Zeitschrift für Kristallographie, Bd. 127, S. 291—308 (1968)

The crystal structure of parawollastonite

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(Received November 2, 1967)

Auszug

Parawollastonit kristallisiert in der Raumgruppe $P2_1/a$ mit folgenden Gitterkonstanten: $a = 15.426$ Å, $b = 7.320$ Å, $c = 7.066$ Å und $\beta = 95°24'15''$. MAMEDOV und BELOVS Koordinaten für Wollastonit, bezogen auf eine doppelte monokline Elementarzelle, wurden verwendet, um vorläufige Strukturfaktoren zu berechnen. Mit Hilfe der Methode der kleinsten Quadrate ergaben sich wesentliche Änderungen in den Koordinaten, so daß sich der R-Wert von anfänglich 52% auf 6,6% verringerte. Einige Autoren haben über ungewöhnliche systematische Auslöschungen, welche nicht durch die Raumgruppe hervorgerufen werden, berichtet. Im Laufe der Untersuchung stellte es sich heraus, daß diese Reflexe nicht ausgelöscht sind, sondern nur sehr schwache Intensität haben.

Abstract

Parawollastonite crystallizes in space group $P2_1/a$ with following cell dimensions: $a = 15.426$ Å, $b = 7.320$ Å, $c = 7.066$ Å, and $\beta = 95°24'15''$. MAMEDOV and BELOV's coordinates for wollastonite, as referred to a doubled monoclinic cell, were used to compute a preliminary set of structure factors for parawollastonite. These coordinates yielded an R value of 52%. Refinement by least squares produced substantial changes in the coordinates which reduced the R value to 6.6%. Unusual systematic absences not required by the space group, reported by previous investigators, turned out not to be true extinctions but rather very weak intensities.

Introduction

Using WARREN's (1931) results of an x-ray investigation of wollastonite, PEACOCK (1935) concluded that two phases of calcium metasilicate exist: triclinic wollastonite and monoclinic parawollastonite. In an attempt to solve the structure of the monoclinic variety, BARNIK (1936) proposed $[Si_3O_9]^{-6}$ rings as the main structural feature for parawollastonite. He also reported the systematic absence of *hkl* reflections of the type $2h + k = 4n + 2$, which are not required by space group $P2_1/a$. His proposal was strongly criticized, mainly because the ring structure could not explain the fibrous character of the crystals.

Structures of several compounds similar to calcium metasilicate were solved by a number of investigators, suggesting that wollastonite as well as parawollastonite have chains of SiO_4 tetrahedra. With the aid of direct methods, MAMEDOV and BELOV (1956) were able to determine the structure of wollastonite in which $[SiO_3]^{-2}$ chains parallel to the *b* axis were found to be a basic structural feature. They used two-dimensional film data and indexed only the strong reflections of layers with *k* even. Their indexing was based on both a triclinic cell, $P\bar{1}$, and on a double monoclinic cell $P2_1/a$. The strong reflections satisfied the condition $2h + k = 4n$; this characterization bears a kind of complementary relation to BARNIK's systematic absence of $2h + k = 4n + 2$, but is not equivalent to it. The Russian authors reported an *R* value of 24⁰/₀ for the strong *h0l* reflections.

TOLLIDAY (1958) proposed a structure for monoclinic parawollastonite. She started the refinement using the centric space group $P2_1/a$. This attempt was not satisfactory, so $P2_1/a$ was replaced by the noncentric space group $P2_1$. After making this change, TOLLIDAY reported that the refinement was progressing well. Unfortunately no coordinates, structure factors, or *R* values were published, so that the validity of her findings can be appraised. In the view of this unsatisfactory state of affairs, a reinvestigation of the structure of parawollastonite appeared desirable.

Material and experimental data

Wollastonite and parawollastonite are often intergrown. Continuous streaks sometimes appear along the a^* direction as seen on precession photographs of odd levels of index *k*, such as *h1l*, *h3l*, etc. JEFFERY (1953) explained this diffration effect in terms of disorder due to stacking faults of alternating sheets of monoclinic and triclinic cells along *b*.

A specimen of parawollastonite crystals from Crestmore, California was kindly provided by Dr. CHARLES T. PREWITT. The crystal used in the present data collection was carefully examined and no continuous streaks or diffuse reflections due to disorder were found.

The space group determined from precession photographs is $P2_1/a$, which is consistent with BARNIK's (1936) result. In addition

Table 1. *Cell dimensions of parawollastonite*

Parameter	BARNIK (1936)	TOLLIDAY (1958)	Present work
a	15.33 Å	15.417 ± 0.004 Å	15.426 ± 0.004 Å
b	7.28	7.321 ± 0.002	7.320 ± 0.003
c	7.07	7.066 ± 0.002	7.066 ± 0.003
β	95°24′30″	95°24′ ± 3′	95°24′15″ ± 50″

to the extinctions caused by the screw axis and the glide plane, reflections *hkl* with $2h + k = 4n + 2$, were found to be very weak or sometimes absent.

Precise lattice constants were obtained by evaluating data from back-reflection Weissenberg films. These data were refined by the least-squares method. The dimensions for the cell of parawollastonite are given in Table 1, which shows that the new values are in good agreement with results published by BARNIK (1936), and by TOLLIDAY (1958).

Nickel-filtered Cu$K\alpha$ radiation was used to record 1290 reflections with an equi-inclination single-crystal diffractometer. In order to obtain accurate experimental data, a proportional counter was employed in connection with pulse-height discrimination. The integrated intensities were improved by correcting for residual white radiation which could not be eliminated through pulse-height discrimination and the Ni filter. The method applied is similar to the procedure outlined by LARSON (1965). These data were corrected for Lorentz and polarization factors as well as for absorption.

Refinement

The coordinates published by MAMEDOV and BELOV (1956) for wollastonite, as referred to a double monoclinic cell, were tested with the present data and a preliminary set of structure factors calculated. With a proper scale factor and an overall isotropic temperature factor of $B = 0.6$ Å^2, R had the rather large value of 52%. MAMEDOV and BELOV's atomic parameters are presented in Table 2. With the exception of their Si I, Si I′, O IV, and O IV′, all positions listed in this table have y coordinates of $(2n + 1)/8$; these coordinates require absences of *hkl* reflections with $2h + k = 4n + 2$. TOLLIDAY (1958) reported having observed this extinction rule. Table 3 gives a representative sample of observed and computed structure factors for those reflections. This table shows that the nonspace-group extinctions are almost obeyed by MAMEDOV and BELOV's model for wollastonite.

Table 2

MAMEDOV *and* BELOV's *coordinates for wollastonite based upon a monoclinic cell*

Atom	x	y	z	Atom	x	y	z
Ca I	0.250	0.375	0.000	O II	0.345	0.125	0.047
Ca II	0.602	0.375	0.263	O II′	0.345	0.625	0.047
Ca II′	0.602	0.875	0.263	O III	0.507	0.125	0.229
Si I	0.406	0.080	0.232	O III′	0.507	0.625	0.229
Si I′	0.406	0.670	0.232	O IV	0.362	0.198	0.406
Si II	0.300	0.375	0.443	O IV′	0.362	0.552	0.406
O I	0.297	0.375	0.667	O V	0.406	0.875	0.232
O I′	0.297	0.875	0.667				

Table 3. *Some observed structure factors with corresponding structure factors based on* MAMEDOV *and* BELOV*'s coordinates and the final refined F_c's for parawollastonite*
Indices with an asterisk refer to "absences" in hkl with $2h + k = 4n + 2$.
All structure factors are in electron units

h k l	F_o parawol-lastonite	F_c Mamedov, Belov	F_c parawol-lastonite	h k l	F_o parawol-lastonite	F_c Mamedov, Belov	F_c parawol-lastonite	h k l	F_o parawol-lastonite	F_c Mamedov, Belov	F_c parawol-lastonite
2 4 0	31.48	57.00	28.17	5 6 0	37.82	-83.52	-34.56	4 4 1	7.03	-32.25	-7.94
* 3	2.00	0.00	-3.80	* 6	0.00	0.00	0.86	-1	25.60	12.49	-25.65
4	38.48	38.24	35.15	7	46.97	-24.68	-45.30	* 5 4 1	1.25	0.04	5.38
* 5	0.00	0.00	-0.26	* 8	0.00	0.00	-5.65	* -1	1.40	0.14	2.13
6	97.96	32.42	97.84	9	52.89	-33.86	-52.43	6 4 1	25.85	-20.39	21.41
* 7	1.48	0.00	1.39	*10	3.11	0.00	-7.54	-1	31.19	74.60	31.80
8	55.76	-92.45	-52.66	0 4 1	43.24	41.01	-36.55	* 7 4 1	0.00	0.14	2.10
* 9	4.02	0.00	1.24	-1	43.59	-41.01	-36.55	* -1	2.21	-0.10	-3.70
10	109.23	-64.59	-114.13	* 1 4 1	1.67	0.02	3.11	8 4 1	98.31	-57.32	-99.14
*11	1.94	0.00	-2.60	* -1	2.02	0.18	0.81	-1	42.36	-81.02	-39.91
12	60.41	13.82	-59.62	2 4 1	60.81	76.14	60.93	* 9 4 1	3.27	-0.06	3.48
*13	4.11	0.00	-1.98	-1	24.20	-44.97	-23.13	* -1	4.82	-0.08	2.37
* 2 6 0	1.40	0.00	-2.99	* 3 4 1	3.02	-0.18	5.84				
* 4	0.71	0.00	-2.55	* -1	0.60	0.08	-5.47				

Actually, as observed in the present investigation, the structure amplitudes of the reflections corresponding to this extinction rule, although small, are not zero.

TOLLIDAY's view that the parawollastonite structure should be refined in the noncentric space group $P2_1$ was tried without success. Accordingly space group $P2_1/a$ was retained and several cycles of least-squares refinement were carried out. An equal weighting scheme was employed and the scattering curves were corrected for anomalous dispersion. Allowing all parameters to vary, the best R value with isotropic temperature factors was $8.4\,^0/_0$.

At this stage of the investigation it became evident that the shifts performed by the least-squares refinement showed no tendency to locate atoms on positions responsible for the nonspace-group extinctions. In continuing the refinement, a weighting scheme was introducted based on a weighting factor $w = |F_{\text{obs}}|$, described by DE VRIES (1965). With anisotropic thermal parameters the final R values were obtained: R (unweighted) $= 6.6\,^0/_0$, R (weighted) $= 4.9\,^0/_0$. The observed and the final calculated structure factors are listed in Table 4.

Table 4. *Observed and calculated structure factors for parawollastonite*

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
5	0	0	0	0.0	10	1	0	- 4.9	- 3.9	15	1	3	11.9	12.7	6	1	7	- 17.8	- 14.2
6	0	0	-110.0	-119.6	11	1	0	3.2	5.3	0	1	-4	- 56.4	- 54.2	6	1	-7	19.5	19.6
7	0	0	0	0.0	12	1	0	5.9	7.7	0	1	4	56.6	54.2	7	1	7	13.2	13.1
8	0	0	109.0	111.9	13	1	0	- 18.4	- 17.1	1	1	-4	29.8	27.5	7	1	-7	- 22.4	- 23.2
9	0	0	0	0.0	14	1	0	- 42.6	- 41.0	1	1	4	- 70.7	- 66.5	8	1	7	20.1	21.1
10	0	0	153.0	142.1	15	1	0	39.2	38.6	2	1	-4	14.0	13.6	8	1	-7	- 25.8	- 25.5
11	0	0	0	0.0	0	1	-1	- 20.5	- 18.2	2	1	4	- 70.4	- 65.6	9	1	-7	25.9	25.7
13	0	0	0	0.0	0	1	1	21.0	18.2	3	1	-4	- 15.7	- 14.3	9	1	7	- 36.9	- 38.0
14	0	0	- 53.2	- 50.4	1	1	-1	- 14.4	- 10.1	3	1	4	47.8	44.6	10	1	-7	21.9	21.9
15	0	0	0	0.0	1	1	1	- 27.1	- 24.1	4	1	-4	- 21.6	- 19.3	11	1	-7	- 16.6	- 17.7
2	0	-1	- 28.5	- 22.6	2	1	-1	- 51.7	- 43.1	4	1	4	7.9	6.6	12	1	-7	- 11.9	- 14.1
2	0	1	- 20.4	- 23.3	2	1	1	- 22.7	- 20.8	5	1	-4	25.4	22.0	2	2	0	0	2.7
4	0	-1	59.7	57.4	3	1	-1	72.0	63.4	5	1	4	7.5	5.1	3	2	0	-317.3	-306.8
4	0	1	49.8	50.4	3	1	1	11.6	10.4	6	1	-4	14.5	13.1	4	2	0	2.3	3.9
6	0	-1	- 14.2	- 9.6	4	1	-1	58.8	52.3	6	1	4	1.7	2.2	5	2	0	119.8	119.2
6	0	1	- 82.4	- 84.5	4	1	1	17.0	16.1	7	1	-4	- 1.5	- 1.5	6	2	0	4.5	0.6
8	0	-1	33.5	30.5	5	1	-1	- 21.8	- 18.4	7	1	4	3.5	3.3	7	2	0	114.5	112.8
8	0	1	95.9	96.6	5	1	1	- 37.9	- 36.7	8	1	-4	14.2	13.6	8	2	0	12.4	2.8
10	0	-1	- 57.8	- 56.6	6	1	-1	- 1.8	- 0.3	8	1	4	19.2	19.1	9	2	0	67.8	66.4
12	0	-1	123.6	131.0	6	1	1	- 42.8	- 41.0	9	1	-4	- 15.8	- 16.4	10	2	0	6.6	3.4
14	0	1	- 41.8	- 39.8	7	1	-1	- 8.0	- 7.6	9	1	4	- 16.7	- 16.0	11	2	0	10.6	8.0
0	0	-2	-159.4	-160.7	7	1	1	40.6	38.2	10	1	-4	- 9.4	- 9.6	12	2	0	3.4	1.5
0	0	2	-159.4	-160.7	8	1	-1	0	- 0.5	11	1	-4	6.6	6.3	13	2	0	- 69.8	- 68.4
2	0	2	-205.6	-193.6	8	1	1	24.6	23.9	12	1	-4	- 7.4	- 1.2	14	2	0	6.8	0.2
4	0	-2	104.5	106.8	9	1	-1	- 18.6	- 16.1	12	1	4	- 8.6	- 9.1	15	2	0	- 61.8	- 60.4
4	0	2	119.5	129.2	9	1	1	0	2.3	13	1	4	1.8	2.5	0	2	-1	- 2.7	- 1.1
6	0	-2	99.3	99.6	10	1	-1	- 11.7	- 9.7	13	1	-4	3.8	5.1	0	2	1	- 2.6	- 1.1
8	0	-2	24.5	20.7	10	1	1	7.4	5.7	14	1	4	- 25.3	- 23.3	1	2	-1	- 49.5	- 39.1
8	0	2	- 49.6	- 50.5	11	1	-1	- 7.0	- 6.9	14	1	-4	6.5	8.3	1	2	1	4.9	3.0
12	0	2	- 34.2	- 33.9	11	1	1	4.4	3.1	15	1	-4	- 15.8	- 17.0	2	2	-1	3.4	3.0
12	0	-2	- 49.2	- 47.3	12	1	-1	- 23.4	- 22.4	15	1	4	26.8	24.7	2	2	1	- 2.9	- 1.4
14	0	-2	- 6.2	- 1.3	12	1	1	1.3	1.3	0	1	-5	- 5.2	- 4.3	3	2	-1	- 72.9	- 67.5
14	0	2	75.4	74.2	13	1	-1	39.8	38.9	0	1	5	5.7	4.3	3	2	1	13.5	13.6
0	0	-3	122.2	114.4	13	1	1	- 10.9	- 9.1	1	1	-5	12.4	13.4	4	2	-1	0	2.7
0	0	3	123.5	114.4	14	1	-1	39.7	37.9	2	1	-5	8.4	10.2	4	2	1	0	1.2
2	0	-3	-204.3	-207.7	14	1	1	- 3.5	- 1.8	2	1	5	14.3	13.0	5	2	-1	- 57.6	- 50.4
2	0	3	29.8	25.4	15	1	-1	- 24.2	- 24.2	3	1	-5	- 8.2	- 9.2	6	2	-1	0	- 3.6
4	0	-3	64.7	59.9	15	1	1	- 16.1	- 16,1	3	1	5	- 19.9	- 17.0	6	2	1	0	0.5
4	0	3	- 51.1	- 46.9	0	1	-2	- 44.7	- 40.1	4	1	-5	- 16.0	- 16.5	7	2	-1	-111.3	-109.7
6	0	-3	- 16.6	- 16.0	0	1	2	45.3	40.1	4	1	5	- 3.6	- 2.6	7	2	1	- 67.7	- 64.2
6	0	3	- 42.7	- 39.8	1	1	-2	85.8	75.0	5	1	-5	28.9	27.5	9	2	-1	96.5	98.1
8	0	-3	47.0	49.4	1	1	2	- 4.2	- 3.2	5	1	5	- 25.6	- 26.0	9	2	1	59.8	55.2
8	0	3	54.3	54.4	2	1	-2	87.9	79.3	6	1	-5	37.0	36.7	10	2	1	0	0.2
10	0	-3	- 96.6	- 98.7	2	1	2	23.5	20.4	6	1	5	- 37.5	- 37.7	11	2	-1	- 39.2	- 39.4
10	0	3	0	- 2.2	3	1	-2	- 61.7	- 55.2	7	1	-5	- 42.6	- 43.3	11	2	1	- 60.6	- 58.0
12	0	-3	- 12.4	- 10.9	3	1	2	- 21.1	- 17.7	7	1	5	48.3	48.2	12	2	-1	3.7	1.6
12	0	3	35.0	33.8	4	1	-2	- 20.1	- 19.1	8	1	-5	- 40.7	- 43.5	12	2	1	0	0.2
2	0	-4	121.9	119.4	4	1	2	8.3	9.9	8	1	5	40.5	40.8	13	2	-1	- 19.6	- 21.3
2	0	4	- 39.8	- 36.9	5	1	-2	0	3.4	9	1	-5	40.8	43.5	13	2	1	101.3	102.1
4	0	-4	- 69.5	- 68.2	5	1	2	- 14.4	- 14.9	9	1	5	- 19.4	- 19.5	14	2	-1	- 3.4	- 1.2
4	0	4	- 39.6	- 37.8	6	1	-2	8.2	8.9	10	1	-5	40.9	42.8	14	2	1	- 7.9	- 1.0
6	0	-4	- 99.5	- 99.2	6	1	2	- 5.9	- 6.5	10	1	5	- 21.0	- 20.4	15	2	-1	- 87.7	- 83.9
8	0	-4	- 23.4	- 18.5	7	1	-2	- 26.4	- 24.7	11	1	5	25.9	25.0	15	2	1	7.5	7.4
10	0	-4	93.6	97.3	7	1	2	- 2.9	- 1.9	11	1	-5	- 40.7	- 41.6	0	2	-2	- 3.0	- 5.2
10	0	4	91.5	93.7	8	1	-2	- 38.8	- 36.5	12	1	5	26.0	25.2	0	2	2	- 3.9	- 5.2
12	0	-4	125.7	138.4	8	1	2	- 19.0	- 17.6	12	1	-5	- 36.3	- 35.7	1	2	-2	70.2	66.7
12	0	4	45.5	45.8	9	1	-2	30.9	30.3	13	1	5	- 36.5	- 36.1	2	2	-2	0	- 3.1
14	0	-4	- 89.1	- 89.3	9	1	2	14.5	12.9	13	1	-5	28.5	28.0	2	2	2	0	- 3.6
14	0	4	- 53.1	- 49.3	10	1	-2	9.6	7.1	14	1	5	- 29.8	- 28.7	3	2	-2	81.3	76.4
0	0	-5	58.5	54.2	10	1	2	- 2.9	- 4.2	14	1	-5	20.2	18.0	3	2	2	81.9	82.4
0	0	5	57.9	54.2	11	1	-2	9.3	8.9	15	1	-5	- 3.5	- 4.5	4	2	-2	2.4	0.3
2	0	5	28.1	25.1	11	1	2	10.2	8.9	0	1	-6	- 39.8	- 38.3	4	2	2	2.6	1.4
6	0	-5	- 33.7	- 34.4	12	1	-2	18.3	17.2	0	1	6	39.6	38.3	5	2	-2	115.0	117.1
6	0	5	33.5	36.4	12	1	2	17.6	16.5	1	1	-6	45.5	44.0	5	2	2	65.0	65.9
8	0	-5	33.2	32.6	13	1	-2	- 20.0	- 19.8	1	1	6	- 41.5	- 40.2	6	2	-2	- 1.9	- 2.0
10	0	-5	- 22.7	- 23.0	13	1	2	- 16.6	- 15.7	2	1	-6	42.5	41.6	6	2	2	0	- 2.4
10	0	5	- 60.8	- 58.9	14	1	-2	- 5.9	- 6.0	2	1	6	- 36.0	- 34.7	8	2	2	0	- 3.8
12	0	-5	68.8	64.8	14	1	2	- 5.3	- 2.6	3	1	-6	- 27.8	- 28.2	9	2	2	- 90.2	- 88.7
12	0	5	11.3	8.3	15	1	2	9.8	8.6	3	1	6	39.1	39.0	10	2	2	0	- 1.8
14	0	5	- 11.1	- 9.1	15	1	-2	3.3	2.7	4	1	-6	- 22.6	- 23.6	11	2	-2	- 28.0	- 27.1
0	0	-6	-117.5	-117.2	0	1	-3	34.3	29.4	4	1	6	49.2	49.0	11	2	2	59.3	57.5
0	0	6	-114.7	-117.2	0	1	3	- 34.4	- 29.4	5	1	-6	16.0	17.2	12	2	2	0	- 0.6
2	0	-6	-131.5	-136.6	1	1	-3	- 28.0	- 24.2	5	1	6	- 38.2	- 37.9	12	2	-2	- 3.8	- 1.1
2	0	6	1.7	1.9	1	1	3	15.6	12.1	6	1	-6	12.5	12.6	13	2	-2	121.3	126.2
4	0	-6	66.2	63.5	2	1	-3	11.1	10.1	6	1	6	- 22.8	- 22.9	13	2	2	109.4	108.2
6	0	-6	95.4	96.2	2	1	3	- 12.7	- 12.4	7	1	-6	- 14.4	- 13.5	15	2	-2	- 16.7	- 13.7
6	0	6	8.8	1.8	3	1	-3	- 37.9	- 34.2	7	1	6	12.1	12.8	0	2	-3	- 1.7	- 1.8
8	0	-6	14.5	11.0	3	1	3	48.6	44.5	8	1	6	- 8.1	- 6.4	0	2	3	- 1.7	- 1.8
8	0	6	- 53.2	- 52.6	4	1	-3	- 43.3	- 40.0	8	1	-6	- 6.7	- 6.4	1	2	-3	15.8	14.5
12	0	6	- 22.0	- 22.8	4	1	3	55.9	52.1	9	1	-6	0	2.2	1	2	3	65.8	61.3
12	0	-6	- 20.5	- 17.4	5	1	-3	27.9	26.3	9	1	6	4.6	3.9	2	2	-3	- 2.6	- 2.0
14	0	-6	- 32.9	- 32.7	5	1	3	- 39.1	- 36.9	10	1	6	- 8.6	- 9.8	2	2	3	3.1	0.3
0	0	-7	38.8	38.3	6	1	-3	5.9	6.8	10	1	-6	- 5.9	- 5.9	3	2	-3	11.4	8.1
0	0	7	38.3	38.3	6	1	3	- 30.5	- 29.6	11	1	6	8.1	10.0	3	2	3	-121.7	-121.8
2	0	7	- 20.0	- 18.0	7	1	-3	- 2.8	- 3.7	11	1	-6	7.2	6.4	4	2	-3	0	0.7
4	0	-7	- 8.1	- 8.0	7	1	3	22.2	22.3	12	1	6	17.1	19.2	4	2	3	0	0.7
4	0	7	- 8.1	- 9.1	8	1	-3	- 6.2	- 5.0	12	1	-6	- 3.8	- 3.5	6	2	3	0	- 2.4
6	0	-7	0	3.8	8	1	3	25.5	25.4	13	1	-6	8.9	7.4	6	2	-3	- 2.6	- 1.6
8	0	-7	16.3	16.5	9	1	-3	20.1	19.3	0	1	-7	- 11.8	- 12.7	7	2	-3	- 97.0	- 97.8
8	0	7	10.1	10.4	9	1	3	- 47.6	- 47.1	0	1	7	11.6	12.7	7	2	3	- 5.9	- 6.0
10	0	-7	3.5	1.4	10	1	-3	28.4	28.7	1	1	-7	12.8	13.0	8	2	-3	1.5	1.4
12	0	-7	- 54.4	- 55.3	10	1	3	- 41.4	- 41.6	1	1	7	- 9.9	- 11.1	8	2	3	0	- 1.7
2	1	0	12.9	7.9	11	1	-3	- 24.5	- 24.0	2	1	-7	25.1	24.9	9	2	-3	2.2	1.0
3	1	0	- 36.5	- 31.0	12	1	-3	- 24.1	- 24.2	2	1	7	- 4.1	- 6.3	9	2	3	15.8	15.1
4	1	0	- 61.2	- 55.1	12	1	3	26.1	25.9	3	1	-7	- 28.1	- 27.0	10	2	-3	0	0.4
5	1	0	60.3	53.2	13	1	-3	14.2	13.6	3	1	7	13.3	15.1	10	2	3	- 1.3	0.4
6	1	0	26.2	22.3	13	1	3	- 5.6	- 7.0	4	1	-7	- 24.1	- 24.1	11	2	-3	12.8	11.6
7	1	0	4.2	1.2	14	1	3	- 5.3	- 6.4	4	1	7	12.1	13.1	11	2	3	- 46.5	- 42.5
8	1	0	24.2	22.0	14	1	-3	7.8	6.6	5	1	-7	21.7	22.5	12	2	-3	0	- 1.0
9	1	0	- 25.1	- 23.5	15	1	-3	- 11.5	- 10.0	5	1	7	- 7.6	- 8.0	12	2	3	0	0.8

Table 4. *(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
13	2	-3	48.1	47.6	8	2	7	-1.1	-1.9	10	3	-3	22.3	20.7	1	3	7	27.5	29.3
13	2	3	4.1	3.4	10	2	-7	-0.8	-0.4	10	3	3	-28.6	-28.5	2	3	-7	-7.0	-7.5
14	2	-3	0	-1.1	11	2	-7	-11.1	-7.5	11	3	-3	25.7	25.6	2	3	7	-20.1	-22.6
14	2	3	0	-1.1	2	3	0	1.8	1.4	11	3	3	-24.5	-24.4	3	3	-7	6.5	6.4
15	2	-3	25.9	28.9	3	3	0	-8.7	-6.9	12	3	-3	-31.6	-33.2	3	3	7	-13.9	-16.1
15	2	3	-69.7	-67.9	4	3	0	6.4	4.3	12	3	3	31.9	32.7	4	3	-7	-30.9	-31.9
0	2	-4	1.6	2.9	5	3	0	-16.5	-13.1	13	3	-3	-13.7	-14.3	4	3	7	2.2	4.2
0	2	4	1.4	2.9	6	3	0	42.8	38.5	13	3	3	17.8	18.1	5	3	-7	-49.2	-51.1
1	2	-4	-5.0	-1.8	7	3	0	61.9	57.8	14	3	-3	-8.2	-8.1	5	3	7	0.7	2.3
1	2	4	-78.2	-77.1	8	3	0	-42.8	-40.4	14	3	3	-4.9	-5.8	6	3	-7	46.0	46.9
2	2	-4	0	2.0	9	3	0	-4.0	-0.2	15	3	-3	-13.2	-13.3	6	3	7	-17.3	-18.0
2	2	4	0.9	0.8	10	3	0	-35.1	-32.6	15	3	3	5.6	4.3	7	3	-7	24.4	25.0
3	2	-4	-104.8	-102.0	11	3	0	-59.5	-57.2	0	3	-4	-53.0	-50.5	7	3	7	-19.7	-19.0
4	2	-4	0	0.3	12	3	0	47.9	45.7	0	3	4	51.8	50.5	8	3	-7	-4.2	-4.9
4	2	4	0	1.9	13	3	0	16.1	14.5	1	3	-4	-65.4	-61.4	9	3	-7	3.8	3.6
6	2	-4	0	-0.4	14	3	0	-4.9	-5.4	1	3	4	19.7	18.3	10	3	-7	8.5	8.1
6	2	4	0	-0.5	15	3	0	-2.0	-2.0	2	3	-4	57.8	54.0	2	4	0	31.5	28.2
7	2	-4	87.4	87.0	0	3	-1	-6.3	-3.2	2	3	4	-3.8	-4.0	3	4	0	-2.0	-3.8
7	2	4	48.5	44.4	0	3	1	6.6	3.2	3	3	-4	27.8	24.5	4	4	0	38.5	35.2
8	2	-4	0	2.7	1	3	-1	-15.9	-12.6	3	3	4	-11.7	-11.9	5	4	0	0	-0.3
8	2	4	0	1.8	1	3	1	-5.0	-3.5	4	3	-4	1.3	2.5	6	4	0	98.0	97.8
9	2	4	69.6	69.4	2	3	-1	14.6	13.2	4	3	4	29.6	28.3	7	4	0	1.5	1.4
10	2	-4	1.8	3.2	2	3	1	-3.5	-4.0	5	3	-4	4.1	5.0	8	4	0	-55.8	-52.7
10	2	4	2.7	2.3	3	3	-1	-6.6	-4.0	5	3	4	50.0	49.1	9	4	0	4.0	1.2
11	2	-4	-8.6	-10.2	3	3	1	-11.5	-12.3	6	3	-4	5.6	6.8	10	4	0	-109.2	-114.1
11	2	4	-69.2	-63.4	4	3	-1	43.3	38.7	6	3	4	-41.4	-41.3	11	4	0	-1.9	-2.6
12	2	-4	0	0.2	4	3	1	17.1	18.0	7	3	-4	14.2	14.0	12	4	0	-60.4	-59.6
12	2	4	0	1.1	5	3	-1	67.9	60.6	7	3	4	-1.7	-3.7	13	4	0	-4.1	-2.0
13	2	-4	-43.5	-39.2	5	3	1	19.7	19.0	8	3	-4	-2.0	-2.3	14	4	0	55.0	55.2
14	2	-4	0	-1.1	6	3	-1	-69.4	-64.9	8	3	4	-18.3	-18.4	15	4	0	4.8	0.9
14	2	4	0	-0.4	6	3	1	-18.7	-16.7	9	3	-4	17.8	18.0	0	4	-1	-43.6	-36.6
15	2	-4	-91.1	-90.9	7	3	-1	-30.7	-29.1	9	3	4	-24.1	-25.4	0	4	1	-43.2	-36.6
15	2	4	10.6	8.2	7	3	1	-30.7	-28.0	10	3	-4	-26.5	-26.7	1	4	-1	2.0	0.8
0	2	-5	-0.7	-0.3	8	3	-1	-17.2	-15.5	10	3	4	16.6	17.2	1	4	1	1.7	3.1
0	2	5	0	-0.3	8	3	1	45.2	42.2	11	3	-4	-20.5	-20.7	2	4	-1	-24.2	-23.1
1	2	-5	-13.8	-12.0	9	3	-1	-34.5	-33.3	11	3	4	-14.1	-12.0	2	4	1	60.8	60.9
1	2	5	-16.3	-19.1	9	3	1	32.9	30.7	12	3	-4	-3.9	-4.3	3	4	-1	-0.6	-5.5
2	2	-5	0.9	2.2	10	3	-1	38.5	37.5	12	3	4	21.9	19.8	3	4	1	3.0	5.8
2	2	5	0	-0.7	10	3	1	-16.8	-16.0	13	3	-4	-27.7	-29.6	4	4	-1	-25.6	-25.7
3	2	-5	-82.2	-80.8	11	3	-1	20.0	19.5	13	3	4	16.3	14.3	4	4	1	7.0	2.1
3	2	5	15.5	12.3	11	3	1	4.8	5.9	14	3	-4	30.7	32.0	5	4	-1	-1.4	-7.9
4	2	-5	1.7	2.7	12	3	-1	0	1.9	14	3	4	-18.5	-18.7	5	4	1	1.3	5.4
4	2	5	0	1.4	12	3	1	-31.4	-31.4	15	3	-4	18.0	18.9	6	4	-1	31.2	31.8
5	2	-5	26.4	26.7	13	3	-1	0	-2.1	0	3	-5	13.0	11.3	6	4	1	25.9	21.4
5	2	5	47.3	45.6	13	3	1	-23.7	-23.5	0	3	5	-12.9	-11.3	7	4	-1	-2.2	-3.7
6	2	-5	-1.4	-1.4	14	3	-1	16.5	17.8	1	3	-5	-3.1	-2.7	7	4	1	0	2.1
6	2	5	0	1.9	14	3	1	3.0	4.1	1	3	5	-13.2	-10.1	8	4	-1	-42.4	-39.9
7	2	-5	-74.8	-71.7	15	3	-1	27.1	27.3	2	3	-5	8.1	9.8	8	4	1	-98.3	-99.1
7	2	5	37.5	40.0	15	3	1	-9.8	-8.4	2	3	5	-7.7	-9.8	9	4	-1	4.8	2.4
8	2	-5	0	-0.6	0	3	-2	11.2	8.9	3	3	-5	9.5	10.8	9	4	1	3.3	3.5
8	2	5	2.1	0.8	0	3	2	-10.7	-8.9	3	3	5	-19.2	-20.9	10	4	-1	54.7	52.7
9	2	-5	63.4	61.5	1	3	-2	21.0	19.3	4	3	-5	-4.5	-6.2	10	4	1	108.8	111.0
9	2	5	-20.7	-24.5	1	3	2	24.1	23.2	4	3	5	23.4	24.9	11	4	-1	0	-3.9
10	2	-5	0	0.6	2	3	-2	4.2	2.8	5	3	-5	-3.2	-5.0	12	4	-1	-95.3	-95.3
10	2	5	0	0.1	2	3	2	-47.2	-47.3	5	3	5	16.1	16.2	12	4	1	-22.7	-20.8
11	2	-5	8.6	6.2	3	3	-2	47.4	43.7	6	3	-5	21.2	22.0	13	4	-1	-4.7	-5.0
11	2	5	-25.4	-23.3	3	3	2	-40.0	-40.6	6	3	5	5.2	5.5	13	4	1	0	5.2
12	2	-5	0	1.8	4	3	-2	-84.3	-77.4	7	3	-5	48.8	49.7	14	4	-1	7.1	5.2
12	2	5	0	0.8	4	3	2	19.0	19.7	7	3	5	-2.6	-2.3	14	4	1	32.4	32.8
13	2	-5	-34.5	-36.6	5	3	-2	-75.5	-71.2	8	3	-5	-67.6	-69.7	15	4	-1	0	-3.2
14	2	-5	0	0.7	5	3	2	-14.4	-13.0	8	3	5	21.9	21.7	15	4	1	1.3	4.1
15	2	-5	-45.6	-46.5	6	3	-2	39.2	36.3	9	3	-5	-63.2	-65.1	0	4	2	113.6	103.0
0	2	-6	-0.5	-2.0	6	3	2	25.5	25.0	9	3	5	37.2	36.4	1	4	-2	0	3.7
1	2	-6	-10.9	-9.1	7	3	-2	-1.4	-2.5	10	3	-5	40.7	43.7	1	4	2	2.7	5.6
2	2	-6	0	0.2	7	3	2	10.7	9.4	10	3	5	-57.1	-57.7	2	4	2	95.1	93.4
2	2	6	0	-1.9	8	3	-2	15.1	14.5	11	3	-5	13.4	15.0	3	4	-2	0	1.7
3	2	6	31.1	27.8	8	3	2	-9.9	-8.9	11	3	5	-50.8	-51.2	3	4	2	0	3.2
4	2	-6	0	0.4	9	3	-2	4.7	4.0	12	3	-5	-4.4	-1.8	4	4	-2	-101.2	-97.2
4	2	6	0	1.0	9	3	2	-7.1	-6.4	12	3	5	25.8	26.5	4	4	2	-101.5	-106.2
5	2	-6	63.8	64.0	10	3	-2	7.8	8.8	13	3	-5	-8.4	-8.0	5	4	-2	0	-2.0
5	2	6	-26.3	-24.6	10	3	2	7.2	6.0	14	3	-5	27.0	27.1	5	4	2	0	-0.1
6	2	6	-2.2	-0.7	11	3	-2	15.6	16.1	15	3	-5	31.2	29.6	6	4	-2	-89.3	-87.4
7	2	-6	-92.9	-94.7	11	3	2	9.1	10.1	0	3	-6	-26.6	-26.9	6	4	2	-51.6	-52.6
7	2	6	-94.5	-98.4	12	3	-2	-3.2	-3.6	0	3	6	26.6	26.9	7	4	-2	-1.7	-2.4
8	2	-6	-1.7	-0.9	12	3	2	8.0	8.0	1	3	-6	-27.1	-27.2	7	4	2	-1.3	-2.0
8	2	6	0	-1.1	13	3	-2	18.0	20.0	1	3	6	41.0	41.3	8	4	-2	9.5	10.4
9	2	-6	-68.6	-68.2	13	3	2	28.9	29.8	2	3	-6	41.0	41.7	8	4	2	31.8	32.0
9	2	6	-7.2	-7.7	14	3	-2	-22.1	-22.9	2	3	6	-48.7	-48.2	9	4	-2	0	-0.2
10	2	-6	-1.3	-1.3	14	3	2	-33.7	-32.9	3	3	-6	46.7	48.0	9	4	2	0	2.1
10	2	6	0	-1.1	15	3	-2	-13.8	-12.2	3	3	6	-42.1	-41.6	10	4	2	129.3	140.6
11	2	-6	-44.6	-43.9	15	3	2	-29.4	-28.3	4	3	-6	-46.4	-47.7	11	4	2	0	2.9
11	2	6	59.7	58.8	0	3	-3	-44.6	-41.6	4	3	6	30.2	31.2	12	4	-2	11.7	11.5
12	2	-6	-2.7	-0.5	0	3	3	43.2	41.6	5	3	-6	-17.7	-18.1	12	4	2	26.6	27.4
13	2	-6	68.8	72.1	1	3	-3	-8.6	-8.1	5	3	6	5.1	6.5	13	4	-2	1.5	2.7
0	2	-7	0	-0.3	1	3	3	50.0	47.8	6	3	-6	-17.5	-17.2	13	4	2	0	0.8
0	2	7	0	-0.3	2	3	-3	-24.5	-21.6	6	3	6	-3.7	-4.6	14	4	-2	-5.7	-3.6
1	2	-7	19.4	15.9	2	3	3	-26.6	-25.0	7	3	-6	-26.8	-27.1	14	4	2	-45.6	-44.0
1	2	7	40.9	37.1	3	3	-3	-37.4	-33.6	7	3	6	-20.5	-22.9	15	4	-2	0	-1.7
2	2	7	-1.4	-0.1	3	3	3	-2.5	-1.5	8	3	-6	15.1	14.8	15	4	2	-1.2	-0.6
3	2	-7	7.1	9.8	4	3	3	-9.5	-9.8	8	3	6	24.9	27.0	0	4	-3	-73.8	-68.4
3	2	7	-47.3	-45.2	5	3	-3	-13.0	-13.8	9	3	-6	-14.2	-14.4	0	4	3	-71.4	-68.4
4	2	-7	0	-0.8	5	3	3	0	1.6	9	3	6	24.2	26.1	1	4	-3	0	3.3
4	2	7	0	0.1	6	3	-3	31.2	31.4	10	3	-6	32.2	32.6	1	4	3	3.5	0.6
5	2	7	-14.2	-11.5	6	3	3	-33.8	-33.8	10	3	6	-11.1	-12.7	2	4	-3	123.2	115.5
5	2	-7	54.4	53.4	7	3	-3	31.3	30.9	11	3	-6	29.1	28.9	2	4	3	-8.7	-7.1
6	2	7	-1.3	-1.4	7	3	3	-43.4	-44.6	12	3	-6	-10.5	-10.2	3	4	-3	1.7	3.2
6	2	-7	0	-0.6	8	3	-3	-17.6	-17.3	13	3	-6	13.6	14.4	3	4	3	0	-2.9
7	2	7	0	-3.1	8	3	3	41.0	42.3	0	3	-7	-14.8	-16.7	4	4	-3	-34.8	-30.7
7	2	-7	-1.3	-3.9	9	3	-3	-15.5	-14.2	0	3	7	15.3	16.7	4	4	3	13.8	10.2
8	2	-7	2.7	1.3	9	3	3	40.8	41.8	1	3	-7	5.8	5.7	5	4	-3	1.9	5.3

Table 4. *(Continued)*

h	k	l	F_o	F_c
5	4	3	-2.3	-5.9
6	4	-3	46.1	43.3
6	4	3	22.3	20.4
7	4	-3	0	1.0
7	4	3	0	-3.1
8	4	-3	-67.3	-65.5
8	4	3	-14.6	-11.6
9	4	-3	0	2.8
9	4	3	0	1.3
10	4	-3	54.6	50.1
10	4	3	16.1	16.4
11	4	-3	0	-0.3
11	4	3	0	-3.0
12	4	-3	24.3	24.6
12	4	3	-56.1	-57.9
13	4	-3	0	3.6
13	4	3	0	-3.3
14	4	-3	31.1	29.9
14	4	3	16.1	15.5
15	4	-3	2.7	4.5
1	4	-4	0	2.3
1	4	4	0	-1.2
2	4	-4	-62.5	-57.5
2	4	4	20.0	15.4
3	4	-4	0	-2.4
3	4	4	-1.6	-3.6
4	4	4	40.3	39.6
4	4	-4	64.3	62.6
5	4	-4	0	-0.3
5	4	4	-2.4	-0.5
6	4	-4	52.7	48.2
6	4	4	111.2	114.0
7	4	-4	0.4	4.9
7	4	4	0	-1.0
8	4	-4	6.7	3.2
8	4	4	-117.6	-124.5
9	4	-4	2.5	2.1
9	4	4	2.3	0.6
10	4	-4	-55.1	-54.4
10	4	4	-72.7	-69.9
11	4	-4	0	-3.2
11	4	4	-1.2	-3.1
12	4	-4	-103.1	-104.7
12	4	4	-17.6	-18.9
13	4	4	0	-2.7
14	4	-4	67.1	66.6
0	4	-5	-13.8	-10.7
0	4	5	-12.0	-10.7
1	4	-5	5.1	1.9
1	4	5	0	0.8
2	4	-5	16.1	16.4
2	4	5	10.5	9.1
3	4	-5	0	-3.5
3	4	5	2.5	3.7
4	4	-5	-91.2	-87.5
4	4	5	24.3	26.0
5	4	-5	-1.5	-4.0
5	4	5	2.4	2.3
6	4	-5	42.0	41.0
6	4	5	-35.1	-37.7
7	4	-5	-0.9	-2.1
7	4	5	1.3	0.9
8	4	-5	-5.1	-3.8
8	4	5	-24.8	-22.8
9	4	-5	2.7	1.6
9	4	5	1.1	1.1
10	4	-5	18.4	18.7
10	4	5	46.5	44.5
11	4	-5	0	-1.6
11	4	5	0	0.8
12	4	-5	-69.2	-65.5
0	4	-6	70.6	69.1
0	4	6	70.6	69.1
1	4	-6	0	1.6
1	4	6	0	3.0
2	4	-6	92.2	93.5
2	4	6	11.4	13.4
3	4	-6	0	0.5
3	4	6	0	3.3
4	4	-6	-32.5	-32.4
4	4	6	-81.7	-82.5
5	4	-6	0	-2.3
5	4	6	1.0	1.1
6	4	-6	-70.4	-69.6
6	4	6	-6.0	-8.3
7	4	-6	0	-2.3
7	4	6	-1.9	-1.5
8	4	-6	-22.6	-19.1
8	4	6	31.4	28.6
9	4	-6	0	-0.3
10	4	-6	82.5	85.2
0	4	-7	-32.4	-32.9
0	4	7	-33.2	-32.9
1	4	-7	0	1.3
1	4	7	0	0.9
2	4	-7	68.9	69.7
2	4	7	-12.4	-15.2
3	4	-7	0	-0.2
3	4	7	-1.4	-0.9
4	4	-7	5.6	8.2
4	4	7	2.0	1.7
5	4	7	0	-2.9
5	4	-7	1.4	3.4
6	4	-7	-4.4	-6.0
7	4	-7	0	1.6
8	4	-7	-12.5	-12.3
2	5	0	14.4	16.3
3	5	0	22.4	21.6
4	5	0	60.8	61.5
5	5	0	-64.6	-64.4
6	5	0	-21.7	-20.8
7	5	0	-24.3	-24.4
8	5	0	-46.1	-47.0
9	5	0	29.8	31.1
10	5	0	-10.6	-9.6
11	5	0	26.8	25.8
12	5	0	19.1	17.1
13	5	0	14.5	14.6
14	5	0	48.2	50.2
15	5	0	-48.7	-49.0
0	5	-1	30.2	28.8
0	5	1	-29.4	-28.8
1	5	-1	-3.0	-0.7
1	5	1	26.8	26.3
2	5	-1	39.5	38.0
2	5	1	6.7	5.5
3	5	1	12.9	15.2
4	5	-1	-41.6	-40.6
4	5	1	0	4.0
5	5	-1	-4.0	-3.8
5	5	1	32.4	33.0
6	5	1	51.4	51.7
6	5	-1	-25.9	-27.1
7	5	-1	18.1	18.8
7	5	1	-47.3	-46.7
8	5	-1	-11.3	-8.7
8	5	1	-15.5	-14.8
9	5	-1	37.4	36.3
9	5	1	-17.6	-18.4
10	5	-1	25.3	26.6
11	5	-1	7.0	5.8
11	5	1	-2.2	-1.5
12	5	-1	33.3	33.2
12	5	1	-16.2	-16.7
13	5	-1	-51.1	-50.7
13	5	1	25.4	25.3
14	5	-1	-33.4	-34.0
14	5	1	6.5	6.7
15	5	-1	8.1	8.0
15	5	1	24.2	25.5
0	5	-2	38.5	36.0
0	5	2	-37.8	-36.0
1	5	2	-18.1	-17.6
2	5	2	-47.4	-46.4
3	5	-2	41.0	38.6
3	5	2	33.6	33.1
4	5	-2	-13.2	-14.4
4	5	2	-13.9	-15.5
5	5	-2	27.3	27.2
5	5	2	34.0	36.6
6	5	-2	1.0	1.2
6	5	2	20.4	21.4
7	5	-2	36.2	35.3
7	5	2	8.4	7.3
8	5	-2	47.0	47.4
8	5	2	32.4	32.7
9	5	-2	-28.0	-28.4
9	5	2	-25.6	-24.4
10	5	-2	9.1	8.5
10	5	2	6.7	8.3
11	5	-2	-29.8	-30.4
11	5	2	-22.8	-24.4
12	5	-2	-24.2	-24.2
12	5	2	-26.1	-26.9
13	5	2	9.5	9.3
14	5	-2	-15.4	-14.9
14	5	2	-15.3	-17.6
15	5	-2	10.2	9.8
0	5	-3	-50.0	-47.8
0	5	3	48.0	47.8
1	5	-3	28.6	26.0
1	5	3	-39.0	-36.6
2	5	-3	-21.2	-21.3
2	5	3	3.3	2.4
3	5	-3	50.0	49.5
3	5	3	-50.3	-48.7
4	5	-3	39.3	38.5
4	5	3	-57.8	-57.8
5	5	-3	-5.7	-6.2
5	5	3	34.5	34.9
6	5	-3	17.1	16.2
6	5	3	10.4	9.3
7	5	-3	-11.8	-10.9
7	5	3	-1.6	-2.1
8	5	-3	11.0	9.6
8	5	3	-15.5	-15.3
9	5	-3	-29.8	-29.3
9	5	3	44.8	46.7
10	5	3	42.5	44.1
10	5	-3	-28.1	-29.1
11	5	-3	14.3	14.7
11	5	3	-26.2	-27.5
12	5	-3	7.3	4.8
12	5	3	-9.0	-9.2
13	5	-3	-5.7	-3.8
14	5	-3	-14.8	-13.3
0	5	-4	26.9	25.4
0	5	4	-26.6	-25.4
1	5	-4	6.7	7.6
1	5	4	61.5	60.7
2	5	4	73.0	73.5
3	5	-4	21.5	20.1
3	5	4	-50.9	-50.1
4	5	-4	44.9	42.1
4	5	4	2.7	3.9
5	5	-4	-41.8	-40.2
5	5	4	-30.4	-31.1
6	5	-4	-9.0	-8.2
6	5	4	-20.3	-21.7
7	5	-4	-20.9	-20.0
7	5	4	-5.6	-6.4
8	5	-4	-29.1	-28.4
8	5	4	-36.3	-37.2
9	5	-4	14.6	14.9
9	5	4	34.4	35.3
10	5	-4	-7.8	-9.2
11	5	-4	12.6	13.8
11	5	4	16.7	16.9
12	5	-4	5.0	5.4
13	5	-4	9.1	8.8
0	5	-5	16.3	15.7
0	5	5	-16.2	-15.7
1	5	-5	-8.5	-11.2
1	5	5	5.3	4.9
2	5	-5	6.4	5.4
2	5	5	-10.5	-11.2
3	5	-5	-5.6	-5.5
3	5	5	30.5	30.8
4	5	-5	14.4	14.9
4	5	5	18.6	18.6
5	5	-5	-37.5	-38.6
5	5	5	18.4	20.3
6	5	-5	-43.9	-44.2
6	5	5	45.0	47.5
7	5	-5	32.5	33.6
8	5	-5	14.1	16.4
9	5	-5	-12.7	-15.0
10	5	-5	-24.4	-24.9
11	5	-5	42.6	43.4
12	5	-5	45.4	46.2
0	5	-6	39.0	39.9
0	5	6	-39.7	-39.9
1	5	-6	-50.0	-52.7
1	5	6	24.7	25.1
2	5	-6	-38.4	-38.6
2	5	6	7.0	7.2
3	5	-6	9.9	10.2
3	5	6	-16.2	-17.0
4	5	-6	-3.9	-3.9
4	5	6	-40.3	-43.5
5	5	-6	-4.3	-5.8
5	5	6	49.1	53.3
6	5	6	34.9	38.0
7	5	-6	33.6	34.7
7	5	6	-10.7	-11.7
8	5	-6	21.0	21.1
9	5	-6	4.8	5.2
0	5	-7	3.6	2.3
0	5	7	-2.1	-2.3
1	5	-7	-13.8	-15.8
1	5	7	-8.2	-7.2
2	5	-7	-33.4	-36.5
4	5	-7	17.7	18.4
2	6	0	-1.4	-3.0
4	6	0	-0.7	-2.8
5	6	0	-37.8	-34.6
6	6	0	0	0.9
7	6	0	-47.0	-45.3
8	6	0	-2.4	-5.7
9	6	0	-52.9	-52.4
10	6	0	-3.1	-7.5
11	6	0	9.0	7.7
12	6	0	-2.2	-2.7
13	6	0	47.3	47.5
0	6	-1	3.2	1.8
0	6	1	2.3	1.8
1	6	-1	-16.7	-17.1
1	6	1	54.7	55.7
2	6	-1	-2.4	-3.1
2	6	1	0	1.6
3	6	-1	67.9	68.2
3	6	1	-15.1	-17.1
4	6	-1	0	-3.9
4	6	1	0	-2.4
5	6	-1	27.7	29.3
6	6	-1	2.4	4.9
6	6	1	0	-0.7
7	6	1	37.3	35.2
7	6	-1	62.2	61.8
8	6	1	0	-3.1
8	6	-1	0.6	1.7
9	6	1	0	2.4
9	6	-1	-63.3	-64.8
10	6	1	0	1.2
10	6	-1	-1.7	-1.6
11	6	1	58.7	57.9
11	6	-1	17.4	16.0
12	6	1	-1.8	-0.8
12	6	-1	-2.2	-3.7
13	6	1	-82.1	-84.7
13	6	-1	-12.8	-10.1
0	6	-2	0	7.3
0	6	2	0	7.3
1	6	-2	-42.4	-37.7
2	6	-2	0	4.2
2	6	2	1.9	6.3
3	6	-2	-59.3	-56.2
3	6	2	-7.7	-7.2
4	6	-2	-2.0	-1.6
4	6	2	-2.6	-3.1
5	6	-2	-53.9	-50.4
6	6	2	3.0	2.1
6	6	-2	0	2.4
7	6	2	71.5	73.2
7	6	-2	104.1	105.3
8	6	-2	0	5.2
8	6	2	0	6.0
9	6	2	27.8	27.7
9	6	-2	45.8	43.5
10	6	2	0	5.1
10	6	-2	0	5.4
11	6	2	-15.4	-14.9
11	6	-2	-3.1	-2.4
12	6	2	0	2.2
12	6	-2	2.0	2.3
13	6	-2	-69.9	-69.4
0	6	-3	4.4	2.2
0	6	3	0	2.2
1	6	-3	-7.9	-6.0
1	6	3	-38.5	-37.2
2	6	-3	2.5	4.1
3	6	-3	21.1	26.6
3	6	3	51.2	48.6
4	6	3	-2.3	-0.8
4	6	-3	-3.0	-1.0
5	6	3	45.6	47.7
5	6	-3	-119.9	-124.2
6	6	-3	0	1.6
6	6	3	1.9	4.8
7	6	3	31.7	35.9
7	6	-3	24.5	20.4
8	6	-3	-3.4	-3.3
8	6	3	0	2.7
9	6	-3	-6.9	-4.1
9	6	3	-35.4	-37.4
10	6	3	0	-0.1
10	6	-3	1.5	2.3
11	6	3	-6.0	-8.5
11	6	-3	44.7	44.6
12	6	-3	0.8	3.0
0	6	-4	0	-5.6
0	6	4	0	-5.6
1	6	4	30.0	30.2
1	6	-4	19.7	22.3
2	6	4	-2.4	-0.6
2	6	-4	-1.5	-4.2
3	6	4	120.5	127.7
3	6	-4	49.1	46.7
4	6	-4	-2.8	-0.5
4	6	4	0	-2.9
5	6	-4	15.2	13.6
5	6	4	-85.3	-87.8
6	6	-4	2.5	1.7
6	6	4	0.2	1.0
7	6	4	-29.7	-31.2
7	6	-4	-42.1	-40.9
8	6	4	0	-3.9
8	6	-4	0	-4.1
9	6	4	-30.7	-29.8
9	6	-4	-64.5	-64.3
11	6	-4	7.4	7.4
0	6	5	-1.9	-0.8
0	6	-5	0	-0.8
1	6	5	7.8	8.2
1	6	-5	-50.0	-50.6
2	6	-5	0	-3.9
3	6	5	-40.7	-43.0
3	6	-5	39.1	39.5
4	6	5	0	-1.9
4	6	-5	-3.7	-3.9
5	6	5	-36.8	-38.6
5	6	-5	18.9	21.7
6	6	5	-3.3	-3.2
6	6	-5	0	3.5
7	6	5	-16.5	-17.0
7	6	-5	72.1	73.3
8	6	-5	0	0.3
9	6	-5	-63.5	-64.0
0	6	-6	0	5.3
0	6	6	1.2	5.3

Table 4. *(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
1	6	6	- 65.7	- 67.1	3	7	1	36.6	38.8	6	7	-2	- 18.9	- 17.4	7	7	-3	- 19.6	- 19.5
1	6	-6	11.1	10.6	4	7	-1	- 10.4	- 9.1	6	7	2	- 28.5	- 28.9	7	7	3	35.5	35.5
2	6	6	0	3.3	4	7	1	- 34.0	- 35.5	7	7	-2	13.0	14.2	8	7	-3	- 1.6	- 0.9
2	6	-6	0	1.0	5	7	-1	- 28.8	- 28.3	7	7	2	3.3	6.3	8	7	3	- 22.6	- 21.1
3	6	-6	- 45.5	- 45.8	5	7	1	- 12.3	- 10.7	8	7	-2	- 16.8	- 17.2	9	7	-3	- 3.5	- 5.6
4	6	-6	0	- 1.6	6	7	-1	38.7	38.8	8	7	2	- 16.3	- 18.1	0	7	-4	50.2	50.2
5	6	-6	- 41.9	- 43.9	7	7	-1	16.7	17.6	9	7	-2	0	1.5	0	7	4	- 49.2	- 50.2
3	7	0	- 14.0	- 13.2	7	7	1	- 4.7	- 5.4	9	7	2	- 13.4	- 14.4	1	7	-4	55.1	56.7
4	7	0	- 11.4	- 14.1	8	7	-1	13.9	14.8	10	7	-2	- 19.4	- 21.2	1	7	4	- 17.2	- 15.9
5	7	0	- 17.4	- 19.8	8	7	1	- 18.6	- 17.4	0	7	-3	23.0	24.9	2	7	-4	- 39.4	- 39.5
6	7	0	- 6.1	- 5.2	9	7	-1	24.8	25.7	0	7	3	- 22.3	- 24.9	2	7	4	0	- 3.3
7	7	0	- 36.6	- 36.1	9	7	1	- 25.7	- 25.9	1	7	-3	1.6	0.9	3	7	4	0	- 1.2
8	7	0	40.4	39.7	10	7	-1	- 23.2	- 24.2	1	7	3	- 26.6	- 27.8	4	7	-4	- 24.4	- 27.0
9	7	0	13.6	13.7	10	7	1	24.9	24.7	2	7	-3	24.8	23.9	4	7	4	- 16.7	- 17.8
10	7	0	17.5	17.9	0	7	-2	8.2	6.8	2	7	3	11.6	11.9	5	7	-4	- 18.3	- 19.1
11	7	0	40.8	42.9	0	7	2	- 7.4	- 6.8	3	7	-3	27.5	27.2	6	7	-4	- 9.4	- 10.8
0	7	-1	- 25.2	- 23.7	2	7	-2	6.9	9.0	3	7	3	- 4.4	- 5.9	7	7	-4	- 30.7	- 31.7
0	7	1	24.5	23.7	2	7	2	45.8	47.3	4	7	-3	- 9.1	- 8.3	0	7	5	13.6	14.6
1	7	1	8.0	8.7	3	7	-2	- 20.8	- 20.0	4	7	3	7.6	6.1	0	7	-5	- 13.9	- 14.6
1	7	-1	- 17.1	- 16.9	3	7	2	21.7	22.4	5	7	-3	21.3	22.3	1	7	-5	7.2	7.7
2	7	-1	2.3	2.0	4	7	-2	50.7	50.5	5	7	3	- 10.1	- 9.7	2	7	-5	- 21.1	- 23.9
2	7	1	20.9	21.4	5	7	-2	47.3	46.5	6	7	-3	- 33.2	- 33.6					
3	7	-1	- 4.0	- 7.0	5	7	2	35.2	36.3	6	7	3	35.8	36.6					

Discussion of the structure

The low residual value of 6.6$^0/_0$ confirms the centric space group $P2_1/a$ as the correct one for parawollastonite. All the atoms in this structure occupy the general position $4e$. The final coordinates are listed in Table 5. Table 6 gives the interatomic distances and Table 7 the bond angles between atoms. A projection of the structure of parawollastonite along c is illustrated in Fig. 1.

The Ca atoms are surrounded by distorted oxygen octahedra which form two different slabs parallel to b. One consists of Ca(1), the other of Ca(2) and Ca(3). Ca(1) is linked to an additional seventh oxygen, O(9), with a rather large distance of 2.895 Å. Similar Ca—O distances

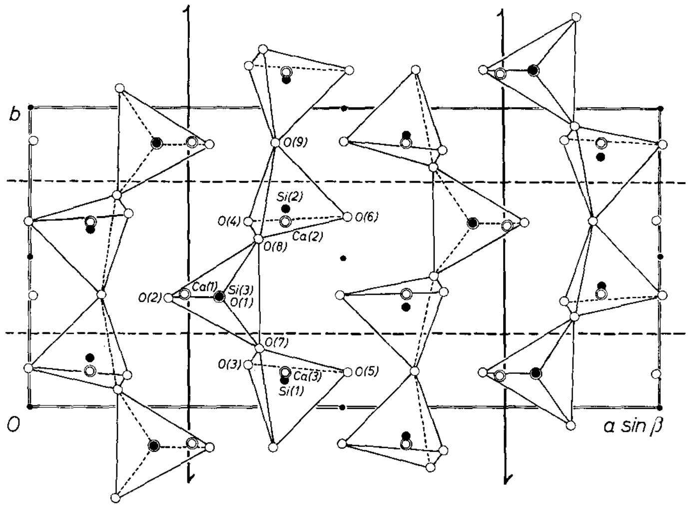

Fig. 1. Projection of the structure of parawollastonite along c. The double circles are Ca atoms, the full circles are Si atoms, and the single circles are O atoms

Table 5. *Positional coordinates for parawollastonite*

Atom	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
Ca(1)	0.2482	0.0001	0.3758	0.0004	0.9712	0.0002
Ca(2)	0.4011	0.0001	0.6265	0.0006	0.7397	0.0002
Ca(3)	0.3987	0.0001	0.1209	0.0006	0.7364	0.0002
Si(1)	0.4076	0.0001	0.0907	0.0003	0.2313	0.0003
Si(2)	0.4075	0.0001	0.6598	0.0003	0.2313	0.0003
Si(3)	0.3016	0.0001	0.3761	0.0004	0.4432	0.0002
O(1)	0.3000	0.0003	0.3747	0.0013	0.6685	0.0006
O(2)	0.2156	0.0003	0.3759	0.0013	0.3031	0.0007
O(3)	0.3490	0.0004	0.1397	0.0014	0.0328	0.0007
O(4)	0.3473	0.0003	0.6157	0.0015	0.0348	0.0007
O(5)	0.5086	0.0003	0.1226	0.0020	0.2388	0.0007
O(6)	0.5078	0.0003	0.6176	0.0019	0.2347	0.0007
O(7)	0.3642	0.0004	0.1962	0.0007	0.4060	0.0007
O(8)	0.3633	0.0004	0.5533	0.0008	0.4067	0.0008
O(9)	0.3906	0.0003	0.8755	0.0010	0.2767	0.0006

Table 6. *Interatomic distances in parawollastonite*

O(3′) is equivalent by symmetry to O(3), and O(4′) to O(4)

Atoms	distance	σ	Atoms	distance	σ
Ca(1)—O(1)	2.214 Å	0.005	Ca(2)—O(1)	2.494 Å	0.008
Ca(1)—O(2)	2.356	0.005	Ca(2)—O(2)	2.598	0.008
Ca(1)—O(3)	2.392	0.008	Ca(2)—O(4)	2.174	0.005
Ca(1)—O(3′)	2.445	0.009	Ca(2)—O(5)	2.318	0.013
Ca(1)—O(4)	2.396	0.009	Ca(2)—O(6)	2.290	0.005
Ca(1)—O(4′)	2.407	0.009	Ca(2)—O(8)	2.537	0.006
Average	2.368		Average	2.402	
Ca(1)—O(9)	2.895				
Ca(3)—O(1)	2.475	0.008	Si(1)—O(3)	1.779	0.007
Ca(3)—O(2)	2.545	0.008	Si(1)—O(5)	1.580	0.006
Ca(3)—O(3)	2.168	0.005	Si(1)—O(7)	1.554	0.005
Ca(3)—O(5)	2.298	0.013	Si(1)—O(9)	1.622	0.007
Ca(3)—O(6)	2.415	0.012	Average	1.634	
Ca(3)—O(7)	2.511	0.005			
Average	2.402				
Si(2)—O(4)	1.788	0.006	Si(3)—O(1)	1.594	0.005
Si(2)—O(6)	1.577	0.006	Si(3)—O(2)	1.732	0.005
Si(2)—O(8)	1.558	0.006	Si(3)—O(7)	1.637	0.006
Si(2)—O(9)	1.626	0.006	Si(3)—O(8)	1.626	0.007
Average	1.637		Average	1.647	

Table 7. *Bond angles between atoms in parawollastonite*
O(3′) is equivalent by symmetry to O(3), and O(4′) to O(4)

Atoms	angle	Atoms	angle
O(1)—Ca(1)—O(2)	171°12′	O(4)—Ca(2)—O(8)	141°51′
O(3)—Ca(1)—O(4)	93°15′	O(1)—Ca(2)—O(2)	92°27′
O(3)—Ca(1)—O(4)	80°48′	O(1)—Ca(2)—O(6)	80°47′
O(3′)—Ca(1)—O(4)	80°01′	O(2)—Ca(2)—O(5)	82°59′
O(3′)—Ca(1)—O(4′)	104°21′	O(5)—Ca(2)—O(6)	103°37′
O(3)—Ca(1)—O(2)	84°07′	O(1)—Ca(2)—O(4)	88°53′
O(3′)—Ca(1)—O(2)	86°33′	O(2)—Ca(2)—O(4)	86°16′
O(4)—Ca(1)—O(2)	83°40′	O(5)—Ca(2)—O(4)	98°06′
O(4′)—Ca(1)—O(2)	86°36′	O(6)—Ca(2)—O(4)	94°17′
O(3)—Ca(3)—O(7)	143°20′	O(3)—Si(1)—O(5)	125°00′
O(1)—Ca(3)—O(2)	93°34′	O(3)—Si(1)—O(7)	108°30′
O(1)—Ca(3)—O(6)	78°47′	O(5)—Si(1)—O(7)	104°25′
O(2)—Ca(3)—O(5)	84°33′	O(3)—Si(1)—O(9)	105°31′
O(5)—Ca(3)—O(6)	103°03′	O(5)—Si(1)—O(9)	106°06′
O(1)—Ca(3)—O(3)	88°34′	O(7)—Si(1)—O(9)	105°59′
O(2)—Ca(3)—O(3)	88°13′		
O(5)—Ca(3)—O(3)	97°57′	O(4)—Si(2)—O(6)	124°07′
O(6)—Ca(3)—O(3)	91°25′	O(4)—Si(2)—O(8)	108°34′
		O(6)—Si(2)—O(8)	104°11′
O(2)—Si(3)—O(7)	112°17′	O(4)—Si(2)—O(9)	104°08′
O(2)—Si(3)—O(8)	112°13′	O(6)—Si(2)—O(9)	109°00′
O(7)—Si(3)—O(8)	107°11′	O(8)—Si(2)—O(9)	105°35′
O(2)—Si(3)—O(1)	129°30′		
O(7)—Si(3)—O(1)	96°39′	Si(1)—O(9)—Si(2)	151°48′
O(8)—Si(3)—O(1)	96°10′	Si(1)—O(7)—Si(3)	135°25′
		Si(2)—O(8)—Si(3)	136°32′

are reported by Peacor and Buerger (1962) for bustamite, such as $\mathrm{Ca_1}$—$\mathrm{O_9}$ = 2.899 Å and $\mathrm{Ca_2}$—$\mathrm{O_9}$ = 2.891 Å. The average Ca—O distances in parawollastonite are the same for Ca(2) and Ca(3), namely 2.402 Å; these atoms form one slab of Ca—O octahedra. The other slab, built up by Ca(1) and its surrounding oxygen atoms, is slightly smaller with an average Ca(1)—O distance of 2.368 Å. Prewitt and Buerger (1963) found almost equal average Ca—O distances for all three calcium atoms in wollastonite.

The Si atoms are tetrahedrally coordinated. The deviation from the ideal tetrahedral angle = 109°28′ are considerable, the values varying between 96°10′ and 129°30′. Prewitt and Buerger (1963) reported three nonequivalent Si—O—Si angles in wollastonite as well as in bustamite. The corresponding angles for parawollastonite lie between those for wollastonite and bustamite:

bustamite	161°, 135°, 137°
parawollastonite	152°, 135°, 137°
wollastonite	149°, 139°, 137°.

Table 8. *Anisotropic temperature coefficients for parawollastonite*

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ca(1)	0.00078	0.00337	0.00157	–0.00001	0.00009	0.00013
σ	0.00006	0.00030	0.00029	0.00012	0.00009	0.00033
Ca(2)	0.00082	0.00283	0.00335	–0.00004	0.00003	–0.00092
σ	0.00007	0.00029	0.00031	0.00032	0.00010	0.00078
Ca(3)	0.00091	0.00265	0.00336	0.00034	0.00009	0.00024
σ	0.00007	0.00029	0.00031	0.00032	0.00010	0.00079
Si(1)	0.00070	0.00076	0.00257	0.00006	–0.00013	–0.00008
σ	0.00010	0.00071	0.00045	0.00016	0.00016	0.00033
Si(2)	0.00072	0.00152	0.00248	–0.00005	–0.00010	0.00004
σ	0.00011	0.00073	0.00045	0.00016	0.00016	0.00032
Si(3)	0.00030	0.00368	0.00209	–0.00003	0.00006	0.00017
σ	0.00008	0.00040	0.00040	0.00021	0.00013	0.00044
O(1)	0.00059	0.00428	0.00015	–0.00017	0.00026	0.00011
σ	0.00024	0.00109	0.00010	0.00067	0.00034	0.00137
O(2)	0.00101	0.00422	0.00144	–0.00007	0.00071	0.00034
σ	0.00025	0.00110	0.00095	0.00072	0.00031	0.00156
O(3)	0.00143	0.00143	0.00101	0.00024	–0.00047	–0.00053
σ	0.00028	0.00028	0.00112	0.00074	0.00041	0.00156
O(4)	0.00126	0.00456	0.00159	0.00007	–0.00058	–0.00056
σ	0.00028	0.00117	0.00113	0.00082	0.00040	0.00173
O(5)	0.00091	0.00335	0.00720	0.00158	0.00023	–0.00012
σ	0.00027	0.00113	0.00120	0.00104	0.00043	0.00241
O(6)	0.00073	0.00258	0.00698	0.00082	0.00004	0.00126
σ	0.00026	0.00109	0.00119	0.00100	0.00041	0.00232
O(7)	0.00141	0.00199	0.00057	0.00082	–0.00058	0.00001
σ	0.00027	0.00111	0.00050	0.00040	0.00041	0.00075
O(8)	0.00114	0.00239	0.00122	–0.00060	–0.00050	0.00020
σ	0.00033	0.00116	0.00117	0.00045	0.00049	0.00089
O(9)	0.00077	0.00215	0.00362	–0.00005	0.00095	0.00033
σ	0.00025	0.00109	0.00108	0.00054	0.00038	0.00114

The interatomic distances within the SiO_4 tetrahedra can be separated into two groups: (*a*) oxygen atoms coordinated by one Si and three Ca, with an average Si—O distance of 1.723 Å; (*b*) oxygen atoms coordinated by one Si and two Ca or by two Si and one Ca, with an average Si—O distance of 1.576 Å. It can be seen that the Si—O distances

Table 9. *Thermal parameters for parawollastonite*

Atom	q_1	B_1	q_2	B_2	q_3	B_3	Equivalent isotropic B
Ca(1)	0.097 Å	0.75 Å^2	0.096 Å	0.72 Å^2	0.063 Å	0.31 Å^2	0.63 Å^2
σ	0.004	0.06	0.004	0.06	0.006	0.06	0.03
Ca(2)	0.102	0.81	0.082	0.52	0.095	0.71	0.71
σ	0.004	0.06	0.006	0.08	0.005	0.08	0.04
Ca(3)	0.106	0.89	0.083	0.54	0.092	0.67	0.70
σ	0.004	0.07	0.006	0.07	0.005	0.07	0.04
Si(1)	0.094	0.70	0.045	0.16	0.078	0.48	0.41
σ	0.006	0.09	0.021	0.15	0.006	0.08	0.06
Si(2)	0.095	0.72	0.064	0.33	0.077	0.47	0.51
σ	0.006	0.09	0.015	0.16	0.007	0.08	0.07
Si(3)	0.060	0.28	0.100	0.79	0.073	0.42	0.49
σ	0.008	0.08	0.005	0.09	0.007	0.08	0.05
O(1)	0.084	0.55	0.108	0.92	0.018	0.02	0.49
σ	0.017	0.23	0.014	0.23	0.072	0.20	0.12
O(2)	0.110	0.96	0.107	0.90	0.058	0.26	0.71
σ	0.013	0.23	0.014	0.23	0.020	0.18	0.12
O(3)	0.133	1.40	0.104	0.86	0.048	0.19	0.82
σ	0.012	0.26	0.016	0.26	0.028	0.22	0.14
O(4)	0.126	1.25	0.111	0.98	0.060	0.28	0.79
σ	0.013	0.25	0.014	0.25	0.023	0.21	0.14
O(5)	0.120	1.14	0.073	0.42	0.136	1.45	1.00
σ	0.016	0.31	0.020	0.23	0.011	0.23	0.15
O(6)	0.101	0.81	0.072	0.41	0.134	1.42	0.88
σ	0.017	0.28	0.021	0.24	0.011	0.24	0.15
O(7)	0.134	1.41	0.071	0.39	0.035	0.10	0.63
σ	0.012	0.25	0.020	0.23	0.036	0.10	0.13
O(8)	0.121	1.16	0.078	0.48	0.042	0.14	0.59
σ	0.015	0.29	0.019	0.24	0.038	0.25	0.15
O(9)	0.086	0.58	0.075	0.45	0.104	0.85	0.63
σ	0.011	0.15	0.018	0.22	0.010	0.16	0.10

are considerably larger if the oxygen atoms are coordinated by three Ca. A similar classification was found for wollastonite by Prewitt and Buerger (1963).

The anisotropic temperature coefficients for parawollastonite are found in Table 8. The orientations of the thermal vibration, ellipsoids expressed by the β_{12}, β_{13}, β_{23} values, are not well refined. In order to improve these parameters a larger number of observed reflections would be necessary. The thermal parameter are listed in Table 9.

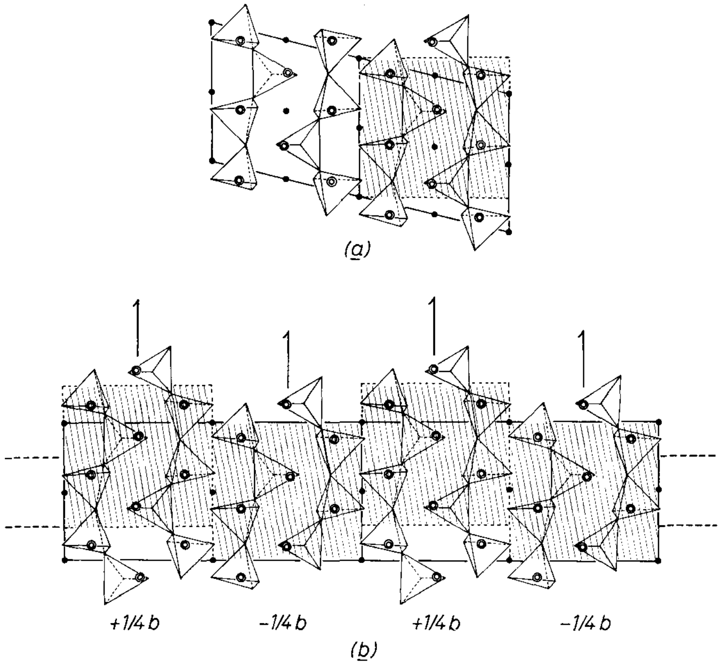

Fig. 2. Structural relation between wollastonite and parawollastonite. Double circles are Ca atoms. Small solid circles are centers of symmetry. (*a*) Selection of the pseudomonoclinic unit, shaded. (*b*) Stacking scheme of the pseudomonoclinic units in parawollastonite

The q_i's ($i = 1$ to 3) are the three principal axes of the vibration ellipsoid. A temperature factor B_i corresponds to each principal axis. The last column in Table 9 lists the average B computed by $B = (B_1 + B_2 + B_3)/3$ which is substantially the usual isotropic temperature factor. The values for parawollastonite are comparable with those for wollastonite published by Buerger and Prewitt (1961).

Precession photographs along the *c* axis of wollastonite and parawollastonite are identical if the odd-numbered reciprocal-lattice levels normal to *b* of parawollastonite are omitted. Based on this observation a structural relation between the two phases can be deduced. ITO (1950) suggested that both the triclinic and monoclinic varieties of calcium metasilicate can be constructed from a pseudomonoclinic cell by alternating shifts of $\pm \frac{1}{4} b$ of a hypothetical monoclinic cell. PREWITT and BUERGER (1963) followed the idea outlined by ITO and proposed the space group $P2_1/a$ for parawollastonite with additional local centers of symmetry which are not required by this space group.

These postulates are approximately verified in the results of the present investigation. Figure 2*a* illustrates how a cell, regarded as having pseudomonoclinic symmetry, can be selected from the structure of wollastonite. When those units are stacked together as shown in Fig. 2*b* a rough model of the structure of parawollastonite is obtained. For example, in wollastonite as well as in the pseudomonoclinic unit, the Ca atoms are related by inversion centers. In parawollastonite, however, these atoms are related by the operations of a 2_1 axis, but they are located in almost the same positions as would be generated

Table 10. *Comparison of the y coordinate of the atoms in parawollastonite with the position* $(2n + 1)/8$

$(2n+1)/8$	1/8 0.1250	3/8 0.3750	5/8 0.6250	7/8 0.8750
Atom	*y*			
Ca(1)		0.3758 ± 0.0004		
Ca(2)			0.6265 ± 0.0006	
Ca(3)	0.1209 ± 0.0006			
Si(1)	0.0906 ± 0.0003			
Si(2)			0.6597 ± 0.0003	
Si(3)		0.3760 ± 0.0004		
O(1)		0.3747 ± 0.0013		
O(2)		0.3759 ± 0.0013		
O(3)	0.1397 ± 0.0014			
O(4)			0.6157 ± 0.0015	
O(5)	0.1226 ± 0.0020			
O(6)			0.6176 ± 0.0019	
O(9)				0.8755 ± 0.0010
O(7)	0.1962 ± 0.0007			
O(8)			0.5533 ± 0.0008	

by the inversion centers of the pseudomonoclinic unit. Both symmetry operations give rise to identical positions if all atoms have y coordinates of $(2n + 1)/8$, except O(7) and O(8). Table 10 shows that the deviations of the y coordinate from $(2n + 1)/8$ for the atoms in parawollastonite are small, but above the limit of error. These specialized locations are responsible for additional symmetry which is discussed in the next section.

Pseudosymmetry and substructure

A close examination of the pseudomonoclinic unit, Fig. 3a, reveals that, in addition to the inversion centers which are a remnant of the symmetry of triclinic wollastonite, a set of pseudosymmetry elements

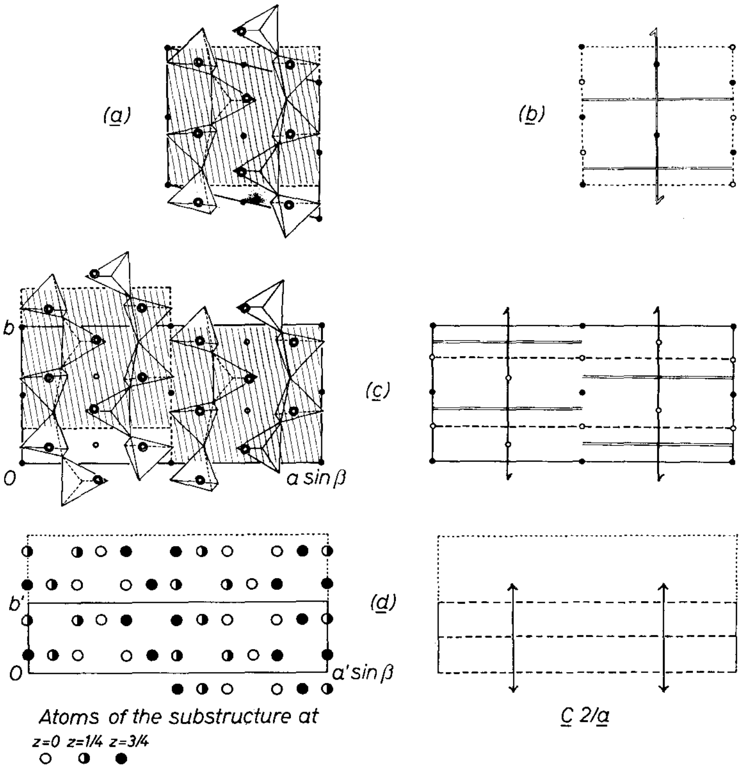

Fig. 3. Symmetry in parawollastonite. The pseudomonoclinic units are shaded, Double circles are Ca atoms. Small solid circles are true centers of symmetry. small open circles are pseudocenters. The pseudomirrors and pseudoscrew axes are represented by thin double lines. (a) Pseudomonoclinic unit. (b) Symmetry in the pseudomonoclinic unit. (c) True and pseudosymmetry in parawollastonite. (d) Symmetry of the subcell as illustrated by the atoms of the substructure.

is also present. Figure 3*b* illustrates the following symmetry elements in this pseudomonoclinic unit: inversion centers, pseudomirror planes, and a pseudo 2_1 axis. There are also pseudoinversion centers which are generated by the combination of a true inversion center and a pseudomirror plane. All these pseudosymmetry elements mentioned above are only approximately obeyed by the atomic configuration.

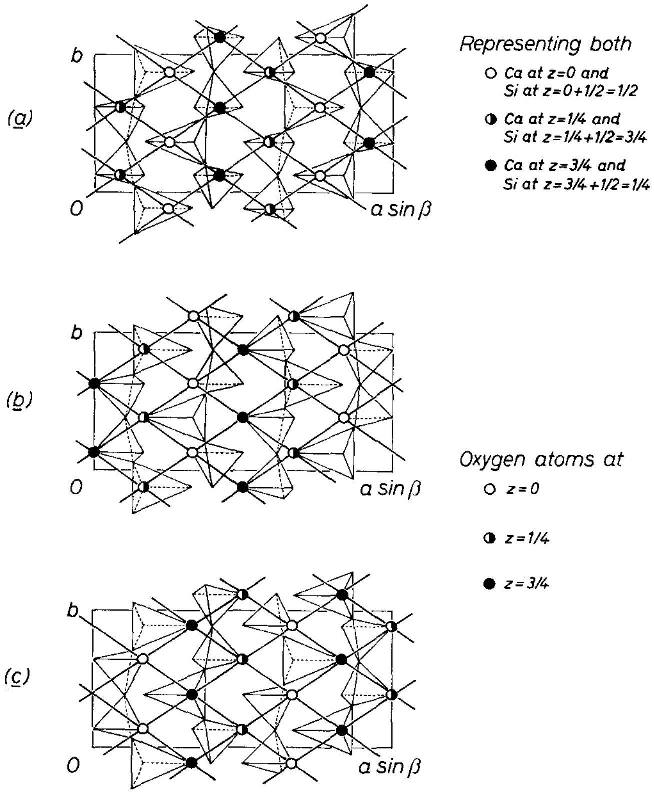

Fig. 4. Projection along *c* of the idealized parawollastonie structure. (*a*) Substructure based on Ca and Si atoms. (*b*) and (*c*) Two substructures based on oxygen atoms

Figure 3*c* shows that certain symmetry elements become pseudosymmetry elements, and vice versa, when those units are stacked together to form the parawollastonite structure. The pseudo 2_1 axis changes to a true 2_1 axis. The combination of the true 2_1 axis with a true inversion center gives rise to a glide plane. The former true centers of symmetry on the pseudo 2_1 axis become pseudoinversion centers.

This pseudosymmetry suggests that parawollastonite might have a substructure. If small changes in the coordinates of some atoms are introduced in the actual parawollastonite structure an idealized structure results which has a distinct substructure. The necessary shifts do not exceed 0.08 of the x, y, or z coordinates. As seen from Fig. 4, this idealized structure is remarkably close to the actual structure of parawollastonite. Figure 4*a* shows that the Ca and Si atoms each conform to a substructure which consists of a simple lattice array. Both sets of atoms have very similar x and y coordinates. In respect to the Ca network, the Si atoms are shifted up along the c direction by the amount $z = \frac{1}{2}$. With the exception of O(7), O(8), and O(9), all oxygen atoms are located on one of two lattice arrays which are between the lattice arrays of the Ca and Si. Figure 3*d* shows how a C-centered subcell, which is half the volume of the true cell of parawollastonite, is outlined by the positions of the atoms of the substructure. Since the Ca and the Si atoms and the majority of the oxygen atoms conform to this substructure, it has a dominant effect on the diffraction pattern. The space group of the subcell is $C2/a$. The glide plane coincides with the a glide in $P2_1/a$; hence no additional absences due to the glide plane are to be expected. The C centering, however, necessitates additional systematic absences of the type $h' + k' = 2n + 1$, where h' and k' are indices referred to the subcell. These indices transform to those for the true cell as follows:

$$h' = h,\ k' = k/2,\ l' = l.$$

The same extinction law, expressed in indices referred to the true cell, is $h + k/2 = 2n + 1$; this implies $2h + k = 4n + 2$. Since the C-centered subcell is based on an idealized structure, this extinction law is only approximately obeyed, so that reflections with the index combination $2h + k = 4n + 2$ are not actually absent but have very weak intensities. A sample of those "extinguished reflections" listed on Table 3 indicates clearly that small but measurable intensities have been observed, ruling out the possibility of systematic absences.

Acknowledgment

I express my thanks to Professor BUERGER for this continued interest and advice during this investigation. I also thank Mrs. LYNEVE WALDROP for valuable discussions. The computations were carried out on an IBM 7094 computer at the Massachusetts Institute of Technology Computation Center. This work was supported by a grant from the National Science Foundation.

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