Lusernaite-(Y), $Y_4Al(CO_3)_2(OH,F)_{11} \cdot 6H_2O$, a new mineral species from Luserna Valley, Piedmont, Italy: Description and crystal structure

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ABSTRACT

The new mineral species lusernaite-(Y), ideally $Y_4Al(CO_3)_2(OH,F)_{11} \cdot 6H_2O$, has been discovered in small fractures of the "Luserna Stone," a leucocratic orthogneiss belonging to the Dora-Maira massif, Western Alps, Italy. It occurs as colorless, thin platelets, with white streak and mica-like pearly luster, elongated along [100] and flattened on {010}, arranged in radiating aggregates. Lusernaite-(Y) is associated with aeschynite-(Y), albite, "chlorite," hematite, pyrite, quartz, and titanite. Lusernaite-(Y) has a perfect cleavage on {010} and a less marked one probably on {100}. Its calculated density is 2.810 g/cm^3. In plane-polarized light, it is transparent, with parallel extinction and positive elongation. Lusernaite-(Y) is biaxial positive; its optical orientation is $\mathbf{a} = Z$, $\mathbf{b} = X$, $\mathbf{c} = Y$. Owing to the crystal morphology, only two refractive indices could be measured, corresponding to $\beta = 1.566(2)$ and $\gamma = 1.577(2)$.

Lusernaite-(Y) is orthorhombic, space group $Pmna$, with $a = 7.8412(3)$, $b = 11.0313(5)$, $c = 11.3870(4)$ Å, $V = 984.96(7)$ Å^3, $Z = 2$. Main diffraction lines of the X-ray powder diffraction pattern are [d in Å, (I), (hkl)]: 11.02 (100) (010), 7.90 (49) (011), 5.66 (25) (002), 5.06 (24) (012), 4.258 (33) (112), 3.195 (27) (220), 3.095 (21) (212). Raman spectroscopy confirmed the presence of CO_3 groups (sharp peak at 1096 cm^{-1}); due to the very strong luminescence, the bands of the OH and H_2O groups could not be seen.

Chemical analyses by electron microprobe gave (wt%) Al_2O_3 6.11, Y_2O_3 43.52, La_2O_3 0.02, Ce_2O_3 0.04, Nd_2O_3 0.03, Sm_2O_3 0.16, Gd_2O_3 1.39, Dy_2O_3 3.46, Er_2O_3 3.15, Yb_2O_3 2.09, CaO 0.33, PbO 0.37, H_2O 22.76, CO_2 9.95, F 1.40, O≡F –0.59, sum 94.19; H_2O and CO_2 were determined from structure refinement. The empirical formula by assuming the presence of 2 $(CO_3)^{2-}$ groups, 11 $(OH,F)^-$ anions, and 6 H_2O groups, in agreement with micro-Raman and structural results, is $(Y_{3.41}Dy_{0.16}Er_{0.15}Yb_{0.09}Gd_{0.07}Ca_{0.05}Pb_{0.02}Sm_{0.01})_{\Sigma3.96}Al_{1.06}(CO_3)_{2.00}(OH_{10.35}F_{0.65})_{\Sigma11.00} \cdot 6H_2O$.

The crystal structure was solved by direct methods and refined on the basis of 840 observed reflections to $R_1 = 6.8\%$. In the structure of lusernaite-(Y), yttrium and REE cations occupy two distinct sites, Y1 and Y2, both in eightfold coordination. The structure is built by layers parallel to (010), formed by chains of edge-sharing Y-centered polyhedra (Y1), which run along [100], and are connected along $\mathbf{c}$ through Al-centered octahedra. These chains are decorated on one side by corner-sharing chains of Y-centered polyhedra (Y2), and on the other side by CO_3 groups. Along [001] the decorated chains alternate their polarity.

Lusernaite-(Y), named after the type locality, the Luserna Valley, shows a new kind of structure among the natural carbonates of REE. Its origin is related to the circulation of hydrothermal solutions during the late-stage Alpine tectono-metamorphic events.

Keywords: Lusernaite-(Y), new mineral species, carbonate, yttrium, crystal structure, Luserna stone, Piedmont, Italy

INTRODUCTION

The "Luserna stone," a leucocratic orthogneiss, has been quarried since the Middle Ages, and it is an important building material for its widespread occurrence and use in historical monuments. The first publications about this stone date back to the beginning of the 19th century, with the studies of Barelli (1835) and De Bartolomeis (1847), focused on the technological and economic importance of the quarrying activities. The first scientific work can be considered that of Gastaldi (1874), who tentatively reconstructed the lithostratigraphic setting of the "Luserna stone." Since then, a large number of studies about this stone have been published (Sandrone 2001). Surprisingly, only recently the mineralogical peculiarities of this formation have been investigated. Vaccio (2002), Piccoli et al. (2007), and Finello et al. (2007) described the minerals occurring in late-stage fractures in the "Luserna stone," reporting more than 40 different

mineral species. A large number of REE and Y phases was listed by the latter authors, including aeschynite-(Y), allanite-(Ce), aluminocerite-(Ce), cerite-(Ce), fergusonite-(Y), hellandite-(Y), kainosite-(Y), monazite-(Ce), synchysite-(Ce), xenotime-(Y), and probably polycrase-(Y). In addition, some unidentified minerals have been described; among these, the mineral UK01, which corresponds to the new mineral species lusernaite-(Y).

The new species and its name have been approved by the IMA-CNMNC (no. 2011-108). It is named after the type locality, the Luserna Valley (Piedmont, Italy); the Levinson suffix (Bayliss and Levinson 1988) indicates the dominance of Y among Y and REE. The type material is deposited in the mineralogical collections of the Museo di Storia Naturale, University of Pisa, via Roma 79, Calci (Pisa, Italy) under the catalog number 19445. A co-type specimen is kept in the mineralogical collections of the Museo Regionale di Scienze Naturali, via Giovanni Giolitti 36, Torino (Italy), with catalog number M/15901.

Geological setting and mineral occurrence

The "Luserna stone" refers to a heterogeneous series of leucocratic gneisses (characterized by a micro-Augen texture and gray-greenish or locally pale blue color) and phengitic schists, cropping out in an area 50 km^2 wide in the Cottian Alps, at the border of the provinces of Torino and Cuneo. This complex forms a flat body structurally located at the top of the Dora-Maira massif, the southernmost of the so-called Internal Crystalline Massif of the Western Alps (Bussy and Cadoppi 1996).

Whereas Vialon (1966) interpreted the "Luserna stone" as a metamorphosed volcano-sedimentary sequence, other authors proposed a granitic origin on the basis of petrographic and geochemical data (Cadoppi 1990; Bussy and Cadoppi 1996; Sandrone et al. 2004). The age of this complex is still unknown; U-Pb dating on zircon indicates that most of the dated metagranites belonging to the Dora-Maira massif were emplaced during the Upper Carboniferous, in relation with the Variscan orogeny (Bussy and Cadoppi 1996).

Mineral assemblages and phase chemistry suggest an Alpine metamorphic evolution characterized by an early eclogite-facies stage at pressures between 1.4 and 2.5 GPa for 550 ± 50 °C; this stage was overprinted by a greenschist-facies metamorphism during the exhumation of the Doira-Maira massif at 35–40 My (Scaillet et al. 1992).

Mineralogically, the "Luserna stone" is composed of quartz (30–45 vol%), K-feldspar (10–25 vol%), albite (15–25 vol%), "phengite" (10–20 vol%), and subordinate "biotite," "chlorite," and epidote-group minerals. Common accessories are opaque phases, titanite, "apatite," and zircon; locally, "tourmaline," carbonates, "axinite," and fluorite are also present (Sandrone et al. 2004).

Finello et al. (2007) described two kinds of mineral occurrence: (1) in small fractures, perpendicular to the main field foliation, probably related to the late-stage tectonic events, and (2) in small aplite dikes, parallel to the main foliation. Lusernaite-(Y) was found only in the first kind of occurrence.

Lusernaite-(Y) was found in the Seccarezze quarries (latitude 44°46′N, longitude 7°12′E), Luserna San Giovanni, Torino, Piedmont, Italy. The first find of lusernaite-(Y) dates back to 1991, when a mineral collector, G. Finello, found two specimens of a

phase that proved to be a possible new mineral species and was described as UK01 (UKGFN009Mugniv) by Finello et al. (2007); a new find of better quality was made in 2006 by the mineral collectors B. Marello and C. Alciati. Other findings of this rare mineral were done in October 2009 (about 15 specimens) and in April–May 2010 (eight collected specimens). The new findings allowed a complete description of the mineral and its approval as a new species. Finally, a last finding of lusernaite-(Y) occurred in March 2012, as radial aggregates of well-developed tabular crystals, in one case associated with calcite.
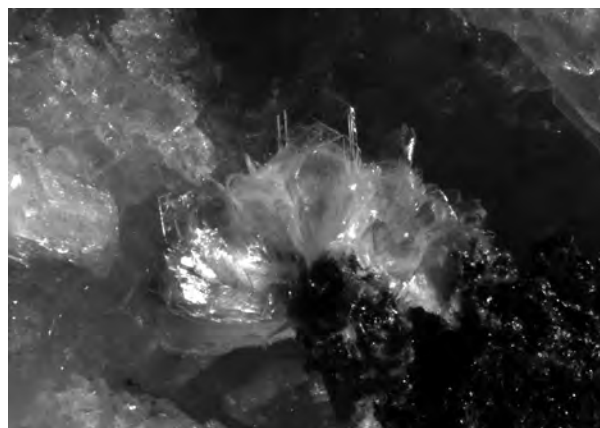
The crystallization of lusernaite-(Y) is probably related to the circulation of hydrothermal fluids in late-stage fractures during the Tertiary Alpine tectono-metamorphic events.

Mineralogical characterization

Appearance and physical properties

Lusernaite-(Y) occurs as thin platelets, up to 1 mm in size, with an indistinct, roughly six-sided outline. Crystals are elongated along **a** and flattened on {010} and are arranged in radiating aggregates (Fig. 1). Associated minerals are aeschynite-(Y), albite, "chlorite," hematite, pyrite, quartz, and titanite.

Lusernaite-(Y) is colorless, with a white streak and a mica-like pearly luster. In plane-polarized light, it is transparent. Between crossed polars, the mineral shows parallel extinction, with a positive elongation parallel to [100]. Birefringence is weak. It is optically biaxial positive, with a low value of 2V. The optical orientation is **a** ∥ Z, **b** ∥ X, **c** ∥ Y. Due to the crystal morphology, only the two refractive indices lying within the (010) plane could be measured in white light using the Becke line method. The measured refractive indices are β = 1.566(2) and γ = 1.577(2). The mean refractive index n of lusernaite-(Y), calculated using the Gladstone-Dale relationship (Mandarino 1979, 1981), using the empirical formula obtained assuming the presence of stoichiometric CO_2 and H_2O (see below), is 1.588. The difference between the measured values and the calculated mean refractive index may be ascribed to chemical variations; for example, the greater the fluorine content, the lower is the

Figure 1. Colorless thin tabular crystals of lusernaite-(Y) associated with "chlorite." Crystal aggregate size: 2 mm. Collection and photo B. Marello.

mean refractive index of lusernaite-(Y). In addition, other possible ionic substitution in the cation sites (e.g., differences in the relative abundance of REE and Y) may be invoked.

Density was not measured due to the small crystal size and the difficulty in observing the mineral in the heavy liquids; the calculated density, based on the empirical formula used for the calculation of the mean refractive index, is 2.810 g/cm³.

Lusernaite-(Y) is brittle, with a perfect {010} cleavage; another cleavage (probably on {100}) was observed perpendicular to the crystal elongation. Owing to the difficulty in preparing a polished surface and to the softness of the mineral, a reliable value of hardness could not be measured.

CHEMICAL AND SPECTROSCOPIC DATA

Chemical data

Preliminary qualitative chemical analysis by energy-dispersive spectroscopy was performed using a Phillips LX30 SEM, equipped with an EDAX DX4 system. It indicated that the only elements with $Z > 8$ occurring in lusernaite-(Y) are Y, Al, F, and minor Dy, Gd, and Er.

Quantitative chemical data were collected using a JEOL JXA-8200 electron-microprobe, using an acceleration voltage of 15 kV and a beam current of 5 nA. The beam size was set to 15 μm to prevent (or limit) the deterioration of the crystal of lusernaite-(Y); notwithstanding this, some surficial damage of the analyzed crystals was observed. Standards were (element, emission line): anorthite (Al$K\alpha$, Ca$K\alpha$), synthetic YPO₄ (Y$L\alpha$), synthetic REEPO₄ set (La$L\alpha$, Ce$L\alpha$, Dy$L\alpha$, Nd$L\alpha$, Er$L\alpha$, Yb$L\alpha$, Gd$L\alpha$, Sm$L\alpha$), galena (Pb$M\alpha$), synthetic RbMnF₃ (F$K\alpha$). Concentrations of the REE were corrected for overlaps. Fluorine concentration was measured on the basis of the F$K\alpha$ peak height; consequently, its measure is probably not accurate, owing to the problems associated with F$K\alpha$ peak shape and breadth:height variability (e.g., Solberg 1982; Raudsepp 1995; Ottolini et al. 2000).

Table 1 gives the weight concentrations obtained on a polished fragment of lusernaite-(Y). The reported H₂O and CO₂ contents were estimated, in agreement with the results of the crystal structure study, showing the presence of 2 $(CO_3)^{2-}$ groups, 11 $(OH,F)^-$ anions, and 6 H₂O groups per formula unit (pfu). The low total, i.e., 94.19 wt%, could be attributed to the surficial damage of the sample and to the difficulty in preparing a good quality polished surface.

The empirical formula of lusernaite-(Y), based on 23 anions pfu, is $(Y_{3.41}Dy_{0.16}Er_{0.15}Yb_{0.09}Gd_{0.07}Ca_{0.05}Pb_{0.02}Sm_{0.01})_{\Sigma 3.96}Al_{1.06}(CO_3)_{2.00}(OH_{10.35}F_{0.65})_{\Sigma 11.00}\cdot 6H_2O$. The empirical formula simplifies to $Y_4Al(CO_3)_2(OH)_{11}\cdot 6H_2O$, which requires (wt%) Y₂O₃ 56.61, Al₂O₃ 6.39, CO₂ 11.03, H₂O 25.97, total 100.00.

Lusernaite-(Y) is slowly soluble in dilute 1:10 HCl, with the development of small gas bubbles, in agreement with the occurrence of carbonate groups in its structure.
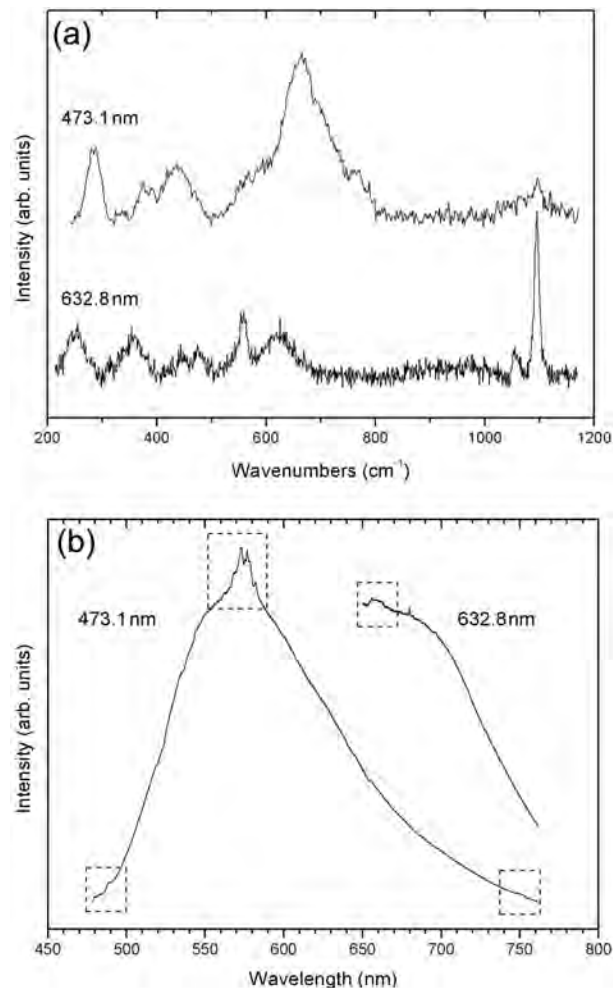
Micro-Raman spectroscopy

Unpolarized micro-Raman spectra (Fig. 2) were obtained on an unpolished crystal of lusernaite-(Y) in nearly backscattered geometry, with a Jobin-Yvon Horiba "Labram" apparatus, equipped with a motorized x-y stage and an Olympus microscope with a 50× objective. The 632.8 nm line of a He-Ne laser and the 473.1 nm line of a Nd:YAG laser were used. The minimum lateral and depth resolution were set to a few micrometers. The system was calibrated using the 520.6 cm⁻¹ Raman peak of silicon before each experimental session. Spectra were collected through multiple acquisitions with single counting times ranging between 20 and 180 s. Both Raman spectra obtained with 473.1 and 632.8 nm excitation lines are dominated by strong luminescence features, in the form of many groups of sharp bands, superimposed on a broad band centered at about 570 nm. The only features ascribable to a Raman band is the sharp peak at 1096 cm⁻¹, confirming the presence of CO_3^{2-} groups in the structure.

The main luminescence peaks are located in the region between 560 and 590 nm; the strongest ones are at 573, 576, and 582 nm. Other weaker groups of luminescence bands are visible in the regions around 488 and 752 nm (using the 473.1 nm excitation) and 660 nm (using the 632.8 nm line). Dy^{3+} could be the cause of these luminescence bands, except the broad ones (Gaft et al. 2005); this observation agrees with the fact that Dy^{3+} is the main substituent of Y^{3+}, as shown by EPMA data. Due to the strong luminescence, even in the region of the bending and stretching of O-H bonds, no detectable Raman signals could be collected.

TABLE 1. Microprobe analyses of lusernaite-(Y): Chemical composition as wt% (average $n = 18$) and number of atoms on the basis of (O+F) = 23 apfu, assuming the presence of 2 (CO₃) and 6 H₂O groups pfu

Oxide	wt% (average $n = 18$)	Range	e.s.d.	apfu (based on 23 anions)
Al₂O₃	6.11	5.94–6.45	0.13	1.060
Y₂O₃	43.52	42.28–44.69	0.77	3.410
La₂O₃	0.02	0.00–0.12	0.03	0.002
Ce₂O₃	0.04	0.00–0.16	0.05	0.002
Nd₂O₃	0.03	0.00–0.12	0.03	0.002
Sm₂O₃	0.16	0.00–0.37	0.10	0.008
Gd₂O₃	1.39	1.06–1.66	0.15	0.068
Dy₂O₃	3.46	2.97–3.77	0.19	0.164
Er₂O₃	3.15	2.84–3.61	0.20	0.146
Yb₂O₃	2.09	1.75–2.53	0.25	0.094
CaO	0.33	0.16–0.58	0.12	0.052
PbO	0.37	0.19–0.57	0.12	0.015
F	1.40	1.19–1.52	0.08	0.652
H₂O(calc)	22.76			6 H₂O
				10.348 OH⁻
CO₂(calc)	9.95			2.000
Subtotal	94.78			
O≡F	−0.59			
Total	94.19			

FIGURE 2. Micro-Raman spectra of lusernaite-(Y) between 200 and 1200 cm⁻¹ (**a**) and the effect of luminescence (**b**) for both 473.1 and 632.8 nm excitation lines.

X-ray crystallography and crystal structure determination

The powder X-ray diffraction pattern of lusernaite-(Y) was obtained using a 114.6 mm Gandolfi camera with Ni-filtered Cu$K\alpha$ radiation (Table 2). Indexing of the reflections was based on a calculated powder pattern obtained by the structural model described below, using the software POWDERCELL (Kraus and Nolze 1996). The unit-cell parameters refined from the powder data with the software UNIT CELL (Holland and Redfern 1997), on the basis of 24 univocally indexed reflections, are $a = 7.839(2)$, $b = 11.023(2)$, $c = 11.383(2)$ Å, and $V = 983.6(2)$ Å^3.

Preliminary Weissenberg photographs were obtained using a small crystal of lusernaite-(Y) and allowed the morphological orientation of the crystal.

Single-crystal X-ray diffraction data were collected using an Oxford Gemini R Ultra diffractometer equipped with a CCD area detector at CrisDi (Interdepartmental Centre for the Research and Development of Crystallography, Torino, Italy). Graphite-monochromatized Mo$K\alpha$ radiation was used. Crystal data and experimental details are reported in Table 3. Some 763 frames were collected in 1.0 slices between ω angles 3.57° and 33.49°. The exposure time was 130 s per frame. Data were integrated and corrected for Lorentz and polarization, background effects, and absorption, using the package CRYSALIS^{Pro} (Oxford Diffraction 2007a, 2007b). Refinement of the unit-cell parameters was based on all measured reflections with $I > 200\sigma(I)$. At room temperature, the unit-cell parameters are $a = 7.8412(3)$, $b = 11.0313(5)$, $c = 11.3870(4)$ Å, $V = 984.96(7)$ Å^3, space group $Pmna$, $Z = 2$. The a:b:c ratio is 0.711:1:1.032. A total of 1081 independent reflections were collected and the structure was solved and refined by means of the SHELX set of programs (Sheldrick 2008).

After having located the Y and Al atoms, the structure was completed through successive difference-Fourier maps. The latter showed the presence of two maxima around one of the two Y-centered sites, i.e., Y1, at 0.80 and 0.98 Å, respectively. On the basis of chemical data, these residuals were attributed to Pb, lowering significantly the R values.

The refined occupancies of the Y1, Y2, Pb1a, and P1b sites were $Y_{0.370(8)}Er_{0.116(8)}$, $Y_{0.457(7)}Dy_{0.043(7)}$, $Pb_{0.007(1)}$, and $Pb_{0.007(1)}$, respectively. This indicates that the other REE measured by EPMA prefer to occupy Y1 and Y2 sites. The two refined Pb occupancies would equal to a Pb content of ~0.06 apfu, a value, which is higher than the measured value of 0.015 Pb pfu. Thus, it may also be possible that some of the measured REE, which have ionic radii fairly different from that of Y^{3+} (e.g., Gd^{3+}, Yb^{3+}), may reside in these satellite positions.

Furthermore, some unacceptably short Pb distances are observed, e.g., Pb1a-O2 1.83(3) Å and Pb1b-O6 2.03(1) Å, and the actual coordination of these split sites cannot be assessed. The total refined site scattering value at the Y1+Y2 sites is 176.5 e^-, to be compared with 167.8 e^- obtained from the chemical data. Two hydrogen positions were located in the difference-Fourier maps; these hydrogen atoms were added to the model but their coordinates and isotropic displacement parameters were not refined. Examination of the bond-valence balance and the hydrogen bonds suggested that two O sites, namely O4 and O5, are possible F-bearing sites. A lower R value was achieved by introducing fluorine at the O4 site. The O:F ratio in the O4 site was fixed taking into account the EPMA data.

TABLE 2. Measured X-ray powder diffraction data for lusernaite-(Y)

I_{obs}	d_{meas} (Å)	I_{calc}	d_{calc} (Å)	$h\,k\,l$	I_{obs}	d_{meas} (Å)	I_{calc}	d_{calc} (Å)	$h\,k\,l$
vs	11.02	100	11.03	0 1 0	w	2.901	11	2.904	1 2 3
s	7.90	49	7.92	0 1 1	w	2.790	15	2.787	2 2 2
m	6.41	15	6.46	1 0 1	vw	2.667*			
m	5.66	25	5.69	0 0 2	vw	2.606	4	2.611	2 3 1
mw	5.06	24	5.06	0 1 2	w	2.526	12	2.530	0 2 4
vw	4.600*				w	2.422	9	2.426	2 3 2
mw	4.258	33	4.251	1 1 2	mw	2.305	11	2.304	2 0 4
w	3.961	9	3.961	0 2 2	w	2.251	5	2.256	2 1 4
vw	3.834						4	2.251	0 3 4
w	3.676	12	3.694	2 1 0	vw	2.185	1	2.182	3 2 2
		10	3.677	0 3 0	w	2.152	3	2.153	3 0 3
vw	3.592	1	3.589	0 1 3	w	2.091	5	2.097	2 4 2
w	3.504	10	3.514	2 1 1	vw	2.010	4	2.005	3 2 3
w	3.416	6	3.416	1 0 3			5	1.995	3 3 2
vw	3.345*				w	1.941	7	1.952	2 3 4
mw	3.195	27	3.196	2 2 0	w	1.824	4	1.822	2 5 2
mw	3.095	21	3.099	2 1 2	w	1.711	5	1.708	2 0 6

Notes: The d_{hkl} values were calculated on the basis of the unit cell refined by using single-crystal data. Intensities ($I/I_{100} \times 100 > 1$ only) were calculated on the basis of the structural model. Observed intensities were visually estimated. vs = very strong; s = strong; ms = medium-strong; m = medium; mw = medium-weak; w = weak; vw = very weak. * indicates three unindexed reflections, probably due to unidentified impurities.

TABLE 3. Crystal data and summary of parameters describing data collection and refinement for lusernaite-(Y)

Crystal data	
Crystal size (mm³)	$0.33 \times 0.09 \times 0.01$
Cell setting, space group	Orthorhombic, $Pmna$
Unit-cell dimensions	
a (Å)	7.8412(3)
b (Å)	11.0313(5)
c (Å)	11.3870(4)
V (Å³)	984.96(7)
Z	2
Data collection and refinement	
Radiation type (λ)	Mo$K\alpha$ (0.71073 Å)
Temperature (K)	~298
Maximum observed 2θ(°)	52.74
Measured reflections	23367
Unique reflections	1081
Reflections $F_o > 4\sigma F_o$	840
R_{int}	0.1131
$R\sigma$	0.0475
Range of h, k, l	$-9 \le h \le 9$
	$-13 \le k \le 13$
	$-14 \le l \le 14$
$R_1 [F_o > 4\sigma F_o]$	0.0682
R_1 (all data)	0.0861
wR_2 (on F_o^2)	0.1990
Goof	1.056
Number of l.s. parameters	90
$\Delta\rho_{max}$ and $\Delta\rho_{min}$	2.67, −1.09

Note: Extinction coefficient was 0. The weighting scheme is defined as w = q/$[\sigma^2(F_o^2) + (a*P)^2 + b*P]$, where $P = [2F_c^2 + Max(F_o^2,0)]/3$. a and b values are 0.1419 and 2.9989.

Refinement converged to $R_1 = 6.82\%$ for 840 observed reflections and 90 parameters. The largest peak and hole in the final difference-Fourier map are 2.67 and −1.09 e Å^{-3}, respectively. Tables 4 and 5 report the atomic coordinates and displacement parameters, and selected bond distances, respectively. CIF^1 is available on deposit.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

General features and cation coordination

The crystal structure of lusernaite-(Y) (Fig. 3) is layered on (010); layering is a common feature of (Y, REE) carbonates (Grice et al. 1994, 2007). In lusernaite-(Y) only one kind of layer occurs; it is composed by two independent Y-centered polyhedra, one Al-centered octahedron, one C-centered triangle, six anion positions, and three H$_2$O groups.

The two Y-centered sites, namely Y1 and Y2, are eightfold coordinated. The average Y-φ bond-lengths are 2.387 and 2.349 Å for Y1 and Y2 sites, respectively, with single values ranging from 2.267 (Y2-O4 bond) to 2.486 (Y1-O5 bond) Å. Pb-atom probably occupies two sub-positions, owing to its stereochemical activity; similar behavior has been observed for lead replacing potassium in synthetic Pb$_2$(Pb,K)$_4$[Si$_8$O$_{20}$]O (Moore et al. 1985) and lead replacing barium in hyalotekite (Moore et al. 1982; Christy et al. 1998). Aluminum is octahedrally coordinated, with an average bond-length of 1.898 Å. The planar carbonate groups (CO$_3$) are inclined with respect to the overall structural layering; they are attached through corner-sharing to two Y1-centered polyhedra.

TABLE 4. Atomic coordinates and displacement parameters for lusernaite-(Y)

Site	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	$U_{eq/iso}$
Y1	¼	0.4975(2)	¾	0.0120(7)	0.0281(13)	0.0111(7)	0	0.0007(4)	0	0.0170(6)
Pb1a	¼	0.570(7)	¾	0.0120(7)	0.0281(13)	0.0111(7)	0	0.0007(4)	0	0.0170(6)
Pb1b	¼	0.409(5)	¾	0.0120(7)	0.0281(13)	0.0111(7)	0	0.0007(4)	0	0.0170(6)
Y2	0	0.2304(1)	0.8487(1)	0.0166(8)	0.0282(9)	0.0160(8)	0.0001(6)	0	0	0.0203(6)
Al	0	½	0	0.012(3)	0.034(4)	0.009(3)	−0.002(2)	0	0	0.018(2)
C	½	0.683(1)	0.915(1)	0.016(8)	0.036(9)	0.012(7)	0.007(6)	0	0	0.021(3)
O1	−0.1624(9)	0.3949(7)	0.9272(6)	0.011(4)	0.046(5)	0.013(4)	−0.001(3)	0.001(3)	0.001(3)	0.023(2)
O2	0.357(1)	0.6424(7)	0.8746(7)	0.017(4)	0.054(6)	0.030(5)	−0.009(4)	0.007(3)	−0.007(4)	0.034(2)
O3	½	0.759(1)	0.9988(9)	0.022(6)	0.038(6)	0.018(5)	−0.011(4)	0	0	0.026(3)
O4	−¼	0.214(1)	¾	0.016(5)	0.046(7)	0.020(5)	0	0.000(3)	0	0.027(3)
O5	0	0.4177(9)	0.1437(8)	0.021(6)	0.033(6)	0.006(5)	0.007(4)	0	0	0.020(2)
O6	0	0.387(1)	0.7091(9)	0.019(6)	0.037(7)	0.007(5)	0.007(4)	0	0	0.021(2)
Ow1	−0.188(2)	0.135(1)	0.9854(9)	0.052(7)	0.063(7)	0.050(7)	0.019(5)	0.016(5)	0.007(6)	0.055(3)
Ow2	0	0.033(2)	0.770(2)	0.09(2)	0.10(2)	0.09(2)	−0.036(12)	0	0	0.093(7)
Ow3	−¼	−0.141(4)	¾							0.101(15)
H1	−0.201	0.037	0.989							0.05
H2	−0.314	0.158	0.014							0.05

TABLE 5. Selected bond distances (Å) for lusernaite-(Y)

Y1-O2	2.297(8) ×2		Y2-O4	2.267(1) ×2
Y1-O6	2.353(6) ×2		Y2-O6	2.350(10)
Y1-O1	2.413(7) ×2		Y2-Ow2	2.354(21)
Y1-O5	2.486(6) ×2		Y2-Ow1	2.387(10) ×2
<Y1-O>	2.387		Y2-O1	2.391(7) ×2
			<Y2-O>	2.349
Al-O5	1.872(9) ×2		C-O3	1.268(19)
Al-O1	1.912(7) ×4		C-O2	1.290(11) ×2
<Al-O>	1.898		<C-O>	1.28
			O2-C-O3	119.8(7)°
			O2-C-O2	120(1)°

The (010) layer is built by chains of edge-sharing Y-centered polyhedra (Y1 site), which run along [100], and are connected along [001] through Al-centered octahedra. These chains are decorated on one side by corner-sharing chains of Y-centered polyhedra (Y2 site), and on the other side by CO_3 groups. Along [001] the decorated chains alternate their polarity. The (010) layers are stacked along [010] by hydrogen bonding (see next section).
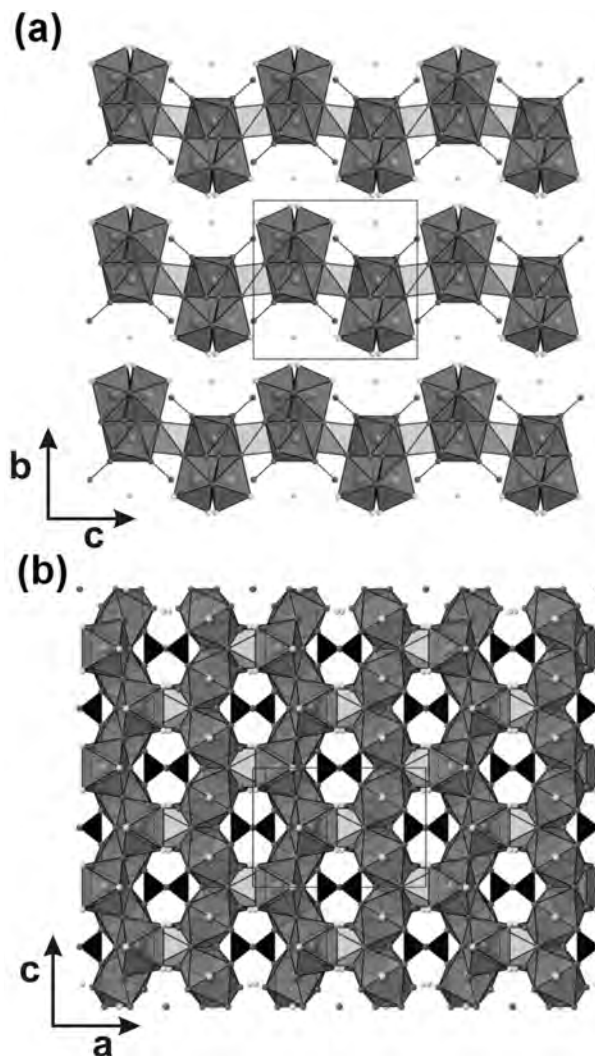
Hydrogen bonding in lusernaite-(Y)

The calculation of the bond-valence sums (BVS) for the nine independent anion sites (Table 6) gives values significantly different from 2 valence units (v.u.) for all these sites. Examination of the O···O distances shorter than 3.0 Å (Table 7) suggests the presence of hydrogen bonds.

The undersaturation of O2 and O3 oxygen atoms, both bonded to CO_3 groups, is removed by their probable hydrogen bonding; O2 is linked to O1 (hosting an OH group), whereas O3 is bonded to O6 (hosting an OH group) and Ow1 (hosting a H_2O group). By applying the equation proposed by Ferraris and Ivaldi (1988), their BVS increase up to 1.99 and 2.01 v.u., indicating their population by oxygen atoms. An additional O2···Ow3 hydrogen bond will be discussed below.

O1 and O6 sites, with BVS of 0.99 and 1.04 v.u., respectively, are occupied by hydroxyl anions, as the O4 and O5 sites. Moreover, the two latter sites are not involved in any plausible hydrogen bond, and they could therefore host also fluorine atoms.

The Ow1 site is occupied by an H_2O group, which is involved in two hydrogen bonds: the Ow1···O3 bond and the Ow1···Ow1′ bond, with the two Ow1 sites belonging to successive layers along [010]. The two hydrogen atoms located during the crystal structure determination, namely H1 and H2, are at 1.09 and 1.08 Å from Ow1. These bond lengths are a little longer than the ex-

FIGURE 3. Crystal structure of lusernaite-(Y), as seen down [100] (**a**) and [010] (**b**). Polyhedra: dark gray = Y-centered polyhedra; light gray = Al-centered octahedra; black = CO_3 groups. Balls: dark gray = O^{2-} or $(OH,F)^-$ anions; light gray = H_2O molecules or mixed H_2O/OH^- occupied site.

TABLE 6. Bond-valence calculations for lusernaite-(Y), according to Brese and O'Keeffe (1991)

	Y1	Y2	Al	C	Σv (O-X)	Σv (O-X) ‡	Species
O1	0.34*	0.36*	0.49†		1.19	0.99	OH⁻
O2	0.47*			1.31*	1.78	1.98	O²⁻
						2.13§	
O3				1.39	1.39	1.99	O²⁻
O4		0.46*			0.92	0.92	OH⁻,F⁻
O5	0.28*		0.55*		1.11	1.11	OH⁻
O6	0.40*	0.40			1.20	1.04	OH⁻
Ow1		0.36*			0.36	0.01‖	H₂O
						0.27#	
Ow2		0.40			0.40	0.20	H₂O
						0.60	OH⁻
Ow3					0.00	–0.15	H₂O
Σv (X-O)	2.98	3.16	3.06	4.01			

* (2x →).
† (4x →).
‡ Bond valence balance after correction for O···O hydrogen bonds.
§ If involved in Ow3···O2 hydrogen bond.
‖ If donor in Ow1···Ow1 hydrogen bond.
If acceptor in Ow1···Ow1 hydrogen bond. For Y1 and Y2 sites, the parameters for Y-O and Y-F bonds were used.

TABLE 7. O···O distances (in angstroms) in the suggested hydrogen-bonding scheme, with corresponding bond-valence values (v.u.)

O···O bond donor → acceptor	d (Å)	v.u.
Ow1 (H₂O) → O3 (O)	2.72(1)	0.22
Ow2 (H₂O/OH) ↔ Ow3 (H₂O)	2.75(4)	0.20
O1 (OH) → O2 (O)	2.76(1)	0.20
O6 (OH) → O3 (O)	2.89(2)	0.16
Ow3 (H₂O) → O2(O)	2.91(4)	0.15
Ow1 (H₂O) ↔ Ow1 (H₂O)	2.99(2)	0.13

pected ones, but taking into account the quality of the refinement and the possible disorder affecting the hydrogen-bond scheme, they could be retained as acceptable. Owing to the presence of a mirror plane, H1 is statistically bonded to the Ow1 of the upper or the lower layer; the H2 takes part in the Ow1-O3 bond. The H1-Ow1-H2 bond angle is ca. 98°.

A more complex situation occurs at the Ow2 and Ow3 sites. The Ow2 site is at 2.75(4) Å from Ow3. The latter has a refined electron density indicating half occupancy. Figure 4 illustrates a possible hydrogen-bonding scheme involving the Ow2 and Ow3 sites. Along [100], every two Ow2, one acts as donor in Ow2···Ow3 hydrogen bond, the other as acceptor. Consequently, the Ow2 site will be occupied, along **a**, by a regular alternation of H₂O and OH⁻ groups. Owing to the lack of any correlation between adjacent columns, the Ow2 site will be statistically occupied by H₂O and OH⁻. In addition, Ow3 is at 2.91(4) Å from two O2 sites. The angle between O2···Ow3···Ow2 is ca. 114° and agrees with a hydrogen bond. It is possible that only one of the two O2 sites is involved in a hydrogen bond with Ow3. In this way, O2 could be slightly oversaturated, with a BVS of 2.13 v.u., whereas Ow3 displays a negative BVS, i.e., –0.15 v.u. The deviation from an ideal valence sum could be related to the disorder occurring along [100], with the statistically occupied Ow3 site probably representing an average position.

In conclusion, hydrogen bonds in lusernaite-(Y) are very important in assuring the link between successive (010) layers, in agreement with its perfect {010} cleavage; the hydrogen bonds linking successive layers are Ow1···Ow1 and, probably, Ow3···O2.
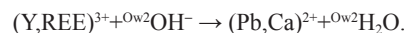

FIGURE 4. The possible hydrogen bonds connecting successive (010) layers. Polyhedra: dark gray = Y-centered polyhedra; light gray = Al-centered octahedra; black = CO₃ groups. Balls: dark gray = O2 sites; gray = Ow1, Ow2, Ow3 sites.

Crystal chemistry of lusernaite-(Y)

Crystal-structure determination and bond-valence analysis indicate that Y1 is coordinated by two oxygen anions and six hydroxyl groups, Y2 is bonded to five (OH,F) anions, two H₂O groups, and a mixed (H₂O/OH) site; Al is octahedrally coordinated by six hydroxyl groups.

Consequently, the layer of lusernaite-(Y) has a composition $Y_4Al(CO_3)_2(OH,F)_{11} \cdot 5H_2O$, being electrostatically neutral; thus the net charge of the interlayer must be zero. In fact, adjacent layers are connected through hydrogen bonding, involving also an additional water molecule, giving the actual formula of lusernaite-(Y), $Y_4Al(CO_3)_2(OH,F)_{11} \cdot 6H_2O$.

The substitution of $(Y,REE)^{3+}$ by $(Pb,Ca)^{2+}$ yields a deficit of charges, compensated through other compositional variations. Taking into account the crystal chemistry of lusernaite-(Y), the most probable mechanism could involve the Ow2 site, i.e., the site with the mixed occupancy by OH⁻ and H₂O groups. Electrostatic neutrality could be achieved through the coupled substitution

$$(Y,REE)^{3+} + {}^{Ow2}OH^- \rightarrow (Pb,Ca)^{2+} + {}^{Ow2}H_2O.$$

Other possible substitution mechanisms (e.g., the substitution of trivalent Y and REE by Pb^{2+} and a tetravalent cation) are less possible and cannot be proven.

CONCLUDING REMARKS

With the discovery of lusernaite-(Y), 20 natural yttrium carbonates are known (Table 8). No yttrium carbonates without additional anions and without H₂O (group 5.A) have been described until now. Lusernaite-(Y), being a carbonate with additional anions and with H₂O, belongs to the 5.D group of Strunz and Nickel (2001). It displays a new kind of layered crystal structure, with an interlayer hosting H₂O molecules; it is also the first natural Y-Al carbonate.

Yttrium carbonates are usually found as late-stage hydrothermal phases in alkaline magmatic rocks (or their metamorphic

TABLE 8. Comparison of natural yttrium carbonates

	Chemical formula	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Space group	Ref.
5.B Carbonates with additional anions, without H$_2$O									
bastnäsite-(Y)	(Y,REE)(CO$_3$)F	6.57	6.57	9.48	90	90	120	$P6$	[1]
horváthite-(Y)	NaY(CO$_3$)F	6.96	9.17	6.30	90	90	90	$Pmcn$	[2]
mineevite-(Y)	Na$_{25}$Ba(Y,Gd,Dy)$_2$(CO$_3$)$_{11}$(HCO$_3$)$_4$(SO$_4$)F$_2$Cl	8.81	8.81	37.03	90	90	120	$P6_3/m$	[3]
reederite-(Y)	Na$_{15}$Y$_2$(CO$_3$)$_9$(SO$_3$F)Cl	8.77	8.77	10.75	90	90	120	$P\bar{6}$	[4]
synchysite-(Y)	Ca(Y,Ce)(CO$_3$)$_2$F	12.04	6.95	18.44	90	102.45	90	$C2/c$	[5]
5.C Carbonates without additional anions, with H$_2$O									
adamsite-(Y)	NaY(CO$_3$)$_2$·6H$_2$O	6.26	13.05	13.22	91.17	103.70	89.99	$P\bar{1}$	[6]
donnayite-(Y)	NaCaSr$_3$Y(CO$_3$)$_6$·3H$_2$O	9.00	9.00	6.79	102.77	116.28	59.99	$P1$	[7]
hizenite-(Y)	Ca$_2$Y$_6$(CO$_3$)$_{11}$·14H$_2$O	6.30	9.09	63.49	90	90	90	UK	[8]
kimuraite-(Y)	CaY$_2$(CO$_3$)$_4$·6H$_2$O	9.25	23.98	6.04	90	90	90	$Imm2$ $Immm$ $I222$ $I2_12_12_1$	[9]
lecoqite-(Y)	Na$_3$Y(CO$_3$)$_3$·6H$_2$O	11.32	11.32	5.93	90	90	120	$P6_3$	[10]
lokkaite-(Y)	CaY$_4$(CO$_3$)$_7$·9H$_2$O	39.07	6.08	9.19	90	90	90	$Pb2m$ $Pbm2$ $Pbmm$	[11]
mckelveyite-(Y)	NaCa(Ba,Sr)$_3$(Y,REE)(CO$_3$)$_6$·3H$_2$O	9.17	9.17	9.15	90	90	90	$P\bar{3}$	[12]
shomiokite-(Y)	Na$_3$Y(CO$_3$)$_3$·3H$_2$O	10.04	17.32	5.94	90	90	90	$Pbn2_1$	[13]
tengerite-(Y)	Y$_2$(CO$_3$)$_3$·2–3H$_2$O	6.08	9.16	15.11	90	90	90	$Bb2_1m$	[14]
5.D Carbonates with additional anions, with H$_2$O									
decrespignyite-(Y)	(Y,REE)$_4$Cu(CO$_3$)$_4$Cl(OH)$_5$·2H$_2$O	8.90	22.77	8.59	90	120.06	90	$P2$ Pm $P2/m$	[15]
kamphaugite-(Y)	Ca(Y,REE)(CO$_3$)$_2$(OH)·H$_2$O	7.43	7.43	21.79	90	90	90	$P4_12_12$	[16]
lusernaite-(Y)	Y$_4$Al(CO$_3$)$_2$(OH,F)$_{11}$·6H$_2$O	7.84	11.03	11.39	90	90	90	$Pmna$	[17]
thomasclarkite-(Y)	(Na,Ce)(Y,REE)(HCO$_3$)(OH)$_3$·4H$_2$O	4.56	13.02	4.56	90	90.15	90	$P2$	[18]
5.E Uranyl carbonates									
bijvoetite-(Y)	(Y,Dy)$_2$(UO$_2$)$_4$(CO$_3$)$_4$(OH)$_6$·11H$_2$O	21.23	12.96	44.91	90	90	90	$B2_1$	[19]
kamotoite-(Y)	Y$_2$U$_4$(CO$_3$)O$_{12}$·14.5H$_2$O	21.22	12.93	12.39	90	115.3	90	$P2_1/n$	[20]

Notes: [1] Mineev et al. 1970; [2] Grice and Chao 1997; [3] Khomyakov et al. 1992; [4] Grice et al. 1995; [5] Wang and Zhou 1995; [6] Grice et al. 2000; [7] Chao et al. 1978; [8] Takai and Uehara 2011; [9] Nagashima et al. 1986; [10] Pekov et al. 2010; [11] Perttunen 1970; [12] Milton et al. 1965; [13] Grice 1996; [14] Miyawaki et al. 1993; [15] Wallwork et al. 2002; [16] Raade and Brastad 1993; [17] this work; [18] Grice and Gault 1998; [19] Li et al. 2000; [20] Deliens and Piret 1986. UK = unknown space group.

derivatives); in some cases, they occur in the oxidation zone of U or Cu deposits. The occurrence of lusernaite-(Y) agrees with the usual genesis of these phases; in fact, it occurs in late-stage fractures as product of hydrothermal activity related to the Alpine tectono-metamorphic events. Owing to the richness of rare minerals in the fractures of the Luserna stone, the quarries exploiting this kind of rock are an interesting field of research for the collection and the study of the crystal chemistry of yttrium and REE minerals.

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_journal_issue 7
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Pb1B Y1 O4 0.000(13) . 6_657 ?
O2 Y1 O4 134.1(2) . 6_657 ?
O2 Y1 O4 134.1(2) 4_556 6_657 ?
O6 Y1 O4 58.9(2) . 6_657 ?
O6 Y1 O4 58.9(2) 6_657 6_657 ?
O1 Y1 O4 62.03(18) 6_657 6_657 ?
O1 Y1 O4 62.03(18) 7 6_657 ?
O5 Y1 O4 112.1(2) 2_564 6_657 ?
O5 Y1 O4 112.1(2) 5_567 6_657 ?
Pb1A Y1 Al 89.54(2) . . ?
Pb1B Y1 Al 90.46(3) . . ?
O2 Y1 Al 72.16(19) . . ?
O2 Y1 Al 107.17(19) 4_556 . ?
O6 Y1 Al 72.2(2) . . ?
O6 Y1 Al 108.3(2) 6_657 . ?
O1 Y1 Al 148.62(18) 6_657 . ?
O1 Y1 Al 32.19(17) 7 . ?
O5 Y1 Al 147.7(2) 2_564 . ?
O5 Y1 Al 31.7(2) 5_567 . ?
O4 Y1 Al 90.46(3) 6_657 . ?
Y1 Pb1A Pb1B 0.000(10) . . ?
Y1 Pb1A O2 116(2) . 4_556 ?
Pb1B Pb1A O2 116(2) . 4_556 ?
Y1 Pb1A O2 116(2) . . ?
Pb1B Pb1A O2 116(2) . . ?
O2 Pb1A O2 128(4) 4_556 . ?
Y1 Pb1A O5 93.4(19) . 2_564 ?
Pb1B Pb1A O5 93.4(19) . 2_564 ?
O2 Pb1A O5 87.6(10) 4_556 2_564 ?
O2 Pb1A O5 89.4(10) . 2_564 ?
Y1 Pb1A O5 93.4(19) . 5_567 ?
Pb1B Pb1A O5 93.4(19) . 5_567 ?
O2 Pb1A O5 89.4(10) 4_556 5_567 ?
O2 Pb1A O5 87.6(10) . 5_567 ?
O5 Pb1A O5 173(4) 2_564 5_567 ?
Y1 Pb1A O6 45.0(11) . . ?
Pb1B Pb1A O6 45.0(11) . . ?
O2 Pb1A O6 82.3(10) 4_556 . ?
O2 Pb1A O6 138.7(16) . . ?
O5 Pb1A O6 123(2) 2_564 . ?
O5 Pb1A O6 62.8(9) 5_567 . ?
Y1 Pb1A O6 45.0(11) . 6_657 ?
Pb1B Pb1A O6 45.0(11) . 6_657 ?
O2 Pb1A O6 138.7(16) 4_556 6_657 ?
O2 Pb1A O6 82.3(10) . 6_657 ?
O5 Pb1A O6 62.8(9) 2_564 6_657 ?
O5 Pb1A O6 123(2) 5_567 6_657 ?
O6 Pb1A O6 90(2) . 6_657 ?
Y1 Pb1A O1 47.9(11) . 6_657 ?
Pb1B Pb1A O1 47.9(11) . 6_657 ?
O2 Pb1A O1 81.9(10) 4_556 6_657 ?
O2 Pb1A O1 136.6(13) . 6_657 ?

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O5 Pb1A O1 128(2) 5_567 6_657 ?
O6 Pb1A O1 64.9(13) . 6_657 ?
O6 Pb1A O1 58.4(12) 6_657 6_657 ?
Y1 Pb1A O1 47.9(11) . 7 ?
Pb1B Pb1A O1 47.9(11) . 7 ?
O2 Pb1A O1 136.6(13) 4_556 7 ?
O2 Pb1A O1 81.9(10) . 7 ?
O5 Pb1A O1 128(2) 2_564 7 ?
O5 Pb1A O1 57.9(8) 5_567 7 ?
O6 Pb1A O1 58.4(12) . 7 ?
O6 Pb1A O1 64.9(13) 6_657 7 ?
O1 Pb1A O1 96(2) 6_657 7 ?
Y1 Pb1A OW3 180.00(2) . 6_667 ?
Pb1B Pb1A OW3 180.000(13) . 6_667 ?
O2 Pb1A OW3 64(2) 4_556 6_667 ?
O2 Pb1A OW3 64(2) . 6_667 ?
O5 Pb1A OW3 86.6(19) 2_564 6_667 ?
O5 Pb1A OW3 86.6(19) 5_567 6_667 ?
O6 Pb1A OW3 135.0(11) . 6_667 ?
O6 Pb1A OW3 135.0(11) 6_657 6_667 ?
O1 Pb1A OW3 132.1(11) 6_657 6_667 ?
O1 Pb1A OW3 132.1(11) 7 6_667 ?
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Y1 Pb1B O6 96.7(15) . . ?
Pb1A Pb1B O6 96.7(15) . . ?
Y1 Pb1B O6 96.7(15) . 6_657 ?
Pb1A Pb1B O6 96.7(15) . 6_657 ?
O6 Pb1B O6 167(3) . 6_657 ?
Y1 Pb1B O1 94.1(14) . 6_657 ?
Pb1A Pb1B O1 94.1(14) . 6_657 ?
O6 Pb1B O1 94.9(4) . 6_657 ?
O6 Pb1B O1 84.1(4) 6_657 6_657 ?
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Pb1A Pb1B O1 94.1(14) . 7 ?
O6 Pb1B O1 84.1(4) . 7 ?
O6 Pb1B O1 94.9(4) 6_657 7 ?
O1 Pb1B O1 172(3) 6_657 7 ?
Y1 Pb1B O4 180.000(4) . 6_657 ?
Pb1A Pb1B O4 180.000(12) . 6_657 ?
O6 Pb1B O4 83.3(15) . 6_657 ?
O6 Pb1B O4 83.3(15) 6_657 6_657 ?
O1 Pb1B O4 85.9(14) 6_657 6_657 ?
O1 Pb1B O4 85.9(14) 7 6_657 ?
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Pb1A Pb1B F4 180.000(12) . 6_657 ?
O6 Pb1B F4 83.3(15) . 6_657 ?
O6 Pb1B F4 83.3(15) 6_657 6_657 ?
O1 Pb1B F4 85.9(14) 6_657 6_657 ?
O1 Pb1B F4 85.9(14) 7 6_657 ?
O4 Pb1B F4 0.000(1) 6_657 6_657 ?
Y1 Pb1B Y2 131.1(8) . . ?
Pb1A Pb1B Y2 131.1(8) . . ?
O6 Pb1B Y2 51.5(8) . . ?
O6 Pb1B Y2 117.9(17) 6_657 . ?
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F4 Pb1B Y2 48.9(8) 6_657 . ?
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Pb1A Pb1B Dy2 131.1(8) . 6_657 ?
O6 Pb1B Dy2 117.9(17) . 6_657 ?
O6 Pb1B Dy2 51.5(8) 6_657 6_657 ?
O1 Pb1B Dy2 52.3(7) 6_657 6_657 ?
O1 Pb1B Dy2 121.1(17) 7 6_657 ?
O4 Pb1B Dy2 48.9(8) 6_657 6_657 ?
F4 Pb1B Dy2 48.9(8) 6_657 6_657 ?
Y2 Pb1B Dy2 97.8(15) . 6_657 ?
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F4 Y2 O6 74.0(3) . . ?
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F4 Y2 OW2 74.6(4) . . ?
O4 Y2 OW2 74.6(4) 6_657 . ?
F4 Y2 OW2 74.6(4) 6_657 . ?
O6 Y2 OW2 115.0(6) . . ?
F4 Y2 OW1 145.1(4) . 7 ?
O4 Y2 OW1 75.8(3) 6_657 7 ?
F4 Y2 OW1 75.8(3) 6_657 7 ?
O6 Y2 OW1 140.0(3) . 7 ?
OW2 Y2 OW1 80.8(5) . 7 ?
F4 Y2 OW1 75.8(3) . . ?
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F4 Y2 OW1 145.1(4) 6_657 . ?
O6 Y2 OW1 140.0(3) . . ?
OW2 Y2 OW1 80.8(5) . . ?
OW1 Y2 OW1 76.1(6) 7 . ?
F4 Y2 O1 135.1(3) . 7 ?
O4 Y2 O1 77.7(3) 6_657 7 ?
F4 Y2 O1 77.7(3) 6_657 7 ?
O6 Y2 O1 72.1(3) . 7 ?
OW2 Y2 O1 147.61(18) . 7 ?
OW1 Y2 O1 76.3(3) 7 7 ?
OW1 Y2 O1 114.8(3) . 7 ?
F4 Y2 O1 77.7(3) . . ?
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F4 Y2 O1 135.1(3) 6_657 . ?
O6 Y2 O1 72.1(3) . . ?
OW2 Y2 O1 147.61(18) . . ?
OW1 Y2 O1 114.8(3) 7 . ?
OW1 Y2 O1 76.3(3) . . ?
O1 Y2 O1 64.4(3) 7 . ?
F4 Y2 Pb1B 115.7(3) . . ?
O4 Y2 Pb1B 45.8(8) 6_657 . ?
F4 Y2 Pb1B 45.8(8) 6_657 . ?
O6 Y2 Pb1B 42.5(4) . . ?
OW2 Y2 Pb1B 117.7(8) . . ?
OW1 Y2 Pb1B 97.6(5) 7 . ?
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O1 Y2 Pb1B 89.4(8) . . ?
F4 Y2 Pb1B 45.8(8) . 6_557 ?
O4 Y2 Pb1B 115.7(3) 6_657 6_557 ?
F4 Y2 Pb1B 115.7(3) 6_657 6_557 ?
O6 Y2 Pb1B 42.5(4) . 6_557 ?
OW2 Y2 Pb1B 117.7(8) . 6_557 ?
OW1 Y2 Pb1B 159.7(6) 7 6_557 ?
OW1 Y2 Pb1B 97.6(5) . 6_557 ?
O1 Y2 Pb1B 89.4(8) 7 6_557 ?
O1 Y2 Pb1B 45.0(5) . 6_557 ?
Pb1B Y2 Pb1B 81.7(12) . 6_557 ?
O5 Al O5 180.000(2) 5_567 . ?
O5 Al O1 85.1(3) 5_567 . ?
O5 Al O1 94.9(3) . . ?
O5 Al O1 94.9(3) 5_567 5_567 ?
O5 Al O1 85.1(3) . 5_567 ?
O1 Al O1 180.0(4) . 5_567 ?
O5 Al O1 94.9(3) 5_567 3_567 ?
O5 Al O1 85.1(3) . 3_567 ?
O1 Al O1 96.4(4) . 3_567 ?
O1 Al O1 83.6(4) 5_567 3_567 ?
O5 Al O1 85.1(3) 5_567 7 ?
O5 Al O1 94.9(3) . 7 ?
O1 Al O1 83.6(4) . 7 ?
O1 Al O1 96.4(4) 5_567 7 ?
O1 Al O1 180.000(2) 3_567 7 ?
O5 Al Y2 88.9(3) 5_567 . ?
O5 Al Y2 91.1(3) . . ?
O1 Al Y2 42.1(2) . . ?
O1 Al Y2 137.9(2) 5_567 . ?
O1 Al Y2 137.9(2) 3_567 . ?
O1 Al Y2 42.1(2) 7 . ?
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O5 Al Dy2 88.9(3) . 5_567 ?
O1 Al Dy2 137.9(2) . 5_567 ?
O1 Al Dy2 42.1(2) 5_567 5_567 ?
O1 Al Dy2 42.1(2) 3_567 5_567 ?
O1 Al Dy2 137.9(2) 7 5_567 ?
Y2 Al Dy2 180.0 . 5_567 ?
O5 Al Y2 91.1(3) 5_567 5_567 ?
O5 Al Y2 88.9(3) . 5_567 ?
O1 Al Y2 137.9(2) . 5_567 ?
O1 Al Y2 42.1(2) 5_567 5_567 ?
O1 Al Y2 42.1(2) 3_567 5_567 ?
O1 Al Y2 137.9(2) 7 5_567 ?
Y2 Al Y2 180.0 . 5_567 ?
Dy2 Al Y2 0.00(4) 5_567 5_567 ?
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O5 Al Er1 135.75(19) . 6_557 ?
O1 Al Er1 42.3(2) . 6_557 ?
O1 Al Er1 137.7(2) 5_567 6_557 ?
O1 Al Er1 89.1(2) 3_567 6_557 ?
O1 Al Er1 90.9(2) 7 6_557 ?
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Dy2 Al Er1 114.82(3) 5_567 6_557 ?
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O5 Al Er1 44.25(19) . 2_565 ?
O1 Al Er1 137.7(2) . 2_565 ?
O1 Al Er1 42.3(2) 5_567 2_565 ?
O1 Al Er1 90.9(2) 3_567 2_565 ?
O1 Al Er1 89.1(2) 7 2_565 ?
Y2 Al Er1 114.82(3) . 2_565 ?
Dy2 Al Er1 65.18(3) 5_567 2_565 ?
Y2 Al Er1 65.18(3) 5_567 2_565 ?
Er1 Al Er1 180.0 6_557 2_565 ?
O3 C O2 119.8(7) . . ?
O3 C O2 119.8(7) . 7_655 ?
O2 C O2 120.3(14) . 7_655 ?
O3 C O5 158.3(11) . 2_564 ?
O2 C O5 63.0(7) . 2_564 ?
O2 C O5 63.0(7) 7_655 2_564 ?
O3 C O1 76.4(5) . 3_667 ?
O2 C O1 143.0(10) . 3_667 ?
O2 C O1 54.0(6) 7_655 3_667 ?
O5 C O1 115.0(4) 2_564 3_667 ?
O3 C O1 76.4(5) . 5_567 ?
O2 C O1 54.0(6) . 5_567 ?
O2 C O1 143.0(10) 7_655 5_567 ?
O5 C O1 115.0(4) 2_564 5_567 ?
O1 C O1 106.2(5) 3_667 5_567 ?
O3 C OW3 92.1(10) . 1_665 ?
O2 C OW3 120.5(9) . 1_665 ?
O2 C OW3 59.3(9) 7_655 1_665 ?
O5 C OW3 70.5(6) 2_564 1_665 ?
O1 C OW3 89.3(3) 3_667 1_665 ?
O1 C OW3 157.6(8) 5_567 1_665 ?
O3 C OW3 92.1(10) . 6_667 ?
O2 C OW3 59.3(9) . 6_667 ?
O2 C OW3 120.5(9) 7_655 6_667 ?
O5 C OW3 70.5(6) 2_564 6_667 ?
O1 C OW3 157.6(8) 3_667 6_667 ?
O1 C OW3 89.3(3) 5_567 6_667 ?
OW3 C OW3 71.8(8) 1_665 6_667 ?
O3 C OW1 49.6(4) . 3_667 ?
O2 C OW1 163.3(10) . 3_667 ?
O2 C OW1 72.3(6) 7_655 3_667 ?
O5 C OW1 121.2(4) 2_564 3_667 ?
O1 C OW1 52.5(3) 3_667 3_667 ?
O1 C OW1 123.6(5) 5_567 3_667 ?
OW3 C OW1 54.1(4) 1_665 3_667 ?
OW3 C OW1 105.5(8) 6_667 3_667 ?
O3 C OW1 49.6(4) . 5_567 ?
O2 C OW1 72.3(6) . 5_567 ?
O2 C OW1 163.3(10) 7_655 5_567 ?
O5 C OW1 121.2(4) 2_564 5_567 ?
O1 C OW1 123.6(5) 3_667 5_567 ?
O1 C OW1 52.5(3) 5_567 5_567 ?
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OW3 C OW1 105.5(8) 1_665 5_567 ?
OW3 C OW1 54.1(4) 6_667 5_567 ?
OW1 C OW1 93.4(6) 3_667 5_567 ?
O3 C O6 54.4(8) . 2_565 ?
O2 C O6 105.8(7) . 2_565 ?
O2 C O6 105.8(7) 7_655 2_565 ?
O5 C O6 147.3(6) 2_564 2_565 ?
O1 C O6 54.1(2) 3_667 2_565 ?
O1 C O6 54.1(2) 5_567 2_565 ?
OW3 C O6 132.8(4) 1_665 2_565 ?
OW3 C O6 132.8(4) 6_667 2_565 ?
OW1 C O6 78.9(4) 3_667 2_565 ?
OW1 C O6 78.9(3) 5_567 2_565 ?
O3 C O6 154.9(10) . 6_657 ?
O2 C O6 62.7(7) . 6_657 ?
O2 C O6 62.7(8) 7_655 6_657 ?
O5 C O6 46.8(3) 2_564 6_657 ?
O1 C O6 88.8(4) 3_667 6_657 ?
O1 C O6 88.8(4) 5_567 6_657 ?
OW3 C O6 108.1(8) 1_665 6_657 ?
OW3 C O6 108.1(8) 6_667 6_657 ?
OW1 C O6 133.0(3) 3_667 6_657 ?
OW1 C O6 133.0(3) 5_567 6_657 ?
O6 C O6 100.5(4) 2_565 6_657 ?
Al O1 Pb1B 125.4(12) . 6_557 ?
Al O1 Y2 105.5(3) . . ?
Pb1B O1 Y2 82.7(11) 6_557 . ?
Al O1 Er1 105.5(3) . 6_557 ?
Pb1B O1 Er1 23.8(14) 6_557 6_557 ?
Y2 O1 Er1 101.3(3) . 6_557 ?
Al O1 Y1 105.5(3) . 6_557 ?
Pb1B O1 Y1 23.8(14) 6_557 6_557 ?
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Al O1 O1 48.2(2) . 7 ?
Pb1B O1 O1 108.74(19) 6_557 7 ?
Y2 O1 O1 57.81(17) . 7 ?
Er1 O1 O1 106.53(17) 6_557 7 ?
Y1 O1 O1 106.53(17) 6_557 7 ?
Al O1 O5 46.8(2) . 5_567 ?
Pb1B O1 O5 78.7(12) 6_557 5_567 ?
Y2 O1 O5 103.3(3) . 5_567 ?
Er1 O1 O5 59.9(2) 6_557 5_567 ?
Y1 O1 O5 59.9(2) 6_557 5_567 ?
O1 O1 O5 60.1(2) 7 5_567 ?
Al O1 O2 96.0(3) . 5_567 ?
Pb1B O1 O2 127.3(4) 6_557 5_567 ?
Y2 O1 O2 119.2(3) . 5_567 ?
Er1 O1 O2 126.7(3) 6_557 5_567 ?
Y1 O1 O2 126.7(3) 6_557 5_567 ?
O1 O1 O2 123.7(2) 7 5_567 ?
O5 O1 O2 130.9(4) 5_567 5_567 ?
Al O1 O5 42.0(2) . . ?
Pb1B O1 O5 167.4(11) 6_557 . ?
Y2 O1 O5 99.0(3) . . ?
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Y1 O1 O5 145.9(4) 6_557 . ?
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O5 O1 O5 88.8(4) 5_567 . ?
O2 O1 O5 62.8(2) 5_567 . ?
Al O1 O6 95.7(3) . . ?
Pb1B O1 O6 46.3(2) 6_557 . ?
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O2 O1 O6 167.6(4) 5_567 . ?
O5 O1 O6 125.5(3) . . ?
Al O1 O1 41.8(2) . 3_567 ?
Pb1B O1 O1 119.4(15) 6_557 3_567 ?
Y2 O1 O1 146.6(2) . 3_567 ?
Er1 O1 O1 96.0(4) 6_557 3_567 ?
Y1 O1 O1 96.0(4) 6_557 3_567 ?
O1 O1 O1 90.000(2) 7 3_567 ?
O5 O1 O1 61.7(3) 5_567 3_567 ?
O2 O1 O1 69.2(3) 5_567 3_567 ?
O5 O1 O1 54.0(3) . 3_567 ?
O6 O1 O1 122.8(4) . 3_567 ?
C O2 Pb1A 145.7(8) . . ?
C O2 O3 29.8(7) . . ?
Pb1A O2 O3 168.4(18) . . ?
C O2 O2 29.8(7) . 7_655 ?
Pb1A O2 O2 117.3(6) . 7_655 ?
O3 O2 O2 59.6(2) . 7_655 ?
C O2 Y1 141.2(8) . . ?
Pb1A O2 Y1 18(2) . . ?
O3 O2 Y1 169.5(5) . . ?
O2 O2 Y1 111.5(2) 7_655 . ?
C O2 O1 103.8(8) . 5_567 ?
Pb1A O2 O1 108.3(8) . 5_567 ?
O3 O2 O1 81.0(3) . 5_567 ?
O2 O2 O1 123.7(2) 7_655 5_567 ?
Y1 O2 O1 101.5(3) . 5_567 ?
C O2 O5 161.2(8) . 5_567 ?
Pb1A O2 O5 53.0(3) . 5_567 ?
O3 O2 O5 132.0(4) . 5_567 ?
O2 O2 O5 166.1(3) 7_655 5_567 ?
Y1 O2 O5 55.9(3) . 5_567 ?
O1 O2 O5 59.1(3) 5_567 5_567 ?
C O2 OW3 98.2(9) . 6_667 ?
Pb1A O2 OW3 81(2) . 6_667 ?
O3 O2 OW3 88.9(7) . 6_667 ?
O2 O2 OW3 106.8(3) 7_655 6_667 ?
Y1 O2 OW3 99.5(6) . 6_667 ?
O1 O2 OW3 111.2(4) 5_567 6_667 ?
O5 O2 OW3 82.7(4) 5_567 6_667 ?
C O2 O5 93.9(7) . 2_564 ?
Pb1A O2 O5 51.9(2) . 2_564 ?
O3 O2 O5 120.7(4) . 2_564 ?
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Y1 O2 O5 55.2(2) . 2_564 ?
O1 O2 O5 155.7(4) 5_567 2_564 ?
O5 O2 O5 104.7(3) 5_567 2_564 ?
OW3 O2 O5 81.9(4) 6_667 2_564 ?
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Pb1A O2 Pb1B 31(2) . . ?
O3 O2 Pb1B 157.5(7) . . ?
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Y1 O2 Pb1B 13.3(5) . . ?
O1 O2 Pb1B 95.8(4) 5_567 . ?
O5 O2 Pb1B 60.4(3) 5_567 . ?
OW3 O2 Pb1B 112.8(8) 6_667 . ?
O5 O2 Pb1B 59.9(3) 2_564 . ?
C O2 O6 96.2(8) . 6_657 ?
Pb1A O2 O6 62.8(18) . 6_657 ?
O3 O2 O6 121.8(4) . 6_657 ?
O2 O2 O6 69.36(15) 7_655 6_657 ?
Y1 O2 O6 47.70(18) . 6_657 ?
O1 O2 O6 108.0(3) 5_567 6_657 ?
O5 O2 O6 96.7(3) 5_567 6_657 ?
OW3 O2 O6 133.3(5) 6_667 6_657 ?
O5 O2 O6 52.9(3) 2_564 6_657 ?
Pb1B O2 O6 37.9(4) . 6_657 ?
C O3 O2 30.4(2) . . ?
C O3 O2 30.4(2) . 7_655 ?
O2 O3 O2 60.7(5) . 7_655 ?
C O3 OW1 109.6(4) . 3_667 ?
O2 O3 OW1 138.3(5) . 3_667 ?
O2 O3 OW1 80.7(3) 7_655 3_667 ?
C O3 OW1 109.6(4) . 5_567 ?
O2 O3 OW1 80.7(3) . 5_567 ?
O2 O3 OW1 138.3(5) 7_655 5_567 ?
OW1 O3 OW1 128.2(6) 3_667 5_567 ?
C O3 O6 104.7(9) . 2_565 ?
O2 O3 O6 101.9(5) . 2_565 ?
O2 O3 O6 101.9(5) 7_655 2_565 ?
OW1 O3 O6 100.7(3) 3_667 2_565 ?
OW1 O3 O6 100.7(3) 5_567 2_565 ?
C O3 O1 81.4(5) . 5_567 ?
O2 O3 O1 56.8(3) . 5_567 ?
O2 O3 O1 105.9(4) 7_655 5_567 ?
OW1 O3 O1 159.9(5) 3_667 5_567 ?
OW1 O3 O1 58.4(3) 5_567 5_567 ?
O6 O3 O1 59.6(2) 2_565 5_567 ?
C O3 O1 81.4(5) . 3_667 ?
O2 O3 O1 105.9(4) . 3_667 ?
O2 O3 O1 56.8(3) 7_655 3_667 ?
OW1 O3 O1 58.4(3) 3_667 3_667 ?
OW1 O3 O1 159.9(5) 5_567 3_667 ?
O6 O3 O1 59.6(2) 2_565 3_667 ?
O1 O3 O1 108.8(4) 5_567 3_667 ?
C O3 O4 132.4(6) . 2_565 ?
O2 O3 O4 149.4(6) . 2_565 ?
O2 O3 O4 106.9(3) 7_655 2_565 ?
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OW1 O3 O4 114.5(4) 5_567 2_565 ?
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O1 O3 O4 106.9(3) 5_567 2_565 ?
O1 O3 O4 51.3(2) 3_667 2_565 ?
C O3 F4 132.4(6) . 2_565 ?
O2 O3 F4 149.4(6) . 2_565 ?
O2 O3 F4 106.9(3) 7_655 2_565 ?
OW1 O3 F4 53.2(3) 3_667 2_565 ?
OW1 O3 F4 114.5(4) 5_567 2_565 ?
O6 O3 F4 50.7(3) 2_565 2_565 ?
O1 O3 F4 106.9(3) 5_567 2_565 ?
O1 O3 F4 51.3(2) 3_667 2_565 ?
O4 O3 F4 0.000(1) 2_565 2_565 ?
C O3 O4 132.4(6) . 5_567 ?
O2 O3 O4 106.9(3) . 5_567 ?
O2 O3 O4 149.4(6) 7_655 5_567 ?
OW1 O3 O4 114.5(4) 3_667 5_567 ?
OW1 O3 O4 53.2(3) 5_567 5_567 ?
O6 O3 O4 50.7(3) 2_565 5_567 ?
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O1 O3 O4 106.9(3) 3_667 5_567 ?
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F4 O3 O4 68.54(19) 2_565 5_567 ?
C O3 F4 132.4(6) . 5_567 ?
O2 O3 F4 106.9(3) . 5_567 ?
O2 O3 F4 149.4(6) 7_655 5_567 ?
OW1 O3 F4 114.5(4) 3_667 5_567 ?
OW1 O3 F4 53.2(3) 5_567 5_567 ?
O6 O3 F4 50.7(3) 2_565 5_567 ?
O1 O3 F4 51.3(2) 5_567 5_567 ?
O1 O3 F4 106.9(3) 3_667 5_567 ?
O4 O3 F4 68.54(19) 2_565 5_567 ?
F4 O3 F4 68.54(19) 2_565 5_567 ?
O4 O3 F4 0.000(1) 5_567 5_567 ?
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Y2 F4 OW2 134.6(5) . 6_557 ?
O6 F4 OW2 165.7(5) . 6_557 ?
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Dy2 F4 OW1 54.0(3) 6_557 4_456 ?
Y2 F4 OW1 54.0(3) 6_557 4_456 ?
Y2 F4 OW1 129.6(3) . 4_456 ?
O6 F4 OW1 100.0(3) . 4_456 ?
O6 F4 OW1 104.2(3) 6_557 4_456 ?
OW2 F4 OW1 65.7(5) 6_557 4_456 ?
OW2 F4 OW1 88.8(5) . 4_456 ?
Pb1B F4 OW1 107.7(3) 6_557 . ?
Dy2 F4 OW1 129.6(3) 6_557 . ?
Y2 F4 OW1 129.6(3) 6_557 . ?
Y2 F4 OW1 54.0(3) . . ?
O6 F4 OW1 104.2(3) . . ?
O6 F4 OW1 100.0(3) 6_557 . ?
OW2 F4 OW1 88.8(5) 6_557 . ?
OW2 F4 OW1 65.7(5) . . ?
OW1 F4 OW1 144.6(6) 4_456 . ?
Pb1B F4 O1 46.8(2) 6_557 4_456 ?
Dy2 F4 O1 53.1(2) 6_557 4_456 ?
Y2 F4 O1 53.1(2) 6_557 4_456 ?
Y2 F4 O1 119.3(4) . 4_456 ?
O6 F4 O1 65.1(3) . 4_456 ?
O6 F4 O1 58.6(3) 6_557 4_456 ?
OW2 F4 O1 105.5(4) 6_557 4_456 ?
OW2 F4 O1 134.9(4) . 4_456 ?
OW1 F4 O1 61.4(3) 4_456 4_456 ?
OW1 F4 O1 153.5(5) . 4_456 ?
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Y1 O5 Y1 104.1(4) 2_565 5_567 ?
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Y1 O5 O1 57.1(2) 5_567 3_567 ?
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O1 O5 O1 64.3(3) 3_567 . ?
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Er1 O5 O1 145.6(3) 5_567 7 ?
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O1 O5 O1 64.3(3) 5_567 7 ?
O1 O5 O1 91.2(3) 3_567 7 ?
O6 O5 O1 127.9(4) 5_567 7 ?
O1 O5 O1 54.4(3) . 7 ?
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Y2 O6 Er1 104.3(3) . 6_557 ?
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Y1 O6 O4 74.7(2) . 6_657 ?
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Y1 O6 O4 155.5(4) 6_557 6_657 ?
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OW3 OW2 OW1 88.8(6) . . ?
OW3 OW2 OW1 131.3(8) 6_657 . ?
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OW3 OW2 OW1 89.7(8) . 5_557 ?
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F4 OW2 OW1 98.0(4) 6_657 5_557 ?
F4 OW2 OW1 134.6(6) . 5_557 ?
OW1 OW2 OW1 51.9(5) 7 5_557 ?
OW1 OW2 OW1 76.6(5) . 5_557 ?
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OW3 OW2 OW1 54.7(4) . 3_557 ?
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F4 OW2 OW1 98.0(4) . 3_557 ?
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OW1 OW3 Pb1A 91.2(10) 2_454 6_547 ?
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OW2 OW3 O3 122.4(7) 6_557 6_547 ?
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O2 OW3 O3 37.7(3) 7_545 1_445 ?
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C OW3 O3 20.5(3) 1_445 1_445 ?
O3 OW3 O3 144.3(15) 6_547 1_445 ?
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C OW3 O5 70.0(8) 6_547 2_454 ?
C OW3 O5 54.0(7) 1_445 2_454 ?
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O3 OW3 O5 74.1(7) 1_445 2_454 ?

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_diffrn_reflns_theta_full               25.00
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_refine_diff_density_max     2.668
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