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# Lutetium ultraphosphate

**Karima Horchani-Naifer and Mokhtar Férid***

Unité de Recherches de Matériaux de Terres Rares, Centre National de Recherches en Sciences des Matériaux, BP 95 Hammam-Lif, 2050, Tunisia
Correspondence e-mail: mokhtar.ferid@inrst.rnrt.tn

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Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(P–O) = 0.002 Å; $R$ factor = 0.019; $wR$ factor = 0.051; data-to-parameter ratio = 15.9.

The structure of the title compound, $LuP_5O_{14}$, comprises puckered eight-membered $PO_4$ rings linked by the lutetium cations in a complex way, forming a three-dimensional framework. Each eight-membered phosphate ring shares a bridging tetrahedron with each of four adjacent tetrahedra, to form layers of $PO_4$ tetrahedra. These layers are $c/2$ in thickness and parallel to the $ab$ plane. Each Lu ion is contained in one such layer, forming bonds to six O atoms in that layer and also to one O atom belonging to a tetrahedron in each of the layers lying above and below it. The $LuO_8$ polyhedra are isolated from one another, since they share no common atoms. The Lu ions lie on twofold axes (special position 4*e*) and the shortest Lu···Lu distance is 5.703 (1) Å.

## Related literature

For related literature, see: Durif (1971); Hong (1974); Hong & Pierce (1974). For the classification of ultraphosphates, see: Bagieu-Beucher & Tranqui (1970).

## Experimental

*Crystal data*

$LuP_5O_{14}$
$M_r$ = 553.82
Monoclinic, $C2/c$
$a$ = 12.8128 (14) Å
$b$ = 12.6821 (13) Å
$c$ = 12.3330 (13) Å
$\beta$ = 91.295 (3)°
$V$ = 2003.5 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 10.74 mm$^{-1}$
$T$ = 298 (2) K
0.20 × 0.19 × 0.18 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.121, $T_{max}$ = 0.145
10422 measured reflections
2912 independent reflections
2734 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
2 standard reflections
every 150 reflections
intensity decay: 2%

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.050
$S$ = 1.08
2912 reflections
183 parameters
$\Delta\rho_{max}$ = 1.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.98 e Å$^{-3}$

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Enraf–Nonius, 1994; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2072).

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# supporting information

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## Lutetium ultraphosphate

**Karima Horchani-Naifer and Mokhtar Férid**

### S1. Comment

The structure of $LuP_5O_{14}$ is a type (II) rare-earth ultraphosphates as classified by Bagieu-Beucher & Tranqui (1970), since it crystallizes in the monoclinic system with space group *C*2/*c*. In this structure, the lutetium ion is surrounded by eight oxygen atoms that form distorted polyhedra. Each of the oxygen atoms in the $LuO_8$ polyhedra are shared exclusively with $PO_4$ tetrahedra to form a three-dimensional framework, which delimits interesting tunnels (Fig.1). The structure is built up from ($PO_4$) tetrahedra (Fig.2) which are cross-linked by bridging O atoms, but these do not form helical ribbons, as in the $NdP_5O_{14}$ structure type (I) (Hong, 1974), and $HoP_5O_{14}$ structure type (III) (Durif, 1971). The anion is being constructed from a succession of eight-membred rings interconnected through the ternary tetrahedra in a complex way (Fig.3a). The members of an individual ring are shown with yellow color. Each ring shares a bridging tetrahedron with each of four adjacent tetrahedra to form layers of $PO_4$ tetrahedra, as illustrated in Fig.3b. These layers are about c/2 in thickness and parallel to the a-b plane. Each Lu ion is contained in one such layer, forming bonds to six oxygen in that layer and also to one oxygen belonging to a tetrahedron in each of the layers lying above and bolow it. the $LuO_8$ polyhedra are isolated from one another, since they share no common atoms. The shortest Lu-Lu distances are 5.703. The $LuP_5O_{14}$ ultraphosphate is isostructural with $YbP_5O_{14}$ (Hong & Pierce, 1974).

### S2. Experimental

Single crystal of $LuP_5O_{14}$ was prepared by flux method. At room temperature, 0.5 g of $Lu_2O_3$ were slowly added to 10 ml of phosphoric acid $H_3PO_4$ (85%). The mixture was then slowly heated to 673 K and kept at this temperature for seven days. colorless, crystals were separated from the excess phosphoric acid by washing the product in boiling water.

### S3. Refinement

The highest peak and the deepest hole are located 0.79Å and 0.54 Å, respectively, from Lu1 and Lu2.

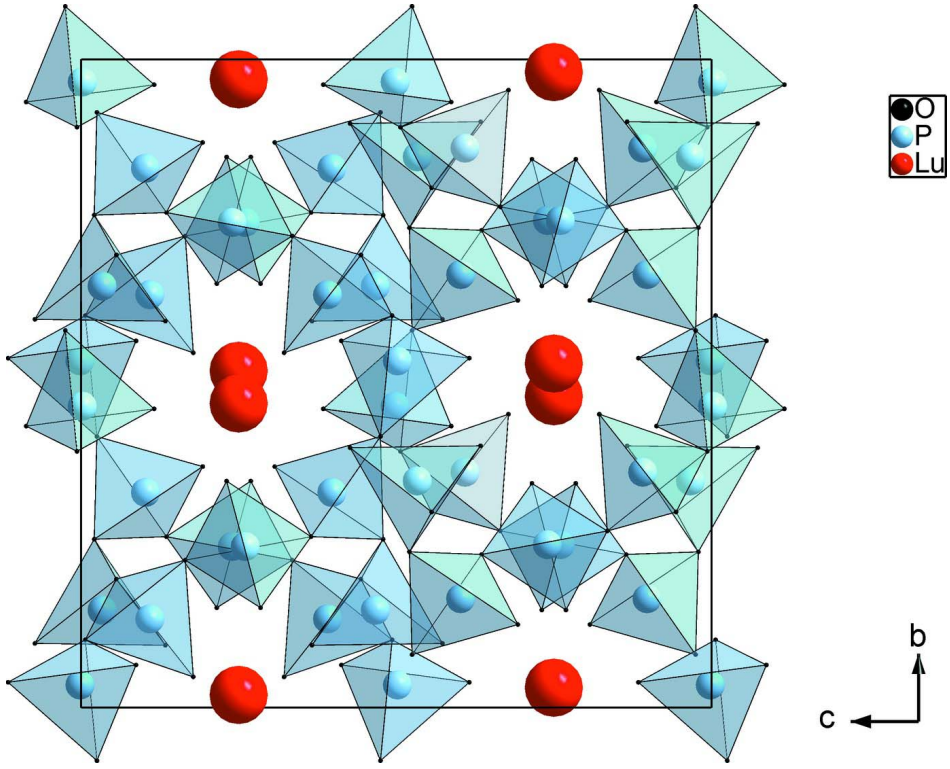


**Figure 1**

The structural arrangement of $LuP_5O_{14}$ along the *a* axis, showing tunnels in which the Lu ions are located.

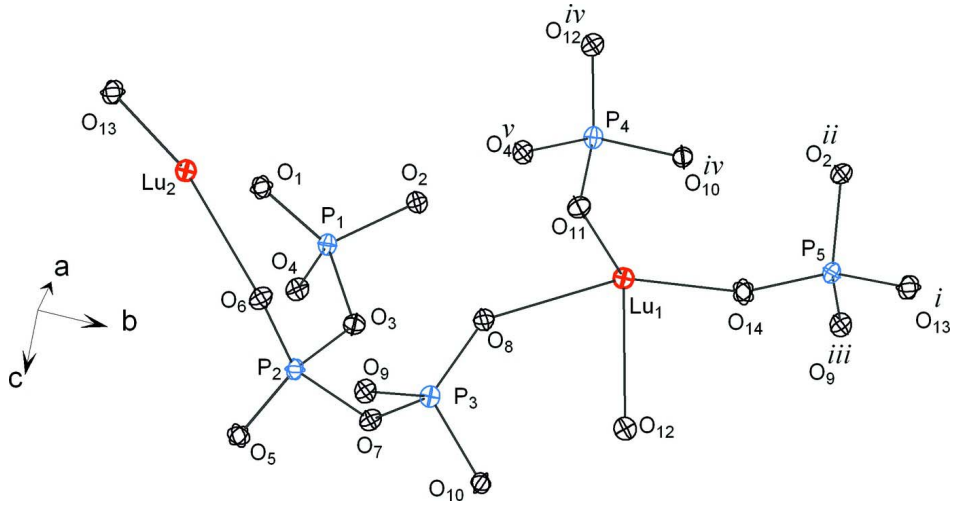


**Figure 2**

Projection of the ultraphosphate with anisotropic displacement parameters drawn at the 50% probability level. [Symmetry codes: (i) x, y+1, z ; (ii)-x+5/2, y+1/2, -z+3/2 ; (iii) x+1/2, y+1/2, z; (iv)x, -y+2, z-1/2 ; (v)x-1/2, -y+3/2, z-1/2.

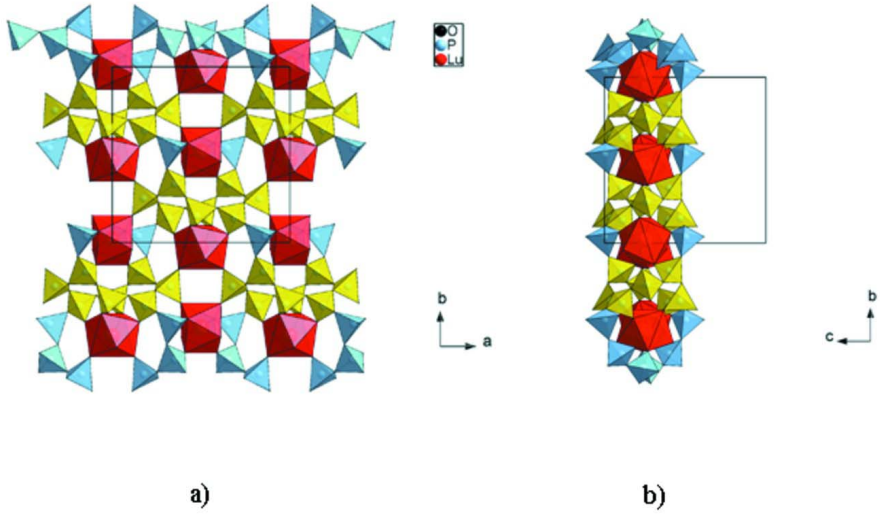


**Figure 3**

a) Projection of one layer showing $LuO_8$ polyhedra and linkage of $PO_4$ tetrahedra forming rings (yellow) in $LuP_5O_{14}$. b) Projection of one layer along the b axis with c/2 thickness.

## lutetium ultraphosphate

*Crystal data*

$LuP_5O_{14}$
$M_r = 553.82$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 12.8128\ (14)$ Å
$b = 12.6821\ (13)$ Å
$c = 12.3330\ (13)$ Å
$\beta = 91.295\ (3)°$
$V = 2003.5\ (4)$ Å$^3$
$Z = 8$
$F(000) = 2064$
$D_x = 3.672$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7043 reflections
$\theta = 2.3–30.0°$
$\mu = 10.74$ mm$^{-1}$
$T = 298$ K
Prism, colorless
0.20 × 0.19 × 0.18 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.121$, $T_{max} = 0.145$
10422 measured reflections
2912 independent reflections
2734 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.3°$
$h = -17\rightarrow18$
$k = -17\rightarrow17$
$l = -17\rightarrow17$
2 standard reflections every 150 reflections
intensity decay: 2%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.050$
$S = 1.08$
2912 reflections
183 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 3.0307P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.98$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00637 (11)

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Lu1 | 1.0000 | 1.019590 (11) | 0.7500 | 0.00946 (6) |
| Lu2 | 1.0000 | 0.469251 (11) | 0.7500 | 0.00947 (6) |
| P1 | 1.18263 (5) | 0.63687 (5) | 0.89095 (5) | 0.01020 (13) |
| P2 | 0.97504 (5) | 0.65029 (5) | 0.96672 (5) | 0.01037 (13) |
| P3 | 0.85012 (5) | 0.83192 (5) | 0.89783 (5) | 0.01042 (13) |
| P4 | 0.85469 (5) | 0.96507 (5) | 0.50182 (6) | 0.01080 (14) |
| P5 | 1.17542 (6) | 1.24856 (5) | 0.76032 (6) | 0.01017 (14) |
| O1 | 1.15332 (15) | 0.54741 (15) | 0.82204 (16) | 0.0131 (4) |
| O2 | 1.24259 (17) | 0.72754 (16) | 0.83475 (17) | 0.0131 (4) |
| O3 | 1.09081 (14) | 0.69824 (15) | 0.94396 (15) | 0.0120 (3) |
| O4 | 1.24970 (13) | 0.60463 (17) | 0.99342 (13) | 0.0121 (4) |
| O5 | 0.97503 (15) | 0.59905 (15) | 1.07328 (15) | 0.0137 (4) |
| O6 | 0.93961 (15) | 0.59620 (15) | 0.86627 (15) | 0.0132 (4) |
| O7 | 0.91291 (17) | 0.75979 (14) | 0.97911 (18) | 0.0114 (4) |
| O8 | 0.90954 (15) | 0.87184 (15) | 0.80717 (15) | 0.0132 (4) |
| O9 | 0.75333 (18) | 0.76371 (15) | 0.86473 (18) | 0.0128 (4) |
| O10 | 0.80606 (15) | 0.91824 (14) | 0.97493 (15) | 0.0123 (4) |
| O11 | 0.88893 (16) | 0.96091 (15) | 0.61582 (16) | 0.0139 (4) |
| O12 | 0.92416 (15) | 1.06579 (15) | 0.91286 (15) | 0.0135 (4) |
| O13 | 1.12590 (16) | 0.34943 (15) | 0.73083 (16) | 0.0142 (4) |
| O14 | 1.11367 (16) | 1.15411 (15) | 0.78473 (16) | 0.0147 (4) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Lu1 | 0.00912 (9) | 0.00934 (9) | 0.00992 (9) | 0.000 | −0.00025 (6) | 0.000 |
| Lu2 | 0.00918 (9) | 0.00909 (8) | 0.01011 (9) | 0.000 | −0.00038 (6) | 0.000 |
| P1 | 0.0100 (3) | 0.0094 (3) | 0.0112 (3) | 0.0001 (2) | −0.0002 (2) | 0.0002 (2) |
| P2 | 0.0100 (3) | 0.0099 (3) | 0.0112 (3) | 0.0004 (2) | 0.0001 (2) | 0.0002 (2) |
| P3 | 0.0103 (3) | 0.0097 (3) | 0.0112 (3) | −0.0001 (2) | −0.0002 (2) | 0.0000 (2) |
| P4 | 0.0108 (3) | 0.0097 (3) | 0.0119 (3) | −0.0006 (2) | −0.0003 (2) | 0.0001 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| P5 | 0.0094 (3) | 0.0099 (3) | 0.0112 (3) | −0.0002 (2) | −0.0004 (3) | −0.0006 (2) |
| O1 | 0.0125 (9) | 0.0125 (8) | 0.0143 (9) | −0.0011 (7) | 0.0008 (7) | −0.0012 (7) |
| O2 | 0.0142 (10) | 0.0108 (8) | 0.0144 (9) | −0.0013 (7) | 0.0030 (7) | 0.0002 (7) |
| O3 | 0.0099 (8) | 0.0113 (8) | 0.0149 (9) | 0.0002 (7) | 0.0013 (7) | −0.0004 (7) |
| O4 | 0.0115 (10) | 0.0129 (9) | 0.0118 (9) | 0.0024 (6) | −0.0014 (7) | −0.0003 (6) |
| O5 | 0.0148 (9) | 0.0127 (8) | 0.0135 (9) | 0.0004 (7) | −0.0001 (7) | 0.0015 (7) |
| O6 | 0.0132 (9) | 0.0135 (8) | 0.0129 (9) | 0.0018 (7) | −0.0009 (7) | −0.0010 (7) |
| O7 | 0.0107 (10) | 0.0119 (8) | 0.0116 (9) | 0.0017 (6) | −0.0008 (7) | −0.0007 (6) |
| O8 | 0.0153 (9) | 0.0122 (8) | 0.0122 (8) | −0.0023 (7) | 0.0012 (7) | −0.0001 (7) |
| O9 | 0.0119 (10) | 0.0136 (8) | 0.0129 (10) | −0.0016 (7) | −0.0012 (8) | 0.0000 (7) |
| O10 | 0.0123 (9) | 0.0098 (8) | 0.0150 (9) | 0.0007 (7) | 0.0013 (7) | −0.0012 (7) |
| O11 | 0.0150 (10) | 0.0142 (8) | 0.0125 (9) | −0.0020 (7) | −0.0014 (7) | 0.0002 (7) |
| O12 | 0.0143 (9) | 0.0129 (8) | 0.0135 (9) | −0.0007 (7) | 0.0013 (7) | 0.0002 (7) |
| O13 | 0.0148 (9) | 0.0137 (8) | 0.0142 (9) | 0.0028 (7) | −0.0001 (7) | 0.0002 (7) |
| O14 | 0.0156 (9) | 0.0131 (8) | 0.0151 (9) | −0.0044 (7) | −0.0009 (7) | 0.0002 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Lu1—O14 | 2.2775 (19) | P2—O7 | 1.6097 (19) |
| Lu1—O14$^{i}$ | 2.2775 (19) | P2—O3 | 1.633 (2) |
| Lu1—O11 | 2.283 (2) | P3—O8 | 1.458 (2) |
| Lu1—O11$^{i}$ | 2.283 (2) | P3—O9 | 1.559 (2) |
| Lu1—O8 | 2.3213 (19) | P3—O10 | 1.5638 (19) |
| Lu1—O8$^{i}$ | 2.3213 (19) | P3—O7 | 1.566 (2) |
| Lu1—O12 | 2.3260 (19) | P4—O11 | 1.464 (2) |
| Lu1—O12$^{i}$ | 2.3260 (19) | P4—O12$^{iv}$ | 1.481 (2) |
| Lu2—O13$^{i}$ | 2.2326 (19) | P4—O4$^{v}$ | 1.6111 (19) |
| Lu2—O13 | 2.2326 (19) | P4—O10$^{iv}$ | 1.637 (2) |
| Lu2—O6 | 2.3016 (19) | P5—O13$^{vi}$ | 1.470 (2) |
| Lu2—O6$^{i}$ | 2.3016 (19) | P5—O14 | 1.470 (2) |
| Lu2—O1 | 2.356 (2) | P5—O2$^{vii}$ | 1.614 (2) |
| Lu2—O1$^{i}$ | 2.356 (2) | P5—O9$^{viii}$ | 1.623 (2) |
| Lu2—O5$^{ii}$ | 2.3604 (19) | O2—P5$^{ix}$ | 1.614 (2) |
| Lu2—O5$^{iii}$ | 2.3604 (19) | O4—P4$^{x}$ | 1.6111 (19) |
| P1—O1 | 1.462 (2) | O5—Lu2$^{iii}$ | 2.3604 (19) |
| P1—O2 | 1.555 (2) | O9—P5$^{xi}$ | 1.623 (2) |
| P1—O3 | 1.5659 (19) | O10—P4$^{xii}$ | 1.637 (2) |
| P1—O4 | 1.5665 (18) | O12—P4$^{xii}$ | 1.481 (2) |
| P2—O5 | 1.466 (2) | O13—P5$^{xiii}$ | 1.470 (2) |
| P2—O6 | 1.479 (2) | | |

| | | | |
|---|---|---|---|
| O14—Lu1—O14$^{i}$ | 82.98 (10) | O13—Lu2—O5$^{iii}$ | 76.40 (7) |
| O14—Lu1—O11 | 140.00 (7) | O6—Lu2—O5$^{iii}$ | 73.85 (7) |
| O14$^{i}$—Lu1—O11 | 73.88 (7) | O6$^{i}$—Lu2—O5$^{iii}$ | 142.33 (7) |
| O14—Lu1—O11$^{i}$ | 73.88 (7) | O1—Lu2—O5$^{iii}$ | 73.25 (7) |
| O14$^{i}$—Lu1—O11$^{i}$ | 140.00 (7) | O1$^{i}$—Lu2—O5$^{iii}$ | 126.65 (7) |
| O11—Lu1—O11$^{i}$ | 141.95 (10) | O5$^{ii}$—Lu2—O5$^{iii}$ | 136.94 (9) |
| O14—Lu1—O8 | 150.35 (7) | O1—P1—O2 | 115.98 (12) |

| | | | |
|---|---|---|---|
| O14$^{i}$—Lu1—O8 | 109.89 (7) | O1—P1—O3 | 116.30 (11) |
| O11—Lu1—O8 | 69.49 (7) | O2—P1—O3 | 101.66 (11) |
| O11$^{i}$—Lu1—O8 | 79.86 (7) | O1—P1—O4 | 113.30 (12) |
| O14—Lu1—O8$^{i}$ | 109.89 (7) | O2—P1—O4 | 106.56 (12) |
| O14$^{i}$—Lu1—O8$^{i}$ | 150.35 (7) | O3—P1—O4 | 101.33 (10) |
| O11—Lu1—O8$^{i}$ | 79.86 (7) | O5—P2—O6 | 122.63 (12) |
| O11$^{i}$—Lu1—O8$^{i}$ | 69.49 (7) | O5—P2—O7 | 106.70 (11) |
| O8—Lu1—O8$^{i}$ | 72.36 (10) | O6—P2—O7 | 109.67 (11) |
| O14—Lu1—O12 | 85.80 (7) | O5—P2—O3 | 109.73 (11) |
| O14$^{i}$—Lu1—O12 | 72.29 (7) | O6—P2—O3 | 106.95 (11) |
| O11—Lu1—O12 | 116.25 (7) | O7—P2—O3 | 98.52 (11) |
| O11$^{i}$—Lu1—O12 | 73.85 (7) | O8—P3—O9 | 114.72 (12) |
| O8—Lu1—O12 | 73.73 (7) | O8—P3—O10 | 115.17 (11) |
| O8$^{i}$—Lu1—O12 | 133.38 (7) | O9—P3—O10 | 104.58 (12) |
| O14—Lu1—O12$^{i}$ | 72.29 (7) | O8—P3—O7 | 115.10 (12) |
| O14$^{i}$—Lu1—O12$^{i}$ | 85.80 (7) | O9—P3—O7 | 103.75 (11) |
| O11—Lu1—O12$^{i}$ | 73.85 (7) | O10—P3—O7 | 101.94 (11) |
| O11$^{i}$—Lu1—O12$^{i}$ | 116.25 (7) | O11—P4—O12$^{iv}$ | 121.99 (12) |
| O8—Lu1—O12$^{i}$ | 133.38 (7) | O11—P4—O4$^{v}$ | 105.88 (11) |
| O8$^{i}$—Lu1—O12$^{i}$ | 73.73 (7) | O12$^{iv}$—P4—O4$^{v}$ | 108.80 (11) |
| O12—Lu1—O12$^{i}$ | 150.82 (9) | O11—P4—O10$^{iv}$ | 109.37 (11) |
| O13$^{i}$—Lu2—O13 | 94.22 (10) | O12$^{iv}$—P4—O10$^{iv}$ | 108.74 (11) |
| O13$^{i}$—Lu2—O6 | 98.99 (7) | O4$^{v}$—P4—O10$^{iv}$ | 99.76 (11) |
| O13—Lu2—O6 | 142.75 (7) | O13$^{vi}$—P5—O14 | 121.90 (13) |
| O13$^{i}$—Lu2—O6$^{i}$ | 142.75 (7) | O13$^{vi}$—P5—O2$^{vii}$ | 104.38 (11) |
| O13—Lu2—O6$^{i}$ | 98.99 (7) | O14—P5—O2$^{vii}$ | 112.10 (11) |
| O6—Lu2—O6$^{i}$ | 91.22 (10) | O13$^{vi}$—P5—O9$^{viii}$ | 110.34 (11) |
| O13$^{i}$—Lu2—O1 | 147.63 (7) | O14—P5—O9$^{viii}$ | 104.96 (11) |
| O13—Lu2—O1 | 74.22 (7) | O2$^{vii}$—P5—O9$^{viii}$ | 101.37 (12) |
| O6—Lu2—O1 | 76.11 (7) | P1—O1—Lu2 | 138.32 (12) |
| O6$^{i}$—Lu2—O1 | 69.60 (7) | P1—O2—P5$^{ix}$ | 141.48 (14) |
| O13$^{i}$—Lu2—O1$^{i}$ | 74.22 (7) | P1—O3—P2 | 125.49 (12) |
| O13—Lu2—O1$^{i}$ | 147.63 (7) | P1—O4—P4$^{x}$ | 129.58 (12) |
| O6—Lu2—O1$^{i}$ | 69.60 (7) | P2—O5—Lu2$^{iii}$ | 170.97 (13) |
| O6$^{i}$—Lu2—O1$^{i}$ | 76.11 (7) | P2—O6—Lu2 | 138.19 (12) |
| O1—Lu2—O1$^{i}$ | 130.25 (10) | P3—O7—P2 | 133.72 (14) |
| O13$^{i}$—Lu2—O5$^{ii}$ | 76.40 (7) | P3—O8—Lu1 | 141.86 (12) |
| O13—Lu2—O5$^{ii}$ | 74.67 (7) | P3—O9—P5$^{xi}$ | 138.16 (14) |
| O6—Lu2—O5$^{ii}$ | 142.33 (7) | P3—O10—P4$^{xii}$ | 127.96 (13) |
| O6$^{i}$—Lu2—O5$^{ii}$ | 73.85 (7) | P4—O11—Lu1 | 148.50 (12) |
| O1—Lu2—O5$^{ii}$ | 126.65 (7) | P4$^{xii}$—O12—Lu1 | 147.46 (12) |
| O1$^{i}$—Lu2—O5$^{ii}$ | 73.25 (7) | P5$^{xiii}$—O13—Lu2 | 151.04 (13) |
| O13$^{i}$—Lu2—O5$^{iii}$ | 74.67 (7) | P5—O14—Lu1 | 156.41 (13) |

Symmetry codes: (i) $-x+2, y, -z+3/2$; (ii) $x, -y+1, z-1/2$; (iii) $-x+2, -y+1, -z+2$; (iv) $x, -y+2, z-1/2$; (v) $x-1/2, -y+3/2, z-1/2$; (vi) $x, y+1, z$; (vii) $-x+5/2, y+1/2, -z+3/2$; (viii) $x+1/2, y+1/2, z$; (ix) $-x+5/2, y-1/2, -z+3/2$; (x) $x+1/2, -y+3/2, z+1/2$; (xi) $x-1/2, y-1/2, z$; (xii) $x, -y+2, z+1/2$; (xiii) $x, y-1, z$.