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Mckelveyite group minerals – Part 1: Nomenclature and new data on donnayite-(Y)

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Abstract. The mckelveyite group consisting of seven carbonate minerals – mckelveyite-(Y), ewaldite, weloganite, donnayite-(Y), alicewilsonite-(YCe), alicewilsonite-(YLa), and bainbridgeite-(YCe) – is formally established. The general formula of the minerals is $A_3B_3(CO_3)_6 \cdot 3H_2O$, where A = Na, Ca, Y, and Zr and B = Sr, Ba, Ce, and La. Different order–disorder modifications are known resulting in triclinic, monoclinic, hexagonal, and trigonal minerals with essentially the same structure. Re-examination of donnayite-(Y) type specimens shows that the original description contains data collected on two different species: donnayite-(Y) and alicewilsonite-(YCe). Donnayite-(Y), NaCaSr₃Y(CO₃)₆ $\cdot 3H_2O$, was found in only one specimen out of seven – CMNMC 39396 – housed at the Canadian Museum of Nature, Ottawa. This specimen becomes the holotype of donnayite-(Y). The crystal structure of donnayite-(Y) was solved and refined to $R_1 = 0.055$ for 3366 reflections with $I > 2\sigma(I)$. Donnayite-(Y) is shown to have a weloganite-type structure confirming its place in the mckelveyite group.

1 Introduction

The terms "donnayite group" (Demartin et al., 2008; Horvath et al., 2019) and "mckelveyite group" (Frost et al., 2013) can be found in the literature describing four related carbonate minerals donnayite-(Y) (Chao et al., 1978), mckelveyite-(Y) (Milton et al., 1965), ewaldite (Donnay et al., 1971), and weloganite (Sabina et al., 1968), but neither the group nor its name had previously been approved by Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA CNMNC).

We conducted a comprehensive investigation of these minerals that resulted in the discovery of three new minerals species – alicewilsonite-(YCe) (IMA 2020-055; Lykova et al., 2023), bainbridgeite-(YCe) (IMA 2020-065), and alicewilsonite-(YLa) (IMA 2021-047) – the holotype redefinition for donnayite-(Y) (proposal 22-F), and the formal establishment of the mckelveyite group (proposal 22-G), all approved by the CNMNC. This paper, the first one in the series on the mckelveyite group minerals, presents the nomenclature of the mckelveyite group and new data on donnayite-(Y), including first known data on its crystal structure.

2 Background

Mckelveyite-(Y), a Na–Ca–Ba–Y carbonate, from the Green River formation, Wyoming, USA, was the first mineral in the group to be described (Milton et al., 1965). Subsequently weloganite from the Francon quarry, Quebec, Canada (Sabina et al., 1968), and ewaldite also from the Green River formation (Donnay et al., 1971) were described.

Solving crystal structures of mckelveyite group minerals proved to be challenging due to the high degree of disorder. The ewaldite structure was determined by Donnay and Preston (1971), and the formula Ba(Ca,REE,Na,K,Sr,U)(CO₃)₂ (Z = 2) was suggested. The new idealised formula BaCa(CO₃)₂ · 2.6H₂O (Z = 2;

 $P6_3mc$) was proposed by Voloshin et al. (1992), who studied material from the Vouriyarvi Massif, Russia. It was suggested that mckelveyite-(Y) and ewaldite may be polymorphs. Both studies provided only limited structural characterisation due to the challenging nature of the material. Weloganite was the first triclinic group member with a determined structure (Chen and Chao, 1975; Grice and Perrault, 1975). The proposed formula was Na₂Sr₃Zr(CO₃)₆ · 3H₂O (Z = 1).

Three vears later donnavite-(Y), $NaCaSr_3Y(CO_3)_6 \cdot 3H_2O$, was described from Mont Saint-Hilaire, Quebec, Canada (Chao et al., 1978). The authors concluded that it is the Ca-Y analogue of weloganite and the Sr analogue of mckelveyite-(Y) and proposed the mckelveyite-(Y) end-member formula: NaCaBa₃Y(CO₃)₆ \cdot 3H₂O. Chao et al. (1978) did not provide structural data on donnayite-(Y). Thi et al. (1984, 1992) reported crystal structures of two "donnayite-(Y)" polymorphs – triclinic P1 and trigonal R3m on material from the Khibiny Massif, Kola Peninsula, Russia. Both phases were characterised by (1) the lack of Ca and (2) the Na: REE ratio close to 1:1, indicating that the crystals were a different species. We are unaware of any published structural work on actual donnayite-(Y).

Demartin et al. (2008) proposed the first model of the crystal structure of mckelveyite-(Y) confirming the NaCaBa₃Y(CO₃)₆ · 3H₂O (Z = 4) formula. It is the only known structural study of a monoclinic *Cc* polymorph with the weloganite-type structure.

Three new minerals with weloganite-type structures (P1) were recently approved by the IMA: alicewilsonite-(YCe), Na₂Sr₂YCe(CO₃)₆ · 3H₂O (IMA 2020-055; Lykova et al., 2023), and bainbridgeite-(YCe), Na₂Ba₂YCe(CO₃)₆ \cdot 3H₂O (IMA 2020-065), from Mont Saint-Hilaire, and alicewilsonite-(YLa), $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$ (IMA 2021-047), from the Paratoo Mine, Australia. It is likely that two "donnayite-(Y)" polymorphs reported by Thi et al. (1984, 1992) were, in fact, alicewilsonite-(YCe), which corroborates with the EMPA we obtained on one of the specimens studied by Thi et al. (Lykova el al, 2023).

3 New data on donnayite-(Y)

Donnayite-(Y), NaCaSr₃Y(CO₃)₆ · 3H₂O, was described by Chao et al. (1978) in several specimens from Mont Saint-Hilaire, Quebec, Canada. According to the original publication there were four cotype specimens deposited at the National Museum of Natural Sciences (now – Canadian Museum of Nature), Ottawa (CMN; specimens CMNMC 39394, CMNMC 39395, and CMNMC 39396), and the Royal Ontario Museum, Toronto (ROM; specimen *M*35222). Three other specimens not mentioned in the article were catalogued as cotypes: two at the Smithsonian National Museum of Natural History, Washington, DC (NMNH; speci-

Table 1. Results of re-investigation of donnayite-(Y) cotypes.

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Catalogue no.	Depository	Species
CMNMC 39394*	CMN	alicewilsonite-(YCe)
CMNMC 39395*	CMN	alicewilsonite-(YCe)
CMNMC 39396*	CMN	donnayite-(Y)
M35222*	ROM	alicewilsonite-(YCe)
M35544	ROM	alicewilsonite-(YCe)
144522	NMNH	alicewilsonite-(YCe)
147191	NMNH	alicewilsonite-(YCe)

 \ast Specimens designated as cotypes in the original publication by Chao et al. (1978).



Figure 1. Colourless transparent donnayite-(Y) crystal, 0.2 mm in size. Specimen CMNMC 39396. Photo: François Génier.

mens 144 522 and 147 191), and one more specimen at the ROM (*M*35544).

Re-examination of donnayite-(Y) type specimens showed that the original description contains data collected on two different phases with simplified formulae NaCaSr₃Y(CO₃)₆ · 3H₂O and Na₂Sr₂YCe(CO₃)₆ · 3H₂O (Table 1). The latter corresponds to the recently approved species alicewilsonite-(YCe) (Lykova et al., 2023). As the original formula of donnayite-(Y) was given as NaCaSr₃Y(CO₃)₆ · 3H₂O, and the mineral with that chemical composition has been consistently labelled as such from various localities around the world, we proposed to keep the name donnayite-(Y) for that phase.

Donnayite-(Y) was found in only one specimen out of seven – CMNMC 39396 – housed at the Canadian Museum of Nature, Ottawa. This specimen becomes the holotype of donnayite-(Y). Results of its investigation are given below.

On the holotype specimen donnayite-(Y) forms transparent colourless hemimorphic barrel-shaped crystals less than 0.3 mm in size (Fig. 1).

3.1 Chemical data

Electron microprobe analyses (EMPAs) for donnavite-(Y) were obtained using a JEOL 8230 SuperProbe electron microscope equipped with five WDS spectrometers (University of Ottawa - Canadian Museum of Nature MicroAnalysis Laboratory, Canada) with an acceleration voltage of 20 kV and a beam current of 10 nA. Donnayite-(Y) is unstable under an electron beam, and so a larger beam diameter of 30 µm was used to minimise element migration. The following reference materials were used: albite or NaInSi₂O₆ (Na $K\alpha$), diopside (Ca $K\alpha$), celestine (Sr $L\alpha$), sanbornite (Ba $L\alpha$), YAG $(YL\alpha)$, LaPO₄ (LaL α), CePO₄ (CeL α), PrPO₄ (PrL β), NdPO₄ (NdL α), SmPO₄ (SmL α), EuPO₄ (EuL α), GdPO₄ $(GdL\alpha)$, TbPO₄ (TbL α), DyPO₄ (DyL β), HoPO₄ (HoL β), ErPO_4 ($\text{Er}L\alpha$), and YbPO_4 ($\text{Yb}L\alpha$). The intensity data were corrected for time-dependent intensity (TDI) loss (or gain) using a self-calibrated correction for NaK α , CaK α , YL α , and LaL α . H₂O and CO₂ contents were not analysed due to the paucity of the available material.

Chao et al. (1978) analysed a number of specimens, but all except one were deemed unsuitable "owing to the presence of intimate syntactic intergrowths with other minerals", which is how analyses corresponding to alicewilsonite-(YCe) were likely interpreted. Therefore, EMPAs were collected on one unspecified crystal only. Donnayite-(Y) from the original description is characterised by a higher content of Sr and lower Ba and Ca, which shows that the analysis was obtained on a different specimen that was not designated as a cotype. Summarising the history behind donnayite-(Y) discovery, Horvath et al. (2019) indicated that due to the nature of the material and its paucity, the species description required the use of several specimens collected, mostly before 1973, by different collectors including Peter Tarassoff, Elsa Pfenninger-Horvath, Laszlo Horvath, Marcelle Weber, William Henderson, and Quintin Wight. This corroborates our data and indicates that original EMPAs were likely collected on a specimen that is no longer identifiable.

3.2 Optical properties

According to Chao et al. (1978) donnayite-(Y) is biaxial negative; however, we measured optical properties of several mckelveyite group minerals, and they all are biaxial positive, including alicewilsonite-(YCe) and donnayite-(Y). Comparative data given in Table 3 show that the original data were likely obtained on alicewilsonite-(YCe).

3.3 Powder X-ray diffraction data

Powder X-ray diffraction (PXRD) data on the holotype were collected at the Canadian Museum of Nature, Canada, using a Bruker D8 Discover microdiffractometer equipped with a DECTRIS EIGER2 R 500K detector and IµS microfocus X-ray source ($\lambda_{CuK\alpha 1} = 1.54060$ Å) with the $K\alpha_2$ contribution removed using the "Strip $K\alpha 2$ " tool in Bruker Diffrac.EVA V4.3. The instrument was calibrated using a statistical calibration method (Rowe, 2009). A powder ball 200µm in diameter, mounted on a fibre pin mount, was analysed with continuous Phi rotation and 10° rocking motion along the Psi axis of the centric Eulerian cradle stage.

Parameters of the triclinic unit cell refined from the PXRD data are as follows: a = 8.9826(5) Å, b = 8.9853(5) Å, c = 6.7932(4) Å, $\alpha = 102.852(5)^{\circ}$, $\beta = 116.083(6)^{\circ}$, $\gamma = 59.935(4)^{\circ}$, and V = 426.20(5) Å³. The PXRD pattern in the xy format is available as a Supplement file.

Comparative data for donnayite-(Y) and alicewilsonite-(YCe) are given in Table 4. The patterns are very similar. The unit cell parameter c of the alicewilsonite-(YCe) unit cell is somewhat smaller than that of donnayite-(Y), and the difference is notable in the basal reflections; however, both minerals are characterised by significant isomorphic substitutions at all cation sites, and thus varying unit cell parameters. The chemistry of the crystal used to collect PXRD data for the original study is unknown, so we cannot confidently tell if it was donnayite-(Y) or alicewilsonite-(YCe).

3.4 Single-crystal X-ray diffraction data and crystal structure of donnayite-(Y)

Single-crystal X-ray diffraction (SXRD) data for the holotype specimen CMNMC 39396 were (Fig. 1) collected at room temperature on a Rigaku XtaLAB Synergy-S diffractometer equipped with a HyPix 6000HE detector $(\lambda_{MoK\alpha} = 0.71073 \text{ Å})$ at the Natural History Museum, University of Oslo, Norway. The data were processed, including face indexed absorption correction, using Rigaku's CrysAlis Pro software (Matsumoto et al., 2021).

The data were indexed in the *P*1 space group with the following unit cell parameters: a = 8.9908(11) Å, b = 9.0067(11) Å, c = 6.8027(8)Å, $\alpha = 102.768(10)^{\circ}, \beta = 116.143(13)^{\circ}, \gamma = 60.000(13)^{\circ}, \text{ and}$ $V = 428.26(11) \text{ Å}^3$.

Multiple domains, strong splitting and complex twinning were observed in every data set we collected. Therefore, we were only able to refine the structure to $R_1 = 0.139$ using the SHELXL 2018/3 program package (Sheldrick, 2015), and thus could not obtain a model of a reasonable quality.

We tested several crystals from different donnayite-(Y) specimens from Mont Saint-Hilaire, and specimen CMNMC 90405 from the Canadian Museum of Nature collection was deemed suitable for a single-crystal X-ray study. The studied donnayite-(Y) occurs as translucent green hemi-

	Donnayite-(Y), specimen CMNMC 39396 (the holotype), average of 17 analyses		Donnayite-(Y), CMNMC 90405, average of 11 analyses	Donnayite-(Y), after Chao et al. (1978)	
Constituent	Mean	Range	SD (2σ)		
Na ₂ O	4.11	3.66-4.58	0.32	4.06	3.37
CaO	7.56	6.20-8.78	1.00	6.13	5.75
SrO	30.11	26.03-32.92	2.03	24.88	35.8
BaO	5.02	3.11-7.96	1.56	14.89	0.85
Y_2O_3	10.18	9.31-10.78	0.41	9.05	13.1
La ₂ O ₃	0.62	0.00 - 1.66	0.54	0.33	0.45
Ce_2O_3	1.17	0.35-2.39	0.70	1.19	-
Nd_2O_3	0.27	0.00-0.54	0.20	0.17	1.83
Gd_2O_3	0.26	0.00-0.43	0.10	0.18	-
Dy_2O_3	1.16	0.82-1.53	0.20	0.73	-
Ho ₂ O ₃	0.25	0.00-0.50	0.14	0.16	-
Er ₂ O ₃	0.9	0.66-1.02	0.09	0.91	_
Yb_2O_3	0.29	0.00-0.52	0.11	0.92	_
CO_2^*	30.86			29.49	30.98
$\mathrm{H}_2\tilde{\mathrm{O}}^*$	6.39			6.1	6.34
Total	99.15			99.19	98.47

Table 2. Chemical data (in wt %) for donnayite-(Y) in comparison with data from Chao et al. (1978).

* Calculated from the stoichiometry.

Table 3. Comparative optical properties of donnayite-(Y) (original and current study) and alicewilsonite-(YCe).

Mineral	Donnayite-(Y), Chao et al. (1978)	Alicewilsonite-(YCe), Lykova et al. (2023)	Donnayite-(Y), CMNMC 39396, this work
α	1.551-1.561(2)	1.554(3)	1.577 (3)
eta	1.646(2)	1.558(3)	1.582(2)
γ	1.652(2)	1.644(2)	1.627(3)
2V, ° (meas.)	0–20	20(3)	16(4)

morphic crystals up to 3 mm in size in a miarolitic cavity (Fig. 2). Chemical data are given in Table 2. The empirical formula calculated on the basis of 6 cations, excluding H^+ , is $Na_{1.15}Ca_{0.96}Sr_{2.11}Ba_{0.85}Y_{0.70}La_{0.02}Ce_{0.06}Nd_{0.01}Gd_{0.01}$ $Dy_{0.04}Ho_{0.01}Er_{0.04}Yb_{0.04}(CO_3)_{5.89}(H_2O)_{3.00}$.

The SXRD data on specimen CMNMC 90405 were collected using a Bruker Kappa APEX II diffractometer equipped with a CCD detector and with an Incoatec Microfocus Source I μ S (30 W, multilayer mirror, $\lambda_{MoK\alpha}$) at the Institute of Mineralogy and Crystallography, University of Vienna, Austria.

The data were indexed in the *P*1 space group with the following unit cell parameters: a = 9.0273(6) Å, b = 9.0317(7) Å, c = 6.8517(7) Å, $\alpha = 102.600(3)^{\circ}$, $\beta = 115.990(4)^{\circ}$, $\gamma = 60.000(3)^{\circ}$, and V = 434.86(7) Å³. The structure was solved and refined to $R_1 = 0.055$ on the basis of 3366 independent reflections with $I > 2\sigma(I)$ using the SHELXT and SHELXL-2018/3 programs (Sheldrick, 2015). Crystal data, data collection, and structure refinement



Figure 2. Green hemimorphic donnayite-(Y) crystal. FOV 9 mm. Specimen CMNMC 90405. Photo: François Génier.

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	Donnayite-(Y), Chao et al. (1978)		Alicev Lyko	wilsonite-(YCe), wa et al. (2023)	Donnayite-(Y), CMNMC 39396, this work	
		Unit cell pa	rameters	s refined from the	PXRD o	lata
a, Å	9	.000		9.004	8.983	
b, Å	8	.999		9.018	:	8.985
<i>c</i> , Å	6	.793		6.771		6.793
α , °	10	2.77		102.72	1	02.85
β , °	11	6.28		116.40	1	16.08
γ, \circ	5	9.99		60.00	:	59.94
$V, Å^3$	427.4			426.5	426.2	
hkl ¹	I _{obs}	$d_{\rm obs}^2$	Iobs	$d_{\rm obs}^2$	I _{obs}	$d_{\rm obs}^2$
010	10	7.77	14	7.81	9	7.76
001	40	6.10	31	6.07	35	6.10
$21\overline{1}, 120, 1\overline{1}0$	70	4.368	100	4.372	100	4.360
$12\overline{1}, 1\overline{11}, 210$	20	4.041	25	4.037	25	4.030
$21\overline{2}, 121, 1\overline{1}1$	30	3.209	25	3.201	32	3.205
002	20	3.050	13	3.032	16	3.052
$1\overline{12}, 12\overline{2}, 211$	100	2.839	67	2.831	100	2.838
$33\overline{1},030,30\overline{1}$	40	2.598	39	2.601	53	2.593
330, 302, 031, 031, 300	20	2.391	19	2.390	21	2.386
$2\overline{21}, 24\overline{1}, 42\overline{1}$	20	2.233	24	2.236	32	2.228
$1\overline{13}, 3\overline{10}, 212, 003^3$	30	2.038	9	2.029	15	2.037
$24\overline{2}, 2\overline{22}, 420, 003^4$	30	2.018	23	2.019	25	2.017
333, 303, 032, 032, 301, 331	30	1.978	24	1.974	32	1.976
423, 241, 221	30	1.916	16	1.915	26	1.914

Table 4. Comparative powder X-ray diffraction data for donnayite-(Y) (original and current study) and alicewilsonite-(YCe).

¹ Selected strongest reflections are given. ² In Å. ³ For donnayite-(Y) (original data and this work). ⁴ For alicewilsonite-(YCe).

details are given in Table 5; atom coordinates, equivalent displacement parameters, site composition, and bond valence sums (BVSs) in Table 6; selected interatomic distances in Table 7. The full bond valence calculations table was uploaded as a Supplement (Table S1).

A crystallographic information file (CIF) for donnayite-(Y) is available as a Supplement file. It was also deposited in the Inorganic Crystal Structure Database (ICSD; no. CSD 2223388).

Donnayite-(Y) is strongly pseudotrigonal. There are six independent large cation sites in the structure (Fig. 3) forming two alternating layers parallel to the *ab* plane (Fig. 4). Na, Ca, Sr, Ba, Y, and Dy were distributed among these sites based on the EMPA, refined site-scattering factors, and charge balance taking into account bond valence sums (BVSs) and interatomic distances (Tables 6–7). Ln (lanthanoids: La–Lu) were formally refined as Dy atoms. One of the layers is formed by the Sr1, Sr2, and Sr3 sites that have 10-fold coordination. The refinement showed that Sr and Ba are distributed between all three sites with the occupancies fixed as Sr_{0.70}Ba_{0.30}. Na4 and Ca5 sites have octahedral coordination, their occupancies were fixed as Na_{0.65}Ca_{0.30}Dy_{0.05}



Figure 3. General view of the crystal structure of donnayite-(Y). Sky-blue spheres are H₂O molecules. The unit cell is outlined.

and $Ca_{0.70}Na_{0.27}Dy_{0.03}$, respectively. The Y6 site is occupied predominantly by Y atoms (75%) with admixed Dy (17%) and Na (8%) atoms.

The three CO_3^{2-} groups centred by carbon atoms C1, C2, and C3 are almost coplanar with {001} as in weloganite,

Specimen	CMNMC 90405
Crystal system, space group, Z	Triclinic, P1, 1
<i>a</i> (Å)	9.0273(6)
b (Å)	9.0317(7)
<i>c</i> (Å)	6.8517(7)
α (°)	102.600(3)
β (°)	115.990(4)
γ (°)	60.000(3)
V (Å ³)	434.86(7)
λ (Mo $K\alpha$) (Å), T (K)	0.71073, 293
Diffractometer	Bruker Kappa APEX II
θ range (°)	3.31-28.28
Crystal size (mm ³)	$0.020 \times 0.030 \times 0.040$
Absorption coefficient $\mu m (mm^{-1})$	12.39
F ₀₀₀	417
h, k, l range	$-12 \le h \le 12, -12 \le k \le 12, -9 \le l \le 9$
Reflections collected	13 700
Unique reflections	4270
Unique reflections $[I > 2\sigma(I)]$	3366
Number of refined parameters	272
Weighting scheme	$1/[\sigma^2(F_0^2) + (0.0497P)^2 + 7.5339P],$
	$P = [\max(F_{\rm o})^2 + 2(F_{\rm c})^2]/3$
R _{int}	0.092
Final <i>R</i> indices $[I > 2\sigma I]$	$R_1 = 0.055, wR_2 = 0.119$
<i>R</i> indices (all data)	$R_1 = 0.071, wR_2 = 0.126$
Goodness of fit	1.019
$\Delta \rho_{\rm max} / \Delta \rho_{\rm min} \ (e {\rm \AA}^{-3})$	$1.58^*/-1.08$

Table 5. Crystal data, data collection information, and structure refinement details for donnayite-(Y).

* Located 1.05 Å away from the O13 site.



Figure 4. A view along [010] of the crystal structure of donnayite-(Y). Sr-, Na-, Ca-, and Y-centred polyhedra are shown in green, yellow, orange, and purple, respectively. Carbonate groups are black triangles. The unit cell is outlined.

Na₂Sr₃Zr(CO₃)₆ · 3H₂O (Grice and Perrault, 1975). In the latter there are three other, non-coplanar CO₃²⁻ groups centred by carbon atoms C4, C5, and C6. In donnayite-(Y) these three sites are split into two alternating sites each marked by letters a and b, e.g. C4a and C4b, forming alternating CO_3^{2-} groups with a shared vertex (Fig. 3). The occupancy of the alternating carbon and oxygen sites was fixed at 50 %. Similar splitting was observed in the recently approved alicewilsonite-(YLa) (IMA 2021-047).

The BVSs at the O19a, O19b, O20a, O20b, O21a, and O21b sites (0.27, 0.25, 0.30, 0.26, 0.28, and 0.28 valence units, respectively) indicate the presence of H_2O^0 molecules. O19a, O20a, and O21a water molecules are bonded to Sr1-and Ca5-centred polyhedra that share a face, while O19b, O20b, and O21b water molecules are bonded to Sr2- and Na4-centred polyhedra.

Only one group of alternating C and O atoms marked by either "a" or "b" is occupied at the same time. Due to the quality of the collected data these atoms were not very reliably localised and were refined with isotropic atomic displacement parameters only.

Site	x	у	Z.	Ueq	site composition	BVS ²
Sr1	0.45854(16)	0.68449(15)	0.36760(19)	0.0108(3)	Sr _{0.70} Ba _{0.30} *	2.38
Sr2	0.12240(18)	0.35597(16)	0.3672(2)	0.0116(3)	Sr _{0.70} Ba _{0.30} *	2.40
Sr3	0.78625(17)	0.01998(16)	0.36631(19)	0.0114(3)	Sr _{0.70} Ba _{0.30} *	2.46
Na4	0.3280(9)	0.3529(8)	0.9772(9)	0.0095(13)	Na _{0.65} Ca _{0.30} Dy _{0.05} *	1.51
Ca5	0.6618(8)	0.6865(7)	0.9787(8)	0.0150(13)	Ca _{0.70} Na _{0.27} Dy _{0.03} *	1.80
Y6	0.9944(5)	0.0204(5)	0.9884(6)	0.0137(3)	Y _{0.75} Dy _{0.17} Na _{0.08} *	2.91
C1	0.412(2)	0.0202(19)	0.233(3)	0.013(3)	1	4.09
C2	0.078(2)	0.6869(19)	0.234(3)	0.011(3)	1	4.00
C3	0.745(2)	0.353(2)	0.233(3)	0.013(3)	1	4.05
C4a	0.020(6)	0.247(6)	0.782(7)	$0.032(9)^{1}$	C _{0.50}	1.87
C4b	0.828(5)	0.341(5)	0.784(6)	$0.026(8)^1$	C _{0.50}	1.90
C5a	0.154(5)	-0.302(5)	0.784(6)	$0.027(8)^1$	C _{0.50}	1.93
C5b	0.254(5)	0.790(5)	0.784(6)	$0.023(7)^1$	C _{0.50}	1.95
C6a	0.603(6)	0.115(6)	0.779(7)	$0.033(9)^1$	C _{0.50}	1.96
C6b	0.699(5)	-0.075(5)	0.783(6)	$0.020(7)^1$	C _{0.50}	2.04
O1	0.2704(16)	0.0203(14)	0.244(2)	0.017(3)	1	2.09
O2	0.4128(18)	0.1588(17)	0.235(3)	0.026(3)	1	2.17
O3	0.5528(18)	0.8797(17)	0.234(2)	0.026(3)	1	2.16
O4	0.9366(18)	0.6874(16)	0.235(2)	0.024(3)	1	2.15
05	0.0815(17)	0.8330(16)	0.248(2)	0.021(3)	1	2.09
O6	0.2169(17)	0.5473(14)	0.231(2)	0.017(3)	1	2.13
O7	0.6056(17)	0.3513(17)	0.236(2)	0.023(3)	1	2.12
O8	0.7426(18)	0.4929(15)	0.229(2)	0.020(3)	1	2.19
O9	0.8937(17)	0.2079(16)	0.250(2)	0.021(3)	1	2.10
O10	0.978(3)	0.306(3)	0.951(4)	$0.073(6)^{1}$	1	1.87
O11a	0.051(4)	0.079(4)	0.708(4)	$0.027(6)^{1}$	O _{0.50}	0.75
O11b	0.746(4)	0.230(3)	0.705(4)	$0.026(6)^1$	O _{0.50}	0.75
O12a	0.051(4)	0.334(4)	0.702(5)	$0.022(6)^1$	O _{0.50}	0.98
O12b	0.746(4)	0.483(4)	0.697(5)	$0.023(7)^1$	O _{0.50}	1.01
O13	0.259(3)	-0.261(3)	0.948(3)	$0.064(5)^1$	1	1.95
O14a	0.214(4)	0.558(4)	0.700(4)	$0.015(6)^1$	O _{0.50}	1.00
O14b	0.364(4)	0.708(4)	0.701(5)	$0.025(7)^1$	O _{0.50}	1.08
O15a	0.955(4)	-0.188(4)	0.704(5)	$0.031(6)^1$	O _{0.50}	0.70
O15b	0.108(4)	-0.040(4)	0.707(5)	$0.031(6)^1$	O _{0 50}	0.74
O16	0.697(3)	0.019(3)	0.950(3)	$0.061(5)^1$	1	1.86
O17a	0.435(4)	0.169(4)	0.699(4)	$0.017(6)^1$	O _{0.50}	1.02
O17b	0.589(4)	0.870(4)	0.704(5)	$0.019(6)^1$	O _{0.50}	1.09
O18a	0.694(4)	0.164(3)	0.710(4)	$0.026(6)^1$	Q0 50	0.83
O18b	0.838(4)	0.875(4)	0.712(5)	$0.031(6)^1$	Q _{0.50}	0.81
$O19a = H_2O$	0.537(5)	0.518(4)	0.704(6)	$0.046(8)^1$	O ₀ 50	0.27
$019b = H_2O$	0.764(4)	0.663(4)	0.704(5)	$0.040(7)^1$	0.50	0.25
$0.020a = H_2O$	0.387(5)	0.875(5)	0.700(6)	$0.051(9)^1$	- 0.50 Oo 50	0.30
$020h - H_2O$	0.037(5)	0.528(5)	0.701(6)	0.031(9)	0.50	0.26
$021a - H_2O$	0.052(5)	0.161(4)	0.703(5)	$0.044(8)^{1}$	0.50	0.28
$021h - H_20$	0.200(5)	0.380(4)	0.702(5)	$0.046(8)^{1}$	0.50	0.28
5210 - 1120	0.402(3)	0.500(+)	0.702(3)	0.040(0)	S0.50	0.20

Table 6. Coordinates and equivalent displacement parameters (U_{eq} , in Å²) of atoms, site occupancies, and bond valence sums (BVSs) for donnayite-(Y).

¹ U_{iso} . ² Bond valence parameters were taken from Brese and O'Keeffe (1991). * The sites occupancies were refined assuming full occupancy, and the best agreement was obtained with Sr_{0.648(15)}Ba_{0.352(15)} for the Sr1 site, Sr_{0.633(15)}Ba_{0.367(15)} for the Sr2 site, Sr_{0.704(16)}Ba_{0.296(16)} for the Sr3 site, Na_{0.863(8)}Dy_{0.137(8)} for the Na4 site, Ca_{0.906(10)}Dy_{0.094(10)} for the Ca5 site, and Y_{0.986(7)} for the Y6 site. In the final refinement cycles the occupancies were fixed based on the site-scattering factors, EMPAs, interatomic distances, bond valence calculations, and the charge-balance.

Sr1	-013	2.64(2)	Na4	-07	2.345(14)	C1	-02	1.25(2)
	-O20a	2.65(3)		-06	2.357(13)		-03	1.268(19)
	-O21a	2.65(4)		-O21b	2.36(3)		-01	1.310(19)
	-O12b	2.66(3)		-02	2.369(15)	< 0	21-0>	1.28
	-O19a	2.67(4)		-O20b	2.38(3)	C2	-06	1.261(19)
	-O14b	2.70(3)		-O19b	2.42(4)		-04	1.277(19)
	-O17b	2.72(3)		-O17a	2.44(3)		-05	1.317(19)
	-08	2.728(12)		-O12a	2.45(3)	< 0	2-0>	1.29
	-07	2.740(13)		-O14a	2.45(3)	C3	-08	1.26(2)
	-01	2.741(12)	< N	a4–O>	2.40/2.37*		-07	1.268(19)
	-05	2.743(12)	Ca5	-04	2.331(14)		-09	1.31(2)
	-03	2.748(14)		-08	2.340(13)	< C	3-0>	1.28
	-06	2.753(12)		-03	2.354(14)	C4a	-O12a	1.24(5)
< S	r1–0>	2.71/2.72*		-O20a	2.36(3)		-O10	1.29(5)
Sr2	-O10	2.61(2)		-O21a	2.40(4)		-O11a	1.42(5)
	-O21b	2.64(3)		-O19a	2.40(3)	< C	4a-O >	1.32
	-O19b	2.67(3)		-O17b	2.43(3)	C4b	-O12b	1.24(5)
	-O20b	2.67(3)		-O12b	2.45(3)		-O10	1.27(4)
	-O14a	2.69(3)		-O14b	2.46(3)		-011b	1.42(5)
	-O17a	2.70(3)	< C	a5-O>	2.36/2.39*	< C-	4b-O>	1.31
	-O12a	2.71(3)	Y6	-05	2.323(13)	C5a	-O14a	1.23(5)
	-04	2.725(13)		-01	2.333(12)		-013	1.24(4)
	-06	2.730(12)		-09	2.338(13)		-O15a	1.46(5)
	-01	2.741(11)		-O18a	2.39(3)	< C	5a-O >	1.31
	-09	2.745(12)		-O18b	2.39(3)	C5b	-014b	1.20(5)
	-02	2.750(13)		-O11a	2.40(3)		-013	1.28(4)
	-08	2.758(13)		-O15b	2.40(3)		-015b	1.44(5)
< S	r2–O>	2.72/2.70*		-011b	2.43(3)	< C.	5b-O>	1.31
Sr3	-016	2.60(2)		-O15a	2.44(3)	C6a	-O17a	1.22(5)
	-O15a	2.68(3)		-013	2.54(2)		-016	1.30(5)
	-O15b	2.69(3)		-010	2.57(2)		-O18a	1.37(5)
	-O18a	2.69(3)		-016	2.59(2)	< C	6a–O >	1.30
	-011b	2.69(3)	< Y	6-0>	2.44/2.43*	C6b	-017b	1.20(4)
	-011a	2.70(3)					-016	1.27(4)
	-O18b	2.70(3)					-O18b	1.38(4)
	-O2	2.712(13)				< C0	6b–O >	1.28
	-03	2.714(13)						
	-09	2.716(13)						
	-05	2.724(12)						
	-07	2.725(14)						
	-04	2.737(13)						

Table 7. Selected interatomic distances (Å) in the structure of donnayite-(Y).

* Calculated for polyhedra with bonds M–O sites marked with appended "a"/M–O sites marked with appended "b".

< Sr3–O >

2.70/2.70*

4 Mckelveyite group nomenclature

According to Mills et al. (2009) "a mineral group consists of two or more minerals with the same or essentially the same structure and composed of chemically similar elements". Seven minerals – alicewilsonite-(YCe), alicewilsonite-(YLa), bainbridgeite-(YCe), donnayite-(Y), ewaldite, mckelveyite-(Y), and weloganite – meet the requirements for formation of a mineral group (Table 8).

Mckelveyite group minerals are carbonates with the general formula $A_3B_3(CO_3)_6 \cdot 3H_2O$, where A = Na, Ca, Y, Zr, and B = Sr, Ba, Ce, and La. Their structure is based on two alternating layers with larger cations *B* forming one layer and smaller cations *A* another. One half of the carbonate groups are coplanar to $\{001\}$, whereas another half is non-

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Name	Formula	Space group	Type locality	References
Alicewilsonite-(YCe)	$Na_2Sr_2YCe(CO_3)_6 \cdot 3H_2O$	P1, R3m ^a	Mont Saint-Hilaire, Quebec, Canada	Lykova et al. (2023); Thi et al. (1984, 1992) ^a
Alicewilsonite-(YLa)	$Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$	<i>P</i> 1	Mont Saint-Hilaire, Quebec, Canada	Proposal IMA 2021-047
Bainbridgeite-(YCe)	$Na_2Ba_2YCe(CO_3)_6 \cdot 3H_2O$	P1	Mont Saint-Hilaire, Quebec, Canada	Proposal IMA 2020-065
Donnayite-(Y)	$NaCaSr_3Y(CO_3)_6 \cdot 3H_2O$	<i>P</i> 1	Mont Saint-Hilaire, Quebec, Canada	Chao et al. (1978), this study
Ewaldite	$BaCa(CO_3)_2 \cdot 2.6H_2O(?)$	P6 ₃ mc ^b	Diamond Alkali Daco No. 3, Wyoming, USA	Donnay et al. (1971), Donnay and Preston (1971); Voloshin et al. (1992)
Mckelveyite-(Y)	NaCaBa $_3$ Y(CO $_3$) $_6 \cdot 3H_2O$	P1, Cc	Diamond Alkali Daco No. 3, Wyoming, USA	Milton et al. (1965), Demartin et al. (2008)
Weloganite	$Na_2Sr_3Zr(CO_3)_6 \cdot 3H_2O$	P1	Francon quarry, Quebec, Canada	Sabina et al. (1968), Grice and Perrault (1975)

Table 8. Mckelveyite group minerals.

^a The trigonal *R3m* polymorph of "donnayite-(Y)" reported by Thi et al. (1992) was very likely triclinic alicewilsonite-(YCe) (Lykova et al., 2023). ^b The studied structures were highly disordered; re-investigation is required to confirm the space group.

coplanar. Different order–disorder modifications occur resulting in triclinic, monoclinic trigonal, and hexagonal minerals with essentially the same structure (Donnay and Preston, 1971; Chen and Chao, 1975; Grice and Perrault, 1975; Thi et al., 1984, 1992; Voloshin et al., 1992; Demartin et al., 2008, our data). There are six independent cation sites in the structure of triclinic and monoclinic members and two sites in the trigonal and hexagonal members.

Although it is suggested "that the group name be that of the first mineral to have been adequately characterised" (Mills et al., 2009), a historical name was proposed for this group after the first mineral discovered in it – mckelveyite-(Y) (Milton et al., 1965). The historical significance should take precedence over the requirement of full structural study for an "adequate" characterisation of a species for this group due to challenges with structural determination because of strong disorder, multiple domains, splitting, and complex twinning. Moreover, although the first structural characterisation of a mckelveyite group mineral should be attributed to ewaldite (Donnay and Preston, 1971), many questions remain about its structure.

Crystal-chemical-driven ordering of lighter and larger Ln at the larger B sites and Y + heavier and smaller Ln at the smaller A sites is observed in the crystal structure of mckelveyite group minerals. In some cases, it leads to two different rare-earth elements being dominant at two different crystal-structure sites (alicewilsonite-(YCe), alicewilsonite-(YLa) and bainbridgeite-(YCe)). In those cases, two chemical symbols are appended to the name in accordance with the nomenclature for rare-earth and Y-mineral species (Levinson, 1966; Bayliss and Levinson, 1988). For the mckelveyite group minerals the first symbol represents the dominant cations at one of the A sites and the second symbol – at one of the B sites.

Data availability. Crystallographic data for donnayite-(Y) and its PXRD pattern in the *xy* format are available in the Supplement.

Supplement. The supplement related to this article is available online at: https://doi.org/10.5194/ejm-35-133-2023-supplement.

Author contributions. IL conceptualised the project. RR collected powder X-ray diffraction data and subsampled the specimens. EM-PAs were obtained by GP. GG and HF collected single-crystal X-ray diffraction data. KO performed the observations of optical properties. IL processed the data and interpreted the results. The manuscript was written by IL with contributions from all coauthors.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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