American Mineralogist, Volume 60, pages 634–641, 1975

The Crystal Structure of Omphacite

TAKEO MATSUMOTO,

Department of Earth Sciences, Faculty of Science, Kanazawa University, Kanazawa 920, Japan

MASAYASU TOKONAMI, AND NOBUO MORIMOTO

Institute of Scientific and Industrial Research, Osaka University, Suita 565, Japan

Abstract

The crystal structure of *P*2/*n* omphacite has been determined by the least squares method using the intensity data collected by a counter method. This *P*2/*n* clinopyroxene has a different space group, but is very similar in structure to the *P*2 omphacite described earlier (Clark and Papike, 1968; Clark, Appleman, and Papike, 1969). The true space group of the Californian omphacite studied by Clark and Papike (1968) and Clark *et al* (1969) has been found to have *P*2/*n*, not *P*2, space group symmetry. In the structure of *P*2/*n* omphacite, only one kind of SiO_3 chain exists in which two crystallographically different Si atoms alternate. This chain is, therefore, different from the chain of *C*2 spodumene, $P2_1/c$ enstatite, and *C*2/*c* diopside. Mg and Al atoms are ordered in the *M*1 and *M*1(2) sites, respectively. Na and Ca atoms are partially ordered in the *M*2 and *M*2(1) sites.

Introduction

Since the first determination of the diopside structure (Warren and Bragg, 1928), five space groups have been reported for the clinopyroxenes. They are *C*2/*c*, $P2_1/c$, $P2_1/n$, *C*2, and *P*2. Clark and Papike (1966, 1968) and Clark *et al* (1969) have published detailed data on *C*2/*c* and *P*2 omphacites. It seemed to us unusual that the rare space group *P*2 should appear in the fairly common mineral omphacite. This idea led to the finding of a new type of omphacite with the space group *P*2/*n* (Matsumoto and Banno, 1970a, b).

In this study, the structure of this new *P*2/*n* omphacite has been precisely determined and is compared with that of omphacites with different space groups. Omphacite from California determined to be of space group *P*2 by Clark and Papike (1968) has been reexamined and found to possess *P*2/*n* space group symmetry.

Experimental

The structure determination was made on omphacite from a hornblende-bearing eclogite of the Iratsu mass, Bessi area, Japan. The Iratsu mass belongs to the epidote amphibolite facies of the Sambagawa metamorphic terrain. The atomic ratios of the pyroxenes were calculated from the results of the wet chemical analysis by Ōki (Matsumoto and Banno, 1970b; Table 1). For comparison, the atomic ratios of omphacite from other localities are also given in Table 1. The similarity in chemical composition between the omphacite from Bessi and from California is remarkable. It is important, however, to record that the omphacite crystals from Bessi possess small differences in chemical composition when examined by the EPMA (±1 wt percent CaO). Omphacite from California was also studied by X-ray diffraction to compare with the Bessi specimens.

The cell dimensions of the Bessi omphacite were determined by a four-circle single crystal diffractometer (Table 1). They are in good agreement with those obtained by Clark and Papike (1966, 1968) and Clark *et al* (1969) for the California omphacite (Table 1).

In order to confirm the space group symmetry of the Bessi material, especially the existence of glide planes, *h*0*l* Weissenberg photographs were taken with an exposure of more than 200 hours. The *h*0*l* reflections are absent when *h*+*l* is odd. Therefore, this omphacite has *n*-glide planes perpendicular to [010], and the diffraction symbol is 2/*m P*-/*n*. The possible

TABLE 1. Crystallographic and Chemical Data for Omphacite

Locality of Minerals		Bessi, Japan	California	Norway
References		This Study	Clark and Papike (1968) Clark *et al* (1969)	Warner (1964), Clark *et al* (1969)
a (Å)		9.585(3)	9.596(5)	9.646(6)
b (Å)		8.776(3)	8.771(4)	8.824(5)
c (Å)		5.260(3)	5.265(6)	5.270(6)
β (°)		106.85(3)	106.93(8)	106.59(8)
Cell volume ($Å^3$)		423.5(3)	423.9(4)	429.9(5)
Space group		*P2/n*	*P2/n* a)	*C2/c*
Cations per 6 oxygen atoms				
Tetrahedral	Si	1.918	1.96	1.995
	Al	0.082	0.04	0.005
	Σ	2.000	2.00	2.000
M cations	Ca	0.516	0.51	0.583
	Na	0.484	0.48	0.325
	Mg	0.392	0.44	0.582
	Fe^{2+}	0.077	0.10	0.116
	Fe^{3+}	0.137	0.10	0.123
	Al	0.398	0.39	0.233
	Ti	0.005	0.01	0.002
	Σ	2.011	2.03	1.964
Z		4	4	4
Cal. density, $g \cdot cm^{-3}$		3.39	3.37	3.36
Reference for chemical analysis		Matsumoto and Banno (1970, analyst. Ōki)	Coleman *et al* (1965)	Schmitt (1963) (from Clark *et al* 1969)

a) *Space group determination by present authors; other data from Clark and Papike (1966, 1968). The standard deviations are in parentheses.*

space group symmetry is thus *P2/n* or *Pn*. Existence of the glide plane was further confirmed by careful examination of the *h0l* reflections using the four-circle diffractometer.

The three-dimensional intensity data were collected with the four-circle automatic diffractometer from a fragment with the dimensions of 0.10×0.16×0.20 mm. The diffractometer was operated by the $\omega/2\theta$ scan technique with the filtered Mo*Kα* radiation (λ=0.7101 Å). The calculated μr of the specimen is 0.21 for the Mo*Kα* radiation.

All 1090 non-equivalent reflections with $\sin\theta<0.65$ were measured, and the number of non-zero reflections is 955. These intensity data were converted into observed structure factors by applying the Lorentz and polarization factors. Absorption corrections were made assuming the crystal to be spherical in shape. The estimated standard deviation of each reflection was computed from counting statistics.

Structure Refinement

The starting atomic parameters for the least squares refinements were the average values of the corresponding parameters reported for *P*2 Californian omphacite by Clark and Papike (1968). In the earlier stage of the refinement, disordered arrangements of $Al_{0.4}Mg_{0.4}Fe_{0.2}$ in the *M*1 and *M*1(1) sites and $Na_{0.5}Ca_{0.5}$ in the *M*2 and *M*2(1) were assumed. The atomic coordinates and isotropic temperature factors were varied utilizing the ORFLS (Busing, Martin, and Levy, 1962) program modified by Iitaka.

At the later stage of the refinement, the site oc-

TABLE 2. Atomic Parameters, Isotropic Temperature Factors, and Site Occupancies of Atoms in *P2/n* Omphacite*

ATOM	X	Y	Z	B	SITE OCCUPANCY
O1(1)	0.3634(4)	0.3382(5)	0.1232(7)	0.73(7)	1.0 for all O
O1(2)	0.3621(4)	0.1767(5)	0.6475(8)	0.74(6)	
O2(1)	0.6138(4)	0.5090(5)	0.3091(8)	0.76(7)	
O2(2)	0.6063(4)	0.9974(5)	0.8054(8)	0.80(7)	
O3(1)	0.6057(4)	0.2663(4)	0.0037(8)	0.65(6)	
O3(2)	0.5981(4)	0.2398(4)	0.4984(8)	0.70(7)	
Si 1	0.5393(2)	0.3465(2)	0.2273(3)	0.37(3)	1.0 for all Si
Si 2	0.5376(2)	0.1621(2)	0.7310(3)	0.36(3)	
M1(1)	0.2500	0.3480(2)	0.7500	0.32(5)	Al 0.868(9),Fe 0.132
M1	0.2500	0.1580(3)	0.2500	0.43(5)	Mg 0.815(9),Fe 0.185
M2	0.2500	0.5521(3)	0.2500	0.86(6)	Ca 0.314(13),Na 0.686
M2(1)	0.2500	0.9502(2)	0.7500	0.82(5)	Ca 0.716,Na 0.284

* If the origin of coordinate is displaced by (.75, .75, 0) and (.75, .75, .75), the values can be directly compared with the coordinate of the C2/c clinopyroxene by Burnahm's(1967) notation, and the P2 omphacite by Clark et al (1969), respectively. Standard deviations in parentheses.

TABLE 3. Observed and Calculated Structure Factors for Omphacite

h	k	F_{obs}	F_{calc}
		ℓ = 0	
2	0	4.518	-1.702
4	0	8.096	13.114
6	0	83.945	-83.975
8	0	70.072	72.125
10	0	58.852	-56.949
12	0	11.917	-10.866
1	1	14.427	-11.751
2	1	3.795	-3.944
3	1	92.079	89.425
4	1	7.735	7.580
5	1	62.438	59.358
6	1	5.157	-5.305
7	1	48.661	45.922
9	1	5.730	-3.533
11	1	35.444	33.825
12	1	4.450	5.923
13	1	10.823	8.334
0	2	42.575	-42.667
1	2	4.590	4.484
2	2	54.027	-53.130
3	2	2.748	-2.988
4	2	18.465	17.158
6	2	15.072	-16.451
7	2	3.821	-3.837
8	2	13.516	14.541
9	2	3.207	3.397
10	2	8.204	7.655
11	2	1.762	-0.683
12	2	15.537	15.560
13	2	3.117	3.210
0	3	3.687	5.178
1	3	1.950	2.821
2	3	1.011	-1.390
3	3	58.000	-55.805
4	3	1.842	-0.843
5	3	31.749	31.214
6	3	7.931	-7.962
7	3	17.157	15.473
8	3	1.840	0.007
9	3	25.570	25.529
10	3	1.006	-0.446
11	3	14.443	-15.170
12	3	2.079	3.580
13	3	3.403	-1.784
0	4	4.084	-6.201
1	4	12.430	11.947
2	4	4.156	-5.574
3	4	2.890	-2.832
4	4	78.230	-78.043
5	4	4.110	-3.468
6	4	22.637	-23.161
7	4	9.948	-10.527
8	4	11.171	11.864
10	4	55.302	54.144
11	4	3.088	-3.290
12	4	13.983	13.553
0	5	17.152	17.300
1	5	90.402	91.158
2	5	3.212	3.281
3	5	74.275	-73.156
4	5	7.319	6.873
5	5	8.470	-9.323
6	5	1.189	-1.956
7	5	105.397	-109.095
8	5	1.512	-0.187
9	5	10.864	10.133
10	5	6.468	-6.423
11	5	40.908	-40.943
0	6	96.901	103.749
1	6	2.092	-2.940
2	6	24.874	24.414
3	6	2.523	2.595
4	6	23.898	22.357
5	6	12.291	12.722
7	6	7.709	7.830
8	6	15.511	14.702
10	6	45.454	-43.258
11	6	2.260	1.120
0	7	13.733	-12.769
1	7	13.408	-14.913
3	7	14.706	-14.674
4	7	2.812	-2.579
5	7	47.613	47.651
7	7	38.940	38.645
8	7	3.235	-2.702
9	7	15.660	15.806
10	7	10.547	10.859
1	8	9.445	9.138
2	8	23.142	22.934
3	8	1.334	2.009
4	8	34.190	-33.613
5	8	2.773	-3.529
6	8	5.325	-5.656
7	8	8.160	-7.781
8	8	5.531	-5.161
9	8	7.211	6.376
0	9	11.958	-9.600
1	9	1.370	1.713
3	9	27.611	28.739
4	9	6.298	-6.078
5	9	8.633	9.443
7	9	19.069	18.038
8	9	4.701	-4.712
0	10	70.186	-72.372
1	10	3.994	4.312
2	10	7.265	6.131
3	10	8.666	-8.609
4	10	53.367	-51.071
5	10	6.465	-5.655
6	10	26.164	25.657
7	10	11.584	-11.171
0	11	16.525	18.464
1	11	1.832	1.743
2	11	8.942	8.050
3	11	37.193	-38.419
5	11	25.103	-23.242
0	12	43.718	45.568
1	12	2.438	-2.962
2	12	24.631	23.492
		ℓ = 1	
1	0	7.879	7.360
3	0	0.578	-0.391
5	0	0.686	0.156
7	0	6.236	-6.403
9	0	3.674	4.310
0	1	2.892	2.929
1	1	3.904	-1.005
2	1	2.675	2.993
3	1	72.962	-71.648
4	1	1.373	0.084
5	1	17.786	-15.222
6	1	5.408	5.226
7	1	16.798	-15.439
8	1	1.298	0.275
9	1	12.962	-12.527
10	1	2.265	-2.694
11	1	29.481	-29.521
12	1	2.294	-1.130
0	2	35.343	34.599
1	2	1.987	2.327
2	2	108.485	111.512
3	2	10.119	-9.700
4	2	27.441	-24.412
5	2	6.455	6.615
6	2	74.290	73.976
7	2	4.363	4.151
8	2	47.897	-45.935
9	2	8.279	8.451
10	2	7.335	-5.919
11	2	2.621	-2.673
12	2	46.099	-45.340
0	3	8.602	-8.835
1	3	18.070	-13.264
2	3	0.578	-0.828
3	3	39.149	-34.619
4	3	6.460	-6.434
5	3	139.223	145.736
6	3	5.588	-5.662
7	3	17.699	18.569
8	3	0.900	2.490
9	3	49.554	49.452
10	3	7.835	7.579
11	3	8.615	-9.568
0	4	87.229	-93.208
1	4	8.202	8.057
2	4	24.265	-22.294
3	4	4.835	-4.756
4	4	27.043	-25.399
5	4	10.635	-10.653
6	4	16.112	-15.868
7	4	3.388	-3.347
8	4	4.752	2.800
9	4	1.331	0.331
10	4	30.212	28.777
0	5	1.589	2.129
1	5	7.577	-7.284
2	5	2.454	1.761
3	5	25.165	-24.432
4	5	3.604	-3.471
5	5	23.357	-22.873
6	5	7.461	7.496
7	5	9.151	9.260
8	5	5.183	-5.212
9	5	4.997	-4.902
10	5	2.513	-2.196
11	5	12.763	-12.026
0	6	37.820	-37.184
1	6	4.110	-4.281
2	6	7.570	7.544
3	6	1.945	-1.878
4	6	16.509	-15.183
5	6	2.848	-2.996
6	6	3.135	2.587
8	6	12.874	-12.335
10	6	11.478	12.279
0	7	7.497	7.895
1	7	62.719	-63.443
2	7	10.599	10.154
3	7	7.172	5.860
4	7	6.597	-6.608
5	7	51.767	-51.511
6	7	7.776	7.500
7	7	12.337	11.175
8	7	0.789	-0.589
9	7	51.638	-50.855
0	8	13.842	14.501
1	8	1.009	-0.450
2	8	61.886	60.813
3	8	3.496	2.869
4	8	10.730	-10.391
5	8	10.903	11.181
6	8	54.623	52.883
7	8	5.317	4.676
8	8	26.322	-27.059
9	8	6.453	6.038
0	9	9.977	-10.233
1	9	16.274	-14.807
2	9	5.111	-4.886
3	9	12.776	11.613
4	9	3.452	-1.799
5	9	36.197	36.326
6	9	6.176	-6.770
7	9	32.905	32.076
8	9	2.402	2.184
0	10	23.558	-23.553
1	10	3.380	-1.441
2	10	5.826	-5.171
3	10	1.868	-0.773
4	10	8.478	8.577
5	10	12.134	-11.409
6	10	21.019	-21.737
0	11	3.341	3.574
1	11	20.756	-18.256
2	11	6.174	-6.111
3	11	6.819	6.507
4	11	6.169	-5.709
0	12	2.152	-0.620
1	12	6.311	-5.386
-1	0	12.797	-12.675
-3	0	7.552	7.705
-5	0	2.745	2.439
-9	0	7.534	-7.906
-11	0	6.582	7.364
-1	1	17.023	15.070
-2	1	1.734	2.369
-3	1	75.565	77.269
-4	1	5.384	-5.212
-5	1	30.557	27.111
-6	1	2.128	2.562
-7	1	27.322	26.882
-8	1	3.749	3.383
-9	1	2.884	0.949
-10	1	2.268	0.470
-11	1	18.305	19.775
-1	2	5.818	-5.774
-2	2	127.170	145.405
-3	2	4.120	4.488
-4	2	63.096	-62.873
-5	2	6.102	-6.541
-6	2	48.442	48.498
-7	2	3.568	4.223
-8	2	44.481	-43.962
-9	2	3.640	-5.175
-10	2	4.644	-2.831
-11	2	4.208	-3.112
-12	2	67.250	-67.350
-1	3	78.382	-83.913
-2	3	5.312	-5.492
-3	3	84.094	88.315
-4	3	1.878	2.354
-5	3	109.664	-118.467
-6	3	2.632	3.046
-7	3	46.716	-45.863
-8	3	1.587	-1.383
-9	3	66.834	-67.778
-10	3	2.518	1.392
-11	3	29.690	29.684
-1	4	3.289	3.280
-2	4	39.523	-38.361
-3	4	1.553	1.370
-4	4	3.826	3.139
-5	4	7.861	7.890
-6	4	7.064	9.218
-7	4	3.929	4.259
-8	4	7.714	-9.668
-9	4	3.204	-3.304
-10	4	26.620	27.063
-11	4	2.910	-2.208
-1	5	29.850	29.410
-2	5	9.745	9.492
-3	5	13.021	13.432
-4	5	10.707	-11.370
-5	5	15.787	16.089
-6	5	3.604	-3.417
-7	5	1.945	-3.446
-8	5	1.334	-1.855
-9	5	5.361	5.439
-10	5	5.537	5.799
-11	5	7.755	8.239
-2	6	14.058	-14.065
-3	6	1.298	1.485
-4	6	24.979	-25.260
-5	6	6.922	7.819
-6	6	19.358	20.068
-7	6	3.171	3.582
-8	6	5.617	4.201
-9	6	2.157	0.896
-10	6	11.891	13.305
-1	7	51.329	52.790
-2	7	15.464	15.785
-3	7	6.019	7.135
-4	7	4.399	-4.541
-5	7	79.554	84.505
-6	7	6.411	6.118
-7	7	5.400	-4.803
-8	7	3.202	-4.516
-9	7	32.446	33.324
-1	8	3.207	-3.055
-2	8	85.862	91.415
-3	8	0.361	-0.007
-4	8	17.330	-16.282
-5	8	12.567	-13.590
-6	8	24.796	24.962
-7	8	10.862	-11.195
-8	8	41.246	-43.302
-1	9	3.421	2.811
-2	9	11.594	-12.328
-3	9	7.776	-6.776
-4	9	1.187	-0.310
-5	9	43.774	-45.275
-7	9	52.226	-50.965
-1	10	5.720	4.959
-2	10	37.833	-38.527
-3	10	4.350	-4.307
-4	10	6.829	5.997
-5	10	13.651	13.448
-1	11	5.746	2.700
-2	11	3.805	4.015
-3	11	4.739	-4.544
		ℓ = 2	
0	0	144.373	-157.510
2	0	79.959	76.559
4	0	109.902	-114.929
6	0	2.632	-4.140
8	0	38.996	-38.940
10	0	72.657	70.547
0	1	7.515	-7.085
1	1	79.216	74.037
2	1	2.456	1.559
3	1	36.422	-33.927
4	1	2.092	1.981
5	1	35.181	-34.925
6	1	5.838	6.006
7	1	57.456	-56.285
8	1	3.385	-3.512
9	1	24.203	-23.642
10	1	2.980	-2.303
11	1	29.621	-28.209
0	2	60.712	-57.579
1	2	4.843	-4.399
2	2	34.164	32.632
3	2	4.401	4.714
4	2	53.937	53.501
5	2	0.578	-1.283
6	2	39.579	38.501
7	2	2.415	2.979
8	2	33.011	-32.131
9	2	1.582	-1.408
10	2	20.431	-19.757
0	3	5.743	5.755
1	3	40.877	-40.336
2	3	1.876	1.055
3	3	9.089	-9.000
4	3	5.552	-5.483
5	3	22.745	-22.154
6	3	6.561	6.168
7	3	18.119	17.658
9	3	9.345	-8.783
10	3	1.293	-0.070
0	4	65.547	65.122
1	4	9.092	-9.379
2	4	34.982	34.056
3	4	7.389	7.240
4	4	47.113	46.319
5	4	1.767	2.564
6	4	7.497	-7.377
7	4	4.933	4.807
8	4	3.596	-3.645
9	4	1.796	-1.679
10	4	15.642	-15.871
0	5	17.237	-17.697
1	5	59.265	-58.799
3	5	108.318	112.119
4	5	5.046	-4.510
5	5	7.750	-6.415
6	5	2.090	-0.050
7	5	55.596	54.432
8	5	3.127	-2.979
9	5	7.144	-5.548
10	5	3.264	2.522
0	6	101.504	-106.478
2	6	7.642	-7.119
3	6	8.578	-9.069
4	6	24.871	-23.630
5	6	5.366	-5.001
6	6	8.349	-7.233
7	6	0.934	-0.307
8	6	16.667	-16.954
9	6	5.813	-5.934
0	7	9.768	9.583
1	7	2.487	2.383
2	7	2.632	-3.602
3	7	29.190	-30.483
4	7	7.420	7.385
5	7	34.370	-33.179
6	7	4.027	3.563
8	7	1.865	1.423
0	8	22.737	22.884
1	8	5.691	-5.973
2	8	10.949	-9.879
3	8	7.704	7.285
4	8	20.939	19.638
5	8	1.331	-1.257
6	8	14.548	-12.901
7	8	1.220	-0.368
8	8	2.939	1.529
0	9	8.313	7.904
1	9	17.487	16.860
2	9	0.828	1.500
3	9	4.208	-4.608
4	9	8.911	7.911
5	9	9.156	-9.061
6	9	1.040	0.143
0	10	48.669	48.119
1	10	10.351	-9.995
2	10	2.874	-2.850
3	10	6.643	6.607
4	10	70.193	67.618
5	10	7.639	7.600
0	11	10.444	-11.145
1	11	14.892	-15.625
2	11	6.135	-4.938
3	11	24.022	23.722
-2	0	38.596	-33.818
-4	0	103.021	-101.434
-6	0	100.209	103.639
-8	0	29.665	-30.806
-10	0	72.167	73.181
-12	0	15.627	11.684
-1	1	3.181	4.824
-2	1	6.143	6.214
-3	1	2.928	-0.504
-4	1	3.684	-4.168
-5	1	29.169	29.429
-6	1	1.370	-0.336
-7	1	97.469	104.824
-8	1	1.981	-2.165
-9	1	19.680	21.193
-11	1	1.545	-1.742
-12	1	3.916	-4.749
-1	2	4.915	-4.856
-2	2	14.961	16.689
-3	2	2.820	-2.643
-4	2	30.807	28.861
-5	2	5.052	5.045
-6	2	42.368	44.400
-7	2	4.757	-4.781
-8	2	23.251	-24.021
-9	2	1.406	1.111
-10	2	33.230	-31.843
-11	2	3.524	2.532
-12	2	28.873	-29.997
		ℓ = 3	
1	0	6.783	-6.733
3	0	9.479	9.902
7	0	3.599	-3.230
9	0	7.828	-7.925
0	1	7.327	-6.831
1	1	11.870	11.340
2	1	2.056	1.765
3	1	30.890	30.273
4	1	5.299	5.192
5	1	8.867	-8.791
6	1	2.306	-1.106
7	1	18.140	16.650
8	1	1.870	-1.940
9	1	26.316	26.480
10	1	2.366	-1.443
0	2	15.083	14.405
1	2	2.237	-1.919
2	2	82.041	-82.579
3	2	0.397	0.271
4	2	10.957	-12.091
5	2	6.308	-5.795
6	2	63.537	-61.170
7	2	3.418	2.566
8	2	37.020	34.487
9	2	3.302	-3.423

TABLE 3, Continued

h	k	F_{obs}	F_{calc}
0	3	2.812	3.659
1	3	18.493	-17.098
2	3	3.568	3.066
3	3	9.409	6.913
4	3	4.577	4.111
5	3	80.477	-78.801
6	3	2.915	-0.332
7	3	2.229	-0.278
9	3	57.268	-54.694
0	4	37.020	35.531
1	4	1.623	1.988
2	4	10.599	10.233
3	4	7.281	7.491
4	4	42.389	41.043
5	4	1.692	0.742
6	4	21.342	22.276
7	4	3.811	-3.923
0	5	5.624	5.837
1	5	26.277	27.060
2	5	4.432	-4.137
3	5	5.694	6.046
4	5	1.981	1.881
5	5	9.899	-9.050
6	5	2.229	-2.794
7	5	5.857	-5.638
8	5	3.553	3.320
0	6	28.044	28.252
1	6	3.029	-3.017
2	6	11.785	12.028
4	6	23.184	21.326
5	6	5.828	5.771
6	6	6.254	-4.995
8	6	5.057	4.625
0	7	3.135	-3.500
1	7	36.527	35.204
2	7	7.201	-6.849
3	7	12.776	-10.966
5	7	42.554	41.066
6	7	11.778	-10.822
7	7	4.448	-3.652
0	8	2.735	1.269
1	8	4.319	3.986
2	8	73.382	-73.245
3	8	3.847	-3.031
4	8	17.425	-16.514
5	8	7.861	-8.405
6	8	37.268	-36.011
0	9	2.518	2.137
1	9	25.880	24.617
2	9	7.797	8.186
3	9	25.459	-23.882
4	9	11.125	10.711
5	9	31.770	-32.634
0	10	5.457	6.153
1	10	2.513	2.090
2	10	17.652	18.554
3	10	0.322	1.703
0	11	3.155	3.597
-1	0	6.969	6.907
-3	0	5.307	6.209
-5	0	2.273	-1.996
-7	0	12.724	-14.149
-9	0	2.487	3.132
-11	0	2.193	-0.568
-1	1	9.097	-7.698
-2	1	8.050	-8.110
-3	1	66.125	-66.700
-4	1	3.393	3.140
-5	1	32.309	-31.216
-6	1	2.343	-3.804
-7	1	28.367	-29.240
-8	1	5.191	-4.559
-10	1	3.132	2.061
-11	1	1.042	-4.188
-12	1	4.381	4.299
-1	2	6.569	6.876
-2	2	97.657	-116.371
-3	2	5.377	-6.527
-4	2	29.071	29.206
-5	2	5.119	5.687
-6	2	10.777	-11.252
-7	2	2.668	2.931
-8	2	69.930	70.781
-9	2	5.764	6.855
-10	2	4.391	-5.177
-11	2	1.870	-1.727
-12	2	57.766	57.312
-1	3	106.548	117.892
-2	3	4.149	4.568
-3	3	27.301	-28.673
-4	3	2.848	3.131
-5	3	78.653	72.394
-6	3	1.514	-2.417
-7	3	27.503	27.997
-8	3	3.929	-3.386
-9	3	74.760	76.304
-10	3	5.000	-5.354
-11	3	37.374	-38.597
-1	4	8.184	-8.699
-2	4	48.697	51.292
-3	4	4.649	-4.946
-4	4	22.276	24.146
-5	4	2.812	-2.082
-6	4	36.767	-38.905
-7	4	5.947	-6.153
-8	4	24.533	-23.233
-9	4	3.346	-2.840
-10	4	14.169	-16.919
-11	4	7.650	7.400
-1	5	8.111	-8.515
-2	5	6.669	-6.817
-3	5	20.222	-21.138
-4	5	1.370	0.921
-5	5	27.177	-29.703
-6	5	2.776	2.445
-7	5	3.891	-4.543
-8	5	10.513	11.093
-9	5	3.274	3.119
-10	5	1.796	-2.509
-1	6	0.973	0.172
-2	6	7.208	-8.197
-3	6	1.876	3.081
-4	6	9.445	9.052
-5	6	5.444	-6.188
-6	6	9.187	-10.877
-7	6	5.219	-5.018
-8	6	1.654	3.196
-9	6	0.792	0.211
-10	6	16.411	-17.020
-1	7	61.409	-63.642
-2	7	13.731	-15.019
-3	7	6.811	-7.772
-4	7	5.402	6.364
-5	7	56.863	-62.084
-7	7	6.295	7.324
-8	7	2.877	2.596
-9	7	37.492	-38.154
-1	8	10.547	11.577
-2	8	53.279	-55.606
-3	8	2.735	2.559
-4	8	21.917	23.238
-5	8	6.081	5.756
-6	8	17.727	-18.057
-7	8	6.218	6.992
-8	8	40.609	42.136
-1	9	36.716	40.765
-2	9	5.789	7.323
-3	9	12.799	13.818
-5	9	5.353	5.702
-6	9	2.371	-4.131
-1	10	12.603	-13.437
-2	10	19.894	20.604
		ℓ = 4	
0	0	110.949	109.810
2	0	17.121	-15.396
4	0	82.500	79.794
6	0	18.736	-15.653
8	0	40.397	38.151
0	1	4.110	4.156
1	1	6.236	-5.380
2	1	5.119	-5.071
3	1	49.492	49.197
6	1	1.509	-2.146
7	1	20.725	21.455
8	1	3.947	2.351
0	2	15.787	-16.259
2	2	50.898	-50.222
3	2	2.018	0.217
4	2	9.185	-10.470
5	2	4.174	4.878
6	2	3.021	3.899
7	2	3.842	-4.123
8	2	12.913	11.360
1	3	1.659	-1.655
2	3	1.981	2.334
3	3	27.203	-25.555
4	3	1.440	-0.724
5	3	18.816	16.923
6	3	7.260	-6.934
7	3	7.575	7.830
8	3	5.449	5.252
0	4	15.067	-13.504
1	4	8.615	8.310
2	4	31.997	-31.303
3	4	8.607	-8.085
4	4	60.601	-59.037
5	4	1.473	-2.468
6	4	4.022	-4.462
7	4	3.767	-2.776
0	5	5.875	5.474
1	5	56.383	55.595
3	5	45.059	-41.806
4	5	9.711	9.206
5	5	22.890	20.274
7	5	65.371	-62.441
0	6	24.884	24.342
1	6	1.404	-0.489
2	6	9.788	9.133
3	6	1.078	1.525
4	6	59.226	57.088
5	6	1.687	1.252
6	6	22.167	20.808
1	7	5.359	-6.407
2	7	2.049	-2.896
3	7	2.012	0.611
4	7	13.176	-12.747
5	7	13.310	11.811
0	8	2.407	2.363
1	8	4.275	3.569
2	8	3.519	2.879
3	8	3.016	-1.799
4	8	31.633	-29.342
0	9	9.154	-9.604
1	9	8.181	-8.558
2	9	2.405	2.046
3	9	13.981	14.845
0	10	55.031	-52.642
-2	0	10.635	11.410
-4	0	66.757	66.887
-6	0	107.562	-118.652
-8	0	5.838	-3.848
-10	0	41.367	-44.066
-1	1	47.291	-47.918
-2	1	1.370	1.035
-3	1	88.313	-87.787
-4	1	1.551	3.023
-5	1	11.932	-10.028
-6	1	1.117	-0.347
-7	1	34.425	-29.736
-8	1	3.963	4.344
-9	1	8.173	-8.215
-11	1	14.515	-13.656
-2	2	13.194	-12.889
-3	2	9.479	10.556
-4	2	21.664	22.950
-5	2	2.632	-2.800
-6	2	3.532	2.638
-7	2	3.965	-4.282
-8	2	10.193	11.794
-9	2	2.988	-3.283
-10	2	1.440	-1.026
-11	2	2.227	2.287
-1	3	10.526	-9.833
-2	3	9.445	-10.463
-3	3	25.341	26.888
-4	3	2.487	2.178
-5	3	19.716	-22.058
-6	3	0.720	-1.098
-7	3	10.449	-9.204
-8	3	3.960	-4.465
-9	3	19.035	-20.887
-10	3	5.787	-5.506
-11	3	13.501	15.653
-1	4	1.587	1.696
-2	4	15.573	16.641
-4	4	30.242	-31.954
-5	4	1.803	-2.376
-6	4	2.018	0.686
-7	4	12.067	13.670
-8	4	13.857	13.541
-9	4	3.021	2.224
-10	4	48.542	48.155
-1	5	14.525	-14.391
-2	5	4.505	4.623
-3	5	77.570	81.970
-4	5	6.561	7.332
-5	5	8.287	-9.681
-6	5	6.592	-6.834
-7	5	75.588	84.074
-8	5	3.524	-3.536
-9	5	3.558	-6.312
-10	5	5.457	-5.792
-1	6	6.950	-7.328
-2	6	23.955	25.209
-3	6	6.053	-7.061
-4	6	41.019	43.504
-5	6	4.427	-4.498
-6	6	37.319	-38.387
-7	6	5.359	-5.243
-8	6	32.745	-33.671
-9	6	2.190	-3.177
-1	7	27.314	-27.313
-2	7	2.988	2.866
-3	7	8.674	-9.203
-4	7	5.397	-6.024
-5	7	12.949	-14.145
-6	7	6.148	7.246
-7	7	26.233	-26.017
-8	7	4.812	4.850
-2	8	22.580	21.716
-3	8	4.889	4.883
-4	8	23.581	-23.334
-5	8	4.814	-5.767
-6	8	0.753	0.148
-1	9	9.515	-10.424
-2	9	2.585	-3.126
-3	9	29.445	-28.881
-4	9	1.615	-1.242
		ℓ = 5	
1	0	2.701	2.651
3	0	9.355	-9.199
5	0	3.341	3.246
0	1	2.918	-2.597
1	1	3.313	1.182
2	1	2.771	-3.222
4	1	3.416	4.793
5	1	9.696	8.045
6	1	4.162	3.797
0	2	12.933	-11.514
1	2	1.512	1.150
2	2	80.402	78.687
3	2	2.841	-2.323
4	2	13.261	13.521
5	2	3.447	3.757
6	2	36.729	35.066
1	3	17.567	16.668
2	3	4.174	-3.911
3	3	17.043	-15.299
4	3	7.221	-6.401
5	3	45.513	43.735
0	4	17.995	-17.129
1	4	1.187	-0.196
2	4	32.474	-33.344
3	4	3.271	3.468
4	4	38.852	-35.570
5	4	2.691	0.982
0	5	5.539	-5.066
1	5	9.025	-9.444
2	5	7.405	6.951
3	5	7.038	6.282
5	5	2.583	2.505
0	6	19.948	-17.480
1	6	1.976	-1.862
2	6	4.131	2.936
3	6	7.250	-6.845
4	6	12.585	-11.988
0	7	1.579	-1.515
1	7	27.998	-27.445
2	7	5.165	4.871
3	7	31.086	28.884
0	8	5.596	-3.922
-1	0	1.731	0.406
-3	0	1.945	-1.263
-5	0	7.350	-7.070
-7	0	10.333	11.080
-9	0	4.316	3.001
-1	1	2.343	2.263
-2	1	8.867	8.770
-3	1	43.976	43.942
-4	1	3.568	3.923
-5	1	28.612	27.808
-6	1	3.279	-3.576
-7	1	17.642	19.570
-8	1	1.798	1.784
-9	1	1.078	-4.935
-10	1	5.101	5.894
-1	2	6.919	-6.623
-2	2	45.552	45.437
-3	2	2.018	1.622
-4	2	25.441	-26.863
-5	2	1.729	-2.152
-6	2	14.657	14.930
-8	2	68.782	-68.412
-9	2	4.889	-5.244
-10	2	6.502	-5.050
-1	3	89.474	-91.476
-2	3	2.665	0.937
-3	3	15.384	-16.260
-5	3	47.933	-47.550
-6	3	2.485	2.977
-7	3	10.436	12.097
-8	3	3.021	2.923
-9	3	60.694	-61.325
-10	3	0.645	1.521
-1	4	2.087	2.811
-2	4	5.402	-4.022
-3	4	6.195	6.302
-4	4	12.853	-12.576
-5	4	2.232	3.192
-6	4	15.114	17.450
-7	4	2.913	-2.710
-8	4	29.799	27.761
-1	5	7.123	7.636
-2	5	2.159	-2.193
-3	5	12.020	13.472
-4	5	4.497	-5.466
-5	5	14.425	15.139
-6	5	2.768	2.758
-7	5	1.545	0.145
-8	5	10.023	-8.235
-1	6	4.422	4.483
-2	6	3.416	-4.669
-3	6	1.870	-1.349
-4	6	8.953	-10.308
-5	6	2.012	0.760
-6	6	17.608	17.963
-7	6	8.906	8.909
-1	7	31.107	32.100
-2	7	13.006	13.220
-3	7	12.286	12.011
-5	7	61.342	66.155
-6	7	3.411	-2.257
		ℓ = 6	
0	0	40.949	-39.115
2	0	3.447	1.973
4	0	76.011	-71.001
0	1	2.012	-0.736
1	1	25.764	25.306
2	1	3.555	3.407
3	1	9.510	6.992
4	1	1.865	-0.850
0	2	5.284	-3.698
1	2	6.502	-6.493
2	2	33.532	31.036
3	2	2.905	-2.698
0	3	5.893	-4.822
1	3	12.675	-11.303
2	3	1.651	2.253
3	3	2.152	-1.882
0	4	41.656	40.901
1	4	2.154	0.972
2	4	30.023	29.017
0	5	3.480	-3.744
1	5	34.471	-32.799
2	5	3.442	-2.567
0	6	29.476	-30.860
-2	0	32.482	30.965
-4	0	62.915	-60.035
-6	0	46.925	47.527
-8	0	26.042	23.251
-1	1	7.371	7.306
-2	1	1.690	-1.933
-3	1	38.669	42.039
-4	1	6.223	-5.575
-5	1	18.630	18.950
-7	1	33.135	31.923
-8	1	1.545	-2.070
-1	2	4.567	4.560
-2	2	6.220	-6.771
-3	2	1.042	-2.589
-4	2	4.136	-4.833
-5	2	2.949	-1.569
-6	2	15.493	15.287
-7	2	1.723	0.904
-8	2	15.908	-16.512
-1	3	22.355	22.173
-2	3	7.730	8.401
-3	3	9.133	8.170
-4	3	4.100	4.517
-5	3	13.228	14.125
-6	3	0.720	-0.664
-7	3	15.983	-16.312
-1	4	4.022	-3.952
-2	4	8.983	-10.444
-3	4	7.007	-7.844
-4	4	12.397	-12.588
-5	4	4.167	4.872
-6	4	24.530	-23.986
-7	4	3.986	-4.866
-1	5	3.661	2.288
-3	5	80.152	-83.650
-4	5	4.525	-4.669
		ℓ = 7	
0	1	2.616	1.259

cupancies of the cations were refined utilizing the RFINE (Finger, 1969) program rewritten by M. Kitamura, using neutral atomic scattering factors (Cromer and Weber, 1965). The magnesium and aluminum atoms were, however, assumed to concentrate in the *M*1 and *M*1(1) sites, respectively. This assumption was based on the bond distances about the *M*1 and *M*1(1) sites. Even if some disordering between the magnesium and aluminum atoms takes place in these sites, it has almost no effect on the calculated structure factors, since the form factors of aluminum and magnesium atoms are practically identical. Sodium and calcium atoms in the *M*2 and *M*2(1) sites were constrained to agree with the result of the chemical analysis (Table 1). Iron contents in *M*1 and *M*1(1) sites were determined without the chemical constraint. The total amount of iron obtained in the refinement is slightly less than that obtained by the wet analysis. This fact suggests slight differences in chemical composition between individual crystals or within crystals or else possible errors of the site occupancies.

The final atomic parameters, isotropic temperature factors, and site occupancies are summarized in Table 2. The final *R* value is 0.058, and the weighted *R* value is 0.054 for the 955 nonzero intensities. The observed and calculated structure factors are shown in Table 3.

Structural Description

The general features of the omphacite structure are similar to those of other clinopyroxenes. However, the structure of the new type of omphacite is different from other pyroxene structures in that there is only one kind of chain in the cell which consists of two crystallographically distinct tetrahedra, Si1 and Si2, alternating along the *c* axis. This structure is in many respects similar to the *P*2 structure proposed by Clark and Papike (1966).

The Si–O distances and the bond angles O–Si–O

TABLE 4. Bond Distances and Bond Angles of the Tetrahedra in *P2/n* Omphacite*

About Si 1		About Si 2	
Si 1 - O1(1)	1.616(4) Å	Si 2 - O1(2)	1.616(4) Å
- O2(1)	1.597(5)	- O2(2)	1.590(5)
- O3(1)	1.649(4)	- O3(1)	1.666(5)
- O3(2)	1.662(4)	O3(2)	1.646(4)
Mean	1.631	Mean	1.630
O1(1) - O2(1)	2.757(5) Å	O1(2) - O2(2)	2.742(6) Å
- O3(1)	2.652(6)	- O3(1)	2.654(6)
- O3(2)	2.670(5)	- O3(2)	2.658(5)
O2(1) - O3(1)	2.655(6)	O2(2) - O3(1)	2.581(6)
- O3(2)	2.585(6)	- O3(2)	2.658(6)
O3(1) - O3(2)	2.634(6)	O3(1) - O3(2)	2.648(6)
Mean	2.659	Mean	2.657
O1(1) - Si1 - O2(1)	118.2(2)°	O1(2) - Si2 - O2(2)	117.6(2)°
O1(1) - Si1 - O3(1)	108.6(2)	O1(2) - Si2 - O3(2)	109.2(2)
O1(1) - Si1 - O3(2)	109.0(2)	O1(2) - Si2 - O3(1)	107.9(2)
O2(1) - Si1 - O3(1)	109.8(2)	O2(2) - Si2 - O3(2)	110.5(2)
O2(1) - Si1 - O3(2)	105.0(2)	O2(2) - Si2 - O3(1)	104.8(2)
O3(1) - Si1 - O3(2)	105.5(2)	O3(2) - Si2 - O3(1)	106.1(2)

* The standard deviations in parentheses are expressed in the unit of the last digit stated.

for Si1 and Si2 tetrahedra are shown in Table 4 and in Figure 1. The difference between the two tetrahedra is slight. The Si–O bonds of the bridging oxygens (O3(1) and O3(2)) are significantly longer than those to other nonbridging oxygens, as in other clinopyroxenes. The angle O1–Si–O2 is 118° for each tetrahedron, compared with 105° for O2–Si–O3, reflecting the long O1(1)–O2(1) and O1(2)–O2(2) distances of 2.757 and 2.742 Å, respectively.

The metal-oxygen bond distances for the four octahedral and eight-fold cation sites are summarized in Table 5.

The Mg and Al atoms are ordered in the *M*1 and *M*1(1) sites, respectively. The Fe atoms are distributed to fill each of these two sites as a minor component. The Na and Ca atoms are partially ordered in the *M*2 and *M*2(1) sites with an isotropic temperature factor of about 0.8 Å^2, and with the ratio of Na/Ca=2/1 and Na/Ca=1/2, respectively. These results are very similar to those found by Clark and Papike (1968) for the *P*2-omphacite.

Discussion

Among the 16 different symmetry types proposed for clinopyroxenes (Matsumoto and Banno, 1970b; Matsumoto, Tokonami, and Morimoto, 1972; Brown, 1972), only five have been reported to exist. They are *C*2/*c*, *P*2/*n*, *C*2, $P2_1/c$, and *P*2. Although $P2_1/n$ was reported for clinoenstatite (Lindeman, 1961), it is considered by Smith (1969) to be erroneously assigned. Furthermore, recent study by Graham on spodumene (1974) has raised a serious doubt of the possibility of *C*2 symmetry for clinopyroxenes. The first three structure types (*C*2/*c*,

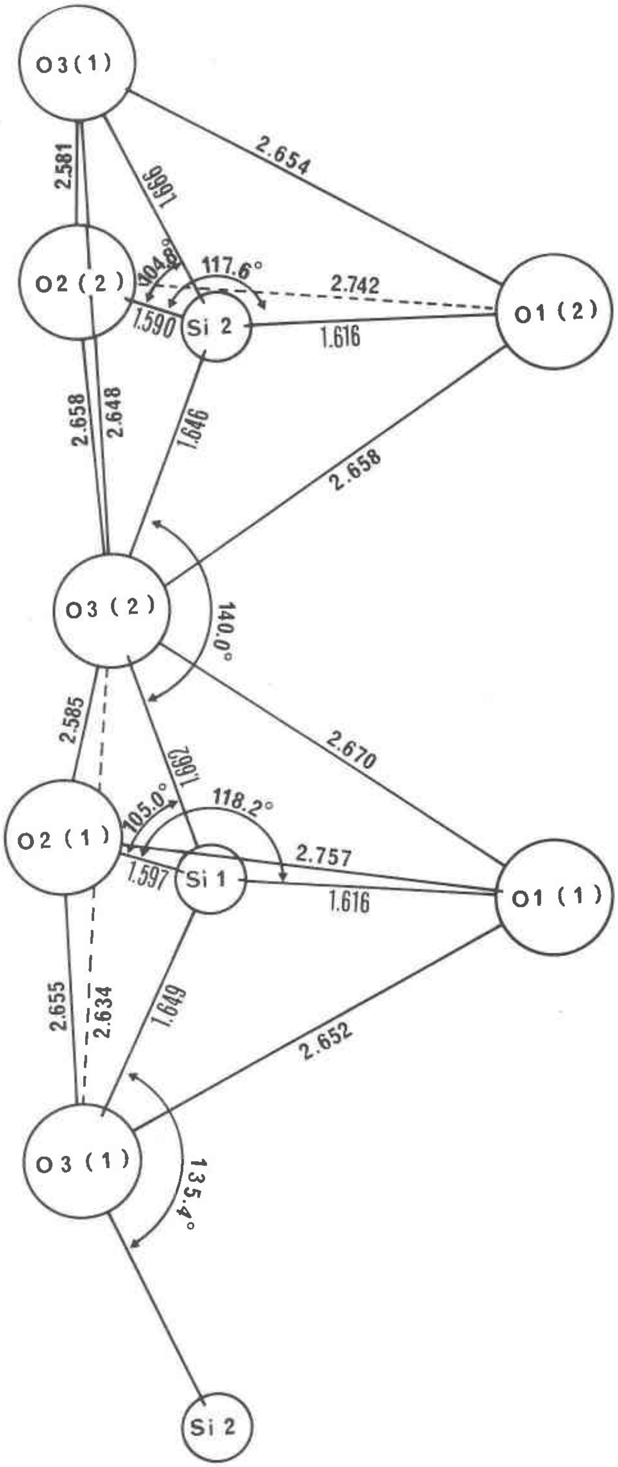

FIG. 1. Silicate chain in *P2/n* omphacite. Bond distances and angles are given.

$P2_1/n$, $C2$) have only one kind of SiO_3 chain, and the other two types have two kinds of chains in the cell. In the structure of the $P2/n$ omphacite, crystallographically different tetrahedra alternate along the c axis and form only one kind of chain in the structure.

According to the present and previous studies, three different space groups for omphacite mineral—$C2/c$, $P2/n$, and $P2$—have been reported. The crystallographic and chemical data for these omphacites are compared in Table 1. The chemical compositions of these three specimens are similar. The Norwegian omphacite, which has the largest cell volume and possesses the higher $C2/c$ space group symmetry, is considered to belong to a high temperature facies (Banno, 1970). The $P2/n$ omphacite is considered to transform to the $C2/c$ omphacite by an order-disorder transition. An antiphase domain structure which has been attributed to this order-disorder transition has been observed for the $P2/n$ omphacite (Champness, 1973; Phakey and Ghose, 1973) as for the $P2_1/c$ pigeonite (Morimoto and Tokonami, 1969).

Because the difference in temperature of omphacite crystallization between the Sambagawa and the Californian occurrences is not large, it seemed necessary to examine the apparent discrepancy in symmetry between the present specimen and the Californian omphacite. Dr. Clark kindly sent us the Californian omphacite which she had studied. We examined the specimen by the precession method at the precession angle of $\bar{\mu}=30°$ with an exposure of 100 hours for Cu$K\alpha$ X-rays at 100 mA. Only four weak reflections (*401* and its equivalent reflections) violating the systematic absences for the n-glide planes appeared in the $h0l$ net. However, these reflections were caused to disappear by changing the precession angle to $\bar{\mu}=25°$ (Fig. 2). The disappearance of *401* and its equivalent reflections by the change of the diffraction geometry indicates that the reflections violating $h+l$=even in

TABLE 5. Metal-Oxygen Bond Distances for the Four M Cation Sites

	M1	M1(1)	M2	M2(1)
O1(1)	2.132(5) Å	1.951(4) Å	2.360(5) Å	Å
O1(2)	2.062(4)	2.010(5)		2.394(5)
O2(1)		1.900(5)	2.370(4)	
O2(2)	2.019(5)			2.390(4)
O3(1)			2.703(5)	2.482(4)
O3(2)			2.468(4)	2.777(4)
Mean of 6	2.071	1.954	2.399	2.422
Mean of 8			2.475	2.511

* The standard deviations in parentheses are expressed in the unit of the last digit stated.

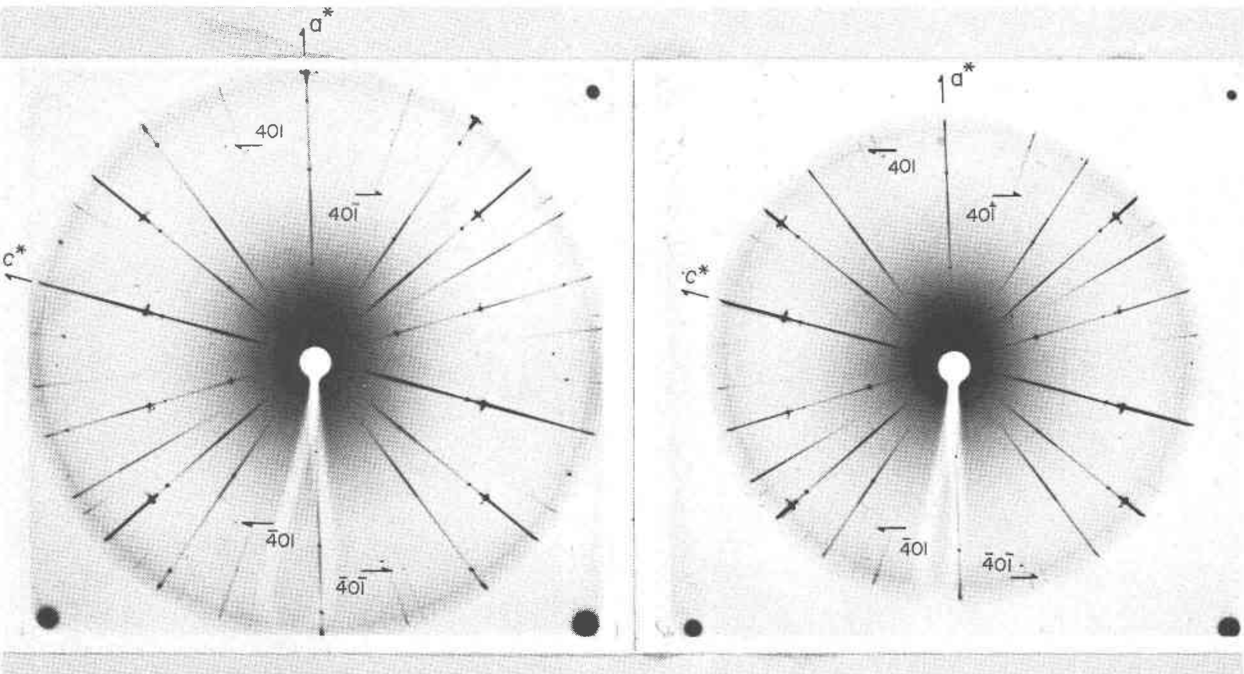

FIG. 2. Precession photographs of $h0l$ *for* $P2/n$ omphacite from California. {*402*} reflections violating $h+k$/even in $h0l$ are shown by arrows in the photograph taken with $\mu=30°$ (left). All {*401*} reflections are not observed in the photograph taken with $\mu=25°$ (right). Both photographs were exposed more than 100 hours with Cu$K\alpha$ radiation of 100 mA.

the *h0l* net observed in the earlier experiment are multiple reflections (Azároff, 1968) and the true space group of the Californian omphacite is not *P*2 but *P*2/*n*. The *h0l* electron diffraction pattern of the Californian omphacite presented by Phakey and Ghose (1973, Fig. 1c) also gives evidence for the presence of an *n*-glide, indicating that the true space group is *P*2/*n*.

The Mössbauer spectrum of the *P*2/*n* omphacites described in the present paper has been reported by Matsui, Syono, and Maeda (1972). The spectrum was similar to those of the *P*2 omphacites reported by Bancroft, Williams, and Essene (1969) with broad absorption bands due to Fe^{2+}. In the calcium-rich pyroxenes, the broad peaks due to Fe^{2+} are better interpreted as due to the variety of local configurations around Fe^{2+} rather than in terms of superposed peaks of Fe^{2+} in nonequivalent positions (Williams *et al*, 1971; Matsui *et al*, 1972; Dowty and Lindsley, 1973). Thus, although it is not possible to decide uniquely the space group of the Ca-rich pyroxenes by the Mössbauer spectrum alone, it is highly probable that the omphacites reported by Bancroft *et al* (1969) actually have the space group *P*2/*n*.

A statistical study of the distribution of crystalline substances with known space groups has shown that only two out of 5572 inorganic crystals are reported to have the *P*2 symmetry (Nowacki, Matsumoto, and Edenharter, 1967a,b). Moreover, the two *P*2 substances, metahewettite and quenselite, have since been found to possess the space groups $P2_1/m$ (Donnay and Ondik, 1973) and $P2_1/c$ (Povarennykh, 1972), respectively. In this statistical distribution, most groups with polar axes (C^x_{2v}, C^x_{4v} and C^x_{6v}) do not appear, and the crystals with only a pure rotation axis (*P*2, *P*3, *P*4, and *P*6), not with a screw axis, are very rare. It therefore seems very unlikely that omphacite would have a rare space group such as *P*2.

In fact, the Bessi omphacite in this study and the Fergusson omphacite (Kanazawa and Matsumoto, 1971) show *P*2/*n* symmetry, and the reexamination of the Californian omphacite reveals that this also has *P*2/*n* symmetry. Although the New Caledonian omphacite with the composition between jadeite and hedenbergite (Black, 1972) and the Venezuela omphacite (Fe-free) were reported to be *P*2, probably all reported *P*2 omphacites actually possess *P*2/*n* symmetry.

Acknowledgments

We thank Professor Y. Iitaka of Tokyo University for his kind assistance with the computation problems; Dr. S. Banno of Kanazawa University and Dr. J. R. Clark of the U.S. Geological Survey for providing with omphacite specimens and the geological information on the specimens; Dr. Y. Matsui of Okayama University for discussions on the Mössbauer spectrum on omphacite; and Mr. M. Kitamura of Tohoku University for his help in computation. We express our thanks to Dr. Malcolm Ross of the U.S. Geological Survey for reviewing the manuscript and providing numerous suggestions for its improvement. Thanks are also due to Mr. Nakamura, Miss Kino, and Miss Hirano for preparing figures and tables and for typing the manuscript. Part of the expenses of this work were defrayed by a research grant from the Ministry of Education of the Japanese Government.

References

AZÁROFF, L. U. (1968) *Elements of X-Ray Crystallography*. McGraw-Hill Book Co., New York, p. 295.

BANCROFT, G. M., P. G. L. WILLIAMS, AND E. J. ESSENE (1969) Mössbauer spectra of omphacites. *Mineral. Soc. Am. Spec. Pap.* **2**, 59–65.

BANNO, S. (1970) Classification of eclogites in terms of physical condition of their origin. *Phys. Earth Planet. Interiors*, **3**, 405–421.

BLACK, PHILLIPPA M. (1970) *P*2 omphacite, intermediate in composition between jadeite and hedenbergite, from metamorphosed acid volcanics, Bouehndep, New Caledonia. *Am. Mineral.* **55**, 512–514.

BROWN, WILLIAM L. (1972) La symetrie et les solutions solides des clinopyroxenes. *Bull. Soc. fr. Mineral. Crystallogr.* **95**, 574–582.

BURNHAM, CHARLES W., JOAN R. CLARK, J. J. PAPIKE, AND C. T. PREWITT (1967) A proposed crystallographic nomenclature for clinopyroxene structures. *Z. Kristallogr.* **125**, 109–119.

BUSING, W. R., K. O. MARTIN, AND H. A. LEVY (1962) ORFLS, a Fortran crystallographic least-squares program. *U.S. Natl. Tech. Inform. Serv.*, **ORNL-TM-305.**

CHAMPNESS, PAMELA E. (1973) Speculation on an order-disorder transformation in omphacite. *Am. Mineral.* **58**, 540–542.

CLARK, JOAN R., AND J. J. PAPIKE (1966) Eclogitic pyroxenes, ordered with *P*2 symmetry. *Science*, **154**, 1003–1004.

———, AND ——— (1968) Crystal-chemical characterization of omphacites. *Am. Mineral.* **53**, 840–868.

———, D. E. APPLEMAN, AND J. J. PAPIKE (1969) Crystal-chemical characterization of clinopyroxenes based on eight new structure refinements. *Mineral. Soc. Am. Spec. Pap.* **2**, 31–50.

COLEMAN, R. G., D. E. LEE, L. B. BEATTY, AND W. W. BRANNOCK (1965) Eclogites and eclogites: their differences and similarities. *Geol. Soc. Am. Bull.* **76**, 483–508.

CROMER, DON T., AND J. T. WEBER (1965) Scattering factors computed from relativistic Dirac-Slater wave functions. *Acta Crystallogr.* **18**, 104–109.

DONNAY, J. D. H., AND H. M. ONDIK (1973) *Crystal Data.* U.S. Dep. Commerce, Nat. Bur. Stand. & JCPDS, **M-211.**

DOWTY, E., AND D. H. LINDSLEY (1973) Mössbauer spectra of synthetic hedenbergite-ferrosilite pyroxenes. *Am. Mineral.* **58**, 850–868.

FINGER, L. W. (1969) Determination of cation distribution by least-squares refinement of single-crystal X-ray data. *Carnegie Inst. Wash. Year Book*, **67**, 216–217.

GRAHAM, J. (1974) Alternation in spodumene and its bearing on the space group problem. *Abstr. Int. Crystallogr. Conf. on Diffraction Studies of Real Atoms and Real Crystals*, p. 163.

KANAZAWA, Y., AND T. MATSUMOTO (1971) The X-ray study for a few clinopyroxenes. *Congr. Mineral. Soc. Japan, (Abstr.).*

LINDEMANN, W. (1961) Gitterkonstanten, Raumgruppe und Parameter des γ-$MgSiO_3$. *Naturwissenschaften,* **48,** 428–429.

MAC GILLAVRY, C. H., AND G. D. RIECK (1962) *International Tables for X-ray Crystallography,* Vol. **3,** The Kynoch Press, Birmingham.

MATSUI, Y., Y. SYONO, AND Y. MAEDA (1972) Mössbauer spectra of synthetic and natural calcium-rich clinopyroxenes. *Mineral. J.* **7,** 88–107.

MATSUMOTO, T., AND S. BANNO (1970a) A natural pyroxene with the space group C^4_{2h}-$P2/n$. *Proc. Japan Acad.* **46,** 173–175.

———, AND ——— (1970b) $P2/n$-omphacite and the possible space groups of clinopyroxenes. *IMA-IAGOD Meeting 1970, Collect. Abstr.,* p. 171.

———, M. TOKONAMI, AND N. MORIMOTO (1972) On the crystal structure of omphacite. *Acta Crystallogr.* **A28,** 71.

MORIMOTO, N., AND M. TOKONAMI (1969) Domain structure of pigeonite and clinoenstatite. *Am. Mineral.* **54,** 725–740.

NOWACKI, W., T. MATSUMOTO, AND A. EDENHARTER (1967a) Classification of crystalline substances by crystal systems, crystal classes, Bravais lattices, and space groups. *Acta Crystallogr.* **22,** 935–940.

———, A. EDENHARTER, AND T. MATSUMOTO (1967b) *Crystal Data, Systematic Tables. Am. Crystallogr. Assoc.,* New York.

PHAKEY, P. P., AND S. GHOSE (1973) Direct observation of antiphase domain structure in omphacite. *Contrib. Mineral. Petrol.* **39,** 239–245.

POVARENNYKH, A. S. (1972) *Crystal Chemical Classification of Minerals.* Plenum Press, New York-London, p. 329.

SMITH, J. V. (1969) Crystal structure and stability of the $MgSiO_3$ polymorphs: Physical properties and phase relations of Mg,Fe pyroxenes. *Mineral Soc. Am. Spec. Pap.* **2,** 3–29.

WARREN, B. E., AND W. L. BRAGG (1928) The structure of diopside, $CaMgSi_2O_6$. *Z. Kristallogr.* **69,** 168–193.

WILLIAMS, P. G. L., G. M. BANCROFT, M. G. BOWN, AND A. C. TURNOCK (1971) Anomalous Mössbauer spectra of $C2/c$ clinopyroxenes. *Nature Phys. Sci.* **230,** 149–151.

Manuscript received, July 29, 1974; accepted for publication, February 13, 1975.