11	10
- 2	- 6	7
- 3	- 8	8
- 4	-15	16
- 5	8	7
- 6	2	
- 7	5	4
- 8	20	21
- 9	-18	18
-10	1	
-11	5	6
-12	- 9	10
-13	4	
5 13 1	4	
12	3	
11	-10	8
10	11	10
9	0	
8	- 8	7
7	14	11
6	-23	20
5	18	17
4	15	16
3	-41	43
2	19	18
1	5	6
0	-11	10
- 1	18	17
- 2	-14	14
- 3	- 1	
- 4	23	23
- 5	-20	18
- 6	7	6
- 7	- 5	
- 8	- 8	7
- 9	9	6
-10	- 2	
-11	4	
-12	- 1	
-13	- 2	
5 13 2	2	
12	2	
11	- 2	
10	- 2	
9	- 2	
8	- 5	7
7	9	10
6	2	
5	- 4	5
4	11	11
3	-12	11
2	16	17
1	-10	9
0	-29	28
- 1	17	15
- 2	14	14
- 3	-10	9
- 4	14	12
- 5	- 8	7
- 6	- 1	
- 7	9	7
- 8	-16	16
- 9	4	
-10	1	
-11	- 3	
-12	7	
5 13 3	- 5	
12	- 9	9
11	10	9
10	- 7	6
9	- 0	
8	11	9
7	-13	12

Table 3 (*continued*)

h k l	F_c	$\|F_o\|$
5 6 3	14	11
5	- 2	
4	- 3	4
3	2	
2	-19	18
1	6	7
0	11	11
- 1	- 2	
- 2	5	5
- 3	- 9	9
- 4	4	
- 5	11	12
- 6	-22	19
- 7	7	
- 8	1	
- 9	- 2	
-10	9	
-11	- 6	
-12	- 0	
5 12 4	- 4	
11	3	
10	- 2	5
9	-11	11
8	16	12
7	- 3	
6	- 5	
5	11	10
4	-15	12
3	9	8
2	5	5
1	-10	11
0	5	5
- 1	- 6	5
- 2	- 2	4
- 3	18	16
- 4	-19	15
- 5	3	
- 6	6	6
- 7	- 4	5
- 8	10	12
- 9	- 4	8
-10	- 2	
-11	8	
5 11 5	- 3	
10	10	7
9	2	
8	- 6	6
7	- 1	4
6	-11	8
5	8	7
4	- 0	
3	- 1	
2	9	8
1	3	
0	3	4
- 1	- 1	
- 2	-13	10
- 3	- 2	
- 4	- 2	
- 5	4	
- 6	11	10
- 7	- 9	6
- 8	7	
- 9	3	
-10	- 6	
5 10 6	- 2	
9	8	8
8	-12	9
7	13	10
6	0	
5	-18	17
4	13	10
3	- 5	4
2	- 2	
1	12	14
0	-15	12
- 1	6	5
- 2	11	9
- 3	-13	12
- 4	10	8
- 5	- 8	7
- 6	- 4	
- 7	7	9
- 8	- 5	5
- 9	2	
5 9 7	1	
8	- 1	
7	- 2	
6	7	7
5	0	
4	8	6
3	- 4	4
2	-13	12
1	4	4
0	0	
- 1	- 7	5
- 2	11	8
- 3	- 4	
- 4	5	
- 5	9	10
- 6	-12	11
- 7	0	
- 8	- 2	
5 7 8	- 1	
6	0	
5	3	
4	- 6	7
3	4	5
2	3	
1	- 4	
0	1	
- 1	- 5	5
- 2	4	
- 3	5	6
- 4	- 9	7
- 5	6	
- 6	- 2	
5 4 9	0	
3	- 7	7
2	6	5
1	- 2	

h k l	F_c	$\|F_o\|$
5 0 9	2	
- 1	9	7
- 2	-12	11
- 3	3	
4 14 0	- 1	
13	5	6
12	- 4	7
11	6	8
10	6	5
9	-17	19
8	- 1	
7	- 3	
6	16	16
5	- 2	
4	- 8	11
3	26	33
2	- 0	
1	- 8	9
0	-12	16
- 1	-30	33
- 2	13	14
- 3	16	17
- 4	-18	19
- 5	34	35
- 6	- 9	7
- 7	-12	11
- 8	16	14
- 9	-13	12
-10	- 7	8
-11	8	8
-12	- 5	6
-13	7	8
4 14 1	- 7	6
13	6	5
12	10	9
11	-13	12
10	14	11
9	- 7	7
8	-10	10
7	14	14
6	-32	34
5	6	7
4	35	34
3	- 9	9
2	0	2
1	5	5
0	-11	13
- 1	16	17
- 2	-32	32
- 3	3	
- 4	7	8
- 5	- 3	4
- 6	12	11
- 7	- 6	6
- 8	4	
- 9	0	
-10	- 8	5
-11	8	5
-12	- 1	
-13	- 8	5
4 14 2	- 3	
13	- 5	5
12	5	6
11	- 6	4
10	- 0	
9	11	9
8	-12	11
7	17	14
6	4	
5	-12	12
4	- 1	3
3	-26	27
2	- 6	4
1	39	38
0	-19	19
- 1	8	7
- 2	29	31
- 3	-13	13
- 4	5	7
- 5	-23	20
- 6	- 7	9
- 7	10	8
- 8	- 8	5
- 9	7	6
-10	12	
-11	- 8	
-12	5	
-13	- 4	
4 13 3	1	
12	- 9	9
11	0	
10	- 8	8
9	9	8
8	0	
7	0	
6	13	12
5	- 9	10
4	2	
3	3	
2	-19	17
1	- 4	4
0	2	
- 1	5	5
- 2	23	22
- 3	-21	18
- 4	7	5
- 5	8	7
- 6	-10	9
- 7	1	
- 8	- 6	5
- 9	2	
-10	6	
-11	- 8	
-12	6	
-13	4	
4 13 4	4	6
12	- 7	6
11	11	8
10	5	5
9	-17	15
8	11	9

h k l	F_c	$\|F_o\|$
4 7 4	- 6	6
6	- 4	5
5	8	8
4	-13	12
3	13	12
2	13	13
1	-18	17
0	25	21
- 1	-22	19
- 2	-19	19
- 3	22	22
- 4	-13	11
- 5	6	6
- 6	7	6
- 7	- 5	6
- 8	12	10
- 9	- 5	
-10	-12	
-11	8	
-12	- 6	
4 12 5	5	
11	- 8	7
10	3	4
9	2	
8	4	5
7	- 7	5
6	- 9	7
5	6	6
4	4	4
3	- 1	
2	5	4
1	- 5	4
0	5	4
- 1	- 0	
- 2	-13	11
- 3	15	11
- 4	-13	9
- 5	- 2	
- 6	17	12
- 7	- 8	4
- 8	- 3	
- 9	6	
-10	- 7	
-11	5	
4 11 6	- 5	6
10	1	4
9	6	5
8	-19	15
7	7	7
6	13	11
5	-10	9
4	4	4
3	0	
2	- 2	
1	9	10
0	-17	14
- 1	5	4
- 2	2	
- 3	- 2	
- 4	7	7
- 5	- 2	4
- 6	2	
- 7	- 3	
- 8	- 5	9
- 9	8	9
-10	- 3	
4 10 7	- 8	6
9	7	8
8	2	
7	- 2	
6	5	
5	-11	12
4	2	
3	13	11
2	-22	15
1	6	4
0	10	11
- 1	- 6	6
- 2	12	11
- 3	-10	8
- 4	- 1	
- 5	5	9
- 6	-12	13
- 7	4	
- 8	6	
- 9	- 7	
4 8 8	4	5
7	- 1	
6	3	
5	5	4
4	- 8	7
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2	- 2	
1	2	
0	7	8
- 1	- 9	7
- 2	7	6
- 3	6	5
- 4	- 5	5
- 5	- 1	
- 6	- 3	
- 7	0	
- 8	2	
4 6 9	- 8	6
5	6	6
4	2	
3	- 5	4
2	15	10
1	-12	13
0	- 3	
- 1	9	10
- 2	-11	9
- 3	3	4
- 4	0	
- 5	- 2	
3 14 0	- 3	
13	6	7
12	- 4	6
11	7	8
10	- 0	
9	- 9	8

h k l	F_c	$\|F_o\|$
3 8 0	- 2	
7	-13	13
6	6	8
5	18	19
4	2	
3	16	20
2	1	
1	-27	30
0	27	34
- 1	-58	67
- 2	- 8	12
- 3	35	38
- 4	- 7	5
- 5	8	10
- 6	12	13
- 7	-11	13
- 8	6	6
- 9	- 9	8
-10	- 9	11
-11	13	16
-12	- 6	8
-13	2	
-14	2	
3 14 1	-10	8
13	9	8
12	6	5
11	-14	13
10	6	7
9	- 6	7
8	3	
7	8	9
6	- 9	9
5	6	7
4	2	4
3	-18	20
2	24	28
1	-33	37
0	10	8
- 1	21	22
- 2	-15	17
- 3	24	24
- 4	-19	17
- 5	- 7	8
- 6	14	12
- 7	-15	9
- 8	0	
- 9	13	10
-10	- 9	5
-11	9	5
-12	- 6	
-13	- 3	
-14	7	
3 14 2	6	
13	-11	10
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11	- 5	4
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9	11	9
8	-14	13
7	3	
6	17	14
5	-21	20
4	10	11
3	- 7	5
2	-13	15
1	31	32
0	-22	24
- 1	21	22
- 2	- 1	
- 3	-19	22
- 4	15	15
- 5	- 8	8
- 6	-12	12
- 7	19	15
- 8	-11	10
- 9	5	5
-10	6	5
-11	-11	
-12	9	
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-14	- 5	
3 14 3	3	
13	- 7	6
12	3	
11	7	6
10	- 9	8
9	10	10
8	8	5
7	- 6	5
6	- 2	
5	-15	13
4	- 7	6
3	14	13
2	-10	10
1	22	23
0	3	6
- 1	6	5
- 2	- 0	
- 3	-19	19
- 4	3	4
- 5	- 4	4
- 6	- 8	8
- 7	16	13
- 8	- 1	
- 9	- 4	
-10	13	11
-11	-15	14
-12	1	
-13	4	
3 13 4	4	
12	-12	11
11	7	6
10	1	
9	- 5	5
8	11	11
7	-11	9
6	0	
5	25	21
4	-27	25
3	7	6
2	5	6

h k l	F_c	$\|F_o\|$
3 1 4	-23	22
0	19	20
- 1	-11	10
- 2	- 0	
- 3	16	16
- 4	- 5	6
- 5	1	
- 6	4	5
- 7	- 9	8
- 8	4	5
- 9	- 9	
-10	4	
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-13	7	
3 12 5	5	5
11	- 3	
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9	- 8	7
8	- 3	
7	5	4
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- 1	6	6
- 2	-18	14
- 3	12	10
- 4	14	10
- 5	- 8	6
- 6	16	12
- 7	- 8	6
- 8	- 9	9
- 9	9	
-10	-12	
-11	3	
-12	3	
3 11 6	- 3	
10	2	
9	5	6
8	- 7	8
7	- 1	
6	1	
5	- 4	
4	8	8
3	-11	8
2	7	7
1	4	6
0	- 4	7
- 1	9	8
- 2	- 9	10
- 3	- 1	
- 4	4	5
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- 6	4	4
- 7	6	6
- 8	- 7	7
- 9	10	
-10	- 5	
-11	0	
3 10 7	-10	8
9	6	5
8	7	5
7	- 6	5
6	13	10
5	-11	8
4	- 7	7
3	9	8
2	-15	13
1	10	9
0	3	5
- 1	- 2	4
- 2	15	14
- 3	- 8	9
- 4	- 6	6
- 5	8	7
- 6	-16	13
- 7	6	7
- 8	3	5
- 9	- 4	
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6	- 2	
5	6	6
4	- 7	6
3	5	5
2	- 3	
1	1	
0	5	6
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- 2	1	
- 3	1	
- 4	- 5	5
- 5	not calc.	6
- 6	- 3	
- 7	- 0	
- 8	8	9
- 9	-11	
3 7 9	6	5
6	-12	9
5	8	5
4	- 1	
3	- 6	6
2	11	9
1	- 6	6
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- 1	4	5
- 2	- 6	7
- 3	2	
- 4	2	
- 5	- 3	
- 6	6	7
- 7	- 4	6
3 4 10	9	
3	- 8	
2	3	

h k l	F_c	$\|F_o\|$
3 1 10	1	
0	-11	11
- 1	7	9
- 2	0	
- 3	- 6	
- 4	12	
2 15 0	3	
14	3	
13	3	
12	-10	11
11	- 0	
10	1	
9	-13	11
8	11	12
7	13	13
6	2	
5	27	28
4	-33	36
3	2	
2	-25	31
1	-51	65
0	21	26
- 1	27	33
- 2	4	8
- 3	38	40
- 4	5	7
- 5	- 7	6
- 6	-14	12
- 7	-22	24
- 8	19	19
- 9	-10	9
-10	- 3	
-11	13	15
-12	2	
-13	2	
-14	- 4	
2 14 1	-10	9
13	7	9
12	3	
11	- 6	6
10	0	
9	-13	12
8	2	
7	17	15
6	-25	24
5	32	34
4	16	17
3	-23	26
2	12	12
1	-31	42
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- 2	-13	10
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- 5	-10	9
- 6	20	15
- 7	-10	8
- 8	- 1	
- 9	- 2	
-10	- 4	5
-11	12	8
-12	-11	5
-13	- 4	
-14	12	
2 14 2	0	
13	- 2	
12	4	4
11	- 5	4
10	6	6
9	17	13
8	-16	15
7	- 0	
6	- 4	
5	-22	20
4	20	21
3	-35	35
2	45	49
1	53	51
0	-41	47
- 1	12	9
- 2	7	8
- 3	-52	54
- 4	13	11
- 5	-13	12
- 6	1	
- 7	27	26
- 8	- 8	8
- 9	12	10
-10	- 4	
-11	-12	6
-12	3	
-13	- 1	
-14	- 1	
2 14 3	6	6
13	- 5	6
12	- 7	7
11	13	9
10	- 0	4
9	- 5	
8	9	8
7	- 5	4
6	6	5
5	-18	17
4	- 1	
3	10	12
2	- 5	4
1	1	
0	3	
- 1	15	17
- 2	6	7
- 3	-27	28
- 4	1	
- 5	22	21
- 6	-25	21
- 7	9	8
- 8	1	
- 9	- 6	6
-10	10	9
-11	- 3	
-12	- 2	

Table 3 (*continued*)

h k l	F_c	$\|F_o\|$
2 -13 3	5	
-14	-6	
2 13 4	4	8
12	-6	6
11	9	9
10	-4	
9	-13	11
8	19	15
7	-15	14
6	-5	4
5	21	18
4	-8	11
3	11	11
2	-11	11
1	-2	4
0	6	8
-1	-23	22
-2	-1	
-3	24	22
-4	-5	4
-5	10	10
-6	-12	11
-7	2	
-8	10	10
-9	-21	17
-10	5	
-11	5	
-12	-4	
-13	8	
2 13 5	4	
12	2	
11	-10	6
10	7	6
9	-3	
8	-4	4
7	11	8
6	-11	9
5	17	13
4	-3	3
3	-18	15
2	14	12
1	-9	9
0	-14	11
-1	21	14
-2	-4	4
-3	6	5
-4	-1	
-5	-10	9
-6	18	15
-7	-16	11
-8	-6	6
-9	9	6
-10	-1	
-11	4	
-12	-2	
2 12 6	1	
11	-5	6
10	0	
9	3	
8	-12	11
7	15	12
6	2	4
5	-7	7
4	8	8
3	-7	9
2	0	
1	-1	
0	-9	9
-1	9	10
-2	3	4
-3	-8	9
-4	15	13
-5	-8	8
-6	-2	
-7	-1	
-8	0	
-9	8	
-10	-9	
-11	-2	
-12	9	
2 11 7	8	8
10	-7	7
9	6	5
8	-0	
7	-6	7
6	4	3
5	-16	12
4	12	11
3	7	10
2	-12	12
1	17	13
0	5	3
-1	-14	13
-2	8	8
-3	-16	15
-4	-0	
-5	8	10
-6	-7	8
-7	13	12
-8	-1	
-9	-5	
-10	5	
-11	-2	
2 10 8	6	6
9	-2	
8	8	6
7	-7	6
6	-2	4
5	3	4
4	-10	10
3	0	
2	5	5
1	3	5
0	not calc.	8
-1	-10	11
-2	5	
-3	8	8
-4	-18	16
-5	8	6
-6	-2	
-7	-4	5

h k l	F_c	$\|F_o\|$
2 $\bar{8}$ 8	10	13
-9	-4	
2 8 9	-1	
7	6	7
6	-3	4
5	6	4
4	-1	
3	0	
2	2	
1	-10	11
0	-2	
-1	7	7
-2	-3	
-3	5	5
-4	-2	
-5	7	5
-6	3	5
-7	-11	12
-8	2	
2 5 10	-3	
4	11	
3	-6	
2	-3	
1	7	8
0	-10	11
-1	4	
-2	-3	
-3	-2	
-4	12	
-5	-9	
1 15 0	-1	
14	-1	
13	6	
12	-7	9
11	-1	
10	3	4
9	-12	13
8	16	16
7	-10	11
6	12	12
5	22	24
4	-26	29
3	-10	16
2	-21	25
1	-2	3
0	48	52
-1	-41	35
-2	4	7
-3	59	72
-4	-45	49
-5	25	25
-6	-14	16
-7	-23	26
-8	24	25
-9	-5	5
-10	-4	
-11	10	13
-12	-11	11
-13	6	7
-14	4	
1 15 1	5	5
14	-8	6
13	1	4
12	3	
11	-15	12
10	14	12
9	-0	
8	-2	
7	23	21
6	-14	15
5	-16	15
4	-3	7
3	4	6
2	-11	14
1	16	19
0	-12	13
-1	35	43
-2	10	13
-3	-7	6
-4	-33	34
-5	3	
-6	15	14
-7	-10	7
-8	8	5
-9	0	
-10	-5	4
-11	9	5
-12	-2	
-13	-10	6
-14	7	5
1 14 2	-3	
13	-4	
12	11	11
11	-12	12
10	5	
9	10	9
8	-30	27
7	25	24
6	-9	7
5	-11	10
4	46	45
3	-29	36
2	-14	21
1	54	53
0	-49	52
-1	-4	7
-2	-11	11
-3	-21	24
-4	49	54
-5	-13	13
-6	3	
-7	4	
-8	-8	7
-9	8	8
-10	-8	6
-11	-10	8
-12	11	6
-13	-4	
-14	6	
1 14 3	1	
13	5	6

h k l	F_c	$\|F_o\|$
1 12 3	-2	
11	11	8
10	-5	6
9	2	
8	-5	5
7	-12	10
6	-1	
5	-10	8
4	18	10
3	32	32
2	3	4
1	7	5
0	-11	14
-1	-41	38
-2	30	21
-3	-28	18
-4	-8	7
-5	20	16
-6	4	
-7	12	9
-8	-3	
-9	-13	11
-10	6	6
-11	-4	4
-12	-1	
-13	4	
-14	-7	
1 14 4	-1	
13	6	6
12	-12	9
11	8	7
10	2	5
9	-7	7
8	13	10
7	-10	9
6	7	5
5	3	4
4	-18	16
3	-1	
2	-5	4
1	-8	5
0	37	38
-1	-11	12
-2	3	3
-3	11	11
-4	-13	14
-5	7	8
-6	-17	14
-7	-10	9
-8	13	9
-9	4	
-10	2	
-11	4	
-12	-6	
-13	5	
1 13 5	4	
12	0	
11	-11	7
10	4	5
9	-10	8
8	9	8
7	11	9
6	-6	7
5	11	9
4	-4	4
3	-12	11
2	not calc.	5
1	-29	23
0	5	5
-1	21	15
-2	-11	10
-3	34	26
-4	-15	12
-5	-13	12
-6	16	12
-7	-14	10
-8	-5	5
-9	6	6
-10	-8	5
-11	14	
-12	1	
-13	-8	
1 12 6	8	6
11	-6	5
10	-1	
9	11	9
8	-13	10
7	-0	
6	8	7
5	-7	3
4	4	5
3	0	
2	-6	6
1	17	14
0	-7	8
-1	-1	3
-2	-9	8
-3	-4	5
-4	7	10
-5	-2	
-6	4	
-7	1	
-8	-4	
-9	10	
-10	-4	
-11	-11	
1 11 7	7	
10	4	4
9	-8	8
8	13	10
7	-7	6
6	-1	
5	8	9
4	-20	17
3	18	16
2	-14	12
1	12	10
0	-3	3
-1	-6	8
-2	12	12

h k l	F_c	$\|F_o\|$
1 $\bar{3}$ 7	-16	15
-4	1	
-5	2	
-6	-1	
-7	10	13
-8	-2	
-9	-5	7
-10	4	
-11	-6	9
1 10 8	-0	
9	-3	
8	3	
7	-8	6
6	-0	
5	9	8
4	-5	4
3	6	5
2	-3	4
1	-5	5
0	15	14
-1	-19	16
-2	-2	
-3	9	9
-4	-4	6
-5	8	8
-6	-1	
-7	-7	8
-8	7	
-9	-6	
-10	1	
1 8 9	1	4
7	3	
6	-5	
5	3	5
4	-2	
3	-4	
2	12	9
1	-11	9
0	-1	3
-1	6	6
-2	-1	3
-3	6	7
-4	-7	7
-5	-4	5
-6	8	7
-7	-4	4
-8	-2	
1 6 10	1	
5	-2	
4	5	
3	-11	
2	0	
1	0	
0	-4	
-1	14	18
-2	-8	
-3	0	
-4	10	
-5	-8	
-6	-2	
1 2 11	-6	
1	4	
0	-2	
-1	-4	
-2	4	
0 15 0	-0	
14	-2	
13	1	
12	-16	17
11	13	12
10	-1	
9	2	
8	30	28
7	-19	21
6	-5	8
5	1	
4	-51	54
3	23	25
2	-33	34
1	-38	36
0 15 1	7	5
14	-10	9
13	-0	
12	9	7
11	-11	11
10	-1	
9	3	3
8	3	5
7	5	6
6	10	12
5	-7	9
4	-5	8
3	-21	24
2	22	21
1	-11	12
0	-13	13
-1	-22	20
-2	17	17
-3	59	52
-4	-27	25
-5	-18	21
-6	22	20
-7	-4	
-8	-11	10
-9	4	6
-10	-11	10
-11	12	10
-12	-1	7
-13	-2	
-14	9	10
-15	-6	
0 14 2	2	
13	-4	5
12	13	16
11	-15	15
10	9	9
9	12	12
8	-30	27
7	-2	4
6	8	8
5	-10	11

h k l	F_c	$\|F_o\|$
0 4 2	39	37
3	4	5
2	1	4
1	7	4
0	-53	54
-1	27	27
-2	-40	36
-3	-21	19
-4	29	28
-5	21	20
-6	9	10
-7	-2	
-8	-18	18
-9	12	8
-10	-5	4
-11	-12	11
-12	9	9
-13	-1	
-14	4	
0 14 3	6	7
13	-8	9
12	5	6
11	11	9
10	-13	12
9	-1	
8	-2	
7	1	
6	15	15
5	-19	19
4	-2	3
3	37	36
2	-36	40
1	21	18
0	-17	15
-1	-15	16
-2	25	27
-3	-11	12
-4	16	15
-5	-1	
-6	-28	23
-7	24	18
-8	2	
-9	-17	13
-10	15	11
-11	-10	8
-12	8	6
-13	3	
-14	-13	7
0 14 4	-0	
13	8	8
12	-7	5
11	1	
10	-4	5
9	-1	
8	12	10
7	-11	11
6	-10	8
5	32	27
4	-10	7
3	-8	8
2	-4	6
1	-11	11
0	20	20
-1	-2	
-2	-4	4
-3	5	4
-4	1	
-5	-6	7
-6	5	5
-7	-5	6
-8	-2	
-9	-3	
-10	13	10
-11	-1	
-12	-9	8
-13	5	
-14	-2	
0 13 5	6	6
12	-7	4
11	0	
10	12	10
9	-10	8
8	7	6
7	7	6
6	-12	13
5	11	9
4	-31	23
3	-11	8
2	51	40
1	-30	26
0	12	10
-1	19	17
-2	-18	16
-3	13	11
-4	-14	12
-5	-21	19
-6	19	17
-7	-8	6
-8	5	4
-9	14	11
-10	-12	9
-11	4	5
-12	-3	
-13	-1	
0 12 6	2	
11	-1	
10	-3	
9	8	8
8	1	
7	1	
6	2	
5	-10	9
4	12	9
3	-10	9
2	-7	6
1	-4	
0	5	4
-1	21	20
-2	-14	11
-3	-8	9
-4	17	14

h k l	F_c	$\|F_o\|$
0 $\bar{5}$ 6	-7	5
-6	-3	
-7	5	5
-8	-13	9
-9	11	6
-10	-4	
-11	-2	
-12	8	
0 11 7	6	
10	-13	11
9	2	
8	-2	
7	-11	8
6	14	12
5	-4	
4	4	3
3	11	9
2	-7	8
1	10	8
0	-16	12
-1	-17	15
-2	6	7
-3	5	6
-4	4	8
-5	5	6
-6	-5	8
-7	12	12
-8	-6	6
-9	-10	11
-10	3	
-11	-4	
0 10 8	-0	
9	1	
8	4	4
7	-14	13
6	2	
5	8	8
4	-10	8
3	15	13
2	-6	5
1	-2	4
0	9	8
-1	-9	10
-2	5	5
-3	-4	3
-4	-13	10
-5	18	13
-6	-3	
-7	-7	8
-8	10	10
-9	-9	10
-10	8	9
0 9 9	-7	6
8	-2	
7	15	10
6	-7	6
5	2	
4	-3	4
3	-9	6
2	8	6
1	-4	3
0	-2	4
-1	9	7
-2	-2	
-3	3	
-4	4	
-5	-10	8
-6	-1	
-7	-4	
-8	6	
-9	1	
0 7 10	7	
6	-10	
5	1	
4	12	
3	-12	
2	4	
1	2	
0	-5	
-1	11	13
-2	-5	
-3	-6	
-4	10	
-5	-8	
-6	3	
-7	4	
0 4 11	-2	
3	-0	
2	2	
1	7	11
0	-6	9
-1	-2	
-2	6	
-3	-6	
-4	2	
$\bar{1}$ 14 1	-9	13
13	-1	
12	1	
11	4	4
10	13	11
9	-5	5
8	-7	5
7	10	8
6	-26	28
5	11	11
4	-12	16
3	-18	16
2	66	77
1	-4	4
0	17	19
-1	-2	4
-2	-51	45
-3	12	9
-4	13	14
-5	-31	30
-6	25	23
-7	-10	9
-8	9	8
-9	6	7
-10	-17	13
-11	12	8

Table 3 (*continued*)

h k l	F_c	$\|F_o\|$
$\bar{1}$ $\overline{12}$ 1	-4	
-13	-6	6
-14	10	10
-15	-5	
$\bar{1}$ 14 2	-0	
13	0	
12	6	
11	-10	12
10	-7	6
9	10	13
8	-2	
7	9	11
6	-0	
5	-3	4
4	31	28
3	-37	38
2	-13	16
1	-23	22
0	-17	15
-1	23	29
-2	37	35
-3	-2	
-4	15	16
-5	-4	4
-6	-6	8
-7	-5	5
-8	-16	14
-9	5	6
-10	1	
-11	7	6
-12	2	
-13	-0	
-14	3	
$\bar{1}$ 14 3	12	13
13	-6	9
12	-1	
11	8	7
10	-11	12
9	-2	5
8	-11	10
7	-8	6
6	40	40
5	-12	9
4	17	12
3	2	2
2	-30	27
1	26	22
0	-51	56
-1	-23	25
-2	48	44
-3	-22	20
-4	21	16
-5	32	28
-6	-40	35
-7	19	14
-8	-5	4
-9	-14	11
-10	12	9
-11	-9	5
-12	2	
-13	9	6
-14	-8	
$\bar{1}$ 14 4	-1	
13	6	
12	-5	
11	2	
10	3	
9	-10	8
8	19	17
7	-3	6
6	-22	22
5	2	5
4	-2	
3	10	12
2	2	
1	6	6
0	12	11
-1	12	11
-2	-14	11
-3	-13	11
-4	-19	16
-5	11	10
-6	-7	4
-7	9	5
-8	17	14
-9	-13	11
-10	7	5
-11	0	
-12	-12	8
-13	3	
-14	-1	
$\bar{1}$ 13 5	4	
12	-7	6
11	-3	
10	16	14
9	-8	9
8	4	5
7	8	8
6	-20	20
5	21	21
4	-19	21
3	-23	20
2	25	16
1	7	7
0	2	
-1	10	9
-2	-13	10
-3	9	7
-4	-6	5
-5	-15	12
-6	11	9
-7	-7	6
-8	6	7
-9	3	5
-10	-1	
-11	3	
-12	-4	
-13	-2	
$\bar{1}$ 12 6	5	
11	-4	
10	1	

h k l	F_c	$\|F_o\|$
$\bar{1}$ 9 6	5	5
8	-11	10
7	13	11
6	-10	10
5	-7	6
4	18	18
3	-7	8
2	11	9
1	-4	
0	-23	21
-1	20	21
-2	-3	
-3	-17	15
-4	22	20
-5	-10	11
-6	11	10
-7	0	
-8	-14	13
-9	11	9
-10	-9	7
-11	-4	
-12	11	
-13	-6	
$\bar{1}$ 12 7	-2	
11	9	
10	-6	7
9	1	4
8	-2	
7	-5	4
6	11	8
5	-5	6
4	4	3
3	1	
2	-11	8
1	5	6
0	6	4
-1	-14	13
-2	7	6
-3	0	
-4	6	6
-5	4	6
-6	-11	11
-7	4	
-8	-0	
-9	-3	
-10	-0	
-11	3	
-12	2	
$\bar{1}$ 10 8	-8	8
9	-3	
8	12	12
7	-11	9
6	9	7
5	3	5
4	-5	5
3	11	10
2	-13	12
1	-5	6
0	8	8
-1	-17	14
-2	16	11
-3	10	8
-4	-19	16
-5	17	15
-6	-6	7
-7	-5	7
-8	6	8
-9	-9	10
-10	5	
-11	6	
$\bar{1}$ 9 9	-5	4
8	-7	5
7	5	
6	-3	
5	3	4
4	-3	
3	-3	
2	8	6
1	1	
0	-0	
-1	3	
-2	-8	6
-3	3	4
-4	-8	7
-5	4	
-6	5	7
-7	-9	9
-8	10	8
-9	2	
$\bar{1}$ 7 10	12	
6	-10	
5	-10	
4	8	
3	-4	
2	-1	
1	8	10
0	-4	
-1	9	8
-2	-2	
-3	-8	
-4	5	
-5	-7	
-6	0	
-7	4	
$\bar{1}$ 4 11	6	
3	-4	
2	-7	
1	11	15
0	-7	
-1	-5	
-2	9	
-3	-6	
-4	8	
$\bar{2}$ 14 1	-7	5
13	7	7
12	1	
11	-16	13
10	21	18
9	-3	5
8	-8	8
7	7	6

h k l	F_c	$\|F_o\|$
$\bar{2}$ 6 1	-16	18
5	27	26
4	-12	14
3	-29	30
2	29	32
1	-1	
0	-19	20
-1	26	27
-2	-22	24
-3	45	49
-4	-24	25
-5	-14	15
-6	27	26
-7	-30	27
-8	3	
-9	12	10
-10	-12	9
-11	12	10
-12	3	
-13	-8	10
-14	10	11
-15	-11	9
$\bar{2}$ 14 2	0	
13	-2	
12	8	8
11	-7	9
10	-1	
9	1	
8	-18	19
7	27	30
6	4	
5	-18	21
4	17	20
3	11	12
2	-32	31
1	-6	5
0	-19	17
-1	18	20
-2	23	25
-3	-13	17
-4	18	19
-5	-1	
-6	-1	
-7	-16	15
-8	-1	
-9	10	10
-10	-6	
-11	0	
-12	10	11
-13	-8	6
-14	4	
$\bar{2}$ 14 3	5	
13	-6	6
12	-2	
11	3	
10	-11	10
9	16	15
8	-4	
7	2	
6	14	13
5	-22	21
4	17	16
3	-12	14
2	-46	42
1	45	45
0	15	17
-1	-30	29
-2	43	37
-3	-20	20
-4	6	6
-5	-6	5
-6	-20	17
-7	15	12
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$\bar{2}$ 13 5	5	
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7	-5	6
6	-9	9
5	2	4
4	4	4
3	8	7
2	20	12
1	-5	6

h k l	F_c	$\|F_o\|$
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-7	-1	
-8	5	
-9	1	
-10	-13	9
-11	1	
-12	1	
-13	0	
$\bar{2}$ 12 6	13	16
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9	4	
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4	13	12
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-8	-12	11
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-11	-4	
-12	10	7
-13	-12	
$\bar{2}$ 11 7	-1	
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9	11	12
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5	2	
4	-4	5
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-5	-4	6
-6	-5	7
-7	0	
-8	-8	8
-9	-1	
-10	8	13
-11	-5	
-12	9	10
$\bar{2}$ 10 8	-6	6
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$\bar{2}$ 9 9	-3	
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4	-3	4
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$\bar{2}$ 7 10	2	
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-8	-6	

h k l	F_c	$\|F_o\|$
$\bar{2}$ 4 11	4	
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$\bar{3}$ 14 1	-6	
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8	1	
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3	-2	
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-2	-51	52
-3	56	55
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-5	-11	11
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-8	3	
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-11	9	7
-12	-3	
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-14	7	
$\bar{3}$ 14 2	-1	
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-9	22	20
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-11	-8	8
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-14	-1	
$\bar{3}$ 14 3	6	
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9	11	12
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7	8	8
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3	5	6
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-7	0	
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-9	-22	19
-10	8	7

h k l	F_c	$\|F_o\|$
$\bar{3}$ $\overline{11}$ 4	3	
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-14	-0	
$\bar{3}$ 13 5	9	10
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11	-2	
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8	-1	
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$\bar{3}$ 12 6	4	
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2	12	11
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-8	-14	11
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-13	-7	
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8	7	7
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$\bar{3}$ 9 9	-9	8
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Table 3 (*continued*)

h k l	F_c	$\lvert F_o \rvert$
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- 3	- 6	
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3̄ 4 11	3	
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- 3	- 5	
- 4	3	
- 5	0	
4̄ 13 1	7	6
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11	0	
10	5	
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8	5	6
7	- 1	
6	- 7	6
5	30	30
4	-28	28
3	- 9	9
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- 4	- 3	4
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-14	4	
4̄ 13 2	- 9	7
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7	13	12
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- 4	14	17
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- 6	2	5
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7	5	
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- 8	-15	15
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-11	- 2	
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6̄ 12 3	9	11
11	5	
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4	3	4
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6̄ 12 4	- 6	
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6̄ 2 4	- 9	8
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