AM-84-241

American Mineralogist, Volume 69, pages 472–480, 1984

Donpeacorite, $(Mn,Mg)MgSi_2O_6$, a new orthopyroxene and its proposed phase relations in the system $MnSiO_3$–$MgSiO_3$–$FeSiO_3$[1]

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Abstract

A Mn-rich orthopyroxene $Mg_{1.41}Mn_{0.56}Ca_{0.03}Si_2O_6$, occurs in a manganiferous pod in the marble units near Balmat, N. Y. The pyroxene coexists with triodite, tourmaline, ferrian braunite, manganoan dolomite, and hedyphane. Refinement of the crystal structure of the pyroxene (space group *Pbca*) shows that as expected virtually all of the Mn is located in the M2 site and the general formula is therefore $(Mn,Mg)MgSi_2O_6$. Because Mn is completely ordered into the M2 site and comprises over 50 percent of that site, the mineral is a new orthopyroxene. It has been named donpeacorite after Donald R. Peacor in recognition of his work on pyroxenes and manganese minerals. The unit cell parameters are a = 18.384(11), b = 8.878(7), c = 5.226(3), Z = 8, D (meas.) = 3.36(1). Donpeacorite is biaxial negative with $2V_x = 88°$, $Z \| c$, α = 1.677(2), β = 1.684(2), γ = 1.692(2). It is yellow-orange with a vitreous luster and has an approximate hardness of 5–6 with perfect (110) cleavages.

The occurrence of donpeacorite and published data for metamorphic pyroxenes and pyroxenoids permit modeling of a phase diagram for the system $MnSiO_3$–$MgSiO_3$–$FeSiO_3$. The diagram is dominated by extensive fields for solid solutions of orthopyroxene and of pyroxmangite, with a small field inferred for kanoite ($MnMgSi_2O_6$, $C2/c$ clinopyroxene) and a three-phase field for ferroan kanoite, manganoan hypersthene, and magnesian pyroxmangite.

Introduction

Several Mn-bearing minerals have been described from the manganoan pods in the Balmat, New York area including tirodite (Ross et al., 1969), magnesian rhodonite (Peacor et al., 1978), calcian kanoite, braunite, and hollandite (Brown et al., 1979; Gordon et al., 1981). Typically these minerals at Balmat form pink- to buff-colored rocks which contrast strikingly with the enclosing rocks. They may fluoresce a deep red when exposed to ultraviolet light and thus have received attention well beyond their abundance. Spectacular yellow-orange rocks containing an unusual Mn-rich pyroxene were collected on the 2500 level of the Balmat No. 4 Mine and provided for our study by John T. Johnson and William deLorraine of the St. Joe Zinc Company, Balmat, N. Y. X-ray diffraction studies and a structure refinement of the pyroxene indicate that it is orthorhombic and completely ordered with over half of the M2 site occupied by Mn. This orthopyroxene therefore qualifies as a new mineral and has been named donpeacorite after Dr. Donald R. Peacor of the University of Michigan Department of Geological Sciences, in recognition of his work with manganese minerals, as well as with pyroxenes and pyroxenoids. The name donpeacorite applies to the ordered orthopyroxene of endmember composition $MnMgSi_2O_6$. Thus the mineral described herein is $Dp_{56}En_{44}$. Both the mineral and the name donpeacorite has been approved by the I.M.A. Commission on New Minerals and Mineral Names (A. Kato, written connunication, 1982). Type material is preserved at the Smithsonian Institution, Washington D. C.

Mn-rich pyroxenes and pyroxenoids have recently received much attention (Peters et al., 1977; Peacor et al., 1978; Albrecht, 1980; Albrecht and Peters, 1980; Brown et al., 1980; Brown and Huebner, 1981; Gordon et al., 1981). Brown et al. (1980) assembled the then available compositional data and inferred phase equilibria at metamorphic temperatures corresponding to the amphibolite facies for three faces of the $RSiO_3$ tetrahedron (R = Ca–Mg–Fe–Mn). With the recent discovery of the unusually Mn-rich orthopyroxene donpeacorite at Balmat, N. Y. it is now possible to infer the general topology of a phase diagram for the remaining Mn–Mg–Fe face of the $RSiO_3$ tetrahedron. In this paper we describe this mineral and evaluate the pertinent metamorphic phase equilibria.

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0003–004X/84/0506–0472$02.00

TABLE 7 Donpeacorite, $(Mn,Mg)MgSi_2O_6$, A new orthopyroxene and its proposed phase relations in the system $MnSiO_3$-$MgSiO_3$-$FeSiO_3$

OPX

. Petersen, E.U., Anovitz, L.M., Essene, E.J.

H	K	L	F(OBS)		F(CALC)
6	0	0	23.7		24.7
10	0	0	2.7	*	2.2
12	0	0	175.7		181.3
14	0	0	30.9		28.8
16	0	0	119.5		124.2
18	0	0	3.1	*	4.4
20	0	0	124.6		126.9
22	0	0	17.4		18.6
8	1	0	2.6	*	4.4
10	1	0	101.2		105.9
12	1	0	5.1		1.2
14	1	0	82.2		84.9
16	1	0	3.2	*	4.8
18	1	0	20.8		19.4
20	1	0	11.1		11.9
22	1	0	22.4		21.6
4	2	0	161.6		169.1
6	2	0	18.5		17.0
8	2	0	68.0		66.6
10	2	0	25.2		25.8
12	2	0	20.5		19.8
14	2	0	3.1	*	1.9
16	2	0	69.7		72.7
18	2	0	11.7		11.4
20	2	0	16.5		18.3
22	2	0	16.4		15.4
23	2	0	7.8		0.0
2	3	0	13.8		13.9
4	3	0	24.4		22.3
6	3	0	66.2		66.1
8	3	0	7.7		3.8
10	3	0	34.8		37.7
12	3	0	7.1		6.1
14	3	0	27.5		28.4
16	3	0	13.8		12.2
18	3	0	22.5		23.0
20	3	0	3.4	*	4.5
22	3	0	20.4		21.0
0	4	0	35.7		31.8
2	4	0	11.9		11.0
4	4	0	92.6		97.2
6	4	0	7.4		1.0
8	4	0	47.2		48.7
10	4	0	38.5		40.7
12	4	0	39.0		39.1
14	4	0	3.2	*	4.3
16	4	0	73.3		76.6
18	4	0	3.2	*	1.5
20	4	0	46.6		44.8
22	4	0	19.9		19.5
2	5	0	140.6		141.6
4	5	0	5.5		3.8
5	5	0	6.2		0.0
6	5	0	117.9		122.9
8	5	0	15.3		15.4
10	5	0	51.9		55.2
12	5	0	6.1		9.1
14	5	0	170.6		173.6
16	5	0	8.9		7.6
18	5	0	37.0		36.7
20	5	0	28.3		28.0
2	6	0	16.3		15.6
4	6	0	14.9		13.2
6	6	0	16.2		14.2
8	6	0	56.6		57.5
14	6	0	22.2		22.9
18	6	0	3.5	*	5.1
20	6	0	110.4		108.8
2	7	0	34.5		33.4
4	7	0	39.7		41.4
6	7	0	11.2		8.6
8	7	0	3.2	*	5.1
10	7	0	95.5		96.4
12	7	0	8.5		7.7
14	7	0	36.8		36.4
16	7	0	19.3		15.8
18	7	0	27.3		27.5
0	8	0	33.4		36.9
2	8	0	21.8		22.4
4	8	0	48.5		47.8
6	8	0	3.2	*	1.1
8	8	0	7.1		5.7
10	8	0	25.4		22.6
12	8	0	21.4		23.3
14	8	0	3.4	*	3.7
16	8	0	44.6		43.1
2	9	0	26.0		27.2
4	9	0	3.2	*	4.6
6	9	0	9.8		6.9
8	9	0	16.8		18.3
10	9	0	42.7		44.7
12	9	0	3.3	*	2.6
14	9	0	9.7		8.2
0	10	0	56.4		50.7
2	10	0	11.3		11.2
4	10	0	29.3		31.1
6	10	0	3.3	*	1.7
8	10	0	41.3		40.3
10	10	0	3.6	*	2.9
2	11	0	61.0		61.5
4	11	0	19.3		18.6
6	11	0	74.2		75.0
5	1	1	90.6		95.1
6	1	1	66.4		68.5
7	1	1	63.0		65.1
8	1	1	48.1		50.6

G OPX

H	K	L	F(OBS)	F(CALC)
9	1	1	5.2	4.4
10	1	1	28.1	28.0
11	1	1	14.1	12.2
12	1	1	10.4	12.0
13	1	1	35.1	35.0
14	1	1	48.8	50.6
15	1	1	30.8	30.4
16	1	1	32.8	33.5
17	1	1	13.1	12.8
18	1	1	13.3	13.7
19	1	1	10.7	11.3
20	1	1	7.0	1.7
21	1	1	29.2	30.7
22	1	1	3.4 *	5.1
23	1	1	16.8	14.9
3	2	1	104.8	108.4
4	2	1	94.0	95.7
5	2	1	92.1	95.4
6	2	1	15.3	16.2
7	2	1	59.3	57.8
8	2	1	58.6	60.6
9	2	1	9.7	10.0
10	2	1	20.1	20.1
11	2	1	22.9	23.6
12	2	1	39.2	40.3
13	2	1	42.2	42.7
14	2	1	8.1	6.8
15	2	1	30.5	31.5
16	2	1	50.3	51.6
17	2	1	37.6	38.6
18	2	1	36.7	36.4
19	2	1	8.4	5.9
20	2	1	3.3 *	4.3
21	2	1	27.4	23.8
22	2	1	45.0	43.6
23	2	1	52.1	49.2
1	3	1	121.7	125.8
2	3	1	71.4	76.1
3	3	1	21.9	18.2
4	3	1	46.9	43.2
5	3	1	109.7	107.8
6	3	1	125.2	125.8
7	3	1	18.4	17.6
8	3	1	65.5	69.9
9	3	1	111.6	113.6
10	3	1	155.1	159.7
11	3	1	164.5	167.7
12	3	1	123.8	129.5
13	3	1	22.2	22.7
14	3	1	17.5	17.7
15	3	1	11.3	12.8
16	3	1	23.4	21.6
17	3	1	67.9	67.0

MG OPX

H	K	L	F(OBS)	F(CALC)
18	3	1	44.5	44.9
19	3	1	20.4	25.3
20	3	1	14.4	14.4
21	3	1	48.9	49.4
22	3	1	67.2	63.7
0	4	1	14.7	16.0
1	4	1	76.9	80.7
2	4	1	80.1	80.9
3	4	1	19.1	20.5
4	4	1	15.5	16.6
5	4	1	53.2	52.9
6	4	1	20.2	21.0
7	4	1	14.6	16.0
8	4	1	25.6	26.6
9	4	1	18.9	18.2
10	4	1	3.0 *	2.0
11	4	1	5.9	4.9
12	4	1	3.2 *	2.6
13	4	1	7.8	9.2
14	4	1	21.2	20.9
15	4	1	3.2 *	7.2
16	4	1	23.1	23.2
17	4	1	17.9	18.2
18	4	1	24.1	24.1
19	4	1	26.6	27.0
20	4	1	28.2	29.1
21	4	1	26.9	25.1
1	5	1	4.9	0.2
2	5	1	50.5	50.5
3	5	1	29.5	29.2
4	5	1	30.9	33.5
5	5	1	51.9	54.0
6	5	1	34.6	34.5
7	5	1	46.7	46.1
8	5	1	26.3	27.1
9	5	1	29.8	30.1
10	5	1	25.3	26.3
11	5	1	3.1 *	2.2
12	5	1	3.0 *	0.2
13	5	1	18.9	17.3
14	5	1	52.7	52.7
15	5	1	20.3	19.6
16	5	1	16.9	19.0
17	5	1	6.0	8.5
18	5	1	7.9	8.4
19	5	1	3.4 *	4.7
20	5	1	3.4 *	1.7
0	6	1	45.0	48.3
1	6	1	34.3	36.8
2	6	1	10.7	11.3
3	6	1	16.2	18.5
4	6	1	11.9	10.6
5	6	1	15.7	16.4

; OPX

H	K	L	F(OBS)	F(CALC)
6	6	1	6.9	7.9
7	6	1	23.4	24.4
8	6	1	3.2 *	4.1
9	6	1	3.1 *	2.9
10	6	1	8.8	8.5
11	6	1	22.8	24.9
12	6	1	30.7	32.1
13	6	1	3.3 *	5.4
14	6	1	13.2	12.8
15	6	1	7.7	0.2
16	6	1	9.4	12.0
17	6	1	9.1	9.3
18	6	1	3.4 *	2.2
19	6	1	16.4	14.5
1	7	1	3.0 *	2.1
2	7	1	17.5	17.0
3	7	1	22.2	23.5
4	7	1	23.1	23.8
5	7	1	43.6	45.7
6	7	1	37.4	38.5
7	7	1	23.4	24.3
8	7	1	36.3	38.4
9	7	1	42.9	43.2
10	7	1	11.8	11.6
11	7	1	20.1	19.0
12	7	1	28.7	28.4
13	7	1	20.9	20.6
14	7	1	3.3 *	2.0
15	7	1	18.5	18.0
16	7	1	24.4	25.4
17	7	1	3.6 *	3.7
18	7	1	3.6 *	4.6
0	8	1	8.7	7.2
1	8	1	14.7	16.6
2	8	1	62.7	65.9
3	8	1	89.5	97.4
4	8	1	83.5	84.0
5	8	1	54.0	54.1
6	8	1	16.8	18.0
7	8	1	31.4	31.6
8	8	1	79.4	78.7
9	8	1	20.0	18.6
10	8	1	11.3	11.4
11	8	1	14.7	13.9
12	8	1	26.6	26.2
13	8	1	46.3	44.0
14	8	1	3.7 *	1.3
15	8	1	46.1	46.2
16	8	1	37.2	36.7
1	9	1	29.3	28.0
2	9	1	38.5	39.2
3	9	1	9.9	5.3
4	9	1	3.4 *	7.5

MG OPX

H	K	L	F(OBS)	F(CALC)
5	9	1	14.1	12.9
6	9	1	3.4 *	5.3
7	9	1	3.3 *	0.4
8	9	1	36.9	37.2
9	9	1	57.9	59.9
10	9	1	57.4	57.5
11	9	1	61.5	61.1
12	9	1	65.6	65.0
13	9	1	22.9	23.6
14	9	1	9.5	11.5
0	10	1	46.8	47.1
1	10	1	46.0	45.7
2	10	1	22.4	22.5
3	10	1	6.3	4.7
4	10	1	3.4 *	5.1
5	10	1	3.5 *	2.2
6	10	1	16.0	16.0
7	10	1	10.3	10.5
8	10	1	18.9	20.4
9	10	1	12.2	10.0
10	10	1	9.7	11.0
1	11	1	9.3	2.9
2	11	1	3.5 *	1.0
3	11	1	3.6 *	2.9
4	11	1	3.5 *	2.8
5	11	1	21.5	19.4
3	0	2	96.9	104.8
4	0	2	12.1	11.7
5	0	2	168.8	174.3
6	0	2	7.7	4.2
7	0	2	109.4	112.0
8	0	2	2.7 *	2.5
9	0	2	119.0	124.0
10	0	2	16.0	17.3
11	0	2	169.8	176.9
12	0	2	21.6	21.4
13	0	2	17.8	17.8
14	0	2	10.9	13.0
15	0	2	37.6	36.1
16	0	2	3.2 *	5.0
17	0	2	68.1	67.5
18	0	2	39.6	40.6
19	0	2	26.6	26.8
20	0	2	3.4 *	9.3
21	0	2	23.8	24.1
22	0	2	86.2	85.6
2	1	2	13.5	11.5
3	1	2	12.7	15.8
4	1	2	41.0	39.0
5	1	2	67.4	67.8
6	1	2	12.5	13.5
7	1	2	2.7 *	5.6
8	1	2	66.4	70.6

MG OPX

H	K	L	F(OBS)	F(CALC)
9	1	2	34.0	34.6
10	1	2	2.8 *	2.7
11	1	2	74.7	77.3
12	1	2	115.9	120.0
13	1	2	26.0	26.6
14	1	2	3.1 *	3.6
15	1	2	3.1 *	3.6
16	1	2	52.9	52.6
17	1	2	54.4	53.8
18	1	2	10.0	8.0
19	1	2	6.8	5.8
20	1	2	6.2	8.3
21	1	2	13.5	13.4
22	1	2	12.2	12.3
0	2	2	2.6 *	4.0
1	2	2	31.0	31.7
2	2	2	9.1	7.0
3	2	2	70.2	70.2
4	2	2	16.3	15.6
5	2	2	22.7	23.2
6	2	2	60.7	61.9
7	2	2	81.2	83.3
8	2	2	12.6	14.5
9	2	2	61.5	62.7
10	2	2	42.2	44.7
11	2	2	8.8	8.3
12	2	2	12.2	13.0
13	2	2	37.8	37.5
14	2	2	17.5	20.7
15	2	2	47.0	48.2
16	2	2	10.0	6.2
17	2	2	19.0	18.6
18	2	2	48.4	47.8
19	2	2	48.6	46.6
20	2	2	10.9	10.0
21	2	2	22.4	20.5
22	2	2	20.1	21.3
1	3	2	27.8	28.2
2	3	2	2.6 *	1.2
3	3	2	20.2	20.3
4	3	2	33.9	33.2
5	3	2	37.5	38.8
6	3	2	9.0	7.6
7	3	2	21.0	21.5
8	3	2	19.3	21.0
9	3	2	3.0 *	7.1
10	3	2	7.2	3.8
11	3	2	20.7	18.9
12	3	2	3.2 *	1.1
13	3	2	11.8	13.0
14	3	2	3.1 *	0.9
15	3	2	3.1 *	3.8
16	3	2	9.5	5.2

MG OPX

H	K	L	F(OBS)	F(CALC)
17	3	2	18.4	19.2
18	3	2	5.5	2.2
19	3	2	6.0	3.3
20	3	2	8.0	4.1
21	3	2	9.8	8.9
0	4	2	16.2	15.8
1	4	2	49.1	51.1
2	4	2	63.5	66.9
3	4	2	23.8	23.6
4	4	2	5.8	3.1
5	4	2	31.1	28.4
6	4	2	39.7	40.5
7	4	2	55.9	57.8
8	4	2	3.0 *	6.0
9	4	2	3.0 *	2.3
10	4	2	3.0 *	1.2
11	4	2	20.3	19.2
12	4	2	3.2 *	7.2
13	4	2	21.1	20.8
14	4	2	21.6	23.6
15	4	2	19.2	18.3
16	4	2	7.3	7.8
17	4	2	3.3 *	7.5
18	4	2	33.9	32.4
19	4	2	18.2	21.8
20	4	2	6.0	4.8
1	5	2	24.4	23.2
2	5	2	15.1	14.4
3	5	2	109.0	112.6
4	5	2	15.9	16.9
5	5	2	55.3	52.8
6	5	2	3.0 *	5.8
7	5	2	30.3	30.5
8	5	2	81.8	85.3
9	5	2	101.3	104.6
10	5	2	3.1 *	1.1
11	5	2	64.2	63.7
12	5	2	89.3	90.4
13	5	2	27.9	25.3
14	5	2	9.3	9.4
15	5	2	28.2	26.6
16	5	2	30.5	30.2
17	5	2	55.2	53.7
18	5	2	13.7	12.0
19	5	2	17.4	17.7
20	5	2	8.7	6.3
0	6	2	7.3	4.8
1	6	2	3.1 *	2.3
2	6	2	131.3	136.2
3	6	2	92.3	94.9
4	6	2	8.6	8.9
5	6	2	72.1	72.2
6	6	2	5.8	2.0

FE OPX

H	K	L	F(OBS)	F(CALC)
7	6	2	54.2	53.6
8	6	2	10.1	9.3
9	6	2	92.7	95.0
10	6	2	31.0	31.2
11	6	2	81.8	80.2
12	6	2	7.4	8.3
13	6	2	6.4	5.3
14	6	2	3.3 *	2.7
15	6	2	21.9	20.9
16	6	2	9.9	9.5
17	6	2	30.2	29.3
18	6	2	16.9	17.9
1	7	2	31.0	31.5
2	7	2	3.2 *	7.9
3	7	2	3.1 *	2.4
4	7	2	16.6	19.2
5	7	2	20.3	19.2
6	7	2	3.1 *	1.1
7	7	2	39.3	41.1
8	7	2	46.2	48.5
9	7	2	7.4	7.5
10	7	2	3.3 *	0.5
11	7	2	9.6	8.5
12	7	2	54.7	52.4
13	7	2	36.7	35.5
14	7	2	3.4 *	2.9
15	7	2	3.4 *	3.1
16	7	2	21.4	21.0
17	7	2	3.6 *	2.0
0	8	2	6.9	3.4
1	8	2	22.7	23.9
2	8	2	3.2 *	2.8
3	8	2	20.2	19.4
4	8	2	6.3	6.7
5	8	2	16.4	16.7
6	8	2	18.3	18.8
7	8	2	26.2	24.6
8	8	2	3.2 *	3.7
9	8	2	16.5	16.3
10	8	2	13.9	10.3
11	8	2	14.9	15.7
12	8	2	3.3 *	0.4
13	8	2	24.4	22.9
14	8	2	12.3	11.8
15	8	2	23.7	22.0
1	9	2	27.8	28.4
2	9	2	11.5	11.3
3	9	2	9.3	5.5
4	9	2	13.2	11.0
5	9	2	13.1	12.9
6	9	2	8.7	5.0
7	9	2	13.1	13.6
8	9	2	14.8	17.8

MG OPX

H	K	L	F(OBS)	F(CALC)
9	9	2	3.3 *	2.9
10	9	2	3.7 *	7.4
11	9	2	3.5 *	4.5
12	9	2	19.4	19.0
0	10	2	3.4 *	5.0
1	10	2	6.5	0.7
2	10	2	41.1	42.3
3	10	2	35.0	32.7
4	10	2	3.4 *	0.1
5	10	2	7.7	4.7
6	10	2	27.1	26.0
7	10	2	21.6	21.7
8	10	2	13.7	12.6
2	1	3	64.0	65.4
3	1	3	65.8	67.1
4	1	3	2.8 *	6.7
5	1	3	33.5	32.3
6	1	3	24.1	24.6
7	1	3	17.6	17.1
8	1	3	2.9 *	9.9
9	1	3	42.5	43.9
10	1	3	55.9	56.4
11	1	3	24.7	24.7
12	1	3	3.0 *	1.7
13	1	3	8.9	7.9
14	1	3	7.5	2.7
15	1	3	19.9	22.7
16	1	3	11.6	11.0
17	1	3	43.0	43.8
18	1	3	29.3	31.9
19	1	3	3.4 *	2.3
20	1	3	3.4 *	1.2
21	1	3	3.4 *	1.7
0	2	3	171.7	179.2
1	2	3	96.3	98.6
2	2	3	2.8 *	6.7
3	2	3	2.8 *	0.2
4	2	3	20.2	21.1
5	2	3	27.0	27.5
6	2	3	15.4	16.0
7	2	3	62.9	62.6
8	2	3	30.8	31.5
9	2	3	17.5	19.6
10	2	3	20.2	21.1
11	2	3	13.6	14.0
12	2	3	42.6	43.8
13	2	3	57.0	60.9
14	2	3	8.6	9.7
15	2	3	47.0	46.5
16	2	3	12.1	12.3
17	2	3	8.1	6.7
18	2	3	12.2	9.0
19	2	3	37.2	39.3

MG OPX

H	K	L	F(OBS)	F(CALC)
20	2	3	57.9	57.9
1	3	3	154.6	158.7
2	3	3	93.4	95.3
3	3	3	22.5	22.1
4	3	3	21.9	22.4
5	3	3	53.9	54.9
6	3	3	102.2	104.3
7	3	3	61.3	62.4
8	3	3	12.2	11.3
9	3	3	6.7	4.5
10	3	3	39.6	43.8
11	3	3	10.2	11.9
12	3	3	24.4	26.2
13	3	3	95.9	95.3
14	3	3	116.4	118.9
15	3	3	55.1	54.8
16	3	3	14.1	14.3
17	3	3	29.0	29.2
18	3	3	40.1	40.1
19	3	3	44.1	47.2
20	3	3	10.9	12.2
0	4	3	95.9	101.4
1	4	3	41.8	44.0
2	4	3	8.6	9.1
3	4	3	46.3	47.4
4	4	3	52.7	54.9
5	4	3	6.1	4.8
6	4	3	8.9	5.5
7	4	3	17.5	16.6
8	4	3	7.9	9.1
9	4	3	38.9	40.1
10	4	3	23.1	24.4
11	4	3	30.4	29.1
12	4	3	13.5	12.7
13	4	3	27.9	28.2
14	4	3	3.4 *	7.8
15	4	3	14.5	13.5
16	4	3	8.1	10.9
17	4	3	10.6	6.6
18	4	3	3.4 *	4.2
19	4	3	3.4 *	4.1
1	5	3	26.6	27.6
2	5	3	56.7	58.6
3	5	3	55.4	56.1
4	5	3	18.4	21.5
5	5	3	19.9	17.5
6	5	3	14.8	16.0
7	5	3	6.4	9.8
8	5	3	3.0 *	4.0
9	5	3	30.8	30.1
10	5	3	33.4	32.9
11	5	3	11.3	13.4
12	5	3	3.3 *	3.5

MG OPX

H	K	L	F(OBS)	F(CALC)
13	5	3	22.1	20.7
14	5	3	25.2	24.2
15	5	3	32.1	29.8
16	5	3	12.9	10.6
17	5	3	29.0	27.6
18	5	3	23.1	23.8
0	6	3	11.5	9.9
1	6	3	12.4	14.9
2	6	3	25.2	24.7
3	6	3	23.1	21.1
4	6	3	21.9	23.8
5	6	3	13.7	11.0
6	6	3	7.6	7.9
7	6	3	3.2 *	1.9
8	6	3	5.6	4.3
9	6	3	5.4	2.4
10	6	3	10.4	10.3
11	6	3	26.7	26.3
12	6	3	15.4	15.4
13	6	3	8.4	5.8
14	6	3	3.4 *	1.9
15	6	3	11.4	9.0
16	6	3	20.3	18.6
17	6	3	14.9	13.5
1	7	3	16.9	16.7
2	7	3	11.8	10.3
3	7	3	21.7	21.2
4	7	3	18.3	19.3
5	7	3	15.6	16.4
6	7	3	25.5	28.2
7	7	3	19.8	18.9
8	7	3	14.8	15.6
9	7	3	17.3	17.8
10	7	3	38.8	37.9
11	7	3	19.9	16.5
12	7	3	3.4 *	8.1
13	7	3	25.1	22.7
14	7	3	33.5	32.1
15	7	3	3.6 *	4.5
0	8	3	109.4	112.3
1	8	3	59.9	60.1
2	8	3	13.6	11.3
3	8	3	22.0	22.7
4	8	3	7.4	0.3
5	8	3	24.5	23.7
6	8	3	3.5 *	7.0
7	8	3	68.5	66.1
8	8	3	48.1	47.5
9	8	3	10.5	7.9
10	8	3	3.4 *	3.3
11	8	3	12.8	12.3
12	8	3	32.8	32.9
13	8	3	48.6	48.4

; OPX

H	K	L	F(OBS)	F(CALC)
1	9	3	66.4	65.1
2	9	3	33.5	33.0
3	9	3	3.5 *	7.3
4	9	3	3.3 *	2.9
5	9	3	7.9	2.3
6	9	3	34.0	32.9
7	9	3	17.5	18.3
8	9	3	3.5 *	2.5
9	9	3	9.2	9.4
10	9	3	39.5	39.7
0	10	3	15.7	14.3
1	10	3	11.1	10.8
2	10	3	6.4	7.5
3	10	3	32.4	30.5
4	10	3	38.0	37.3
3	0	4	58.6	63.1
4	0	4	137.3	140.8
5	0	4	26.8	27.4
6	0	4	14.0	13.6
7	0	4	39.8	44.1
8	0	4	99.6	102.4
9	0	4	34.7	37.9
10	0	4	3.3 *	3.9
11	0	4	89.0	90.2
12	0	4	92.2	90.6
13	0	4	40.2	38.6
14	0	4	6.0	4.1
15	0	4	3.2 *	2.6
16	0	4	74.0	72.8
17	0	4	3.4 *	6.2
18	0	4	22.5	21.2
2	1	4	16.1	15.1
3	1	4	32.5	33.6
4	1	4	5.4	1.7
5	1	4	51.0	52.5
6	1	4	26.4	25.3
7	1	4	45.5	48.7
8	1	4	3.2 *	1.1
9	1	4	27.4	25.2
10	1	4	63.4	64.2
11	1	4	56.8	58.7
12	1	4	6.5	3.9
13	1	4	12.3	13.9
14	1	4	17.6	19.4
15	1	4	24.6	24.4
16	1	4	7.7	6.0
17	1	4	3.4 *	2.7
18	1	4	22.7	20.8
0	2	4	44.8	45.7
1	2	4	31.5	33.3
2	2	4	8.7	0.3
3	2	4	3.1 *	2.2
4	2	4	39.9	39.4

/MG OPX

H	K	L	F(OBS)	F(CALC)
5	2	4	53.7	55.6
6	2	4	7.2	0.8
7	2	4	27.7	27.2
8	2	4	68.0	66.8
9	2	4	13.1	11.7
10	2	4	9.0	10.3
11	2	4	7.7	3.4
12	2	4	31.2	29.3
13	2	4	3.2 *	2.2
14	2	4	13.5	14.7
15	2	4	14.1	16.9
16	2	4	14.4	12.7
17	2	4	6.3	4.9
18	2	4	9.4	7.0
1	3	4	8.4	10.3
2	3	4	9.0	6.9
3	3	4	8.8	9.0
4	3	4	3.1 *	3.0
5	3	4	13.0	11.7
6	3	4	25.4	25.2
7	3	4	16.1	17.6
8	3	4	3.3 *	3.2
9	3	4	15.0	15.4
10	3	4	7.6	7.9
11	3	4	9.0	8.1
12	3	4	6.4	7.7
13	3	4	14.6	14.9
14	3	4	7.3	4.8
15	3	4	20.6	19.3
16	3	4	6.0	2.6
17	3	4	3.5 *	3.7
0	4	4	50.2	52.1
1	4	4	10.5	7.1
2	4	4	3.2 *	2.6
3	4	4	10.5	10.9
4	4	4	3.2 *	3.9
5	4	4	43.1	42.6
6	4	4	3.3 *	3.5
7	4	4	9.6	7.2
8	4	4	26.2	25.6
9	4	4	44.9	45.0
10	4	4	3.2 *	3.3
11	4	4	3.3 *	3.2
12	4	4	22.2	22.9
13	4	4	24.7	26.2
14	4	4	11.7	12.0
15	4	4	33.6	34.6
16	4	4	3.5 *	4.1
17	4	4	13.0	14.3
1	5	4	43.8	44.8
2	5	4	68.0	68.1
3	5	4	48.8	49.3
4	5	4	6.4	3.2

G OPX

H	K	L	F(OBS)	F(CALC)
5	5	4	27.5	25.5
6	5	4	46.5	44.5
7	5	4	22.2	24.0
8	5	4	6.6	3.3
9	5	4	23.8	23.3
10	5	4	93.3	92.5
11	5	4	54.4	51.7
12	5	4	9.5	8.0
13	5	4	45.1	43.4
14	5	4	23.6	22.6
15	5	4	42.1	42.4
0	6	4	11.5	10.6
1	6	4	52.4	54.1
2	6	4	3.3 *	3.6
3	6	4	35.7	37.0
4	6	4	87.5	87.8
5	6	4	19.7	17.8
6	6	4	7.6	7.3
7	6	4	11.3	12.4
8	6	4	66.8	66.7
9	6	4	48.4	46.3
10	6	4	3.4 *	1.4
11	6	4	52.9	51.3
12	6	4	48.5	46.5
13	6	4	46.9	44.0
14	6	4	3.6 *	1.3
1	7	4	30.7	29.0
2	7	4	22.3	21.0
3	7	4	30.6	28.7
4	7	4	3.3 *	1.7
5	7	4	10.7	12.0
6	7	4	28.7	28.6
7	7	4	3.3 *	0.8
8	7	4	3.4 *	3.8
9	7	4	23.8	24.1
10	7	4	6.9	6.2
11	7	4	39.2	37.5
12	7	4	3.6 *	2.9
0	8	4	18.5	20.0
1	8	4	8.6	5.9
2	8	4	3.3 *	1.9
3	8	4	12.7	12.7
4	8	4	21.4	19.1
5	8	4	23.7	21.7
6	8	4	3.4 *	2.4
7	8	4	3.4 *	3.5
8	8	4	32.3	32.2
9	8	4	16.2	15.9
1	9	4	7.4	4.8
2	9	4	14.6	13.8
3	9	4	3.4 *	4.6
2	1	5	22.4	22.6
3	1	5	3.1 *	6.8

/MG OPX

H	K	L	F(OBS)	F(CALC)
4	1	5	22.0	22.6
5	1	5	7.3	3.6
6	1	5	48.6	48.9
7	1	5	26.4	25.5
8	1	5	18.6	18.8
9	1	5	25.4	24.5
10	1	5	9.9	10.4
11	1	5	9.2	10.0
12	1	5	24.7	24.3
13	1	5	18.9	19.8
14	1	5	28.3	29.9
15	1	5	12.3	10.9
0	2	5	10.4	9.9
1	2	5	22.7	19.4
2	2	5	49.1	50.4
3	2	5	14.3	13.5
4	2	5	62.7	62.1
5	2	5	14.6	16.1
6	2	5	18.1	19.5
7	2	5	3.3 *	3.4
8	2	5	24.9	26.4
9	2	5	56.3	54.9
10	2	5	7.2	8.7
11	2	5	61.0	62.1
12	2	5	33.8	30.5
13	2	5	31.4	31.3
14	2	5	3.5 *	3.3
15	2	5	14.9	12.4
1	3	5	19.6	19.9
2	3	5	54.6	55.1
3	3	5	81.0	80.2
4	3	5	14.5	14.6
5	3	5	44.5	42.4
6	3	5	56.1	55.9
7	3	5	29.5	27.3
8	3	5	42.0	42.3
9	3	5	33.5	34.9
10	3	5	102.5	98.7
11	3	5	8.7	11.9
12	3	5	58.3	58.4
13	3	5	34.4	33.3
14	3	5	8.4	7.4
0	4	5	36.9	38.1
1	4	5	3.2 *	2.1
2	4	5	35.2	35.8
3	4	5	7.3	2.8
4	4	5	18.4	16.4
5	4	5	6.9	2.9
6	4	5	18.3	17.8
7	4	5	14.4	15.3
8	4	5	3.6 *	5.8
9	4	5	32.9	31.2
10	4	5	3.6 *	4.4

/MG OPX

H	K	L	F(OBS)		F(CALC)
11	4	5	32.0		30.9
12	4	5	3.4	*	0.7
13	4	5	37.7		36.7
1	5	5	3.4	*	7.5
2	5	5	23.1		22.7
3	5	5	6.2		4.3
4	5	5	8.5		8.9
5	5	5	8.7		4.4
6	5	5	38.6		35.8
7	5	5	33.6		31.5
8	5	5	10.6		4.9
9	5	5	29.0		29.2
10	5	5	21.3		19.4
11	5	5	3.4	*	3.7
0	6	5	29.5		28.9
1	6	5	3.6	*	6.4
2	6	5	19.2		19.1
3	6	5	3.7	*	3.2
4	6	5	3.4	*	5.7
5	6	5	19.7		19.5
6	6	5	3.7	*	4.4
7	6	5	23.9		24.3
8	6	5	14.2		14.7
9	6	5	3.5	*	4.1
1	7	5	29.3		30.4
2	7	5	3.6	*	3.1
3	7	5	19.3		20.2
4	7	5	25.7		27.6
5	7	5	18.5		19.0
6	7	5	24.3		24.4