## Article



# Zincorietveldite, $Zn(UO_2)(SO_4)_2(H_2O)_5$ , the zinc analogue of rietveldite from the Blue Lizard mine, San Juan County, Utah, USA

### Anthony R. Kampf<sup>1</sup>, Travis A. Olds<sup>2</sup>, Jakub Plášil<sup>3</sup> b and Joe Marty<sup>1</sup>

<sup>1</sup>Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA, USA; <sup>2</sup>Section of Minerals and Earth Sciences, Carnegie Museum of Natural History, 4400 Forbes Avenue, Pittsburgh, PA, USA and <sup>3</sup>Institute of Physics of the CAS, Na Slovance 1999/2, 18200 Prague 8, Czech Republic

#### Abstract

The new mineral zincorietveldite (IMA2022-070), Zn(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>5</sub>, was found in the Blue Lizard mine, San Juan County, Utah, USA, where it occurs as yellow to orange–yellow blades in a secondary assemblage with bobcookite, coquimbite, halotrichite, libbyite, metavoltine, rhomboclase, römerite, tamarugite and voltaite. The streak is very pale yellow. Crystals are transparent with vitreous lustre. The tenacity is brittle, the Mohs hardness is ~2½ and the fracture is curved. Cleavage is excellent on {010}, good on {100} and fair on {001}. The mineral is easily soluble in H<sub>2</sub>O and has a calculated density of 3.376 g·cm<sup>-3</sup>. The mineral is optically biaxial (+) with  $\alpha = 1.568(2)$ ,  $\beta = 1.577(2)$  and  $\gamma = 1.595(2)$ ;  $2V = 70(1)^{\circ}$ . Electron microprobe analyses provided (Zn<sub>0.720</sub>Mg<sub>0.109</sub>Fe<sub>0.091</sub>Mn<sub>0.046</sub>Co<sub>0.035</sub>)<sub>\S1.00</sub>(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>5</sub>. Zincorietveldite is orthorhombic, *Pmn2*<sub>1</sub>, *a* = 12.8712(9), *b* = 8.3148(4), *c* = 11.2959(4) Å, *V* = 1208.90(11) Å<sup>3</sup> and *Z* = 4. Zincorietveldite is the Zn analogue of rietveldite. The structural unit is a uranyl-sulfate chain that is also found in the structures of bobcookite, odpsite, oppenheimerite and svornostite.

**Keywords:** zincorietveldite, rietveldite, new mineral, uranyl sulfate, crystal structure, Raman spectroscopy, Blue Lizard mine, Red Canyon, Utah, USA

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#### Introduction

Uranyl-sulfate minerals are widespread phases found in nearly all sandstone-hosted uranium-vanadium deposits in the southwestern United States, and worldwide. In Red Canyon, Utah, sulfates dominate the secondary uranyl mineralisation occurring on mine walls; in fact, many of the deposits in this region were first located by prospectors who noticed bright yellow and green encrustations on the uranium-bearing layers exposed at the surface. In the decades since mining ceased in Red Canyon, the remaining exposed (and unexposed) ore has undergone numerous periods of dissolution, crystallisation, and fluctuations in humidity and pH, which have led to an explosion in the diversity of uranyl species found underground.

Zincorietveldite, the new mineral described herein, is the 25<sup>th</sup> new mineral to be first described from the Blue Lizard mine in southeast Utah, USA, all within the last 10 years (see, for instance, Plášil *et al.*, 2023; Kampf *et al.*, 2023a). Zincorietveldite is named as the zinc analogue of rietveldite with Zn dominant in each of the two octahedrally coordinated cation sites. The new mineral and name (symbol Zrvd) were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA2022-070, Kampf *et al.*, 2023b). The description is based

Corresponding author: Anthony R. Kampf; Email: akampf@nhm.org

on five cotype specimens, all micromounts, deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue numbers 76262, 76264, 76265, 76266 and 76267. Specimen 76267 is also a cotype for libbyite (Kampf *et al.*, 2023c).

#### Occurrence

Zincorietveldite was found by two of the authors (ARK and JM) in efflorescent crusts on mine walls underground in the Blue Lizard mine (37°33'26"N, 110°17'44"W), Red Canvon, White Canyon District, San Juan County, Utah, USA. The mine is ~72 km west of the town of Blanding, Utah, and ~22 km southeast of Good Hope Bay on Lake Powell. Detailed historical and geological information on the Blue Lizard mine is described elsewhere (e.g. Kampf et al., 2015a), and is primarily derived from a report by Chenoweth (1993). Abundant secondary uranium mineralisation in Red Canyon is associated with post-mining oxidation of asphaltite-rich sandstone beds laced with uraninite and sulfides in the damp underground environment. Zincorietveldite is a relatively rare mineral found in association with bobcookite, coquimbite, halotrichite, libbyite, metavoltine, rhomboclase, römerite, tamarugite, voltaite and other potentially new minerals on matrix comprised mostly of subhedral to euhedral, equant quartz crystals that are recrystallised counterparts of the original grains of the sandstone.

We have also confirmed the occurrence of zincorietveldite at the Widowmaker mine, on Fry Mesa, also in the White Canyon district; however, our description of the species is based solely

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on material from the Blue Lizard mine. The Widowmaker mine should not be considered a cotype locality.

#### Morphology, physical properties and optical properties

Zincorietveldite occurs as subparallel groups of yellow to orangeyellow blades up to  $\sim 1$  mm in length (Fig. 1). Blades are elongate on [001], flattened on {010} and exhibit the forms {100}, {010},  $\{110\}, \{011\}, \{01\overline{1}\}, \{101\}, \{\overline{1}0\overline{1}\}, \{111\} \text{ and } \{11\overline{1}\} \text{ (Fig. 2). No}$ twinning was observed, but merohedral twinning is likely because of the noncentrosymmetric space group. The streak is very pale vellow and the mineral is nonfluorescent. Crystals are transparent with a vitreous lustre. The tenacity is brittle and the fracture is curved. The Mohs hardness is  $\sim 2\frac{1}{2}$  based on scratch tests. There are three cleavages: excellent on {010}, good on {100} and fair on {001}. Crystals sink very slowly in pure methylene iodide  $(3.32 \text{ g} \cdot \text{cm}^{-3})$ . The mineral is soluble in Clerici solution, so the density could not be measured. The calculated density based upon the empirical formula is 3.376 g·cm<sup>-3</sup>. The mineral is easily soluble in room-temperature H<sub>2</sub>O. Zincorietveldite is optically biaxial (+) with  $\alpha = 1.568(2)$ ,  $\beta = 1.577(2)$  and  $\gamma = 1.595(2)$  measured in white light. The 2V measured directly on a spindle stage is 70(1)°; the calculated 2V is 71.2°. Dispersion is strong, r > v. The optical orientation is  $X = \mathbf{b}$ ,  $Y = \mathbf{a}$  and  $Z = \mathbf{c}$ . The mineral is pleochroic with X = yellow, Y = colourless and Z = light yellow; Y < Z < X. The Gladstone-Dale compatibility (Mandarino, 2007) 1 –  $(K_p/K_c)$  is –0.002 (superior) based on the empirical formula using  $k(UO_3) = 0.118$ , as provided by Mandarino (1976).

#### Raman spectroscopy

Raman spectroscopy was done on a Horiba XploRA PLUS micro-Raman spectrometer using an incident wavelength of 532 nm, laser slit of 100  $\mu$ m, 1800 gr/mm diffraction grating and a 100× (0.9 NA) objective. The spectrum, recorded from 4000 to 60 cm<sup>-1</sup>, is shown in Fig. 3.

The spectrum of zincorietveldite is very similar to that of rietveldite and the band assignments indicated in Fig. 3 are the same as those previously proposed for rietveldite (Kampf *et al.*, 2017). Using the empirically derived equation of Libowitzky (1999),



**Figure 1.** Zincorietveldite blades on cotype specimen #76263. The field of view is 1.12 mm across.

the sharp band at 3540 cm<sup>-1</sup> is consistent with hydrogen bond O···O distances of ~2.96 Å. This value matches well with our proposed hydrogen bonding scheme for which 14 of the 18 O···O distances are in the range 2.92 to 3.00 Å (see Table 4). According to the empirical relationship of Bartlett and Cooney (1989), the v<sub>1</sub> UO<sub>2</sub><sup>2+</sup> band at 860 cm<sup>-1</sup> corresponds to a U-O<sub>Ur</sub> bond length of ~1.75 Å, in excellent agreement with U-O<sub>Ur</sub> bond lengths from the X-ray data: 1.750(6) and 1.766(6) Å.



Figure 2. Crystal drawing of zincorietveldite; clinographic projection.



Figure 3. Raman spectrum of zincorietveldite recorded using a 532 nm diode laser.

#### **Chemical composition**

Electron probe microanalyses (6 points) were done using a JEOL JXA-8230 electron microprobe operating in wavelength dispersive spectroscopy mode using *Probe for EPMA* software (https://www.probesoftware.com). Analytical conditions were 15 kV accelerating voltage, 1 nA beam current and a beam diameter of 10  $\mu$ m. Because insufficient material is available for a direct determination of H<sub>2</sub>O, it has been calculated based upon the structure determination (S = 2 and O = 15 atoms per formula unit). The analytical results are given in Table 1.

The empirical formula (based on 15 O apfu) is  $(Zn_{0.675} Mg_{0.102}Fe_{0.085}Mn_{0.043}Co_{0.033})_{\Sigma 0.938}(U_{1.028}O_2)(SO_4)_2(H_{1.991}O)_5$ . Adjusting for full occupancy of the Zn and U sites, the empirical

| Table 1. Analytica | l data (i | n wt.%) f | for zincorietveldite. |
|--------------------|-----------|-----------|-----------------------|
|--------------------|-----------|-----------|-----------------------|

| Constituent       | Mean   | Range       | S.D.  | Probe standard  |
|-------------------|--------|-------------|-------|-----------------|
| MgO               | 0.68   | 0.65-0.70   | 0.033 | MgO             |
| MnO               | 0.50   | 0.37-0.62   | 0.104 | spessartine     |
| FeO               | 1.01   | 0.65-1.28   | 0.231 | hematite        |
| CoO               | 0.41   | 0.27-0.55   | 0.114 | Co metal        |
| ZnO               | 9.10   | 8.28-9.59   | 0.526 | ZnS             |
| SO <sub>3</sub>   | 26.53  | 24.78-28.14 | 1.148 | anhydrite       |
| UO <sub>3</sub>   | 48.73  | 46.26-50.26 | 1.394 | UO <sub>2</sub> |
| H <sub>2</sub> O* | 14.86  |             |       |                 |
| Total             | 101.82 |             |       |                 |
|                   |        |             |       |                 |

\* Based on structure

S.D. - standard deviation

Table 2. Data collection and structure refinement details for zincorietveldite.

| Crystal data   |  |
|--|--|
| Structural formula                                     | $(Zn_{0.88}Mg_{0.12})_{\Sigma 1.00}US_2O_{15}$         |
| Space group  | Pmn2 <sub>1</sub> (#31)                                |
| Unit cell dimensions (Å)                               | <i>a</i> = 12.8712(9)                                  |
|  | b = 8.3148(4)  |
|  | <i>c</i> = 11.2959(4)                                  |
| V (Å <sup>3</sup> )                                    | 1208.90(11)  |
| Z  | 4  |
| Density (for above formula) (g·cm <sup>-3</sup> )      | 3.365  |
| Absorption coefficient (mm <sup>-1</sup> )             | 15.553   |
| Data collection  |  |
| Diffractometer   | Rigaku R-Axis Rapid II                                 |
| X-ray radiation/power                                  | $MoK\alpha$ ( $\lambda = 0.71075$ Å)/50 kV, 40 mA      |
| Temperature (K)  | 293(2)   |
| F(000)   | 1127   |
| Crystal size (µm)                                      | 190 × 80 × 20  |
| θ range (°)  | 3.04 to 27.48  |
| Index ranges   | $-14 \le h \le 16, -10 \le k \le 10, -12 \le l \le 14$ |
| Reflections collected/unique                           | 6954/2485; R <sub>int</sub> = 0.035                    |
| Reflections with $l > 2\sigma l$                       | 2174   |
| Completeness to $\theta = 27.48^{\circ}$               | 99.7%  |
| Refinement   |  |
| Refinement method                                      | Full-matrix least-squares on F <sup>2</sup>            |
| Parameter/restraints                                   | 189/1  |
| GoF  | 1.074  |
| Final R indices $[l > 2\sigma l]$                      | $R_1 = 0.0308, wR_2 = 0.0683$                          |
| R indices (all data)                                   | $R_1 = 0.0361, wR_2 = 0.0716$                          |
| Absolute structure parameter                           | 0.000(9)   |
| Largest diff. peak/hole ( <i>e</i> – Å <sup>–3</sup> ) | +4.45/-0.99  |

$$\begin{split} R_{\text{int}} &= \Sigma |F_o^2 - F_o^2(\text{mean})| / \Sigma [F_o^2]. \text{ GoF} = S = \{\Sigma [w(F_o^2 - F_o^2)^2] / (n-p)\}^{V_0}. R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|. wR_2 = \{\Sigma [w(F_o^2 - F_o^2)^2] / \Sigma [w(F_o^2)^2]\}^{V_2}; w = 1 / [\sigma^2 (F_o^2) + (aP)^2 + bP] \text{ where } a \text{ is } 0.0325, b \text{ is } 0.5911 \text{ and } P \text{ is } [2F_c^2 + \text{Max} (F_o^2, 0)]/3. \end{split}$$

Table 3. Atom coordinates and displacement parameters  $(Å^2)$  for zincorietveldite.

|      | x/a         | y/b        | z/c         | U <sub>eq</sub> | U <sup>11</sup> | U <sup>22</sup> | U <sup>33</sup> | U <sup>23</sup> | U <sup>13</sup> | U <sup>12</sup> |
|------|-------------|------------|-------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Zn1* | 0           | 0.6777(3)  | 0.28060(17) | 0.0263(8)       | 0.0134(10)      | 0.0395(16)      | 0.0260(13)      | 0.0072(9)       | 0               | 0               |
| Zn2* | 1/2         | 0.6643(2)  | 0.24863(16) | 0.0204(7)       | 0.0155(10)      | 0.0253(13)      | 0.0204(11)      | 0.0011(8)       | 0               | 0               |
| U    | 0.24791(2)  | 0.88701(3) | 0.93401(15) | 0.01318(13)     | 0.01588(19)     | 0.01445(19)     | 0.00921(19)     | 0.0009(3)       | -0.00065(17)    | -0.00114(11     |
| S1   | 0.2737(2)   | 0.7625(4)  | 0.6263(3)   | 0.0178(6)       | 0.0223(10)      | 0.0214(15)      | 0.0097(13)      | 0.0008(11)      | 0.0003(14)      | 0.0011(11)      |
| S2   | 0.24643(15) | 0.7436(4)  | 0.2456(3)   | 0.0139(6)       | 0.0161(12)      | 0.0144(15)      | 0.0112(15)      | 0.0006(11)      | 0.0008(9)       | -0.0007(8)      |
| 01   | 0.1607(5)   | 0.7507(11) | 0.6238(8)   | 0.0343(18)      | 0.019(3)        | 0.051(5)        | 0.033(4)        | -0.001(4)       | 0.000(4)        | -0.011(3)       |
| 02   | 0.3250(7)   | 0.6194(8)  | 0.5794(8)   | 0.036(2)        | 0.048(5)        | 0.020(5)        | 0.041(5)        | -0.009(4)       | 0.001(4)        | 0.012(3)        |
| 03   | 0.3103(6)   | 0.9011(8)  | 0.5553(7)   | 0.0317(19)      | 0.037(5)        | 0.022(5)        | 0.037(5)        | 0.014(3)        | 0.001(4)        | 0.005(3)        |
| 04   | 0.3133(5)   | 0.7867(9)  | 0.7503(5)   | 0.0279(18)      | 0.030(4)        | 0.047(5)        | 0.007(3)        | -0.002(3)       | -0.010(3)       | -0.004(3)       |
| 05   | 0.3376(6)   | 0.6417(9)  | 0.2524(8)   | 0.031(2)        | 0.020(4)        | 0.022(4)        | 0.052(6)        | 0.008(4)        | -0.001(4)       | 0.002(3)        |
| 06   | 0.2674(7)   | 0.8970(12) | 0.3040(12)  | 0.041(3)        | 0.048(6)        | 0.040(7)        | 0.034(7)        | -0.016(4)       | -0.004(5)       | -0.004(4)       |
| 07   | 0.1602(6)   | 0.6624(11) | 0.3040(7)   | 0.033(2)        | 0.020(4)        | 0.050(5)        | 0.028(5)        | 0.019(4)        | 0.006(4)        | -0.001(3)       |
| 08   | 0.2171(6)   | 0.7758(9)  | 0.1221(7)   | 0.0296(16)      | 0.043(3)        | 0.032(5)        | 0.015(3)        | 0.005(3)        | 0.003(4)        | -0.002(4)       |
| 09   | 0.1184(5)   | 0.8428(9)  | 0.8997(6)   | 0.0234(15)      | 0.021(3)        | 0.034(4)        | 0.015(3)        | -0.009(3)       | 0.001(3)        | -0.004(3)       |
| 010  | 0.3786(5)   | 0.9331(8)  | 0.9678(6)   | 0.0269(17)      | 0.025(3)        | 0.025(4)        | 0.031(4)        | -0.010(3)       | 0.001(3)        | -0.007(3)       |
| OW1  | 0.2884(7)   | 0.5950(8)  | 0.9473(9)   | 0.0350(19)      | 0.061(5)        | 0.019(4)        | 0.025(5)        | 0.003(3)        | 0.012(6)        | -0.001(3)       |
| OW2  | 0           | 0.6385(19) | 0.0970(16)  | 0.056(5)        | 0.038(8)        | 0.085(12)       | 0.044(10)       | -0.002(8)       | 0               | 0               |
| OW3  | 0           | 0.7112(15) | 0.4649(9)   | 0.035(3)        | 0.021(5)        | 0.066(9)        | 0.018(7)        | -0.015(5)       | 0               | 0               |
| OW4  | 0           | 0.9259(17) | 0.2402(16)  | 0.060(5)        | 0.041(7)        | 0.030(8)        | 0.108(14)       | -0.003(8)       | 0               | 0               |
| OW5  | 0           | 0.4130(19) | 0.2895(16)  | 0.044(4)        | 0.027(6)        | 0.059(9)        | 0.045(9)        | -0.012(8)       | 0               | 0               |
| OW6  | 1/2         | 0.6355(16) | 0.0670(13)  | 0.036(4)        | 0.042(8)        | 0.044(8)        | 0.024(7)        | 0.009(5)        | 0               | 0               |
| OW7  | 0           | 0.5845(16) | 0.7677(14)  | 0.036(4)        | 0.032(7)        | 0.026(7)        | 0.051(10)       | -0.007(6)       | 0               | 0               |
| OW8  | 1/2         | 0.7151(15) | 0.4277(14)  | 0.047(3)        | 0.034(5)        | 0.087(10)       | 0.019(6)        | -0.013(8)       | 0               | 0               |
| OW9  | 1/2         | 0.9138(13) | 0.2119(12)  | 0.033(3)        | 0.032(6)        | 0.024(6)        | 0.041(8)        | -0.004(5)       | 0               | 0               |

\* Refined occupancies: Zn1 = Zn<sub>0.875(14)</sub>Mg<sub>0.125(14)</sub>; Zn2 = Zn<sub>0.856(13)</sub>Mg<sub>0.144(13)</sub>

Table 4. Selected bond distances (Å) for zincorietveldite.

| Zn1–07 (×2)     | 2.083(7)  | U-09                      | 1.750(6)  | S1-01         | 1.458(6)  | Hydrogen bonds           |           |
|-----------------|-----------|---------------------------|-----------|---------------|-----------|--------------------------|-----------|
| Zn1–OW2         | 2.099(18) | U-010                     | 1.766(6)  | S1-02         | 1.461(7)  | OW102                    | 2.745(12) |
| Zn1-OW3         | 2.101(10) | U-06                      | 2.328(10) | S1-03         | 1.481(8)  | OW107                    | 2.764(12) |
| Zn1–OW4         | 2.114(14) | U-08                      | 2.351(8)  | S1-04         | 1.504(7)  | OW2 <sup></sup> O9 (×2)  | 3.190(17) |
| Zn1-OW5         | 2.204(16) | U-03                      | 2.354(7)  | <\$1-0>       | 1.459     | OW301 (×2)               | 2.758(10) |
| <zn1-0></zn1-0> | 2.114     | U-04                      | 2.390(7)  |               |           | OW4 <sup></sup> O10 (×2) | 3.229(16) |
|                 |           | U-OW1                     | 2.488(7)  | S2-05         | 1.450(8)  | OW5 <sup></sup> O4 (×2)  | 2.954(12) |
| Zn2–OW6         | 2.065(15) | <u-0<sub>Ur&gt;</u-0<sub> | 1.758     | S2-07         | 1.457(8)  | OW6 <sup></sup> O10 (×2) | 3.134(13) |
| Zn2–OW8         | 2.067(15) | <u-o<sub>eg&gt;</u-o<sub> | 2.382     | S2-06         | 1.461(10) | OW701 (×2)               | 2.971(13) |
| Zn2–OW7         | 2.079(14) | -1                        |           | S2-08         | 1.469(9)  | OW8 <sup></sup> O2 (×2)  | 2.940(13) |
| Zn2–05 (×2)     | 2.099(8)  |                           |           | <s2-0></s2-0> | 1.476     | OW9 <sup></sup> O10 (×2) | 3.174(14) |
| Zn2–OW9         | 2.116(11) |                           |           |               |           |                          |           |
| <zn2-0></zn2-0> | 2.088     |                           |           |               |           |                          |           |

formula is  $(Zn_{0.720}Mg_{0.109}Fe_{0.091}Mn_{0.046}Co_{0.035})_{\Sigma1.00}(UO_2)$  $(SO_4)_2(H_2O)_5$ . The simplified formula is (Zn,Mg,Fe,Mn,Co) $(UO_2)(SO_4)_2(H_2O)_5$ . The ideal formula is  $Zn(UO_2)(SO_4)_2$  $(H_2O)_5$ , which requires ZnO 13.18, UO<sub>3</sub> 46.31, SO<sub>3</sub> 25.93,  $H_2O$  14.58, total 100 wt.%.

#### X-ray crystallography

Powder X-ray diffraction (PXRD) data were recorded using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer with monochromatised MoK $\alpha$  radiation. A Gandolfi-like motion on the  $\varphi$  and  $\omega$  axes was used to randomise the sample. Observed *d* values and intensities were derived by profile fitting using *JADE Pro* software (Materials Data, Inc.). The powder data are presented in Supplementary Table S1 (see below). The unit-cell parameters refined from the powder data using *JADE Pro* with whole pattern fitting are *a* = 12.871(3), *b* = 8.343(2), *c* = 11.314(2) Å and *V* = 1214.9(4) Å<sup>3</sup>.

The single-crystal structure data were collected at room temperature using the same diffractometer and radiation noted above. The Rigaku CrystalClear software package was used for processing the structure data, including the application of an empirical absorption correction using the multi-scan method with ABSCOR (Higashi, 2001). The structure was solved using the intrinsic-phasing algorithm of SHELXT (Sheldrick, 2015a). SHELXL-2016 (Sheldrick, 2015b) was used for the refinement of the structure. The structure solution located all non-hydrogen atoms, which were refined with anisotropic displacement parameters. The Zn1 and Zn2 sites were refined with joint occupancies by Zn and Mg yielding Zn<sub>0.875</sub>Mg<sub>0.125(14)</sub> and Zn<sub>0.856</sub>Mg<sub>0.144(13)</sub>, respectively. These correspond to site scattering values of 55.500 and 54.816, respectively, for a total site scattering of 110.316. For comparison, the total site-scattering value corresponding to full site occupancies with the cation ratios indicated by the electron probe microanalyses is 109.476. The H atoms locations could not be found in the difference-Fourier maps. The two largest electron density residuals, 4.44 and 3.55 e<sup>-</sup>, located 0.89 and 0.87 Å from the U site, respectively, are presumed to be ripple effects. Data collection and refinement details are given in Table 2,

|     |                     |                     |      |      |      | Hydrogen         | bonds                | Σ     |
|-----|---------------------|---------------------|------|------|------|------------------|----------------------|-------|
|     | Zn1                 | Zn2                 | U    | S1   | S2   | Accepted         | Donated              | 2     |
| 01  |                     |                     |      | 1.55 |      | 0.20, 0.14       |                      | 1.89  |
| 02  |                     |                     |      | 1.54 |      | 0.21, 0.14       |                      | 1.89  |
| 03  |                     |                     | 0.52 | 1.47 |      |                  |                      | 1.99  |
| 04  |                     |                     | 0.48 | 1.39 |      | 0.14             |                      | 2.01  |
| 05  |                     | 0.34 <sup>×2↓</sup> |      |      | 1.59 |                  |                      | 1.92  |
| 06  |                     |                     | 0.55 |      | 1.54 |                  |                      | 2.09  |
| 07  | 0.35 <sup>×2↓</sup> |                     |      |      | 1.56 | 0.20             |                      | 2.11  |
| 08  |                     |                     | 0.52 |      | 1.51 |                  |                      | 2.03  |
| 09  |                     |                     | 1.87 |      |      | 0.10             |                      | 1.97  |
| O10 |                     |                     | 1.81 |      |      | 0.10, 0.10, 0.11 |                      | 2.12  |
| OW1 |                     |                     | 0.39 |      |      |                  | -0.21, -0.20         | -0.02 |
| OW2 | 0.34                |                     |      |      |      |                  | -0.10 <sup>×2→</sup> | 0.14  |
| OW3 | 0.34                |                     |      |      |      |                  | -0.20 <sup>×2→</sup> | -0.06 |
| OW4 | 0.33                |                     |      |      |      |                  | -0.10 <sup>×2→</sup> | 0.13  |
| OW5 | 0.26                |                     |      |      |      |                  | -0.14 <sup>×2→</sup> | -0.02 |
| OW6 |                     | 0.37                |      |      |      |                  | -0.11 <sup>×2→</sup> | 0.15  |
| OW7 |                     | 0.36                |      |      |      |                  | -0.14 <sup>×2→</sup> | 0.08  |
| OW8 |                     | 0.37                |      |      |      |                  | -0.14 <sup>×2→</sup> | 0.09  |
| OW9 |                     | 0.32                |      |      |      |                  | -0.10 <sup>×2→</sup> | 0.12  |
| Σ   | 1.97                | 2.10                | 6.14 | 5.95 | 6.20 |                  |                      |       |

Table 5. Bond valence analysis for zincorietveldite. Values are expressed in valence units.\*

U<sup>+6</sup>-O and S<sup>+6</sup>-O bond-valence parameters from Gagné and Hawthorne (2015). Hydrogen-bond strengths based on O-O bond lengths from Ferraris and Ivaldi (1988). Negative values indicate donated hydrogen-bond contributions.

atom coordinates and displacement parameters in Table 3, selected bond distances in Table 4 and a bond-valence analysis in Table 5. The crystallographic information file has been deposited with the Principal Editor of *Mineralogical Magazine* and is available as Supplementary material (see below).

#### **Description of the structure**

Zincorietveldite is isostructural with rietveldite. The U site in the structure is surrounded by seven O atoms forming a squat  $UO_7$  pentagonal bipyramid. This is the most typical coordination for  $U^{6+}$ , particularly in uranyl sulfates, where the two short apical bonds of the bipyramid constitute the uranyl group. Four of the five equatorial O atoms of the  $UO_7$  bipyramid participate in  $SO_4$  tetrahedra; the other is an  $H_2O$  group. The linkages of pentagonal bipyramids and tetrahedra form an infinite  $[(UO_2)(SO_4)_2(H_2O)]^{2-}$  chain along [001] (Fig. 4). The chains are linked in the [100] direction by  $Zn1O_2(H_2O)_4$  and  $Zn2O_2(H_2O)_4$  octahedra, which share O vertices with  $SO_4$  tetrahedra in the chains (Fig. 5). A heteropolyhedral sheet parallel to {010} is thereby formed. Adjacent sheets are linked only by hydrogen bonding (Fig. 4).

The  $[(UO_2)(SO_4)_2(H_2O)]^{2-}$  chain in the structures of rietveldite and zincorietveldite is also found in the structures of bobcookite, Na(H<sub>2</sub>O)<sub>2</sub>Al(H<sub>2</sub>O)<sub>6</sub>[(UO<sub>2</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>]·8H<sub>2</sub>O (Kampf *et al.* 2015a), oldsite, K<sub>2</sub>Fe[(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>]<sub>2</sub>·8H<sub>2</sub>O (Plášil *et al.*, 2023), oppenheimerite, Na<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>[(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>]<sub>2</sub>·8H<sub>2</sub>O (Plášil *et al.*, 2015b), svornostite, K<sub>2</sub>Mg[(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>]<sub>2</sub>·8H<sub>2</sub>O (Plášil *et al.* 2015b), synthetic K<sub>2</sub>[(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)](H<sub>2</sub>O) (Ling *et al.*, 2010) and synthetic Mn(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>5</sub> (Tabachenko *et al.*, 1979). The chains in bobcookite and oppenheimerite are geometrical isomers of the chain in the structures of oldsite, rietveldite and zincorietveldite.

Studies of the synthetic phases of general formula  $M(UO_2)$  (SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>5</sub>, in which M = Mg, Mn, Fe, Co, Ni, Cu, Zn or Cd (Kornyakov *et al.*, 2021; Serezhkin and Serezhkina, 1978; Soares Rocha, 1960; Tabachenko *et al.*, 1979), show that these phases occur in two polytypes (Table 6). Rietveldite and zincorietveldite



Figure 4. The structure of zincorietveldite viewed down [100]. Hydrogen bonds are shown as black lines. The unit-cell outline is shown by dashed lines.



Figure 5. The structure of zincorietveldite viewed down [010]. Hydrogen bonds are shown as black lines. The unit-cell outline is shown by dashed lines

Table 6. Comparison of related minerals and synthetic phases.

| Phase   | Polytype   | Space group       | a (Å)  | b (Å)  | c (Å)  | β (°)  | Reference                       |
|---|------------|-------------------|--------|--------|--------|--------|---------------------------------|
| Zincorietveldite  | 20         | Pmn2 <sub>1</sub> | 12.871 | 8.315  | 11.296 |        | This work                       |
| Rietveldite   | 20         | $Pmn2_{1}$        | 12.958 | 8.318  | 11.297 |        | Kampf <i>et al.</i> (2017)      |
| $Zn(UO_{2})(SO_{4})_{2}(H_{2}O)_{5}$  | 20         | $Pmn2_{1}$        | 12.869 | 8.282  | 11.292 |        | Kornyakov et al. (2021)         |
| Fe(UO <sub>2</sub> )(SO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>5</sub> | 20         | $Pmn2_{1}$        | 12.958 | 11.28  | 8.297  |        | Kornyakov et al. (2021)         |
| Fe(UO <sub>2</sub> )(SO <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>5</sub> | 1 <i>M</i> | P21               | 6.489  | 11.28  | 8.297  | 90.78  | Serezhkin and Serezhkina (1978) |
| $Mg(UO_2)(SO_4)_2(H_2O)_5$  | 1 <i>M</i> | P21               | 6.388  | 11.304 | 8.231  | 90.345 | Kornyakov et al. (2021)         |
| $Co(UO_2)(SO_4)_2(H_2O)_5$  | 20         | Pmn21             | 12.920 | 8.299  | 11.296 |        | Kornyakov et al. (2021)         |
| $Mn(UO_2)(SO_4)_2(H_2O)_5$  | 1 <i>M</i> | P21               | 6.511  | 11.383 | 8.344  | 90.773 | Kornyakov et al. (2021)         |

are isostructural with the synthetic phases with space group  $Pmn2_1$  and have double the *a* cell parameter of the phases with space group  $P2_1$ .

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