research communications

Crystal structure of lutetium aluminate (LUAM), Lu$_4$Al$_2$O$_9$

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The crystal structure of the title compound containing lutetium, the last element in the lanthanide series, was determined using a single crystal prepared by heating a pressed pellet of a 2:1 molar ratio mixture of Lu$_2$O$_3$ and Al$_2$O$_3$ powders in an Ar atmosphere at 2173 K for 4 h. Lu$_4$Al$_2$O$_9$ is isostructural with Eu$_4$Al$_2$O$_9$ and composed of Al$_2$O$_7$ ditetrahedra and Lu-centered six- and sevenfold oxygen polyhedra. The unit-cell volume, 787.3 (3) Å^3, is the smallest among the volumes of the rare-earth (RE) aluminates, RE_4Al$_2$O$_9$. The crystal studied was refined as a two-component pseudo-merohedric twin.

1. Chemical context

In the Al$_2$O$_3$-Lu$_2$O$_3$ system, where Lu has the largest atomic number among the rare-earth elements (RE), the following three phases have been reported: Lu$_3$Al$_5$O$_{12}$, LuAlO$_3$, and Lu$_4$Al$_2$O$_9$. These phases have been actively investigated as host materials, not only for phosphors (Ding *et al.*, 2011; Xiang *et al.*, 2016; Wang *et al.*, 2018), but also for scintillators, owing to their large radiation absorption cross sections arising from the presence of Lu. Various scintillation properties of Ce- and Pr-doped Lu$_3$Al$_5$O$_{12}$ and LuAlO$_3$ crystals have been characterized (Wojtowicz, 1999; Nikl, 2000; Wojtowicz *et al.*, 2006; Nikl *et al.*, 2013), and the luminescence properties of Ce- and Pr-doped Lu$_4$Al$_2$O$_9$ evaluated (Lempicki *et al.*, 1996; Zhang *et al.*, 1997, Zhang *et al.*, 1998; Drozdowski *et al.*, 2005). The crystal structures of the lutetium aluminates Lu$_3$Al$_5$O$_{12}$ (Euler & Bruce, 1965) and LuAlO$_3$ (Dernier & Maines, 1971; Shishido *et al.*, 1995) have been determined as garnet-type (LUAG) and perovskite-type (LUAP), respectively. However, to date, there have been no reports of the lattice constants of Lu$_4$Al$_2$O$_9$, although Shirvinskaya & Popova (1977) treated it as isotypic with Y$_4$Al$_2$O$_9$ and have reported the d-spacings and relative peak intensities in the powder X-ray diffraction pattern (PDF#00-033-0844).

Many REAl$_2$O$_9$ compounds have been investigated in detail. After Warshaw & Roy (1959) first reported the existence of Y$_4$Al$_2$O$_9$, Reed & Chase (1962) determined the space group of this material as $P2_1/c$ using X-ray Weissenberg and precession photography. Christensen & Hazell (1991) later determined the crystal structure of Y$_4$Al$_2$O$_9$ using powder synchrotron X-ray and neutron diffraction. Brandle & Steinfink (1969) also prepared crystals of REAl$_2$O$_9$ (RE = Sm, Gd, Eu, Dy, Ho) and determined the crystal structure of Eu$_4$Al$_2$O$_9$ using X-ray diffraction.

Al$_2$O$_7$ ditetrahedra

Lu-centered O polyhedra

Lu   O
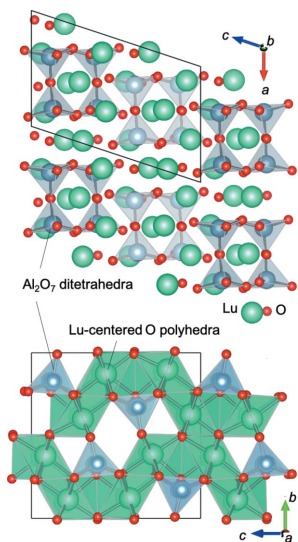
The lattice parameters of $RE_4Al_2O_9$ have previously been reported for RE = Y (Lehmann *et al.*, 1987; Reed & Chase, 1962; Christensen & Hazell, 1991; Yamane *et al.*, 1995b; Talik *et al.*, 2016), La (Dohrup *et al.*, 1996), Pr (Dohrup *et al.*, 1996), Nd (Dohrup *et al.*, 1996), Sm (Brandle & Steinfink, 1969; Mizuno *et al.*, 1977a; Yamane *et al.*, 1995a), Eu (Brandle & Steinfink, 1969; Mizuno *et al.*, 1977b; Yamane *et al.*, 1995a), Gd (Brandle & Steinfink, 1969; Mizuno *et al.*, 1977b; Yamane *et al.*, 1995a; Dohrup *et al.*, 1996; Martín-Sedeño *et al.*, 2006), Tb (Jero & Kriven, 1988; Yamane *et al.*, 1995a; Dohrup *et al.*, 1996; Li *et al.*, 2009), Dy (Brandle & Steinfink, 1969; Mizuno *et al.*, 1978; Yamane *et al.*, 1995a), Ho (Brandle & Steinfink, 1969; Mizuno, 1979; Yamane *et al.*, 1995a), Er (Mizuno, 1979; Yamane *et al.*, 1995a), Tm (Yamane *et al.*, 1995a), and Yb (Mizuno & Noguchi, 1980; Yamane *et al.*, 1995a).

Wu & Pelton (1992) investigated the phase diagram of the Lu_2O_3–Al_2O_3 system and showed that $Lu_4Al_2O_9$ melted congruently at 2313 K under an inert atmosphere. Petrosyan *et al.* (2006) studied the same system under a reducing atmosphere and reported that $Lu_4Al_2O_9$ could be formed by reaction of Lu_2O_3 and $Lu_3Al_5O_{12}$ at 1923 K, but decomposed into Lu_2O_3 and a melt at 2273 K. Subsequently, Petrosyan *et al.* (2013) observed incongruent melting of $Lu_4Al_2O_9$ at 2123 K under an Ar / 2% H_2 atmosphere using differential thermal analysis (DTA). Klimm (2010) employed DTA to investigate $LuAlO_3$ melting behavior in a 5 N pure Ar flow and concluded that the congruent and incongruent melting of $LuAlO_3$ depended on the atmospheric conditions. The author also concluded that the phase diagram at around Lu:Al = 1:1 under an inert atmosphere, previously reported by Wu & Pelton (1992), is correct. Yamane *et al.* (1995a) reported that only a very small amount of $Lu_4Al_2O_9$ can be obtained by reactions in air at 1673–2073 K, even though $RE_4Al_2O_9$ (RE = Y, Sm–Yb) can be synthesized under the same conditions.
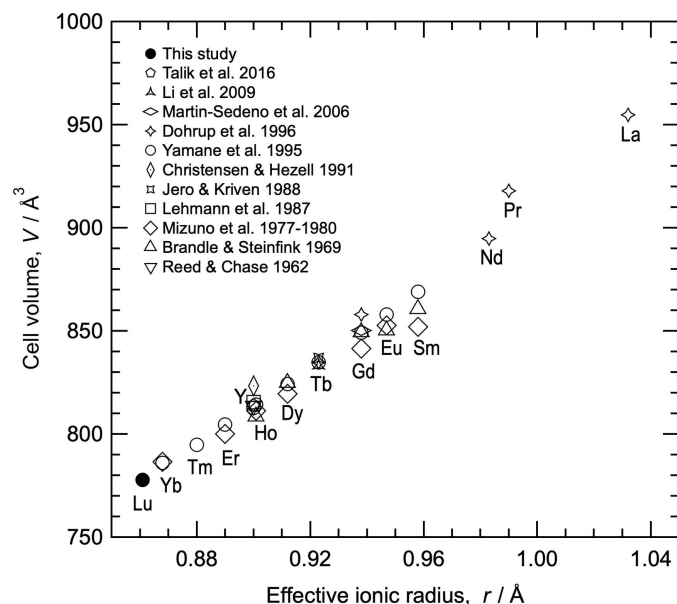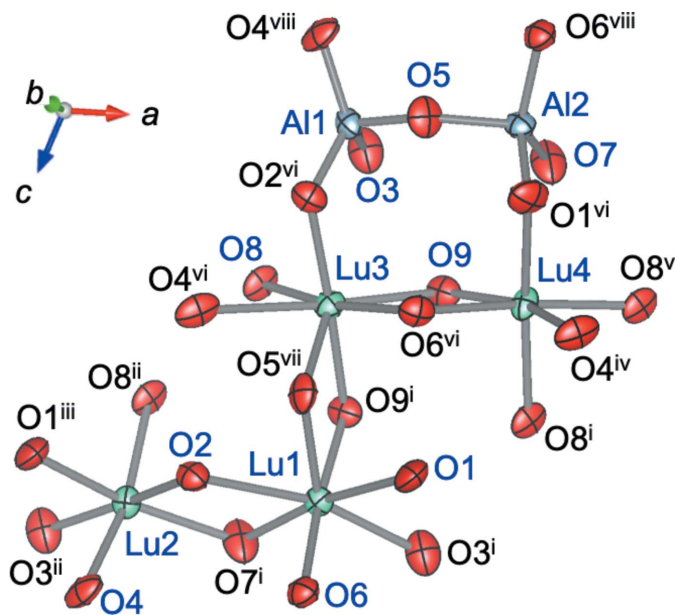

Figure 2
The atomic arrangement of $Lu_4Al_2O_9$ depicted with displacement ellipsoids at the 99% probability level. [Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $-x, -y, 1 - z$; (iii) $x - 1, y, z$; (iv) $1 + x, -y + \frac{1}{2}, z - \frac{1}{2}$; (v) $x + 1, y, z$; (vi) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (vii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (viii) $x, y, z - 1$.]

Following these reports, the present authors also attempted to synthesize $Lu_4Al_2O_9$ by heating a 2:1 molar ratio powder mixture of Lu_2O_3 and Al_2O_3 at 2073 K for 2 h in air, but the sample obtained was a mixture of $LuAlO_3$ and Lu_2O_3 (see Fig. S1a in the supporting information). The method used to prepare the single crystals of $Lu_4Al_2O_9$ used for the present diffraction study is described below.

2. Structural commentary

X-ray diffraction spots from the $Lu_4Al_2O_9$ single crystal were indexed on the basis of a monoclinic unit cell with lattice parameters: $a = 7.236\,(2)$ Å, $b = 10.333\,(2)$ Å, $c = 11.096\,(3)$ Å, and $\beta = 108.38\,(2)^\circ$. As shown in Fig. 1, the unit-cell volume of $Lu_4Al_2O_9$ calculated from these parameters lies on the extrapolated line of $RE_4Al_2O_9$ volumes plotted against the effective ionic radii for sixfold coordination of the trivalent rare-earth anions (RE^{3+}) (Shannon, 1976). In other words, $Lu_4Al_2O_9$ containing Lu, which has the smallest effective ionic radius of the RE atoms, has the smallest unit-cell volume in the $RE_4Al_2O_9$ series, in line with predictions arising from the lanthanide contraction.

The crystal structure of $Lu_4Al_2O_9$ (space group $P2_1/c$), determined using $Eu_4Al_2O_9$ (Brandle & Steinfink, 1969) as the starting model, contains two crystallographically distinct Al sites, four Lu sites, and nine O sites. The two Al sites are tetrahedrally coordinated by oxygen atoms. The two Al tetrahedra are connected through a shared O5 atom, forming an Al_2O_7 ditetrahedral oxy-aluminate group (Fig. 2). The Al_2O_7 dimers lie parallel to the *a* axis, and are related by the *c* glide symmetry operation (Fig. 3). The average Al1—O and

Figure 1
Unit-cell volume of $RE_4Al_2O_9$ *versus* effective ionic radius for the trivalent rare-earth anion (RE^{3+}) with sixfold coordination.

Al2—O distances in $Lu_4Al_2O_9$ are 1.744 and 1.756 Å, respectively, which are comparable to values found in $Eu_4Al_2O_9$ (1.741 and 1.755 Å, Brandle & Steinfink, 1969) and $Y_4Al_2O_9$ (1.739 and 1.769 Å, Lehmann *et al.*, 1987). The bond-valence sums (BVS; Brown & Altermatt, 1985) calculated using the Al—O distances and bond-valence parameters recently reported by Gagne & Hawthorne (2015) ($r_0 = 1.634$ Å, $b = 0.39$) are 3.02 and 2.93 for Al1 and Al2, respectively. These BVS values are close to those expected for trivalent Al. The Al1—O5—Al2 angle of the Al_2O_7 dimer is 134.9 (3)°, which is smaller than the corresponding angles in $Eu_4Al_2O_9$ (141.9°; Brandle & Steinfink, 1969) and $Y_4Al_2O_9$ (137.6°; Lehmann *et al.*, 1987).

Of the four crystallographically distinct Lu atoms, Lu1 and Lu3 are coordinated by seven oxygen atoms with five Lu—O distances in the range 2.219 (5)–2.344 (5) Å and two in the range 2.461 (6)–2.573 (6) Å. The remaining Lu atoms, Lu2 and Lu4, are coordinated by six oxygen atoms in distorted octahedra with Lu—O distances in the range 2.172 (6)–2.337 (6) Å.
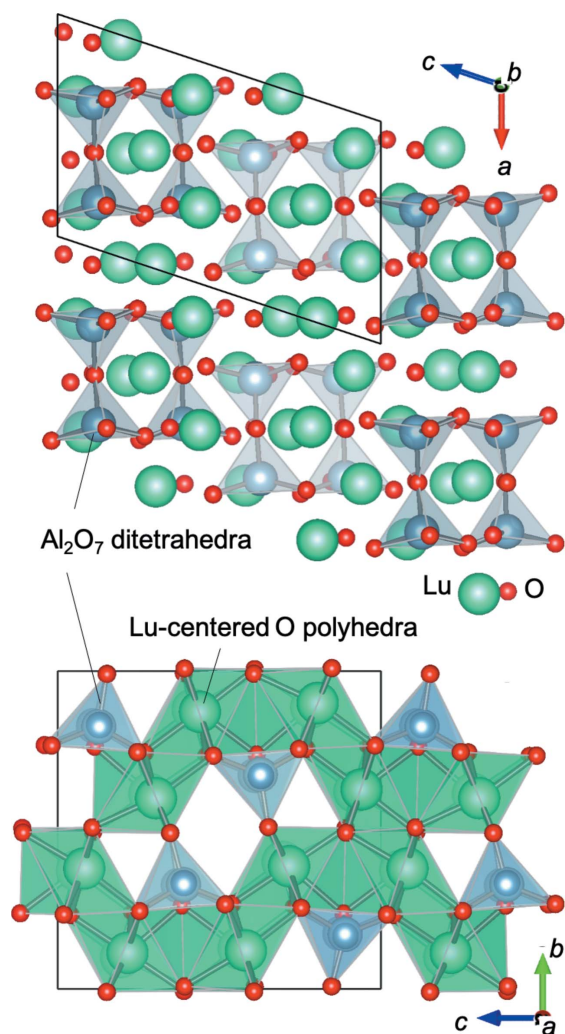
The averages Lu—O distances for the six-fold coordinated Lu atoms in $Lu_4Al_2O_9$ are 2.250 and 2.260 Å for Lu2 and Lu4, respectively. These values are 0.02–0.10 Å shorter than those for the LuO_6 octahedra found in $Lu_3Al_5O_{12}$ (2.352 Å; Euler & Bruce, 1965) and $LuAlO_3$ (2.330 Å; Shishido *et al.*, 1995).

The average values for the Eu—O and Y—O distances in $Eu_4Al_2O_9$ and $Y_4Al_2O_9$ lie in the ranges 2.328–2.439 Å (Brandle & Steinfink, 1969) and 2.286–2.387 Å (Lehmann *et al.*, 1987), respectively. The differences between the RE—O lengths in $RE_4Al_2O_9$ when RE = Eu and Lu (0.07–0.09 Å), and when RE = Y and Lu (0.02–0.05 Å) correspond to the differences between $^{VI}r_{Eu} - {}^{VI}r_{Lu}$ (0.086 Å) and $^{VI}r_{Y} - {}^{VI}r_{Lu}$ (0.039 Å), where $^{VI}r_{Eu}$, $^{VI}r_{Lu}$, and $^{VI}r_{Lu}$ are the effective ionic radii in sixfold coordination of Lu^{3+} (0.861 Å), Eu^{3+} (0.947 Å), and Y^{3+} (0.900 Å), respectively (Shannon, 1976). The BVS for Lu1, Lu2, Lu3, and Lu4, calculated using the bond-valence parameters ($r_0 = 1.939$ Å, $b = 0.403$) of Gagné & Hawthorne (2015), are 2.766, 2.796, 2.642, and 2.714, respectively, which are smaller than the expected valence value of +3 for the Lu atoms. The polyhedral volumes of $Lu1O_7$ (18.18 Å^3), $Lu2O_6$ (14.29 Å^3), $Lu3O_7$ (18.56 Å^3), and $Lu4O_6$ (14.24 Å^3) are 1.1–1.7 Å^3 and 0.5–0.8 Å^3 smaller than those for $Eu_4Al_2O_9$ ($Eu1O_7$:19.85 Å^3, $Eu2O_6$:15.38 Å^3, $Eu3O_7$:20.14 Å^3, and $Eu4O_6$:15.71 Å^3) and for $Y_4Al_2O_9$ ($Y1O_7$:18.66 Å^3, $Y2O_6$: 14.77 Å^3, $Y3O_7$:19.33 Å^3, and $Y4O_6$:14.98 Å^3), respectively. These differences in polyhedral volumes correlate with the differences in ionic radii of the lanthanides.

3. Synthesis and crystallization

The starting powders Al_2O_3 (Sumitomo Chemicals, AKP20, 99.99%) and Lu_2O_3 (Nippon Yttrium, 99.999%) were mixed in a molar ratio of Lu:Al = 2:1, ground with ethanol in an agate mortar, and pressed into a pellet. The pellet was placed in a BN crucible with an inner diameter of 18 mm and a height of 20 mm. The BN crucible was covered with a BN lid, and heated in a chamber with a carbon heater (Shimadzu Mectem, Inc., VESTA). The pellet was heated slowly under vacuum ($\sim10^{-2}$ Pa) from room temperature to 1273 K. During the 5 min. hold at 1273 K, the chamber was filled with Ar (99.9995%) up to 0.15 MPa. The temperature was then raised to 2173 K at a heating rate of 300 Kh^{-1}. After being held at 2173 K for 4 h, the sample was cooled to 1473 K at a rate of 20 Kh^{-1}, and then to room temperature by shutting off the heater. A part of the obtained sample was pulverized in the agate mortar, and powder X-ray diffraction measurements (Bruker D2 Phaser, Cu Kα radiation) confirmed that the major crystalline phase present in the sample was $Lu_4Al_2O_9$, together with small amounts of $LuAlO_3$ and unreacted Lu_2O_3 (Fig. S1a). Colorless crystals of $Lu_4Al_2O_9$ were selected for single-crystal X-ray diffraction studies.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The Eu atoms in the rare-earth metal sites in the structural model of $Eu_4Al_2O_9$ (Brandle &

Figure 3
The crystal structure of $Lu_4Al_2O_9$ highlighting the Al_2O_7 ditetrahedra viewed down the *b* axis (upper), and the Al_2O_7 ditetrahedra and Lu-centered polyhedra viewed down the *a* axis (lower).

Table 1
Experimental details.

Crystal data	
Chemical formula	$Lu_4Al_2O_9$
M_r	897.84
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	301
a, b, c (Å)	7.2360 (11), 10.3330 (19), 11.096 (3)
β (°)	108.381 (11)
V (Å^3)	787.3 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	49.97
Crystal size (mm)	$0.12 \times 0.05 \times 0.04$
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.451, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32672, 2795, 2719
R_{int}	0.035
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.748
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.043, 1.17
No. of reflections	2795
No. of parameters	138
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.49, -1.81

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2017), *SHELXL2014/7* (Sheldrick, 2015), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

Steinfink, 1969) were replaced by Lu atoms to generate the initial model. Several iterations of refinement yielded an R value of 10.07% and a residual electron density of ~10 e Å^{-3}. A subsequent refinement, performed by implementing the (100) twin plane observed in a study of $Y_4Al_2O_9$ (Yamane *et al.*, 1995*b*), yielded an $R(F^2 > 2\sigma(F^2))$ value of 1.92% with an approximate volume ratio of 6:4 for the twin domains.

Acknowledgements

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References

Brandle, C. D. & Steinfink, H. (1969). *Inorg. Chem.* **8**, 1320–1324.
Brown, I. D. & Altermatt, D. (1985). *Acta Cryst.* B**41**, 244–247.
Bruker (2016). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2017). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2018). *APEX3*. Bruker AXS Inc., Madison, Wisconsin, USA.
Christensen, A. N. & Hazell, R. G. (1991). *Acta Chem. Scand.* **45**, 226–230.
Dernier, P. D. & Maines, R. G. (1971). *Mater. Res. Bull.* **6**, 433–439.
Ding, L., Zhang, Q., Luo, J., Liu, W., Zhou, W. & Yin, S. (2011). *J. Alloys Compd.* **509**, 10167–10171.
Dohrup, J., Hoyvald, A., Mogensen, G., Jacobsen, C. J. H. & Villadsen, J. (1996). *J. Am. Ceram. Soc.* **79**, 2959–2960.
Drozdowski, W., Lukasiewicz, T., Wojtowicz, A. J., Wisniewski, D. & Kisielewski, J. (2005). *J. Cryst. Growth*, **275**, e709–e714.
Euler, F. & Bruce, J. A. (1965). *Acta Cryst.* **19**, 971–978.
Gagné, O. C. & Hawthorne, F. C. (2015). *Acta Cryst.* B**71**, 562–578.
Jero, P. D. & Kriven, W. M. (1988). *J. Am. Ceram. Soc.* **71**, C454–C455.
Klimm, D. (2010). *J. Cryst. Growth*, **312**, 730–733.
Lehmann, M. S., Christensen, A. N., Fjellvåg, H., Feidenhans'l, R. & Nielsen, M. (1987). *J. Appl. Cryst.* **20**, 123–129.
Lempicki, A., Brecher, C., Wisniewski, D., Zych, E. & Wojtowicz, A. J. (1996). *IEEE Trans. Nucl. Sci.* **43**, 1316–1320.
Li, Y. Q., Hirosaki, N., Xie, R. J., Takeda, T., Lofland, S. E. & Ramanujachary, K. V. (2009). *J. Alloys Compd.* **484**, 943–948.
Martín-Sedeño, M. C., Marrero-López, D., Losilla, E. R., Bruque, S., Núñez, P. & Aranda, M. A. G. (2006). *J. Solid State Chem.* **179**, 3445–3455.
Mizuno, M. (1979). *J. Ceram. Soc. Jpn*, **87**, 405–412.
Mizuno, M. & Noguchi, T. (1980). *J. Ceram. Soc. Jpn*, **88**, 322–327.
Mizuno, M., Yamada, T. & Noguchi, T. (1977*a*). *J. Ceram. Soc. Jpn*, **85**, 374–379.
Mizuno, M., Yamada, T. & Noguchi, T. (1977*b*). *J. Ceram. Soc. Jpn*, **85**, 543–548.
Mizuno, M., Yamada, T. & Noguchi, T. (1978). *J. Ceram. Soc. Jpn*, **86**, 359–364.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Nikl, M. (2000). *Phys. Status Solidi A*, **178**, 595-620.
Nikl, M., Yoshikawa, A., Kamada, K., Nejezchleb, K., Stanek, C. R., Mares, J. A. & Blazek, K. (2013). *Prog. Cryst. Growth Charact. Mater.* **59**, 47–72.
Petrosyan, A. G., Popova, V. F., Gusarov, V. V., Shirinyan, G. O., Pedrini, C. & Lecoq, P. (2006). *J. Cryst. Growth*, **293**, 74–77.
Petrosyan, A. G., Popova, V. F., Ugolkov, V. L., Romanov, D. P. & Ovanesyan, K. L. (2013). *J. Cryst. Growth*, **377**, 178–183.
Reed, J. W. & Chase, A. B. (1962). *Acta Cryst.* **15**, 812.
Shannon, R. D. (1976). *Acta Cryst.* A**32**, 751–767.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Shirvinskaya, A. K. & Popova, V. F. (1977). *Dokl. Akad. Nauk SSSR*, **233**, 1110–1113.
Shishido, T., Nojima, S., Tanaka, M., Horiuchi, H. & Fukuda, T. (1995). *J. Alloys Compd.* **227**, 175–179.
Talik, E., Guzik, A., Zajdel, P., Lipifska, L., Baran, M. & Szubka, M. (2016). *Mater. Res. Bull.* **83**, 56–64.
Wang, Z., Zou, J., Zhang, C., Yang, B., Shi, M., Li, Y., Zhou, H., Liu, Y., Li, M. & Liu, Z. (2018). *J. Non-Cryst. Solids*, **489**, 57–63.
Warshaw, I. & Roy, R. (1959). *J. Am. Ceram. Soc.* **42**, 434–438.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wojtowicz, A. J. (1999). *Acta Phys. Pol. A*, **95**, 165–178.
Wojtowicz, A. J., Drozdowski, W., Wisniewski, D., Lefaucheur, J.-L., Galazka, Z., Gou, Z., Lukasiewicz, T. & Kisielewski, J. (2006). *Opt. Mater.* **28**, 85–93.
Wu, P. & Pelton, A. D. (1992). *J. Alloys Compd.* **179**, 259–287.
Xiang, R., Liang, X., Li, P., Di, X. & Xiang, W. (2016). *Chem. Eng. J.* **306**, 858–865.
Yamane, H., Ogawara, K., Omori, M. & Hirai, T. (1995*a*). *J. Am. Ceram. Soc.* **78**, 2385–2390.
Yamane, H., Omori, M. & Hirai, T. (1995*b*). *J. Mater. Sci. Lett.* **14**, 561–563.
Zhang, L., Madej, C., Pedrini, C., Dujardin, C., Kamenskikh, I., Belsky, A., Shaw, D. A., Mesnard, P. & Fouassier, C. (1998). *J. Electrochem. Soc.: Proceedings of the Sixth International Conference on Luminescent materials* **97**, 342-351.
Zhang, L., Madej, C., Pédrini, C., Moine, B., Dujardin, C., Petrosyan, A. & Belsky, A. N. (1997). *Chem. Phys. Lett.* **268**, 408–412.

Crystal structure of lutetium aluminate (LUAM), $Lu_4Al_2O_9$

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *APEX3* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2017); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Lutetium aluminate

Crystal data

$Lu_4Al_2O_9$	$F(000) = 1528$
$M_r = 897.84$	$D_x = 7.575$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.2360$ (11) Å	Cell parameters from 1294 reflections
$b = 10.3330$ (19) Å	$\theta = 2.8–38.5°$
$c = 11.096$ (3) Å	$\mu = 49.97$ mm^{-1}
$\beta = 108.381$ (11)°	$T = 301$ K
$V = 787.3$ (3) Å^3	Chip, colourless
$Z = 4$	$0.12 \times 0.05 \times 0.04$ mm

Data collection

Bruker D8 QUEST diffractometer	2795 independent reflections
	2719 reflections with $I > 2\sigma(I)$
Detector resolution: 7.3910 pixels mm^{-1}	$R_{int} = 0.035$
ω and σcans	$\theta_{max} = 32.1°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$h = -10\rightarrow10$
	$k = -15\rightarrow15$
$T_{min} = 0.451$, $T_{max} = 0.746$	$l = -16\rightarrow16$
32672 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + 17.273P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.019$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.043$	$\Delta\rho_{max} = 1.49$ e Å^{-3}
$S = 1.17$	$\Delta\rho_{min} = -1.81$ e Å^{-3}
2795 reflections	Extinction correction: *SHELXL2014/7*
138 parameters	(Sheldrick 2015b),
0 restraints	$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00026 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a two-component inversion twin

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Al1	0.2142 (4)	0.1742 (2)	0.1270 (2)	0.0058 (4)
Al2	0.6551 (4)	0.1717 (2)	0.1108 (2)	0.0059 (4)
Lu1	0.52225 (7)	0.11375 (3)	0.78409 (2)	0.00572 (6)
Lu2	0.02236 (6)	0.10027 (3)	0.80405 (2)	0.00574 (6)
Lu3	0.34172 (7)	0.12783 (3)	0.44005 (2)	0.00605 (6)
Lu4	0.83940 (6)	0.12082 (3)	0.41774 (3)	0.00610 (6)
O1	0.7934 (8)	0.2450 (6)	0.7469 (5)	0.0102 (11)
O2	0.2314 (8)	0.2439 (5)	0.7699 (5)	0.0072 (11)
O3	0.2106 (13)	0.0095 (5)	0.1516 (5)	0.0102 (10)
O4	0.0720 (8)	0.2340 (6)	0.9813 (6)	0.0092 (11)
O5	0.4326 (10)	0.2381 (4)	0.1156 (5)	0.0085 (8)
O6	0.6371 (8)	0.2328 (5)	0.9599 (5)	0.0072 (11)
O7	0.6926 (13)	0.0084 (5)	0.1529 (5)	0.0111 (10)
O8	0.0764 (12)	−0.0082 (5)	0.3927 (5)	0.0072 (9)
O9	0.5643 (13)	0.0063 (5)	0.3906 (5)	0.0069 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0071 (12)	0.0044 (8)	0.0067 (9)	0.0012 (8)	0.0032 (8)	0.0005 (7)
Al2	0.0074 (12)	0.0050 (8)	0.0055 (8)	0.0010 (8)	0.0021 (8)	0.0012 (7)
Lu1	0.00622 (14)	0.00463 (12)	0.00594 (10)	0.00019 (12)	0.00140 (14)	−0.00101 (8)
Lu2	0.00566 (13)	0.00433 (12)	0.00733 (10)	−0.00031 (13)	0.00218 (14)	−0.00058 (8)
Lu3	0.00647 (13)	0.00518 (11)	0.00625 (10)	0.00024 (13)	0.00165 (13)	0.00101 (9)
Lu4	0.00538 (14)	0.00435 (10)	0.00863 (10)	0.00048 (13)	0.00231 (15)	0.00137 (9)
O1	0.008 (3)	0.013 (3)	0.008 (2)	0.0039 (19)	0.0002 (18)	0.002 (2)
O2	0.009 (3)	0.006 (2)	0.007 (2)	0.0012 (18)	0.0030 (19)	0.0010 (17)
O3	0.011 (3)	0.006 (2)	0.015 (2)	0.000 (3)	0.007 (3)	0.0006 (17)
O4	0.009 (3)	0.007 (2)	0.009 (2)	0.0039 (18)	−0.0009 (18)	−0.0003 (19)
O5	0.008 (2)	0.0064 (18)	0.012 (2)	−0.003 (2)	0.004 (2)	−0.0003 (15)
O6	0.008 (3)	0.007 (2)	0.007 (2)	0.0017 (18)	0.0018 (18)	0.0009 (17)
O7	0.013 (3)	0.008 (2)	0.016 (2)	0.003 (3)	0.009 (3)	0.0059 (18)
O8	0.005 (3)	0.006 (2)	0.009 (2)	−0.003 (2)	0.000 (3)	−0.0002 (16)
O9	0.010 (3)	0.0042 (19)	0.007 (2)	0.001 (3)	0.003 (3)	0.0001 (16)

Geometric parameters (Å, º)

Al1—O3	1.724 (6)	Lu3—O5^{iv}	2.310 (5)
Al1—O4^{i}	1.733 (6)	Lu3—O6^{ii}	2.529 (5)
Al1—O5	1.754 (7)	Lu3—O4^{ii}	2.573 (6)
Al1—O2^{ii}	1.767 (6)	Lu3—Al2^{iv}	3.211 (2)
Al1—Lu1^{ii}	3.219 (2)	Lu3—Al1^{iv}	3.247 (2)
Al1—Lu3^{ii}	3.247 (2)	Lu3—Lu3^{iii}	3.4748 (8)
Al1—Lu3	3.336 (2)	Lu3—Lu4^{iii}	3.4803 (7)
Al2—O7	1.749 (6)	Lu4—O4^{ix}	2.198 (6)
Al2—O1^{ii}	1.753 (6)	Lu4—O9	2.253 (8)
Al2—O6^{i}	1.755 (6)	Lu4—O6^{ii}	2.255 (6)
Al2—O5	1.767 (7)	Lu4—O8^{v}	2.257 (8)
Al2—Lu3^{ii}	3.211 (2)	Lu4—O1^{ii}	2.287 (6)
Al2—Lu1^{ii}	3.272 (2)	Lu4—O8^{iii}	2.311 (5)
Al2—Lu4	3.285 (2)	Lu4—Lu3^{iii}	3.4804 (7)
Lu1—O9^{iii}	2.219 (5)	Lu4—Lu4^{x}	3.5061 (8)
Lu1—O6	2.233 (5)	Lu4—Lu2^{ix}	3.5641 (7)
Lu1—O3^{iii}	2.236 (8)	Lu4—Lu3^{v}	3.5652 (7)
Lu1—O7^{iii}	2.277 (8)	Lu4—Lu1^{ii}	3.5836 (7)
Lu1—O5^{iv}	2.344 (5)	O1—Al2^{iv}	1.753 (6)
Lu1—O2	2.461 (6)	O1—Lu2^{v}	2.172 (6)
Lu1—O1	2.524 (6)	O1—Lu4^{iv}	2.287 (6)
Lu1—Al1^{iv}	3.219 (2)	O2—Al1^{iv}	1.767 (6)
Lu1—Al2^{iv}	3.272 (2)	O2—Lu3^{iv}	2.238 (5)
Lu1—Lu2^{v}	3.5579 (7)	O3—Lu2^{vii}	2.213 (8)
Lu1—Lu4^{iv}	3.5836 (7)	O3—Lu1^{iii}	2.236 (8)
Lu1—Lu3	3.6270 (9)	O4—Al1^{xi}	1.733 (6)
Lu2—O1^{vi}	2.172 (6)	O4—Lu4^{viii}	2.198 (6)
Lu2—O3^{vii}	2.213 (8)	O4—Lu3^{iv}	2.573 (6)
Lu2—O2	2.235 (6)	O5—Lu3^{ii}	2.310 (5)
Lu2—O7^{iii}	2.263 (8)	O5—Lu1^{ii}	2.344 (5)
Lu2—O8^{vii}	2.280 (5)	O6—Al2^{xi}	1.754 (6)
Lu2—O4	2.337 (6)	O6—Lu4^{iv}	2.255 (6)
Lu2—Lu1^{vi}	3.5579 (7)	O6—Lu3^{iv}	2.529 (5)
Lu2—Lu4^{viii}	3.5641 (7)	O7—Lu2^{iii}	2.263 (8)
Lu2—Lu3^{iv}	3.6485 (7)	O7—Lu1^{iii}	2.277 (8)
Lu2—Lu4^{iii}	3.7187 (7)	O8—Lu4^{vi}	2.257 (8)
Lu2—Lu3^{vii}	3.9156 (7)	O8—Lu2^{vii}	2.280 (5)
Lu3—O2^{ii}	2.238 (5)	O8—Lu4^{iii}	2.311 (5)
Lu3—O9	2.242 (8)	O9—Lu1^{iii}	2.219 (5)
Lu3—O9^{iii}	2.260 (5)	O9—Lu3^{iii}	2.260 (5)
Lu3—O8	2.302 (7)		
O3—Al1—O4^{i}	117.7 (3)	O2^{ii}—Lu3—O8	96.84 (19)
O3—Al1—O5	116.2 (4)	O9—Lu3—O8	102.35 (18)
O4^{i}—Al1—O5	94.7 (3)	O9^{iii}—Lu3—O8	80.0 (2)
O3—Al1—O2^{ii}	109.3 (3)	O2^{ii}—Lu3—O5^{iv}	106.69 (18)

O4[i]—Al1—O2[ii]	121.3 (3)	O9—Lu3—O5[iv]	120.4 (2)
O5—Al1—O2[ii]	94.3 (3)	O9[iii]—Lu3—O5[iv]	74.68 (16)
O3—Al1—Lu1[ii]	128.9 (3)	O8—Lu3—O5[iv]	123.6 (2)
O4[i]—Al1—Lu1[ii]	111.6 (2)	O2[ii]—Lu3—O6[ii]	78.65 (19)
O5—Al1—Lu1[ii]	45.30 (17)	O9—Lu3—O6[ii]	71.8 (2)
O2[ii]—Al1—Lu1[ii]	49.24 (19)	O9[iii]—Lu3—O6[ii]	104.6 (2)
O3—Al1—Lu3[ii]	138.1 (3)	O8—Lu3—O6[ii]	171.4 (2)
O4[i]—Al1—Lu3[ii]	52.0 (2)	O5[iv]—Lu3—O6[ii]	65.0 (2)
O5—Al1—Lu3[ii]	43.34 (18)	O2[ii]—Lu3—O4[ii]	74.48 (19)
O2[ii]—Al1—Lu3[ii]	108.5 (2)	O9—Lu3—O4[ii]	176.2 (2)
Lu1[ii]—Al1—Lu3[ii]	68.24 (5)	O9[iii]—Lu3—O4[ii]	103.8 (2)
O3—Al1—Lu3	72.9 (2)	O8—Lu3—O4[ii]	75.8 (2)
O4[i]—Al1—Lu3	155.5 (2)	O5[iv]—Lu3—O4[ii]	63.1 (2)
O5—Al1—Lu3	99.75 (19)	O6[ii]—Lu3—O4[ii]	109.64 (15)
O2[ii]—Al1—Lu3	38.37 (18)	O2[ii]—Lu3—Al2[iv]	96.50 (15)
Lu1[ii]—Al1—Lu3	67.47 (5)	O9—Lu3—Al2[iv]	94.44 (18)
Lu3[ii]—Al1—Lu3	135.61 (8)	O9[iii]—Lu3—Al2[iv]	86.21 (17)
O7—Al2—O1[ii]	104.2 (3)	O8—Lu3—Al2[iv]	155.68 (16)
O7—Al2—O6[i]	124.1 (3)	O5[iv]—Lu3—Al2[iv]	32.39 (17)
O1[ii]—Al2—O6[i]	119.7 (3)	O6[ii]—Lu3—Al2[iv]	32.95 (13)
O7—Al2—O5	115.6 (4)	O4[ii]—Lu3—Al2[iv]	88.36 (14)
O1[ii]—Al2—O5	93.5 (3)	O2[ii]—Lu3—Al1[iv]	93.90 (15)
O6[i]—Al2—O5	95.4 (3)	O9—Lu3—Al1[iv]	151.60 (17)
O7—Al2—Lu3[ii]	143.2 (3)	O9[iii]—Lu3—Al1[iv]	85.82 (16)
O1[ii]—Al2—Lu3[ii]	107.2 (2)	O8—Lu3—Al1[iv]	98.38 (18)
O6[i]—Al2—Lu3[ii]	51.62 (19)	O5[iv]—Lu3—Al1[iv]	31.41 (17)
O5—Al2—Lu3[ii]	44.47 (16)	O6[ii]—Lu3—Al1[iv]	89.32 (13)
O7—Al2—Lu1[ii]	123.1 (2)	O4[ii]—Lu3—Al1[iv]	32.07 (14)
O1[ii]—Al2—Lu1[ii]	49.8 (2)	Al2[iv]—Lu3—Al1[iv]	60.46 (5)
O6[i]—Al2—Lu1[ii]	111.7 (2)	O2[ii]—Lu3—Al1	29.36 (15)
O5—Al2—Lu1[ii]	43.89 (17)	O9—Lu3—Al1	79.05 (14)
Lu3[ii]—Al2—Lu1[ii]	68.03 (5)	O9[iii]—Lu3—Al1	149.97 (14)
O7—Al2—Lu4	65.8 (2)	O8—Lu3—Al1	85.02 (13)
O1[ii]—Al2—Lu4	41.4 (2)	O5[iv]—Lu3—Al1	134.72 (12)
O6[i]—Al2—Lu4	158.5 (2)	O6[ii]—Lu3—Al1	87.58 (13)
O5—Al2—Lu4	96.12 (18)	O4[ii]—Lu3—Al1	97.42 (14)
Lu3[ii]—Al2—Lu4	134.03 (8)	Al2[iv]—Lu3—Al1	115.70 (7)
Lu1[ii]—Al2—Lu4	66.26 (5)	Al1[iv]—Lu3—Al1	122.25 (5)
O9[iii]—Lu1—O6	174.8 (3)	O2[ii]—Lu3—Lu3[iii]	142.19 (14)
O9[iii]—Lu1—O3[iii]	86.4 (2)	O9—Lu3—Lu3[iii]	39.67 (13)
O6—Lu1—O3[iii]	89.4 (2)	O9[iii]—Lu3—Lu3[iii]	39.30 (19)
O9[iii]—Lu1—O7[iii]	85.8 (2)	O8—Lu3—Lu3[iii]	91.43 (16)
O6—Lu1—O7[iii]	98.0 (2)	O5[iv]—Lu3—Lu3[iii]	98.91 (14)
O3[iii]—Lu1—O7[iii]	101.03 (18)	O6[ii]—Lu3—Lu3[iii]	87.86 (13)
O9[iii]—Lu1—O5[iv]	74.76 (17)	O4[ii]—Lu3—Lu3[iii]	143.06 (13)
O6—Lu1—O5[iv]	105.69 (19)	Al2[iv]—Lu3—Lu3[iii]	90.40 (5)
O3[iii]—Lu1—O5[iv]	128.4 (2)	Al1[iv]—Lu3—Lu3[iii]	121.35 (4)
O7[iii]—Lu1—O5[iv]	124.3 (2)	Al1—Lu3—Lu3[iii]	116.13 (4)

O9^{iii}—Lu1—O2	104.5 (2)	O2^{ii}—Lu3—Lu4^{iii}	137.27 (15)
O6—Lu1—O2	80.21 (19)	O9—Lu3—Lu4^{iii}	95.71 (15)
O3^{iii}—Lu1—O2	165.4 (2)	O9^{iii}—Lu3—Lu4^{iii}	39.5 (2)
O7^{iii}—Lu1—O2	70.7 (2)	O8—Lu3—Lu4^{iii}	41.12 (12)
O5^{iv}—Lu1—O2	64.9 (2)	O5^{iv}—Lu3—Lu4^{iii}	96.21 (14)
O9^{iii}—Lu1—O1	100.2 (2)	O6^{ii}—Lu3—Lu4^{iii}	144.07 (12)
O6—Lu1—O1	75.68 (19)	O4^{ii}—Lu3—Lu4^{iii}	85.06 (13)
O3^{iii}—Lu1—O1	73.7 (2)	Al2^{iv}—Lu3—Lu4^{iii}	120.37 (4)
O7^{iii}—Lu1—O1	171.6 (2)	Al1^{iv}—Lu3—Lu4^{iii}	87.25 (5)
O5^{iv}—Lu1—O1	63.4 (2)	Al1—Lu3—Lu4^{iii}	123.92 (4)
O2—Lu1—O1	112.92 (16)	Lu3^{iii}—Lu3—Lu4^{iii}	64.036 (14)
O9^{iii}—Lu1—Al1^{iv}	87.18 (17)	O4^{ix}—Lu4—O9	163.0 (2)
O6—Lu1—Al1^{iv}	95.83 (15)	O4^{ix}—Lu4—O6^{ii}	87.53 (18)
O3^{iii}—Lu1—Al1^{iv}	160.44 (18)	O9—Lu4—O6^{ii}	77.1 (2)
O7^{iii}—Lu1—Al1^{iv}	96.91 (18)	O4^{ix}—Lu4—O8^{v}	84.7 (2)
O5^{iv}—Lu1—Al1^{iv}	32.14 (17)	O9—Lu4—O8^{v}	110.30 (17)
O2—Lu1—Al1^{iv}	32.95 (13)	O6^{ii}—Lu4—O8^{v}	171.9 (2)
O1—Lu1—Al1^{iv}	89.26 (14)	O4^{ix}—Lu4—O1^{ii}	75.4 (2)
O9^{iii}—Lu1—Al2^{iv}	85.38 (16)	O9—Lu4—O1^{ii}	108.45 (19)
O6—Lu1—Al2^{iv}	92.47 (15)	O6^{ii}—Lu4—O1^{ii}	80.3 (2)
O3^{iii}—Lu1—Al2^{iv}	100.91 (19)	O8^{v}—Lu4—O1^{ii}	100.0 (2)
O7^{iii}—Lu1—Al2^{iv}	155.76 (18)	O4^{ix}—Lu4—O8^{iii}	95.5 (2)
O5^{iv}—Lu1—Al2^{iv}	31.50 (17)	O9—Lu4—O8^{iii}	79.9 (2)
O2—Lu1—Al2^{iv}	89.77 (14)	O6^{ii}—Lu4—O8^{iii}	98.7 (2)
O1—Lu1—Al2^{iv}	32.02 (14)	O8^{v}—Lu4—O8^{iii}	79.7 (3)
Al1^{iv}—Lu1—Al2^{iv}	60.13 (5)	O1^{ii}—Lu4—O8^{iii}	170.9 (2)
O9^{iii}—Lu1—Lu2^{v}	91.9 (2)	O4^{ix}—Lu4—Al2	104.05 (15)
O6—Lu1—Lu2^{v}	82.89 (14)	O9—Lu4—Al2	83.86 (13)
O3^{iii}—Lu1—Lu2^{v}	36.67 (18)	O6^{ii}—Lu4—Al2	91.72 (14)
O7^{iii}—Lu1—Lu2^{v}	137.63 (18)	O8^{v}—Lu4—Al2	92.45 (14)
O5^{iv}—Lu1—Lu2^{v}	95.47 (17)	O1^{ii}—Lu4—Al2	30.48 (15)
O2—Lu1—Lu2^{v}	149.10 (13)	O8^{iii}—Lu4—Al2	158.20 (14)
O1—Lu1—Lu2^{v}	37.17 (13)	O4^{ix}—Lu4—Lu3^{iii}	135.90 (15)
Al1^{iv}—Lu1—Lu2^{v}	125.28 (5)	O9—Lu4—Lu3^{iii}	39.61 (13)
Al2^{iv}—Lu1—Lu2^{v}	65.26 (5)	O6^{ii}—Lu4—Lu3^{iii}	92.25 (14)
O9^{iii}—Lu1—Lu4^{iv}	139.2 (2)	O8^{v}—Lu4—Lu3^{iii}	91.67 (16)
O6—Lu1—Lu4^{iv}	37.22 (14)	O1^{ii}—Lu4—Lu3^{iii}	147.82 (15)
O3^{iii}—Lu1—Lu4^{iv}	85.85 (17)	O8^{iii}—Lu4—Lu3^{iii}	40.93 (18)
O7^{iii}—Lu1—Lu4^{iv}	135.01 (15)	Al2—Lu4—Lu3^{iii}	120.03 (4)
O5^{iv}—Lu1—Lu4^{iv}	79.07 (14)	O4^{ix}—Lu4—Lu4^{x}	90.25 (15)
O2—Lu1—Lu4^{iv}	91.80 (13)	O9—Lu4—Lu4^{x}	96.21 (15)
O1—Lu1—Lu4^{iv}	39.37 (13)	O6^{ii}—Lu4—Lu4^{x}	137.47 (14)
Al1^{iv}—Lu1—Lu4^{iv}	86.95 (5)	O8^{v}—Lu4—Lu4^{x}	40.44 (13)
Al2^{iv}—Lu1—Lu4^{iv}	57.05 (4)	O1^{ii}—Lu4—Lu4^{x}	139.71 (15)
Lu2^{v}—Lu1—Lu4^{iv}	59.875 (14)	O8^{iii}—Lu4—Lu4^{x}	39.3 (2)
O9^{iii}—Lu1—Lu3	36.30 (13)	Al2—Lu4—Lu4^{x}	129.75 (4)
O6—Lu1—Lu3	143.97 (15)	Lu3^{iii}—Lu4—Lu4^{x}	61.365 (15)
O3^{iii}—Lu1—Lu3	110.32 (15)	O4^{ix}—Lu4—Lu2^{ix}	39.59 (15)

Atoms	Angle	Atoms	Angle
O7^{iii}—Lu1—Lu3	106.94 (16)	O9—Lu4—Lu2^{ix}	142.06 (14)
O5^{iv}—Lu1—Lu3	38.47 (12)	O6^{ii}—Lu4—Lu2^{ix}	82.47 (14)
O2—Lu1—Lu3	83.91 (13)	O8^{v}—Lu4—Lu2^{ix}	93.01 (16)
O1—Lu1—Lu3	81.20 (13)	O1^{ii}—Lu4—Lu2^{ix}	35.84 (15)
Al1^{iv}—Lu1—Lu3	56.26 (4)	O8^{iii}—Lu4—Lu2^{ix}	135.12 (17)
Al2^{iv}—Lu1—Lu3	55.19 (4)	Al2—Lu4—Lu2^{ix}	65.06 (4)
Lu2^{v}—Lu1—Lu3	95.095 (18)	Lu3^{iii}—Lu4—Lu2^{ix}	172.933 (13)
Lu4^{iv}—Lu1—Lu3	112.083 (15)	Lu4^{x}—Lu4—Lu2^{ix}	120.06 (2)
O1^{vi}—Lu2—O3^{vii}	81.6 (2)	O4^{ix}—Lu4—Lu3^{v}	45.83 (16)
O1^{vi}—Lu2—O2	89.32 (19)	O9—Lu4—Lu3^{v}	149.15 (16)
O3^{vii}—Lu2—O2	169.1 (2)	O6^{ii}—Lu4—Lu3^{v}	133.35 (14)
O1^{vi}—Lu2—O7^{iii}	164.5 (2)	O8^{v}—Lu4—Lu3^{v}	39.02 (17)
O3^{vii}—Lu2—O7^{iii}	113.97 (17)	O1^{ii}—Lu4—Lu3^{v}	85.63 (15)
O2—Lu2—O7^{iii}	75.2 (2)	O8^{iii}—Lu4—Lu3^{v}	88.7 (2)
O1^{vi}—Lu2—O8^{vii}	91.6 (2)	Al2—Lu4—Lu3^{v}	98.07 (5)
O3^{vii}—Lu2—O8^{vii}	88.2 (2)	Lu3^{iii}—Lu4—Lu3^{v}	120.326 (15)
O2—Lu2—O8^{vii}	98.0 (2)	Lu4^{x}—Lu4—Lu3^{v}	58.961 (16)
O7^{iii}—Lu2—O8^{vii}	89.1 (3)	Lu2^{ix}—Lu4—Lu3^{v}	61.562 (13)
O1^{vi}—Lu2—O4	74.9 (2)	O4^{ix}—Lu4—Lu1^{ii}	86.32 (15)
O3^{vii}—Lu2—O4	92.4 (2)	O9—Lu4—Lu1^{ii}	85.60 (15)
O2—Lu2—O4	79.5 (2)	O6^{ii}—Lu4—Lu1^{ii}	36.81 (14)
O7^{iii}—Lu2—O4	103.2 (2)	O8^{v}—Lu4—Lu1^{ii}	144.42 (14)
O8^{vii}—Lu2—O4	166.2 (2)	O1^{ii}—Lu4—Lu1^{ii}	44.44 (15)
O1^{vi}—Lu2—Lu1^{vi}	44.59 (16)	O8^{iii}—Lu4—Lu1^{ii}	135.46 (19)
O3^{vii}—Lu2—Lu1^{vi}	37.11 (17)	Al2—Lu4—Lu1^{ii}	56.69 (4)
O2—Lu2—Lu1^{vi}	133.86 (14)	Lu3^{iii}—Lu4—Lu1^{ii}	117.97 (2)
O7^{iii}—Lu2—Lu1^{vi}	150.92 (17)	Lu4^{x}—Lu4—Lu1^{ii}	173.404 (16)
O8^{vii}—Lu2—Lu1^{vi}	87.2 (2)	Lu2^{ix}—Lu4—Lu1^{ii}	59.705 (14)
O4—Lu2—Lu1^{vi}	84.98 (14)	Lu3^{v}—Lu4—Lu1^{ii}	121.266 (15)
O1^{vi}—Lu2—Lu4^{viii}	38.06 (15)	Al2^{iv}—O1—Lu2^{v}	139.9 (3)
O3^{vii}—Lu2—Lu4^{viii}	86.66 (16)	Al2^{iv}—O1—Lu4^{iv}	108.1 (3)
O2—Lu2—Lu4^{viii}	82.52 (14)	Lu2^{v}—O1—Lu4^{iv}	106.1 (2)
O7^{iii}—Lu2—Lu4^{viii}	137.89 (15)	Al2^{iv}—O1—Lu1	98.2 (3)
O8^{vii}—Lu2—Lu4^{viii}	129.58 (17)	Lu2^{v}—O1—Lu1	98.2 (2)
O4—Lu2—Lu4^{viii}	36.84 (14)	Lu4^{iv}—O1—Lu1	96.2 (2)
Lu1^{vi}—Lu2—Lu4^{viii}	60.420 (13)	Al1^{iv}—O2—Lu2	127.6 (3)
O1^{vi}—Lu2—Lu3^{iv}	85.18 (17)	Al1^{iv}—O2—Lu3^{iv}	112.3 (3)
O3^{vii}—Lu2—Lu3^{iv}	136.93 (14)	Lu2—O2—Lu3^{iv}	109.3 (2)
O2—Lu2—Lu3^{iv}	35.36 (14)	Al1^{iv}—O2—Lu1	97.8 (2)
O7^{iii}—Lu2—Lu3^{iv}	83.02 (17)	Lu2—O2—Lu1	103.7 (2)
O8^{vii}—Lu2—Lu3^{iv}	133.14 (18)	Lu3^{iv}—O2—Lu1	101.5 (2)
O4—Lu2—Lu3^{iv}	44.56 (15)	Al1—O3—Lu2^{vii}	126.3 (5)
Lu1^{vi}—Lu2—Lu3^{iv}	119.653 (15)	Al1—O3—Lu1^{iii}	123.9 (5)
Lu4^{viii}—Lu2—Lu3^{iv}	59.233 (14)	Lu2^{vii}—O3—Lu1^{iii}	106.2 (2)
O1^{vi}—Lu2—Lu1	128.85 (16)	Al1^{xi}—O4—Lu4^{viii}	135.4 (3)
O3^{vii}—Lu2—Lu1	149.48 (17)	Al1^{xi}—O4—Lu2	117.6 (3)
O2—Lu2—Lu1	40.30 (14)	Lu4^{viii}—O4—Lu2	103.6 (2)
O7^{iii}—Lu2—Lu1	35.63 (17)	Al1^{xi}—O4—Lu3^{iv}	95.9 (3)

O8vii—Lu2—Lu1	88.6 (2)	Lu4viii—O4—Lu3iv	96.4 (2)
O4—Lu2—Lu1	97.74 (14)	Lu2—O4—Lu3iv	95.9 (2)
Lu1vi—Lu2—Lu1	172.025 (12)	Al1—O5—Al2	134.9 (3)
Lu4viii—Lu2—Lu1	118.072 (14)	Al1—O5—Lu3ii	105.3 (3)
Lu3iv—Lu2—Lu1	59.438 (13)	Al2—O5—Lu3ii	103.1 (3)
O1vi—Lu2—Lu4iii	124.70 (15)	Al1—O5—Lu1ii	102.6 (3)
O3vii—Lu2—Lu4iii	102.42 (15)	Al2—O5—Lu1ii	104.6 (3)
O2—Lu2—Lu4iii	87.60 (14)	Lu3ii—O5—Lu1ii	102.39 (18)
O7iii—Lu2—Lu4iii	54.38 (15)	Al2xi—O6—Lu1	122.0 (3)
O8vii—Lu2—Lu4iii	34.8 (2)	Al2xi—O6—Lu4iv	125.6 (3)
O4—Lu2—Lu4iii	156.67 (14)	Lu1—O6—Lu4iv	106.0 (2)
Lu1vi—Lu2—Lu4iii	117.607 (14)	Al2xi—O6—Lu3iv	95.4 (2)
Lu4viii—Lu2—Lu4iii	159.792 (10)	Lu1—O6—Lu3iv	99.6 (2)
Lu3iv—Lu2—Lu4iii	118.642 (17)	Lu4iv—O6—Lu3iv	100.7 (2)
Lu1—Lu2—Lu4iii	60.716 (12)	Al2—O7—Lu2iii	126.1 (5)
O1vi—Lu2—Lu3vii	85.85 (16)	Al2—O7—Lu1iii	123.6 (5)
O3vii—Lu2—Lu3vii	56.75 (14)	Lu2iii—O7—Lu1iii	109.0 (2)
O2—Lu2—Lu3vii	128.77 (14)	Lu4vi—O8—Lu2vii	110.1 (3)
O7iii—Lu2—Lu3vii	102.54 (16)	Lu4vi—O8—Lu3	102.9 (2)
O8vii—Lu2—Lu3vii	31.5 (2)	Lu2vii—O8—Lu3	117.4 (3)
O4—Lu2—Lu3vii	146.03 (14)	Lu4vi—O8—Lu4iii	100.3 (3)
Lu1vi—Lu2—Lu3vii	62.045 (13)	Lu2vii—O8—Lu4iii	125.0 (2)
Lu4viii—Lu2—Lu3vii	119.182 (17)	Lu3—O8—Lu4iii	97.9 (2)
Lu3iv—Lu2—Lu3vii	161.782 (11)	Lu1iii—O9—Lu3	120.0 (4)
Lu1—Lu2—Lu3vii	116.038 (15)	Lu1iii—O9—Lu4	113.8 (3)
Lu4iii—Lu2—Lu3vii	55.607 (13)	Lu3—O9—Lu4	110.2 (2)
O2ii—Lu3—O9	102.6 (2)	Lu1iii—O9—Lu3iii	108.2 (2)
O2ii—Lu3—O9iii	176.7 (3)	Lu3—O9—Lu3iii	101.0 (3)
O9—Lu3—O9iii	79.0 (3)	Lu4—O9—Lu3iii	100.9 (3)

Symmetry codes: (i) $x, y, z-1$; (ii) $x, -y+1/2, z-1/2$; (iii) $-x+1, -y, -z+1$; (iv) $x, -y+1/2, z+1/2$; (v) $x+1, y, z$; (vi) $x-1, y, z$; (vii) $-x, -y, -z+1$; (viii) $x-1, -y+1/2, z+1/2$; (ix) $x+1, -y+1/2, z-1/2$; (x) $-x+2, -y, -z+1$; (xi) $x, y, z+1$.