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THE CRYSTAL STRUCTURE OF MCKELVEYITE-(Y)-2*M*, A NEW MONOCLINIC POLYTYPE FROM VAL MALENCO, ITALIAN ALPS

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Abstract

A new monoclinic (*Cc*) polytype, mckelveyite-(Y)-2*M*, $\mathrm{NaBa_3CaY(CO_3)_6 \cdot 3H_2O}$, was found in "Cava Fabi", a talc quarry near Lanzada in Val Malenco, Lombardy, Italy, associated with anatase, brookite, brucite, calcite, dolomite, ilmenite, lindsleyite, magnesite, magnetite, pyrite, quartz, redledgeite and rutile, in hydrothermal carbonate veins intercalated in ultrabasic rocks and dolomitic marble in contact with serpentinites. The origin of the mineral is related to circulation of $\mathrm{CO_2}$-rich fluids in serpentinites, during the latest stages of Alpine metamorphism. The monoclinic mineral, space group *Cc*, has cell parameters *a* 15.8213(7), *b* 9.1364(4), *c* 13.7522(6) Å, β 112.44(1)°, *V* 1837.35(15) Å^3, with marked pseudorhombohedral symmetry. The crystals are pseudopyramidal, up to 4 mm in length, with distinct trigonal character derived from intergrowth of three individuals twinned about a pseudo-threefold axis, in some cases showing re-entrant angles. The chemical analysis obtained by wavelength-dispersion electron-microprobe analysis, supplemented by structural data for $\mathrm{CO_2}$ and $\mathrm{H_2O}$, gave (wt%): $\mathrm{Na_2O}$ 3.50, CaO 5.68, SrO 3.45, BaO 45.33, $\mathrm{Y_2O_3}$ 8.82, $\mathrm{Sm_2O_3}$ 0.05, $\mathrm{Gd_2O_3}$ 0.45, $\mathrm{Dy_2O_3}$ 1.10, $\mathrm{Er_2O_3}$ 0.85, $\mathrm{Yb_2O_3}$ 0.08, $\mathrm{CO_2}$ 27.13, $\mathrm{H_2O}$ 5.55, total 101.99, corresponding to the empirical formula (calculated on the basis of six metal sites in the asymmetric unit, as shown in the structure solution): $\mathrm{Na_{1.00}(Ca_{0.83}Na_{0.07}Sr_{0.11})_{\Sigma 1.01}(Ba_{2.79}Sr_{0.20})_{\Sigma 2.99}(Y_{0.74}REE_{0.13}Ca_{0.12})_{\Sigma 0.99}[CO_3]_6 \cdot 3H_2O}$. The crystal structure has been refined to a final $R = 0.0283$ for 4454 observed reflections [$I > 2\sigma(I)$], and corresponds to the first accurate determination of the structure of mckelveyite-(Y). The unit cell contains three independent atomic sites occupied by Ba plus minor Sr, and three sites occupied almost exclusively by $\mathrm{Na^+}$, $\mathrm{Ca^{2+}}$, and $\mathrm{Y^{3+}}$ (plus the REE), respectively; there are alternate double layers of pseudo-hexagonal rings perpendicular to the *c** axis containing either the Ba atoms or the other metal atoms, with no substantial disorder; each double layer is the mirror image on {010} of the adjacent ones. The strongest six lines in the X-ray powder-diffraction pattern [d_{obs} in Å(*I*)*hkl*] are: 3.106(100)(312), 4.299(48)(310), 6.369(36)(002), 2.029(29)(602), 3.180(28)(004), 2.635(27)(60$\bar{2}$). The pattern shows significant differences with respect to type triclinic mckelveyite-(Y).

Keywords: mckelveyite-(Y)-2*M*, new monoclinic polytype, crystal structure, donnayite group, Val Malenco, Italian Alps.

Sommaire

Nous décrivons un nouveau polytype monoclinique (*Cc*), mckelveyite-(Y)-2*M*, $\mathrm{NaBa_3CaY(CO_3)_6 \cdot 3H_2O}$, découvert dans la carrière de talc "Cava Fabi", près de Lanzada, dans le Val Malenco, Lombardie, Italie, associé à anatase, brookite, brucite, calcite, dolomite, ilménite, lindsleyite, magnésite, magnétite, pyrite, quartz, redledgeite et rutile, dans des veines hydrothermales carbonatées intercalées dans des roches ultrabasiques et des marbres dolomitiques en contact avec des serpentinites. Le minéral a cristallisé lors de la circulation de fluides riches en $\mathrm{CO_2}$ dans les serpentinites, au cours des stades ultimes du métamorphisme alpin. Le minéral monoclinique, groupe spatial *Cc*, possède les paramètres réticulaires *a* 15.8213(7), *b* 9.1364(4), *c* 13.7522(6) Å, β 112.44(1)°, *V* 1837.35(15) Å^3, avec symétrie pseudo-rhomboédrique marquée. Les cristaux sont pseudo-pyramidaux, atteignant une longueur de 4 mm, et possèdent un aspect distinctement trigonal, dérivé de l'intercroissance de trois individus maclés selon un pseudo-axe 3, dans certains cas avec des angles rentrants. L'analyse chimique, obtenue avec une microsonde électronique en dispersion d'énergie, et complétée avec données sur la teneur en $\mathrm{CO_2}$ et $\mathrm{H_2O}$ obtenues par ébauche de la structure, a donné (en %, base pondérale): $\mathrm{Na_2O}$ 3.50, CaO 5.68, SrO 3.45, BaO 45.33, $\mathrm{Y_2O_3}$ 8.82, $\mathrm{Sm_2O_3}$ 0.05, $\mathrm{Gd_2O_3}$ 0.45, $\mathrm{Dy_2O_3}$ 1.10, $\mathrm{Er_2O_3}$ 0.85, $\mathrm{Yb_2O_3}$ 0.08, $\mathrm{CO_2}$ 27.13, $\mathrm{H_2O}$ 5.55, total 101.99, ce qui correspond à la formule empirique (calculée sur une base de six sites pour métaux dans l'unité asymétrique, telle qu'indiquée dans la solution de la structure): $\mathrm{Na_{1.00}(Ca_{0.83}Na_{0.07}Sr_{0.11})_{\Sigma 1.01}(Ba_{2.79}Sr_{0.20})_{\Sigma 2.99}(Y_{0.74}REE_{0.13}Ca_{0.12})_{\Sigma 0.99}[CO_3]_6 \cdot 3H_2O}$. Nous en avons affiné la structure cristalline

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jusqu'à un résidu R final de 0.0283 pour 4454 réflexions observées [$I > 2\sigma(I)$], et elle est en fait la première détermination exacte de la structure de la mckelveyite-(Y). La maille élémentaire contient trois sites indépendants qu'occupe le Ba et, en proportion mineure, le Sr, et trois sites remplis presqu'exclusivement par Na^+, Ca^{2+}, et Y^{3+} (avec les terres rares), respectivement; il y a une alternance de couches doubles d'anneaux pseudo-hexagonaux perpendiculaires à l'axe c^* contenant soit les atomes de Ba ou les autres atomes métalliques, sans grand désordre; chaque couche double est l'image miroir sur {010} des couches adjacentes. Les six lignes les plus intenses du spectre de diffraction, méthode des poudres [d_{obs} en Å(I)hkl] sont: 3.106(100)(312), 4.299(48)(310), 6.369(36)(002), 2.029(29)(602), 3.180(28)(004), 2.635(27)(60$\bar{2}$). Le spectre de diffraction diffère de façon importante de celui de la mckelveyite-(Y) triclinique holotypique.

(Traduit par la Rédaction)

Mots-clés: mckelveyite-(Y)-2*M*, nouveau polytype monoclinique, structure cristalline, groupe de la donnayite, Val Malenco, Alpes italiennes.

INTRODUCTION

In recent times, several interesting minerals have been found in the Cava Fabi talc quarry, near Lanzada, Val Malenco, Sondrio, Lombardy, northern Italy, within hydrothermal carbonate veins intercalated in ultrabasic rocks and dolomitic marble in contact with serpentinites. Among the rarer minerals found there are lindsleyite and redledgeite, occurring together with anatase, brookite, brucite, calcite, dolomite, ilmenite, magnesite, magnetite, pyrite, quartz and rutile (Bedogné *et al.* 1993). These minerals are attributed to the circulation of CO_2-rich fluids in serpentinites, during the last stages of Alpine metamorphism.

A sample of another unusual mineral occurring in this suite was submitted to our attention by Dr. Francesco Bedogné of Sondrio. A preliminary chemical analysis using an energy-dispersion electron-microprobe instrument and infrared data showed the main components to be Ba, Y, Ca, Na, Sr, carbonates and H_2O, the composition being similar to that of mckelveyite-(Y). Since no other mineral found in the Alpine region shows such a composition, a detailed study of this material appeared to be rewarding, especially in view of the availability of crystals of particularly good quality and of the lack of an accurate determination of the structure of some members of the donnayite group, including mckelveyite-(Y) itself.

As is shown below in detail, the crystal-structure determination and the X-ray powder-diffraction data (see below) showed that the mineral is a new modification of mckelveyite-(Y) for which a new name might be proposed; however, following the advice of the Chairman of CNMNC Commission of IMA, we accept the suggestion that material is simply a polytype: mckelveyite-(Y)-2*M*. Consequently, the "old" triclinic modification should be called, from now on, "mckelveyite-(Y)-1*A*".

PHYSICAL PROPERTIES AND CHEMICAL DATA

The mineral occurs as pseudopyramidal crystals up to 4 mm long, showing in some cases re-entrant angles, with a distinct trigonal character derived by intergrowth of three individuals twinned about a pseudo-threefold axis. The crystals are photosensitive and metameric; the color is pale pink under sunlight and pale blue under fluorescent light. On exposure to sunlight, the color turns from pale pink to almost colorless; the color is restored after keeping the mineral in the dark for some time.

Chemical analyses were carried out by means of an ARL–SEMQ electron microprobe (20 kV, 15 nA, 0.15 μm beam diameter). The mean analytical results are reported in Table 1.

The empirical formula (calculated on the basis of six metal sites in the asymmetric unit and accounting for the presence of CO_2 and H_2O as revealed by structure solution) is: $Na_{1.00}(Ca_{0.83}Na_{0.07}Sr_{0.11})_{\Sigma 1.01}(Ba_{2.79}Sr_{0.20})_{\Sigma 2.99}(Y_{0.74}REE_{0.13}Ca_{0.12})_{\Sigma 0.99}[CO_3]_6 \cdot 3H_2O$. The composition is nearly identical with that of mckelveyite $NaBa_3(Ca,U)Y(CO_3)_6 \cdot 3H_2O$ (Milton *et al.* 1965, Desautels 1967, Chao *et al.* 1978, Voloshin *et al.* 1990, Pekov & Podlesnyi 2004), the main difference with respect to the specimens from the other (non-Alpine) occurrences being the absence of uranium and thorium in appreciable amounts.

The infrared spectrum recorded on small fragments cut from a single crystal using a Perkin–Elmer FTIR spectrometer shows sharp absorptions at 665, 722, 865, 1066 and 1075 cm^{-1} due to the carbonate anion,

TABLE 1. CHEMICAL COMPOSITION OF MCKELVEYITE-(Y)-2*M*

		Range	Stand. dev.	Probe standard
Na_2O wt.%	3.50	3.22 – 3.74	0.08	Albite natural standard
CaO	5.68	5.40 – 5.89	0.06	Kaersutite natural standard
SrO	3.45	2.35 – 5.18	0.05	Celestine natural standard
BaO	45.33	41.82 – 46.55	0.05	Celsian natural standard
Y_2O_3	8.82	7.72 – 10.10	0.04	Synthetic glass
Sm_2O_3	0.05	0.00 – 0.10	0.15	Synthetic glass
Gd_2O_3	0.45	0.20 – 0.55	0.15	Synthetic glass
Dy_2O_3	1.10	1.04 – 1.51	0.08	Synthetic glass
Er_2O_3	0.85	0.59 – 1.09	0.08	Synthetic glass
Yb_2O_3	0.08	0.04 – 0.12	0.10	Synthetic glass
CO_2 *	27.13			
H_2O *	5.55			
Total	101.99			

Number of analyses: 12; * determined from structure solution.

and wider bands in the range 1399–1700 cm^{-1} and 2800–3400 cm^{-1} containing a series of minor absorptions at 1766, 1786, 2423, 2450, 2539 cm^{-1}. The first of such bands includes the contribution of the bending modes in the carbonate anions as well as the H–O–H flexing modes. The second band includes all the OH stretching modes.

X-Ray Data and Structure Refinement

Single-crystal diffraction data were collected from a crystal fragment measuring 0.10 × 0.06 × 0.03 mm with Mo*K*α radiation (λ = 0.71073 Å), using a BRUKER Apex II diffractometer equipped with a 2K CCD detector. A one-minute frame-time and 0.3° frame width were used. A total of 11329 reflections were measured up to 2θ = 58.64°. The unit-cell dimensions were obtained by least-squares fit from 7465 reflections with $I > 5\sigma(I)$; the refined values are given in Table 2. The intensities and the extinctions comply with the requirements of the *Cc* or *C*2/*c* space-group symmetry.

TABLE 2. MISCELLANEOUS STRUCTURE-REFINEMENT DATA FOR MCKELVEYITE-(Y)-2*M*

Crystal system	monoclinic	Space group	*Cc* (no. 9)
a (Å)	15.8213(7)	β (°)	112.44(1)
b (Å)	9.1364(4)	*V* (Å^3)	1837.35(15)
c (Å)	13.7522(6)	Z	4
D_{calc} (g cm^{-3})[#]	3.536	μ (Mo*K*α) (mm^{-1})[#]	9.89
Scan mode	ω	θ range (°)	2.63 -29.32
Measured reflections		11329	
Independent reflections		4618	
Observed reflections [$I > 2\sigma(I)$]		4454	
Minimum transmission factor		0.536	
Parameters refined		271	
Final *R* and w*R*2[§]		0.0283, 0.0829	
Largest diffraction peak and hole (e Å^{-3})		1.27, -1.40	

[§] $R = \Sigma \| Fo | - | Fc \| / \Sigma | Fo |$; $wR2 = \{\Sigma[w(Fo^2 - Fc^2)^2] / \Sigma[w(Fo^2)^2]\}^{1/2}$.

[#] Calculated from the idealized formula $NaBa_3CaY(CO_3)_6{\cdot}3H_2O$.

A triclinic cell, closely comparable with that of the triclinic members of the donnayite-(Y) group, including type mckelveyite-(Y) (Chao *et al.* 1978), can be derived from the monoclinic cell using the transformation matrix $\mathbf{A}^{-1} = [\overline{\tfrac{1}{2}}\ \overline{\tfrac{1}{2}}\ 0 / 0\ \overline{1}\ 0 / \tfrac{1}{2}\ \tfrac{1}{2}\ 1]$ (see Table 3). Interestingly enough, at least *one other* equivalent triclinic primitive unit-cell with nearly exactly the same parameters exists [*a* 9.1353(4), *b* 9.1332(4), *c* 13.7639(7) Å, α 109.466°(5), β 109.377(5)°, γ 60.000(5)°], the transformation matrix $\mathbf{A}'^{-1}$ from the monoclinic reference being $[0\ 1\ 0 / \overline{\tfrac{1}{2}}\ \tfrac{1}{2}\ 0 / \tfrac{1}{2}\ \overline{\tfrac{1}{2}}\ 1]$. Such a strict resemblance, which indicates the existence of remarkable pseudosymmetry, caused notable confusion and consequent difficulty in establishing the actual relationships with the already known phases. Difficulties of the same kind also appear in the "classic" works by Donnay & Donnay (1971), who described type mckelveyite-(Y) as trigonal instead of triclinic, with many specimens showing twinning by merohedry, giving twin symmetry 6*'m'm*.

A comparison of the unit cell of our mineral with those of minerals in the donnayite group is reported in Tables 3 and 4. Similarities are evident: for instance, the unit-cell volume is about four times as large as that of triclinic mckelveyite-(Y)-1*A*, and is about six times as large as that of ewaldite, the *a* and *b* parameters in the triclinic setting being almost equal to those of mckelveyite-(Y)-1*A*, and *c* nearly double in length.

However, surprisingly enough, in spite of nearly doubling in length, the **c**-axis *vector* in our mineral *does not correspond* to double the **c**-axis *vector* in mckelveyite-(Y)-1*A* (see the transformation matrix $\mathbf{A}^{-1}$ reported above, and also below). The most useful data for comparison in this respect are instead the values of the *c** parameters: the inverse of these values, as for

TABLE 3. UNIT-CELL DATA FOR MEMBERS OF THE DONNAYITE GROUP

	Mckelveyite-(Y)-2*M* present work	Mckelveyite-(Y)-1*A* Chao *et al.* (1978)	Donnayite-(Y)-1*A* Chao *et al.* (1978)	Weloganite Grice & Perrault (1975)
Formula	$NaBa_3CaY$ $(CO_3)_6{\cdot}3H_2O$	$NaBa_3(Ca,U)Y$ $(CO_3)_6{\cdot}3H_2O$	$Na\ Sr_3CaY$ $(CO_3)_6{\cdot}3H_2O$	Na_2Sr_3Zr $(CO_3)_6{\cdot}3H_2O$
Crystal system	monoclinic [§]	triclinic	triclinic	triclinic
Space group	*Cc*	*P*1	*P*1	*P*1
a (Å)	9.1349(3)	9.170(3)	9.000(1)	8.966(1)
b (Å)	9.1364(3)	9.169(3)	8.999(1)	8.980(2)
c (Å)	13.7660(8)	7.075(2)	6.793(1)	6.730(1)
α (°)	109.381(4)	102.50(3)	102.77(1)	102.72(2)
β (°)	109.469(4)	115.63(3)	116.28(1)	116.65(1)
γ (°)	59.995(5)	59.99(3)	59.99(1)	60.06(1)
*c** (Å^{-1})	0.07868	0.15678	0.16417	0.16624
Distance (Å)[%]	12.710/2 = 6.355	6.378	6.091	6.015
V (Å^3)	918.65(7)	464.4(3)	427.2(1)	419.7(1)
Z	2	1	1	1

[§] the data above are for a pseudotriclinic unit-cell obtained by application of the transformation matrix $\mathbf{A}^{-1} = [\overline{\tfrac{1}{2}}\ \overline{\tfrac{1}{2}}\ 0 / 0\ \overline{1}\ 0 / \tfrac{1}{2}\ \tfrac{1}{2}\ 1]$ to the monoclinic *C*-centered cell adopted in this work; $\mathbf{A} = [\overline{2}\ 1\ 0 / 0\ \overline{1}\ 0 / \overline{1}\ 0\ 1]$. %: the distance between successive double layers.

all the minerals in the group, are multiples of a unit distance of about 6.36 Å between successive double layers of metal atoms (see Tables 3, 4 and below). Such a distance is slightly smaller for the phases where Sr prevails over Ba, such as donnayite-(Y) and weloganite.

Besides the possibilities described above, the cell can also be transformed into a pseudorhombohedral counterpart (see Table 4), although the symmetry of the reflections is not accounted for. A marked similarity in this respect with other species in the donnayite group [some of which show similar problems of pseudosymmetry: see for instance Donnay & Donnay (1971), Chen & Chao (1975), Grice & Perrault (1975)] is also shown in the same table.

An absorption correction was applied using the SADABS program (Sheldrick 2000). After having merged the multiple measurements and the equivalent reflections but not the Friedel pairs (R_{int} = 0.057), 4618 unique reflections were obtained. The absence of a center of symmetry was first suggested by the distinctly hemimorphic habit of the crystals and, notwithstanding the distribution of the *E* values ($E^2 - 1 = 1.178$), the structure solution and refinement fully confirm the space group to be *Cc* (see also below).

The structure was solved by direct methods with SIR97 (Altomare *et al.* 1999) and refined on F^2 using the SHELXL97 program (Sheldrick 1997) implemented in the WINGX suite (Farrugia 1999). A total of 4454 reflections with $I > 2\sigma(I)$ were used for the structure refinement. Since the possibility of dealing with a twin was indicated by SHELXL97, a twin matrix [$\bar{1}$ 0 0 / 0 $\bar{1}$ 0 / 0 0 $\bar{1}$] was applied; after the refinement, the relative percentage of twins was found to be 0.83 and 0.17, thereby confirming twinning and excluding the presence of a center of symmetry. Furthermore, a check carried out using the MISSYM algorithm in the program PLATON (Le Page 1987, 1988) excluded the presence of a higher symmetry than that of the proposed space-group *Cc*. To account for possible compositional variation, the occupancies of the metal sites were also refined, and the results are in agreement with the empirical formula

TABLE 4. UNIT-CELL DATA FOR Y-RICH MEMBERS OF THE DONNAYITE GROUP

	Mckelveyite-(Y)-2*M* present work	Mckelveyite-(Y)-1*A* Chao *et al.* (1978)	Donnayite-(Y)-1*A* Trinh *et al.* (1992)	Donnayite-(Y)-3*R* Trinh *et al.* (1992)
Formula	$NaBa_3CaY$ $(CO_3)_6 \cdot 3H_2O$	$NaBa_3(Ca,U)Y$ $(CO_3)_6 \cdot 3H_2O$	$NaSr_3CaY$ $(CO_3)_6 \cdot 3H_2O$	$Na\ Sr_3CaY$ $(CO_3)_6 \cdot 3H_2O$
Crystal system	monoclinic	triclinic	triclinic	trigonal
Space group	*Cc*	*P*1	*P*1	*R*3*m*
a (Å)	15.8213(7)	9.170(3)	8.993(2)	5.211(1)
b (Å)	9.1364(4)	9.169(3)	8.985(2)	
c (Å)	13.7522(6)	7.075(2)	6.780(2)	18.357(7)
α (°)		102.50(3)	116.25(2)	
β (°)	112.44(1)	115.63(3)	102.76(2)	
γ (°)		59.99(3)	60.00(1)	
V(Å^3)	1837.3(2)	464.4(3)	425.5(2)	431.7(2)
Z	4	1	1	1

TABLE 4 (cont'd). UNIT-CELL DATA REFERRED TO HEXAGONAL AXES

	Mckelveyite-(Y)-2*M* pseudo-trigonal *R*-centered	Mckelveyite-(Y)-1*A* pseudo-trigonal *P*31*m* Donnay & Donnay (1971)	Donnayite-(Y)-1*A* Trinh *et al.* (1992) pseudotrigonal *R* From the triclinic cell through 010/1$\bar{1}$0/$\bar{1}$0$\bar{3}$	Donnayite-(Y)-3*R* rhombohedral *R*3*m* Trinh *et al.* (1992)	Ewaldite Donnay & Donnay (1971a, b), Voloshin *et al.* (1992) hexagonal *P*6$_3$*mc*
Formula	$NaBa_3CaY$ $(CO_3)_6 \cdot 3H_2O$	$NaBa_3(Ca,U)Y$ $(CO_3)_6 \cdot 3H_2O$	$NaSr_3CaY$ $(CO_3)_6 \cdot 3H_2O$	$NaSr_3CaY$ $(CO_3)_6 \cdot 3H_2O$	$Ba(Ca,Y,Na)$ $(CO_3)_2 \cdot nH_2O$
a (Å)	9.1351(4)	9.16(1)= 5.297√3	8.987	5.211(1)	5.284-5.320 $^{\$}$
c (Å)	38.1316(18)	19.13(2)	18.242	18.357(7)	12.78-12.84 $^{\$\$}$
*c** (Å^{-1})	0.0262	0.0523	0.0548	0.0545	0.0782-0.0779
Distance $^{\%}$	38.1316/6 = 6.355	19.13/3 = 6.377	18.242/3 = 6.081	18.357/3 = 6.119	*c*/2 = 6.39-6.42
V (Å^3)	2775.8(2)	1390(3)	1275.9	431.7(2)	309.0 – 314.7
Z	6	3	3	1	2

$^{\$}$: *a* (mckelveyite-1*A*) / √3. $^{\$\$}$: *c* (mckelveyite-1*A*) × 2/3. $^{\%}$: distance (Å) between successive double layers.

proposed above. Other details concerning the data collection and refinement are reported in Table 2. The final coordinates and the displacement parameters of the atoms are reported in Tables 5 and 6, respectively. Tables of observed and calculated structure-factors may be obtained from The Depository of Unpublished Data on the MAC web site [document Mckelveyite CM46_195].

X-ray powder-diffraction data (Table 7) were obtained using a Rigaku D/MAX diffractometer with Cu*K*α radiation (λ = 1.54059 Å) and a graphite monochromator on the reflected beam; the pattern shows significant differences with respect to those of type mckelveyite-(Y)-1*A* (see Table 7) . Using these data, the program UNIT CELL (Holland & Redfern 1997) has provided the following unit-cell parameters: *a* 15.8203(7) Å, *b* 9.1277(3) Å, *c* 13.7708(7) Å, β 112.544(3)°, *V* = 1836.58(9) Å^3 after correction of the zero shift on a best-fit basis.

RESULTS AND DISCUSSION

A perspective view of the structure is shown in Figure 1. The asymmetric unit contains three independent sites occupied by Ba plus minor Sr and three additional sites, each one of them occupied in strong

TABLE 5. FRACTIONAL COORDINATES OF THE ATOMS IN MCKELVEYITE-(Y)-2*M*

Atom	*X/a*	*Y/b*	*Z/c*
Ba(1)	0.06707(7)	0.07929(3)	0.19538(8)
Ba(2)	-0.10600(8)	0.58255(4)	0.19136(9)
Ba(3)	0.23060(8)	0.58870(3)	0.18838(3)
Y	0.00000	0.41563(4)	0.00000
Ca	-0.16659(17)	-0.08353(13)	-0.0044(2)
Na	0.1646(3)	-0.0834(2)	-0.0068(4)
C(1)	0.0387(4)	-0.2510(6)	0.1166(5)
C(2)	0.2053(4)	0.2559(6)	0.1164(4)
C(3)	-0.1264(4)	0.2531(6)	0.1174(4)
C(4)	0.0126(4)	0.1476(6)	-0.0991(4)
C(5)	0.0784(4)	0.6198(6)	-0.0978(4)
C(6)	-0.1899(4)	0.4833(6)	-0.0984(4)
O(11)	-0.0320(3)	-0.1849(5)	0.1164(4)
O(12)	0.1048(3)	-0.1844(5)	0.1119(4)
O(13)	0.0425(3)	-0.3951(4)	0.1288(4)
O(21)	0.2033(3)	0.1135(5)	0.1086(4)
O(22)	0.1388(3)	0.3243(5)	0.1265(3)
O(23)	0.2754(3)	0.3257(5)	0.1208(4)
O(31)	-0.1253(3)	0.1086(4)	0.1176(4)
O(32)	-0.0546(3)	0.3215(4)	0.1242(3)
O(33)	-0.1956(3)	0.3197(5)	0.1152(4)
O(41)	0.0271(3)	0.2765(4)	-0.1328(4)
O(42)	-0.0163(3)	0.1482(4)	-0.0238(3)
O(43)	0.0263(3)	0.0294(5)	-0.1399(4)
O(51)	0.1292(3)	0.5399(5)	-0.0242(3)
O(52)	-0.0099(3)	0.5954(4)	-0.1309(4)
O(53)	0.1100(3)	0.7210(5)	-0.1379(3)
O(61)	-0.1377(3)	0.5629(5)	-0.0233(4)
O(62)	-0.1506(3)	0.3792(5)	-0.1315(4)
O(63)	-0.2764(3)	0.5017(5)	-0.1385(4)
OW(1)	-0.1062(3)	-0.1522(5)	-0.1350(4)
OW(2)	-0.2303(3)	0.1071(5)	-0.1335(4)
OW(3)	-0.2976(3)	-0.2077(5)	-0.1330(4)

TABLE 6. DISPLACEMENT PARAMETERS *U*(i,j) FOR MCKELVEYITE-(Y)-2*M*

Atom	U_{11},U	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Ba(1)	0.0084(2)	0.0077(1)	0.0111(2)	-0.0003(2)	0.0043(2)	-0.0001(1)	0.0089(1)
Ba(2)	0.0101(2)	0.0092(2)	0.0112(2)	-0.0007(1)	0.0046(2)	0.0003(1)	0.0100(1)
Ba(3)	0.0112(2)	0.0115(2)	0.0153(3)	-0.0007(2)	0.0059(2)	-0.0008(2)	0.0124(1)
Y	0.0061(2)	0.0061(2)	0.0088(2)	-0.0001(2)	0.0033(2)	-0.0001(1)	0.0068(1)
Ca	0.0173(7)	0.0167(7)	0.0160(8)	0.0005(4)	0.0070(6)	0.0009(4)	0.0165(5)
Na	0.021(1)	0.012(1)	0.023(2)	0.001(1)	0.010(1)	-0.000(7)	0.018(1)
O(11)	0.009(2)	0.013(2)	0.022(2)	0.001(2)	0.006(2)	0.008(2)	0.014(1)
O(12)	0.016(2)	0.008(2)	0.026(2)	0.003(2)	0.012(2)	-0.002(2)	0.015(2)
O(13)	0.015(2)	0.005(2)	0.019(2)	-0.002(2)	0.009(2)	0.002(2)	0.012(1)
O(21)	0.018(2)	0.007(2)	0.026(3)	-0.003(2)	0.011(2)	-0.001(2)	0.016(1)
O(22)	0.007(2)	0.011(2)	0.015(2)	0.004(2)	0.002(2)	0.005(2)	0.011(1)
O(23)	0.013(2)	0.007(2)	0.022(2)	0.003(2)	0.009(2)	-0.001(2)	0.013(1)
O(31)	0.018(2)	0.005(2)	0.023(2)	0.000(2)	0.013(2)	0.001(2)	0.014(1)
O(32)	0.013(2)	0.006(2)	0.013(2)	0.002(2)	0.007(2)	0.000(2)	0.010(1)
O(33)	0.011(2)	0.010(2)	0.032(3)	0.005(2)	0.012(2)	0.008(2)	0.016(2)
O(41)	0.018(2)	0.013(2)	0.026(3)	0.000(2)	0.012(2)	0.001(2)	0.018(2)
O(42)	0.027(2)	0.022(2)	0.012(2)	-0.002(2)	0.011(2)	0.002(2)	0.019(1)
O(43)	0.026(2)	0.017(2)	0.021(2)	-0.004(2)	0.012(2)	0.001(2)	0.020(2)
O(51)	0.017(2)	0.020(2)	0.018(2)	0.008(2)	0.007(2)	0.000(2)	0.018(1)
O(52)	0.015(2)	0.018(2)	0.027(2)	0.004(2)	0.009(2)	0.000(2)	0.019(2)
O(53)	0.021(2)	0.020(2)	0.022(2)	0.005(2)	0.010(2)	-0.004(2)	0.021(2)
O(61)	0.015(2)	0.026(2)	0.021(2)	-0.006(2)	0.005(2)	0.000(2)	0.021(2)
O(62)	0.013(2)	0.021(2)	0.024(2)	-0.004(2)	0.009(2)	-0.001(2)	0.019(1)
O(63)	0.011(2)	0.025(2)	0.026(2)	-0.003(2)	0.004(2)	0.003(2)	0.022(1)
OW(1)	0.018(2)	0.021(2)	0.022(2)	0.001(2)	0.009(2)	0.004(2)	0.020(1)
OW(2)	0.018(2)	0.019(2)	0.024(2)	0.003(2)	0.005(2)	0.002(2)	0.021(2)
OW(3)	0.016(2)	0.024(2)	0.022(2)	-0.003(2)	0.007(2)	-0.002(2)	0.021(1)
C(1)	0.014(1)						
C(2)	0.011(1)						
C(3)	0.012(1)						
C(4)	0.015(1)						
C(5)	0.014(1)						
C(6)	0.014(1)						

The anisotropic displacement factor exponent takes the form: $-2\pi^2(U_{11}h^2(a^*)^2 + ... + 2U_{12}hka^*b^* + ...)$; Ueq = $1/3(U_{11} + U_{22} + U_{33})$.

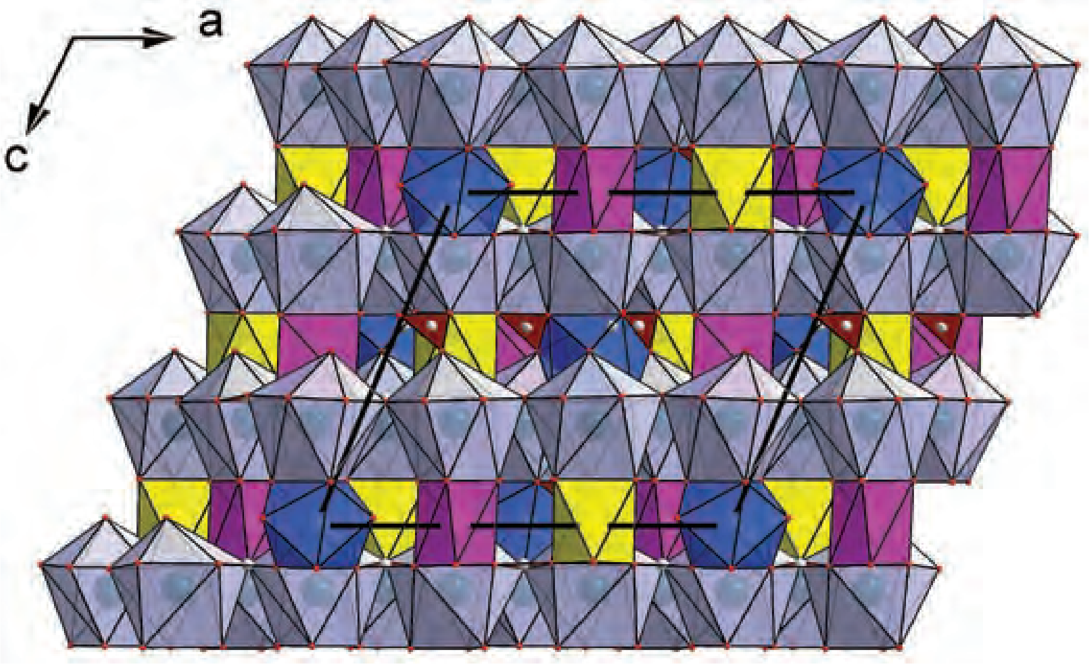

FIG. 1. Perspective view along [010]. The double layers perpendicular to **c*** are evident: barium atoms are represented at the center of gray polyhedra. The polyhedra around Y, Ca and Na sites are shown in blue, magenta and yellow, respectively. The carbonate ions are shown as red triangles.

prevalence by Na^+, Ca^{2+}, or Y^{3+} (with the REE), respectively. Six carbonate anions are also present, together with three H_2O molecules.

Each barium atom is bonded to 10 oxygen atoms: the Ba(1)–O distances range from 2.753(5) to 2.861(4) Å, with an average of 2.823 Å, the Ba(2)–O distances range from 2.782(5) to 2.845(5) Å, with an average of 2.810 Å, and the Ba(3)–O distances range from 2.765 (4) to 2.903(5) Å, with an average of 2.810 Å. Both these values of bond distances and the equivalent displacement-parameters of atoms show that there is little compositional difference between the independent sites, although the site of Ba(1) is probably poorer in strontium than the other two. The bond-valence sums, according to Brown & Wu (1976), are 2.37, 2.44 and 2.46 valence units (*vu*), respectively; these high values are probably due to the presence of Sr. The nine Y–O distances range from 2.351(4) to 2.476(4) Å, with an average of 2.412 Å, a value close to the average (2.428 Å) of the Y–O distances observed in a series of crystals of Alpine gadolinite by Demartin *et al*. (1993); the bond-valence sum is 3.11 *vu*. The values of the six Ca–O distances (below 3 Å) are in comparison more scattered, in agreement with their less covalent character; they range from 2.334(5) to 2.431(5) Å, with an average of 2.388 Å, and define a distorted trigonal prism. The bond-valence sum is 1.80 *vu*. The six shortest Na–O distances (below 3 Å) range from 2.322(6) to 2.477(7) Å, with an average of 2.408 Å. They define a distorted octahedron; the bond-valence sum is 1.11 *vu*.

As for all the members of the donnayite group, there are couples of adjacent layers of metal atoms perpendicular to the **c*** axis. In each couple, where all the metal atoms follow a pseudohexagonal arrangement (Fig. 2), one layer contains barium atoms only, with minor Sr; in the other layer, there are instead sites with a prevalence of Y, Ca, or Na atoms, respectively. The non-equivalence of all the metal sites in the same layer (especially those concerning Y, Na and Ca) and their different coordination-polyhedra are the main reasons for lowering the symmetry with respect to the true hexagonal or trigonal counterparts of the group, such as ewaldite or donnayite-(Y)-3*R*-like structures (Trinh *et al*. 1992). For these species of higher symmetry, disorder renders all these sites equivalent, apparently notwithstanding the opinion of Donnay & Donnay (1971) and Donnay & Preston (1971). On the other hand, Ba(3) also does not show exactly the same environment as Ba(1) and Ba(2), being linked to the three H_2O molecules and not exclusively to carbonate groups (see below).

The arrangement of these layers is very similar to that of weloganite (Grice & Perrault 1975), the unit-cell *vectors* being related by the following transformation

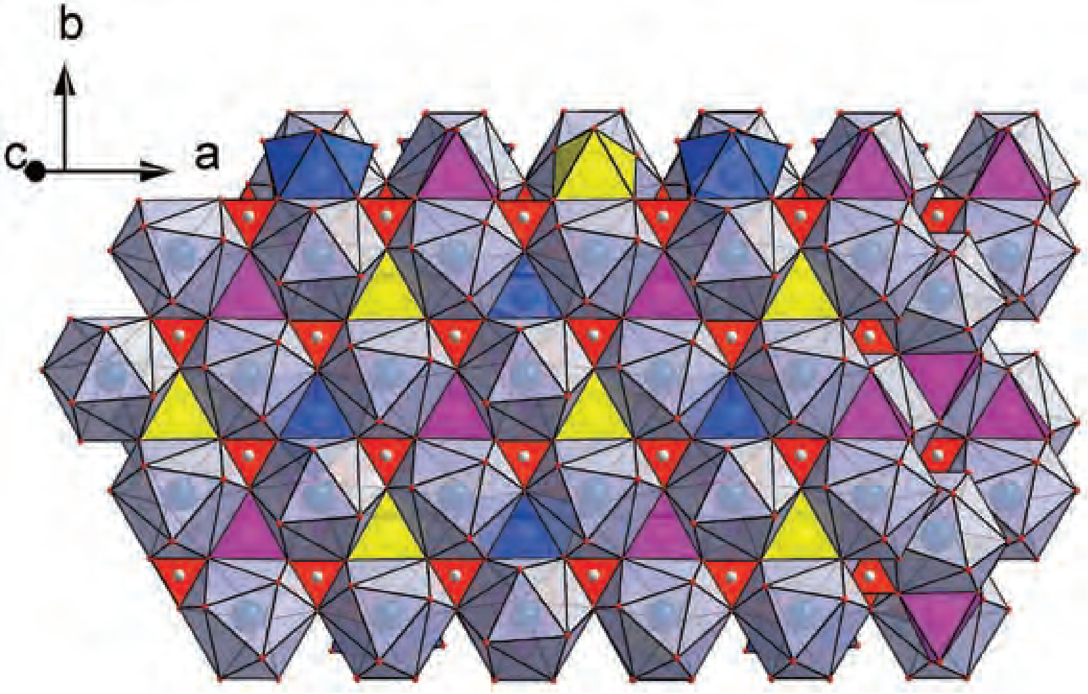

FIG. 2. View of the structure along **c***. The same conventions as for Figure 1 have been adopted.

(our mineral to weloganite): ***a'*** = – ½ ***a*** – ½ ***b***; ***b'*** = – ***b***; ***c'*** = ¼ ***a*** + ¼ ***b*** + ½ ***c***. The major differences with respect to weloganite (and to the other triclinic members of the donnayite group) are the presence of *C*-centering and of a *c*-glide, which renders the alternate double layers reflections of each other on (010); in other words, the monoclinic unit-cell can be described as derived from a triclinic cell corresponding to weloganite by an "internal twinning" with respect to a glide, as also happens in a notable number of polymorphic substances, such as for instance the zoisite–clinozoisite pair. This "internal twinning" almost doubles the *c* parameter; owing to the obliquity of the unit cells, however, it is interesting to note that the ***c*** *vectors* are not related by the transformation ***c'*** = **2*c*** (see above), although the moduli are almost related by: $c'^* = c^*/2$ (see Table 3). Similar simple relationships involving the reciprocal parameter c^* hold for the whole donnayite-(Y) group, including the trigonal–hexagonal phases as well; such analogies are reflected in the distances between corresponding layers of metal atoms, which are similar throughout the group (see the entry "*Distance*" in Tables 3 and 4). Owing also to these reasons, even for all the lowest-symmetry members of the donnayite group, there is a marked pseudohexagonal symmetry.

The bond arrangement of the six carbonate ions is similar to that occurring in weloganite (Grice & Perrault 1975). The average C–O distance is not significantly different from the corresponding value of 1.29 Å observed in weloganite, and coincides with the mean C–O bond length (1.284 ± 0.004 Å) reported by Zemann (1981) for 30 different carbonates. The three ions centered by carbon atoms C(1), C(2) and C(3) are almost coplanar with {001}, the other three [centered on C(4), C(5) and C(6)] are not coplanar, and are involved in forming hydrogen bonds with the three H_2O molecules, which belong to the coordination spheres of Ca and Ba(3) (Table 8, Figs. 1, 2). It is interesting to note that the H_2O molecules are not bonded to either Ba(1), Ba(2) or Y. For Y and the REE in general, this behavior can be accounted for by their preference to complex with carbonates, six of the nine bonds with oxygen arising from bidentate coordination of the non-coplanar carbonate ions. Such a coordination is an important factor in accounting for the deviation of such CO_3 planes from {001}.

CONCLUSIONS

The present work is the first accurate determination of the structure of mckelveyite-(Y) minerals and fully confirms the general features of the whole 5.CC.05 Donnayite group reported by Strunz & Nickel (2001), which have been best illustrated by Donnay & Donnay

TABLE 7. X-RAY POWDER-DIFFRACTION PATTERNS OF MCKELVEYITE-(Y)

Mckelveyite-(Y)-2*M*				Mckelveyite-(Y)-1*A*		
I(obs.)	*d*(meas.)	*d*(calc.)*	*h k l*	*d*(meas.)	*I*(obs.)	*h k l*
36	6.369	6.359	0 0 2	7.98	5	1 0 0
15	4.569	4.564	0 2 0	6.40	35	0 0 3
48	4.299	4.297	3 1 0	5.03	5	1 0 3
4	3.708	3.708	0 2 2	4.64	<5	0 0 4, 1 1 0
28	3.180	3.180	0 0 4	4.47	85	1 1 1
100	3.106	3.106	3 1 2	4.15	20	1 1 2
27	2.635	2.637	6 0 $\bar{2}$	3.88	<5	2 0 1
35	2.609	2.609	3 1 3	3.73	<5	1 1 3
14	2.435	2.435	6 0 0	3.32	30	1 1 4
8	2.283	2.282	0 4 0	3.19	10	0 0 6
17	2.246	2.246	0 4 1	2.942	100	1 1 5
14	2.222	2.222	3 1 4	2.648	40	3 0 0
4	2.148	2.149	6 2 0	2.445	15	3 0 3
12	2.119	2.120	0 0 6	2.349	5	1 1 7
29	2.029	2.029	6 0 2	2.276	20	2 2 1
27	2.010	2.010	6 2 1	2.229	5	2 2 2
14	1.922	1.922	0 2 6	2.127	15	0 0 9, 1 1 8
5	1.854	1.854	6 2 2	2.069	15	2 2 4
5	1.726	1.725	6 4 $\bar{2}$	2.040	30	3 0 6
10	1.710	1.709	3 5 0	2.001	<5	3 1 4
20	1.688	1.688	3 1 6	1.967	15	2 2 5
13	1.652	1.652	6 0 $\bar{8}$	1.767	10	
12	1.598	1.598	3 5 2	1.728	10	
3	1.553	1.553	0 4 6	1.659	10	
4	1.518	1.521	0 6 0	1.629	10	
3	1.501	1.501	3 1 7	1.578	5	
3	1.480	1.480	9 3 $\bar{5}$	1.527	5	
4	1.428	1.428	3 5 4	1.466	5	
5	1.422	1.421	0 4 7			
4	1.373	1.373	9 3 1			
3	1.361	1.361	6 0 6			
7	1.350	1.350	3 1 8			
4	1.339	1.338	6 4 4			
4	1.318	1.318	6 6 $\bar{2}$			
8	1.251	1.251	9 1 4			
4	1.236	1.236	0 6 6			
5	1.214	1.213	9 5 $\bar{6}$			

* (Cu*K*α radiation, λ = 1.54059 Å). Calculated from XRPD cell refinement, with parameters *a* 15.8203(7), *b* 9.1277(3), *c* 13.7708(7) Å, β 112.544(3)°, *V* 1836.58(9) Å^3. The *d* values are expressed in Å.

TABLE 8. INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN MCKELVEYITE-(Y)-2*M*

Coordination around the metal ions					
Ba(1)-O(11)	2.857(5)	Ba(2)-O(32)	2.789(4)	Ba(3)-O(22)	2.779(4)
Ba(1)-O(12)	2.829(4)	Ba(2)-O(33)	2.782(5)	Ba(3)-O(23)	2.765(4)
Ba(1)-O(21)	2.851(5)	Ba(2)-O(61)	2.805(5)	Ba(3)-O(51)	2.782(5)
Ba(1)-O(22)	2.832(4)	Ba(2)-O(11)^{a}	2.805(5)	Ba(3)-O(12)^{a}	2.787(4)
Ba(1)-O(31)	2.827(5)	Ba(2)-O(13)^{a}	2.801(5)	Ba(3)-O(13)^{a}	2.773(5)
Ba(1)-O(32)	2.850(4)	Ba(2)-O(21)^{e}	2.803(5)	Ba(3)-O(31)^{f}	2.806(5)
Ba(1)-O(42)	2.861(4)	Ba(2)-O(23)^{e}	2.829(4)	Ba(3)-O(33)^{f}	2.780(5)
Ba(1)-O(43)^{b}	2.766(5)	Ba(2)-O(41)^{c}	2.838(5)	Ba(3)-OW(1)^{d}	2.849(5)
Ba(1)-O(53)^{c}	2.803(4)	Ba(2)-O(52)^{c}	2.845(5)	Ba(3)-OW(2)^{d}	2.903(5)
Ba(1)-O(63)^{d}	2.753(5)	Ba(2)-O(62)^{c}	2.805(5)	Ba(3)-OW(3)^{d}	2.872(5)
Average	2.823		2.810		2.810
Y-O(22)	2.373(4)	Ca-O(11)	2.334(5)	Na-O(12)	2.364(6)
Y-O(32)	2.351(4)	Ca-O(31)	2.342(5)	Na-O(21)	2.322(6)
Y-O(41)	2.394(4)	Ca-OW(1)	2.417(6)	Na-O(43)	2.477(7)
Y-O(42)	2.466(4)	Ca-OW(2)	2.416(5)	Na-O(33)^{i}	2.379(6)
Y-O(51)	2.469(4)	Ca-OW(3)	2.431(5)	Na-O(53)^{g}	2.449(6)
Y-O(52)	2.397(4)	Ca-O(23)^{g}	2.387(5)	Na-O(63)^{i}	2.459(7)
Y-O(61)	2.476(4)				
Y-O(62)	2.401(4)				
Y-O(13)^{a}	2.381(4)				
Average	2.412		2.388		2.408
The carbonate ions					
C(1)-O(11)	1.270(7)	C(3)-O(31)	1.320(6)	C(5)-O(51)	1.258(7)
C(1)-O(12)	1.233(8)	C(3)-O(32)	1.268(7)	C(5)-O(52)	1.313(7)
C(1)-O(13)	1.325(7)	C(3)-O(33)	1.242(7)	C(5)-O(53)	1.272(7)
Average	1.276	Average	1.277	Average	1.281
C(2)-O(21)	1.305(7)	C(4)-O(41)	1.317(7)	C(6)-O(61)	1.276(7)
C(2)-O(22)	1.276(7)	C(4)-O(42)	1.283(7)	C(6)-O(62)	1.310(7)
C(2)-O(23)	1.261(7)	C(4)-O(43)	1.273(7)	C(6)-O(63)	1.276(6)
Average	1.281	Average	1.291	Average	1.287
O(11)-C(1)-O(12)		121.9(5)	O(21)-C(2)-O(22)		120.1(5)
O(11)-C(1)-O(13)		118.1(6)	O(21)-C(2)-O(23)		120.2(5)
O(12)-C(1)-O(13)		119.9(6)	O(22)-C(2)-O(23)		119.6(5)
O(31)-C(3)-O(32)		118.8(5)	O(41)-C(4)-O(42)		116.3(5)
O(31)-C(3)-O(33)		120.1(5)	O(41)-C(4)-O(43)		121.5(5)
O(32)-C(3)-O(33)		121.1(5)	O(42)-C(4)-O(43)		122.2(5)
O(51)-C(5)-O(52)		116.6(5)	O(61)-C(6)-O(62)		116.7(5)
O(51)-C(5)-O(53)		122.4(5)	O(61)-C(6)-O(63)		122.0(5)
O(52)-C(5)-O(53)		121.0(5)	O(62)-C(6)-O(63)		121.3(5)
Hydrogen-bond interactions					
OW(1)...O(43)		2.695(7)	OW(1)...O(52)^{h}		2.752(6)
OW(2)...O(53)^{g}		2.713(7)	OW(2)...O(62)		2.782(7)
OW(3)...O(41)^{g}		2.779(7)	OW(3)...O(63)^{h}		2.681(6)

Symmetry operations: a = x, y + 1, z; b = x, –y, ½ + z ; c = x, 1 – y, ½ + z ; d = ½ + x, ½ – y, ½ + z ; e = x – ½, y + ½, z ; f = ½ + x, ½ + y, z; g = x – ½, y – ½, z ; h = x, y – 1, z ; i = x + ½, y – ½, z.

(1971) and Donnay & Preston (1971), and with more detail for weloganite by Grice & Perrault (1975). Because of the relationships to type mckelveyite-(Y), and in agreement with suggestions from the IMA CNMCN Commission, the mineral here studied should be considered as a new polytype, *i.e.* mckelveyite-(Y)-2*M*, to be distinguished from type mckelveyite-(Y), which is triclinic and should now be called mckelveyite-(Y)-1*A*. The almost complete ordering of the metal sites with respect to the more symmetrical REE-containing species in the group may be ascribed to a low temperature of formation, and applies in general to minerals in the Alpine-fissure environment.

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REFERENCES

ALTOMARE, A., BURLA, M.C., CAMALLI, M., CASCARANO, G.L., GIACOVAZZO, C, GAGLIARDI, A., MOLITERNI, A.G.G., POLIDORI, G. & SPAGNA, R. (1999): SIR97: a new tool for crystal structure determination and refinement. *J. Appl. Crystallogr.* **32**, 115-119.

BEDOGNÉ, F., MONTRASIO, A. & SCIESA, E. (1993): *I minerali della provincia di Sondrio: Valmalenco*. Bettini Publisher, Sondrio, Italy (113-119).

BROWN, I.D. & WU, K.K. (1976): Empirical parameters for calculating cation–oxygen bond valences. *Acta Crystallogr.* **B32**, 1957-1959.

CHAO, G.Y., MAINWARING, P.R. & BAKER, J. (1978): Donnayite, $NaCaSr_3Y(CO_3)_6 \bullet 3H_2O$, a new mineral from Mont St.-Hilaire, Quebec. *Can. Mineral.* **16**, 335-340.

CHEN, T.T. & CHAO, G.Y. (1975): X-ray crystallography of weloganite. *Can. Mineral.* **13**, 22-26.

DEMARTIN, F., PILATI, T., DIELLA, V., GENTILE, P. & GRAMACCIOLI, C.M. (1993): A crystal-chemical investigation of Alpine gadolinite. *Can. Mineral.* **30**, 127-136.

DESAUTELS, P.E. (1967): The morphology of mckelveyite. *Am. Mineral.* **52**, 860-864.

DONNAY, G. & DONNAY, J.D.H. (1971): Ewaldite, a new barium calcium carbonate. I. Occurrence of ewaldite in syntactic intergrowth with mckelveyite. *Tschermaks Mineral. Petrogr. Mitt.* **15**, 185-200.

DONNAY, G. & PRESTON, H. (1971): Ewaldite, a new barium calcium carbonate. II. Its crystal structure. *Tschermaks Mineral. Petrogr. Mitt.* **15**, 201-212.

FARRUGIA, L. J. (1999): WINGX suite for small-molecule single-crystal crystallography. *J. Appl. Crystallogr.* **32**, 837-838.

GRICE, J.D. & PERRAULT, G. (1975): The crystal structure of triclinic weloganite. *Can. Mineral.* **13**, 209-216.

HOLLAND, T.J.B. & REDFERN, S.A.T. (1997): Unit cell refinement from powder diffraction data: the use of regression diagnostics. *Mineral. Mag.* **61**, 65-77.

LE PAGE, Y. (1987): Computer derivation of the symmetry elements implied in a structure description. *J. Appl. Crystallogr.* **20**, 264-269.

LE PAGE, Y. (1988): MISSYM1.1 – a flexible new release. *J. Appl. Crystallogr.* **21**, 983-984.

MILTON, C., INGRAM, B., CLARK, J.R. & DWORNIK, E.J. (1965): Mckelveyite, a new hydrous sodium barium rare-earth uranium carbonate mineral from the Green River Formation, Wyoming. *Am. Mineral.* **50**, 593-612.

PEKOV, I.V. & PODLESNYI, A.S. (2004): Kukisvumchorr deposit: mineralogy of alkaline pegmatites and hydrothermalites. *Mineralogical Almanac* **7**.

SHELDRICK, G.M. (1997): SHELXL97, *Program for Crystal Structure Refinement*. University of Göttingen, Göttingen, Germany.

SHELDRICK, G.M. (2000): SADABS, *Area-Detector Absorption Correction Program*. Bruker AXS Inc., Madison, Wisconsin.

STRUNZ, H. & NICKEL, E.H. (2001): *Strunz Mineralogical Tables*. E. Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, Germany.

TRINH, THI LE THU, POBEDINSKAYA, E.A., NADEZHINA, T.N. & KHOMYAKOV, A.P. (1992): Polymorphism of donnayite $(Na,REE)Sr(CO_3)_2 \bullet H_2O$. *Moscow Univ. Geol. Bull.* **47**(5), 68-78 (in Russ.).

VOLOSHIN, A.V., SUBBOTIN, V.V., YAKOVENCHUK, V.N., PAKHOMOVSKY, YA.A., MENSHIKOV, YU.P., NADEZHINA, T.N. & PUSHCHAROVSKIY, D.YU. (1992): New data on ewaldite *Zap. Vses. Mineral. Obshchest.* **121**, 56-66 (in Russ.).

VOLOSHIN, A.V., SUBBOTIN, V.V., YAKOVENCHUK, V.N., PAKHOMOVSKY, YA.A., MENSHIKOV, YU.P. & ZAITSEV, A.N. (1990): Mckelveyite from carbonatites and hydrothermalites of Kola peninsula (the first finds in the USSR). *Zap. Vses. Mineral. Obshchest.* **119**(6), 76-86 (in Russ.).

ZEMANN, J. (1981): Zur Stereochemie der Karbonate. *Fortschr. Mineral.* **59**, 95-116.

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