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Crystal structure and hydrogen bonding of copiapite

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Auszug

Copiapit, $MgFe_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, ist triklin, Raumgruppe $P\bar{1}$, mit $a = 7{,}342$ Å, $b = 18{,}818$ Å, $c = 7{,}389$ Å, $\alpha = 91{,}45°$, $\beta = 102{,}15°$ und $\gamma = 98{,}85°$. In der Struktur sind $Fe(O,OH,H_2O)_6$-Koordinationsoktaeder und Sulfattetraeder zu eindimensional-unendlichen Komplexen parallel [101] verknüpft. $Mg(H_2O)_6$-Oktaeder und nicht an Kationen gebundene Wassermoleküle liegen zwischen den Komplexen. Die einzelnen Struktureinheiten sind nur über Wasserstoffbrücken miteinander verknüpft.

Abstract

The structure of copiapite, $MgFe_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, is triclinic, space group $P\bar{1}$, with $a = 7.342$ Å, $b = 18.818$ Å, $c = 7.389$ Å, $\alpha = 91.45°$, $\beta = 102.15°$, and $\gamma = 98.85°$. $Fe(O,OH,H_2O)_6$ octahedra and sulfate tetrahedra are connected to form one-dimensional infinite complexes along [101]. $Mg(H_2O)_6$ octahedra and water molecules not bound to cations lie between the complexes. These structural groups are interconnected only by hydrogen bonds.

Introduction

Copiapite, a greenish-yellow secondary mineral found in the oxidation zone of sulfidic iron-ore deposits, is the commonest of the natural ferric sulfates. It was first described by Rose (1833). Considered to be monoclinic by Linck (1889), it was later found to be triclinic by Palache *et al.* (1946). The general chemical formula (Berry, 1947) is $AB_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, where A is usually Fe^{2+}, Mg, Cu, Zn and B is Fe^{3+}, Al.

Experimental

The crystals used for this investigation are from Alcaparrosa, Chile. The cation chemistry was assumed to be $A = Mg$ and $B = Fe^{3+}$, which was later confirmed during the structure refinement.

Single-crystal x-ray photographs showed triclinic symmetry. The lattice constants were measured on NaCl-calibrated photographs and refined by the method of least squares. They are in good agreement with those determined earlier on crystals from other localities, as shown in Table 1.

The unit cell has a volume of 984.4 Å^3 and contains 1 × [$MgFe_4(OH)_2(SO_4)_6 \cdot 20H_2O$]. The calculated density is 2.05 g · cm^{-3}; the measured density is 2.04 g · cm^{-3}.

Table 1. *Cell constants of copiapites*

Cell dimensions	Chuquicamata, Chile, PALACHE *et al.* (1946)	Alaska, JOLLY and FOSTER (1967)	Alcaparrosa, Chile, this work
a	7.34 Å	7.251 Å	7.342 ± .007 Å
b	18.19	18.161	18.818 ± .010
c	7.28	7.267	7.389 ± .004
α	93° 51′	93° 59′ 35″	91.45 ± .04°
β	101° 30′	102° 17′ 16″	102.15 ± .11°
γ	99° 23′	97° 57′ 46″	98.85 ± .09°

Intensities were measured with an automated two-circle diffractometer on a square tabular crystal of dimensions 0.3 × 0.3 × 0.07 mm, rotated about the a axis. The reflected Zr-filtered Mo$K\alpha$ radiation was detected by a scintillation counter. Within the hemisphere out to $(\sin\theta)/\lambda = 0.55$ Å^{-1}, 2902 reflections were measured, of which 184 had intensities below the detectable limit and were assigned intensities of one-third the value of the weakest measurable reflection. The intensities were corrected for Lorentz, polarization, and absorption effects.

Structure determination and refinement

A three-dimensional Patterson synthesis was used to determine approximate positions of the two iron and three sulfur atoms. Through a subsequent structure-factor calculation yielding an R value of 46%, correct signs could be found for about two-thirds of the observed F's. They were used to compute a three-dimensional Fourier synthesis, which revealed the positions of all atoms except hydrogen. In the subsequent structure-factor calculation the R value dropped to 20%. A full-matrix, least-squares refinement with isotropic temperature

Table 2. *Atom parameters of copiapite*

Atom	x	y	z
Mg	0	0	0
Fe(1)	0.6861 (2)	0.3326 (1)	0.4944 (2)
Fe(2)	.6833 (2)	.6800 (1)	.8980 (2)
S(1)	.9461 (4)	.7338 (1)	.3113 (3)
S(2)	.7221 (4)	.4200 (1)	.1318 (3)
S(3)	.5945 (4)	.2057 (1)	.1675 (3)
O(1)	.774 (1)	.6993 (4)	.172 (1)
O(2)	.881 (1)	.7607 (4)	.469 (1)
O(3)	.944 (1)	.3248 (4)	.631 (1)
O(4)	.943 (1)	.2103 (4)	.771 (1)
O(5)	.551 (1)	.3702 (4)	.037 (1)
O(6)	.671 (1)	.4905 (4)	.166 (1)
O(7)	.807 (1)	.3917 (4)	.311 (1)
O(8)	.857 (1)	.4254 (4)	.011 (1)
O(9)	.580 (1)	.1272 (4)	.178 (1)
O(10)	.597 (1)	.7757 (4)	.893 (1)
O(11)	.712 (1)	.2317 (4)	.038 (1)
O(12)	.682 (1)	.2406 (4)	.357 (1)
O(13)	.567 (1)	.6562 (4)	.635 (1)
O(14)	.572 (1)	.2788 (4)	.694 (1)
O(15)	.706 (1)	.4262 (4)	.647 (1)
O(16)	.758 (1)	.9491 (5)	.076 (1)
O(17)	.778 (1)	.5834 (4)	.919 (1)
O(18)	.854 (1)	.9923 (5)	.728 (1)
O(19)	.919 (1)	.7206 (4)	.818 (1)
O(20)	.912 (1)	.0976 (5)	.035 (1)
O(21)	.725 (1)	.8934 (5)	.418 (1)
O(22)	.768 (1)	.5601 (4)	.509 (1)
O(23)	.657 (1)	.1007 (5)	.570 (1)

factors brought the R value down to 11%. Finally, anisotropic thermal parameters were varied in the least-squares refinement. This led to a final R value of 0.096 for all data. Table 2 lists the refined atom parameters and their standard deviations. Mg occupies the special position in the cell origin; all other atoms are in general positions. The thermal parameters and their standard deviations are given in Table 3. Table 4 lists the corresponding root-mean-square amplitudes along principal axes. The temperature factor is defined as $\exp\left[-\frac{1}{4}\left(B_{11}a^{*2}h^2 + B_{22}b^{*2}k^2 + B_{33}c^{*2}l^2 + 2B_{23}b^*c^*kl + 2B_{13}a^*c^*hl + 2B_{12}a^*b^*hk\right)\right]$. The equivalent isotropic temperature coefficients B_{iso} were computed from

Table 3. *Thermal parameters of atoms in copiapite*

Atom	B_{11}	B_{22}	B_{33}	B_{23}	B_{13}	B_{12}	B_{iso}
Mg	1.70(26) Å^2	2.19(22) Å^2	2.07(21) Å^2	0.34(17) Å^2	0.35(18) Å^2	0.52(18) Å^2	1.95 Å^2
Fe(1)	0.83(07)	1.47(06)	0.71(05)	0.22(04)	0.02(04)	0.21(05)	0.95
Fe(2)	0.48(07)	1.47(06)	1.00(05)	0.24(04)	− 0.04(05)	0.18(05)	0.89
S(1)	0.89(12)	1.77(10)	0.93(09)	0.31(07)	0.13(08)	0.15(08)	1.13
S(2)	0.87(12)	1.57(10)	0.97(09)	0.32(07)	0.11(08)	0.11(08)	1.09
S(3)	0.77(12)	1.52(10)	1.20(09)	0.16(07)	0.09(08)	0.24(08)	1.12
O(1)	0.71(36)	2.81(36)	2.41(34)	0.27(27)	0.07(26)	0.01(27)	1.72
O(2)	2.87(42)	2.11(32)	1.18(28)	0.30(24)	0.72(27)	0.72(28)	1.81
O(3)	1.51(38)	1.56(31)	2.96(36)	0.54(26)	0.42(28)	0.64(26)	1.79
O(4)	1.76(40)	2.59(34)	1.76(31)	0.61(25)	0.58(27)	− 0.35(28)	1.87
O(5)	0.39(34)	2.65(34)	1.04(27)	0.24(24)	− 0.37(23)	− 0.04(26)	0.90
O(6)	3.15(44)	1.06(30)	1.88(32)	0.06(24)	0.32(29)	0.44(28)	1.84
O(7)	1.26(37)	1.88(31)	1.06(28)	0.25(23)	0.02(25)	0.22(26)	1.37
O(8)	1.18(37)	3.06(36)	1.32(30)	1.06(26)	0.72(25)	0.15(28)	1.30
O(9)	1.57(39)	1.17(29)	2.69(35)	0.05(25)	0.13(28)	0.30(26)	1.72
O(10)	0.71(34)	1.95(30)	0.88(26)	0.01(22)	− 0.07(23)	0.08(24)	1.09
O(11)	1.02(37)	2.61(35)	1.45(30)	0.26(25)	0.38(26)	0.29(27)	1.54
O(12)	1.75(39)	2.06(33)	1.15(28)	0.21(24)	0.14(26)	0.75(27)	1.55
O(13)	1.41(37)	2.00(31)	1.18(28)	0.31(23)	0.51(25)	− 0.20(26)	1.41
O(14)	2.11(40)	2.30(33)	1.30(30)	− 0.03(25)	0.76(27)	0.19(28)	1.74
O(15)	2.05(39)	2.22(33)	1.51(30)	0.41(25)	0.28(26)	0.52(27)	1.87
O(16)	2.02(43)	3.35(41)	2.87(38)	− 0.07(31)	0.59(31)	− 0.31(32)	2.69
O(17)	1.22(37)	1.84(31)	2.52(34)	0.76(26)	0.44(27)	0.60(26)	1.64
O(18)	4.49(55)	3.30(43)	2.88(40)	0.41(33)	0.30(37)	1.31(38)	3.42
O(19)	1.30(38)	2.62(35)	2.35(34)	0.63(27)	0.75(27)	− 0.11(27)	1.85
O(20)	4.37(54)	2.07(36)	3.62(43)	0.25(31)	1.35(38)	0.96(34)	3.04
O(21)	3.43(49)	2.70(38)	3.09(40)	0.11(31)	0.51(35)	0.36(33)	3.10
O(22)	3.16(45)	1.91(33)	2.04(33)	0.35(26)	0.95(30)	0.35(29)	2.22
O(23)	3.70(52)	2.78(39)	3.37(42)	1.25(32)	0.51(36)	0.53(34)	3.11

Table 4. *Parameters for the ellipsoids of vibration*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	b*	c*
Mg	.14 Å	29.4°	107.4°	67.9°
	.16	66.1	61.1	133.8
	.17	74.0	34.7	51.9
Fe(1)	.11	37.7	78.0	114.7
	.14	86.6	13.3	76.2
	.09	52.5	95.7	28.8
Fe(2)	.14	91.9	156.3	113.9
	.12	72.9	66.3	142.4
	.07	17.2	89.1	62.8
S(1)	.11	41.4	72.2	116.9
	.15	90.7	18.5	73.5
	.10	48.6	94.8	32.3
S(2)	.15	86.2	154.6	111.7
	.11	48.0	65.1	120.2
	.10	42.3	94.6	38.6
S(3)	.14	97.2	166.3	106.2
	.13	77.3	76.3	151.5
	.10	14.6	90.6	67.2
O(1)	.20	86.7	152.4	114.6
	.18	88.8	65.5	150.7
	.09	3.5	78.1	75.0
O(2)	.11	87.6	85.5	164.0
	.16	105.4	25.0	88.6
	.19	15.6	65.5	74.1
O(3)	.20	96.6	104.8	166.3
	.11	129.3	49.3	103.3
	.15	40.1	44.4	93.0
O(4)	.20	70.0	145.8	103.3
	.12	53.3	57.6	120.7
	.16	43.6	80.1	34.0

Table 4. *(Continued)*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	**b***	**c***
O(5)	.13 Å	67.0°	74.5°	141.8°
	.19	94.5	17.7	78.9
	.05	23.5	81.6	54.0
O(6)	.20	16.4	82.9	93.8
	.11	87.7	7.2	87.2
	.15	73.8	88.8	4.7
O(7)	.14	37.4	69.2	111.8
	.16	94.7	21.3	74.1
	.11	53.0	94.1	27.5
O(8)	.21	93.3	158.0	112.9
	.07	58.2	68.8	113.5
	.14	32.0	95.5	50.2
O(9)	.19	80.6	87.8	158.0
	.12	96.6	16.0	90.4
	.14	11.5	74.2	68.0
O(10)	.12	60.4	85.6	137.9
	.16	91.3	10.7	89.9
	.09	29.6	80.2	47.9
O(11)	.11	19.4	83.8	96.7
	.18	85.2	7.3	82.0
	.13	71.3	93.8	10.5
O(12)	.14	57.0	119.8	118.2
	.12	120.9	76.6	151.7
	.17	48.5	33.3	88.0
O(13)	.17	67.5	147.3	93.6
	.10	58.7	66.1	130.6
	.14	40.2	69.0	40.8
O(14)	.11	74.7	93.5	151.7
	.18	121.1	43.2	108.6
	.16	35.5	47.0	69.5

Table 4. *(Continued)*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	b*	c*
O(15)	.16	34.2	101.3	105.7
	.13	108.7	71.1	155.0
	.17	62.4	22.2	71.1
O(16)	.19	93.2	101.6	166.6
	.22	109.9	30.9	102.2
	.15	20.2	61.8	84.4
O(17)	.11	34.0	113.8	73.6
	.14	58.8	41.8	113.0
	.19	77.8	58.0	28.8
O(18)	.25	24.7	66.1	96.6
	.18	114.6	57.2	136.5
	.20	88.4	42.6	47.2
O(19)	.11	32.5	65.6	104.9
	.17	122.4	71.9	146.1
	.20	91.3	31.2	60.3
O(20)	.20	71.3	80.5	147.7
	.15	96.6	16.6	85.5
	.24	19.9	76.5	58.1
O(21)	.21	31.4	93.5	106.7
	.20	115.0	78.8	158.5
	.18	72.3	11.8	76.9
O(22)	.16	87.9	140.5	127.7
	.14	78.3	50.7	133.6
	.20	11.9	86.3	67.2
O(23)	.24	68.1	118.6	131.6
	.15	93.9	39.9	126.3
	.21	22.3	64.8	62.7

hypothetical spheres of vibration having the same volume as the corresponding ellipsoids. The observed and calculated structure factors are compiled in Table 5.

Table 5. *Observed and calculated structure factors of copiapite*

h	k	l	F_o	F_c
0	0	0		566.0
	1			-86.5
	2			-116.0
	3		116.0	100.2
	4		29.3	17.5
	5		24.3	-14.3
	6		42.1	-34.9
	7		21.4	12.5
	8		33.7	-32.2
	9		124.7	117.4
	10		51.5	35.6
	11		66.6	-59.8
	12		67.3	62.8
	13		44.5	-38.2
	14			0.6
	15		30.8	28.4
	16		12.7	3.9
	17		31.2	-30.3
	18		26.3	26.6
	19		35.5	35.2
1	0	0		-30.3
	1			62.1
	2			6.9
	3		49.9	53.9
	4		16.4	-17.6
	5		5.5	1.8
	6		12.2	- 8.0
	7		22.0	23.3
	8		12.7	-12.1
	9		35.6	-37.4
	10		23.9	22.3
	11		24.4	24.3
	12		29.5	26.6
	13		16.4	16.0
	14		28.7	-27.8
	15		31.6	36.5
	16		2.8	1.0
	17		8.7	0.0
	18		2.8	2.5
	19		9.3	13.3
	20		5.1	-14.9
	21		2.7	2.9
	-1			- 3.2
	-2			46.3
	-3		27.5	-26.4
	-4		148.1	137.5
	-5		34.6	22.6
	-6		87.9	-82.2
	-7		111.0	100.7
	-8		56.3	53.9
	-9		33.0	-28.8
	-10		15.3	-14.2
	-11		58.5	57.7
	-12		11.1	4.5
	-13		7.6	- 3.0
	-14		32.7	32.0
	-15		34.0	-31.8
	-16		6.8	6.0
	-17		14.6	9.7
	-18		2.8	3.4
	-19		2.8	0.2
	-20		27.8	28.7
	-21		5.2	- 8.3
	-22		5.6	- 7.7
2	0	0		-89.3
	1			7.0
	2			-61.1
	3			8.3
	4		58.1	58.5
	5		37.5	-34.3
	6		20.2	19.6
	7		9.3	9.3
	8		59.3	55.7
	9		67.3	-66.2
	10		13.4	10.4
	11		75.8	74.0
	12		75.5	-75.6
	13		13.4	12.9
	14		57.4	54.6
	15		2.8	0.1
	16		14.7	-13.7
	17		5.7	- 4.8
	18		6.8	- 0.3
	19		3.9	- 6.8
	20		18.4	19.7
	21		22.2	-25.7
	-1			140.4
	-2			-44.2
	-3			-63.4
	-4		30.9	28.3
	-5		62.9	55.9
	-6		13.0	10.3
	-8		94.9	86.2
	-9		10.8	-10.0
	-10		18.1	-14.5
	-11		75.7	74.8
	-12		23.9	-21.4
	-13		9.6	- 7.7
	-14		9.2	- 6.7
	-15		48.0	49.2
2	-16	0	10.5	- 6.2
	-17		1.7	- 4.8
	-18		5.3	5.5
	-19		2.8	3.2
	-20		2.5	4.5
	-21		9.5	-10.0
	-22		12.5	10.9
3	0	0		104.2
	1		7.0	- 6.5
	2		17.5	-14.9
	3		75.3	75.1
	4		23.2	21.7
	5		84.3	-79.9
	6		40.4	40.7
	7		12.4	8.8
	8		51.1	-48.5
	9		31.9	26.8
	10		11.8	11.2
	11		13.4	8.1
	12		42.3	41.8
	13		37.5	-35.9
	14		14.6	-16.2
	15		4.5	6.0
	16		14.8	11.5
	17		21.3	-20.1
	18		10.3	1.1
	-1			-32.6
	-2			-105.5
	-3		6.2	- 4.7
	-4		5.2	0.6
	-5		36.7	-34.8
	-6		61.7	60.7
	-7		62.0	-59.0
	-8		14.4	-13.1
	-9		112.7	110.6
	-11		99.0	-99.7
	-12		59.3	56.2
	-13		22.2	16.8
	-14		37.3	-35.9
	-15		47.2	43.6
	-16		2.9	- 6.2
	-17		36.6	-35.6
	-18		37.3	36.0
	-19		35.9	32.6
	-20		29.4	-30.3
	-21		2.7	- 0.0
4	0	0	12.9	5.0
	1		22.9	-22.2
	2		24.7	19.2
	3		52.2	54.1
	4		33.0	-31.9
	5		7.7	9.4
	6		6.0	7.8
	7		46.0	47.9
	8		46.8	-51.1
	9		13.0	-16.4
	10		33.4	35.6
	11		40.2	-40.6
	12		10.5	8.8
	13		12.7	12.2
	14			- 0.0
	15		15.5	18.4
	-1			-18.8
	-2			46.4
	-3		5.1	-12.3
	-4		2.0	4.0
	-5		6.6	4.7
	-6		38.4	-38.2
	-7		18.2	16.4
	-8		37.2	35.2
	-9		11.9	- 9.3
	-10		58.7	-59.9
	-11		42.1	46.0
	-12		21.3	14.3
	-13		33.4	-34.1
	-14		7.7	5.4
	-15		36.2	-37.5
	-16		35.5	38.3
	-17		26.5	25.4
	-18		25.4	-24.6
	-19		2.7	3.5
5	0	0	43.2	-45.0
	1		31.4	30.4
	2		21.4	20.2
	3		41.8	-42.7
	4		6.3	1.0
	5		26.3	27.2
	6		2.8	- 0.6
	7		2.0	5.3
	8		18.1	16.2
	9		41.1	-43.0
	10		34.5	34.2
	11		40.6	43.0
	12		63.6	-68.2
	13		2.7	1.8
	14		34.4	43.4
	15		2.7	- 0.3
	-1		33.0	41.0
	-2		12.4	19.0
	-3			-39.5
5	-4	0	19.0	25.8
	-5		70.8	72.8
	-6		30.8	-32.3
	-7		13.1	- 9.4
	-8		34.2	33.8
	-9		21.2	-21.4
	-10		3.6	0.3
	-11		17.9	19.0
	-12		38.5	-40.4
	-13		14.7	13.4
	-14		19.6	18.6
	-15		10.7	11.1
	-16		4.9	- 5.2
	-17		6.7	- 5.7
	-18		2.7	- 4.6
	-19		2.7	- 4.8
6	0	0	8.8	-10.9
	1		34.6	-36.0
	2		40.0	43.2
	3		28.3	26.5
	4		4.1	- 2.0
	5		49.1	-49.0
	6		55.7	56.9
	7		13.3	14.7
	8		26.4	-28.5
	9		15.7	14.6
	10		2.7	- 3.0
	11		15.2	9.7
	12		18.0	17.0
	13		20.3	23.2
	14		16.0	-15.6
	-1		12.0	8.5
	-2		15.2	-14.4
	-3		55.7	52.4
	-4		24.5	-25.8
	-5		10.6	7.3
	-6		43.7	40.0
	-7		26.1	-25.0
	-8		18.0	19.7
	-9		25.9	25.9
	-10		2.8	- 0.2
0	0	1		43.3
	1		34.2	-35.8
	2		65.6	61.1
	3		51.9	-55.8
	4		66.6	66.2
	5		83.9	80.3
	6		57.3	-52.0
	7		3.5	3.0
	8		6.7	6.2
	9		16.2	-13.9
	10		6.8	6.7
	11		41.8	-41.6
	12		8.8	4.9
	13		4.0	10.2
	14		33.5	33.1
	15		27.5	-24.5
	16		18.1	17.8
	17		5.7	- 6.1
	18		24.0	-28.2
	19		28.6	31.3
1	0	1	18.4	18.4
	1		44.6	49.0
	2		102.6	103.6
	3		49.1	-48.9
	4		137.8	-133.1
	5		34.7	43.2
	6		9.6	- 9.6
	7		48.0	-48.0
	8		10.4	- 6.3
	9		9.7	6.5
	10		8.9	5.8
	11		31.1	33.0
	12		30.7	32.3
	13		51.9	-63.8
	14		12.4	7.0
	15		14.8	17.3
	16		18.5	-24.5
	17			41.7
	18		10.1	- 8.0
	19		24.1	-23.4
	20		30.5	33.1
	21		19.6	21.1
	-1		18.0	-26.2
	-2		13.9	-10.5
	-3		14.8	- 6.0
	-4		101.1	100.8
	-5		62.4	-61.8
	-6		75.2	-68.9
	-7			62.2
	-8		56.6	50.1
	-9		47.0	-42.5
	-10		11.1	8.7
	-11		2.9	3.2
	-12		12.4	-14.3
	-13		14.4	13.0
	-14		21.7	19.6
	-15		24.1	-22.5
	-16		0.8	- 4.7
	-17		2.4	- 5.7
1	-18	1	13.9	12.5
	-19		2.8	1.1
	-20		7.4	2.6
	-21		3.6	4.2
	-22		2.2	5.6
2	0	1	5.8	- 6.1
	1		74.7	83.8
	2		63.0	-70.4
	3		1.4	6.3
	4		10.2	- 8.7
	5		7.0	- 7.9
	6		23.9	-25.9
	7		7.2	7.6
	8		4.8	1.7
	9		4.6	- 0.1
	10		26.1	27.8
	11		12.2	- 7.3
	12		6.3	- 6.7
	13		61.3	70.6
	14		26.2	-24.1
	15		9.9	-14.2
	16		12.8	17.9
	17		14.7	-14.1
	18		3.9	1.4
	19		5.5	9.9
	20		2.7	2.5
	-1		78.5	-88.4
	-2		52.0	62.0
	-3		56.5	64.3
	-4		79.8	-80.8
	-5		57.3	-58.3
	-6		26.9	26.6
	-7		12.2	-10.5
	-8		40.4	37.8
	-9		42.5	40.4
	-10		73.0	-72.6
	-11		99.1	100.2
	-12		29.3	22.9
	-13		61.5	-60.3
	-14		18.9	-19.0
	-15		20.8	19.7
	-16		29.9	-30.5
	-17		10.3	- 7.6
	-18		55.8	56.0
	-19		39.3	-39.1
	-20		2.7	1.9
	-21		37.1	36.2
	-22		17.9	-20.7
3	0	1	32.0	-33.7
	1		46.7	43.9
	2		6.4	- 6.7
	3		13.1	-11.3
	4		50.5	48.8
	5		2.9	0.3
	6		35.5	35.0
	7		5.9	- 2.5
	8		12.9	11.3
	9		14.3	11.6
	10		3.1	2.6
	11		2.8	- 4.3
	12		2.8	4.4
	13		14.1	17.3
	14		17.8	-20.1
	15		8.8	6.7
	16		50.0	48.6
	17		25.2	-25.3
	-1		6.1	- 4.1
	-2		9.6	8.4
	-3		60.5	-71.3
	-4		21.6	21.4
	-5		45.3	41.8
	-6		18.3	-18.7
	-7		22.2	20.8
	-8		5.3	6.6
	-9		19.3	-15.8
	-10		32.6	33.1
	-11		6.4	- 6.8
	-12		44.4	-42.3
	-13		24.6	22.5
	-14		19.6	18.5
	-15		14.2	12.4
	-16		8.7	9.1
	-17		15.2	-10.2
	-18		15.5	-14.5
	-19		22.6	26.8
	-20		2.7	1.2
4	0	1	5.1	- 4.8
	1		19.0	-20.2
	2		95.0	90.3
	3			- 7.1
	4		13.9	- 8.3
	5		70.8	71.9
	6		22.5	-21.3
	7		30.3	-30.0
	8		67.2	70.3
	9		16.2	-16.8
	10		59.2	-62.1
	11		48.2	50.2
	12		37.7	41.2
	13		38.4	-42.7
4	14	1	16.4	15.8
	15		10.2	8.0
	-1		25.3	32.0
	-2		49.2	-50.5
	-3		36.2	33.3
	-4			87.3
	-5		42.2	-53.1
	-6		45.0	-44.2
	-7		69.8	72.0
	-8		18.3	20.2
	-9		41.2	-40.7
	-10		14.6	14.9
	-11		23.9	-24.9
	-12		35.5	34.3
	-13		19.4	19.4
	-14		2.8	4.0
	-15		28.8	-33.2
	-16		8.0	11.5
	-17		32.0	35.9
	-18		13.0	-13.7
5	0	1	35.7	34.0
	1		59.5	54.9
	2		50.9	-50.8
	3		10.8	13.0
	4		51.4	49.4
	5		10.0	-11.9
	6		26.6	-27.6
	7		13.3	16.6
	8		2.8	1.9
	9		7.6	10.7
	10		7.7	8.1
	11		13.1	-16.5
	12		2.4	5.7
	13		9.1	14.1
	14		2.7	2.2
	-1		12.4	-11.0
	-2		26.3	28.4
	-3		17.8	17.2
	-4		45.1	-42.5
	-5		27.8	26.7
	-6		40.7	37.9
	-7		11.4	-10.9
	-8		23.5	22.5
	-9		26.3	27.9
	-10		21.2	-20.5
	-11		29.6	30.1
	-12		12.6	10.9
	-13		43.1	-44.2
	-14		6.3	- 3.9
	-15		35.8	39.7
	-16		9.3	0.3
	-17		6.2	- 2.5
	-18		17.5	17.9
6	0	1	2.8	- 2.1
	1		2.8	- 2.4
	2		2.2	0.9
	3		13.0	13.7
	4		18.7	17.2
	5		40.5	-40.6
	6		19.4	20.2
	7		39.4	40.8
	8		13.8	-15.9
	9		16.1	-19.0
	10		11.3	12.6
	11		8.5	14.9
	12		6.7	9.7
	13		2.9	4.1
	-1		2.8	- 0.8
	-2		16.6	-17.3
	-3		32.5	35.1
	-4		22.2	23.2
	-5		5.9	- 6.4
	-6		20.5	20.1
	-7		6.8	3.0
	-8		22.9	22.8
	-9		6.7	-11.1
0	1	-1	40.6	44.5
	2		10.0	- 4.4
	3		13.6	13.4
	4		21.2	-25.8
	5		24.1	25.2
	6		19.3	19.5
	7		25.3	25.6
	8		46.2	-45.5
	9		33.2	-32.8
	10		106.9	103.4
	12		53.5	-56.8
	13		31.4	32.5
	14		28.1	26.6
	15		11.6	-10.7
	16		17.5	19.0
	17		24.3	26.8
	18		24.3	-26.5
	19		31.8	37.2
	20		13.1	- 7.6
	21		10.8	-15.8
	22		23.2	26.1
1	0	-1		-43.3
	1		99.7	-95.0
	2		104.5	96.2

Table 5. *(Continued)*

h	k	l	F_o	F_c
1	3	-1	131.9	127.0
	4			-117.8
	5		37.4	33.3
	6		15.4	18.5
	7		47.9	-46.8
	8		25.2	22.7
	9		59.1	56.4
	10		56.6	-57.2
	11		48.0	48.9
	12		76.9	78.3
	13		35.1	-34.8
	14		31.6	35.5
	15		28.3	32.9
	16		60.1	-61.8
	17		20.1	16.6
	18		41.3	43.0
	19		23.1	-19.9
	20		7.2	- 8.1
	21		24.6	28.3
	-1			150.0
	-2		15.2	- 9.1
	-3		3.8	- 1.5
	-4		73.2	68.6
	-5		104.1	-99.5
	-6		64.2	61.5
	-7		135.7	122.9
	-8		95.6	-90.1
	-9		25.8	25.0
	-10		66.9	63.1
	-11		13.1	11.3
	-12		7.4	- 8.9
	-13		37.2	37.3
	-14		40.6	-41.0
	-15		19.9	-19.8
	-16		36.5	34.9
	-17		11.4	- 6.1
	-18		8.4	- 7.9
	-19		15.0	11.6
	-20		4.1	6.5
	-21		7.3	0.1
	-22		7.5	7.9
2	0	-1		16.0
	1		87.1	69.1
	2		50.2	60.8
	3		49.5	-49.5
	4		48.9	45.1
	5		34.0	29.9
	6		2.5	4.2
	7		8.8	- 8.7
	8		5.2	- 5.8
	9		41.7	39.1
	10		49.4	49.2
	11		12.2	14.6
	12		22.4	-18.4
	13		10.1	4.8
	14		43.4	42.9
	15		8.3	- 2.7
	16		6.1	- 1.3
	17		15.9	-17.2
	18		16.0	17.4
	19		14.0	-10.1
	20		4.9	0.7
	21		13.6	15.9
	-1			27.6
	-2			7.3
	-3		81.9	-66.7
	-4		61.7	-61.0
	-5		59.7	61.5
	-6		66.5	59.3
	-7			-51.8
	-8		99.9	93.7
	-9		62.1	60.4
	-10		19.6	-13.4
	-11			53.8
	-12		29.4	-25.4
	-13		19.2	-16.0
	-14		4.1	8.3
	-15		30.2	28.2
	-16		2.8	0.3
	-17		18.2	16.5
	-18		10.7	10.2
	-19		20.8	-21.2
	-20		35.6	35.6
	-21		8.2	8.3
	-22		31.4	-32.9
3	0	-1		15.5
	1		52.2	49.2
	2		30.1	-25.5
	3		6.8	4.4
	4		98.0	90.4
	5		16.2	-14.4
	6		17.7	17.6
	7		56.2	54.4
	8		31.4	-26.5
	9		21.4	-17.6
	10		48.7	46.6
	11		26.5	-23.3
	12		31.0	-29.3
	13		50.6	46.9
	14		6.0	- 1.6
3	15	-1	36.3	-35.9
	16		14.1	11.4
	17		32.5	31.9
	18		13.6	-12.5
	-1			-54.5
	-2			23.9
	-3			41.1
	-4		10.3	8.4
	-5		35.5	34.4
	-6		4.0	4.7
	-7		28.0	-28.3
	-8		25.0	26.2
	-9		8.5	- 0.4
	-10		9.8	6.8
	-11		13.3	- 9.9
	-12		30.0	26.5
	-13		28.8	26.2
	-14		25.3	24.8
	-15		12.7	-13.1
	-16		2.8	1.5
	-17		17.9	12.8
	-18		16.8	13.8
	-19		10.1	4.9
	-20		2.7	1.4
4	0	-1		21.9
	1		69.2	-66.0
	2		36.2	33.8
	3		53.8	54.1
	4		85.6	-85.4
	5		69.3	72.8
	6		32.9	31.5
	7		78.2	-80.4
	8		30.1	29.1
	9		21.7	21.6
	10		16.5	-17.3
	11		24.3	-23.4
	12		4.7	- 2.9
	13		13.0	14.9
	14		4.6	3.8
	15		24.2	25.7
	16		25.7	-28.6
	-1			89.9
	-2			-52.9
	-3			11.0
	-4		42.0	45.1
	-5		48.3	-49.1
	-6		26.1	26.8
	-7		75.5	76.4
	-8		83.0	-85.1
	-9		6.8	6.1
	-10		69.1	71.9
	-11		37.0	-39.7
	-12		23.3	-21.3
	-13		40.0	42.9
	-14		25.5	-26.4
	-15		16.1	-17.3
	-16		60.8	61.1
	-17		6.2	- 2.1
	-18		24.1	-25.2
	-19		23.3	25.6
5	0	-1		0.5
	1		35.8	35.3
	2		2.9	- 4.9
	3		3.0	3.2
	4		10.7	-11.7
	5		8.7	- 3.0
	6		47.3	45.2
	7		48.0	-46.9
	8		23.6	-26.6
	9		24.4	24.6
	10		2.8	4.3
	11		5.6	5.4
	12		10.3	12.9
	13		5.4	- 7.2
	14		2.7	2.4
	15		4.1	11.9
	-1			-26.5
	-2			-18.9
	-3			-19.1
	-4			26.5
	-5		46.6	46.9
	-6		2.9	- 4.3
	-7		2.2	-23.9
	-8		48.1	48.0
	-9		23.6	17.2
	-10		23.5	-24.2
	-11		16.8	-12.2
	-12		10.8	-13.3
	-13		4.1	2.0
	-14		19.3	21.9
	-15		8.8	17.0
	-16		39.0	-43.2
	-17		22.1	21.7
	-18		23.4	26.9
	-19		24.6	-26.4
6	0	-1	28.2	-27.9
	1		6.2	5.5
	2		2.8	3.3
	3		41.1	-40.3
	4		56.0	54.3
6	5	-1	14.0	-14.3
	6		22.3	-23.2
	7		51.8	51.4
	8		5.3	- 5.6
	9		10.4	9.2
	10		2.1	2.6
	11		14.8	-14.8
	12		2.7	- 2.3
	-1			-16.3
	-2			51.0
	-3			20.3
	-4			8.4
	-5		22.8	24.3
	-6		31.4	32.1
	-7		29.5	-31.7
	-8		6.8	6.5
	-9		7.1	0.8
	-10		6.7	3.8
	-11		3.4	4.8
0	0	2	57.8	49.7
	1		155.3	-149.3
	2		58.5	56.2
	3		32.8	37.0
	4		55.8	-50.9
	5		37.1	-37.5
	6		66.2	63.1
	7		20.8	-20.0
	8		19.7	-21.5
	9		131.7	129.3
	10		79.8	-80.6
	11		31.5	-31.9
	12		43.4	44.3
	13		8.8	- 7.1
	14		3.0	- 5.1
	15		22.2	-21.9
	16		6.9	- 5.5
	17		9.8	-12.8
	18		54.9	59.6
1	0	2	2.2	- 4.1
	1		42.5	45.2
	2		92.2	92.0
	3		73.2	-77.2
	4		25.1	23.2
	5		10.0	- 2.5
	6		21.7	-23.9
	7		43.4	43.7
	8		39.0	-42.9
	9		21.9	-22.3
	10		36.6	43.1
	11			17.9
	12			-20.5
	13		13.1	-20.5
	14			52.6
	15		16.1	-12.4
	16		10.7	9.5
	17		18.6	21.2
	18		21.8	-23.4
	19		10.2	6.8
	20		17.8	14.2
	-1		12.2	-14.5
	-2		87.9	93.3
	-3		71.2	-75.3
	-4		21.4	-18.7
	-5		76.6	76.5
	-6		42.8	-42.8
	-7		2.1	- 0.7
	-8		27.1	27.0
	-9		9.6	12.4
	-10		13.5	-11.9
	-11		8.5	- 4.8
	-12		6.3	- 7.2
	-13		37.8	-38.6
	-14		65.8	62.0
	-15		39.0	-37.0
	-16		18.0	-11.9
	-17		39.5	37.6
	-18		22.0	-17.7
	-19			-13.8
	-20		22.6	22.7
	-21		16.1	13.7
2	0	2		-91.6
	1		17.0	16.5
	2		22.8	30.5
	3			72.2
	4		27.4	-34.3
	5		14.8	17.2
	6		6.2	- 6.6
	7		5.1	2.8
	8		23.7	27.4
	9			-42.3
	10			39.7
	11		5.1	- 5.4
	12		13.0	15.7
	13			69.3
	14		22.0	-25.1
	15		14.5	-13.2
	16		6.3	5.3
	17		30.6	42.5
	18			-25.6
	19		2.7	- 3.9
2	20	2	14.1	21.2
	-1		22.6	31.1
	-2		36.9	45.8
	-3		11.2	-13.2
	-4		27.7	28.8
	-5		19.6	-19.6
	-6		84.0	90.4
	-7		2.9	- 1.2
	-8		19.0	-18.6
	-9		50.3	53.2
	-10		15.1	-13.8
	-11		12.7	-11.7
	-12		5.3	- 5.5
	-13		58.6	62.7
	-14		21.9	-16.6
	-15		54.7	-52.5
	-16		53.1	49.3
	-17		15.8	-13.1
	-18		13.8	12.6
	-19		7.0	1.2
	-20		21.9	-20.6
	-21		14.3	15.6
	-22		8.9	12.6
3	0	2	42.7	41.8
	1		38.4	-38.4
	2		6.0	- 1.7
	3		94.0	93.5
	4		75.5	-74.1
	5		15.6	- 7.6
	6		97.4	94.7
	7		76.2	-72.0
	8		21.7	21.8
	9		94.3	92.4
	10		22.7	-22.5
	11		19.8	-21.3
	12		42.5	41.0
	13		2.2	1.7
	14		16.3	-18.9
	15		35.1	35.8
	16		16.5	-16.2
	17		16.9	-16.7
	-1		81.6	82.4
	-2		34.6	-33.1
	-3		31.9	29.9
	-4		36.0	-35.7
	-5		62.2	-63.0
	-6		100.6	95.6
	-7		13.6	11.8
	-8		45.8	-43.1
	-9		38.9	38.2
	-10		77.8	77.0
	-11		2.8	3.5
	-12		21.2	-19.2
	-13		34.4	34.5
	-14		51.7	-51.0
	-15		42.1	41.8
	-16		18.5	14.8
	-17		20.1	-16.8
	-18		13.0	11.7
	-19		5.0	3.5
	-20		14.6	10.2
4	0	2	35.8	-31.2
	1		54.6	54.8
	2		83.2	84.9
	3		64.6	-66.8
	4		31.4	27.8
	5		41.8	47.7
	6		17.0	-17.2
	7		17.3	18.5
	8		11.3	-11.5
	9		2.8	1.3
	10		0.1	10.8
	11		6.5	4.6
	12		4.0	5.8
	13		2.7	- 2.1
	-1		50.0	-52.4
	-2		64.6	67.4
	-3		2.9	2.5
	-4		39.1	-41.3
	-5		57.4	60.0
	-6		14.2	-13.1
	-7		6.9	- 3.7
	-8		41.9	42.4
	-9		12.2	-12.6
	-10		16.4	15.6
	-11		2.8	- 3.7
	-12		3.8	4.3
	-13		3.9	- 0.3
	-14		51.6	50.8
	-15		10.1	-10.6
	-16		42.6	-43.2
	-17		57.2	58.7
	-18		9.4	5.6
5	0	2	10.2	- 9.8
	1		14.7	11.7
	2		16.2	-17.2
	3		7.6	7.2
	4		37.0	35.9
	5		12.5	14.9
	6		29.7	-30.5
5	7	2	12.4	14.8
	8		9.5	11.5
	9		10.8	- 6.3
	10		4.5	-10.7
	11		10.0	-17.5
	12		7.4	- 7.8
	13		25.8	29.9
	-1		22.6	-22.1
	-2		70.4	69.1
	-3		2.8	4.2
	-4		38.0	-35.8
	-5		19.9	23.8
	-6		32.2	28.9
	-7		24.9	25.4
	-8		34.1	-35.9
	-9		2.8	- 1.6
	-10		11.3	13.4
	-11		7.5	2.4
	-12		7.2	11.8
	-13		15.5	-15.8
	-14		3.8	4.6
	-15		2.7	1.4
	-16		22.7	25.5
	-17		2.7	2.5
6	0	2	26.1	24.1
	1		9.4	14.8
	2		13.5	-12.2
	3		9.3	8.0
	4		22.1	-22.8
	5		5.6	1.3
	6		42.0	40.8
	7		52.2	-52.6
	8		7.2	- 0.9
	9		31.1	34.8
	10		8.1	- 7.2
	11		2.7	- 2.2
	-1		6.9	7.3
	-2		71.0	-69.7
	-3		59.2	55.2
	-4		29.1	27.9
0	1	-2	114.5	109.2
	2		9.3	3.5
	3		49.6	49.7
	4		91.1	-80.8
	5		7.4	7.6
	6		50.6	-43.5
	7		47.0	-45.3
	8		43.9	-44.0
	9			24.5
	10		26.3	21.4
	11		25.9	-23.8
	12		60.3	58.7
	13		30.8	31.4
	14		53.9	-56.2
	15		10.6	- 7.0
	16		4.8	11.0
	17		16.3	20.2
	18		25.9	-31.1
	19		5.6	12.3
	20		13.2	16.7
	21		2.7	- 2.6
1	0	-2	40.4	-38.5
	1		14.7	17.6
	2		71.6	-67.4
	3		45.4	-38.0
	4		97.1	93.2
	5		49.1	-45.4
	6		24.8	-24.4
	7		17.4	13.1
	8		3.0	4.8
	9		50.7	49.8
	10		7.5	-10.0
	11		66.2	-68.9
	12		35.2	38.5
	13		73.3	75.0
	14		44.2	-43.5
	15		11.1	9.1
	16		26.9	26.9
	17		23.1	-24.2
	18		17.4	16.0
	19		2.7	2.7
	20		8.3	-12.9
	21		7.0	- 7.3
	-1		21.0	25.4
	-2		17.0	18.4
	-3		27.0	26.4
	-4		92.5	-86.6
	-5		19.8	14.3
	-6		22.8	25.6
	-7		2.1	- 1.4
	-8		20.3	19.0
	-9		14.0	-12.3
	-10		24.9	22.9
	-11		40.4	40.5
	-12		20.4	-24.9
	-13		6.8	- 2.3
	-14		17.7	-17.5
	-15		2.0	- 7.8
	-16		2.8	1.4
	-17		20.4	25.9

Table 5. *(Continued)*

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
1	-18	-2	4.6	-13.2	4	15	-2	36.0	42.0	1	5	3	40.3	47.8	3	-10	3	31.6	28.0	1	2	-3	20.5	16.4
	-19		10.0	-14.3		-1		1.7	- 1.5		6		10.6	-13.3		-11		44.9	46.3		3		32.0	29.0
	-20		20.6	17.2		-2		19.1	-16.8		7			- 9.4		-12		46.7	-44.3		4		65.2	-61.5
	-21		7.4	- 0.8		-3		29.6	29.1		8		30.5	34.1		-13		27.4	25.0		5		30.0	28.5
2	0	-2	41.3	-36.3		-4		22.1	21.2		9		17.4	17.5		-14		8.6	4.1		6		27.7	25.4
	1		12.2	13.5		-5			-22.1		10		12.2	13.7		-15		40.9	-38.9		7		44.7	-42.8
	2		126.8	118.3		-6		75.2	74.5		11			7.0		-16		54.1	50.2		8		3.3	- 5.2
	3		116.8	-110.7		-7		23.3	22.0		12			-22.4		-18		32.5	-30.0		9		31.1	31.0
	4		19.6	16.0		-8		12.0	-10.6		13		23.1	-30.0		-19		5.7	0.3		10		10.0	9.2
	5		111.8	102.6		-9		17.4	17.6		14			64.3	4	0	3	9.1	4.7		11		11.1	-10.3
	6		50.6	-49.3		-10		13.6	-14.1		15		17.8	- 1.0		1		6.2	6.9		12		31.2	32.6
	7		16.5	-11.2		-11		49.2	54.7		16			-18.7		2		37.0	40.2		13		19.5	-23.5
	8		112.6	106.7		-12		42.2	-47.5		17		6.5	6.9		3		49.3	-51.3		14		16.3	17.8
	9		36.1	-34.5		-13		19.3	-21.8		18		13.8	16.0		4		13.4	16.9		15		30.2	27.0
	10		31.3	-29.6		-14		29.0	30.4		19		1.8	13.2		5		32.6	34.9		16		6.2	- 4.8
	12		6.0	- 6.3		-15		28.3	26.1		-1		13.1	12.5		6		4.9	- 5.9		17		38.7	-38.5
	13		51.3	-52.8		-16		6.4	3.4		-2		69.8	73.4		7		19.2	-17.4		18		16.4	10.5
	14		46.9	40.4		-17		7.3	- 0.3		-3		3.8	2.7		8		12.7	9.3		19		10.2	12.7
	15		13.1	-11.5		-18		11.2	10.9		-4		14.3	12.2		9		2.8	3.4		20		7.0	-10.1
	16		14.2	14.6	5	1	-2	5.7	6.0		-5		7.6	- 1.2		10		9.2	12.4		-1		15.2	-11.4
	17		20.1	19.2		2		91.3	88.9		-6		6.8	- 4.7		11		22.9	23.2		-2		51.4	-50.8
	18		21.6	-23.0		3		99.3	-95.9		-7		10.2	7.9		12		28.1	-27.9		-3		16.0	16.3
	19		5.4	- 5.6		4		20.8	19.0		-8		2.9	3.0		-1		39.8	39.8		-4		15.2	12.5
	20		30.7	27.6		5			29.5		-9		21.9	18.3		-2		59.7	-59.4		-5		88.6	-87.2
	21		2.7	3.0		6		13.0	- 9.4		-10		4.5	3.5		-3		27.2	-25.1		-6		75.6	72.1
	-1		14.2	-12.2		7		2.8	- 2.6		-11		7.6	8.0		-4		19.5	17.2		-7		60.9	62.3
	-2		4.3	- 0.1		8		36.4	37.3		-12		45.8	45.7		-5		46.1	46.2		-8		66.8	-65.3
	-3		19.0	15.9		9		5.8	-11.0		-13		16.1	-19.5		-6		28.7	-28.1		-9		45.2	47.9
	-4		27.7	-22.1		10		33.8	-33.2		-14		44.7	-43.3		-7		41.9	-45.0		-10		57.8	58.9
	-5		12.6	8.3		11		59.8	65.3		-15		53.5	51.2		-8		57.1	60.3		-11		44.6	-43.1
	-6		10.5	- 9.6		12		9.8	- 8.0		-16		15.2	16.9		-9		5.9	9.4		-12		17.1	18.4
	-7			34.4		13		22.4	-24.6		-17		17.0	-12.7		-10		8.1	- 6.7		-13		19.6	19.6
	-8		17.7	16.0		14		20.9	26.0		-18		3.5	- 5.3		-11		19.2	-20.4		-14		56.8	-62.0
	-9		93.4	-89.4		15		6.1	- 6.4		-19		9.6	8.3		-12		2.8	2.3		-16		28.6	32.2
	-10		99.3	96.1		-1			46.7		-20		13.2	11.9		-13		16.7	15.9		-17		44.6	-48.8
	-11		2.9	1.4		-2		4.1	9.4		-21		10.6	15.1		-14		3.7	- 3.1		-18		3.7	2.6
	-12		50.1	-47.9		-3		3.6	1.4	2	0	3		94.1		-15		22.0	23.7		-19		33.2	36.0
	-13		31.0	30.0		-4		55.2	61.8		1		17.9	24.6		-16		12.9	-13.3		-20		8.6	-11.5
	-14		48.7	47.0		-5		9.1	10.4		2			-64.8	5	0	3		32.9	2	0	-3	25.7	25.8
	-15		10.2	-10.8		-6		63.1	-65.0		3			89.9		1		13.7	-14.2		1		25.7	-27.7
	-16		23.0	-22.7		-7		63.5	65.3		4		5.4	- 8.8		2		16.2	-15.4		2		40.7	39.0
	-17		20.8	22.0		-8		46.1	46.5		5			-82.7		3		54.6	53.0		3		98.1	94.1
	-18		22.0	-19.4		-9		84.5	-88.1		6			38.8		4		3.2	4.6		4		15.1	-12.8
	-19		2.7	4.0		-10		46.8	48.1		7			48.8		5		50.6	-49.9		5		49.7	-47.1
	-20		14.9	13.5		-11		27.5	30.8		8			-54.6		6		18.3	19.5		6		40.2	41.2
	-21		17.6	-14.1		-12		16.7	-14.5		9		5.6	5.6		7		34.8	33.9		7		31.8	26.5
	-22		8.0	8.3		-13		15.1	18.4		10			61.3		8		27.8	-30.7		8		41.4	-40.4
3	0	-2	20.6	19.5		-14		19.9	23.3		11		22.8	-24.0		9		2.7	- 2.8		9		12.4	-12.1
	1		52.3	46.4		-15		17.5	-16.9		12			21.4		10		10.6	13.4		10		31.6	-29.0
	2		55.8	-55.0		-16		7.7	- 4.2		13		8.1	17.4		11		6.8	-15.7		11		41.8	38.0
	3		125.6	120.7		-17		11.1	15.9		14			-33.6		-1		35.8	-35.3		12		60.8	58.3
	4		63.5	61.4		-18		12.5	-15.6		15		13.9	20.0		-2		31.3	31.7		13		56.1	-47.4
	5		3.4	- 0.7		-19		6.3	20.5		16		9.0	16.4		-3		45.6	44.5		14		16.6	-21.1
	6		36.6	-31.4	6	0	-2	46.6	48.5		17		9.2	-10.2		-4		68.2	-65.1		15		35.4	31.6
	7		31.5	29.0		1		53.0	-51.4		18		9.0	9.5		-5		6.2	6.7		16		9.7	3.5
	8		15.5	15.0		2		11.2	-13.3		19		18.1	19.1		-6		40.3	38.7		17		27.2	-25.5
	9		19.6	-18.2		3		5.9	5.6		-2		31.0	41.8		-7		40.9	-38.0		18		9.2	8.2
	10		12.0	- 6.3		4		45.7	'44.8		-3		40.9	50.0		-8		2.8	1.3		19		8.7	2.8
	11		20.2	-20.1		5		8.7	8.8		-4		4.4	- 1.1		-9		23.0	21.0		20		27.1	-25.2
	12		43.4	43.4		6		47.7	-47.0		-5		17.8	-19.7		-10		15.7	- 7.7		-1		97.7	-93.0
	13		33.5	33.6		7		36.1	38.8		-6		63.4	74.5		-11		23.7	-23.3		-2		27.0	-24.9
	14		9.9	-10.4		8		10.1	14.4		-7		33.7	-37.9		-12		50.2	52.7		-3		16.3	14.0
	15		3.9	- 8.0		9		10.1	6.4		-8		7.8	- 8.2		-13		17.3	-17.5		-4		20.1	-16.7
	16		9.9	- 5.2		10		14.3	-15.5		-9		92.1	99.8		-14		29.8	-31.2		-5		16.2	-14.7
	17		18.9	20.9		11		2.7	2.7		-10		53.8	-56.6		-15		21.2	24.1		-6		2.7	- 1.2
	-1		30.5	-35.5		12		8.5	6.4		-11		13.1	10.3		-16		8.7	-12.9		-7		31.2	32.4
	-2		54.8	54.7		-1		5.1	3.8		-12		64.4	68.1	6	0	3		-14.5		-8		33.3	30.5
	-3		17.7	-15.5		-2			-17.7		-14		9.4	12.7		1		3.9	7.9		-9		23.7	-23.0
	-4		4.3	- 5.9		-3			23.6		-15		6.6	6.3		2		7.7	- 8.1		-10		15.5	-12.1
	-5		17.0	-14.4		-4		39.4	-42.2		-16		8.5	- 1.0		3		5.9	2.8		-11		2.9	0.0
	-6		61.5	61.1		-5		22.7	26.2		-17		28.1	-29.2		4		6.6	- 2.9		-12		11.1	8.4
	-7		15.7	16.6		-6		19.2	21.7		-18		21.3	22.0		5		10.6	15.0		-13		23.7	-19.7
	-8		30.9	-30.2		-7		2.9	5.1		-19		12.5	13.7		6		2.8	2.7		-14		30.0	28.4
	-9		47.8	47.1		-8		10.9	-12.2		-20		5.6	0.5		7		5.1	- 1.2		-15		3.1	3.5
	-10		12.3	-12.3		-9		3.2	- 2.9		-21		3.4	10.6		8		8.5	- 9.4		-16		15.5	-13.8
	-11		3.6	- 4.9		-10		8.6	15.0	3	0	3	43.7	-45.1		9			- 1.2		-17		21.5	16.4
	-12		23.8	22.1	0	0	3	34.2	-37.3		1		23.5	-21.9		10		24.1	23.9		-18		8.2	8.6
	-13		18.1	-16.6		1		49.3	-46.9		2		3.0	- 1.5	0	1	-3	96.9	94.8		-19		5.7	4.0
	-14		2.8	0.0		2		101.7	96.8		3		25.7	24.3		2		42.2	-40.9		-20		3.6	8.1
	-15		21.1	19.8		3		55.3	55.6		4		33.5	35.2		3		14.8	-15.1		-21		17.9	-19.7
	-16		10.8	-10.4		4		16.2	16.7		5		3.1	9.7		4		3.9	4.2	3	0	-3	41.3	-41.5
	-17		3.4	1.2		5		32.2	32.5		6		30.1	-28.6		5		34.2	31.7		1		80.1	78.4
	-18		57.1	60.2		6		50.9	-49.0		7		6.5	5.6		6		55.7	-55.4		2		50.3	-48.8
	-19		14.4	-14.3		7		11.1	9.1		8		31.6	31.9		7		46.2	47.1		3		49.4	-46.9
	-20		33.4	-31.5		8		71.3	68.8		9		18.5	-14.8		8		51.9	49.2		4		88.7	88.7
4	0	-2	57.3	60.7		9		18.5	-19.2		10		17.2	-15.3		9		77.0	-73.5		5		2.9	2.9
	1		51.3	54.3		10		51.4	-47.2		11		18.4	18.0		10		19.3	19.1		6		56.2	-55.8
	2		86.4	-87.3		11		69.9	69.8		12		2.8	- 2.9		11		35.5	34.2		7		39.9	37.5
	3		58.4	59.5		12		19.4	19.2		13		26.8	26.1		12		16.5	-13.9		8		33.3	36.9
	4		38.8	36.9		13		2.8	3.5		14		13.6	13.1		13		26.7	25.3		9		27.6	-25.6
	5		26.5	-24.2		14		2.8	3.8		15		11.5	3.2		14		6.3	- 7.1		10		4.4	1.9
	6		26.2	24.2		15		15.4	-18.0		-1		75.3	74.5		15		5.7	- 7.5		11		3.8	- 6.1
	7		20.3	-19.5		16		2.8	- 3.8		-2		7.0	- 4.7		16		9.2	11.9		12		42.5	-42.0
	8		9.4	9.4		17		3.5	6.8		-3		68.3	-68.3		17		19.5	24.3		13		40.6	40.0
	9		17.6	16.3		18		14.9	13.4		-4		41.3	39.9		18		16.5	-20.3		14		10.1	11.1
	10		4.5	9.5	1	0	3	46.7	49.2		-5		23.6	22.4		19		8.7	12.5		15		17.2	-20.0
	11		22.9	-24.1		1		75.3	76.9		-6		23.0	-22.5		20		15.8	18.2		16		2.7	- 1.0
	12		5.1	2.3		2		16.1	-17.1		-7		54.2	55.5		21		23.9	-28.6		17		22.2	23.4
	13		27.3	27.1		3		42.8	-46.2		-8		12.6	11.6	1	0	-3	60.2	59.9		18		9.7	- 8.7
	14		32.6	-34.2		4		26.6	27.7		-9		25.9	-25.1		1		40.6	-38.6		-1		33.8	35.4

Table 5. *(Continued)*

h	k	l	F_o	F_c
3	-2	-3	45.1	40.9
	-3		25.5	-24.3
	-4		3.0	4.3
	-5		20.9	19.3
	-6		49.9	-48.7
	-7		6.3	- 8.1
	-8		34.8	35.8
	-9			- 2.5
	-10		53.1	-53.5
	-11		44.1	45.2
	-12		17.1	14.5
	-13		31.4	-33.3
	-14		1.7	2.1
	-15		11.2	-10.6
	-16		10.0	10.0
	-17		23.3	23.9
	-18		7.8	- 4.6
	-19		13.3	-15.7
4	0	-3	23.8	21.1
	1		6.5	4.1
	2		2.9	- 2.4
	3		24.6	25.1
	4		9.4	- 7.9
	5		23.2	-22.5
	6		50.2	49.9
	7		24.2	-25.3
	8		2.8	0.5
	9		7.6	- 8.0
	10		18.3	18.9
	11		14.7	14.2
	12		11.2	- 8.9
	13		2.3	5.6
	14		3.9	- 5.6
	15		23.1	25.1
	-1		27.2	27.0
	-2		67.8	-68.8
	-3		44.6	46.1
	-4		51.5	54.5
	-5		36.4	-37.8
	-6		40.7	42.5
	-7		2.9	- 2.9
	-8			9.1
	-9		13.8	11.9
	-10		12.7	-12.3
	-11		15.7	-13.4
	-12		2.8	3.9
	-13		28.1	28.5
	-14		33.9	-39.1
	-15		22.3	24.3
	-16		31.5	32.9
	-17		44.9	-50.3
5	0	-3	2.8	4.2
	1		53.0	-53.9
	2		19.4	17.7
	3		54.0	51.1
	4		2.8	- 1.5
	5		21.0	-20.6
	6		32.1	31.7
	7		17.3	18.1
	8		3.3	1.4
	9		10.9	13.0
	10		37.6	-39.8
	11		15.0	14.5
	12		43.6	51.2
	13		22.3	-22.7
	14		2.7	4.9
	-1		5.5	- 6.9
	-2		4.2	- 1.2
	-3		47.7	50.0
	-4		5.2	- 6.6
	-5			- 4.5
	-6		33.0	35.7
	-7		15.7	15.0
	-8		21.3	19.2
	-9		11.9	-13.4
	-10		5.3	3.4
	-11		14.7	-14.3
	-12		33.8	38.2
	-13		11.2	7.3
	-14		20.0	-21.6
	-15		7.0	12.7
	-16		3.8	4.0
	-17		16.9	21.0
	-18		6.7	1.3
6	0	-3	20.3	22.1
	1		7.7	4.8
	2		14.4	-16.5
	3		18.2	-16.3
	4		50.5	52.3
	5		19.3	17.2
	6		64.7	-66.6
	7		63.5	66.4
	8		8.2	8.6
	9		19.5	-17.7
	10		40.0	42.7
	11		7.1	- 3.0
	-1		14.8	11.1
	-2		41.8	40.2
	-3		61.2	-58.9
	-4		20.2	-22.0
6	-5	-3	104.3	105.0
	-6		39.7	-42.9
	-7		20.8	-23.2
	-8		27.4	31.7
	-9		9.7	13.7
0	0	4	23.1	-20.0
	1		12.4	12.7
	2		33.7	30.6
	3			-15.1
	4		9.8	- 3.6
	5		39.2	38.7
	6		2.6	5.9
	7		6.3	5.7
	8		55.7	55.6
	9		23.1	22.1
	10		44.0	-44.1
	11		34.9	32.9
	12		34.1	29.2
	13		21.5	-19.7
	14		37.9	-41.1
	15		25.1	27.8
	16		8.2	13.1
	17		2.7	- 1.3
	18		10.5	12.2
1	0	4	17.1	13.5
	1			75.7
	2		32.2	-38.3
	3		41.8	-48.7
	4		98.3	124.0
	5		8.9	-13.6
	6		42.9	-54.4
	7		24.3	27.4
	8		2.8	- 1.7
	9		5.5	5.8
	10		7.1	- 0.4
	11			- 5.1
	12			-18.3
	13		26.1	42.5
	14		2.8	4.3
	15		16.6	-31.8
	16		5.3	23.5
	17		6.4	-18.0
	18		5.1	- 8.1
	-1		16.7	-15.6
	-2		53.3	56.8
	-3		9.4	11.2
	-4		76.9	-79.6
	-5		89.6	92.8
	-6		28.8	-26.4
	-7		43.5	-44.9
	-8		56.7	55.1
	-9		10.3	-10.1
	-10		8.3	- 8.8
	-11		48.5	46.0
	-12		3.3	6.3
	-13		30.1	-28.2
	-14		15.8	13.2
	-15		23.7	20.9
	-16		35.2	-32.3
	-17		32.1	33.3
	-18		20.0	16.3
	-19		17.4	-18.5
	-20		13.6	8.8
2	0	4		73.2
	1		2.9	- 3.4
	2		9.8	20.3
	3		8.8	-12.6
	4			-28.4
	5			43.1
	6			-37.0
	7		6.4	-20.8
	8		10.6	23.9
	9		24.0	-25.2
	10		13.3	14.0
	11		14.0	14.7
	12		12.5	13.1
	13			-30.3
	14		4.6	3.7
	15			18.0
	16		7.1	7.4
	17		9.6	- 1.4
	-1		17.1	-23.1
	-2			-41.7
	-3		3.9	4.3
	-4			55.4
	-5		39.2	-49.3
	-6		2.9	- 0.7
	-7		71.7	84.1
	-8		48.5	-56.3
	-9		6.7	5.9
	-10		58.1	66.2
	-11		39.7	-45.1
	-12		18.5	-21.9
	-13		3.4	2.0
	-14		21.4	21.1
	-15		2.8	- 4.7
	-16		16.5	20.2
	-17		27.7	-27.4
	-18		8.9	- 5.9
	-19		58.0	54.8
2	-20	4	31.4	-26.6
3	0	4	14.5	-13.2
	1		5.9	- 6.2
	2		26.9	-25.5
	3		57.1	56.2
	4		54.9	-56.3
	5		8.4	1.7
	6		19.7	19.7
	7		25.5	-21.8
	8		42.7	39.0
	9		8.4	- 2.7
	10		31.7	-27.7
	11		20.5	18.8
	12		39.3	40.9
	13		24.9	-29.3
	-1		1.1	0.3
	-2		21.4	21.8
	-3		1.3	1.5
	-4		39.0	37.2
	-5		60.0	-60.9
	-6		7.5	4.5
	-7		39.4	41.0
	-8		22.5	-23.0
	-9			-16.2
	-10		3.1	9.3
	-11		43.3	42.0
	-12		5.0	- 9.0
	-13		6.2	0.4
	-14		6.3	5.2
	-15		14.8	-14.7
	-16		2.7	- 2.0
	-17		8.3	-10.8
4	0	4	7.5	10.7
	1		50.8	49.7
	2		51.6	-49.1
	3		32.6	-31.8
	4		85.1	84.7
	5		18.7	-18.5
	6		19.4	-20.6
	7		26.4	28.7
	8		4.6	- 1.3
	9		2.4	- 5.7
	10		20.0	21.1
	-1		16.8	17.2
	-2		35.3	-34.1
	-3		10.8	-11.8
	-4		9.2	- 1.7
	-5		24.9	27.1
	-6		4.1	- 3.8
	-7		46.9	-46.5
	-8		57.2	54.5
	-9		6.0	2.5
	-10		23.7	-23.5
	-11		46.9	47.4
	-12		22.2	-21.7
	-13		32.9	-32.7
	-14		21.1	19.2
5	0	4	7.9	14.6
	1		4.1	- 7.6
	2		47.2	46.5
	3		6.4	- 6.8
	4		7.5	14.1
	5		2.7	- 3.8
	6		9.1	9.6
	7		10.4	18.7
	8		10.8	-17.0
	-1		11.5	-15.1
	-2		33.8	-33.3
	-3		38.6	39.5
	-4		24.1	23.1
	-5		13.9	-12.1
	-6		28.6	-26.1
	-7		42.0	40.2
	-8		23.4	25.8
	-9		33.5	-35.6
	-10		8.0	11.1
	-11		22.8	-21.6
	-12		13.4	15.0
	-13		22.1	20.5
	-14		12.4	-18.7
6	0	4	32.5	31.8
	1		43.3	-42.6
	2		6.2	9.6
	3		34.6	33.0
	4		31.6	-32.8
	5		19.5	21.1
	6		3.6	4.5
	7		19.0	-16.8
0	1	-4	32.2	32.7
	2		3.0	1.3
	3		42.1	40.3
	4		18.6	18.9
	5		13.1	-12.1
	6		31.6	31.3
	7		21.5	-20.8
	8		6.9	- 2.9
	9		9.2	- 6.7
	10		11.5	11.2
	11		41.8	44.5
	12		30.5	-28.9
0	13	-4	37.3	36.7
	14		49.1	53.3
	15		7.7	- 4.9
	16		24.5	-28.4
	17		4.6	1.3
	18		29.9	35.7
	19		20.0	-30.0
	20		6.5	6.4
1	0	-4	79.6	77.0
	1		34.4	31.9
	2		18.1	-16.0
	3		18.4	-13.6
	4		67.5	68.7
	5		47.5	-48.1
	6		32.8	32.2
	7		62.7	63.7
	8		70.5	-70.8
	9		27.9	27.7
	10		76.8	79.8
	11		21.6	-18.3
	12		15.1	-15.6
	13		16.1	12.5
	14		11.5	8.6
	15		7.6	- 7.2
	16		34.6	35.8
	17		16.5	-18.3
	18		12.5	-11.7
	19		30.4	27.4
	-1		44.8	-44.0
	-2		8.5	- 6.2
	-3		3.3	- 3.0
	-4		28.2	-23.6
	-5		73.0	70.2
	-6		16.0	12.9
	-7		37.6	-38.3
	-8		30.8	30.6
	-9		71.2	69.6
	-10		2.8	1.9
	-11		38.3	-37.9
	-12		36.5	39.5
	-13		13.2	-14.8
	-14		24.1	28.3
	-15		3.0	11.6
	-16		4.3	-12.1
	-17		20.7	19.0
	-18		6.2	-10.7
	-19		8.8	9.3
2	0	-4	37.1	-37.8
	1		71.2	-67.6
	2		100.3	95.6
	3		50.7	51.2
	4		82.5	-82.4
	5		69.4	65.3
	6		3.7	1.3
	7		6.1	3.3
	8		32.0	30.1
	9		15.7	-14.4
	10		13.2	-11.5
	11		4.8	4.2
	12		33.2	30.4
	13		8.8	-11.9
	14		6.0	4.0
	15		20.3	-15.3
	16		21.5	-18.9
	17		54.5	50.7
	18		27.4	-26.1
	19		2.4	- 5.7
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	-2		2.9	2.9
	-3		60.1	-58.2
	-4		81.9	77.2
	-5		7.1	- 6.7
	-6		63.9	-60.5
	-7		48.4	46.0
	-8		4.9	- 4.8
	-9		10.3	- 8.2
	-10		38.6	40.0
	-11		13.0	-10.1
	-12		2.8	- 1.5
	-13		65.2	59.1
	-14		2.8	- 3.3
	-20		5.6	5.9
3	0	-4	37.4	-38.3
	1		31.9	31.0
	2		1.9	3.1
	3		11.5	11.2
	4		16.4	-14.8
	5		40.4	40.3
	6		31.1	30.9
	7		56.7	-57.3
	8		4.6	6.8
	9		1.4	- 0.3
	10		9.5	- 3.7
	11		9.3	- 8.6
	12		12.4	-13.4
	13		8.3	- 5.0
	14		22.4	24.0
	15		32.3	34.3
	16		37.8	-38.5
	17		14.8	11.7
3	-1	-4	48.9	47.4
	-2		16.8	-16.4
	-3		32.6	-28.8
	-4		25.3	24.3
	-5		14.1	13.5
	-6		45.4	47.1
	-7		36.7	-37.0
	-8		15.4	16.4
	-9			25.9
	-10		30.0	-29.6
	-11		11.1	9.0
	-12		26.9	-29.3
	-13		9.6	15.3
	-14		10.3	- 8.9
	-15		24.2	23.5
	-16		3.4	5.8
	-17		5.8	3.8
	-18		18.8	18.2
4	0	-4	30.2	-29.2
	1		23.3	22.2
	2		17.5	17.5
	3		14.2	-15.1
	4		16.2	12.9
	5		43.1	-46.5
	6		44.9	48.9
	7		16.6	13.0
	8		43.8	-43.1
	9		2.1	- 5.4
	10		22.8	20.6
	11		8.8	5.8
	12		13.2	-14.2
	13		37.7	39.5
	14		26.4	-29.2
	-1		50.2	-51.7
	-2		31.8	31.0
	-3		43.2	46.0
	-4		53.7	-57.9
	-5		45.3	47.0
	-6		59.9	61.4
	-7		72.3	-76.7
	-8		29.0	28.9
	-9		34.5	33.3
	-10		20.6	-21.4
	-11		35.1	-37.1
	-12		8.5	13.3
	-13		25.1	23.2
	-14		2.5	- 5.8
	-15		9.3	9.8
	-16		19.2	-21.3
5	0	-4	18.7	-20.0
	1		36.4	-36.4
	2			44.6
	3			- 9.1
	4		24.4	-24.7
	5		14.5	12.5
	6		4.2	0.3
	7		10.8	15.9
	8		8.3	4.0
	9		25.5	25.9
	10		12.5	-14.9
	11		2.7	3.8
	12		9.6	10.2
	13		2.7	- 2.2
	14		10.6	10.9
	-1		22.9	22.0
	-2		30.7	31.9
	-3		13.5	-11.4
	-4		13.6	-11.5
	-5		6.0	- 4.7
	-6		25.7	-28.5
	-7		70.2	74.1
	-8		36.0	-37.3
	-9			-29.3
	-10		59.2	66.1
	-11		14.2	-17.0
	-12		9.6	- 3.2
	-13			14.0
	-14		5.0	- 1.5
	-15		31.3	-36.4
	-16		30.2	33.8
	-17		17.1	22.0
6	0	-4	4.2	0.6
	1		10.2	8.7
	2		25.8	26.9
	3		5.8	- 9.1
	4		36.1	-38.5
	5		66.8	70.2
	6		10.1	10.7
	7		34.5	-36.1
	8		25.1	25.9
	9		7.0	8.7
	10		2.7	- 4.4
	11		6.2	6.2
	-1		6.0	- 6.1
	-2		2.0	- 5.0
	-3		2.8	4.8
	-4		19.7	19.1
	-5		5.8	- 4.0
	-6		8.9	9.2
	-7		11.5	11.9