European Journal of
**Mineralogy**

Open Access

# Mckelveyite group minerals – Part 4: Alicewilsonite-(YLa), $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$, a new lanthanum-dominant species from the Paratoo mine, Australia

**Inna Lykova**[1], **Ralph Rowe**[1], **Glenn Poirier**[1], **Henrik Friis**[2], and **Kate Helwig**[3]

[1]Canadian Museum of Nature, Ottawa, K1P 6P4, Canada
[2]Natural History Museum, University of Oslo, Oslo, 0318, Norway
[3]Canadian Conservation Institute, Ottawa, K1B 4S7, Canada

**Correspondence:** Inna Lykova (ilykova@nature.ca)

**Abstract.** The new mckelveyite group mineral, alicewilsonite-(YLa), $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$, was found together with kamphaugite-(Y), paratooite-(Y), bastnäsite-(La), and decrespignyite-(Y) coating along fractures in dolomite at the Paratoo copper mine, South Australia, Australia. It occurs as pale pink to colourless pseudohexagonal tabular crystals up to 150 μm in size. The streak is white; the lustre is vitreous. The mineral has no cleavage. $D_{calc}$ is $3.37\,\text{g cm}^{-3}$. Alicewilsonite-(YLa) is optically biaxial $(-)$, $\alpha = 1.556(2)$, $\beta = 1.582(2)$, $\gamma = 1.592(2)$, 2V (meas.) $= 60(2)°$, 2V (calc.) $= 63°$ (589 nm). The IR spectrum is reported. The composition (wt %, average of seven analyses) is $Na_2O$ 7.43, CaO 2.00, SrO 18.43, BaO 1.64, $Y_2O_3$ 9.59, $La_2O_3$ 11.74, $Pr_2O_3$ 1.29, $Nd_2O_3$ 5.74, $Sm_2O_3$ 0.44, $Eu_2O_3$ 0.09, $Gd_2O_3$ 0.95, $Dy_2O_3$ 1.15, $Ho_2O_3$ 0.25, $Er_2O_3$ 0.89, $Yb_2O_3$ 0.29, $CO_2$ 29.78, $H_2O$ 6.18, total 97.88. The empirical formula calculated on the basis of six cations with 3 $H_2O$ molecules is as follows: $Na_{2.10}Ca_{0.31}Sr_{1.56}Ba_{0.10}Y_{0.74}La_{0.63}Pr_{0.07}Nd_{0.30}Sm_{0.03}Eu_{0.01}Gd_{0.04}Dy_{0.05}Ho_{0.01}Er_{0.04}Yb_{0.01}(CO_3)_{5.92}(H_2O)_3$. The mineral is triclinic, $P1$, $a = 8.9839(2)$, $b = 8.9728(3)$, $c = 6.7441(2)$ Å, $\alpha = 102.812(2)°$, $\beta = 116.424(2)°$, $\gamma = 60.128(2)°$, and $V = 422.17(2)$ Å$^3$ and $Z = 1$. The strongest reflections of the powder X-ray diffraction pattern $[d,\text{Å}(I)(hkl)]$ are 6.03(43)(001), 4.355(100)($1\bar{1}0$, $\bar{2}11$, 120), 4.020(30)($\bar{1}11$, 210, $\bar{1}21$), 3.188(29)($\bar{2}12$, $1\bar{1}1$, 121), 2.819(96)(002, $\bar{1}12$, 211, $\bar{1}22$), 2.592(40)($\bar{3}01$, 030, $\bar{3}31$), 2.228(33)($\bar{2}21$, $\bar{4}21$, $\bar{2}41$). 2.011(36)($\bar{2}22$, 003, 420, $\bar{2}42$), 1.9671(32)($\bar{3}03$, 301, $0\bar{3}2$, 032, $\bar{3}33$, 331). The crystal structure was solved and refined from single-crystal X-ray diffraction data ($R_1 = 0.058$).

## 1 Introduction

This paper describes alicewilsonite-(YLa), $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$, the first lanthanum-dominant member of the mckelveyite group which consists of rare carbonates with the general formula $A_3B_3(CO_3)_6 \cdot 3H_2O$, where $A =$ Na, Ca, Y, and Zr, and $B =$ Sr, Ba, Ce, and La (Lykova et al., 2023a).

Alicewilsonite-(YLa) is named as the La analogue of alicewilsonite-(YCe), $Na_2Sr_2YCe(CO_3)_6 \cdot 3H_2O$. The parenthesised Levinson suffix -(YLa) was added in accordance with the nomenclature for rare-earth and Y mineral species (Levinson, 1966; Bayliss and Levinson, 1988) and the nomenclature of the mckelveyite group; the first symbol

represents the dominant cations at one of the $A$ sites and the second symbol at one of the $B$ sites (Lykova et al., 2023a).

Both the new mineral and the name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA CNMNC), proposal IMA 2021-047. The holotype of alicewilsonite-(YLa) was deposited in the collection of the Canadian Museum of Nature, Ottawa, Canada. The catalogue number is CMNMC 89063. A part of the holotype used for structure determination is kept at the Natural History Museum in Oslo under catalogue number KNR 44330.

**Figure 1.** Transparent pale pink to colourless alicewilsonite-(YLa) crystals up to 150 μm in size, with white globular kamphaugite-(Y). FOV 1.5 mm. Specimen CMNMC 89063. Canadian Museum of Nature collection. Photos: François Génier.

## 2    Occurrence and general appearance

Alicewilsonite-(YLa) occurs at the Paratoo copper mine, Yunta, Olary Province, South Australia, Australia. It was found together with kamphaugite-(Y) as coating along fractures in dolomite. The new mineral forms pseudohexagonal tabular crystals up to 150 μm in size (Fig. 1). Similar crystals have been previously reported from Paratoo as "donnayite-(Y)" and are known to be associated with kamphaugite-(Y), paratooite-(Y), bastnäsite-(La) (Pring et al., 2006), and decrespignyite-(Y) (Wallwork et al., 2002). No analytical data were published on that phase, but electron microprobe analyses shared with us by Allan Pring (personal communication, 2023) correspond to alicewilsonite-(YLa). No specimen with conclusively identified donnayite-(Y) from the Paratoo mine is known to us.

At Paratoo, dolomites, sandstones, and shales of the Torrensian Burra Group were disrupted by several dolerite bodies and were brecciated forming the "Paratoo Diapir". At its surface, the bulk of the copper mineralisation occurs in the quartz–magnetite veins, and as impregnations and fissure fillings of secondary copper minerals in sedimentary rocks. The secondary Cu-*REE* mineralisation, including alicewilsonite-(YLa), associated with the intensely weathered base metal and magnetite ores, occurs as thin coatings along bedding joints and fractures and is most abundant near the surface ($< 3$ m) (Brugger et al., 2006).

## 3    Physical and optical properties

Alicewilsonite-(YLa) is pale pink to colourless with a white streak and vitreous lustre. The mineral has no cleavage, and its fracture is uneven. The Mohs hardness could not be determined as the crystals are very small; it is expected to be ca. 3, based on data for other members of the mckelveyite group. The mineral is non-fluorescent under ultraviolet light. The density calculated using the empirical formula and unit-cell volume refined from the single-crystal XRD data is $3.37$ g cm$^{-3}$.

Alicewilsonite-(YLa) is optically biaxial $(-)$, $\alpha = 1.556(2)$, $\beta = 1.582(2)$, $\gamma = 1.592(2)$, 2 V (meas.) $= 60(2)°$ (from a spindle-stage extinction curve), 2 V (calc.) $= 63°$. The mineral is non-pleochroic.

## 4    Experimental methods

Electron microprobe analyses (EMPAs) for alicewilsonite-(YLa) were obtained using a JEOL 8230 SuperProbe electron microscope equipped with five WDS spectrometers (University of Ottawa – Canadian Museum of Nature MicroAnalysis Laboratory, Canada) using an accelerating voltage of 20 kV, a beam current of 10 nA, and a beam diameter of 30 μm depending on the grain size. Alicewilsonite-(YLa) is unstable under an electron beam, and so a large beam diameter was used to minimise element migration. The following reference materials were used: albite (Na$K\alpha$), diopside (Ca$K\alpha$), celestine (Sr$L\alpha$), sanbornite (Ba$L\alpha$), YAG (Y$L\alpha$), LaPO$_4$ (La$L\alpha$), PrPO$_4$ (Pr$L\beta$), NdPO$_4$ (Nd$L\alpha$), SmPO$_4$ (Sm$L\alpha$), EuPO$_4$ (Eu$L\alpha$), GdPO$_4$ (Gd$L\alpha$), DyPO$_4$ (Dy$L\beta$), HoPO$_4$

(Ho$L\beta$), ErPO$_4$ (Er$L\alpha$), (Yb$L\alpha$). The intensity data were corrected for time-dependent intensity loss (or gain) using a self-calibrated correction for Na$K\alpha$, Ca$K\alpha$, Y$L\alpha$, and La$L\alpha$. H$_2$O and CO$_2$ contents were not analysed due to the paucity of the available material.

The Fourier transform infrared (FTIR) spectrum of alicewilsonite-(YLa) was obtained using a Bruker Hyperion 2000 microscope interfaced to a Tensor 27 spectrometer with a wide-band mercury cadmium telluride (MCT) detector (Canadian Conservation Institute, Canada). A small fragment of alicewilsonite-(YLa) was mounted on a low-pressure diamond anvil microsample cell and analysed in transmission mode. The spectrum was collected between 4000–400 cm$^{-1}$ with the co-addition of 150 scans at a 4 cm$^{-1}$ resolution.

Powder X-ray diffraction (PXRD) data were collected at the Canadian Museum of Nature, Canada, using a Bruker D8 Discover microdiffractometer equipped with a DECTRIS EIGER2 R 500K detector and I$\mu$S microfocus X-ray source ($\lambda_{\mathrm{Cu}K\alpha1} = 1.54060$ 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 of alicewilsonite-(YLa) $\sim 200\,\mu$m 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.

Single-crystal X-ray diffraction (SXRD) studies were carried out at the Natural History Museum, University of Oslo, Norway, using a Rigaku XtaLAB Synergy-S diffractometer equipped with a HyPix 6000HE detector ($\lambda_{\mathrm{Mo}K\alpha} = 0.71073$) operating at 50 kV and 1 mA. The data were processed, including absorption correction, using Rigaku's CrysAlis Pro software (Matsumoto et al., 2021).

## 5 Results

### 5.1 Chemical data

Chemical data on alicewilsonite-(YLa) are given in Table 1. The contents of Ce, Tb, Tm, U, Th, and Hf are below the detection limit.

The empirical formula calculated on the basis of six cations with 3 H$_2$O molecules is Na$_{2.10}$Ca$_{0.31}$Sr$_{1.56}$Ba$_{0.10}$Y$_{0.74}$La$_{0.63}$Pr$_{0.07}$Nd$_{0.30}$ Sm$_{0.03}$Eu$_{0.01}$Gd$_{0.04}$Dy$_{0.05}$Ho$_{0.01}$Er$_{0.04}$Yb$_{0.01}$ (CO$_3$)$_{5.92}$(H$_2$O)$_3$. The simplified formula is Na$_2$(Sr,Ca,Ba)$_2$(Y,Dy,Er)(La,Nd,Pr)(CO$_3$)$_6 \cdot$ 3H$_2$O.

The ideal end-member formula is Na$_2$Sr$_2$YLa(CO$_3$)$_6 \cdot$ 3H$_2$O, which requires Na$_2$O 7.18, SrO 24.01, Y$_2$O$_3$ 13.08, La$_2$O$_3$ 18.88, CO$_3$ 30.59, H$_2$O 6.26, total 100 wt %.

Alicewilsonite-(YLa) dissolves in an aqueous HCl solution at room temperature with strong effervescence.

**Table 1.** Chemical data for alicewilsonite-(YLa) (average of seven analyses).

| Constituent | Mean | Range | SD ($2\sigma$) |
|---|---|---|---|
| Na$_2$O | 7.43 | 6.79–8.05 | 0.51 |
| CaO | 2.00 | 1.68–2.28 | 0.25 |
| SrO | 18.43 | 17.77–19.59 | 0.64 |
| BaO | 1.64 | 1.18–2.19 | 0.42 |
| Y$_2$O$_3$ | 9.59 | 9.29–9.83 | 0.19 |
| La$_2$O$_3$ | 11.74 | 10.57–13.43 | 0.90 |
| Pr$_2$O$_3$ | 1.29 | 0.94–1.73 | 0.27 |
| Nd$_2$O$_3$ | 5.74 | 4.41–7.44 | 1.10 |
| Sm$_2$O$_3$ | 0.44 | 0.33–0.53 | 0.09 |
| Eu$_2$O$_3$ | 0.09 | 0.00–0.25 | 0.12 |
| Gd$_2$O$_3$ | 0.95 | 0.68–1.29 | 0.24 |
| Dy$_2$O$_3$ | 1.15 | 0.91–1.37 | 0.17 |
| Ho$_2$O$_3$ | 0.25 | 0.09–0.44 | 0.13 |
| Er$_2$O$_3$ | 0.89 | 0.83–0.91 | 0.03 |
| Yb$_2$O$_3$ | 0.29 | 0.26–0.32 | 0.02 |
| CO$_2^*$ | 29.78 | | |
| H$_2$O$^*$ | 6.18 | | |
| Total | 97.88 | | |

$^*$ Calculated from the stoichiometry.

### 5.2 Infrared spectroscopy

The IR spectrum of alicewilsonite-(YLa) (Fig. 2) shows IR bands of O–H stretching (in the range from 3300–3400 cm$^{-1}$) and H–O–H bending (at 1687 cm$^{-1}$) vibrations of H$_2$O molecules and C–O stretching (in the range 1369–1554 cm$^{-1}$) vibrations of CO$_3^{2-}$ group molecules. The band at 1066 cm$^{-1}$ can be assigned to the non-degenerate mode of C–O stretching vibrations, indicating polarisation of CO$_3^{2-}$ groups. If only symmetric non-polarised carbonate groups (with a 3-fold axis) were present, this mode would be inactive. The band at 855 cm$^{-1}$ could correspond to the non-degenerate mode of out-of-plane O–C–O bending vibrations, and its high intensity may be attributed to a high degree of distortion of the CO$_3^{2-}$ groups. The band assignment was made after Chukanov and Chervonnyi (2016) and Kasatkin et al. (2021).

### 5.3 X-ray diffraction data and description of the crystal structure

The indexed PXRD data are given in Table 2. Parameters of the triclinic unit cell refined from the data are as follows: $a = 8.9839(2)$, $b = 8.9728(3)$, $c = 6.7441(2)$ Å, $\alpha = 102.812(2)°$, $\beta = 116.424(2)°$, $\gamma = 60.128(2)°$, and $V = 422.17(2)$ Å$^3$. The PXRD pattern in the $xy$ format is available as a Supplement.

The SXRD data were indexed in the $P1$ space group with the following unit-cell parameters: $a = 8.9793(3)$ Å, $b = 8.9734(2)$ Å, $c = 6.74044(19)$ Å, $\alpha = 102.829(2)°$,
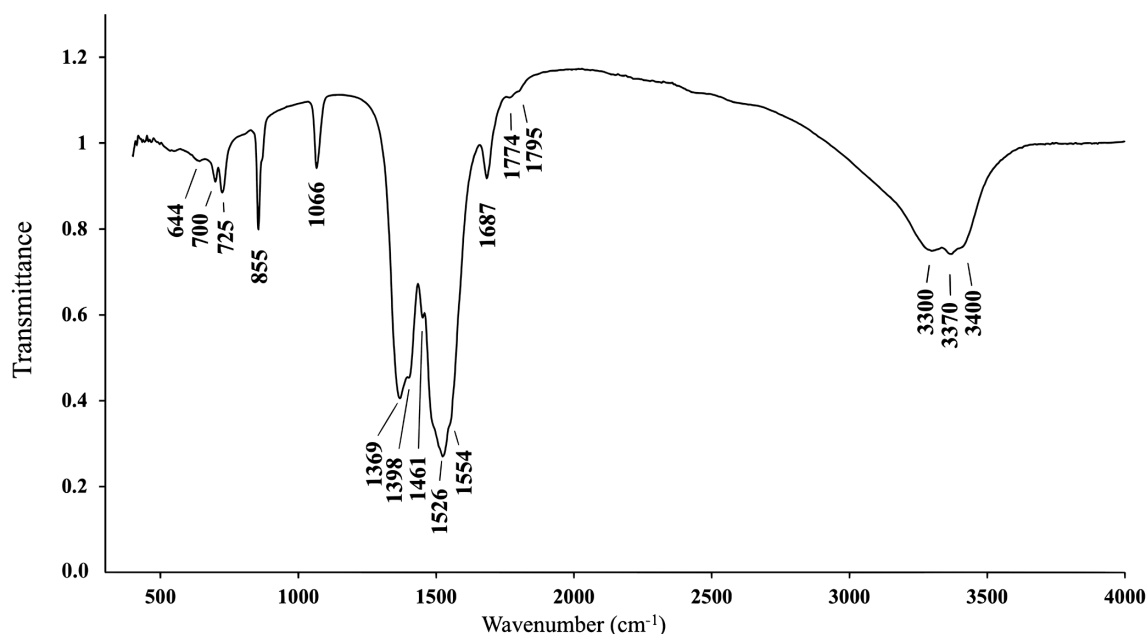
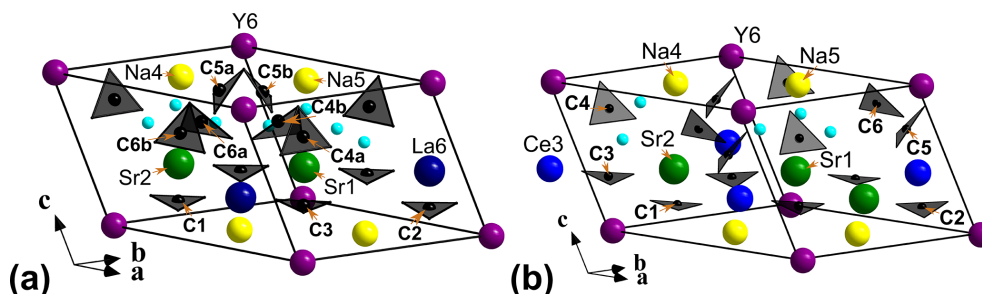**Figure 2.** Infrared spectrum of alicewilsonite-(YLa).



**Figure 3.** General view of the crystal structure of (**a**) alicewilsonite-(YLa) and (**b**) alicewilsonite-(YCe). The unit cells are outlined.

$\beta = 116.382(3)°$, $\gamma = 60.109(3)°$, and $V = 421.82(2)$ Å$^3$. The structure was solved and refined to $R_1 = 0.058$ on the basis of 3640 independent reflections with $I > 2\sigma(I)$ using the SHELXL-2018/3 program package (Sheldrick, 2015). Crystal data, data collection information, and structure refinement details are given in Table 3, atom coordinates, equivalent displacement parameters, site composition, and bond-valence sums (BVSs) in Table 4, and selected inter-atomic distances in Table 5. The studied crystal demonstrated twinning by merohedry Class I (Nespolo and Ferraris, 2000), with twin domains ratio of 22 : 78. The crystallographic information file (CIF) for alicewilsonite-(YLa) is available as a file in the Supplement. It was also deposited in the Inorganic Crystal Structure Database (ICSD; no. 2308960).

Due to the poor quality of alicewilsonite-(YLa) crystals resulting in multiple split reflections and streaks, the structure could only be refined to $R_1 = 0.058$. The mineral is strongly pseudotrigonal. There are six independent large cation sites in the structure (Fig. 3a) forming two alternating layers par-

allel to the *ab* plane (Fig. 4). Na, Sr, Y, La, Ca, Dy, and Ba cations were distributed among these sites based on the microprobe data, refined site-scattering factors ($e_{ref}$, in electrons per site), and charge balance taking into account bond-valence sums (BVSs) and interatomic distances (Tables 4–5). Lighter lanthanoids (Ln, La–Lu) were formally refined as La atoms and heavier Ln as Dy atoms. One of the layers is formed by the Sr1, Sr2, and La3 sites that have a 10-fold coordination. The refinement showed that Sr and La are distributed between all three sites; the best agreement was obtained with the refined site-occupation factor $Sr_{0.617(7)}La_{0.383(7)}$ for the Sr1 site, $Sr_{0.541(7)}La_{0.459(7)}$ for the Sr2 site, and $La_{0.584(8)}Sr_{0.416(8)}$ for the La3 site. The occupancies were assigned as $Sr_{0.65}La_{0.25}Ba_{0.10}$, $Sr_{0.57}La_{0.43}$, and $La_{0.58}Sr_{0.42}$ for the Sr1, Sr2, and La3 sites, respectively. Na4 and Na5 sites have octahedra coordination; their occupancies were fixed as $Na_{0.90}Dy_{0.05}Ca_{0.05}$. The Y6 site is occupied predominantly by Y atoms (67 %) with admixed Na

**Table 2.** X-ray powder diffraction data (*d* in Å) for alicewilsonite-(YLa). The strongest reflections are given in bold.

| $I_{\text{meas}}^1$ | $d_{\text{meas}}$ | $I_{\text{calc}}^1$ | $d_{\text{calc}}^2$ | *hkl* |
|---|---|---|---|---|
| 11 | 7.76 | 13 | 7.78 | 010 |
| 6 | 7.15 | 9, 8 | 7.16, 7.14 | 100, 110 |
| **43** | **6.03** | 100 | 6.04 | 001 |
| **100** | **4.355** | 71, 73, 75 | 4.37, 4.36, 4.35 | $0\bar{1}1$, $\bar{2}\bar{1}1$, 120 |
| **30** | **4.020** | 25, 24, 24 | 4.03, 4.03, 4.02 | $\bar{1}11$, 210, $\bar{1}\bar{2}1$ |
| 29 | 3.188 | 24, 24, 23 | 3.192, 3.192, 3.187 | $\bar{2}\bar{1}2$, $1\,\bar{1}1$, 121 |
| 18 | 3.018 | 36 | 3.020 | 002 |
| **96** | **2.819** | 60, 60, 59 | 2.823, 2.820, 2.820 | $\bar{1}12$, 211, $\bar{1}\bar{2}2$ |
| **40** | **2.592** | 36, 35, 35 | 2.598, 2.594, 2.591 | $\bar{3}01$, 030, $\bar{3}\bar{3}1$ |
| 25 | 2.381 | 9, 9, 10, 10, 9, 9 | 2.387, 2.386, 2.383, 2.383, 2.382, 2.380 | $\bar{3}02$, 300, $0\bar{3}1$, 031, $\bar{3}\bar{3}2$, 330 |
| 7 | 2.242 | 5, 5, 5 | 2.244, 2.243, 2.241 | $\bar{2}\bar{1}3$, $1\,\bar{1}2$, 122 |
| **33** | **2.228** | 23, 23, 23 | 2.232, 2.230, 2.226 | $\bar{2}21$, $\bar{4}\bar{2}1$, $\bar{2}41$ |
| 10 | 2.179 | 8, 7, 8 | 2.183, 2.181, 2.177, | $2\bar{2}0$, $\bar{4}\bar{2}2$, 240 |
| 13 | 2.021 | 9, 9, 9 | 2.023, 2.022, 2.022 | $\bar{1}13$, $\bar{1}\bar{2}3$, 212 |
| **36** | **2.011** | 19, 20, 18, 18 | 2.015, 2.013, 2.012, 2.011 | $\bar{2}22$, 003, 420, $\bar{2}\bar{4}2$ |
| **32** | **1.9671** | 11, 12, 12, 12, 11, 11 | 1.9701, 1.9688, 1.9676, 1.9674, 1.9671, 1.9655 | $\bar{3}03$, 301, $0\bar{3}2$, 032, $\bar{3}\bar{3}3$, 331 |
| 25 | 1.9084 | 19, 20, 19 | 1.9109, 1.9104, 1.9069, | $2\bar{2}1$, $\bar{4}\bar{2}3$, 241 |
| 12 | 1.6898 | 6, 6, 5, 6, 6, 6 | 1.6935, 1.6929, 1.6915, 1.6896, 1.6895, 1.6881 | $\bar{4}11$, $\bar{5}\bar{1}2$, $1\,\bar{4}0$, $\bar{5}42$, 150, $\bar{4}51$ |
| 9 | 1.6794 | 8, 8, 8 | 1.6809, 1.6805, 1.6797 | $\bar{2}14$, $1\,\bar{1}2$, 123 |
| 17 | 1.5895 | 2, 3, 3, 4, 3, 5, 5, 4, 5, 5, 5, 4, 5, 3, 4 | 1.5958, 1.5958, 1.5933, 1.5922, 1.5922, 1.5919, 1.5908, 1.5907, 1.5904, 1.5903, 1.5902, 1.5895, 1.5891, 1.5889, 1.5876 | $\bar{4}24$, $2\bar{2}2$, 242, $\bar{5}13$, $4\bar{1}0$, $\bar{3}04$, 302, $1\bar{4}1$, $0\bar{3}3$, $\bar{3}34$, 033, $\bar{5}43$, 332, 151, 450 |
| 5 | 1.5460 | 3, 3, 4, 4 | 1.5469, 1.5465, 1.5461, 1.5402 | $\bar{1}14$, $\bar{1}\bar{2}4$, 213, $\bar{4}13$ |
| 9 | 1.5368 | 4, 4, 4, 4, 4 | 1.5388, 1.5383, 1.5369, 1.5362, 1.5362 | 510, $\bar{1}42$, $\bar{1}52$, 540, $\bar{4}53$ |

$^1$ Calculated from the crystal structure determination; only reflections with intensities > 1 are given. $^2$ Calculated from PXRD Rietveld unit-cell refinement with
$a = 8.9839(2)$, $b = 8.9728(3)$, $c = 6.7441(2)$ Å, $\alpha = 102.812(2)°$, $\beta = 116.424(2)°$, $\gamma = 60.128(2)°$, and $V = 422.17(2)$ Å$^3$.
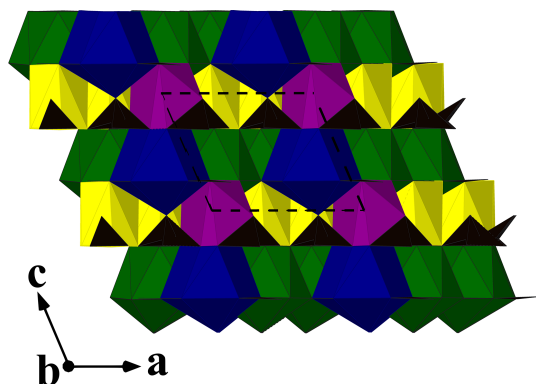


**Figure 4.** A view along [010] of the crystal structure of alicewilsonite-(YLa). Sr-, La-, Y-, and Na-centred polyhedra are shown in green, blue, purple, and yellow, respectively. Carbonate groups are black triangles. The unit cell is outlined.

(23 %) and Ca (10 %) atoms. The Y6-centred nine-fold polyhedron has an average < Y6–O > distance of 2.44/2.46 Å.

The three $CO_3^{2-}$ groups centred by carbon atoms C1, C2, and C3 are almost coplanar with {001} as in alicewilsonite-(YCe) (Lykova et al., 2023b). In the latter, as well as in most other member of the mckelveyite group (Lykova et

al., 2023a, 2024), there are three other, not coplanar $CO_3^{2-}$ groups centred by carbon atoms C4, C5, and C6 (Fig. 3b). In alicewilsonite-(YLa) 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. 3a). The occupancy of the alternating carbon and oxygen sites was fixed at 50 %. Similar splitting of carbon sites was observed in donnayite-(Y) (Lykova et al., 2023a).

The BVSs at the O19a, O19b, O20a, O20b, O21a, and O21b sites (0.19, 0.20, 0.21, 0.21, 0.21, and 0.22 valence units, respectively) indicate the presence of $H_2O^0$ molecules, also confirmed by the presence of the bands of O–H-stretching and H–O–H bending vibrations in the IR spectrum of alicewilsonite-(YLa). O19a, O20a, and O21a water molecules are bonded to Sr1- and Na5-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 most were refined with isotropic atomic displacement parameters only.

The resulting structural formula of alicewilsonite-(YLa) is $(Na_{1.80}Dy_{0.10} \quad Ca_{0.10})_{\sum 2}$

**Table 3.** Crystal data, data collection information, and structure refinement details for alicewilsonite-(YLa).

| Crystal system, space group, $Z$ | Triclinic, $P1$, 1 |
|---|---|
| $a$ (Å) | 8.9793(3) |
| $b$ (Å) | 8.9734(2) |
| $c$ (Å) | 6.74044(19) |
| $\alpha$ (°) | 102.829(2) |
| $\beta$ (°) | 116.382(3) |
| $\gamma$ (°) | 60.109(3) |
| $V$ (Å$^3$) | 421.82(2) |
| $\lambda$ (MoK$\alpha$) (Å), $T$ (K) | 0.71073, 293 |
| Diffractometer | Rigaku XtaLAB Synergy-S |
| $\theta$ range (°) | 2.62–28.27 |
| Crystal size (mm$^3$) | $0.019 \times 0.031 \times 0.044$ |
| Absorption coefficient μm (mm$^{-1}$) | 11.47 |
| $F_{000}$ | 409 |
| $h, k, l$ range | $-11 \leq h \leq 11,\ -11 \leq k \leq 11,\ -8 \leq l \leq 8$ |
| Reflections collected | 11980 |
| Unique reflections | 4133 |
| Unique reflections [$I > 2\sigma(I)$] | 3640 |
| Number of refined parameters | 307 |
| Weighting scheme | $1/[\sigma^2(F_o^2) + (0.1008P)^2 + 1.6718P], P = [\max(F_o)^2 + 2(F_c)^2]/3$ |
| Final $R$ indices [$I > 2\sigma I$] | $R_1 = 0.058, wR_2 = 0.156$ |
| $R$ indices (all data) | $R_1 = 0.061, wR_2 = 0.161$ |
| Goodness of fit | 1.016 |
| $\Delta\rho_{max}/\Delta\rho_{min}$ ($e$ Å$^{-3}$) | 2.50*/−1.16 |

\* Located 0.14 Å away from the Sr1 site.

$(Sr_{1.22}La_{0.68}Ba_{0.10})_{\sum 2}(Y_{0.67}Na_{0.23}Ca_{0.10})_{\sum 1}$ $(La_{0.58}Sr_{0.42})_{\sum 1}(CO_3)_6(H_2O)_3$, which leads to the ideal formula $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$. Combining structural and chemical data results in the following formula: $(Na_{1.90}HREE_{0.10})_{\sum 2}(Sr_{1.14}LREE_{0.51}Ca_{0.25}Ba_{0.10})_{\sum 2}$ $(Y_{0.74}Na_{0.20}Ca_{0.06})_{\sum 1}(LREE_{0.52}Sr_{0.42}HREE_{0.06})_{\sum 1}$ $(CO_3)_{5.92}(H_2O)_3$, where $LREE = La_{0.63}Nd_{0.30}Pr_{0.07}Sm_{0.03}$, and $HREE = Dy_{0.05}Gd_{0.04}Er_{0.04}Eu_{0.01}Ho_{0.01}Yb_{0.01}$.

## 6 Discussion

Alicewilsonite-(YLa), $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$, is a member of the mckelveyite group (Lykova et al., 2023a). It is the La analogue of alicewilsonite-(YCe), $Na_2Sr_2YCe(CO_3)_6 \cdot 3H_2O$ (Lykova et al., 2023b), and the SrLa analogue of bainbridgeite-(YCe), $Na_2Ba_2YCe(CO_3)_6 \cdot 3H_2O$ (Lykova et al., 2024; Table 6).

The absence of Ce in alicewilsonite-(YLa) suggests that it was separated and deposited elsewhere as highly insoluble Ce$^{4+}$. Whole-rock geochemical analyses of fresh and mineralised host rock and of vein material at Paratoo conducted by Brugger et al. (2006) revealed a strong enrichment in light rare-earth elements (*LREE*) and a strong negative Ce anomaly in secondary *REE* minerals and mineralised rock samples. This indicates that Ce was present as Ce$^{4+}$ and left behind during either the transport from

the unknown source rock to the Paratoo deposit or the deep weathering and remobilisation of *REE* elements. That the latter may result in preferential leaching of trivalent *REE* was demonstrated by Taunton et al. (2000) in a granite. The fractionation of Ce$^{4+}$ led to the formation of La-dominant secondary *REE* carbonates, such as paratooite-(La), $(La,Sr,Ca)_4CuCa(Na,Ca)_2(CO_3)_8$ (Pring et al., 2006; Krivovichev et al., 2019), bastnäsite-(La), $La(CO_3)F$ (Pring et al., 2006), and alicewilsonite-(YLa).

We have previously shown the penchant of the mckelveyite structure type to incorporate lighter and larger Ln at the larger cation sites and Y+ heavier and smaller Ln at the smaller cation sites (Lykova et al., 2023a, b, 2024). Alicewilsonite-(YLa) is another example of such crystal-chemically driven ordering and the first one with La as the dominant cation at one of the sites.

The splitting of carbon sites observed in donnayite-(Y) (Lykova et al., 2023a) and alicewilsonite-(YLa) likely represents structural variations within one species and is expected to be found in other mckelveyite group minerals. In fact, we anticipate it to be relatively common, but the poor quality of crystals in this group resulting in multiple split reflections and streaks in SXRD data sets often does not allow for a proper localisation of half-occupied carbon and oxygen sites. Thus, the structures of these minerals are usually solved on crystals where the splitting is not observed.

**Table 4.** Coordinates and equivalent displacement parameters ($U_{eq}$, in Å$^2$) of atoms, site occupancies, and bond-valence sums (BVSs) for alicewilsonite-(YLa).

| Site | $x$ | $y$ | $z$ | $U_{eq}$ | Site composition | BVS[2] |
|---|---|---|---|---|---|---|
| Sr1 | 0.45784(16) | 0.68467(15) | 0.36704(18) | 0.0250(3) | $Sr_{0.65}La_{0.25}Ba_{0.10}$ * | 1.95 |
| Sr2 | 0.12210(13) | 0.35597(11) | 0.36658(12) | 0.0249(3) | $Sr_{0.57}La_{0.43}$ * | 2.12 |
| La3 | 0.78605(13) | 0.02041(13) | 0.36465(14) | 0.0252(3) | $La_{0.58}Sr_{0.42}$ * | 2.43 |
| Na4 | 0.3280(9) | 0.3537(8) | 0.9846(10) | 0.0196(11) | $Na_{0.90}Dy_{0.05}Ca_{0.05}$ * | 1.07 |
| Na5 | 0.6615(8) | 0.6850(7) | 0.9836(9) | 0.0177(11) | $Na_{0.90}Dy_{0.05}Ca_{0.05}$ * | 1.04 |
| Y6 | 0.9982(6) | 0.0200(6) | 0.9912(7) | 0.0201(3) | $Y_{0.67}Na_{0.23}Ca_{0.10}$ * | 2.25 |
| C1 | 0.419(2) | 0.0205(17) | 0.251(2) | 0.023(2) | 1 | 4.23 |
| C2 | 0.0814(18) | 0.6872(18) | 0.248(2) | 0.023(2) | 1 | 4.12 |
| C3 | 0.7500(18) | 0.3520(18) | 0.247(2) | 0.023(2) | 1 | 4.11 |
| C4a | 0.031(6) | 0.235(6) | 0.783(7) | 0.064(9)[1] | $C_{0.50}$ | 1.79 |
| C4b | 0.788(12) | 0.354(11) | 0.808(14) | 0.19(4)[1] | $C_{0.50}$ | 1.59 |
| C5a | 0.142(13) | 0.685(13) | 0.795(15) | 0.16(3)[1] | $C_{0.50}$ | 1.52 |
| C5b | 0.247(6) | 0.806(6) | 0.787(7) | 0.064(9)[1] | $C_{0.50}$ | 1.94 |
| C6a | 0.605(7) | 0.127(6) | 0.797(8) | 0.072(11)[1] | $C_{0.50}$ | 1.69 |
| C6b | 0.700(9) | 0.917(8) | 0.782(10) | 0.097(16)[1] | $C_{0.50}$ | 1.97 |
| O1 | 0.2753(16) | 0.0202(15) | 0.2544(19) | 0.031(2) | 1 | 1.98 |
| O2 | 0.4170(18) | 0.1620(17) | 0.252(3) | 0.043(3) | 1 | 2.02 |
| O3 | 0.5577(18) | 0.8812(17) | 0.250(3) | 0.041(3) | 1 | 2.05 |
| O4 | 0.9399(18) | 0.6897(16) | 0.253(2) | 0.037(3) | 1 | 1.98 |
| O5 | 0.0844(17) | 0.8322(15) | 0.260(2) | 0.033(2) | 1 | 2.00 |
| O6 | 0.2204(18) | 0.5465(17) | 0.241(2) | 0.037(3) | 1 | 1.98 |
| O7 | 0.6103(17) | 0.3495(16) | 0.250(2) | 0.037(3) | 1 | 1.98 |
| O8 | 0.7487(17) | 0.4935(15) | 0.243(2) | 0.034(2) | 1 | 1.97 |
| O9 | 0.8994(17) | 0.2078(15) | 0.262(2) | 0.031(2) | 1 | 2.01 |
| O10 | 0.982(3) | 0.312(3) | 0.956(3) | 0.090(5)[1] | 1 | 1.45 |
| O11a | 0.049(5) | 0.073(5) | 0.698(5) | 0.068(9) | $O_{0.50}$ | 0.78 |
| O11b | 0.738(6) | 0.231(4) | 0.698(5) | 0.081(12) | $O_{0.50}$ | 0.80 |
| O12a | 0.051(5) | 0.338(4) | 0.706(6) | 0.060(8)[1] | $O_{0.50}$ | 0.89 |
| O12b | 0.747(4) | 0.485(3) | 0.698(4) | 0.042(6) | $O_{0.50}$ | 0.78 |
| O13 | 0.269(3) | 0.737(3) | 0.954(4) | 0.095(5)[1] | 1 | 1.64 |
| O14a | 0.226(5) | 0.543(4) | 0.690(4) | 0.052(7) | $O_{0.50}$ | 0.78 |
| O14b | 0.361(4) | 0.714(4) | 0.701(5) | 0.050(6) | $O_{0.50}$ | 0.94 |
| O15a | 0.947(6) | 0.820(3) | 0.699(5) | 0.068(10) | $O_{0.50}$ | 0.68 |
| O15b | 0.104(4) | -0.037(4) | 0.697(5) | 0.054(6)[1] | $O_{0.50}$ | 0.77 |
| O16 | 0.696(3) | 0.025(3) | 0.960(4) | 0.093(5)[1] | 1 | 1.75 |
| O17a | 0.420(4) | 0.168(4) | 0.696(5) | 0.074(12) | $O_{0.50}$ | 0.75 |
| O17b | 0.588(5) | 0.870(4) | 0.705(6) | 0.056(7)[1] | $O_{0.50}$ | 1.15 |
| O18a | 0.702(4) | 0.163(4) | 0.707(5) | 0.059(7)[1] | $O_{0.50}$ | 0.73 |
| O18b | 0.834(5) | 0.882(5) | 0.694(6) | 0.075(9)[1] | $O_{0.50}$ | 0.74 |
| O19a = $H_2O$ | 0.559(5) | 0.499(5) | 0.696(6) | 0.065(9)[1] | $O_{0.50}$ | 0.19 |
| O19b = $H_2O$ | 0.763(4) | 0.657(4) | 0.699(5) | 0.050(6)[1] | $O_{0.50}$ | 0.20 |
| O20a = $H_2O$ | 0.390(5) | 0.867(4) | 0.700(6) | 0.060(8)[1] | $O_{0.50}$ | 0.21 |
| O20b = $H_2O$ | 0.038(4) | 0.527(4) | 0.700(5) | 0.053(7)[1] | $O_{0.50}$ | 0.21 |
| O21a = $H_2O$ | 0.256(4) | 0.163(4) | 0.700(5) | 0.051(6)[1] | $O_{0.50}$ | 0.21 |
| O21b = $H_2O$ | 0.405(5) | 0.371(5) | 0.701(6) | 0.072(9)[1] | $O_{0.50}$ | 0.22 |

[1] $U_{iso}$. [2] Bond-valence parameters were taken from Gagne and Hawthorne (2015). * The sites occupancies were refined assuming full occupancy; the best agreement was obtained with $Sr_{0.617(7)}La_{0.383(7)}$ for the Sr1 site, $Sr_{0.541(7)}La_{0.459(7)}$ for the Sr2 site, $La_{0.584(8)}Sr_{0.416(8)}$ for the La3 site, $Na_{0.918(7)}Dy_{0.082(7)}$ for the Na4 site, $Na_{0.916(6)}Dy_{0.084(6)}$ for the Na5 site, and $Y_{0.716(16)}Na_{0.284(16)}$ for the Y6 site. In the final refinement cycles the occupancies were fixed based on the $e_{ref}$ values, electron microprobe data, interatomic distances, bond-valence calculations, and the charge balance.

**Table 5.** Selected interatomic distances (Å) in the structure of alicewilsonite-(YLa).

| Sr1 | O13 | 2.54(2) | Na4 | O6 | 2.325(14) | C1 | O3 | 1.253(19) |
|---|---|---|---|---|---|---|---|---|
| | O21a | 2.58(3) | | O7 | 2.352(14) | | O2 | 1.260(19) |
| | O20a | 2.59(3) | | O20b | 2.36(3) | | O1 | 1.301(18) |
| | O19a | 2.62(4) | | O2 | 2.361(15) | < C1–O > | | 1.27 |
| | O12b | 2.63(2) | | O21b | 2.36(4) | C2 | O6 | 1.269(19) |
| | O14b | 2.67(3) | | O19b | 2.39(3) | | O4 | 1.275(18) |
| | O17b | 2.68(3) | | O12a | 2.41(4) | | O5 | 1.299(18) |
| | O8 | 2.702(12) | | O17a | 2.42(3) | < C2–O > | | 1.28 |
| | O1 | 2.705(12) | | O14a | 2.45(3) | C3 | O8 | 1.271(19) |
| | O7 | 2.710(13) | < Na4–O > | | 2.39/2.36* | | O7 | 1.274(18) |
| | O6 | 2.713(13) | Na5 | O8 | 2.324(14) | | O9 | 1.300(18) |
| | O5 | 2.713(12) | | O21a | 2.36(3) | < C3–O > | | 1.28 |
| | O3 | 2.714(13) | | O4 | 2.364(14) | C4a | O12a | 1.27(5) |
| < Sr1–O > | | 2.66/2.68* | | O3 | 2.373(15) | | O10 | 1.35(4) |
| Sr2 | O10 | 2.51(2) | | O20a | 2.38(3) | | O11a | 1.39(6) |
| | O14a | 2.56(3) | | O19a | 2.43(4) | < C4a–O > | | 1.34 |
| | O21b | 2.58(4) | | O17b | 2.43(3) | C4b | O12b | 1.33(7) |
| | O20b | 2.60(3) | | O14b | 2.43(3) | | O11b | 1.35(7) |
| | O19b | 2.61(3) | | O12b | 2.44(3) | | O10 | 1.46(7) |
| | O17a | 2.61(3) | < Na5–O > | | 2.37/2.39* | < C4b–O > | | 1.38 |
| | O6 | 2.688(13) | Y6 | O1 | 2.327(12) | C5a | O14a | 1.34(11) |
| | O12a | 2.69(3) | | O5 | 2.350(12) | | O13 | 1.38(7) |
| | O9 | 2.692(12) | | O9 | 2.356(12) | | O15a | 1.48(10) |
| | O4 | 2.692(13) | | O18a | 2.36(3) | < C5a–O > | | 1.40 |
| | O2 | 2.695(14) | | O15a | 2.40(3) | C5b | O14b | 1.24(5) |
| | O8 | 2.704(12) | | O11a | 2.40(3) | | O13 | 1.30(4) |
| | O1 | 2.706(12) | | O18b | 2.41(4) | | O15b | 1.38(5) |
| < Sr2–O > | | 2.65/2.65* | | O15b | 2.42(3) | < C5b–O > | | 1.31 |
| La3 | O16 | 2.48(2) | | O11b | 2.47(3) | C6a | O16 | 1.28(5) |
| | O18b | 2.55(3) | | O13 | 2.56(2) | | O17a | 1.36(6) |
| | O15a | 2.59(3) | | O16 | 2.61(2) | | O18a | 1.44(5) |
| | O11a | 2.60(3) | | O10 | 2.61(2) | < C6a–O > | | 1.36 |
| | O15b | 2.61(3) | < Y6–O > | | 2.44/2.46* | C6b | O17b | 1.15(7) |
| | O18a | 2.61(3) | | | | | O16 | 1.37(6) |
| | O11b | 2.64(3) | | | | | O18b | 1.44(7) |
| | O3 | 2.660(13) | | | | < C6b–O > | | 1.32 |
| | O7 | 2.663(13) | | | | | | |
| | O4 | 2.669(13) | | | | | | |
| | O2 | 2.677(13) | | | | | | |
| | O5 | 2.679(12) | | | | | | |
| | O9 | 2.680(12) | | | | | | |
| < La3–O > | | 2.63/2.63* | | | | | | |

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

**Table 6.** Comparative data for alicewilsonite-(YLa) and related mckelveyite group minerals.

| Mineral | Alicewilsonite-(YLa) | Alicewilsonite-(YCe) | Bainbridgeite-(YCe) |
|---|---|---|---|
| Formula | $Na_2Sr_2YLa(CO_3)_6 \cdot 3H_2O$ | $Na_2Sr_2YCe(CO_3)_6 \cdot 3H_2O$ | $Na_2Ba_2YCe(CO_3)_6 \cdot 3H_2O$ |
| Space group | $P1$ | $P1$ | $P1$ |
| $a$, Å | 8.979 | 9.004 | 9.108 |
| $b$, Å | 8.973 | 9.018 | 9.107 |
| $c$, Å | 6.740 | 6.771 | 6.933 |
| $\alpha$, ° | 102.83 | 102.72 | 102.86 |
| $\beta$, ° | 116.38 | 116.40 | 116.15 |
| $\gamma$, ° | 60.11 | 60.00 | 60.18 |
| $V$, Å$^3$ | 421.8 | 426.5 | 447.9 |
| $Z$ | 1 | 1 | 1 |
| $D$, g cm$^{-3}$ | 3.37 (calc.) | 3.37 (calc.) | 3.49 (calc.) |
| Strongest reflections of the PXRD pattern: $d$, Å ($I$) | 6.03 (43) | 6.07 (31) | 6.22 (42) |
| | 4.36 (100) | 4.37 (100) | 4.43 (100) |
| | 4.02 (30) | 4.04 (25) | 4.09 (37) |
| | 3.188 (29) | 3.201 (25) | 3.263 (26) |
| | 2.819 (96) | 2.831 (67) | 2.888 (67) |
| | 2.592 (40) | 2.601 (39) | 2.633 (38) |
| | 2.228 (33) | 2.236 (24) | 2.236 (23) |
| | 2.011(36) | 2.019 (23) | 2.010 (20) |
| | 1.967 (32) | 1.974 (24) | |
| References | This paper | Lykova et al. (2023b) | Lykova et al. (2024) |

*Data availability.* Crystallographic data for alicewilsonite-(YLa) 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-36-301-2024-supplement.

*Author contributions.* IL conceptualised the project. RR collected powder X-ray diffraction data. EMPAs were obtained by GP. HF collected single-crystal X-ray diffraction data. KH obtained the IR spectrum. IL processed the data and interpreted the results. The manuscript was written by IL with contributions from all co-authors.

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

*Disclaimer.* Publisher's note: Copernicus Publications remains neutral with regard to jurisdictional claims made in the text, published maps, institutional affiliations, or any other geographical representation in this paper. While Copernicus Publications makes every effort to include appropriate place names, the final responsibility lies with the authors.

## References

Bayliss, P. and Levinson, A. A.: A system of nomenclature for rare-earth mineral species; revision and extension, Am. Mineral., 73, 422–423, 1988.

Brugger, J., Ogierman, J., Pring, A., Waldron, H., and Kolitsch, U.: Origin of the secondary REE-minerals at the Paratoo copper deposit near Yunta, South Australia, Mineral. Mag., 70, 609–627, 2006.

Chukanov, N. V. and Chervonnyi, A. D.: Infrared Spectroscopy of Minerals and Related Compounds, Springer Cham, Switzerland, 1109 pp., https://doi.org/10.1007/978-3-319-25349-7, 2016.

Gagne, O. C. and Hawthorne, F. C.: Comprehensive derivation of bond-valence parameters for ion pairs in-

volving oxygen, Acta Crystallogr. B, 71, 562–578, https://doi.org/10.1107/s2052520615016297, 2015.

Kasatkin, A. V., Zubkova, N. V., Pekov, I. V., Chukanov, N. V., Škoda, R., Agakhanov, A. A., Belakovskiy, D. I., Britvin, S. N., and Yu. Pushcharovsky, D.: The mineralogy of the historical Mochalin Log REE deposit, South Urals, Russia. Part IV. Alexkuznetsovite-(La), $La_2Mn(CO_3)(Si_2O_7)$, alexkuznetsovite-(Ce), $Ce_2Mn(CO_3)(Si_2O_7)$ and biraite-(La), $La_2Fe^{2+}(CO_3)(Si_2O_7)$, three new isostructural minerals and a definition of the biraite group, Mineral. Mag., 85, 772–783, https://doi.org/10.1180/mgm.2021.64, 2021.

Krivovichev, S.V., Panikorovskii, T.L., Zolotarev, A.A., Bocharov, V.N., Kasatkin, A.V., and Škoda, R.: Jahn-teller distortion and cation ordering: the crystal structure of paratooite-(La), a superstructure of carbocernaite, Minerals, 9, 1–11, https://doi.org/10.3390/min9060370, 2019.

Levinson, A. A.: A system of nomenclature for rare-earth minerals, Am. Mineral., 51, 152–158, 1966.

Lykova, I., Rowe, R., Poirier, G., Giester, G., Ojaste, K., and Friis, H.: Mckelveyite group minerals – Part 1: Nomenclature and new data on donnayite-(Y), Eur. J. Mineral., 35, 133–142, https://doi.org/10.5194/ejm-35-133-2023, 2023a.

Lykova, I., Rowe, R., Poirier, G., Friis, H., and Helwig, K.: Mckelveyite group minerals – Part 2: Alicewilsonite-(YCe), $Na_2Sr_2YCe(CO_3)_6 \cdot 3H_2O$, a new species, Eur. J. Mineral., 35, 143–155, https://doi.org/10.5194/ejm-35-143-2023, 2023b.

Lykova, I., Rowe, R., Poirier, G., Friis, H., and Helwig, K.: Mckelveyite group minerals – Part 3: Bainbridgeite-(YCe), $Na_2Ba_2YCe(CO_3)_6 \cdot 3H_2O$, a new species from Mont Saint-Hilaire, Canada, Eur. J. Mineral., 36, 183–194, https://doi.org/10.5194/ejm-36-183-2024, 2024.

Matsumoto, T., Yamano, A., Sato, T., Ferrara, J. D., White, F. J., and Meyer, M.: "What is This?" A structure analysis tool for rapid and automated solution of small molecule structures, J. Chem. Crystallogr., 51, 438–450, https://doi.org/10.1007/s10870-020-00867-w, 2021.

Nespolo, M. and Ferraris, G.: Twinning by syngonic and metric merohedry. Analysis, classification and effects on the diffraction pattern, Z. Krist.-Cryst. Mater., 215, 77–81, https://doi.org/10.1524/zkri.2000.215.2.77, 2000.

Pring, A., Wallwork, K., Brugger, J., and Kolitsch, U.: Paratooite-(La), a new lanthanum-dominant rare-earth copper carbonate from Paratoo, South Australia, Mineral. Mag., 70, 131–138, 2006.

Rowe, R.: New statistical calibration approach for Bruker AXS D8 Discover microdiffractometer with Hi-Star detector using GADDS software, Powder Diffr., 24, 263–271, https://doi.org/10.1154/1.3193683, 2009.

Sheldrick, G. M.: Crystal structure refinement with SHELXL, Acta Crystallogr. C, 71, 3–8, https://doi.org/10.1107/s2053229614024218, 2015.

Taunton, A. E., Welch, S. A., and Banfield, J. F.: Microbial controls on phosphate and lanthanide distributions during granite weathering and soil formation, Chem. Geol., 169, 371–382, https://doi.org/10.1016/S0009-2541(00)00215-1, 2000.

Wallwork, K., Kolitsch, U., Pring, A., and Nasdala, L.: Decrespignyite-(Y), a new copper yttrium rare earth carbonate chloride hydrate from Paratoo, South Australia, Mineral. Mag., 66, 181–188, https://doi.org/10.1180/0026461026610021, 2002.