early absolute data which are probably incorrect'. Rather surprisingly, however, it is now apparent that Wollan & Harvey's final results are by far the closer to the true values.

We thank the Science Research Council for a Research Studentship (R.W.M.).

References

BARRON, T. H. K., LEADBETTER, A. J., MORRISON, J. A. & SALTER, L. S. (1966). *Acta Cryst.* **20**, 125.

BARRON, T. H. K. & MUNN, R. W. (1966). *Phil. Mag.* In the press.

BENSON, G. C. & GILL, E. K. (1966). *Canad. J. Phys.* **44**, 674.

BLACKMAN, M. (1956). *Acta Cryst.* **9**, 734.

BORGONOVI, G., CAGLIOTI, G. & ANTAL, J. J. (1963). *Phys. Rev.* **132**, 683.

BRINDLEY, G. W. (1936). *Phil. Mag.* **21**, 790.

DEWAMES, R. E., WOLFRAM, T. & LEHMAN, G. W. (1965). *Phys. Rev.* **138**, A717.

FELDMAN, J. L. & HORTON, G. K. (1963). *Phys. Rev.* **132**, 644.

GUPTA, R. P. & DAYAL, B. (1966). *Phys. Stat. Sol.* **13**, 519.

HOLAS, A. (1965). *Inelastic Scattering of Neutrons* (1964). Vol. I, p. 205. Vienna: International Atomic Energy Agency.

HOUSLEY, R. M. & NUSSBAUM, R. H. (1965). *Phys. Rev.* **138**, A753.

International Tables for X-ray Crystallography (1962). Vol. III, p. 237. Birmingham: Kynoch Press.

JAMES, R. W. (1948). *The Optical Principles of the Diffraction of X-rays*, p. 264. London: Bell.

JAUNCEY, G. E. M. & BRUCE, W. A. (1936). *Phys. Rev.* **50**, 408.

JAUNCEY, G. E. M. & BRUCE, W. A. (1937). *Phys. Rev.* **51**, 1067.

MALISZEWSKI, E., ROSOLOWSKI, J., SLEDZIEWSKA, D. & CZACHOR, A. (1965). *Lattice Dynamics* (1963). Ed. Wallis, R. F. p. 33. London: Pergamon Press.

MARADUDIN, A. A. & FLINN, P. A. (1963). *Phys. Rev.* **129**, 2529.

OWEN, E. A. & YATES, E. L. (1934). *Phil. Mag.* **17**, 113.

RYBA, E. R. (1960). Thesis, Iowa State Univ.

SACK, R. A., MARADUDIN, A. A. & WEISS, G. H. (1961). *Phys. Rev.* **124**, 717.

SALTER, L. S. (1965). *Adv. Phys.* (*Phil. Mag. Supp.*), **14**, 1.

WOLLAN, E. O. & HARVEY, G. G. (1937). *Phys. Rev.* **51**, 1054.

ZENER, C. (1936). *Phys. Rev.* **49**, 122.

Acta Cryst. (1967). **22**, 173

The Crystal Structure of Beraunite

BY L. FANFANI AND P. F. ZANAZZI

Istituto di Mineralogia dell'Università di Perugia, Italy

(*Received* 14 *July* 1966)

Beraunite, a basic hydrated iron phosphate, crystallizes in the monoclinic space group $C2/c$ with $a_0 = 20{\cdot}646 \pm 0{\cdot}005$, $b_0 = 5{\cdot}129 \pm 0{\cdot}007$, $c_0 = 19{\cdot}213 \pm 0{\cdot}005$ Å, $\beta = 93°37' \pm 4'$ and $Z = 8$. Crystallochemical considerations and a chemical analysis of the ratio Fe^{II}/Fe^{III} suggest the formula

$$Fe^{II}_{0{\cdot}5}\,Fe^{III}_{2{\cdot}5}\,(OH)_{2{\cdot}5}\,(PO_4)_2 . 3H_2O$$

as the most representative for the mineral.

The intensities from *h*0*l* to *h*4*l* were collected by Weissenberg techniques. The analysis of the crystal structure was carried out by interpretation of the Patterson function and by three-dimensional Fourier syntheses. An isotropic refinement gave a final R index of 0·066 for 898 measured reflexions.

Fe and P show the usual octahedral and tetrahedral coordination respectively. The average bond length is 2·01 Å for Fe–O and 1·54 Å for P–O.

The crystal structure can be outlined as a three-dimensional framework of Fe and P coordination polyhedra with empty channels along the screw axes, where free water molecules are located. The existence of thick sheets normal to **a** explains the good cleavage {100}.

Introduction

Beraunite is a hydrated basic phosphate of iron, which occurs in secondary iron deposits and as an alteration product of primary phosphates in pegmatites.

The mineral was first found by A. Breithaupt in 1841. Bořicky (1867) assigned it to the monoclinic system from morphological studies and gave the first chemical analysis. Later Frondel (1949), on the basis of a small but significant content of ferrous iron revealed by the analysis, suggested that beraunite, like dufrenite and rockbridgeite, is properly a basic phosphate of both divalent and trivalent iron with a ratio Fe/P of 5:4. Beraunite was also studied from morphological, optical and chemical points of view under the name eleonorite (Nies, 1877; Streng, 1881; König, 1890); Fischer in 1956

demonstrated the identity of the two minerals and gave the space group, the lattice constants and the chemical formula. This formula, $Fe_6(OH)_6(PO_4)_4.5H_2O$, containing only trivalent iron, was assumed at the beginning of the present work. During the structural determination, we chose the limit formula

$$Fe^{II}Fe^{III}_5(OH)_5(PO_4)_4.6H_2O$$

as correct for beraunite, though the mineral is known ordinarily in a differently oxidized condition.

Experimental

For the structural study of beraunite, a sample from the Eleonore iron mine near Giessen (Germany) was used. The crystals are reddish brown, translucent, elongated along [010], with prismatic or tabular shape. The cell dimensions, redetermined from precession and Weissenberg photographs using a method proposed by Christ (1956), are:

$$a_0 = 20{\cdot}646 \pm 0{\cdot}005 \text{ Å}$$
$$b_0 = 5{\cdot}129 \pm 0{\cdot}007$$
$$c_0 = 19{\cdot}213 \pm 0{\cdot}005$$
$$\beta = 93°37' \pm 4'$$

From systematic extinctions, two space groups were possible: *Cc* and *C2/c*. For the present investigation the centrosymmetric space group was assumed and the structure determination confirmed this. The calculated density for eight units $Fe^{II}_{0.5}Fe^{III}_{2.5}(OH)_{2\cdot5}(PO_4)_2.3H_2O$ in the cell is $D_x = 2{\cdot}970$ g.cm^{-3}; the measured densities are from 2·80 to 3·08 g.cm^{-3} (Dana, 1951). The linear absorption coefficient is $\mu = 383{\cdot}8$ cm^{-1} for the Cu $K\alpha$ radiation.

For the intensity collection, a crystal with nearly rhombic section measuring approximately $0{\cdot}04 \times 0{\cdot}11 \times 0{\cdot}45$ mm was chosen.

Weissenberg multiple-film integrated photographs from the zero layer to the fourth layer were taken about [010] with the equi-inclination setting, using Ni-filtered Cu $K\alpha$ radiation. A total of 1823 independent reflexions were collected; of these, 925 were not observed.

Intensities were measured with a microdensitometer and different layers were put on the same relative scale taking into account their exposure times. Empirical corrections for $\alpha_1 - \alpha_2$ doublet resolution were applied; then Lorentz-polarization and absorption corrections were calculated with the use of the Burnham general absorption program adapted for the IBM 7090 computer by Stewart (1964).

Structure determination

Location of the heavy atoms

A three-dimensional Patterson synthesis was computed. The most striking features of the maps were the highest peaks at $v = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$. This suggested that the y coordinates of the heavy atoms were about $\frac{1}{8}; \frac{3}{8}$ or $0; \frac{1}{4}$. The latter y values were verified on further interpretation of the Patterson function. In fact the occurrence of peaks at $(\frac{1}{4},\frac{1}{4},0)$, $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$, $(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},\frac{1}{2},0)$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ allowed us to locate two iron ions in special positions at inversion centers $(0,0,0)$ and $(\frac{1}{4},\frac{1}{4},0)$. Two more iron ions were then located in general positions at $y=0$ and $\frac{1}{4}$ respectively.

A three-dimensional Fourier synthesis, computed with the phase signs given by the iron ions, revealed the locations of the phosphorus atoms. By successive electron density maps, thirteen oxygen atoms in general position and one oxygen atom in a special position on the twofold axis were located to complete the asymmetric unit.

With this set of atomic coordinates, structure factors were calculated, the Fe, P and O atoms being given isotropic thermal parameters of 0·8, 0·6 and 1·5 Å^2 respectively. A discrepancy index $R = \Sigma \, ||F_o| - |F_c|| / \Sigma \, |F_o|$ of 0·13 was obtained for all observed reflexions.

The least-squares refinement was performed with a program written by Albano, Bellon, Pompa & Scatturin (1963) for the IBM 1620 computer. The weighting scheme suggested by Cruickshank (1961) was employed and the unobserved reflexions were excluded from the calculations, together with the two strongest reflexions (314 and 10,2,0) showing extinction.

After three cycles of isotropic refinement, each followed by a proper rescaling of F_o's, the R value fell to 0·068.

Derivation of the new chemical formula

In an attempt to locate the hydrogen atoms in the structure more easily, a distinction between oxygen atoms, hydroxyl groups and water molecules was made, assuming Fischer's formula to be correct. The results based on this assumption were not in agreement with Pauling's electrostatic valence rule.

On the basis of Fischer's chemical formula the oxygen atom on the twofold axis is part of an H_2O molecule. This would require three of the five oxygen atoms in general positions not linked to phosphorus to be identified as belonging to OH groups and two as belonging to H_2O molecules. According to a charge balance only two of these oxygen atoms seem to be in OH groups and three in H_2O molecules. It could thus be that Fischer's formula with all the iron oxidized is not completely correct, and that in beraunite there is a small amount of Fe^{2+}, as revealed in Frondel's analysis.

A microchemical analysis was performed in order to determine the Fe^{II}/Fe^{III} ratio in the sample of beraunite under examination, a small amount of the mineral being dissolved in hydrochloric acid. A colorimetric test with α,α'-dipyridyl before and after reduction of Fe^{III} gave results in a large range with an average ratio Fe^{II}/Fe^{III} of 1:5·9. This fact suggests the formula $Fe^{II}Fe^{III}_5(OH)_5(PO_4)_4.6H_2O$ as more probable for beraunite, though the mineral usually occurs in a more or less oxidized state; the result of this

Table 1(*a*). *Fractional atomic coordinates, with their standard deviations and isotropic thermal parameters*

	x	$10^4\sigma(x)$	y	$10^4\sigma(y)$	z	$10^4\sigma(z)$	B(Å^2)
Fe(1)	0·0000	—	0·0000	—	0·0000	—	0·79
Fe(2)	0·2500	—	0·2500	—	0·0000	—	1·28
Fe(3)	0·0438	1	0·2689	5	0·1725	1	0·77
Fe(4)	0·1075	1	0·0312	5	0·4127	1	0·74
P(1)	0·1050	2	0·4787	9	0·0267	2	0·56
P(2)	0·4073	2	0·0378	9	0·1822	2	0·67
O(1)	0·1777	5	0·4819	23	0·0140	5	0·55
O(2)	0·4286	5	0·2460	24	0·0181	5	0·64
O(3)	0·4246	5	0·2447	26	0·4979	6	1·37
O(4)	0·0942	6	0·4379	26	0·1028	6	1·35
O(5)	0·4792	5	0·0443	25	0·1676	6	1·12
O(6)	0·1022	5	0·4759	26	0·2405	6	1·22
O(7)	0·3786	5	0·3081	25	0·1651	6	1·04
O(8)	0·1295	5	0·3453	24	0·3645	6	1·00
OH(1)	0·0070	5	0·0493	24	0·3967	6	1·13
OH(2)	0·1914	5	0·0179	25	0·4633	6	1·13
OH(3)	0·0000	—	0·0989	33	0·2500	—	0·85
$H_2O(1)$	0·3851	5	0·4707	27	0·3205	6	1·56
$H_2O(2)$	0·2482	6	0·0903	27	0·0969	7	1·66
$H_2O(3)$	0·2323	7	0·3509	30	0·2512	7	2·78

Table 1(*b*). *The assumed hydrogen atom parameters*

	x	y	z
H(1)	0·187	0·184	0·480
H(2)	0·012	0·882	0·375
H(3)	0·244	0·184	0·238
H(4)	0·189	0·391	0·224
H(5)	0·289	0·010	0·110
H(6)	0·233	0·176	0·136
H(7)	0·111	0·807	0·200
H(8)	0·144	0·005	0·156
H(9)	0·000	0·912	0·250

oxidation is the loss of the hydrogen content without damage to the crystal structure.

This last structural hypothesis requires that the oxygen on the twofold axis must be considered as belonging to an OH group. A better agreement with Pauling's rule is so achieved.

Final refinement

A three-dimensional difference synthesis was calculated in an attempt to locate the hydrogen atoms in the structure. The positions at which they would be expected fell in regions of positive electron density, but since peaks were poorly defined we located them from stereochemical considerations, taking into account the conditions for the existence of hydrogen bond.

Then a last cycle of refinement of the heavy atom positions was carried out, including also the contributions of the hydrogen atoms. The final R value for all observed reflexions was 0·066.

The coordinates and isotropic thermal parameters of Fe, P, and O are given in Table 1(*a*) with their standard deviations. The hydrogen locations are reported in Table 1(*b*). The observed and calculated structure factors are listed in Table 2. For the calcula-

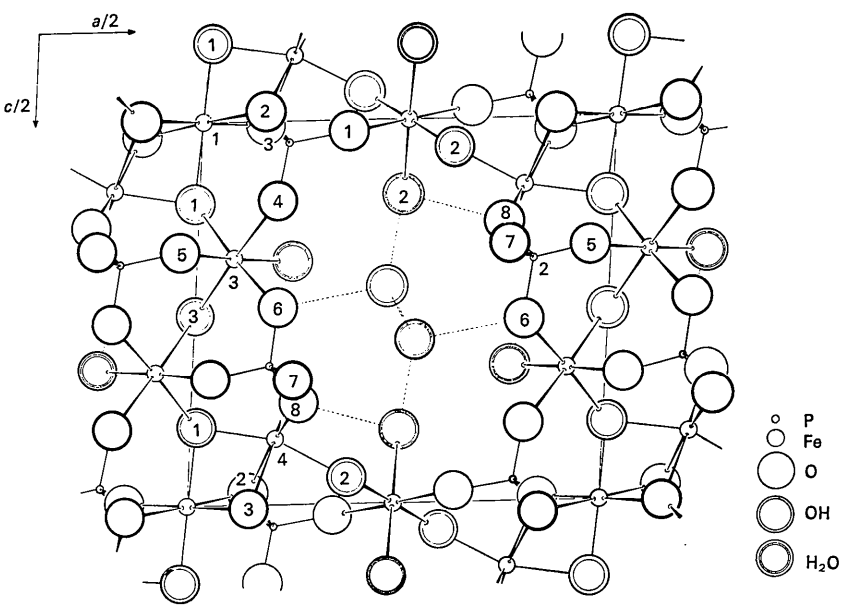

Fig. 1. Projection of the structure along the *b* axis.

Table 2. *Observed and calculated structure factors*

h	k	l	FO	FC
0	0	2	201,1	208,2
0	0	4	118,4	130,8
0	0	6	351,5	384,2
0	0	8	90,0	88,6
0	0	10	291,2	288,8
0	0	12	413,3	425,2
0	0	14	190,6	-152,2
0	0	16		- 12,4
0	0	18		28,4
0	0	20		- 59,0
0	0	22	112,0	122,8
0	0	24	75,0	70,4
2	0	0	340,1	316,4
2	0	2	61,7	47,4
2	0	-2	229,0	-251,6
2	0	4		- 14,6
2	0	-4	162,7	-175,6
2	0	6	85,0	68,8
2	0	-6	282,0	288,0
2	0	8	155,9	-164,6
2	0	-8		30,4
2	0	10	134,3	-132,8
2	0	-10	153,1	142,6
2	0	12	185,1	169,4
2	0	-12	250,9	242,2
2	0	14	170,5	-140,0
2	0	-14	137,5	-138,6
2	0	16	100,5	107,6
2	0	-16		- 36,6
2	0	18		3,6
2	0	-18	84,0	87,2
2	0	20	167,3	-153,2
2	0	-20		37,4
2	0	22		0,8
2	0	-22		31,0
2	0	24	50,7	77,8
2	0	-24		- 29,2
4	0	0	124,4	-120,4
4	0	2		- 16,8
4	0	-2	41,5	46,4
4	0	4	184,2	187,6
4	0	-4	96,0	107,4
4	0	6	109,2	93,4
4	0	-6	114,3	114,8
4	0	8		22,8
4	0	-8	240,9	269,2
4	0	10	79,9	76,4
4	0	-10	98,7	69,6
4	0	12	50,7	51,6
4	0	-12		33,4
4	0	14	108,3	104,0
4	0	-14	93,2	91,2
4	0	16	225,8	219,2
4	0	-16		- 11,6
4	0	18	231,2	224,0
4	0	-18	199,3	210,4
4	0	20	102,4	97,4
4	0	-20	123,4	128,8
4	0	22		58,2
4	0	-22		- 54,8
4	0	-24		29,8
6	0	0	336,4	-358,0
6	0	2	243,6	-248,0
6	0	-2	212,1	189,8
6	0	4	142,1	132,0
6	0	-4	171,4	-174,4
6	0	6	115,2	97,4
6	0	-6	63,1	- 65,4
6	0	8	123,0	114,2
6	0	-8		- 1,0
6	0	10	88,2	79,4
6	0	-10	354,7	-386,2
6	0	12	97,8	- 79,0
6	0	-12	115,8	-109,2
6	0	14		- 14,6
6	0	-14	128,8	123,2
6	0	16		52,6
6	0	-16		19,6
6	0	18		40,4
6	0	-18	75,8	95,0
6	0	20	73,8	69,2
6	0	-20		36,4
6	0	22		8,0
6	0	-22	124,8	-119,0
6	0	-24	123,4	129,6
8	0	0	315,4	343,4
8	0	2	101,9	- 96,0
8	0	-2	137,1	129,8
8	0	4		5,2
8	0	-4	157,2	-137,6
8	0	6	120,2	-112,4
8	0	-6	101,9	- 89,2
8	0	8	109,2	113,6
8	0	-8	149,0	143,6
8	0	10	355,7	370,2
8	0	-10	115,6	-115,6
8	0	12		57,2
8	0	-12	193,3	200,4
8	0	14		31,4
8	0	-14	104,7	113,6
8	0	16		15,2
8	0	-16		- 25,8
8	0	18		- 76,4
8	0	-18		44,0
8	0	20	122,5	122,2
8	0	-20		28,4
8	0	22	90,5	97,2
8	0	-22		11,8
10	0	0	276,5	272,2
10	0	2	179,6	170,0
10	0	-2	73,6	62,8
10	0	4	150,8	139,8
10	0	-4		- 36,2
10	0	6	279,2	-294,6
10	0	-6		- 2,4
10	0	8		- 32,8
10	0	-8	99,6	85,0
10	0	10	53,9	58,6
10	0	-10	102,8	90,0
10	0	12		- 16,8
10	0	-12	88,6	81,4
10	0	14		- 32,2
10	0	-14	117,5	-119,0
10	0	16		- 4,0
10	0	-16	96,4	- 96,4
10	0	18	186,9	-176,8
10	0	-18	85,0	- 96,2
10	0	20		14,2
10	0	-20		- 0,2
10	0	-22		2,4
12	0	0	109,2	96,0
12	0	2	336,0	355,2
12	0	-2	71,3	66,0
12	0	4	186,9	194,8
12	0	-4	257,8	257,0
12	0	6		- 36,2
12	0	-6		20,6
12	0	8	81,5	92,6
12	0	-8	358,9	351,0
12	0	10		0,6
12	0	-10	596,3	607,0
12	0	12		29,0
12	0	-12		47,8
12	0	14	102,8	97,6
12	0	-14	45,5	69,6
12	0	16	64,8	60,8
12	0	-16	149,5	135,2
12	0	18		- 18,8
12	0	-18	77,2	80,4
12	0	20	58,9	66,4
12	0	-20	181,4	184,2
12	0	-22	93,7	89,2
14	0	0	276,0	-295,6
14	0	2		39,8
14	0	-2	57,5	- 61,6
14	0	4	78,5	- 83,2
14	0	-4	211,7	208,0
14	0	6		19,6
14	0	-6		- 35,6
14	0	8	141,4	167,8
14	0	-8	87,2	80,2
14	0	10	186,5	-192,2
14	0	-10	132,5	127,4
14	0	12		- 45,0
14	0	-12	205,7	-201,6
14	0	14	107,8	107,4
14	0	-14	130,7	122,4
14	0	16		21,2
14	0	-16	183,2	178,2
14	0	18	154,3	128,4
14	0	-18		- 14,4
14	0	-20	88,6	99,4
16	0	0	76,3	63,6
16	0	2	225,8	232,8
16	0	-2	79,0	75,6
16	0	4		- 41,6
16	0	-4	234,5	242,4
16	0	6	158,2	158,6
16	0	-6		- 50,2
16	0	8	328,2	342,2
16	0	-8		- 22,4
16	0	10	105,3	94,6
16	0	-10		- 4,2
16	0	12	101,0	107,4
16	0	-12		- 50,2
16	0	14	127,5	158,4
16	0	-14	90,9	89,8
16	0	16		- 37,8
16	0	-16	118,9	116,8
16	0	18	119,3	125,6
16	0	-18		- 28,4
16	0	-20		53,4
18	0	0	92,7	105,2
18	0	2	89,1	98,2
18	0	-2		- 46,2
18	0	4		- 27,2
18	0	-4		36,6
18	0	6	72,6	- 68,0
18	0	-6		- 59,2
18	0	8	91,4	106,6
18	0	-8	118,4	-118,6
18	0	10		47,2
18	0	-10		2,0
18	0	12	69,7	74,6
18	0	-12		54,0
18	0	14		41,2
18	0	-14	70,9	- 72,0
18	0	16	104,5	-113,8
18	0	-16		8,0
18	0	-18	54,7	- 57,4
20	0	0	190,1	194,8
20	0	2	131,6	119,4
20	0	-2		- 25,2
20	0	4		53,2
20	0	-4		6,8
20	0	6		- 47,0
20	0	-6	43,5	58,0
20	0	8	75,8	- 77,4
20	0	-8	85,4	75,6
20	0	10		5,8
20	0	-10	152,2	151,0
20	0	12	94,0	93,0
20	0	-12	106,0	105,0
20	0	14		10,4
20	0	-14	144,4	-155,4
20	0	-16		12,8
22	0	0		43,6
22	0	2		- 55,6
22	0	-2	124,8	-129,0
22	0	4		4,4
22	0	-4		- 24,0
22	0	6	61,2	63,0
22	0	-6	101,0	104,6
22	0	8	87,2	- 91,4
22	0	-8		23,2
22	0	10	94,0	- 94,8
22	0	-10	69,5	77,4
22	0	12		23,8
22	0	-12		- 10,4
22	0	-14	67,2	- 66,8
24	0	0		22,4
24	0	2		- 41,0
24	0	-2		- 35,4
24	0	4	58,9	- 62,8
24	0	-4	54,2	54,6
24	0	6	128,4	121,2
24	0	-6	132,5	118,6
24	0	8		20,4
24	0	-10		41,6
1	1	1	245,4	-281,8
1	1	2	193,5	195,2
1	1	-2	79,9	89,8
1	1	3		- 9,0
1	1	-3	48,4	49,6
1	1	4	152,9	158,6
1	1	-4	222,2	-249,0
1	1	5	81,4	- 81,6
1	1	-5	190,8	-222,6
1	1	6	44,3	- 48,6
1	1	-6	253,0	-279,8
1	1	7		- 31,0
1	1	-7	44,7	- 47,0
1	1	8		29,8
1	1	-8	61,8	44,6
1	1	9		6,2
1	1	-9	71,7	- 83,4
1	1	10	236,5	225,2
1	1	-10		24,6
1	1	11		- 28,0
1	1	-11	151,2	-153,4
1	1	12	138,4	133,2
1	1	-12	74,7	76,8
1	1	13	121,2	-107,0
1	1	-13		25,4
1	1	14	259,5	239,4
1	1	-14		- 5,0
1	1	15	74,4	68,6
1	1	-15		- 20,6
1	1	16		48,2
1	1	-16	49,3	- 65,0
1	1	17		- 20,6
1	1	-17	94,9	- 89,0
1	1	18		- 21,6
1	1	-18		58,4
1	1	19		- 54,4
1	1	-19		- 22,0
1	1	20	94,2	88,4
1	1	-20	101,8	100,0
1	1	21		58,4
1	1	-21		- 37,2
1	1	22		35,2
1	1	-22	71,3	88,8
1	1	23		- 3,6
1	1	-23		- 32,0
3	1	0	108,3	111,8
3	1	1	54,9	- 33,4
3	1	-1	122,5	130,6
3	1	2	204,2	217,8
3	1	-2		- 21,8
3	1	3	210,1	229,6
3	1	-3	126,3	134,2
3	1	4	409,0	504,2
3	1	-4	150,3	-157,2
3	1	5		49,2
3	1	-5	136,7	-151,0
3	1	6		- 42,8
3	1	-6	137,1	126,0
3	1	7	71,7	- 90,0
3	1	-7	88,8	93,4
3	1	8	80,7	65,4
3	1	-8	359,2	393,8
3	1	9	265,1	279,6
3	1	-9	175,7	178,8
3	1	10	138,4	125,0
3	1	-10		44,7
3	1	11	48,3	64,0
3	1	-11	101,4	- 90,6
3	1	12		41,4
3	1	-12		- 42,8
3	1	13		- 5,8
3	1	-13	173,6	174,2
3	1	14	231,2	217,0
3	1	-14	138,4	-130,8
3	1	15	208,8	202,8
3	1	-15	75,6	83,6
3	1	16	141,4	133,6
3	1	-16		24,6
3	1	17		9,4
3	1	-17	65,6	- 68,0
3	1	18		- 56,2
3	1	-18	102,7	108,4
3	1	19		11,0
3	1	-19	105,1	108,2
3	1	20		11,8
3	1	-20	82,5	77,4
3	1	21	95,3	102,0
3	1	-21	83,2	78,0
3	1	22		- 25,8
3	1	-22		2,0
3	1	23		37,4
3	1	-23		6,8
5	1	0	184,7	186,6
5	1	1	262,9	-278,0
5	1	-1	123,5	-128,2
5	1	2		15,0
5	1	-2	135,4	123,4
5	1	3	187,3	184,4
5	1	-3	54,1	50,2
5	1	4	132,8	124,4
5	1	-4	274,1	289,0
5	1	5	115,6	-122,4
5	1	-5	140,1	-155,8
5	1	6	87,2	85,4
5	1	-6	116,9	129,6
5	1	7	171,0	-168,8
5	1	-7		32,4
5	1	8	153,3	149,2
5	1	-8	177,0	171,0
5	1	9		17,6
5	1	-9		23,0
5	1	10		0,4
5	1	-10		- 40,2
5	1	11	103,5	-109,4
5	1	-11	120,7	-119,4
5	1	12	137,1	-132,0
5	1	-12		- 32,6
5	1	13	90,2	- 79,4
5	1	-13		13,6
5	1	14	180,0	-186,4
5	1	-14		- 49,2
5	1	15		57,4
5	1	-15		13,0
5	1	16		71,2
5	1	-16	94,6	100,2
5	1	17	42,4	- 66,8
5	1	-17	73,8	- 78,4
5	1	18		14,4
5	1	-18		9,0
5	1	19		- 34,8
5	1	-19		49,4
5	1	20		23,6
5	1	-20		1,0
5	1	21		6,0
5	1	-21		28,4
5	1	-22		- 14,6
5	1	-23	61,8	- 65,8
7	1	0	198,1	206,2
7	1	1	78,6	81,6
7	1	-1		- 22,2
7	1	-2	61,8	- 60,0
7	1	3	119,4	122,8
7	1	-3	198,1	209,8
7	1	4	95,4	-101,4
7	1	-4	223,5	228,4
7	1	5		- 39,0
7	1	-5	61,4	66,6
7	1	6		51,8
7	1	-6		13,4
7	1	7		56,2
7	1	-7		- 34,8
7	1	8	167,1	161,8
7	1	-8	76,9	- 68,4
7	1	9	90,6	91,6
7	1	-9	211,0	224,6
7	1	10	101,8	93,4
7	1	-10	140,5	140,6
7	1	11	80,7	- 76,6
7	1	-11		25,4
7	1	12	114,3	110,4
7	1	-12	86,5	63,4
7	1	13		31,0
7	1	-13		4,8
7	1	14	164,9	-156,6
7	1	-14	120,5	124,2
7	1	15		44,2
7	1	-15	97,5	85,2
7	1	16		- 4,6
7	1	-16	120,3	124,8
7	1	17	90,6	- 77,4
7	1	-17		40,6
7	1	18	101,8	102,2
7	1	-18		- 29,2
7	1	19	65,0	69,6
7	1	-19		28,8
7	1	20		60,4
7	1	-20		- 0,6
7	1	-21	73,0	68,0
7	1	-22		- 9,4
7	1	-23		- 13,8
9	1	0	138,8	134,8
9	1	1		- 30,2
9	1	-1	153,8	-167,8
9	1	2		33,8
9	1	-2	202,4	198,6
9	1	3		- 34,8
9	1	-3	64,4	58,4
9	1	4	201,1	-195,4
9	1	-4	92,3	65,8
9	1	5	261,6	-262,8
9	1	-5		16,2
9	1	6		- 48,8
9	1	-6	73,0	- 68,0
9	1	7	95,8	88,8
9	1	-7	211,4	-213,0
9	1	8		9,2
9	1	-8		34,8
9	1	9		- 34,6
9	1	-9		55,4
9	1	10	73,8	70,2
9	1	-10	220,9	229,8
9	1	11	208,0	-199,0
9	1	-11		- 31,2
9	1	12	165,4	166,4
9	1	-12	188,6	194,6
9	1	13		- 17,0
9	1	-13	130,6	-142,0
9	1	14		15,6
9	1	-14	165,8	162,4
9	1	15		- 52,2
9	1	-15	83,3	83,0
9	1	16		- 12,0
9	1	-16		37,2
9	1	17	116,9	-111,0
9	1	-17		- 35,6
9	1	18	77,8	73,0
9	1	-18		- 13,6
9	1	19		6,8
9	1	-19	126,8	-128,4
9	1	20	65,6	70,2
9	1	-20	82,0	69,4
9	1	21		- 30,6
9	1	-21		31,8
9	1	-22	70,8	75,0
11	1	0		18,2
11	1	1	189,9	197,0
11	1	-1		- 39,2
11	1	2	177,4	181,0
11	1	-2		- 41,4
11	1	3		41,4
11	1	-3	114,3	116,0
11	1	4	189,5	188,8
11	1	-4	226,9	-221,0
11	1	5	126,3	-109,4
11	1	-5	114,7	109,2
11	1	6		- 53,6
11	1	-6	78,9	- 78,6
11	1	7	142,2	131,8
11	1	-7	127,2	-117,6
11	1	8		- 25,8
11	1	-8	159,8	156,6
11	1	9		58,8
11	1	-9	124,2	122,4
11	1	10		55,2
11	1	-10		0,6
11	1	11		- 4,4
11	1	-11	66,6	70,2
11	1	12	94,9	99,2
11	1	-12		- 29,8
11	1	13		65,4

Table 2 (*cont.*)

h	k	l	Fo	Fc
11	1	-13		- 17,2
11	1	14	218,3	201,6
11	1	-14		- 13,0
11	1	15		3,2
11	1	-15	71,1	76,2
11	1	16		31,2
11	1	-16		- 55,4
11	1	17		- 19,8
11	1	-17		- 8,4
11	1	18		- 19,8
11	1	-18	90,6	88,0
11	1	19		64,0
11	1	-19	76,9	- 64,4
11	1	20		- 0,0
11	1	-20	152,4	137,0
11	1	-21	83,5	86,4
13	1	0		- 3,0
13	1	1		5,6
13	1	- 1	103,5	-109,0
13	1	2	94,9	90,4
13	1	- 2		14,8
13	1	3		- 29,4
13	1	- 3	105,7	- 97,4
13	1	4	278,4	287,6
13	1	- 4	59,6	- 49,4
13	1	5		- 60,2
13	1	- 5		24,6
13	1	6	82,0	86,8
13	1	- 6	114,3	103,8
13	1	7		47,4
13	1	- 7	146,5	-145,6
13	1	8	102,2	95,6
13	1	- 8	204,1	199,6
13	1	9	93,6	- 87,8
13	1	- 9	88,9	- 83,4
13	1	10	104,0	97,6
13	1	-10	143,5	-127,2
13	1	11		- 18,6
13	1	-11		10,8
13	1	12		5,4
13	1	-12		- 22,0
13	1	13		62,8
13	1	-13	96,6	-101,8
13	1	14	87,2	95,4
13	1	-14		- 70,6
13	1	15		- 60,4
13	1	-15		- 52,2
13	1	16	112,1	117,4
13	1	-16		- 23,4
13	1	17		1,8
13	1	-17		- 27,0
13	1	18		9,4
13	1	-18	82,0	77,4
13	1	19		27,8
13	1	-19	64,8	- 62,4
15	1	0	168,0	169,2
15	1	1	139,2	137,8
15	1	- 1		33,4
15	1	2		- 51,4
15	1	- 2	104,8	96,8
15	1	3		- 11,6
15	1	- 3		- 30,0
15	1	4	133,6	134,0
15	1	- 4	174,4	170,0
15	1	5	91,9	96,2
15	1	- 5	108,7	100,8
15	1	6		68,4
15	1	- 6	223,0	219,2
15	1	7	121,2	127,0
15	1	- 7		21,8
15	1	8		7,2
15	1	- 8	113,0	110,4
15	1	9		- 34,2
15	1	- 9		- 1,0
15	1	10		44,0
15	1	-10		- 20,8
15	1	11	85,9	83,2
15	1	-11	99,2	92,4
15	1	12		- 41,4
15	1	-12		50,2
15	1	13	102,7	108,2
15	1	-13		- 19,0
15	1	14	139,7	-141,4
15	1	-14		- 11,6
15	1	15		3,0
15	1	-15		- 48,0
15	1	16		20,2
15	1	-16	75,0	68,2
15	1	17		50,6
15	1	-17	103,5	98,8
15	1	18		6,2
15	1	-18	62,7	62,6
15	1	-19		- 1,0
15	1	-20		- 44,0
17	1	0	159,4	155,6
17	1	1		- 16,2
17	1	- 1		18,4
17	1	2	103,1	-105,8
17	1	- 2	80,7	81,4
17	1	3	108,7	-114,2
17	1	- 3	134,4	-128,0
17	1	4	123,7	-121,4
17	1	- 4		43,0
17	1	5		13,8
17	1	- 5		49,4
17	1	6		19,8
17	1	- 6		15,4
17	1	7		21,2
17	1	- 7		- 10,0
17	1	8		5,0
17	1	- 8	74,7	- 72,0
17	1	9	70,1	- 74,8
17	1	- 9	89,8	- 84,6
17	1	10		65,4
17	1	-10	88,5	85,4
17	1	11		- 6,6
17	1	-11		13,2
17	1	12	71,0	75,0
17	1	-12	138,8	134,4
17	1	13		- 26,4
17	1	-13		- 38,4
17	1	14	128,3	-138,0
17	1	-14	74,7	67,2
17	1	15		- 44,0
17	1	-15		- 49,4
17	1	16		- 5,8
17	1	-16	75,4	86,4
17	1	-17	52,5	57,4
17	1	-18		2,0
17	1	-19		- 38,4
19	1	0	82,0	80,4
19	1	1		29,4
19	1	- 1	101,4	107,2
19	1	2	46,1	60,2
19	1	- 2		- 12,4
19	1	3		- 52,2
19	1	- 3		- 30,2
19	1	4		- 62,0
19	1	- 4		- 45,4
19	1	5		49,2
19	1	- 5		41,6
19	1	6		- 27,2
19	1	- 6		- 42,8
19	1	7		- 5,4
19	1	- 7	80,3	47,6
19	1	8		- 14,8
19	1	- 8		44,8
19	1	9		- 0,8
19	1	- 9		- 22,4
19	1	10		54,2
19	1	-10	155,2	129,8
19	1	11	86,3	100,2
19	1	-11	49,5	48,8
19	1	12	128,0	140,8
19	1	-12	68,3	67,2
19	1	13	55,3	- 54,8
19	1	-13	83,7	89,0
19	1	14	75,7	81,0
19	1	-14	47,4	49,2
19	1	15		- 8,8
19	1	-15		- 13,8
19	1	-16		7,0
19	1	-17		58,0
19	1	-18		4,4
21	1	0		- 23,0
21	1	1	96,2	- 89,4
21	1	- 1		53,4
21	1	2	141,4	142,4
21	1	- 2		- 2,4
21	1	3		- 68,4
21	1	- 3	65,7	- 69,4
21	1	4	120,7	105,0
21	1	- 4		- 35,2
21	1	5		18,0
21	1	- 5		- 44,4
21	1	6		10,6
21	1	- 6		- 21,8
21	1	7	99,2	- 97,0
21	1	- 7		12,4
21	1	8		44,0
21	1	- 8	101,8	99,0
21	1	9	54,1	- 58,0
21	1	- 9		- 54,8
21	1	10		0,2
21	1	-10		- 3,2
21	1	11		36,0
21	1	-11		- 6,8
21	1	12		39,0
21	1	-12		- 32,4
21	1	13	77,3	- 82,8
21	1	-13		54,4
21	1	-14		8,6
21	1	-15		- 53,8
21	1	-16		- 33,0
23	1	0		- 33,4
23	1	1		- 23,6
23	1	- 1	65,1	73,4
23	1	2		40,0
23	1	- 2		- 3,8
23	1	3		32,2
23	1	- 3		16,0
23	1	4	140,5	151,6
23	1	- 4		30,0
23	1	5		54,8
23	1	- 5		- 45,2
23	1	6	57,1	55,6
23	1	- 6		50,2
23	1	7		- 22,4
23	1	- 7	68,1	72,0
23	1	8		58,6
23	1	- 8	86,3	95,2
23	1	9		2,4
23	1	- 9		25,2
23	1	-10	93,8	- 88,0
23	1	-11		- 8,0
23	1	-12		- 51,8
23	1	-13		40,4
25	1	0	94,5	97,0
25	1	1	71,3	- 69,4
25	1	- 1		- 1,2
25	1	2		- 38,4
25	1	- 2	78,1	95,4
25	1	- 3		1,4
25	1	- 4	95,4	94,8
25	1	- 5	72,1	- 59,0
25	1	- 6	105,2	111,8
0	2	2	114,7	125,0
0	2	3	77,4	- 80,6
0	2	4		- 16,2
0	2	5	45,8	- 55,4
0	2	6	241,8	-257,4
0	2	7	82,5	71,8
0	2	8		- 7,4
0	2	9	114,2	94,2
0	2	10	130,8	108,2
0	2	11		19,6
0	2	12		15,8
0	2	13		- 58,0
0	2	14	106,4	- 97,4
0	2	15		10,2
0	2	16	45,3	- 41,4
0	2	17		- 4,2
0	2	18	155,4	-158,4
0	2	19		48,4
0	2	20		5,4
0	2	21		9,2
0	2	22		34,2
2	2	0	78,1	92,2
2	2	1	46,9	55,4
2	2	- 1	151,2	141,8
2	2	2	146,0	177,0
2	2	- 2		- 33,4
2	2	3	63,4	60,4
2	2	- 3	61,4	- 42,8
2	2	4	50,2	49,4
2	2	- 4	78,1	98,4
2	2	5		- 5,2
2	2	- 5		37,4
2	2	6	74,2	- 65,4
2	2	- 6		- 4,0
2	2	7	83,9	- 72,4
2	2	- 7	85,0	- 90,8
2	2	8		4,2
2	2	- 8	245,1	245,4
2	2	9		10,4
2	2	- 9		9,4
2	2	10	138,4	-115,4
2	2	-10	330,9	346,8
2	2	11	102,5	96,2
2	2	-11	98,1	98,4
2	2	12	66,8	61,2
2	2	-12		46,4
2	2	13		- 2,2
2	2	-13		- 32,6
2	2	14	107,4	92,0
2	2	-14	84,8	95,2
2	2	15		- 44,4
2	2	-15		- 52,8
2	2	-16	93,2	95,6
2	2	17		20,2
2	2	-17		4,8
2	2	18		- 4,8
2	2	-18		30,8
2	2	19		- 36,0
2	2	-19		- 36,2
2	2	20		11,0
2	2	-20	139,4	141,2
2	2	21		- 3,2
2	2	-21		15,4
2	2	22		- 11,4
2	2	-22	85,9	95,8
4	2	0	207,4	-245,4
4	2	1		- 9,2
4	2	- 1	137,1	127,4
4	2	2	151,2	145,0
4	2	- 2	123,4	-142,0
4	2	3	137,4	-132,2
4	2	- 3		- 22,4
4	2	4	190,8	-191,2
4	2	- 4	138,6	145,0
4	2	5		25,8
4	2	- 5	48,0	- 57,8
4	2	6		- 0,8
4	2	- 6	55,6	47,4
4	2	7	35,6	53,0
4	2	- 7		- 40,0
4	2	8	122,0	110,2
4	2	- 8	96,1	102,4
4	2	9	135,2	-121,2
4	2	- 9		57,0
4	2	10	285,5	-273,2
4	2	-10	144,7	156,6
4	2	11		60,0
4	2	-11	46,9	71,6
4	2	12		- 39,6
4	2	-12	122,9	-134,2
4	2	13		- 58,8
4	2	-13		- 61,6
4	2	14		- 15,8
4	2	-14	78,1	93,0
4	2	15		27,0
4	2	-15		22,4
4	2	16		32,6
4	2	-16	136,1	151,8
4	2	17		- 18,8
4	2	-17		- 31,4
4	2	18	90,0	84,4
4	2	-18	83,0	86,6
4	2	19		- 32,0
4	2	-19		39,2
4	2	20	71,7	- 74,2
4	2	-20		- 6,4
6	2	0	67,8	71,8
6	2	1		- 19,4
6	2	- 1		32,4
6	2	- 2	330,9	329,6
6	2	- 3	79,1	71,4
6	2	- 4		- 28,2
6	2	- 5	134,4	-131,8
6	2	6		22,4
6	2	- 6	380,2	422,2
6	2	- 7		28,0
6	2	- 8	85,4	82,8
6	2	- 9	309,0	305,6
6	2	- 10	151,7	162,4
6	2	- 11	79,1	71,2
6	2	- 12		54,2
6	2	- 13	416,3	414,4
6	2	- 14		- 32,8
6	2	- 15	97,4	- 92,6
6	2	- 16		22,0
6	2	- 17	61,8	58,0
6	2	- 18	91,2	88,2
6	2	- 19		- 50,0
6	2	- 20		- 34,2
8	2	0	95,1	93,2
8	2	- 1		26,4
8	2	- 2		16,2
8	2	- 3		0,2
8	2	- 4	195,7	167,0
8	2	- 5	116,2	126,4
8	2	- 6		15,8
8	2	- 7		- 6,0
8	2	- 8		- 39,2
8	2	- 9	212,8	226,8
8	2	- 10		56,0
8	2	- 11		1,6
8	2	- 12	172,8	184,0
8	2	- 13	93,7	107,4
8	2	- 14		15,4
8	2	- 15	111,3	132,0
8	2	- 16		43,6
8	2	- 17		- 55,0
8	2	- 18		6,4
8	2	- 19	57,0	62,6
8	2	- 20	221,0	228,8
8	2	- 21	61,9	- 65,4
8	2	- 22		- 52,4
8	2	1	61,9	52,0
8	2	- 2		- 12,0
8	2	- 3		- 36,4
8	2	- 4	115,7	-117,4
8	2	- 5		52,8
8	2	- 6		- 18,8
8	2	- 7		47,8
8	2	- 8		32,8
8	2	- 9	154,2	121,2
8	2	- 10	146,4	-180,4
8	2	- 11	98,5	-106,4
8	2	10	145,0	127,0
8	2	-10		58,0
8	2	11		- 5,2
8	2	-11		- 55,6
8	2	12	172,8	151,4
8	2	-12	106,4	114,2
8	2	13		- 48,2
8	2	-13	75,5	80,6
8	2	14		- 15,0
8	2	-14	109,8	-110,8
8	2	15		5,6
8	2	-15		5,6
8	2	16	126,8	-109,8
8	2	-16		57,8
8	2	17		39,4
8	2	-17		15,6
8	2	18		8,0
8	2	-18		- 53,8
8	2	19		49,8
8	2	-19		20,2
8	2	20		57,0
8	2	-20	96,6	-105,6
8	2	-21		- 10,4
8	2	-22		53,2
10	2	0	467,3	536,0
10	2	1	58,1	- 62,2
10	2	- 1		57,8
10	2	- 2	155,6	160,6
10	2	- 3	57,3	61,4
10	2	2		12,0
10	2	- 3		- 4,0
10	2	4	133,2	121,6
10	2	- 4		37,0
10	2	5		29,2
10	2	- 5		- 10,4
10	2	6	154,7	138,4
10	2	- 6	175,7	174,4
10	2	7	82,5	- 70,2
10	2	- 7		- 29,4
10	2	8		- 42,2
10	2	- 8		40,6
10	2	9		50,8
10	2	- 9		- 55,6
10	2	10	121,5	108,0
10	2	-10	156,1	158,6
10	2	11		55,6
10	2	-11		- 14,8
10	2	12	240,1	224,8
10	2	-12	178,2	187,6
10	2	13		- 8,4
10	2	-13		32,6
10	2	14		- 16,6
10	2	-14	167,4	-169,2
10	2	15		- 5,8
10	2	-15		- 35,0
10	2	16		31,6
10	2	-16		- 9,2
10	2	17		- 22,8
10	2	-17		5,6
10	2	18		2,2
10	2	-18		5,8
10	2	19		8,0
10	2	-19		8,0
10	2	20		- 11,8
10	2	-20	72,7	- 78,8
12	2	0	143,0	144,4
12	2	1		1,4
12	2	- 1	175,7	178,4
12	2	2		- 26,2
12	2	- 2	198,6	-198,6
12	2	3		- 14,4
12	2	- 3		- 8,0
12	2	4		- 39,0
12	2	- 4	126,4	-129,2
12	2	5		25,8
12	2	- 5	95,1	- 99,2
12	2	6	63,9	61,4
12	2	- 6	156,6	146,2
12	2	7		- 33,4
12	2	- 7		25,8
12	2	8	176,7	-158,0
12	2	- 8		16,6
12	2	9		0,8
12	2	- 9		- 2,4
12	2	10	134,7	-119,6
12	2	-10	111,3	111,2
12	2	11	68,6	73,4
12	2	-11		30,6
12	2	12	72,1	77,2
12	2	-12	72,7	68,2
12	2	13		- 45,0
12	2	-13		36,4
12	2	14	109,3	- 85,4
12	2	-14	114,7	-112,8
12	2	15		- 1,0
12	2	-15	67,4	- 72,2
12	2	16		57,6
12	2	-16		12,4
12	2	17		- 19,6
12	2	-17		- 11,8

Table 2 (*cont.*)

h	k	l	FO	FC
12	2	18		28,0
12	2	-18	97,1	94,0
12	2	19		- 40,2
12	2	-19		- 26,8
12	2	-20		15,6
14	2	0	98,5	- 97,4
14	2	1		31,2
14	2	- 1		46,4
14	2	2		- 62,8
14	2	- 2	85,3	- 90,8
14	2	3		- 9,0
14	2	- 3	112,7	-108,4
14	2	4		- 55,8
14	2	- 4		59,0
14	2	5		6,2
14	2	- 5		13,2
14	2	6	107,4	121,2
14	2	- 6	148,4	144,6
14	2	7		- 31,2
14	2	- 7		41,6
14	2	8		8,8
14	2	- 8		34,8
14	2	9		- 45,4
14	2	- 9		62,4
14	2	10		- 40,2
14	2	-10		24,2
14	2	11		- 0,2
14	2	-11		10,4
14	2	12		58,4
14	2	-12		29,0
14	2	13		- 22,2
14	2	-13		12,8
14	2	14		18,0
14	2	-14	73,7	80,4
14	2	15		20,6
14	2	-15		- 33,6
14	2	16	117,5	114,0
14	2	-16	100,5	104,0
14	2	17		5,6
14	2	-17		5,2
14	2	18		175,0
14	2	-18	147,9	148,8
14	2	-19		25,4
14	2	-20	70,4	66,4
16	2	0		- 63,6
16	2	1		- 34,2
16	2	- 1		- 56,8
16	2	2		- 60,2
16	2	- 2	95,6	92,2
16	2	3		- 6,4
16	2	- 3		25,6
16	2	4		17,2
16	2	- 4		- 17,8
16	2	5		- 57,0
16	2	- 5		45,0
16	2	6		20,6
16	2	- 6	65,8	- 65,2
16	2	7	73,4	69,2
16	2	- 7		- 37,0
16	2	8	89,2	82,2
16	2	- 8	75,1	- 58,8
16	2	9		- 17,0
16	2	- 9		- 0,0
16	2	10	110,8	113,0
16	2	-10	143,0	-144,2
16	2	11		- 35,2
16	2	-11		5,6
16	2	12		- 5,2
16	2	-12		- 31,0
16	2	13		- 29,6
16	2	-13		2,8
16	2	14		- 10,8
16	2	-14	61,9	57,8
16	2	15		4,0
16	2	-15		13,8
16	2	16		1,2
16	2	-16		- 15,0
16	2	17		41,8
16	2	-17		- 4,6
16	2	-18		26,8
16	2	-19		19,2
18	2	0	145,9	143,0
18	2	1		- 31,4
18	2	- 1		- 50,4
18	2	2		55,6
18	2	- 2	251,8	244,4
18	2	3		19,8
18	2	- 3		64,4
18	2	4	174,7	182,0
18	2	- 4		- 10,8
18	2	5		- 14,0
18	2	- 5		13,2
18	2	6		- 24,4
18	2	- 6		15,6
18	2	7		45,6
18	2	- 7	79,6	- 72,4
18	2	8		61,4
18	2	- 8	151,7	151,8
18	2	9		30,4
18	2	- 9		17,6
18	2	10	204,5	214,0
18	2	-10		- 20,4
18	2	11		- 15,6
18	2	-11		- 40,8
18	2	12		33,0
18	2	-12	134,6	147,0
18	2	13		17,2
18	2	-13		- 7,2
18	2	14		37,4
18	2	-14	100,5	102,8
18	2	-15		34,2
18	2	-16		- 21,0
18	2	-17		1,8
20	2	0	107,9	105,4
20	2	1		- 15,8
20	2	- 1		47,6
20	2	2		49,0
20	2	- 2	80,5	92,8
20	2	3		5,6
20	2	- 3		37,6
20	2	4	127,8	133,4
20	2	- 4	71,8	- 67,2
20	2	5		- 37,0
20	2	- 5		- 45,4
20	2	6	124,4	-128,4
20	2	- 6		33,8
20	2	7		19,2
20	2	- 7		- 27,0
20	2	8	69,3	- 79,0
20	2	- 8	124,8	166,0
20	2	9		36,6
20	2	- 9		0,2
20	2	10		48,4
20	2	-10		34,8
20	2	11		- 0,0
20	2	-11		- 6,2
20	2	12		- 42,0
20	2	-12		47,8
20	2	-13		17,8
20	2	-14		- 25,8
20	2	-15		5,8
22	2	0		6,4
22	2	1		52,6
22	2	- 1		30,2
22	2	- 2	111,8	110,4
22	2	3		28,4
22	2	- 3		19,6
22	2	- 3		- 47,0
22	2	4	116,2	117,0
22	2	- 4	86,8	87,4
22	2	5		- 13,6
22	2	- 5		- 3,8
22	2	6		30,2
22	2	- 6	90,7	82,2
22	2	7		- 26,0
22	2	- 7		19,6
22	2	8		44,4
22	2	- 8	150,2	142,8
22	2	9		- 5,4
22	2	- 9		19,4
22	2	-10	121,5	115,8
22	2	-11		5,6
22	2	-12		- 6,2
24	2	0	150,7	-149,8
24	2	- 1		- 4,4
24	2	- 2		- 43,6
24	2	- 3		- 35,8
24	2	- 4	80,0	82,4
24	2	- 5		45,2
24	2	- 6		- 59,0
1	3	1	102,4	109,2
1	3	2	111,7	128,0
1	3	- 2		39,0
1	3	3	90,4	- 91,0
1	3	- 3	155,6	146,2
1	3	4	116,1	115,8
1	3	- 4	252,0	-248,4
1	3	5	151,5	-141,4
1	3	- 5	228,4	214,4
1	3	6	43,1	- 43,4
1	3	- 6	39,8	- 36,4
1	3	7	233,3	232,4
1	3	- 7	129,0	-142,4
1	3	8		19,4
1	3	- 8		24,8
1	3	9	93,6	- 77,8
1	3	- 9	49,7	53,4
1	3	10	199,4	174,6
1	3	-10		10,8
1	3	11		- 45,2
1	3	-11	126,8	139,8
1	3	12	99,9	105,0
1	3	-12		49,4
1	3	13	75,1	72,4
1	3	-13		49,4
1	3	14	142,4	154,0
1	3	-14		22,6
1	3	15	82,5	- 82,0
1	3	-15	124,6	130,0
1	3	16	71,5	74,4
1	3	-16	59,7	56,0
1	3	17		- 9,6
1	3	-17		41,4
1	3	18		9,2
1	3	-18		53,6
1	3	19	98,0	96,2
1	3	-19	64,1	- 67,8
1	3	20		8,6
1	3	-20	78,5	91,6
1	3	21	46,8	- 53,0
1	3	-21	57,5	62,0
3	3	0	58,2	61,2
3	3	1	80,3	87,8
3	3	- 1	62,3	- 79,6
3	3	2	92,5	97,6
3	3	- 2		40,0
3	3	3	106,5	-108,0
3	3	- 3	134,1	-164,4
3	3	4	278,0	288,4
3	3	- 4	66,4	- 78,0
3	3	5	149,3	-149,6
3	3	- 5	43,1	- 47,0
3	3	6	109,9	107,6
3	3	- 6	129,3	133,0
3	3	7		10,6
3	3	- 7	152,3	-169,4
3	3	8		- 39,2
3	3	- 8	168,5	183,4
3	3	9	119,8	-104,0
3	3	- 9	57,5	- 70,0
3	3	10	183,2	167,8
3	3	-10	51,6	- 51,8
3	3	11		- 16,6
3	3	-11	67,8	66,0
3	3	12		40,8
3	3	-12	65,6	72,4
3	3	13	57,5	74,4
3	3	-13		- 45,0
3	3	14	73,8	79,0
3	3	-14	81,4	- 75,8
3	3	15	64,5	- 61,0
3	3	-15	86,2	- 95,8
3	3	16	122,4	135,6
3	3	-16		- 53,0
3	3	17	78,2	- 73,4
3	3	-17		- 24,6
3	3	18		5,4
3	3	-18	103,2	113,8
3	3	19		11,8
3	3	-19		- 57,4
3	3	20		- 28,8
3	3	-20		50,0
3	3	21	47,5	- 89,0
3	3	-21		- 6,8
5	3	0	98,8	102,8
5	3	1	80,3	85,8
5	3	- 1		30,4
5	3	2	59,7	- 54,8
5	3	- 2	92,1	96,8
5	3	3	96,9	100,8
5	3	- 3	78,1	- 80,2
5	3	4	170,7	176,0
5	3	- 4	122,1	132,6
5	3	5	154,8	155,0
5	3	- 5	91,0	102,6
5	3	6	118,7	108,4
5	3	- 6	153,4	170,8
5	3	7	63,4	62,6
5	3	- 7	102,5	110,2
5	3	8		17,8
5	3	- 8	56,0	44,2
5	3	9		- 27,2
5	3	- 9		- 39,6
5	3	10		- 6,4
5	3	-10		- 7,6
5	3	11		50,0
5	3	-11	69,9	65,6
5	3	12		- 55,8
5	3	-12		- 19,2
5	3	13	90,3	71,8
5	3	-13		- 24,8
5	3	14	105,1	- 96,8
5	3	-14		- 45,4
5	3	15	67,1	72,6
5	3	-15	86,2	- 96,2
5	3	16		24,2
5	3	-16		42,6
5	3	17		52,4
5	3	-17	92,9	85,6
5	3	18		16,8
5	3	-18	59,3	60,2
5	3	19		- 2,4
5	3	-19		7,2
5	3	20		1,0
5	3	-20		- 21,4
5	3	-21		- 24,4
7	3	0	66,4	69,2
7	3	1		- 47,0
7	3	- 1	61,2	54,4
7	3	2		- 39,4
7	3	- 2	130,1	135,4
7	3	3	99,9	-105,4
7	3	- 3	139,3	-146,0
7	3	4	106,9	-100,4
7	3	- 4	119,5	121,2
7	3	5	97,3	94,8
7	3	- 5		- 3,2
7	3	6	70,4	67,6
7	3	- 6		1,0
7	3	7		- 19,4
7	3	- 7		- 7,6
7	3	8	106,2	102,2
7	3	- 8		11,0
7	3	9	54,9	- 49,2
7	3	- 9	114,5	-122,6
7	3	10	68,2	65,4
7	3	-10	70,4	67,0
7	3	11		39,8
7	3	-11		- 44,4
7	3	12		19,0
7	3	-12		38,4
7	3	13	130,8	-124,8
7	3	-13	40,8	- 77,0
7	3	14	92,9	- 75,8
7	3	-14	119,8	121,0
7	3	15		- 45,4
7	3	-15	136,4	-152,6
7	3	16		23,4
7	3	-16	91,8	95,8
7	3	17		47,8
7	3	-17		38,2
7	3	18		29,6
7	3	-18		- 26,0
7	3	19		- 34,8
7	3	-19		- 37,0
7	3	-20		- 22,0
9	3	0	56,4	46,6
9	3	1		- 28,2
9	3	- 1	183,9	197,0
9	3	2		57,2
9	3	- 2	115,8	121,8
9	3	3	105,4	- 93,6
9	3	- 3		31,0
9	3	4	71,2	- 65,4
9	3	- 4		2,8
9	3	5	119,1	114,4
9	3	- 5	125,6	118,0
9	3	6	132,5	-124,8
9	3	- 6		- 26,6
9	3	7	98,4	101,6
9	3	- 7		45,0
9	3	8		13,6
9	3	- 8	85,8	80,4
9	3	9		32,0
9	3	- 9		- 39,8
9	3	10	117,5	106,0
9	3	-10	141,2	147,2
9	3	11	133,0	128,4
9	3	-11		56,0
9	3	12	84,4	48,0
9	3	-12	76,2	77,6
9	3	13	64,4	- 69,0
9	3	-13	107,3	103,8
9	3	14		50,8
9	3	-14	177,6	193,0
9	3	15		- 2,6
9	3	-15		24,8
9	3	16		21,8
9	3	-16		4,0
9	3	17	135,6	127,2
9	3	-17		56,0
9	3	18		28,8
9	3	-18		- 11,4
9	3	19		- 18,6
9	3	-19		- 5,4
9	3	-20	96,2	92,4
11	3	0	63,0	- 67,2
11	3	1	69,7	- 75,6
11	3	- 1	80,7	82,6
11	3	2	147,8	150,8
11	3	- 2		49,4
11	3	3	112,4	-118,0
11	3	- 3		- 27,4
11	3	4	131,2	124,0
11	3	- 4	131,9	-129,2
11	3	5	108,8	-106,2
11	3	- 5	104,7	-103,8
11	3	6		- 42,4
11	3	- 6	84,7	- 83,0
11	3	7	89,2	- 84,6
11	3	- 7	66,4	- 68,8
11	3	8		- 6,6
11	3	- 8	107,6	97,4
11	3	9		- 24,6
11	3	- 9		- 11,2
11	3	10	107,6	89,2
11	3	-10		- 9,4
11	3	11		47,4
11	3	-11		16,4
11	3	12		50,6
11	3	-12		3,4
11	3	13	84,0	- 87,8
11	3	-13	105,2	101,2
11	3	14	124,9	125,0
11	3	-14		21,6
11	3	15		- 31,4
11	3	-15		- 21,2
11	3	16		37,8
11	3	-16	63,8	- 68,2
11	3	17		- 0,4
11	3	-17	65,6	- 62,8
11	3	-18	57,9	61,8
13	3	0		- 7,2
13	3	1	70,4	- 78,4
13	3	- 1		28,0
13	3	2	83,5	80,8
13	3	- 2		22,6
13	3	3	137,1	141,1
13	3	- 3	62,3	60,0
13	3	4	209,8	211,4
13	3	- 4		15,2
13	3	5		16,2
13	3	- 5	107,6	-102,8
13	3	6	95,5	89,8
13	3	- 6	56,8	48,0
13	3	7		- 54,4
13	3	- 7	57,1	52,4
13	3	8	79,2	79,4
13	3	- 8	126,8	120,6
13	3	9	60,0	64,2
13	3	- 9	85,1	77,8
13	3	10		51,0
13	3	-10		- 24,2
13	3	11		5,0
13	3	-11		- 31,6
13	3	12		11,6
13	3	-12	70,8	- 57,6
13	3	13		12,0
13	3	-13	111,0	102,6
13	3	14	115,4	125,4
13	3	-14	44,2	- 47,8
13	3	15	104,0	111,4
13	3	-15		29,2
13	3	-16		- 10,6
13	3	-17		- 39,0
13	3	-18	58,2	66,8
15	3	0	100,3	88,8
15	3	1	128,2	-131,6
15	3	- 1	54,5	- 42,2
15	3	2		26,6
15	3	- 2	111,7	103,2
15	3	3	117,6	117,6
15	3	- 3		28,0
15	3	- 4		31,0
15	3	- 4	161,5	157,4
15	3	5		- 17,2
15	3	- 5	149,3	-148,8
15	3	6	76,6	72,2
15	3	- 6	147,5	140,6
15	3	7	113,6	-112,0
15	3	- 7		47,4
15	3	8	77,3	77,0
15	3	- 8	70,4	65,8
15	3	9		48,4
15	3	- 9	65,0	59,0
15	3	10		- 17,0
15	3	-10		28,2
15	3	11	80,7	- 80,6
15	3	-11	134,9	-136,4
15	3	12		- 55,2
15	3	-12		9,8
15	3	13	69,5	- 65,0
15	3	- 13		- 8,8
15	3	14		- 56,4
15	3	-14		5,6
15	3	15	64,1	68,6
15	3	-15		- 43,2
15	3	-16	96,2	93,2
15	3	-17	61,9	- 67,8
17	3	0	92,1	89,8
17	3	1		- 50,0
17	3	- 1		53,6
17	3	2		- 17,4
17	3	- 2		7,2
17	3	3	98,8	92,8
17	3	- 3	117,6	110,2
17	3	4	97,7	- 96,4
17	3	- 4	75,1	70,2
17	3	5		36,8
17	3	- 5		34,6
17	3	6		- 4,6
17	3	- 6		25,2
17	3	7		15,2
17	3	- 7	59,0	58,8
17	3	8		13,8
17	3	- 8	52,7	- 51,8
17	3	9	80,7	85,0
17	3	- 9	86,6	57,8
17	3	10		45,0
17	3	-10	65,6	85,0

Table 2 (*cont.*)

h	k	l	FO	FC
17	3	11		- 48.6
17	3	-11	70.4	- 64.6
17	3	12		29.0
17	3	-12	66.5	62.4
17	3	13	64.3	- 68.8
17	3	-13		16.4
17	3	-14	76.6	77.8
17	3	-15	57.5	45.4
19	3	0		36.2
19	3	1		- 10.2
19	3	- 1		- 0.2
19	3	2		53.0
19	3	- 2		- 5.4
19	3	3		- 49.4
19	3	- 3		17.4
19	3	4	62.7	- 59.2
19	3	- 4		- 25.2
19	3	5	104.7	-106.4
19	3	- 5		- 19.8
19	3	6		- 3.4
19	3	- 6		- 11.6
19	3	7		4.6
19	3	- 7	101.7	-109.9
19	3	- 8		- 13.8
19	3	- 9		13.2
19	3	-10	115.0	112.8
19	3	-11		- 3.4
19	3	-12	71.9	72.0
21	3	0		16.8
21	3	1	74.9	68.4
21	3	- 1		- 4.6
21	3	2	97.3	91.4
21	3	- 2		- 26.4
21	3	3		21.4
21	3	- 3	53.4	50.2
21	3	4	56.4	54.2
21	3	- 4		- 28.4
21	3	5	65.4	- 59.6
21	3	- 5	39.6	34.0
21	3	6	75.1	64.8
21	3	- 6		- 2.2
21	3	7	73.4	70.0
21	3	- 7	82.9	- 89.0
21	3	- 8	56.0	47.2
21	3	- 9	82.5	75.4
0	4	1	145.1	-155.2
0	4	2	152.5	145.2
0	4	3	45.7	- 57.0
0	4	4	135.4	127.0
0	4	5	72.9	84.4
0	4	6	201.5	215.6
0	4	7		- 25.8
0	4	8		4.8
0	4	9	112.7	119.6
0	4	10	111.9	122.4
0	4	11	72.1	71.8
0	4	12	179.3	197.2
0	4	13	85.5	- 75.6
0	4	14	61.4	- 55.0
0	4	15		15.6
0	4	16		17.8
0	4	17		25.2
2	4	0	159.5	149.6
2	4	1	69.7	84.0
2	4	- 1	221.7	208.0
2	4	2		- 20.8
2	4	- 2	32.3	- 45.0
2	4	3	34.6	- 40.2
2	4	- 3	34.2	- 42.4
2	4	4		23.6
2	4	- 4	75.7	- 89.6
2	4	5	51.6	44.2
2	4	- 5	50.4	- 65.2
2	4	6	66.6	50.8
2	4	- 6	95.8	98.2
2	4	7	68.9	- 62.4
2	4	- 7		19.2
2	4	8	135.6	-155.2
2	4	- 8	55.1	58.2
2	4	9		34.8
2	4	- 9		- 30.0
2	4	10		- 26.4
2	4	-10	95.7	106.4
2	4	11	108.7	114.6
2	4	-11		35.4
2	4	12	75.6	72.2
2	4	-12	85.9	78.0
2	4	13	61.8	- 58.4
2	4	-13		54.2
2	4	14		- 45.0
2	4	-14		- 36.6
2	4	15		- 21.0
2	4	-15	81.1	- 76.2
2	4	16		13.4
2	4	-16		- 30.2
2	4	17		- 30.4
2	4	-17		- 32.4
4	4	0		- 46.2
4	4	1		27.2
4	4	- 1		45.8
4	4	2		8.2
4	4	- 2		58.8
4	4	3		4.4
4	4	- 3		- 46.4
4	4	4	81.9	78.2
4	4	- 4		- 31.0
4	4	5	51.2	- 49.4
4	4	- 5		0.8
4	4	6	108.7	107.0
4	4	- 6	146.2	171.4
4	4	7	54.7	- 45.4
4	4	- 7		- 31.4
4	4	8		9.0
4	4	- 8	121.0	132.0
4	4	9		- 37.6
4	4	- 9	82.7	81.8
4	4	10		24.2
4	4	-10		2.4
4	4	11		- 5.4
4	4	-11	73.3	77.4
4	4	12		33.2
4	4	-12		19.0
4	4	13		- 34.6
4	4	-13		19.4
4	4	14	78.4	77.4
4	4	-14	83.9	84.0
4	4	15		10.2
4	4	-15		- 35.8
4	4	16	131.6	153.2
4	4	-16		21.0
4	4	-17		- 50.0
6	4	0	99.7	-105.8
6	4	1	67.8	- 75.2
6	4	- 1	115.5	-118.0
6	4	2	78.4	- 76.4
6	4	- 2	59.5	50.6
6	4	3	81.5	82.8
6	4	- 3	70.9	75.8
6	4	4		20.2
6	4	- 4	76.0	- 79.2
6	4	5		- 28.0
6	4	- 5		9.6
6	4	6		11.0
6	4	- 6		- 43.6
6	4	7		34.8
6	4	- 7		- 6.4
6	4	8		43.8
6	4	- 8		- 27.4
6	4	9	57.1	- 51.6
6	4	- 9	113.9	115.6
6	4	10	139.9	127.8
6	4	-10	150.5	-158.4
6	4	11	86.7	- 85.0
6	4	-11		- 49.8
6	4	12	64.6	- 65.8
6	4	-12		- 31.0
6	4	13		- 5.4
6	4	-13		- 23.6
6	4	14		- 0.0
6	4	-14	83.1	74.2
6	4	15		54.4
6	4	-15		40.2
6	4	-16		- 44.2
8	4	-17		- 19.6
8	4	0		24.0
8	4	1	118.2	-130.6
8	4	- 1	61.8	- 54.2
8	4	2		- 15.0
8	4	- 2	171.4	180.4
8	4	3		- 9.4
8	4	- 3	105.6	110.0
8	4	4	98.1	98.2
8	4	- 4		- 12.6
8	4	5		- 10.8
8	4	- 5		- 17.8
8	4	6		- 10.0
8	4	- 6		- 12.4
8	4	7	104.8	101.8
8	4	- 7		- 43.0
8	4	8	75.6	66.0
8	4	- 8		21.4
8	4	9	78.8	69.0
8	4	- 9		- 3.8
8	4	10	198.2	180.4
8	4	-10		- 36.6
8	4	11	71.7	- 76.8
8	4	-11	111.1	- 95.8
8	4	12		19.2
8	4	-12	89.8	84.2
8	4	13		0.8
8	4	-13		33.4
8	4	-14	88.6	78.8
8	4	-15	89.8	95.0
8	4	-16		- 6.4
8	4	-17		- 10.6
10	4	0	102.0	102.8
10	4	1		15.2
10	4	- 1	52.0	40.4
10	4	2		61.2
10	4	- 2	106.4	104.8
10	4	3		- 44.6
10	4	- 3		9.6
10	4	4	61.3	65.6
10	4	- 4		- 15.4
10	4	5		- 40.6
10	4	- 5		- 33.0
10	4	6	89.8	- 85.8
10	4	- 6		- 40.2
10	4	7		32.6
10	4	- 7		- 21.0
10	4	8		- 51.8
10	4	- 8	100.1	87.4
10	4	9		59.6
10	4	- 9	87.9	- 79.0
10	4	10		44.2
10	4	-10	56.3	54.0
10	4	11		20.0
10	4	-11		- 18.4
10	4	12		- 35.4
10	4	-12		10.6
10	4	-13		29.8
10	4	-14		- 24.6
10	4	-15		- 15.2
10	4	-16	65.0	- 71.2
12	4	0		28.6
12	4	1	122.2	126.4
12	4	- 1	102.0	103.6
12	4	2	170.2	147.8
12	4	- 2	63.3	63.0
12	4	3		- 13.0
12	4	- 3		- 51.4
12	4	4	114.7	100.6
12	4	- 4	126.5	110.8
12	4	5		- 14.0
12	4	- 5		29.2
12	4	6		15.4
12	4	- 6	117.0	111.6
12	4	7		- 17.4
12	4	- 7	62.2	- 45.4
12	4	8		57.4
12	4	- 8	178.9	179.0
12	4	9		15.6
12	4	- 9		- 26.4
12	4	10		- 25.4
12	4	-10	162.0	186.0
12	4	11		45.8
12	4	-11	102.0	101.2
12	4	-13		- 6.2
12	4	-14	101.7	108.2
12	4	-15	95.7	- 97.8
12	4	16	96.9	95.4
14	4	0	137.9	-141.8
14	4	1	57.5	59.4
14	4	- 1		- 5.8
14	4	2	68.1	71.4
14	4	- 2	60.5	- 55.4
14	4	3		- 7.4
14	4	- 3	81.9	- 76.2
14	4	4	81.5	- 76.2
14	4	- 4	96.9	96.2
14	4	5		- 4.0
14	4	- 5	49.2	53.2
14	4	6		- 11.0
14	4	- 6		- 14.6
14	4	7		- 5.2
14	4	- 7		- 5.0
14	4	8	68.5	63.2
14	4	- 8		32.8
14	4	9	97.7	- 99.6
14	4	- 9	72.5	66.0
14	4	10		- 48.0
14	4	-10	79.6	79.0
14	4	-11	95.8	105.2
14	4	-12	71.3	- 76.4
14	4	-13	54.3	- 50.6
14	4	-14	68.9	69.6
16	4	0		0.0
16	4	1		- 26.2
16	4	- 1	60.3	- 44.4
16	4	2	118.6	122.8
16	4	- 2	68.5	69.4
16	4	3	109.5	- 84.0
16	4	- 3		- 20.2
16	4	4		21.2
16	4	- 4	139.9	135.0
16	4	5		5.2
16	4	- 5	59.9	57.8
16	4	6	101.7	106.0
16	4	- 6		- 14.8
16	4	7	74.8	80.4
16	4	- 7		- 29.8
16	4	8	188.8	186.8
16	4	- 8	54.7	- 48.2
16	4	9	89.3	- 74.0
16	4	- 9		16.4
16	4	-10		36.2
16	4	-11		3.4
18	4	0	61.1	66.2
18	4	1		- 10.2
18	4	- 1		- 8.4
18	4	2	53.6	54.8
18	4	- 2		14.2
18	4	3	49.2	- 51.6
18	4	- 3		6.8
18	4	4		- 40.2
18	4	- 4		0.4
18	4	5		1.0
18	4	- 5		19.2
18	4	- 6		11.8
18	4	6	53.6	- 55.6
18	4	- 7	103.6	97.8
18	4	7		- 19.8
18	4	- 8	60.7	- 52.8
18	4	- 9	72.9	- 68.8
20	4	0	120.2	111.6
20	4	1		12.4
20	4	- 1	45.7	55.6
20	4	2	63.0	55.0
20	4	- 2		- 9.0
20	4	- 3		9.6
20	4	- 4		14.8
20	4	- 5		- 24.4
20	4	- 6	84.7	83.4

tions the scattering factor values from the self-consistent model as listed in *International Tables for X-ray Crystallography* (1962) for Fe^{3+}, P, O^- and H were used. Corrections for the real part of the anomalous dispersion were applied for Fe^{3+} with values of $\Delta f'$ reported for the Cu $K\alpha$ wave-length by Cromer (1965). An overall temperature factor of 5·0 Å^2 was applied to the hydrogen atoms.*

Discussion of the structure

The atomic arrangement projected along the *b* axis is shown in Fig. 1. The lists of bond lengths and bond angles with their standard deviations are included in Tables 3 and 4. The standard deviations are estimated by Cruickshank's (1953) formula for the bond lengths and by Darlow's (1961) formula for bond angles.

Both PO_4 tetrahedra in the structure are nearly regular. O–P–O angles are in the range 106°45′–111°29′; the average P–O distances are 1·54 and 1·53 Å. These are in agreement with the generally accepted values.

Each of the four non-equivalent iron ions in the cell is bound to six oxygen atoms to form distorted octahedra. The average Fe–O distances are 2·02, 1·97, 2·00, and 2·03 Å. These values can be compared with the 1·99 Å average ferric iron–oxygen distance in laueite (Moore, 1965) and 2·00 Å in metastrengite (Fanfani & Zanazzi, 1966).

The configuration shown by the iron–oxygen complexes is as follows:

Fe(1) links 4 O and 2 OH
Fe(2) 2 O, 2 OH and 2 H_2O
Fe(3) 3 O, 2 OH and 1 H_2O
Fe(4) 4 O and 2 OH .

The octahedron of the iron ion at the origin of the cell shares two opposite faces with the Fe(4) coordination polyhedron; furthermore the same octahedron links two opposite Fe(3) coordination octahedra by a corner. This group of five octahedra is joined to others, related to the first one by the twofold axis, to form an infinite chain along the *c* axis. Connexions occur through an oxygen atom on the twofold axis.

* All the calculations were performed on an IBM 1620 computer, except the computations for the absorption correction, which were carried out with the IBM 7090 computer of the Centro Nazionale Universitario di Calcolo Elettronico at Pisa University.

The Fe(2) coordination octahedra on the inversion center $(\frac{1}{4},\frac{1}{4},0)$ and on the equivalent positions link these infinite chains together, sharing opposite corners with Fe(4) octahedra in the **a** direction.

Each of the PO_4 tetrahedra shares the four corners with different Fe octahedra connecting them inside the chain in the **c** direction and between different chains in the **b** direction to form a thick sheet parallel to (100).

The Fe(2) octahedron is linked to the chain by a vertex of a PO_4 tetrahedron, as well as by the corner shared with the Fe(3) polyhedron.

The three-dimensional network of Fe polyhedra is shown in Fig. 2.

This atomic array accounts for the good {100} cleavage in beraunite. In the crystal structure there are empty channels along the screw axes, where the free water molecules are located. The presence of non-cation coordinated water has already been found in laueite (Moore, 1965) and can explain the weight loss which occurs when the mineral is heated below 150 °C (Fischer, 1956). These water molecules are hydrogen-bonded together and to the framework of Fe polyhedra; in the structure other hydrogen bridges connect oxygen atoms of different Fe and P coordination polyhedra. Lengths of O–H···O bonds are in the range 2·67–2·96 Å; they are listed in Table 5.

Table 3. *Bond lengths in beraunite*

(I) x, y, z
(II) $-x, y, \frac{1}{2}-z$
(III) $x, -y, -\frac{1}{2}+z$
(IV) $\frac{1}{2}-x, \frac{1}{2}-y, -z$
(V) $-\frac{1}{2}+x, -\frac{1}{2}+y, z$
(VI) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
(VII) $-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$
(VIII) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
(IX) $-\frac{1}{2}+x, \frac{1}{2}+y, z$
(X) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$
(XI) $x, 1-y, \frac{1}{2}+z$

Fe(1)(I)–OH(1)(III)	2·01 Å	Fe(2)(I)–O(1)(I)	1·94 Å
–O(2)(IV)	2·01	–OH(2)(VIII)	1·93
–O(3)(VI)	2·03	–H_2O(2)(I)	2·04
Fe(3)(I)–OH(3)(I)	1·99	Fe(4)(I)–OH(1)(I)	2·08
–O(5)(IX)	1·94	–O(7)(VI)	1·92
–O(6)(I)	2·02	–O(8)(I)	1·93
–H_2O(1)(VI)	2·12	–OH(2)(I)	1·93
–O(4)(I)	1·95	–O(2)(VI)	2·14
–OH(1)(II)	1·99	–O(3)(X)	2·20
P(1)(I)—O(1)(I)	1·53	P(2)(I)—O(5)(I)	1·53
–O(2)(IV)	1·57	–O(6)(VI)	1·54
–O(3)(VIII)	1·56	–O(7)(I)	1·53
–O(4)(I)	1·51	–O(8)(VI)	1·51

Estimated standard deviations for Fe–O and P–O bond lengths are 0·01. Å

Table 4. *Bond angles in beraunite*

OH(1)(III)	–Fe(1)(I)–O(2)(IV)	79·2°	O(1)(I)	—Fe(2)(I)–OH(2)(VIII)	89·0°
–	–O(3)(VI)	80·6	–	–H_2O(2)(I)	93·5
O(2)(IV)	—O(3)(VI)	81·4	H_2O(2)(I)–	–OH(2)(VIII)	91·0
OH(3)(I)	—Fe(3)(I)–O(5)(IX)	90·7	OH(1)(I)	–Fe(4)(I)–O(7)(VI)	96·2
–	–O(6)(I)	91·6	–	–O(8)(I)	98·9
–	–H_2O(1)(VI)	89·0	–	–OH(2)(I)	158·4
–	–O(4)(I)	174·4	–	–O(2)(VI)	74·9
–	–OH(1)(II)	90·4	–	–O(3)(X)	75·3
O(5)(IX)—	–O(6)(I)	91·7	O(7)(VI)—	–O(8)(I)	94·2
–	–H_2O(1)(VI)	179·0	–	–OH(2)(I)	101·4
–	–O(4)(I)	92·2	–	–O(2)(VI)	98·7
–	–OH(1)(II)	92·7	–	–O(3)(X)	170·3
O(6)(I)—	–H_2O(1)(VI)	87·5	O(8)(I)	—OH(2)(I)	92·3
–	–O(4)(I)	83·6	–	–O(2)(VI)	166·2
–	–OH(1)(II)	175·2	–	–O(3)(X)	91·7
H_2O(1)(VI)–	–O(4)(I)	88·1	OH(2)(I)–	–O(2)(VI)	90·0
–	–OH(1)(II)	88·1	–	–O(3)(X)	86·0
O(4)(I)—	–OH(1)(II)	94·3	O(2)(VI)—	–O(3)(X)	74·9

Estimated standard deviations for O–Fe–O angles are 0·5°

O(1)(I)—	—P(1)(I)—O(2)(IV)	108·8°	O(5)(I)	—P(2)(I)—O(6)(VI)	111·4°
–	–O(3)(VIII)	108·1	–	–O(7)(I)	107·9
–	–O(4)(I)	111·2	–	–O(8)(VI)	111·3
O(2)(IV)	—O(3)(VIII)	109·0	O(6)(VI)—	–O(7)(I)	108·7
–	–O(4)(I)	110·0	–	–O(8)(VI)	110·4
O(3)(VIII)—	–O(4)(I)	109·7	O(7)(I)	—O(8)(VI)	106·9

Estimated standard deviations for O–P–O angles are 0·7°.

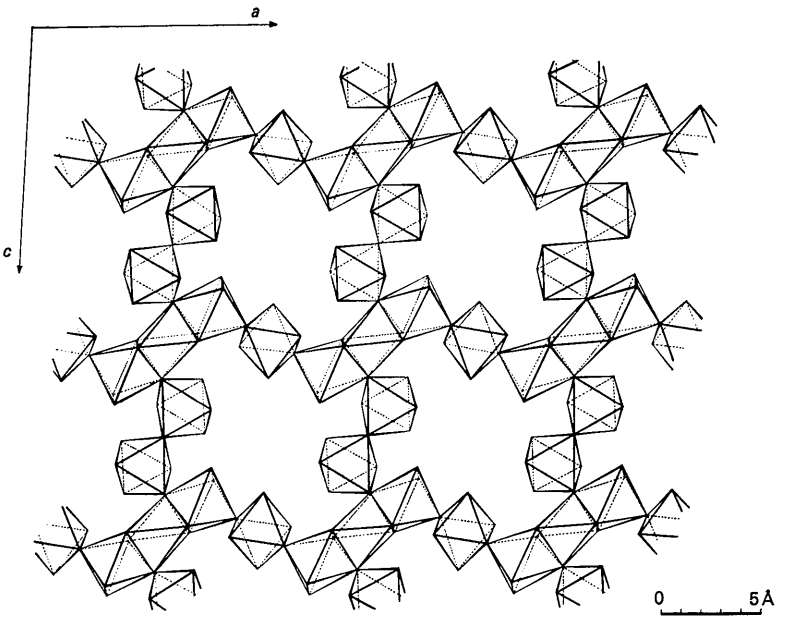

Fig. 2. The arrangement of Fe coordination polyhedra in beraunite. Projection along the *b* axis.

Table 5. *Hydrogen bond distances*

OH(1)(I)—O(5)(VI)	2·89 Å
OH(2)(I)—O(1)(XI)	2·77
$H_2O(1)(I)$–O(6)(VI)	2·81
$H_2O(2)(I)$–$H_2O(3)(I)$	2·67
–O(8)(VI)	2·88
$H_2O(3)(I)$–O(6)(I)	2·83
–$H_2O(3)(VI)$	2·96

A further distance of 3·33 Å which occurs between the oxygen atoms of $H_2O(1)(I)$ and $H_2O(2)(VIII)$ is too large to be considered as an H bond but suggests that the H atom of the $H_2O(1)$ points towards the neighbouring oxygen atom of $H_2O(2)$.

References

ALBANO, V., BELLON, P. L., POMPA, F. & SCATTURIN, V. (1963). *Ric. Sci.* **3A**, 1067.

BOŘICKY, E. (1867). *Sitzber. Akad. Wiss. Wien. Math. Nat. Kl.*, I, **56**, 7.

BREITHAUPT, A. (1841). *Handbuch der Mineralogie*, **2**, 152.

CHRIST, C. L. (1956). *Amer. Min.* **41**, 569.

CROMER, D. T. (1965). *Acta Cryst.* **18**, 17.

CRUICKSHANK, D. W. J. (1961). In *Computing Methods and the Phase Problem in X-ray Crystal Analysis*, p. 32. Oxford: Pergamon Press.

CRUICKSHANK, D. W. J. & ROBERTSON, A. P. (1953). *Acta Cryst.* **6**, 698.

Dana's system of Mineralogy, Vol. II, p. 959. New York: John Wiley.

DARLOW, S. F. (1961). *Acta Cryst.* **14**, 160.

FANFANI, L. & ZANAZZI, P. F. (1966). *Rend. Acc. Naz. Lincei.* In the press.

FISCHER, E. (1956). *Heid. Beitr. zur Mineralogie und Petrographie*, **5**, 204.

FRONDEL, C. (1949). *Amer. Min.* **34**, 513.

International Tables for X-ray Crystallography (1962). Vol. III, p. 202. Birmingham: Kynoch Press.

KÖNIG, G. A. (1890). *Z. Kristallogr.* **17**, 91.

MOORE, P. B. (1965). *Amer. Min.* **50**, 2052.

NIES, A. (1877). *Neues Jb. Mineral. Geol. Paläont.*, 176.

STEWART, J. M. (1964). Technical Report TR – 64 – 6. Univ. of Maryland.

STRENG, A. (1881). *Neues Jb. Mineral, Geol. Paläont.*, I, 102.