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$K_3Gd(PO_4)_2$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(P–O) = 0.004 Å; R factor = 0.027; wR factor = 0.065; data-to-parameter ratio = 12.4.

The title compound, tripotassium gadolinium(III) bis[orthophosphate(V)], was synthesized by a high-temperature solution reaction. Of the 12 atoms of the asymmetric unit (1 × Gd, 2 × P, 3 × K, 6 × O), all but two O atoms (which are in general positions) lie on mirror planes. The crystal structure features sheets of composition $[Gd(PO_4)_2]^{3-}$ which extend parallel to (100) and are built up from isolated PO_4 tetrahedra and GdO_7 monocapped prisms through corner- and edge-sharing. The K^+ ions, which have coordination numbers of 10, 9 and 11, help to stack the anionic sheets along [100] into a three-dimensional structure.

Related literature

For the structures, properties and applications of phosphates with general formula $M_3RE(PO_4)_2$ (M = alkali metal, RE = rare earth metal), see: $K_3Lu(PO_4)_2$ (Efremov *et al.*, 1981); $K_3(La_{0.99}Nd_{0.01})(PO_4)_2$ (Hong & Chinn, 1976); $Na_3Ce(PO_4)_2$ (Karpov *et al.*, 1980); $K_3Eu(PO_4)_2$ (Morozov *et al.*, 2001); $K_3Sm(PO_4)_2$ (Toumi *et al.*, 1999); $K_3Ce(PO_4)_2$ (Zah-Letho *et al.*, 1988).

Experimental

Crystal data

$K_3Gd(PO_4)_2$
M_r = 464.49
Monoclinic, $P2_1/m$
a = 7.4153 (15) Å
b = 5.6206 (11) Å
c = 9.445 (2) Å
β = 90.723 (14)°
V = 393.62 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 10.43 mm^{-1}
T = 293 K
0.30 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury70 CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.304, T_{max} = 0.624
3036 measured reflections
993 independent reflections
946 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.03
993 reflections
80 parameters
$\Delta\rho_{max}$ = 2.38 e Å^{-3}
$\Delta\rho_{min}$ = −2.68 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2378).

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supporting information

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$K_3Gd(PO_4)_2$

Dan Zhao and Fei Fei Li

S1. Comment

Inorganic phosphates with general formula $M_3RE(PO_4)_2$ have been investigated in the past years due to their interesting optical properties, in which *M* is a alkali metal cation and *RE* is a trivalent rare-earth cation: $K_3Lu(PO_4)_2$, space group $P\bar{3}$ (Efremov *et al.*, 1981); $K_3(La_{0.99}Nd_{0.01})(PO_4)_2$, $P2_1/m$ (Hong & Chinn, 1976); $Na_3Ce(PO_4)_2$, $Pca2_1$ (Karpov *et al.*, 1980); $K_3Eu(PO_4)_2$, $P2_1/m$ (Morozov *et al.*, 2001); $K_3Sm(PO_4)_2$, $P2_1/m$ (Toumi *et al.*, 1999); $K_3Ce(PO_4)_2$, $P2_1/m$ (Zah-Letho *et al.*, 1988). We report herein the synthesis and crystal structure of $K_3Gd(PO_4)_2$ which is isotypic with all structures crystallizing in space group $P2_1/m$.

As shown in Fig. 1, the crystal structure of $K_3Gd(PO_4)_2$ features two-dimensional sheets with composition $[Gd(PO_4)_2]^{3-}$ extending in the *bc* plane and constructed from isolated PO_4 tetrahedra and isolated GdO_7 monocapped prisms through corner- and edge-sharing. The K^+ cations, with coordination numbers of 10 (K1), 9 (K2) and 11 (K3), are situated between these sheets and join them through coulombic action to the O^{2-} anions, eventually forming the three-dimensional framework of $K_3Gd(PO_4)_2$ (Fig. 2).

S2. Experimental

The finely ground reagents K_2CO_3, Gd_2O_3, and $NH_4H_2PO_4$ were mixed in the molar ratio K: Gd: P = 12: 1: 10, placed in a Pt crucible, and heated at 573 K for 4 h. The mixture was re-ground and heated at 1173 K for 20 h, then cooled to 573 K at a rate of 4 K h^{-1}, and finally quenched to room temperature. A few colorless crystals of the title compound with prismatic shape were obtained.

S3. Refinement

The highest peak in the difference electron density map is 1.10 Å from Gd1 while the deepest hole is 0.85 Å from the same atom.

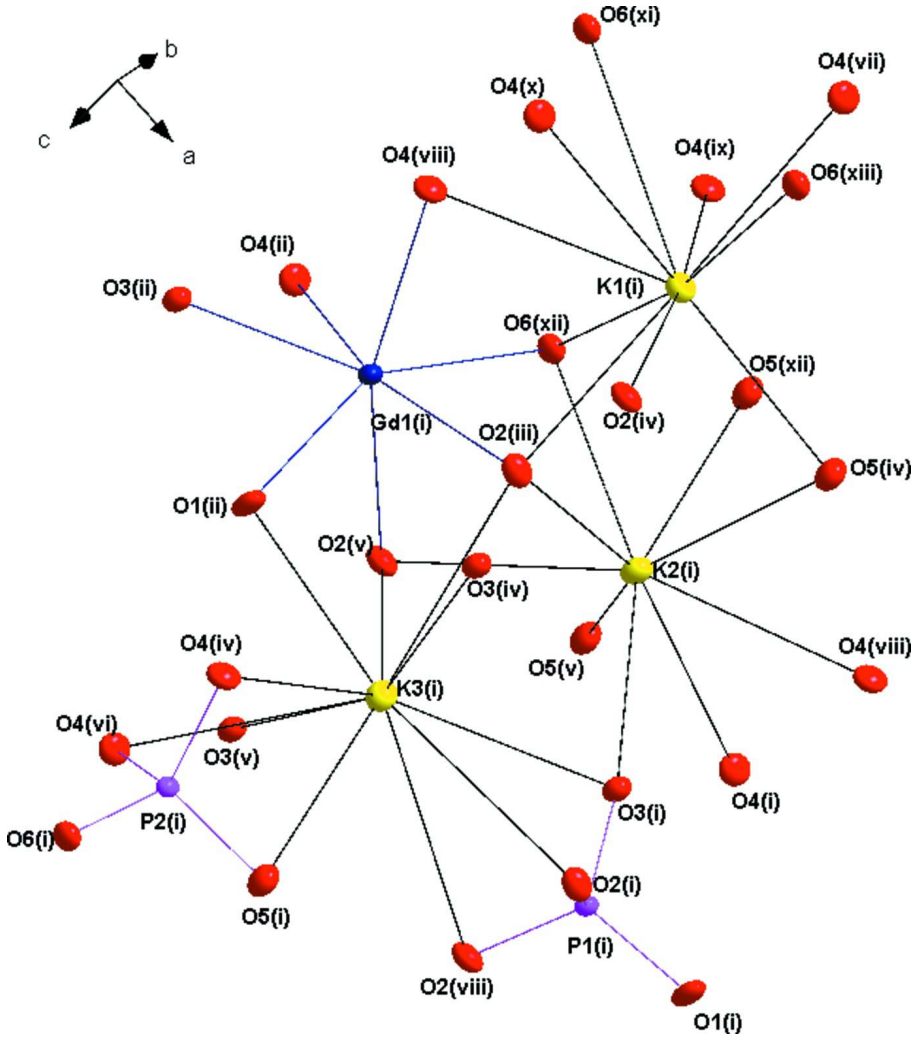

Figure 1

Section of the structure of $K_3Gd(PO_4)_2$ with the atom labelling scheme. The displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) x, y, z; (ii) -1+x, y, z; (iii) 1-x, 1-y, 1-z; (iv) 1-x, 0.5+y, 1-z; (v) 1-x, -0.5+y, 1-z; (vi) 1-x, -y, 1-z; (vii) 1-x, 1-y, -z; (viii) x, 0.5-y, z; (ix) 1-x, 0.5+y, -z; (x) -1+x, 1+y, z; (xi) -x, 0.5+y, 1-z; (xii) x, y, -1+z; (xiii) x, 1+y, -1+z.]

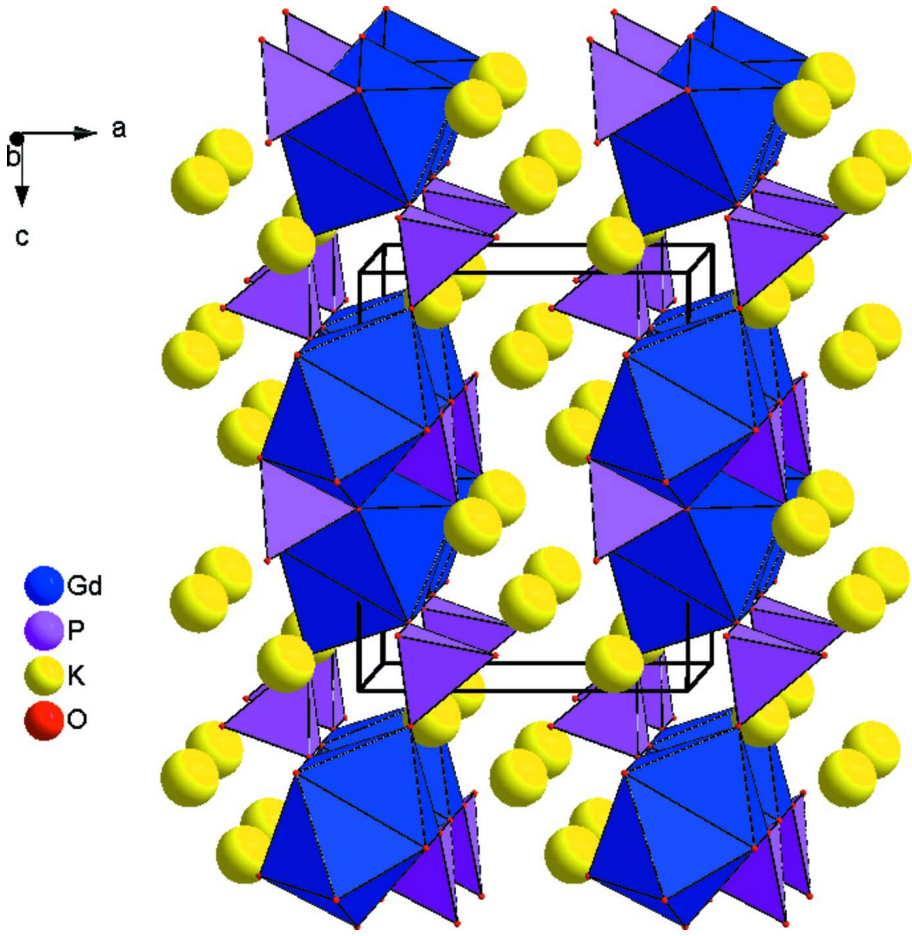

Figure 2

View of the crystal structure of $K_3Gd(PO_4)_2$. K—O bonds were omitted for clarity.

tripotassium gadolinium(III) bis[orthophosphate(V)]

Crystal data

$K_3Gd(PO_4)_2$
M_r = 464.49
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
a = 7.4153 (15) Å
b = 5.6206 (11) Å
c = 9.445 (2) Å
β = 90.723 (14)°
V = 393.62 (14) Å^3
Z = 2
$F(000)$ = 430
D_x = 3.919 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1264 reflections
θ = 2.2–27.5°
μ = 10.43 mm^{-1}
T = 293 K
Prism, colourless
0.30 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury70 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite Monochromator monochromator
Detector resolution: 14.6306 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.304, T_{max} = 0.624
3036 measured reflections
993 independent reflections
946 reflections with $I > 2\sigma(I)$

R_{int} = 0.045
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −9→9
k = −7→7
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.03
993 reflections
80 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.38 e Å^{-3}
$\Delta\rho_{min}$ = −2.68 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0314 (17)

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Gd1	0.00699 (3)	0.2500	0.29011 (3)	0.00731 (15)
P1	0.80967 (19)	0.2500	0.57350 (15)	0.0076 (3)
P2	0.2303 (2)	0.2500	0.91166 (15)	0.0066 (3)
K1	0.20438 (17)	0.7500	0.08160 (13)	0.0119 (3)
K2	0.50495 (17)	0.2500	0.19219 (13)	0.0142 (3)
K3	0.36353 (18)	0.2500	0.59102 (14)	0.0142 (3)
O1	1.0137 (6)	0.2500	0.5478 (4)	0.0169 (10)
O2	0.7564 (4)	0.4735 (5)	0.6577 (3)	0.0123 (6)
O3	0.7177 (6)	0.2500	0.4266 (4)	0.0116 (9)
O4	0.8481 (4)	−0.0269 (5)	0.1623 (3)	0.0129 (6)
O5	0.4337 (6)	0.2500	0.8991 (5)	0.0163 (9)
O6	0.1744 (6)	0.2500	1.0689 (4)	0.0113 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.0066 (2)	0.0068 (2)	0.0085 (2)	0.000	−0.00097 (12)	0.000
P1	0.0065 (7)	0.0086 (8)	0.0076 (7)	0.000	−0.0012 (5)	0.000
P2	0.0070 (7)	0.0052 (7)	0.0076 (6)	0.000	−0.0009 (5)	0.000
K1	0.0137 (6)	0.0100 (7)	0.0118 (6)	0.000	−0.0001 (5)	0.000
K2	0.0101 (7)	0.0186 (8)	0.0138 (6)	0.000	−0.0021 (5)	0.000
K3	0.0126 (6)	0.0136 (7)	0.0165 (6)	0.000	−0.0002 (5)	0.000

O1	0.007 (2)	0.031 (3)	0.012 (2)	0.000	−0.0023 (16)	0.000
O2	0.0176 (16)	0.0087 (15)	0.0105 (14)	−0.0023 (12)	0.0007 (12)	−0.0019 (11)
O3	0.0087 (19)	0.015 (2)	0.0110 (19)	0.000	−0.0010 (16)	0.000
O4	0.0152 (15)	0.0081 (15)	0.0152 (14)	−0.0033 (12)	−0.0016 (12)	−0.0018 (12)
O5	0.010 (2)	0.021 (3)	0.018 (2)	0.000	0.0017 (16)	0.000
O6	0.013 (2)	0.014 (2)	0.0076 (19)	0.000	0.0012 (16)	0.000

Geometric parameters (Å, º)

Gd1—O4^{i}	2.287 (3)	K1—O4^{xii}	3.030 (3)
Gd1—O4^{ii}	2.287 (3)	K1—O6^{xiii}	3.132 (4)
Gd1—O2^{iii}	2.390 (3)	K2—O6^{v}	2.700 (4)
Gd1—O2^{iv}	2.390 (3)	K2—O3	2.702 (4)
Gd1—O1^{i}	2.434 (4)	K2—O5^{v}	2.812 (4)
Gd1—O6^{v}	2.444 (4)	K2—O2^{iv}	2.872 (3)
Gd1—O3^{i}	2.517 (4)	K2—O2^{iii}	2.872 (3)
P1—O1	1.535 (4)	K2—O5^{vii}	2.9761 (15)
P1—O3	1.538 (4)	K2—O5^{iii}	2.9761 (16)
P1—O2	1.541 (3)	K2—O4^{vi}	2.999 (3)
P1—O2^{vi}	1.541 (3)	K2—O4	2.999 (3)
P2—O5	1.515 (4)	K3—O1^{i}	2.621 (4)
P2—O6	1.547 (4)	K3—O3^{vii}	2.8785 (11)
P2—O4^{vii}	1.545 (3)	K3—O3^{iii}	2.8785 (11)
P2—O4^{viii}	1.545 (3)	K3—O2^{iv}	2.945 (3)
K1—O5^{iii}	2.687 (5)	K3—O2^{iii}	2.945 (3)
K1—O2^{viii}	2.776 (3)	K3—O5	2.949 (4)
K1—O2^{iii}	2.776 (3)	K3—O3	3.067 (4)
K1—O4^{ix}	2.803 (3)	K3—O4^{viii}	3.092 (3)
K1—O4^{x}	2.803 (3)	K3—O4^{vii}	3.092 (3)
K1—O6^{v}	2.8215 (7)	K3—O2	3.227 (3)
K1—O6^{xi}	2.8215 (7)	K3—O2^{vi}	3.227 (3)
K1—O4^{ii}	3.030 (3)		
O4^{i}—Gd1—O4^{ii}	85.75 (15)	O3^{vii}—K3—O5	95.24 (9)
O4^{i}—Gd1—O2^{iii}	157.36 (10)	O3^{iii}—K3—O5	95.24 (9)
O4^{ii}—Gd1—O2^{iii}	92.20 (11)	O2^{iv}—K3—O5	146.60 (6)
O4^{i}—Gd1—O2^{iv}	92.20 (11)	O2^{iii}—K3—O5	146.60 (6)
O4^{ii}—Gd1—O2^{iv}	157.36 (10)	O1^{i}—K3—O3	140.64 (13)
O2^{iii}—Gd1—O2^{iv}	81.09 (14)	O3^{vii}—K3—O3	98.65 (8)
O4^{i}—Gd1—O1^{i}	122.12 (9)	O3^{iii}—K3—O3	98.65 (8)
O4^{ii}—Gd1—O1^{i}	122.12 (9)	O2^{iv}—K3—O3	81.26 (9)
O2^{iii}—Gd1—O1^{i}	77.78 (10)	O2^{iii}—K3—O3	81.26 (9)
O2^{iv}—Gd1—O1^{i}	77.78 (10)	O5—K3—O3	110.96 (12)
O4^{i}—Gd1—O6^{v}	79.20 (10)	O1^{i}—K3—O4^{viii}	66.82 (11)
O4^{ii}—Gd1—O6^{v}	79.20 (10)	O3^{vii}—K3—O4^{viii}	109.38 (10)
O2^{iii}—Gd1—O6^{v}	78.27 (10)	O3^{iii}—K3—O4^{viii}	62.60 (10)
O2^{iv}—Gd1—O6^{v}	78.27 (10)	O2^{iv}—K3—O4^{viii}	131.63 (9)
O1^{i}—Gd1—O6^{v}	148.30 (14)	O2^{iii}—K3—O4^{viii}	103.66 (8)

O4^{i}—Gd1—O3^{i}	80.43 (10)	O5—K3—O4^{viii}	48.81 (9)
O4^{ii}—Gd1—O3^{i}	80.43 (10)	O3—K3—O4^{viii}	145.84 (9)
O2^{iii}—Gd1—O3^{i}	121.51 (9)	O1^{i}—K3—O4^{vii}	66.82 (11)
O2^{iv}—Gd1—O3^{i}	121.51 (9)	O3^{vii}—K3—O4^{vii}	62.60 (10)
O1^{i}—Gd1—O3^{i}	59.63 (13)	O3^{iii}—K3—O4^{vii}	109.38 (10)
O6^{v}—Gd1—O3^{i}	152.07 (14)	O2^{iv}—K3—O4^{vii}	103.66 (8)
O1—P1—O3	106.5 (2)	O2^{iii}—K3—O4^{vii}	131.63 (9)
O1—P1—O2	109.94 (15)	O5—K3—O4^{vii}	48.81 (9)
O3—P1—O2	110.60 (15)	O3—K3—O4^{vii}	145.84 (9)
O1—P1—O2^{vi}	109.94 (15)	O4^{viii}—K3—O4^{vii}	47.86 (11)
O3—P1—O2^{vi}	110.60 (15)	O1^{i}—K3—O2	156.87 (6)
O2—P1—O2^{vi}	109.2 (2)	O3^{vii}—K3—O2	125.38 (10)
O5—P2—O6	110.7 (2)	O3^{iii}—K3—O2	79.56 (10)
O5—P2—O4^{vii}	109.50 (16)	O2^{iv}—K3—O2	128.60 (6)
O6—P2—O4^{vii}	109.28 (15)	O2^{iii}—K3—O2	102.30 (8)
O5—P2—O4^{viii}	109.50 (16)	O5—K3—O2	70.11 (10)
O6—P2—O4^{viii}	109.28 (15)	O3—K3—O2	47.34 (8)
O4^{vii}—P2—O4^{viii}	108.5 (2)	O4^{viii}—K3—O2	99.24 (8)
O5^{iii}—K1—O2^{viii}	81.16 (11)	O4^{vii}—K3—O2	118.45 (9)
O5^{iii}—K1—O2^{iii}	81.16 (11)	P2—K3—O2	95.98 (7)
O2^{viii}—K1—O2^{iii}	53.82 (12)	O1^{i}—K3—O2^{vi}	156.87 (6)
O5^{iii}—K1—O4^{ix}	100.61 (10)	O3^{vii}—K3—O2^{vi}	79.56 (10)
O2^{viii}—K1—O4^{ix}	172.75 (9)	O3^{iii}—K3—O2^{vi}	125.38 (10)
O2^{iii}—K1—O4^{ix}	119.30 (8)	O2^{iv}—K3—O2^{vi}	102.30 (8)
O5^{iii}—K1—O4^{x}	100.61 (10)	O2^{iii}—K3—O2^{vi}	128.60 (6)
O2^{viii}—K1—O4^{x}	119.30 (8)	O5—K3—O2^{vi}	70.11 (10)
O2^{iii}—K1—O4^{x}	172.75 (9)	O3—K3—O2^{vi}	47.34 (8)
O4^{ix}—K1—O4^{x}	67.45 (12)	O4^{viii}—K3—O2^{vi}	118.45 (9)
O5^{iii}—K1—O6^{v}	94.64 (9)	O4^{vii}—K3—O2^{vi}	99.24 (8)
O2^{viii}—K1—O6^{v}	119.72 (11)	P2—K3—O2^{vi}	95.98 (7)
O2^{iii}—K1—O6^{v}	66.06 (10)	O2—K3—O2^{vi}	45.82 (11)
O4^{ix}—K1—O6^{v}	53.27 (10)	P1—O1—Gd1^{xiv}	98.6 (2)
O4^{x}—K1—O6^{v}	120.53 (11)	P1—O1—K3^{xiv}	162.0 (3)
O5^{iii}—K1—O6^{xi}	94.64 (9)	Gd1^{xiv}—O1—K3^{xiv}	99.39 (14)
O2^{viii}—K1—O6^{xi}	66.06 (10)	P1—O2—Gd1^{iii}	116.36 (16)
O2^{iii}—K1—O6^{xi}	119.72 (11)	P1—O2—K1^{iii}	93.68 (14)
O4^{ix}—K1—O6^{xi}	120.53 (11)	Gd1^{iii}—O2—K1^{iii}	92.46 (10)
O4^{x}—K1—O6^{xi}	53.27 (10)	P1—O2—K2^{iii}	151.02 (17)
O6^{v}—K1—O6^{xi}	169.79 (18)	Gd1^{iii}—O2—K2^{iii}	92.56 (9)
O5^{iii}—K1—O4^{ii}	148.85 (8)	K1^{iii}—O2—K2^{iii}	82.58 (8)
O2^{viii}—K1—O4^{ii}	92.65 (9)	P1—O2—K3^{iii}	95.46 (13)
O2^{iii}—K1—O4^{ii}	70.83 (9)	Gd1^{iii}—O2—K3^{iii}	92.00 (9)
O4^{ix}—K1—O4^{ii}	82.21 (9)	K1^{iii}—O2—K3^{iii}	166.79 (12)
O4^{x}—K1—O4^{ii}	108.90 (7)	K2^{iii}—O2—K3^{iii}	84.80 (9)
O6^{v}—K1—O4^{ii}	61.97 (10)	P1—O2—K3	79.54 (13)
O6^{xi}—K1—O4^{ii}	110.76 (11)	Gd1^{iii}—O2—K3	162.12 (12)
O5^{iii}—K1—O4^{xii}	148.85 (8)	K1^{iii}—O2—K3	94.66 (9)
O2^{viii}—K1—O4^{xii}	70.83 (9)	K2^{iii}—O2—K3	72.18 (7)

O2^{iii}—K1—O4^{xii}	92.65 (9)	K3^{iii}—O2—K3	77.70 (8)
O4^{ix}—K1—O4^{xii}	108.90 (7)	P1—O3—Gd1^{xiv}	95.21 (19)
O4^{x}—K1—O4^{xii}	82.21 (9)	P1—O3—K2	170.6 (2)
O6^{v}—K1—O4^{xii}	110.76 (11)	Gd1^{xiv}—O3—K2	94.17 (13)
O6^{xi}—K1—O4^{xii}	61.97 (10)	P1—O3—K3^{vii}	98.18 (9)
O4^{ii}—K1—O4^{xii}	48.89 (11)	Gd1^{xiv}—O3—K3^{vii}	98.59 (8)
O5^{iii}—K1—O6^{xiii}	156.91 (13)	K2—O3—K3^{vii}	80.39 (9)
O2^{viii}—K1—O6^{xiii}	119.07 (9)	P1—O3—K3^{iii}	98.18 (9)
O2^{iii}—K1—O6^{xiii}	119.07 (9)	Gd1^{xiv}—O3—K3^{iii}	98.59 (8)
O4^{ix}—K1—O6^{xiii}	60.83 (9)	K2—O3—K3^{iii}	80.39 (9)
O4^{x}—K1—O6^{xiii}	60.83 (9)	K3^{vii}—O3—K3^{iii}	155.01 (17)
O6^{v}—K1—O6^{xiii}	84.90 (9)	P1—O3—K3	85.20 (16)
O6^{xi}—K1—O6^{xiii}	84.90 (9)	Gd1^{xiv}—O3—K3	179.59 (17)
O4^{ii}—K1—O6^{xiii}	48.27 (9)	K2—O3—K3	85.42 (12)
O4^{xii}—K1—O6^{xiii}	48.27 (9)	K3^{vii}—O3—K3	81.34 (8)
O6^{v}—K2—O3	150.53 (13)	K3^{iii}—O3—K3	81.34 (8)
O6^{v}—K2—O5^{v}	54.35 (12)	P2^{vii}—O4—Gd1^{xiv}	168.2 (2)
O3—K2—O5^{v}	155.12 (13)	P2^{vii}—O4—K1^{x}	91.81 (14)
O6^{v}—K2—O2^{iv}	66.32 (9)	Gd1^{xiv}—O4—K1^{x}	96.97 (10)
O3—K2—O2^{iv}	89.20 (10)	P2^{vii}—O4—K2	98.57 (15)
O5^{v}—K2—O2^{iv}	111.49 (10)	Gd1^{xiv}—O4—K2	91.67 (10)
O6^{v}—K2—O2^{iii}	66.32 (9)	K1^{x}—O4—K2	71.34 (8)
O3—K2—O2^{iii}	89.20 (10)	P2^{vii}—O4—K1^{xv}	82.80 (13)
O5^{v}—K2—O2^{iii}	111.49 (10)	Gd1^{xiv}—O4—K1^{xv}	88.25 (10)
O2^{iv}—K2—O2^{iii}	65.51 (12)	K1^{x}—O4—K1^{xv}	97.79 (9)
O6^{v}—K2—O5^{vii}	90.93 (9)	K2—O4—K1^{xv}	169.05 (11)
O3—K2—O5^{vii}	98.48 (9)	P2^{vii}—O4—K3^{vii}	79.62 (13)
O5^{v}—K2—O5^{vii}	75.07 (9)	Gd1^{xiv}—O4—K3^{vii}	98.11 (10)
O2^{iv}—K2—O5^{vii}	74.84 (10)	K1^{x}—O4—K3^{vii}	141.08 (12)
O2^{iii}—K2—O5^{vii}	139.49 (10)	K2—O4—K3^{vii}	72.55 (7)
O6^{v}—K2—O5^{iii}	90.93 (9)	K1^{xv}—O4—K3^{vii}	118.30 (10)
O3—K2—O5^{iii}	98.48 (9)	P2—O5—K1^{iii}	171.6 (3)
O5^{v}—K2—O5^{iii}	75.07 (9)	P2—O5—K2^{xvi}	95.6 (2)
O2^{iv}—K2—O5^{iii}	139.49 (10)	K1^{iii}—O5—K2^{xvi}	76.00 (12)
O2^{iii}—K2—O5^{iii}	74.84 (10)	P2—O5—K3	85.06 (19)
O5^{vii}—K2—O5^{iii}	141.57 (16)	K1^{iii}—O5—K3	103.34 (14)
O6^{v}—K2—O4^{vi}	136.55 (9)	K2^{xvi}—O5—K3	179.34 (17)
O3—K2—O4^{vi}	65.80 (10)	P2—O5—K2^{vii}	100.29 (10)
O5^{v}—K2—O4^{vi}	93.23 (10)	K1^{iii}—O5—K2^{vii}	82.16 (9)
O2^{iv}—K2—O4^{vi}	154.93 (10)	K2^{xvi}—O5—K2^{vii}	104.93 (9)
O2^{iii}—K2—O4^{vi}	110.14 (8)	K3—O5—K2^{vii}	74.93 (9)
O5^{vii}—K2—O4^{vi}	109.26 (11)	P2—O5—K2^{iii}	100.29 (10)
O5^{iii}—K2—O4^{vi}	49.45 (10)	K1^{iii}—O5—K2^{iii}	82.16 (9)
O6^{v}—K2—O4	136.55 (9)	K2^{xvi}—O5—K2^{iii}	104.93 (9)
O3—K2—O4	65.80 (9)	K3—O5—K2^{iii}	74.93 (9)
O5^{v}—K2—O4	93.23 (10)	K2^{vii}—O5—K2^{iii}	141.57 (16)
O2^{iv}—K2—O4	110.14 (8)	P2—O6—Gd1^{xvi}	165.0 (3)
O2^{iii}—K2—O4	154.93 (10)	P2—O6—K2^{xvi}	99.3 (2)

O5^{vii}—K2—O4	49.45 (10)	Gd1^{xvi}—O6—K2^{xvi}	95.71 (14)
O5^{iii}—K2—O4	109.26 (11)	P2—O6—K1^{xvi}	91.08 (8)
O4^{vi}—K2—O4	62.52 (12)	Gd1^{xvi}—O6—K1^{xvi}	90.24 (8)
O1^{i}—K3—O3^{vii}	77.59 (8)	K2^{xvi}—O6—K1^{xvi}	84.90 (9)
O1^{i}—K3—O3^{iii}	77.59 (8)	P2—O6—K1^{xvii}	91.08 (8)
O3^{vii}—K3—O3^{iii}	155.01 (17)	Gd1^{xvi}—O6—K1^{xvii}	90.24 (8)
O1^{i}—K3—O2^{iv}	65.64 (10)	K2^{xvi}—O6—K1^{xvii}	84.90 (9)
O3^{vii}—K3—O2^{iv}	51.52 (10)	K1^{xvi}—O6—K1^{xvii}	169.79 (18)
O3^{iii}—K3—O2^{iv}	114.09 (11)	P2—O6—K1^{xiii}	79.26 (17)
O1^{i}—K3—O2^{iii}	65.64 (10)	Gd1^{xvi}—O6—K1^{xiii}	85.73 (12)
O3^{vii}—K3—O2^{iii}	114.09 (11)	K2^{xvi}—O6—K1^{xiii}	178.56 (15)
O3^{iii}—K3—O2^{iii}	51.52 (10)	K1^{xvi}—O6—K1^{xiii}	95.10 (9)
O2^{iv}—K3—O2^{iii}	63.70 (12)	K1^{xvii}—O6—K1^{xiii}	95.10 (9)
O1^{i}—K3—O5	108.39 (13)		

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