

Structure of walstromite, $\text{BaCa}_2\text{Si}_3\text{O}_9$, and its relationship to CaSiO_3 -walstromite and wollastonite-II

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ABSTRACT

The crystal structure of walstromite, ideally $\text{BaCa}_2\text{Si}_3\text{O}_9$, was refined with data from single-crystal X-ray diffraction on a natural specimen from the type locality Esquire No. 8 claim, Big Creek, Fresno County, California, U.S.A. It is triclinic, with space group $P\bar{1}$ and unit-cell parameters $a = 6.7335(2)$, $b = 9.6142(3)$, $c = 6.6859(2)$ Å, $\alpha = 69.638(2)^\circ$, $\beta = 102.281(2)^\circ$, $\gamma = 96.855(2)^\circ$, and $V = 396.01(2)$ Å³. The only previously published structure for walstromite was based on photographic film intensity data collected from synthetic $\text{BaCa}_2\text{Si}_3\text{O}_9$ (Dent Glasser and Glasser 1968). Due to uncertainty in oxygen positions, the reported final R-factor was 0.16. The current refinement yielded an R-factor of 0.030 with the inclusion of anisotropic displacement parameters.

Walstromite is a Ba-Ca cyclosilicate characterized by Si_3O_9 three-membered rings. It is related to the important calcium silicate group of minerals, especially to CaSiO_3 -walstromite, through the substitution of Ba into one of the three distinct Ca sites. Joswig et al. (2003) suggested that the structural changes caused by the replacement of Ba^{2+} by Ca^{2+} are minimal and that walstromite is isomorphic with CaSiO_3 -walstromite, but topologically different from high-pressure wollastonite-II ($\text{Ca}_3\text{Si}_3\text{O}_9$). Our study demonstrates that wollastonite-II and CaSiO_3 -walstromite are identical phases, and are isostructural with walstromite. This isomorphism implies that the high-pressure CaSiO_3 phase may be a potential host for large cations in deep Earth environments.

Keywords: Walstromite, CaSiO_3 -walstromite, wollastonite-II, crystal structure, single-crystal X-ray diffraction

INTRODUCTION

The CaSiO_3 polymorphs and walstromite, $\text{BaCa}_2\text{Si}_3\text{O}_9$, are important in the ceramic and biomedical industries. CaSiO_3 -containing ceramics are used as glass-ceramic seals in solid oxide fuel cells (Badding et al. 2008) and have been investigated for potential use as bioactive material for bone regeneration (Wu et al. 2007). Calcium-bearing minerals, especially CaSiO_3 -walstromite, are also vital to our understanding of the physical and chemical characteristics of the Earth's mantle because they eventually adopt the perovskite structure with increased pressure and temperature, and are generally considered the dominant Ca-bearing phase in the Earth's lower mantle (Mao et al. 1977; Irifune et al. 1989; Tamai and Yagi 1989). According to Akaogi et al. (2004), CaSiO_3 -walstromite is the intermediate phase in the high-pressure and temperature transformation sequence:

wollastonite-1A \rightarrow CaSiO_3 -walstromite \rightarrow β - Ca_2SiO_4 + CaSi_2O_5
 \rightarrow CaSiO_3 -perovskite.

Wollastonite-1A, a chain silicate, [also known as β -wollastonite,

wollastonite-1T, wollastonite I, CaSiO_3 (I)] is stable at ambient conditions and transforms to CaSiO_3 -walstromite, with its three membered rings, at ~ 3 GPa (Swamy and Dubrovinsky 1997). The reaction appears to be insensitive to temperature. In nature, CaSiO_3 -walstromite has been discovered as inclusions in diamonds (Joswig et al. 1999; Jambor et al. 2000; Brenker et al. 2005). However, to date no one has applied to IMA for an official mineral name, so in this paper we will refer to it as CaSiO_3 -walstromite, following the nomenclature of Kanzaki et al. (1991) and Gasparik et al. (1994). CaSiO_3 -walstromite decomposes to β - Ca_2SiO_4 (larnite) + CaSi_2O_5 (or ϵ -phase) in the range of 10–12 GPa at 1500 °C (Kanzaki et al. 1991). This mixture is stable to 15 GPa. At about 15 GPa and 1500 °C, Ca_2SiO_4 + CaSi_2O_5 forms CaSiO_3 perovskite [or CaSiO_3 (IV)] (Gasparik et al. 1994). Additional studies of the stability of CaSiO_3 -perovskite include those by Shim and Duffy (2000), Mao et al. (1989), Wang et al. (1996), and Li et al. (2006).

$\text{BaCa}_2\text{Si}_3\text{O}_9$ (walstromite) is related to the CaSiO_3 group of minerals, especially to CaSiO_3 -walstromite, with the substitution of 1/3 of the Ca atoms by Ba. Joswig et al. (2003) showed that CaSiO_3 -walstromite is isomorphic with walstromite and the structural changes caused by the replacement of Ca^{2+} by Ba^{2+} are minimal, demonstrating that a CaSiO_3 phase can accommodate

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large cations, such as Ba, without destabilizing its structure (Dörsam et al. 2009; Mikirticheva et al. 2001).

Walstromite was first described by Alfors et al. (1965) along with six other new Ba-bearing minerals from the Esquire No. 8 claim, Big Creek, Fresno County, California. Based on optical properties and powder X-ray diffraction data, Alfors et al. (1965) concluded that walstromite is identical to the BaCa₂Si₃O₉ phase synthesized by Eskola (1922). Dent Glasser and Glasser (1968) obtained a walstromite structural model from synthetic BaCa₂Si₃O₉ using photographic X-ray diffraction data with $R = 0.16$. Basciano (1999) completed a refinement of the walstromite structure as part of a Master's study on the mineralogy and crystal structures of barium silicate minerals from Fresno County, California; however, the findings were not published.

Trojer (1969) determined the structure of a high-pressure CaSiO₃ phase synthesized at 6.5 GPa and 1300 °C from glass, which appeared to be the same phase as previously synthesized by Ringwood and Major (1967) at pressures above 3 GPa from both glass and wollastonite as starting materials. From precession photographs, Trojer (1969) obtained triclinic symmetry with space group of $P\bar{1}$ and cell dimensions of $a = 6.695(5)$, $b = 9.257(7)$, $c = 6.666(6)$ Å, $\alpha = 86^\circ 38'$, $\beta = 76^\circ 08'$, and $\gamma = 70^\circ 23'$. According to Trojer (1969), this high-pressure CaSiO₃ phase and walstromite (Glasser and Dent Glasser 1961) are polytypes, differing from each other in their stacking sequences. Trojer (1969) claimed that the high-pressure phase has three Ca layers parallel to (111), while walstromite has only two layers parallel to (101). In subsequent studies, this high-pressure CaSiO₃ phase has been given four different names: wollastonite-II (Essene 1974), walstromite-like CaSiO₃ or CaSiO₃(III) (Liu and Bassett 1986), CaSiO₃-II (Tamai and Yagi 1989), and CaSiO₃-walstromite (Kanzaki et al. 1991; Gasparik et al. 1994).

Joswig et al. (2003) found a natural CaSiO₃ inclusion in a diamond and called it CaSiO₃-walstromite. They further reported apparent differences between the CaSiO₃-walstromite and wollastonite-II structures, leading them to propose the existence of a new kind of isomorphism where the Si₃O₉ ring unit is replaced by the same ring, but with the non-bridging apices of the tetrahedra pointing in opposite directions, and applied the term "inverse axiality." Joswig et al. (2003) concluded that CaSiO₃-walstromite and wollastonite-II are different in the axiality of their Si₃O₉ rings, but they are energetically identical based on quantum mechanical calculations. Thus the stability relations between CaSiO₃-walstromite and wollastonite-II remained unknown (Dörsam et al. 2009). The nomenclature of Joswig et al. (2003) was adopted by Dörsam et al. (2009) in their study of an intermediate member of the high-pressure (Ca,Sr)SiO₃ solid-solution series. Dörsam et al. (2009) noted a difference in volume between the intermediate (Ca,Sr)SiO₃-walstromite series and the (Ca,Sr)-wollastonite-II series.

In this study, we report a structure refinement of walstromite from a natural specimen and demonstrate that the structures of walstromite, CaSiO₃-walstromite, and wollastonite-II are all actually isomorphic.

EXPERIMENTAL METHODS

The sample used in this study is from the type locality Esquire No. 8 claim, Big Creek, Fresno County, California, and is in the collection of the RRUFF

project (deposition no. R070634; <http://truff.info/R070634>). The sample appears as a colorless mass with pronounced cleavage and shows a strong orange-pink fluorescence under long-wave ultraviolet light. Celsian and quartz inclusions, as reported by Alfors et al. (1965), were not observed in this sample. The chemical composition, Ca_{1.998(11)}Ba_{0.958(5)}Mn_{0.029(2)}Sr_{0.019(0)}Si_{2.998(6)}O₉, or structurally (Ba_{0.96}Sr_{0.02}Ca_{0.02})_{Σ=1}(Ca_{1.98}Mn_{0.02})_{Σ=2}Si_{3.00}O₉, was determined with the Cameca SX-50 microprobe (15 point analyses), which is consistent with that reported by Alfors et al. (1965), but slightly different from the one, Ba_{1.021}(Ca_{1.947}Na_{0.011})_{Σ=1.958}(Si_{2.995}Al_{0.023})_{Σ=3.018}O₉, by Basciano (1999).

An equant, euhedral crystal, approximately 0.06 × 0.05 × 0.04 mm, was selected and mounted on a Bruker X8 APEX2 CCD X-ray diffractometer equipped with graphite-monochromatized MoK α radiation. X-ray diffraction data were collected to $2\theta \leq 70^\circ$ with frame widths of 0.5° in ω and 30 s counting time per frame. Cell refinement and data reduction were completed using SAINT (Bruker 2005). The intensity data were corrected for X-ray absorption using the Bruker program SADABS (Sheldrick 2001). SHELX97 (Sheldrick 2008) was used for both structure determination and refinement. A summary of the data collection, crystallographic data, and refinement statistics is given in Table 1. Final coordinates and isotropic displacement parameters of all atoms are listed in Table 2. Anisotropic displacement parameters are recorded in Table 3¹, and selected bond distances in Table 4¹.

¹ Deposit item AM-11-027, Tables 3 and 4 (Anisotropic displacement parameters and selected bond distances). Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at <http://www.minsocam.org>, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

TABLE 1. Summary of data collection and refinement parameters, and crystallographic data for walstromite

Structural formula	BaCa ₂ Si ₃ O ₉
Space group	$P\bar{1}$
a (Å)	6.7335(2)
b (Å)	9.6142(3)
c (Å)	6.6859(2)
α (°)	69.638(2)
β (°)	102.281(2)
γ (°)	96.855(2)
V (Å ³)	396.01(2)
Z	2
ρ_{calc} (g/cm ³)	3.738
θ range for data collection (°)	2.4 to 35.0
No. of reflections collected	9266
No. of independent reflections	3372
No. of reflections with $F > 4\sigma(F)$	2818
R_{int}	0.028
R [$F^2 > 4\sigma(F^2)$]	0.030
wR (F^2)	0.067
Goodness-of-fit	1.044
No. of parameters refined	137

TABLE 2. Coordinates and isotropic displacement parameters (Å²) of atoms in walstromite

Atom	x	y	z	U_{eq}
Ca1	0.27564(10)	0.50942(7)	0.76296(10)	0.01177(12)
Ca2	0.43704(9)	0.82810(7)	0.94439(10)	0.00973(12)
Ba1	0.04730(3)	0.84865(2)	0.32147(3)	0.01220(6)
Si1	0.09661(13)	0.22212(10)	0.15253(14)	0.0086(2)
Si2	0.23397(13)	0.48134(10)	0.28615(14)	0.0087(2)
Si3	0.44128(13)	0.19622(10)	0.51332(14)	0.0088(2)
O1	0.2334(3)	0.2611(3)	-0.0293(4)	0.0118(4)
O2	-0.1009(3)	0.1228(3)	0.1041(4)	0.0118(4)
O3	0.0457(3)	0.3714(3)	0.2005(4)	0.0117(4)
O4	0.3730(3)	0.5563(3)	0.1071(4)	0.0115(4)
O5	0.1349(4)	0.5860(3)	0.3697(4)	0.0146(5)
O6	0.3598(4)	0.3559(2)	0.5060(4)	0.0122(4)
O7	0.6141(3)	0.2341(3)	0.3686(4)	0.0114(4)
O8	0.5080(4)	0.0916(3)	0.7570(4)	0.0129(4)
O9	0.2305(3)	0.1245(2)	0.3932(4)	0.0107(4)

RESULTS AND DISCUSSION

Structure of walstromite

Thus far, two different triclinic unit-cell settings in $P\bar{1}$ symmetry have been reported for walstromite: $a = 6.72$, $b = 6.73$, $c = 9.62$ Å, $\alpha = 88^\circ$, $\beta = 111^\circ$, $\gamma = 102^\circ$ by Glasser and Dent Glasser (1961) and $a = 6.743$, $b = 9.607$, $c = 6.687$ Å, $\alpha = 69^\circ$, $\beta = 102^\circ$, $\gamma = 97^\circ$ by Alfors et al. (1965), Dent Glasser and Glasser (1968), and Basciano (1999). We adopt the latter setting in this study and our unit-cell parameters (Table 1) are consistent with those determined by Alfors et al. (1965), Dent Glasser and Glasser (1968), and Basciano (1999).

Walstromite is characterized by three-membered rings of silicate tetrahedra that occur in layers with the apices of alternating rings pointing in opposite directions (Fig. 1). There are three unique Si sites (Si1, Si2, and Si3) in each ring. The average Si-O distances associated with Si1, Si2, and Si3 are 1.633(2), 1.630(2), and 1.633(2) Å, respectively, and are consistent with those determined by Basciano (1999). The Si-O distances reported by Dent Glasser and Glasser (1968) are longer ($\langle R(\text{Si1-O}) \rangle = 1.65$ Å, $\langle R(\text{Si2-O}) \rangle = 1.66$ Å, $\langle R(\text{Si3-O}) \rangle = 1.66$ Å) than we found; however, they suggest that their Si-O bond lengths may not be very accurate due to uncertainty in the

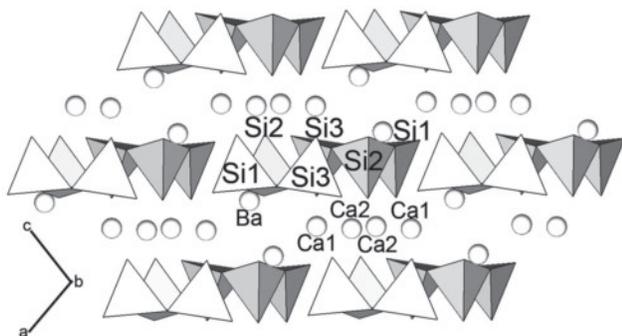


FIGURE 1. The structure of walstromite. Rings of silicate tetrahedra occupy layers with the apices of alternating rings pointing in opposite directions.

oxygen positions. There are two nonequivalent Ca sites in walstromite. Ca1O₈ polyhedra share edges to form chains parallel to [101] and lie on the (010) plane halfway between planes of Ca2 and Ba atoms (Fig. 1). The Ca1-O distances range between 2.325(2) and 2.861(3) Å, with a mean distance of 2.545(2) Å. Ca2 is 6-coordinated with the Ca2-O distances varying between 2.299(2) and 2.480(2) Å, and an average value of 2.370(2) Å. Barium is 8-coordinated and forms edge-sharing chains parallel to [001]. The Ba-O distances range from 2.556(2) to 3.101(2) Å, with a mean value of 2.841(2) Å.

Structural relationships among walstromite, CaSiO₃-walstromite, and wollastonite-II

For purposes of comparison, we converted the atomic coordinates of walstromite obtained in this study and the coordinates of wollastonite-II (Trojer 1969) into the setting of CaSiO₃-walstromite given by Joswig et al. (2003).

The atomic coordinates of the asymmetric unit of walstromite (this study) were transformed to the setting of CaSiO₃-walstromite (Joswig et al. 2003) according to $T[v]_B = [v]_J$, where $[v]_B$ and $[v]_J$ represent atomic coordinates in the settings of this study and Joswig et al. (2003), respectively, and

$$T = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0.5 \\ -1 & 0 & 0 & 0 \end{bmatrix}$$

This transformation represents a quarter-turn rotation about [010], with an origin shift of $[0 \frac{1}{2} 0]$. Not all atoms in the asymmetric unit of walstromite in this study correspond to atoms in the asymmetric unit of Joswig et al. (2003), so some of the transformed coordinates represent symmetry equivalents. The transformed coordinates are given in Table 5. The corresponding unit-cell parameters of walstromite after the transformation are $a = 6.686$, $b = 9.614$, $c = 6.734$ Å, $\alpha = 83.145^\circ$, $\beta = 77.719^\circ$, $\gamma = 69.638^\circ$, matching the setting adopted by Joswig et al. (2003).

By the same token, the atomic coordinates of the asymmetric unit of wollastonite-II (Trojer 1969) can also be transformed to the setting of CaSiO₃-walstromite (Joswig et al. 2003) with

TABLE 5. Coordinates of wollastonite-II from Trojer (1969) transformed to the setting of CaSiO₃-walstromite (Joswig et al. 2003), CaSiO₃-walstromite from (Joswig et al. 2003), and walstromite (this study) transformed into the setting of CaSiO₃-walstromite (Joswig et al. 2003)

Atom	x			y			z		
	wollast.-II	CaSiO ₃ -walstr.	walstr.	wollast.-II	CaSiO ₃ -walstr.	walstr.	wollast.-II	CaSiO ₃ -walstr.	walstr.
Ca111	0.7557(3)	0.7566(1)	0.76296(10)	0.0002(3)	0.0014(1)	0.00942(7)	0.7377(3)	0.7369(1)	0.72436(10)
Ca322	0.9201(3)	0.9256(1)	0.94439(10)	0.3356(3)	0.3345(1)	0.32810(7)	0.5755(3)	0.5716(1)	0.56296(9)
Ca23Ba	0.2698(3)	0.2790(1)	0.32147(3)	0.3513(3)	0.3531(1)	0.34865(2)	0.9154(3)	0.9186(1)	0.95270(3)
Si313	0.4773(4)	0.4771(2)	0.48668(14)	0.3009(4)	0.3027(1)	0.30378(10)	0.4584(4)	0.4540(2)	0.44128(13)
Si222	0.7255(4)	0.7234(2)	0.71385(14)	0.0162(4)	0.0154(1)	0.01866(10)	0.2299(4)	0.2279(2)	0.23397(13)
Si131	0.8365(4)	0.8382(2)	0.84747(14)	0.2951(4)	0.2941(1)	0.27788(10)	0.1084(4)	0.1024(2)	0.09661(13)
O818	0.2319(10)	0.2315(4)	0.2430(4)	0.4031(9)	0.4054(3)	0.4083(3)	0.5460(10)	0.5401(4)	0.5080(4)
O727	0.6089(10)	0.6143(5)	0.6314(4)	0.2629(9)	0.2649(3)	0.2658(3)	0.6409(9)	0.6385(4)	0.6141(3)
O636	0.4953(10)	0.4918(4)	0.4940(4)	0.1386(9)	0.1381(3)	0.1440(2)	0.3647(10)	0.3597(4)	0.3598(4)
O545	0.6561(10)	0.6535(5)	0.6303(4)	0.9068(9)	-0.0976(3)	0.9139(3)	0.1140(10)	0.1129(4)	0.1349(4)
O454	0.9003(10)	0.8990(5)	0.8929(4)	0.9388(9)	-0.0589(3)	0.9437(3)	0.3715(10)	0.3728(4)	0.3729(3)
O363	0.8085(10)	0.8069(5)	0.7995(4)	0.1359(8)	0.1344(3)	0.1286(3)	0.0482(9)	0.0418(4)	0.0457(3)
O272	0.8805(9)	0.8815(5)	0.8959(4)	0.4055(9)	0.4069(3)	0.3772(3)	0.9157(9)	-0.0914(4)	0.8991(3)
O181	0.0286(10)	1.0301(5)	0.0293(4)	0.2564(9)	0.2567(3)	0.2388(3)	0.2344(9)	0.2317(4)	0.2334(3)
O999	0.5993(10)	0.5951(5)	0.6067(4)	0.3853(9)	0.3870(3)	0.3755(3)	0.2574(9)	0.2463(4)	0.2305(3)

Notes: The atoms are labeled with three digit numbers. The first digit refers to the atom number assigned by Trojer (1969) for wollastonite-II, and the second digit refers to the atom number assigned by Joswig et al. (2003) for CaSiO₃-walstromite, and the third digit is the atom number assigned in this study for walstromite.

$$T = \begin{bmatrix} -1 & -1 & 0 & 0.5 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0.5 \end{bmatrix}$$

This transformation represents a redefinition of the *b* axis and an origin shift of $[\frac{1}{2} 0 \frac{1}{2}]$. Just as in the previous transformation, not all atoms in the asymmetric unit of wollastonite-II correspond to atoms in the asymmetric unit of CaSiO₃-walstromite, so some of the transformed coordinates represent symmetry equivalents. The corresponding unit-cell parameters for wollastonite-II after the transformation are $a = 6.695$, $b = 9.429$, $c = 6.666$ Å, $\alpha = 83.671^\circ$, $\beta = 76.133^\circ$, $\gamma = 67.639^\circ$. The transformed atomic coordinates for wollastonite-II are also given in Table 5 for comparison. An examination of Table 5 indicates that the transformed coordinates are virtually identical in value to those reported by Joswig et al. (2003). Figure 2 shows the projection of the structures of CaSiO₃-

walstromite and transformed wollastonite-II.

The fact that the atomic coordinates of both walstromite and wollastonite-II can be converted by a linear transformation to those of CaSiO₃-walstromite demonstrates that all three of these phases are isostructural. This accounts for the identical total energies of the CaSiO₃-walstromite and wollastonite-II and the lack of significant structural differences between the two phases (Joswig et al. 2003). This also explains the similarities in the calculated powder X-ray diffraction patterns of wollastonite-II (Trojer 1969), and CaSiO₃-walstromite (Joswig et al. 2003) (Fig. 3). The transformation was also undertaken between the (Ca,Sr)SiO₃-walstromite and (Ca,Sr)-wollastonite-II (Dörsam et al. 2009), and shows that these two are likely the same phase, reported in different settings. Furthermore, our demonstration that walstromite, CaSiO₃-walstromite, and high-pressure wollastonite-II are all isostructural suggests that CaSiO₃-walstromite could be a potential storage for appropriate cations larger than Ca under deep Earth conditions.

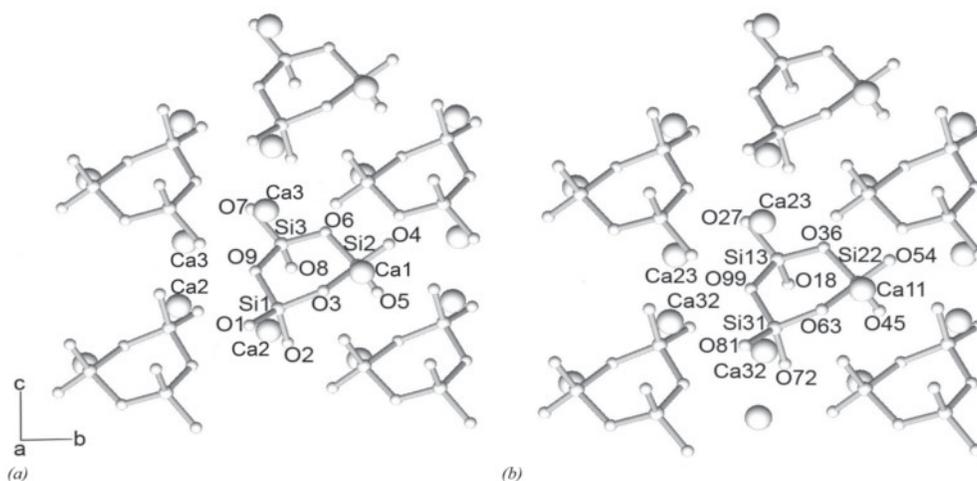


FIGURE 2. Comparison of (a) the structure of CaSiO₃-walstromite (Joswig et al. 2003) and (b) transformed wollastonite-II (Trojer 1969). For the transformed wollastonite-II, the atoms are labeled with two digit numbers. The first digit refers to the atom number assigned by Trojer (1969), and the second digit refers to the atom number assigned by Joswig et al. (2003).

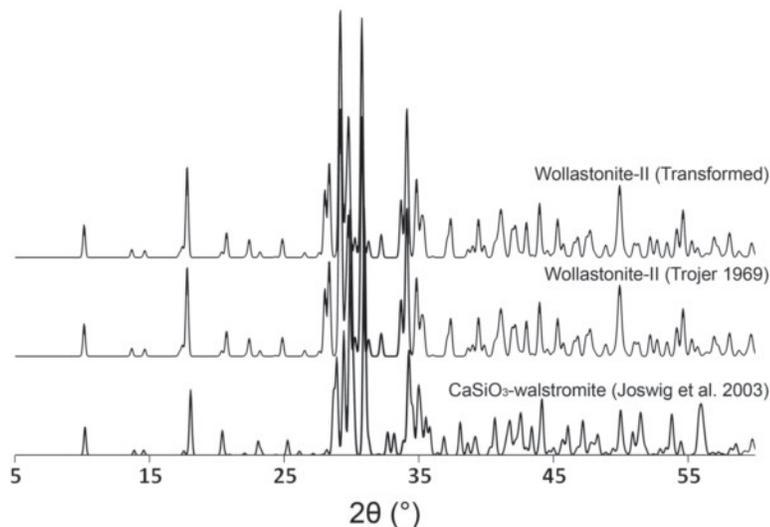


FIGURE 3. Calculated powder X-ray diffraction patterns (CuK α) for CaSiO₃-walstromite (Joswig et al. 2003), wollastonite-II in the setting of Trojer (1969). Note that the transformed pattern of wollastonite-II is identical to the pattern in the setting of Trojer demonstrating that the correct transformation was used.

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TABLE 3. Anisotropic displacement parameters (\AA^2) for walstromite
(FOR DEPOSIT)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0133 (3)	0.0107 (3)	0.0109 (3)	0.0005 (2)	0.0040 (2)	-0.0019 (2)
Ca2	0.0087 (3)	0.0116 (3)	0.0106 (3)	0.0009 (2)	0.0032 (2)	-0.0047 (2)
Ba1	0.0137 (1)	0.0109 (1)	0.01248 (9)	0.00202 (6)	0.00236 (6)	-0.00413 (7)
Si1	0.0082 (4)	0.0087 (4)	0.0093 (4)	-0.0004 (3)	0.0033 (3)	-0.0028 (3)
Si2	0.0084 (4)	0.0094 (4)	0.0097 (4)	0.0009 (3)	0.0036 (3)	-0.0035 (3)
Si3	0.0085 (4)	0.0100 (4)	0.0079 (4)	0.0005 (3)	0.0022 (3)	-0.0024 (3)
O1	0.0109 (10)	0.0126 (11)	0.0124 (10)	0.0001 (8)	0.0054 (8)	-0.0031 (8)
O2	0.0099 (10)	0.0115 (11)	0.0138 (10)	-0.0004 (8)	0.0024 (8)	-0.0043 (9)
O3	0.0106 (10)	0.0115 (11)	0.0131 (10)	0.0014 (8)	0.0032 (8)	-0.0032 (8)
O4	0.0112 (10)	0.0128 (11)	0.0106 (10)	-0.0016 (8)	0.0050 (8)	-0.0029 (8)
O5	0.0183 (12)	0.0119 (11)	0.0159 (11)	0.0025 (9)	0.0064 (9)	-0.0047 (9)
O6	0.0150 (11)	0.0104 (11)	0.0112 (10)	0.0013 (9)	0.0030 (8)	-0.0034 (8)
O7	0.0113 (10)	0.0133 (11)	0.0112 (10)	-0.0010 (8)	0.0054 (8)	-0.0045 (8)
O8	0.0163 (11)	0.0120 (11)	0.0097 (10)	0.0018 (9)	0.0026 (9)	-0.0025 (8)
O9	0.0107 (10)	0.0101 (10)	0.0107 (10)	0.0004 (8)	0.0024 (8)	-0.0026 (8)

TABLE 4. Selected atomic distances [\AA] sfor walstromite. **(FOR DEPOSIT)**

Ba1	— O1	2.809 (2)
	— O2	2.720 (2)
	— O2	2.858 (2)
	— O5	2.557 (2)
	— O7	2.721 (2)
	— O8	3.101 (2)
	— O9	2.939 (2)
	— O9	3.030 (2)
	Avg.	2.842
Si1	— O1	1.595 (2)
	— O2	1.586 (2)
	— O3	1.662 (2)
	— O9	1.678 (2)
	Avg.	1.630
Ca1	— O1	2.325 (2)
	— O3	2.658 (2)
	— O4	2.419 (2)
	— O4	2.436 (2)
	— O5	2.472 (3)
	— O5	2.862 (3)
	— O6	2.798 (2)
	— O7	2.395 (2)
	Avg.	2.546
Si2	— O3	1.687 (2)
	— O4	1.595 (2)
	— O5	1.575 (2)
	— O6	1.677 (2)
	Avg.	1.634
Ca2	— O1	2.358 (2)
	— O2	2.300 (2)
	— O4	2.480 (2)
	— O7	2.317 (2)
	— O8	2.326 (2)
	— O8	2.444 (2)
	Avg.	2.371
Si3	— O6	1.673 (2)
	— O7	1.599 (2)
	— O8	1.589 (2)
	— O9	1.674 (2)
	Avg.	1.634