

## New mineral names\*

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### CALCIOPETERSITE\*

J. Sejkora, P. Novotný, M. Novák, V. Šrein, P. Berlepsch (2005)  
Calciopetersite from Domašov nad Bystřicí, northern Moravia, Czech Republic, a new mineral species of the mixite group. *Can. Mineral.*, 43, 1393–1400.

Calciopetersite forms translucent to transparent minute acicular crystals, up to 0.4 mm in length and 5–20 μm in width, with a hexagonal outline, clustered in fine radiating sprays (up to 0.1–0.5 mm). The mineral is brittle and soft (hardness not measured), olive green, light olive green streak, vitreous, nonfluorescent, with uneven fracture and no observed cleavage. Calciopetersite is pleochroic, light green with yellowish tint (O) to dark green (E), uniaxial positive with  $\omega$  1.674(5) and  $\epsilon > 1.739$  (~1.75) in Na light (590 nm). An average of eight electron microprobe analyses gave K<sub>2</sub>O 0.09, CaO 4.39, CuO 51.25, Y<sub>2</sub>O<sub>3</sub> 1.61, La<sub>2</sub>O<sub>3</sub> 0.64, Ce<sub>2</sub>O<sub>3</sub> 1.98, Pr<sub>2</sub>O<sub>3</sub> 0.25, Nd<sub>2</sub>O<sub>3</sub> 1.40, Dy<sub>2</sub>O<sub>3</sub> 0.33, Yb<sub>2</sub>O<sub>3</sub> 0.21, Bi<sub>2</sub>O<sub>3</sub> 0.09, SiO<sub>2</sub> 0.52, P<sub>2</sub>O<sub>5</sub> 20.98, As<sub>2</sub>O<sub>5</sub> 2.70, H<sub>2</sub>O (calc.) 12.45, sum 98.89 wt%, corresponding to (Ca<sub>0.58</sub>Y<sub>0.13</sub>Ce<sub>0.11</sub>Nd<sub>0.08</sub>La<sub>0.04</sub>K<sub>0.02</sub>Dy<sub>0.02</sub>Pr<sub>0.01</sub>Yb<sub>0.01</sub>)<sub>Σ1.00</sub>(Cu<sub>5.90</sub>Ca<sub>0.14</sub>)<sub>Σ6.04</sub>[(PO<sub>4</sub>)<sub>2.06</sub>(PO<sub>3</sub>OH)<sub>0.65</sub>(AsO<sub>4</sub>)<sub>0.22</sub>(SiO<sub>4</sub>)<sub>0.08</sub>]<sub>Σ3.01</sub>(OH)<sub>6</sub>·3.00 H<sub>2</sub>O on the basis of 21 anions, ideally CaCu<sub>6</sub>[(PO<sub>4</sub>)<sub>2</sub>(PO<sub>3</sub>OH)](OH)<sub>6</sub>·3H<sub>2</sub>O.

A single-crystal X-ray study showed the mineral to be a member of the mixite group: hexagonal, space group *P6<sub>3</sub>/m* (inferred),  $a = 13.3045(18)$ ,  $c = 5.8711(8)$  Å,  $V = 900.0(4)$  Å<sup>3</sup>, but did not permit refinement of a structure model to an acceptable level of precision. Powder diffraction data were collected with a Philips APD diffractometer (3–66° 2θ, CuKα radiation) and yielded refined unit cell parameters  $a = 13.284(4)$  Å,  $c = 5.902(4)$  Å,  $V = 902.0(6)$  Å<sup>3</sup>, and the strongest lines [ $d$  in Å ( $I, hkl$ ): 11.51 (100,100), 4.346 (88,210), 4.140 (46,201), 3.837 (38,300), 3.321 (44,220), 3.184 (35,130), 2.888 (53,221), 2.877 (37,400), 2.510 (37,140), and 1.965 (31,322)]. Density was not measured;  $D_{\text{calc}} = 3.337$  for the empirical formula, 3.179 g/cm<sup>3</sup> for the idealized formula and  $Z = 2$ . The infrared absorption spectrum (<0.05 mg sample in KBr) is interpreted to be consistent with the presence of H<sub>2</sub>O, PO<sub>4</sub><sup>3-</sup>, and PO<sub>3</sub>OH<sup>2-</sup>.

Calciopetersite occurs in cavities in quartz veins in an abandoned quarry near Domašov nad Bystřicí, 20 km northeast of

Olomouc, northern Moravia, Czech Republic. It forms as a result of the weathering of chalcopyrite and other copper sulfides, and is associated with chrysocolla, a Ce-dominant analogue of petersite-(Y), malachite, allophane, goethite, lepidocrocite, chalcopyrite, pyrite, covellite, chalcocite and quartz. The name is derived from its composition and relationship to petersite-(Y), YCu<sub>6</sub>[(PO<sub>4</sub>)<sub>3</sub>](OH)<sub>6</sub>·3H<sub>2</sub>O. The holotype specimen is deposited in the mineralogical collection of the Natural History Museum, National Museum, Prague, Czech Republic, under the number P1p–20/2000. The mineral corresponds to IMA mineral no. 2001-004.

**Discussion.** The atomic proportions of Si in the empirical formula are misstated in the abstract and in the text of the paper; the corrected value is given above. **A.J.L.**

### Cu<sub>8</sub>(OH)<sub>12</sub>(SiO<sub>4</sub>)·8H<sub>2</sub>O

K. Walenta, T. Theye, T. (2005) A new copper silicate mineral from the Clara mine, Central Black Forest. *Der Erzgräber*, 19, 1–4 (in German with English abstract).

The secondary mineral was found on the dumps of the Clara mine, Central Black Forest, Germany. It forms bluish green to turquoise crusts on fluorite and quartz; the latter contains partially corroded galena. The crusts are fine-grained, with angular fragments seen at high magnification, and are partly composed of spherulitic aggregates with a maximum diameter of 10 μm. The mineral has a bluish green to turquoise streak, is translucent, has a vitreous luster, and no discernible cleavage. The hardness could not be determined accurately, but is estimated to be approximately 2. The mineral is optically isotropic or weakly birefringent,  $n_{\text{mean}} = 1.735 \pm 0.003$ . The spherulitic aggregates show a radiating internal structure, with negative optical elongation. The optical properties infer cubic symmetry if the weak birefringence is considered as anomalous.

Electron microprobe analyses (H<sub>2</sub>O by difference) gave CuO 63.9, PbO 7.09, SiO<sub>2</sub> 4.15, SO<sub>3</sub> 0.52, H<sub>2</sub>O 24.34, sum 100.00 wt%, corresponding to the empirical formula Cu<sub>8.23</sub>Pb<sub>0.33</sub>Si<sub>0.71</sub>S<sub>0.07</sub>H<sub>27.67</sub>O<sub>24</sub>, on the basis of 24 O atoms. Neglecting Pb and S, the idealized formula is Cu<sub>8</sub>(OH)<sub>12</sub>(SiO<sub>4</sub>)·8H<sub>2</sub>O for  $Z = 4$ ,  $D_{\text{calc}} = 3.74$  g/cm<sup>3</sup>.

The strongest lines of the unindexed powder pattern (57.3 mm camera, FeKα radiation, intensities visually estimated) include 3.04(10), 2.74(3), 2.50(0.5), 2.15(3), 1.890(1), 1.573(10). The pattern shows relations to those of andradite and pyrochlore, and can be indexed on the basis of a cubic cell with  $a = 12.20$  Å. However, the imperfect agreement between measured and

\* Before publication, minerals marked with an asterisk were approved by the Commission on New Minerals and Mineral Names, International Mineralogical Association.

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calculated *d*-spacings may indicate a pseudocubic cell. Lack of suitable material precluded a full and more accurate description of the mineral, and therefore the authors did not submit a proposal to the CNMMN IMA. **U.K.**

**FLUOROPARGASITE\***

M.V. Lupulescu, J. Rakovan, G.W. Robinson, J.M. Hughes (2005) Fluoropargasite, a new member of the calcic amphiboles from Edenville, Orange County, New York. *Can. Mineral.*, 43, 1423–1428.

Fluoropargasite occurs as stubby prismatic crystals up to 13 cm in dimension. The mineral is brittle, has Mohs hardness of ~6, is transparent to translucent in very thin fragments, black, gray to greenish gray streak, vitreous, nonfluorescent, with perfect {110} cleavage and a conchoidal fracture. Fluoropargasite is biaxial positive, with  $\alpha = 1.634(2)$ ,  $\beta = 1.642(2)$ ,  $\gamma = 1.654(2)$ ,  $2V_{\text{meas}} = 68^\circ$ ,  $2V_{\text{calc}} = 79^\circ$ ,  $Y = b$  and  $Z \wedge c = 24^\circ$  (acute), dispersion  $r > v$ , weak, pleochroic:  $X =$  colorless to light brown,  $Y =$  light brown, and  $Z =$  brown. An average of six electron microprobe analyses of the type material gave SiO<sub>2</sub> 43.30, MgO 14.44, FeO 9.73, CaO 12.29, Al<sub>2</sub>O<sub>3</sub> 12.11, Na<sub>2</sub>O 2.88, TiO<sub>2</sub> 0.90, MnO 0.08, K<sub>2</sub>O 0.91, V<sub>2</sub>O<sub>3</sub> 0.18, Cr<sub>2</sub>O<sub>3</sub> 0.01, F 2.71, Cl 0.12, O = (F + Cl) – 1.17, H<sub>2</sub>O (calc.) 0.71, sum 99.20 wt%, corresponding to (Na<sub>0.75</sub> K<sub>0.17</sub>)<sub>Σ0.92</sub>(Ca<sub>1.94</sub>Na<sub>0.06</sub>)<sub>Σ2</sub>(Mg<sub>3.18</sub>Fe<sub>1.18</sub>Al<sub>0.50</sub>Ti<sub>0.10</sub>Fe<sub>0.02</sub>V<sub>0.02</sub>Mn<sub>0.01</sub>)<sub>Σ5</sub>(Si<sub>6.39</sub>Al<sub>1.61</sub>)<sub>Σ8</sub>O<sub>22</sub>[F<sub>1.26</sub>(OH)<sub>0.71</sub>Cl<sub>0.03</sub>]<sub>Σ2</sub>, determined on the basis of 13 cations and 24 anions (Schumacher 1997; *Can. Mineral.*, 35, 238–246) with Fe<sup>3+</sup> and OH calculated by stoichiometry, ideally NaCa<sub>2</sub>(Mg<sub>4</sub>Al)Si<sub>6</sub>Al<sub>2</sub>O<sub>22</sub>F<sub>2</sub>.

Single crystal X-ray structure study ( $R_1 = 0.019$ ) showed the mineral to be a member of the calcic amphibole subgroup of the amphibole group: monoclinic, space group *C2/m*,  $a = 9.8771(6)$ ,  $b = 18.041(1)$ ,  $c = 5.3092(3)$  Å,  $\beta = 105.133(1)^\circ$ ,  $V = 913.25(3)$  Å<sup>3</sup>. Powder diffraction data were collected with a Scintag X-2 diffractometer (quartz internal standard, CuK $\alpha$  radiation) and yielded refined unit cell parameters  $a = 9.879(2)$ ,  $b = 18.043(2)$ ,  $c = 5.308(1)$  Å,  $\beta = 105.13(1)^\circ$ ,  $V = 913.4$  Å<sup>3</sup>, and the strongest lines [ $d$  in Å ( $hkl$ ): 8.44 (100,110), 3.38 (19,131), 3.28 (41,240), 3.13 (80,310), 3.04 (16,311), 2.810 (32,330), 2.746 (17,331), 2.706 (19,151), 2.385 (21,350), and 2.345 (41,351)]. Density was measured by gas displacement using an AccuPyc 1330 (helium):  $D_{\text{meas}} = 3.18$ ,  $D_{\text{calc}} = 3.20$  for the empirical formula, and 3.05 g/cm<sup>3</sup> for the ideal formula and  $Z = 2$ .

The type locality of fluoropargasite is the Franklin Marble, at Edenville, Orange County, New York. It has also been identified from Russell, St. Lawrence County, and Monroe, Orange County, New York. It occurs in granulite-facies metacarbonates of late Precambrian age, and is associated with calcite, actinolite, titanite, phlogopite and diopside. The name is for the composition and the relationship to pargasite, NaCa<sub>2</sub>(Mg<sub>4</sub>Al)Si<sub>6</sub>Al<sub>2</sub>O<sub>22</sub>(OH)<sub>2</sub>. The holotype specimen is deposited in the mineral collection at the New York State Museum (NYSM 338.92). The mineral corresponds to IMA mineral No. 2003-050.

**Discussion.** Minor rounding errors in the empirical formula have been ignored. The composition of the type specimen is close to the boundary at 6.5 Si apfu between fluoropargasite, NaCa<sub>2</sub>(Mg<sub>4</sub>Al)Si<sub>6</sub>Al<sub>2</sub>O<sub>22</sub>F<sub>2</sub>, and fluoro-edenite NaCa<sub>2</sub>Mg<sub>5</sub>Si<sub>7</sub>AlO<sub>22</sub>F<sub>2</sub>. The name fluoropargasite is in agreement with

current IMA amphibole nomenclature (Burke and Leake 2004; *Can. Mineral.*, 42, 1881–1883); the terms fluorpargasite, fluorparagasite and F-pargasite are not to be used. **A.J.L.**

**KINGSTONITE\***

C.J. Stanley, A.J. Criddle, J. Spratt, A.C. Roberts, J.T. Szymański, M.D. Welch (2005) Kingstonite, (Rh,Ir,Pt)<sub>3</sub>S<sub>4</sub>, a new mineral species from Yubdo, Ethiopia. *Mineral. Mag.*, 69, 447–453.

Kingstonite occurs as subhedral to anhedral, elongate, tabular inclusions between 15 and 40  $\mu\text{m}$  in size in Pt-Fe alloys from the Bir Bir river, Yubdo district, Wallaga province, Ethiopia. It is opaque, has a metallic luster, black streak, is brittle with a subconchoidal fracture and one good cleavage parallel to [100]. Indentation measurements gave  $VHN_{25} = 895$  (871–920) kg/mm<sup>2</sup>, corresponding to a Mohs hardness of approximately 6. In plane polarized light, the mineral is pale brownish gray, has weak birefringence and pleochroism, and has no internal reflections. It is weakly anisotropic, with weak to moderate rotation tints in dull gray and brown. Reflectance percentages for  $R_{\text{min}}$  and  $R_{\text{max}}$  in air (and in oil) are 47.2, 48.9 (33.2, 34.7) (470 nm), 48.4, 50.3 (34.3, 36.1) (546 nm), 49.1, 50.7 (35.0, 36.5) (589 nm), 49.8, 51.0 (35.6, 36.7) (650 nm), respectively.

Electron microprobe analyses [WDS, average of 20 analyses on four grains (range)] gave Rh = 46.5 (46.5–46.9), Pt = 11.2 (10.8–11.3), Ir = 16.4 (15.6–16.9), S = 25.6 (25.2–25.7), sum 99.7 wt%, corresponding to (Rh<sub>2.27</sub>Ir<sub>0.43</sub>Pt<sub>0.29</sub>)<sub>Σ2.99</sub>S<sub>4.01</sub>, based on 7 atoms pfu. The simplified formula is (Rh,Ir,Pt)<sub>3</sub>S<sub>4</sub> with  $D_{\text{calc}} = 7.52$  g/cm<sup>3</sup> ( $Z = 6$ ).

The crystal structure of kingstonite was solved and refined using a  $35 \times 10 \times 10$   $\mu\text{m}$  fragment to  $R_1 = 0.0378$  for 830 reflections with  $F_o > 2.5\sigma(F_o)$ . Kingstonite is monoclinic, *C2/m*,  $a = 10.4616(5)$ ,  $b = 10.7527(5)$ ,  $c = 6.2648(3)$  Å,  $\beta = 109.000(5)^\circ$ ,  $V = 666.34(1)$  Å<sup>3</sup>,  $Z = 6$ . The strongest lines on the powder X-ray diffraction pattern (114.6 mm Debye-Scherrer camera, CuK $\alpha$  radiation, 39 lines given) include 5.23(20,111), 4.97(20,200), 3.500(20,221), 3.156(100,310), 3.081(100,131), 2.957(90,002), 2.805(40,221), 2.601(40,401), 2.471(20,400), 2.449(30,041), 2.353(132), 2.234(60,132), 2.000(20,242), 1.941(50,223), 1.918(40,421), 1.885(40,312), 1.871(80,441), 1.791(90,060), 1.722(30,332), 1.692(30,602), 1.678(20,352), 1.656(20,203), 1.631(40,441), and 1.532(70,062). The structure of kingstonite is unique among natural minerals, but is essentially identical to that of synthetic Rh<sub>3</sub>S<sub>4</sub> [Beck & Hilbert (2000), *Zeit. Anorganische Allgemeine Chem.*, 626, 72–79] and consists of edge-sharing RhS<sub>6</sub> octahedra that form ribbons parallel to *c*, as well as Rh<sub>6</sub> rings with sites coordinated by 4S+2Rh and 5S+2Rh. The RhS<sub>6</sub> ribbons alternate with columns of Rh<sub>6</sub> rings linked by S atoms.

Kingstonite was discovered in a 1.5 cm nugget, the type specimen of “prassoite.” The sample is from the platinum deposits of the Yubdo district, Wallaga province, Ethiopia which cover an area of >30 km<sup>2</sup>. The primary PGM occur in fresh and altered dunite and pyroxenite, as well as in secondary placer deposits in the Alfe, Bir Bir, and Deressa rivers. The deposits are dominated by isoferroplatinum and less tetraferroplatinum with minor PGE alloys, antimonides, arsenides, and sulphides. Kingstonite occurs as inclusions in a Pt-Fe alloy, as either a single-phase or intergrown with bowieite, ferrorhodsite, or cuprorhodsite. As-

sociated minerals include isoferroplatinum, tetraferroplatinum, Cu-bearing Pt-Fe alloy, osmium, and enriched oxide remnants of osmium and laurite. The mineral is named in honor of Gordon Andrew Kingston (b. 1939), senior lecturer in the Department of Geology, University of Wales, College of Cardiff, Wales, U.K., for his contribution to PGE mineralogy. Type material has been deposited at the Natural History Museum, London, U.K. (BM 2004,56) and a single-crystal and two powder mounts at the National Mineral Collection of Canada, Geological Survey of Canada, Ottawa, Canada (IMA 2004-56). **P.C.P.**

#### MANGANILVAITE\*

I.K. Bonev, R.D. Vassileva, N. Zotov, K. Kouzmanov (2005) Manganilvaite,  $\text{CaFe}^{2+}\text{Fe}^{3+}(\text{Mn},\text{Fe}^{2+})(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$ , a new mineral of the ilvaite group from Pb-Zn skarn deposits in the Rhodope Mountains, Bulgaria. *Can. Mineral.*, 43, 1027–1042

Manganilvaite occurs as black euhedral, striated dipyrnidal prismatic crystals up to 1–2 mm in length, elongated along the *c*-axis. The mineral is opaque, has a vitreous luster and a black to brownish streak. It is brittle with a distinct {100} cleavage and an uneven fracture. Microindentation measurements with (VHN<sub>100</sub>) gave a mean value of 868 kg/mm<sup>2</sup>, corresponding to a Mohs hardness of 5.5 to 6. Manganilvaite is opaque, gray to bluish gray in reflected light, with a red internal reflection and a bluish gray to lilac brown pleochroism. It shows distinct anisotropism under crossed polars. Electron microprobe analyses (average of 62 analyses) of manganilvaite from the Ossikovo deposit (Madan ore district) gave MgO 0.48, Al<sub>2</sub>O<sub>3</sub> 0.20, SiO<sub>2</sub> 29.65, CaO 12.62, TiO<sub>2</sub> 0.02, MnO 11.99, (FeO + Fe<sub>2</sub>O<sub>3</sub>) 40.93, H<sub>2</sub>O 2.21, sum 98.10 corresponding to  $(\text{Ca}_{0.92}\text{Mn}_{0.08}^{2+})(\text{Fe}_{0.97}^{2+}\text{Mg}_{0.05})\text{Fe}_{0.96}^{3+}\text{Al}_{0.02}(\text{Mn}_{0.61}^{2+}\text{Fe}_{0.39}^{2+})(\text{Si}_{2.00}\text{O}_7)\text{O}(\text{OH})$ . Electron microprobe analyses (17 analyses) of manganilvaite from the Govedarnika deposit (Laki district) gave MgO 0.45, Al<sub>2</sub>O<sub>3</sub> 0.34, SiO<sub>2</sub> 29.48 CaO 13.06, TiO<sub>2</sub> 0.04, MnO 13.54, (FeO+Fe<sub>2</sub>O<sub>3</sub>) 39.31, H<sub>2</sub>O 2.21, sum 98.43 corresponding to  $(\text{Ca}_{0.94}\text{Mn}_{0.06}^{2+})(\text{Fe}_{0.94}^{2+}\text{Mg}_{0.05})\text{Fe}_{0.99}^{3+}\text{Al}_{0.03}(\text{Mn}_{0.71}^{2+}\text{Fe}_{0.29}^{2+})(\text{Si}_{1.99}\text{O}_7)\text{O}(\text{OH})$ . The ideal formula is  $\text{CaFe}^{2+}\text{Fe}^{3+}(\text{Mn},\text{Fe}^{2+})(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$ . The IR spectrum of the mineral has absorption bands at 3446, 1739, 1635, 1454, 1377, 1121, 1040, 1005, 981, 950, 900, 880, 820, 700, 571, 534, 513, 503, 493, 480, 449, and 424 cm<sup>-1</sup>. There were no designations for the bands. Reflectance percentages for *R*<sub>min</sub> and *R*<sub>max</sub> in air are 8.2, 9.9 (480 nm), 7.5, 9.7 (546 nm), 6.9, 9.7 (589 nm), 6.0, 9.4 (650 nm), respectively.

Manganilvaite is monoclinic, *P2<sub>1</sub>/a*, with unit-cell parameters refined from powder X-ray data *a* = 13.025(7), *b* = 8.8514(5), *c* = 5.8486(3) Å, β = 90.167(1)°, *V* = 674.28 Å<sup>3</sup>, *Z* = 4, *D*<sub>obs</sub> = 3.92 g/cm<sup>3</sup>, *D*<sub>calc</sub> = 3.93 g/cm<sup>3</sup>. The strongest lines on the X-ray powder diffraction pattern (Stoe powder diffractometer, CoKα radiation, 78 lines) include 7.34(18,110), 3.901(24,211), 3.257(20,400, 311), 2.920(16,002), 2.875(85,130), 2.848(90,401,401), 2.737(27,321,321) 2.718(100,112, 112), 2.687(70,230), 2.624(15,420), 2.553(17,212), 2.442(33,231), 2.395(23, 122), 2.337(24,312), 2.180(48,140), 2.111(47,322,412,412), 1.973(25,241,241,340), 1.897(20,512), 1.716(39,720), 1.673(29,631,403,403), 1.635(19,251,342), 1.623(22,532,532,800), 1.527(20,820), 1.499(35,632,641), 1.475(48,060,252,523), 1.462(28,004).

The mineral was found in marble-hosted skarn-type orebodies at the Ossikovo and Mogilata deposits (Madan ore district) and the Govedarnika deposit (Laki district) in the central Rhodope Mountains, Bulgaria. Manganilvaite is invariably closely related to Pb-Zn-(Mn) skarns and the products of their retrograde alteration. It is often found replacing primary Mn-enriched clinopyroxenes (hedenbergite-johannsenite) and closely associated with bustamite, which is often found to replace the clinopyroxenes. It is also associated with manganoan ferro-actinolite, rhodonite, rhodochrosite, manganoan calcite, andradite, manganoan chlorite, sphalerite, galena, quartz, and magnetite. The presence of manganilvaite is thought to indicate the evolution of retrograde, hydrothermal processes from reduced to more oxidized. Manganilvaite is the Mn analogue of ilvaite with which it forms a continuous solid solution. The name is given for its composition and relation to other ilvaite-group minerals. Type material has been deposited in the collections of the Geological Institute, Bulgarian Academy of Sciences, Sofia (catalogue no. M1.2003.5-6, IMA no. 2002-016). **R.R.**

#### PAUTOVITE \*

I.V. Pekov, A.A. Agakhanov, M.M. Boldyreva, V.G. Grishin, (2005) Pautovite,  $\text{CsFe}_2\text{S}_3$ , a new mineral species from the Lovozero alkaline complex, Kola peninsula, Russia. *Can. Mineral.*, 43, 965–972.

Pautovite occurs as crudely prismatic to acicular crystals up to 120 μm in length and 5 μm in thickness. The crystals are thought to be elongated in the direction [001], and no twinning was observed. It is usually found as individuals, and clusters are rarely observed. The mineral is relatively soft, but the exact hardness could not be measured due to the small crystal size. The cleavage is perfect on {110}, the fracture is splintery, and the crystals split easily into flexible needles. Pautovite is opaque with a dark steel-gray color and a very strong metallic luster, but in moist air, it becomes dull black. In plane polarized reflected light, it is grayish white to grey and strongly birefractant. It is pleochroic from grayish-white to grey with a slightly pinkish tint. Pautovite is anisotropic with no internal reflections. Reflectance percentages for *R*<sub>min</sub> and *R*<sub>max</sub> are 13.95, 24.6 (470 nm), 14.65, 23.45 (546 nm), 15.15, 24.55 (589 nm), 16.0, 27.05 (650 nm), respectively. Electron microprobe analyses of pautovite (16 analyses) gave K 0.21, Rb 1.31, Cs 36.12, Tl 0.50, Fe 33.8, S 28.85, sum 100.79 wt%, corresponding to  $(\text{Cs}_{0.91}\text{Rb}_{0.05}\text{K}_{0.02}\text{Tl}_{0.01})_{\Sigma 0.99}\text{Fe}_{2.02}\text{S}_{2.99}$ , based on the sum of 6 atoms. The ideal formula is  $\text{CsFe}_2\text{S}_3$ , *Z* = 4.

Single-crystal diffraction study of pautovite was not successful due to the minute size and poor quality of the crystals. Pautovite is orthorhombic, *Cmcm*, with refined unit-cell parameters from the powder diffraction pattern *a* = 9.477(4), *b* = 11.245(4), *c* = 5.485(2) Å, *V* = 584.5(6) Å<sup>3</sup>, *Z* = 4, *D*<sub>calc</sub> of 3.85 g/cm<sup>3</sup>. The strongest lines on the X-ray diffraction pattern (144.6 mm RKU camera, Mn filtered FeKα radiation, 24 lines) include 4.69(30,200), 4.28(20,111), 2.981(100,221), 2.723(40,002), 2.629(15,311), 2.003(30,312,151,421), 1.910(60,042,060), 1.862(20,510,350), 1.785(30,402), 1.565(40,313), 1.514(20,171,442), 1.279(20,443,224,134). Pautovite is isostructural with rasvumite  $\text{KFe}_2\text{S}_3$ , and picotpaulite  $\text{TlFe}_2\text{S}_3$ . They all have a rasvumite-type structure, which is found

in chalcogenides and halides with general formula  $AB_2X_3$ .

Pautovite was discovered in the Palitra peralkaline pegmatite, Kedykverpakjk Mountain, Lovozero alkaline complex, Kola Peninsula, Russia. The Palitra is a thick lens-shaped pegmatite of 7 m in length and up to 1.5 m in thickness, within complex layered urtite-foyaite-lujavrite rocks. Pautovite is an extremely rare mineral present in the hydrothermal assemblage, typically as an overgrowth on needle-shaped to hair-like crystals of belovite-(Ce), but also observed on ussingite, microcline, nordite-(Ce) and bornemanite, and as inclusions in massive villiaumite in vugs. Other minerals associated with pautovite include aegirine, natrosilite, sodalite, potassicarfvedsonite, serandite, ferronordite-(Ce), vuonnemite, lomonosovite, vitusite-(Ce), phosinaite-(Ce), barytolamprophyllite, mangan-neptunite, manaksite, chkalovite, kapustinite, kazakovite, steenstrupine-(Ce), thorostenstrupine, bario-oligite, nalipoite, sphalerite, löllingite, wurtzite, bartonite, chlorbartonite, and zakharovite. The mineral name is for Leonid Anatol'evich Pautov, a Russian mineralogist affiliated with the Fersman Mineralogical Museum of Russian Academy of Sciences, Moscow, in recognition of his contribution to the study of minerals by physical methods, the mineralogy of alkaline pegmatites and the mineralogy of cesium. The holotype specimen has been deposited at the Fersman Mineralogical Museum of Russian Academy of Sciences, Moscow (catalogue no. 3168/1, IMA no. 2004-005). **R.R.**

**PLUMBOAGARDITE\***

K. Walenta, T. Theye (2005) Plumboagardite, a new mineral of the mixite group from an occurrence in the Southern Black Forest, Germany. *N. Jb. Mineral. Abh.*, 181, 219–222.

Plumboagardite occurs as spherulitic aggregates up to 0.12 mm (average 0.05 to 0.08 mm) with a radial fibrous structure consisting of acicular crystals (0.05 mm long, 2 μm thick). The crystals are elongated along [0001]. The mineral is grass green, has a greenish streak, is translucent with a vitreous luster, has a Mohs hardness of 3, and does not show cleavage. It is uniaxial positive,  $\omega = 1.726(5)$  and  $\epsilon = 1.805(5)$ . It is soluble in dilute HCl and HNO<sub>3</sub>.

Electron microprobe analyses (average of 3 analyses) gave PbO 8.99, La<sub>2</sub>O<sub>3</sub> 1.91, Nd<sub>2</sub>O<sub>3</sub> 1.17, Ce<sub>2</sub>O<sub>3</sub> 0.96, Sm<sub>2</sub>O<sub>3</sub> 0.20, Pr<sub>2</sub>O<sub>3</sub> 0.19, Gd<sub>2</sub>O<sub>3</sub> 0.17, Dy<sub>2</sub>O<sub>3</sub> 0.10, Y<sub>2</sub>O<sub>3</sub> 0.96 CaO 1.44, CuO 40.49, Fe<sub>2</sub>O<sub>3</sub> 1.54, As<sub>2</sub>O<sub>5</sub> 29.74, P<sub>2</sub>O<sub>5</sub> 0.30, SiO<sub>2</sub> 1.46, H<sub>2</sub>O (by difference) 10.38, sum 100.00 wt%, corresponding to the empirical formula [Pb<sub>0.44</sub>(La<sub>0.13</sub>Nd<sub>0.08</sub>Ce<sub>0.06</sub>Pr<sub>0.01</sub>Sm<sub>0.01</sub>Gd<sub>0.01</sub>Dy<sub>0.01</sub>Y<sub>0.09</sub>)<sub>ΣREE0.40</sub>Ca<sub>0.28</sub>]<sub>Σ1.12</sub>(Cu<sub>5.59</sub>Fe<sub>0.21</sub>)<sub>Σ5.80</sub>(As<sub>2.84</sub>Si<sub>0.27</sub>P<sub>0.05</sub>)<sub>Σ3.16</sub>O<sub>12</sub>(OH)<sub>6</sub>·3.33H<sub>2</sub>O based on 12O + 6(OH). The simplified formula is (Pb,REE,Ca)Cu<sub>6</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>6</sub>·3H<sub>2</sub>O,  $D_{\text{calc}} = 3.471 \text{ g/cm}^3$ .

Plumboagardite is hexagonal,  $P6_3/m$ , with unit-cell parameters refined from powder X-ray diffraction data  $a = 13.77(2)$ ,  $c = 5.94(1) \text{ \AA}$ ,  $V = 975.4(2) \text{ \AA}^3$ ,  $c:a = 0.4314$ . The strongest lines on the powder X-ray diffraction pattern (57.3 mm camera, FeK $\alpha$  radiation, 42 lines given) include 12.01(100,10 $\bar{1}$ 0), 4.51(60,21 $\bar{3}$ 0,11 $\bar{2}$ 1), 4.23(40,20 $\bar{2}$ 1), 3.60(80,21 $\bar{3}$ 1), 3.31(50,31 $\bar{4}$ 0,30 $\bar{3}$ 1), 2.98(60,40 $\bar{4}$ 0,22 $\bar{4}$ 1,0002), 2.89(40,31 $\bar{4}$ 1,10 $\bar{1}$ 2), 2.74(50,32 $\bar{5}$ 0,11 $\bar{2}$ 2), 2.61(50,41 $\bar{5}$ 0), 2.49(70,32 $\bar{5}$ 1,21 $\bar{3}$ 2), 1.817(50,61 $\bar{7}$ 0,52 $\bar{7}$ 1,33 $\bar{6}$ 2), 1.792(40,42 $\bar{6}$ 2), 1.648(40,40 $\bar{4}$ 3), and 1.485(40,4263,0004). The mineral is isostructural with other

members of the mixite group.

Plumboagardite was found in an abandoned mine, Aitern-Süd, near Schönau in the Southern Black Forest. A hydrothermal Pb-Zn vein with abundant chalcopyrite was the main ore body cutting through Upper Devonian schists and granite. The resultant waste dumps are a source of secondary Cu and Pb minerals. Plumboagardite was formed in an oxidized zone, the product of alteration of primary Pb, Cu, REE, and As minerals such as chalcopyrite, fluorite, fahlore, and galena. It is associated with fluorite, limonite, and quartz. The name is for its chemistry and relation to agardite. Type material has been deposited at the Staatliches Museum für Naturkunde, Stuttgart, Germany. **P.C.P.**

**SELENOJALPAITE\***

L. Bindi, G. Pratesi (2005) Selenojalpaite, Ag<sub>3</sub>CuSe<sub>2</sub>, a new mineral species from the Skrikerum Cu-Ag-Tl selenide deposit, Småland, southeastern Sweden. *Can. Mineral.*, 43, 1373–1377.

Selenojalpaite is typically intergrown with eucairite and berzelianite to form aggregates up to several hundred micrometers across, and also occurs as anhedral to subhedral grains, up to 200 μm in length. The mineral is brittle, VHN<sub>25</sub> = 37 kg/mm<sup>2</sup> (range 36–40),  $H = 4\text{--}4\frac{1}{2}$ , opaque, dark gray with a black streak, metallic luster, an uneven fracture and no cleavage. Light gray under reflected light, weakly to moderately birefractant, weakly pleochroic from brownish gray to a slightly darker greenish gray, anisotropic, without characteristic rotation-tints or internal reflections. Reflectance values for randomly oriented grains (in air, SiC standard) are ( $R_1$ - $R_2$ ) 33.5–37.1 (471.1 nm), 31.8–35.1 (548.3 nm), 30.4–34.0 (586.6 nm), and 29.3–32.4 (652.3 nm). An average of fifteen electron microprobe analyses for the same grain gave Ag 59.20, Cu 11.81, Se 29.01, (Fe, Mn, and S below detection), sum 100.02 wt%, corresponding to Ag<sub>2.99</sub>Cu<sub>1.01</sub>Se<sub>2.00</sub> for six atoms, ideally Ag<sub>3</sub>CuSe<sub>2</sub>.

Examination by single-crystal X-ray methods revealed the diffraction profiles to be too broad to yield a structure refinement. Powder diffraction data were collected with a Gandolfi camera (114.6 mm, CuK $\alpha$  radiation) and showed the mineral to be tetragonal, with refined unit-cell parameters  $a = 8.939(1)$ ,  $c = 11.844(2) \text{ \AA}$ ,  $V = 946.4(2) \text{ \AA}^3$ ; systematic absences are consistent with space group  $I4_1/amd$ . The strongest lines are [ $d$  in  $\text{Å}$  ( $l,hkl$ )]: 7.14 (45,101), 4.47 (60,200), 2.891 (85,301), 2.813 (80,213), 2.552 (50,312), 2.473 (75,204), 2.426 (100,321), 2.292 (45,105), 2.162 (70,224), and 2.034 (65,215). Density was not measured;  $D_{\text{calc}} = 7.64$  for the empirical formula, 7.65 g/cm<sup>3</sup> for the idealized formula and  $Z = 8$ . The most closely related species is jalpaite, Ag<sub>3</sub>CuS<sub>2</sub>. The authors suggest that selenojalpaite and jalpaite may be isotypic, but caution that not all chemically corresponding phases in the Cu-Ag-Se-S system are isostructural.

The mineral occurs in a hydrothermal calcite vein in the Skrikerum Cu-Ag-Tl selenide deposit, near Valdermarsvik, Småland, southeastern Sweden; this deposit is also the type locality for berzelianite (Cu<sub>2</sub>Se), crookesite (Cu<sub>2</sub>TlSe<sub>4</sub>) and eucairite (CuAgSe). Associated minerals in the vein include copper, Au-Ag alloy, Se-bearing chalcopyrite, Se-bearing bornite, berzelianite, covellite, umangite, athabascaite, klockmannite, ferroselite, eucairite, naumannite, fischesserite, crookesite, buko-

vite, clausenthalite, Se-bearing sphalerite, Se-bearing stromeyerite, and Se-bearing chalcocite. The name is for the composition and the relationship to jalpaite,  $\text{Ag}_3\text{CuS}_2$ . Type material is deposited in the mineralogical collection of the Museo di Storia Naturale, Università di Firenze, Italy, under catalogue number 1768/I. The mineral corresponds to IMA mineral No. 2004-48.

**Discussion.** The reflectance values listed above are given at wavelengths within 3 nm of the four standard wavelengths recommended by the IMA Commission on Ore Mineralogy: 470, 546, 589, and 650 nm. **A.J.L.**

#### WATERHOUSEITE\*

A. Pring, U. Kolitsch, W.D. Birch (2005) Description and unique crystal-structure of waterhouseite, a new hydroxy manganese phosphate species from the Iron Monarch deposit, Middleback Ranges, South Australia. *Can. Mineral.*, 43, 1401–1410.

Waterhouseite occurs as divergent sprays of bladed crystals up to 1.0 mm in length and elongated along [001]. Forms observed include {100} (dominant), {010}, {011}, and on most crystals, {001}. The crystals show contact twinning on (100), and show pseudo-orthorhombic morphology. The mineral is brittle, *H*4, transparent, with color ranging from resinous orange-brown to dark clove-brown, and a yellowish brown streak. The luster is pearly on cleavages and vitreous to pearly on crystal faces, fracture is splintery to conchoidal, and there is a perfect cleavage on (100) and a probable cleavage on (001). Waterhouseite is biaxial negative, with  $\alpha$  1.730(3),  $\beta$  ~1.738,  $\gamma$  1.738(4), *2V* not measured but inferred to be close to 0°,  $X = b$ ,  $Y = a$  and  $Z = c$ , pleochroic: *X* pale brown, *Y* brown-yellow, and *Z* pale brown, with absorption  $Z = X > Y$ . An average of seven electron microprobe analyses for multiple crystals gave MnO 69.70, ZnO 0.02,  $\text{P}_2\text{O}_5$  17.37,  $\text{As}_2\text{O}_5$  1.09,  $\text{V}_2\text{O}_5$  0.50,  $\text{H}_2\text{O}$  (calc.) 9.49, sum 98.17 wt%, corresponding to  $\text{Mn}_{7.28}[\text{P}_{1.81}\text{As}_{0.07}\text{V}_{0.04}]\text{O}_{41.92}(\text{OH})_{7.81}\text{O}_{0.51}$  on the basis of 16 oxygen atoms, ideally  $\text{Mn}_7(\text{PO}_4)_2(\text{OH})_8$ . Single crystal X-ray structure study ( $R_1 = 0.052$ ) showed the mineral to be twinned by non-merohedry and to have an unique complex framework composed of  $\text{Mn}(\text{O},\text{OH})_6$  octahedra and  $\text{PO}_4$  tetrahedra, which are linked by both edges and corners. Waterhouseite is monoclinic, space group  $P2_1/c$ ,  $a$  11.364(2),  $b$  5.570(1),  $c$  10.455(2) Å,  $\beta$  96.61(3)°,  $V$  657.3(2) Å<sup>3</sup>. Powder diffraction data were collected with a Guinier-Hägg camera (100 mm, 10–90° 2 $\theta$ , Si internal standard,  $\text{CrK}\alpha$  radiation) and yielded refined-cell parameters  $a$  11.364(6),  $b$  5.570(2),  $c$  10.455(3) Å,  $\beta$  96.61(3)°,  $V$  657.4(2) Å<sup>3</sup>, and the strongest lines [ $d$  in Å (*hkl*)]: 4.980 (15,110), 4.436 (70,111), 3.621 (100,202), 3.069 (50,311), 2.941 (40,013), 2.890 (20,302), 2.842 (20,400), 2.780 (35,020), 2.718 (20,213), and 2.596 (20,004). Density was measured by suspension in diluted Clerici solution:  $D_{\text{meas}}$  3.55(5),  $D_{\text{calc}}$  3.67 for the empirical formula, 3.59 g/cm<sup>3</sup> for the ideal formula and *Z* 2. The single-crystal Raman spectrum is interpreted to be consistent with the presence of OH<sup>-</sup> and  $\text{PO}_4^{3-}$ , and Mn–O bonds. Waterhouseite is not structurally related to any other mineral species. Allactite,  $\text{Mn}_7(\text{AsO}_4)_2(\text{OH})_8$  and raadeite,  $\text{Mg}_7(\text{PO}_4)_2(\text{OH})_8$ , have similar stoichiometries, but their structures are different.

Waterhouseite occurs in cavities in a matrix consisting of hematite, hausmannite, barite, manganoan calcite and rhodo-

chrosite, from the 130-meter level on the eastern side of the Iron Monarch mine, a Proterozoic sedimentary iron ore deposit in the Middleback Ranges, at Iron

Knob, South Australia. Shigaite, gatehouseite, seamanite, rhodochrosite, barite, hausmannite and hematite are found in close association with waterhouseite. Metaswitzerite, sussexite, arsenoclasite, collinsite, pyrobelonite, triploidite and a new, unnamed hexagonal calcium–manganese carbonate–phosphate have been noted from the immediate area of the open cut, but not in direct association with the mineral. Waterhouseite was noted in Pring et al. (2000; *Aust. J. Mineral.*, 6, 9–23) as an unidentified phase designated UK02. The mineral is named after Frederick George Waterhouse (1815–1898), first Director of the South Australian Museum (Adelaide), in recognition of his contribution to the preservation of the natural history of South Australia, and celebrates the continuing work of the Waterhouse Club in their support of the South Australian Museum. The type specimen and additional material are deposited in the collections of the South Australian Museum, Adelaide (SAM 28408 and 28409). The mineral corresponds to IMA mineral No. 2004–035.

**Discussion.** The optical orientation given for waterhouseite is not consistent with its monoclinic symmetry, but refers to the observed pseudo-orthorhombic morphology; a pseudo-orthorhombic unit cell is not presented. The analytical total reported for the electron microprobe analysis is erroneous; the correct sum is given above. The calculated densities for the empirical formula and for the simplified formula  $\text{Mn}_7(\text{PO}_4)_2(\text{OH})_8$  reported are erroneous; corrected values are given above. **A.J.L.**

#### NEW DATA

##### BOHDANOWICZITE, PD-AG-BI-TE PHASE

T. Augé, R. Petrunov, L. Bailly (2005) On the origin of the PGE mineralization in the Elatsite Porphyry Cu–Au deposit, Bulgaria: comparison with the Baula–Nuasahi complex, India, and other alkaline PGE-rich porphyries. *Can. Mineral.*, 43, 1355–1372.

An Ag–Bi–Se phase with a composition similar to that of bohdanowiczite ( $\text{Ag}_2\text{Bi}_2\text{Se}_4$ ) occurs in contact with merenskyite,  $\text{PdTe}_2$ . Electron microprobe analysis gave Cu 1.86, Ag 20.47, Pb 0.17, Fe 1.33, Bi 40.28, S 0.28, Se 33.01, Te 3.45, sum 100.85 wt%, which corresponds (on the basis of 8 atoms) to:  $(\text{Ag}_{1.71}\text{Cu}_{0.26})_{\Sigma 1.97}(\text{Bi}_{1.73}\text{Fe}_{0.21}\text{Pb}_{0.01})_{\Sigma 1.95}(\text{Se}_{3.76}\text{Te}_{0.24}\text{S}_{0.08})_{\Sigma 4.08}$ . The copper content of the bohdanowiczite from the Elatsite deposit falls within the range (1.60–7.37 wt% Cu) of Cu-rich bohdanowiczite recently reported from the Niederschlema–Alberoda U–Se–polymetallic deposit, Erzgebirge, Germany (Förster et al. 2005; *Can. Mineral.*, 43, 899–908).

An undetermined Pd–Ag–Te–Bi phase occurs in a composite grain associated with merenskyite, palladoarsenide, and hessite. Electron microprobe analysis gave Pt 0.54, Fe 0.14, Pd 19.76, Pb 0.16, Cu 0.35, Sb 0.10, Se 0.23, Te 41.79, Bi 28.27, Ag 10.48, sum 101.82 wt%, corresponding to  $(\text{Pd}_{0.73}\text{Ag}_{0.38}\text{Cu}_{0.02}\text{Pt}_{0.01}\text{Fe}_{0.01})_{\Sigma 1.15}(\text{Te}_{1.29}\text{Bi}_{0.53}\text{Se}_{0.01})_{\Sigma 1.83}$  on the basis of three atoms, and simplified as  $(\text{Pd},\text{Ag})(\text{Te},\text{Bi})_2$ . The composition given for the merenskyite, ideally  $\text{PdTe}_2$ , with which this unidentified phase occurs, has

much lower Bi (0–2.16 wt%, mean 0.56) and Ag (0–3.1 wt%, mean 0.4) contents.

These minerals occur associated with platinum-group-element minerals in a magnetite–bornite–chalcopyrite assemblage in the Elatsite porphyry-copper deposit, Bulgaria. **A.J.L.**

### COBALTARTHURITE

A.R. Kampf (2005) The crystal structure of cobaltarthurite from the Bou Azzer district, Morocco: the location of hydrogen atoms in the arthurite structure-type. *Can. Mineral.*, 43, 1387–1391.

Re-investigation of the structure of cobaltarthurite,  $\text{Co}^{2+}\text{Fe}^{3+}(\text{AsO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ , by single-crystal X-ray methods ( $R1 = 0.018$ ), showed that it is monoclinic, space group  $P2_1/c$ , with cell dimensions  $a = 10.2635(9)$ ,  $b = 9.7028(8)$ ,  $c = 5.5711(5)$  Å,  $\beta = 94.207(1)^\circ$ ,  $V = 553.30(8)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_{\text{calc}} = 3.33$  g/cm<sup>3</sup>. The data reveal the hydrogen positions in a mineral of the arthurite group for the first time. All of the hydrogen positions were located, and refined with fixed isotropic displacement parameters, but without constraints on the O–H distances. The hydrogen bonding revealed is in accord with the scheme previously inferred (Moore et al. 1974; *Amer. Mineral.*, 59, 900–905) for the isostructural phosphate whitmoreite,  $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ , with one change: OW2–H··OW1. Electron-microprobe analysis of crystals associated with that used in the structure analysis (average of 3 analyses), gave for the cations: Co 6.4, Fe 21.9, Ca 0.2, and As 27.1 wt%, equivalent to CoO 8.14, Fe<sub>2</sub>O<sub>3</sub> 31.31, CaO 0.28, As<sub>2</sub>O<sub>5</sub> 41.57, sum 81.30 wt%. These data yield low cation proportions ( $\text{Co}_{0.60}\text{Fe}_{2.17}\text{Ca}_{0.03}\text{As}_{2.80}$ ) on the basis of two As apfu. Details of the electron-microprobe analysis and reasons for the low cation total are not given.

**Discussion.** The atomic proportions of Ca and Fe given in the text, ( $\text{Co}_{0.60}\text{Fe}_{2.16}\text{Ca}_{0.01}\text{As}_{2.77}$ ) are not in agreement with the weight abundances presented. Recalculated proportions are given above. **A.J.L.**

### DIVERSILITE-(Ce)\*

S.V. Krivovichev, Y.N. Yakovenchuk (2005) Crystal structure of diversilite-(Ce). *Zap. Vser. Mineral. Obshch.*, 134(1), 113–117 (in Russian, English abstract).

The crystal structure of diversilite-(Ce) from the type locality (Khibiny massif, Kola Peninsula, Russia), was re-investigated (see also Dokl. Akad. Nauk, 388, 64–68 and Zeits. Kristallogr., 218, 392–396). Diversilite-(Ce) is shown to be twinned on (001), and to have space group  $R32$ ,  $a = 10.708(2)$ ,  $c = 60.073(11)$  Å, ideal formula  $(\text{Ba,K,Na,Ca})_{-11-12}(\text{REE,Fe,Th})_4(\text{Ti,Nb})_6[\text{Si}_6\text{O}_{18}]_4(\text{OH, O})_{12} \cdot n\text{H}_2\text{O}$ ,  $Z = 3$ , based on a refinement of 1762 independent reflections ( $F > 4\sigma[F]$ ;  $R = 0.077$ ). Instead of a structure hosting both  $\text{SiO}_3(\text{OH})$  tetrahedra and  $\text{Si}_3\text{O}_9$  triple-rings (the origin of its name), the structure would seem to contain *only*  $\text{Si}_6\text{O}_{18}$  rings. The crystal structure of diversilite is described in analogy with its Nb-analogue, ilímaussite-(Ce), as consisting of three sets of (001) layers. The *A* layer consists of  $\text{Si}_6\text{O}_{18}$  rings and  $\text{CeO}_6$  trigonal prisms. The *O* layer consists of  $\text{Si}_6\text{O}_{18}$  rings and  $\text{TiO}_5(\text{OH})$  octahedra. The remaining layer, denoted *A'*, consists of a superimposition of three *A* layers displaced relative to each other by  $\pm 1/3$  ( $a + 2b$ ), hence the low occupancies of the Ce and Si sites (2/3), and positional disorder of anions at  $z \sim 0.135$  in the layer. **T.S.E.**

### PASCOITE

J.M. Hughes, M. Schindler, C. Francis (2005) The  $C2/m$  disordered structure of pascoite,  $\text{Ca}_3[\text{V}_{10}\text{O}_{28}] \cdot 17\text{H}_2\text{O}$ : bonding between structural units and interstitial complexes in compounds containing the  $[\text{V}_{10}\text{O}_{28}]^{6-}$  decavanadate polyanion. *Can. Mineral.*, 43, 1387–1391.

Re-investigation of the structure of pascoite,  $\text{Ca}_3[\text{V}_{10}\text{O}_{28}] \cdot 17\text{H}_2\text{O}$ , by single-crystal X-ray methods ( $R1 = 0.026$ ), showed that it is monoclinic, space group  $C2/m$ , with cell dimensions  $a = 19.5859(6)$ ,  $b = 10.1405(3)$ ,  $c = 10.9110(3)$  Å,  $\beta = 120.815(1)^\circ$ ,  $V = 1861.11$  Å<sup>3</sup>,  $Z = 2$ ,  $D_{\text{calc}} = 2.47$  g/cm<sup>3</sup>. The alternative setting of the space group (with  $\beta$  close to  $90^\circ$ ) is  $I2/m$ ,  $a = 10.911(3)$ ,  $b = 10.141(3)$ ,  $c = 16.844(5)$ ,  $\beta = 92.987(1)^\circ$ . The data reveal the hydrogen bonding in the structure for the first time. All of the hydrogen positions were located, and refined with fixed isotropic displacement parameters but without constraints on the O–H distances. The centrosymmetric and disordered description of the structure of pascoite in space group  $C2/m$  is preferred over a noncentrosymmetric and ordered model in space group  $C2$ , as the centric model has a better agreement index. **A.J.L.**