1	Revision 1					
2	Jingwenite–(Y) from the Yushui Cu deposit, South China: the first					
3	occurrence of a V–HREE–bearing silicate mineral					
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ABSTRACT

Jingwenite–(Y), $Y_2AI_2V^{4+}_2(SiO_4)O_4(OH)_4$ 22 the first V-HREE-bearing silicate mineraldiscovered in nature, is an abundant component of a sediment-hosted stratiform Cu 23 (SSC) deposit, Yushui, in South China. The mineral occurs in bedded/massive sulfide-24 bearing ore and is associated with bornite, chalcopyrite, galena, xenotime-(Y), nolanite, 25 thortveitite, roscoelite, barite, and quartz. Optically, jingwenite–(Y) is biaxial (+), with α = 26 1.92(4), $\beta = 1.95(2)$, $\gamma = 1.99(3)$ (white light), and 2V (calculated) = 83°. The dispersion is 27 medium with r<v, and the pleochroism is with X = light brown, Y = brown, Z = dark brown. 28 29 The colour, streak, lustre, and hardness (Mohs) are light brown, yellowish grey, vitreous, and 30 $4\frac{1}{2}$ -5, respectively. Jingwenite–(Y) is monoclinic, with space group I2/a, Z = 4, and unit–cell parameters a =31 9.4821(2) Å, b = 5.8781(1) Å, c = 19.3987(4) Å, $\beta = 90.165(2)^{\circ}$, and V = 1081.21(4) Å³. The 32 structure of jingwenite-(Y) has chains of edge-sharing AI (V, Fe)-O octahedra and V (Ti)-O 33 octahedra extending along the *b*-axis and linked by insular Si-O tetrahedra, leaving open 34 35 channels occupied by HREEs. Jingwenite-(Y) is a new nesosilicate structural type. Sm–Nd dating and Nd isotope signatures of jingwenite–(Y) reveal an epigenetic origin 36

and suggest that HREEs and V were added to the SSC system via leaching of abundant heavy minerals in the footwall red sandstone by oxidized basinal brines. The abundance of jingwenite–(Y) at Yushui indicates that it could potentially be a valuable resource for HREE and V. Moreover, HREE and V mineralization can also occur in the same sediment–hosted Cu mineral system.

42 *Keywords*: New mineral; Jingwenite–(Y); Heavy Rare Earth Elements; Yushui;

43

INTRODUCTION

44	Both heavy rare earth elements (HREE: Gd–Lu + Y) and vanadium (V) are critical and highly
45	valuable metals increasingly needed for high-technology applications, e.g., in the aerospace
46	industry and in the transition to low-carbon energy generation (Hatch, 2012). Here we report
47	a new mineral, jingwenite–(Y), ideally $Y_2Al_2V^{4+}_2(SiO_4)_2O_4(OH)_4$, the first V–HREE–bearing
48	silicate mineral discovered in nature. It occurs as an abundant phase in a sediment-hosted
49	stratiform Cu deposit (SSC) (Liu et al., 2022), the Yushui deposit, South China, which could
50	potentially be a valuable resource of HREE and V. Jingwenite–(Y) has been approved by the
51	International Mineralogical Association Commission on New Minerals, Nomenclature and
52	Classification (IMA2021-070). The new mineral jingwenite-(Y) is named in honor of
53	Professor Jingwen Mao (born in 1956). He is a leading Chinese economic geologist at the
54	China University of Geosciences (Beijing), with global impact from his publication output and
55	significant contribution to international professional associations. Type material is deposited
56	in the mineralogical collections of the Geological Museum of China, catalog number
57	M16122.

58

OCCURRENCE AND ASSOCIATED MINERALS

Jingwenite–(Y) is found in Cu–sulfide ore from the Yushui deposit, an SSC ore system located about 16 km northeast of Meizhou City, Guangdong Province, China (24°25'18"N, 116°11'48"E) (Fig. 1A). The Yushui deposit is concealed beneath Late–Jurassic volcanic cover and is hosted mainly within sedimentary rocks at the unconformity between Upper Carboniferous dark–grey dolostone and a >300 m–thick sequence of Lower Carboniferous red sandstone (Fig. 1B) characterized by an abundance of heavy minerals including

65	xenotime-(Y), rutile, zircon, and hematite. There are three ore types: I) bedded/massive; II)
66	disseminated; and III) vein-type. Jingwenite-(Y) occurs mainly in bedded/massive ore
67	(orebody V_1), where associated minerals are bornite, chalcopyrite, galena, xenotime–(Y),
68	nolanite, thortveitite, roscoelite, barite, quartz, and an as-yet unnamed V-HREE-Sc-
69	bearing silicate mineral phase (Fig. 2).

70

ANALYTICAL METHODS

Polished sections were prepared from the jingwenite–(Y) specimen for major element and

72 Sm–Nd isotope analysis.

73 Chemical composition analysis

Quantitative major-element analysis of minerals was done at the State Key Laboratory of 74 75 Mineral Deposits Research, School of Earth Sciences and Engineering, Nanjing University, using a JEOL JXA-8530F electron microprobe. All measurements were done using an 76 accelerating voltage of 15 kV, a beam current of 50 nA, and a beam size of 2 µm. The 77 analyzing crystals were PETJ (V and Y), LIFH (Fe, Nd, Sm, Gd, Tb and Ti), LIFL (Dy, Ho, Er, 78 Tm, Yb and Lu), LDE1L (F) and TAP (Si and Al). The $K\alpha$ line was chosen for analysis of Si, 79 Al, Fe, V and Ti; the $L\alpha$ line for Sm, Nd, Tb, Gd, Dy, Er, Tm, Yb and Y; and the $L\beta$ line for Ho 80 and Lu. The counting times on peaks were 10 s for Si, Al and F; 20 s for Fe, V, Ti, Sm, Gd, 81 Dy, Er, Ho, and Y; and 30 s for Nd, Tb, Tm, Yb, and Lu. Background intensities were 82 measured on both sides of the peak for half of the peak time. The standards were REE1 for 83 Gd, Tb, and Tm, REE2 for Nd, Sm, Yb, and Lu, and REE4 for Dy, Ho, and Er; albite for Si; 84 amphibole (B5) for AI, Fe, Ca, and Ti; synthetic YPO₄ for Y; Ca₃(VO₄)₂ for V. 85

86 Crystal–structure analysis

X–ray powder and single–crystal diffraction was done at the School of Geosciences and Info–Physics, Central South University, China, with a Rigaku XtaLAB Synergy diffractometer (CuK α radiation) in powder Gandolfi mode at 50 kV and 1 mA, and a Rigaku XtaLAB Synergy diffractometer equipped with Cu $K\alpha$ radiation at 50 kV and 1 mA.

91 Raman spectroscopy analysis

Raman spectroscopy of jingwenite–(Y) was done on a Horiba LabRAMIS spectrometer using the 532 nm line of laser at the State Key Laboratory for Mineral Deposits Research, Nanjing University. The laser beam (532 nm, laser power 20 mW) was focused to 1 μ m with a 100× objective in an Olympus microscope. The time of each scan in the range 100–4000 cm⁻¹ was 20–60 s (3 accumulated times) with a resolution of 2 cm⁻¹.

97 LA–MC–ICP–MS Sm–Nd isotope analysis

Neodymium isotopic ratios of jingwenite-(Y) were measured by LA-MC-ICP-MS at Nanjing 98 FocuMS Technology Co. Ltd, Jiangsu province, China, with an Australian Scientific 99 Instruments RESOlution LR laser-ablation system (Canberra, Australia) and Nu Instruments 100 Nu Plasma II MC-ICP-MS (Wrexham, Wales, UK). The 193 nm ArF excimer laser, 101 homogenized by a set of beam delivery systems, was focused on the surface with fluence of 102 103 4.5 J/cm². Helium (370ml/min) was used as carrier gas to transport aerosol out of the ablation cell, and was mixed with argon (~0.97 L/min) via T-connector before entering ICP 104 torch. Integration time of Nu Plasma II was set to 0.3 s (equating to 133 cycles during the 40 105 s). For Sm–Nd isotope analyses, each acquisition incorporated 20 s background (gas blank), 106 followed by ablation with spot diameters of 40 µm, and 75 µm, respectively, at 5 Hz repetition 107

108 rate for 40 s.

109	The isobaric interference of ¹⁴⁴ Sm on ¹⁴⁴ Nd is significant. The ¹⁴⁷ Sm/ ¹⁴⁹ Sm ratio (1.0868)
110	and the measured ¹⁴⁷ Sm/ ¹⁴⁹ Sm ratio were used to calculate the Sm fractionation factor, and
111	then used the measured ¹⁴⁷ Sm intensity and the natural ¹⁴⁷ Sm/ ¹⁴⁴ Sm ratio were used to
112	correct the Sm interference on mass 144. The interference-corrected ¹⁴⁶ Nd/ ¹⁴⁴ Nd ratio was
113	then normalized to 0.7219 to calculate the Nd fractionation factor. Then the ¹⁴³ Nd/ ¹⁴⁴ Nd and
114	¹⁴⁵ Nd/ ¹⁴⁴ Nd ratios were normalized using the exponential law. Standard monazites (44069,
115	M2, M4, Trebilcock, and Namaqualand-2) and apatites (MAD, Durango, OtterLake, AP1,
116	and AP2) were treated as quality control every ten unknown samples. The ¹⁴⁷ Sm/ ¹⁴⁴ Nd ratio
117	was calculated using the exponential law after correcting for the isobaric interference of
118	¹⁴⁴ Sm on ¹⁴⁴ Nd as described above, and then was externally calibrated against the
119	¹⁴⁷ Sm/ ¹⁴⁴ Nd ratio of the standard monazite (Namaqualand-2: ¹⁴⁷ Sm/ ¹⁴⁴ Nd=0.0980±3, ID-
120	TIMS by Liu et al. 2012).

121

RESULTS

122 Optical, morphological, and physical properties of Jingwenite–(Y)

Jingwenite–(Y) occurs as brown aggregates up to 280 μ m in size consisting of platy and columnar crystals, individually ranging from 5 to 30 μ m. The method of the measurement of refractive index allows the Fresnel equations to be directly used to calculate the refractive index with the measured diffuse reflectance. More details are provided in Tolosa et al. (2011). Optically, jingwenite–(Y) is biaxial (+), with α = 1.92(4), β = 1.95(2), γ = 1.99(3) (white light), and 2V (calculated) = 83°. The dispersion is medium with r<v, and the pleochroism is with X = light brown, Y = brown, Z = dark brown. The *a:b:c* ratio from single–crystal X–ray diffraction data is 0.489:0.303:1. The colour, streak, lustre, and hardness (Mohs) are light brown, yellowish grey, vitreous, and $4\frac{1}{2}$ -5, respectively. The calculated density is 4.475 g/cm⁻³ based on the empirical formula and unit cell volume determined from single crystal XRD data.

134 Chemical composition

- Jingwenite–(Y) displays narrow ranges of SiO_2 and Al_2O_3 contents of 16.07–16.67 wt% and
- 136 10.10–11.66 wt%, respectively, and variable contents of VO₂, TiO₂, Y_2O_3 , Dy_2O_3 , Er_2O_3 ,
- 137 Yb_2O_3 , and Lu_2O_3 ranging from 25.06 to 28.31 wt%, 0.06 to 3.74 wt%, 21.97 to 27.43 wt%,
- 138 2.54 to 4.23 wt%, 2.80 to 4.37 wt%, 2.86 to 5.86 wt%, and 1.21–4.01 wt%, respectively, with
- 139 low Fe₂O₃, Gd₂O₃, Tb₂O₃, Ho₂O₃, and Tm₂O₃ contents of ~1.87 wt%, 0.45–0.94 wt%, 0.22–
- 140 0.52 wt%, 0.63–1.04 wt%, and 0.39–0.87 wt% (Table S1).
- 141 The empirical formula, calculated on the basis of 16 apfu O, is
- 142 $(Y_{1.54}Yb_{0.14}Er_{0.14}Dy_{0.12}Lu_{0.08}Ho_{0.04}Gd_{0.02}Tm_{0.02}Tb_{0.02})_{\Sigma 2.12}(AI_{1.5}V_{0.38}Fe_{0.08})_{\Sigma 1.96}(V_{1.84}Ti_{0.16})_{\Sigma 2}(Si_{0.02}Ti_{0.02}Ti_{0.02})_{\Sigma 2.12}(AI_{1.5}V_{0.38}Fe_{0.08})_{\Sigma 1.96}(V_{1.84}Ti_{0.16})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0.02}Ti_{0.02})_{\Sigma 2}(Si_{0$
- 143 $O_4)_{1.94}O_{4.6}(OH)_{3.64}$, which can be simplified to 144 $(Y,Yb,Er,Dy)_2(AI,V^{3+},Fe^{3+})_2(V^{4+},Ti)_2(SiO_4)_2O_4(OH)_4$. The type and amount of OH were 145 determined from bond–valence calculations of O atoms in the crystal structure, and the 146 Raman spectrum of jingwenite–(Y) (Fig. S1).

147 Crystal structure

Unit–cell parameters obtained from the single–crystal and powder X–ray diffraction data (Fig. S2; Tables S2, S3) are: a = 9.4821(2) Å, b = 5.8781(1) Å, c = 19.3987(4) Å, $\beta = 90.165(2)^{\circ}$, and V = 1081.21(4) Å³, and a = 9.5166(6) Å, b = 5.8967(3) Å, c = 19.4557(8) Å, $\beta = 90.111(4)^{\circ}$, and V = 1090.63(7) Å³, respectively. The crystal structure of jingwenite–(Y) was

determined and refined using SHELX (Sheldrick, 2015a, b); crystallographic data and 152 refinement statistics are given in Table S3. The structure was solved in space group /2/a and 153 refined with anisotropic vibrations for all sites. The occupancies of atoms are refined toward 154 minimum R1 and show good agreement with chemical composition. For simplicity, only Y, Dy, 155 Er and Yb are considered in the refinement for rare earth elements (REE) as they are the 156 157 dominant elements according to microprobe analyses. The final anisotropic full-matrix least-squares refinement on F^2 for 111 parameters converged at R1 = 2.46%, wR2 = 6.92% 158 for 874 independent reflections ($I > 4\sigma(I)$) and R1 = 2.67%, wR2 = 6.99% for all 5274 159 160 reflections. The final atomic coordinates and displacement parameters are listed in Table 1, and selected bond lengths and angles are presented in Table 2. The bond-valence sums of 161 atoms were calculated using parameters given by Brese and O'Keeffe (1991) (Table 3; Fig. 162 163 3).

164 Raman spectrum

The Raman spectrum of jingwenite–(Y) shows the bands of O–H stretching vibrations at 2937, 3176, 3486 and 3568 cm⁻¹, the bands of Si–O stretching vibrations at 824, 847, 897 and 1008 cm⁻¹, the bands of Al–O, V–O, Y–O vibrations in the range of 100–700 cm⁻¹(Fig. S1).

169 In-situ Sm-Nd isotope composition

Twenty *in–situ* spot analyses of jingwenite–(Y) gave a Sm–Nd isochron age of 217 ± 25 Ma (2 σ , MSWD=4.0) (Fig. 4A), which is comparable, within uncertainty, to the HREE and U mineralization age of ca. 223 Ma using U–Pb and Sm–Nd dating of uraninite, xenotime–(Y) and hingganite–(Y) (Liu et al., 2022). The $\varepsilon_{Nd(t)}$ values were calculated using an age of 223

174 Ma for HREE mineralization and range from –13.0 to –9.7 (Fig. 4B; Table S4).

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DISCUSSION

The structure of jingwenite-(Y) is composed of b-axis-oriented chains of octahedra 176 consisting of edge-sharing AI (V, Fe)-O octahedra and V (Ti)-O octahedra linked by insular 177 178 Si-O tetrahedra, leaving open channels occupied by rare earth elements (Fig. 3). In the chains of Al-O octahedra chain, two alternative cation sites, Al1 and Al2, share edges O4-179 O4 and O7–O7. Both sites are dominated by AI but with incorporation of Fe^{3+} , V^{3+} , more in 180 Al2 than in Al1. In the chains of V–O octahedra, the V–O octahedra share the edge O5–O6 181 and are strongly distorted with respect to the major difference between the shortest V-O6 182 183 distance (1.664 Å) and the longest V–O6 distance (2.406 Å). The Si–O tetrahedra share O2, O4 with two separate chains of Al–O octahedra and share O1, O3 with two neighboring V–O 184 octahedra in the same chains of V-O octahedra. Rare earth elements are 8-coordinated 185 and occupy open channels along the *b*-axis with the REE-O distances ranging from 2.302 Å 186 to 2.409 Å (average 2.353 Å). Bond valence calculations show that V1 site is dominated by 187 V^{4+} and hydrogen atoms are attached with two oxygen atoms (O7, O8), leading to the ideal 188 crystal chemical formula $Y_2AI_2V^{4+}_2(SiO_4)_2O_4(OH)_4$. The edge-sharing chains of $V^{4+}_2O_4(OH)_4$. 189 190 octahedra also occur in synthetic VO₂ (C2/m) (Marezio et al. 1972) and VO₂ ($P2_1/c$) (Longo and Kierkegaard, 1970), in which V–O bond lengths vary from 1.73 Å to 2.13 Å. The crystal 191 192 structure of jingwenite-(Y) may represent a new structural type of nesosilicate and could therefore be classified as a new group with a Dana classification number 52.4.10.1, or a new 193 194 series with a Strunz classification number 8/B.39.1.

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IMPLICATIONS

The Sm–Nd isochron age of 217 \pm 25 Ma for jingwenite–(Y) indicates an epigenetic origin. 196 Furthermore, our recent studies (Liu et al., 2022) showed that the HREEs and U were 197 leached from the footwall sandstone, which contains abundant heavy minerals, by oxidized 198 basinal brines, and mobilized into the SSC system. The similar $\varepsilon_{Nd(t)}$ values (-13.0 to -9.7) of 199 jingwenite-(Y) also support an identical sedimentary source. Vanadium can be dissolved 200 and transported in oxidized fluids as V^{5+} , whereas V^{4+} and V^{3+} are insoluble in hydrothermal 201 fluids and preferentially partition into mineral phases (Fischer, 1973; Huang et al., 2015a). In 202 jingwenite–(Y), V occurs mainly as V^{4+} while the crystal structure indicates that V^{3+} can 203 substitute for AI^{3+} in Y₂AI₂V⁴⁺₂(SiO₄)₂O₄(OH)₄. Thus, just like HREE and U, V is also likely 204 leached and transported as V^{5+} by oxidized fluids, then reduced to insoluble V^{4+} or V^{3+} by 205 organic-rich beds in the overlying dolostone/limestone, where it is precipitated and forms 206 into jingwenite–(Y). 207

208 Collectively, the abundance of jingwenite–(Y) at Yushui not only indicates that it could 209 potentially be a valuable resource for HREE and V but also highlights that HREE and V 210 mineralization can also occur in the same sediment–hosted Cu mineral system.

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ACKNOWLEDGMENTS

We thank Guoguang Wang, Xiaochun Li, Changhui Ke, Wei Jian, and Liang Li for their insightful discussion and technical assistance with EPMA and Sm–Nd isotope analysis. We appreciate the careful editing and constructive comments from Prof. Frank Hawthorne and one anonymous reviewer.

216

FUNDING

- This research was jointly funded by the National Natural Science Foundation of China (grants 42130102, 42072054 and 41902072).
- 219

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Figure captions

- Fig. 1. A. Geological map of the Yushui deposit (After Huang et al., 2015b). B. Geological
- cross section of the exploration line a–b in the Yushui deposit (Chen et al., 2021).
- **Fig. 2.** Photomicrographs showing the occurrence and mineral association of jingwenite–(Y)
- 258 (Jw-Y). A. euhedral jingwenite-(Y) crystals with bornite (Bn) and chalcopyrite (Ccp). B.
- anhedral jingwenite-(Y), roscoelite (Rcl), V-HREE-Sc-bearing mineral phase (HREE-V-

- Sc), quartz and colloidal thortveitite (Tvt) in a matrix of bornite (Bn), chalcopyrite (Ccp), and
- nolanite (Nol), in reflected light, parallel nicols.
- Fig. 3. Crystal structure of jingwenite-(Y) (unit cell outlined in black lines), plotted with
- VESTA (Momma and Izumi, 2011). A. Crystal structure viewed along the *b*-axis, showing the
- chains of Al–O octahedra (Al1, Al2) and V–O octahedra (V1) linked through isolated Si–O
- tetrahedra (Si1), forming open cavities occupied by REE (Y1), with hydrogen attached with
- 266 O7, O8. B. Edge-sharing chains of Al-O octahedra and V-O octahedra parallel to the b-
- axis viewed along the *c*-axis.
- **Fig. 4.** A. Sm–Nd isochron plot of jingwenite–(Y). B. $\varepsilon_{Nd}(t)$ vs. t plot of jingwenite–(Y). Data of
- hingganite–(Y), xenotime and red sandstone are from Liu et al. (2022).
- 270

Table captions

- Table 1. Fractional atomic coordinates and displacement parameters ($Å^2$) of atoms in jingwenite–(Y).
- Table 2. Selected bond lengths (Å) and angles (°) for jingwenite–(Y).
- Table 3. Calculated bond–valence (*v.u.*) sums for atoms in jingwenite–(Y).

 Table 1 (revision 1)

Sites	Wyck. x		У	Z	Occupancy	$U_{ m eq}$
Y1	8f	0.25637(3)	0.13540(5)	0.65492(2)	Y _{0.76} Yb _{0.13} Dy _{0.06} Er _{0.08}	5 0.0118(1)
Al1	4e	0.25	0.87474(25)	0.5	$AI_{0.916(15)}V_{0.084(15)}$	0.0136(6)
Al2	4e	0.25	0.38344(22)	0.5	$AI_{0.66}V_{0.28}Fe_{0.06}$	0.0149(3)
V1	8f	0.53026(8)	0.34497(11)	0.74258(4)	$V_{0.95} Ti_{0.05}$	0.0134(2)
Si1	8f	0.46320(11)	0.62923(17)	0.60704(6)	Si _{1.00}	0.0118(2)
O1	8f	0.42846(31)	0.85038(42)	0.65639(14)	O _{1.00}	0.0132(6)
O2	8f	0.62861(30)	0.63001(43)	0.58226(15)	O _{1.00}	0.0150(6)
O3	8f	0.43379(29)	0.40254(47)	0.65354(14)	O _{1.00}	0.0136(5)
O4	4f	0.35800(30)	0.62789(42)	0.54030(15)	O _{1.00}	0.0141(6)
O5	8f	0.62633(30)	0.63971(42)	0.73683(15)	O _{1.00}	0.0133(6)
O6	8f	0.63489(33)	0.13009(45)	0.72027(16)	O _{1.00}	0.0166(6)
07(OH)	8f	0.14883(31)	0.13014(44)	0.45881(15)	O _{1.00}	0.0141(6)
O8(OH)	8f	0.36204(31)	0.88768(49)	0.42323(15)	O _{1.00}	0.0152(6)
	<i>U</i> ¹¹	U ²²	U ³³	U^{23}	<i>U</i> ¹³	U ¹²
Y1	0.0127(2)	0.0138(2)	0.0089(2)	0.0006(0)	0.0010(1)	-0.00004(1)
Al1	0.0164(9)	0.0151(9)	0.0093(8)	0	0.0001(6)	0
Al2	0.0174(7)	0.0163(7)	0.0110(6)	0	0.0011(5)	0
V1	0.0155(3)	0.0147(3)	0.0102(3)	0.0008(2)	0.0003(3)	-0.0021(2)
Si1	0.0124(5)	0.0135(5)	0.0094(5)	-0.0005(3)	0.0004(4)	0.0003(3)
O1	0.0187(14) 0.0137(15	6) 0.0072(13	3) 0.0004(9)	0.0013(11)	0.0018(10)
O2	0.0145(14) 0.0190(15	6) 0.0115(13	6) -0.0001(10)	0.0016(11)	-0.0007(10)
O3	0.0141(13	6) 0.0145(13	6) 0.0123(13	3) 0.0008(10)	-0.0026(11)	-0.0006(10)
O4	0.0164(14) 0.0137(14) 0.0122(13	3) -0.0005(9)	-0.0011(12)	0.0007(10)
O5	0.0132(13	6) 0.0147(14) 0.0119(14) 0.0010(9)	0.0007(11)	0.0003(10)
O6	0.0161(13	6) 0.0199(16	6) 0.0137(14) -0.0037(9)	0.0014(12)	0.0020(10)
07(OH)	0.0137(14	·) 0.0170(15	5) 0.0116(13	6) 0.0007(9)	0.0016(12)	0.0011(10)
08(OH)	0.0177(14) 0.0166(14) 0.0114(13	6) 0.0005(10)	0.0031(11)	0.0022(11)

Table 2 (revision 1)							
Bond Length Bond		Length	Bond	Length			
Al1—O8 ^{×2} (OH)	1.833(3)	Al2—04 ^{×2}	1.929(3)	Si1—O4	1.632(3)		
04 ^{×2}	1.939(3)	—07 ^{×2} (OH)	1.942(3)	—O3	1.634(3)		
—07 ^{×2} (OH)	1.951(3)		1.972(3)	—O2	1.642(3)		
			—O1		1.648(3)		
average	1.908	average	1.948	average	1.639		
V1—O6	1.664(3)	Y1—O3	2.302(3)	Si1—O4—Al1	3.234(1)		
—O5	1.955(3)	02	2.312(3)		3.427(1)		
—O5	1.961(3)	—O6	2.319(3)	O1V1	3.181(1)		
—O3	1.982(3)	<u> </u> 01	2.339(3)	—O3—V1	3.178(1)		
—O1	1.998(3)	—O5	2.374(3)	Al1—Al2(0707)	2.990(2)		
—O6	2.406(3)	—O8(OH)	2.381(3)	Al1—Al2(O4O4)	2.888(2)		
		—07(OH)	2.385(3)	V1—V1(O5O6)	3.009(4)		
		—O5	2.409(3)				
average	1.994	average	2.353				
_							
Bond	Angle	Bond	Angle	Bond	Angle		
Si1—O4—Al1	129.6(2)	Si1—O2—Al2	142.2(1.8)	Si1—O1—V1	151.7(2)		
Si1—O3—V1 122.8(2) Al1—O7-		AI1—07—AI2	100.3(1)	AI1—04—AI2	96.6(1)		
V1—O5—V1	100.4(1)	V1—O6—V1	93.5(1)				

Table 3 (revision 1)							
	Y1	AI1	Al2	V1	Si1	Sum	
01	$0.391^{\times 1\downarrow 1 ightarrow}$			$0.562^{\times 1\downarrow 1 \rightarrow}$	$0.957^{\times 1\downarrow 1 \rightarrow}$	1.910	
O2	$0.427^{\times 1 \downarrow 1 \rightarrow}$		$0.442^{\times 2\downarrow 1 \rightarrow}$		$0.979^{\times 1\downarrow 1 \rightarrow}$	1.848	
O3	$0.433^{\times 1\downarrow 1 ightarrow}$			$0.586^{\times 1\downarrow 1 \rightarrow}$	$0.995^{\times 1\downarrow 1 \rightarrow}$	2.014	
O4		$0.453^{\star 2 \downarrow 1 \rightarrow}$	$0.502^{\times2\downarrow1\rightarrow}$		$0.995^{\times 1\downarrow 1 \rightarrow}$	1.950	
O5	$0.341^{\star 2\downarrow 2 ightarrow}$			$0.626^{\times 2 \downarrow 2 \rightarrow}$		1.934	
O6	$0.414^{\times 1\downarrow 1 \rightarrow}$			$0.786^{\times 2 \downarrow 2 \rightarrow}$		1.986	
O7(OH)	0.344 ^{×1↓1}	$0.438^{\times 2\downarrow 1 \rightarrow}$	$0.482^{\times 2\downarrow 1 \rightarrow}$			1.264	
O8(OH)	0.353 ^{×1↓1}	$0.595^{\star 2\downarrow 1 ightarrow}$				0.948	
Sum.	3.044	2.972	2.852	3.972	3.926		





Fig. 1 (revision 1)



Fig. 2 (revision 1)



В

a

b



Fig. 3 (revision 1)

