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$RbYb(PO_3)_4$

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ(P–O) = 0.005 Å; R factor = 0.043; wR factor = 0.078; data-to-parameter ratio = 16.4.

Rubidium ytterbium(III) tetrakis(polyphosphate), $RbYb(PO_3)_4$, was synthesized by solid-state reaction. It adopts structure type IV of the $MRE(PO_3)_4$ (M = alkali metal and RE = rare earth metal) family of compounds. The structure is composed of a three-dimensional framework made up from double spiral polyphosphate chains parallel to $[10\bar{1}]$ and irregular $[YbO_8]$ polyhedra. There are eight PO_4 tetrahedra in the repeat unit of the polyphosphate chains. The Rb^+ cation is located in channels extending along [100] that are delimited by the three-dimensional framework. It is surrounded by 11 O atoms, defining an irregular polyhedron.

Related literature

For background to applications of condensed rare earth phosphates, see: Malinowski (1989); Miyazawa *et al.* (1979). For the structures of other ytterbium phosphate compounds, see: Rghioui *et al.* (2002); Fang *et al.* (2008); Hong (1974); Jansen *et al.* (1991). For an isotypic structure, see: Zhu *et al.* (2009).

Experimental

Crystal data

$RbYb(PO_3)_4$
M_r = 574.40
Monoclinic, $P2_1/n$
a = 10.2022 (15) Å
b = 8.7975 (13) Å
c = 10.9300 (16) Å
β = 106.323 (2)°
V = 941.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 15.80 mm^{-1}
T = 296 K
0.10 × 0.07 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.725, T_{max} = 0.854
9912 measured reflections
2676 independent reflections
2024 reflections with $I > 2\sigma(I)$
R_{int} = 0.143

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.078
S = 1.00
2676 reflections
163 parameters
$\Delta\rho_{max}$ = 2.95 e Å^{-3}
$\Delta\rho_{min}$ = −2.99 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2707).

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supporting information

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$RbYb(PO_3)_4$

Jing Zhu and Hui Chen

S1. Comment

Extensive studies on structures and properties of condensed rare earth phosphates have been carried out in the past owing to their potential application in the optics domain (Miyazawa *et al.*, 1979; Malinowski *et al.*, 1989). Furthermore, their chemical and thermal stability ensures the feasibility of possible applications. Numerous rare-earth phosphates with ytterbium, such as YbP_3O_9 (Hong, 1974), $CsYbP_2O_7$ (Jansen *et al.*, 1991), and $K_2CsYb(PO_4)_2$ (Rghioui *et al.*, 2002) have been synthesized and structurally determined. However, the literature shows that in the polyphosphate family with general formula $MRE(PO_3)_4$ (*M* = monovalent cation, *RE* = rare earth cation), only a few examples with ytterbium are known [$LiYb(PO_3)_4$ (Fang *et al.*, 2008)]. The reason for this situation is probably the difficulty in obtaining crystals of high quality. Accordingly, our research group is paying attention to the preparation of new polyphosphates $MYb(PO_3)_4$. We successfully grew single crystals of rubidium ytterbium polyphosphate, $RbYb(PO_3)_4$, the structure of which is reported here.

The crystal structure of $RbYb(PO_3)_4$ is shown in Figs. 1 and 2. It is isostructural with $CsEu(PO_3)_4$ (Zhu *et al.*, 2009) and belongs to type IV of the $MRE(PO_3)_4$ (*M* = alkali metal and RE = rare earth) family of compounds. The structure can be described as a three-dimensional framework made up from polyphosphate double spiral chains extending parallel to $[10\bar{1}]$ and YbO_8 polyhedra. The Rb^+ cations are located in infinite tunnels along [100] delimited by the three-dimensional framework. As illustrated in Fig. 3, the P atom is four-coordinated, and four crystallographically distinct PO_4 tetrahedra form the $(PO_3)_\infty^-$ double spiral chains by corner-sharing. The P–O bond lengths and O—P—O bond angles show normal values for catena-polyphosphates. There are eight PO_4 tetrahedra in the repeating unit of the double spiral chain. The Yb^{III} cation is eight-coordinated in form of a distorted polyhedron with Y—O bond lengths ranging from 2.253 (5) to 2.412 (5) Å, which are consistent with those reported previously (Fang *et al.*, 2008). The shortest Yb···Yb contact is 6.3540 (8) Å. The Rb^+ cation are located in the intersecting channels and are surrounded by eleven O atoms, with Rb—O bond lengths in the range of 2.915 (5)–3.504 (5) Å. Neighboring two RbO_{11} polyhedra are connected by corner-sharing.

S2. Experimental

Single crystals of $RbYb(PO_3)_4$ were grown by solid state reactions. All reagents were purchased commercially and used without further purification. The starting materials $RbNO_3$, Yb_2O_3 and $NH_4H_2PO_4$ were weighed in the molar ratio of Rb/Yb/P = 7/1/18 and finely ground in an agate mortar to ensure the best homogeneity and reactivity, and were then placed in a corundum crucible and preheated at 373 K for 6 h. Afterwards, the material was reground and heated to 723 K for 36 h and then cooled to 393 K at a rate of 6 K/h and finally air-quenched to room temperature. A few colourless block-shaped crystals were obtained from the reaction product.

S3. Refinement

EDX spectrometry using a JSM6700F scanning electron microscope confirmed the composition. The remaining maximum and minimum electron densities are located 0.87 Å and 0.81 Å, respectively, from the Rb atom.

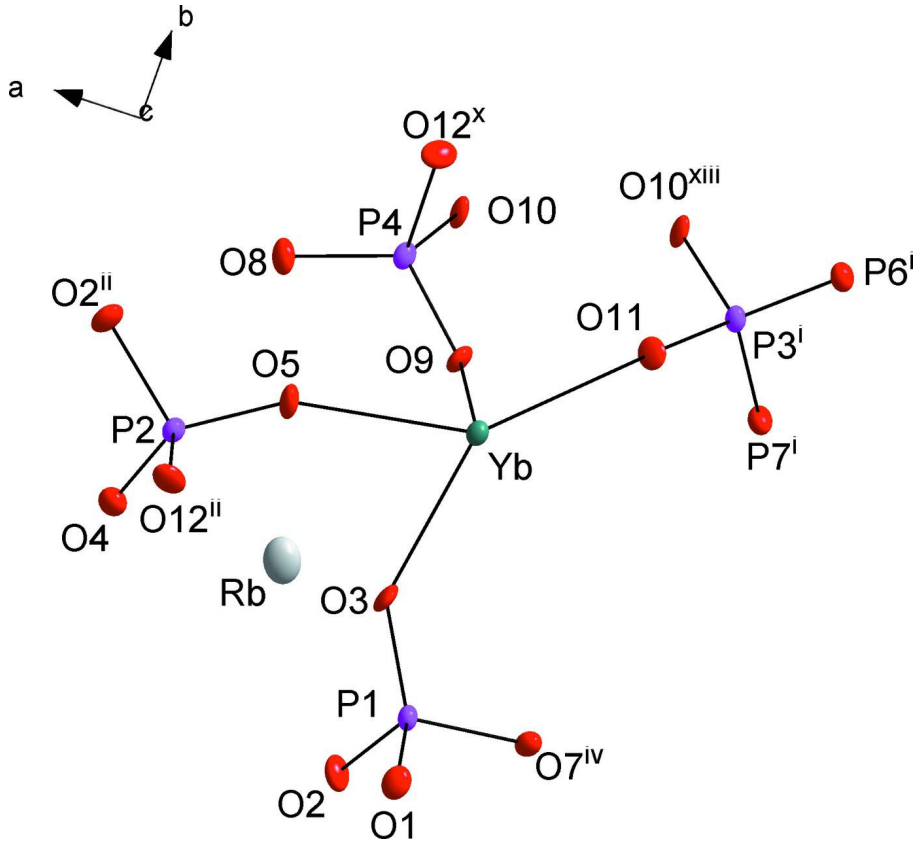

Figure 1

View of a part of the title structure. Ellipsoids are shown at the 50% probability level. [Symmetry code: (i) -0.5 + *x*, 0.5 - *y*, -0.5 + *z*; (ii) 1.5 - *x*, 0.5 + *y*, 1.5 - *z*; (iv) 1 - *x*, -*y*, 2 - *z*; (*x*) *x*, 1 + *y*, *z*; (xiii) 1 - *x*, 1 - *y*, 2 - *z*;]

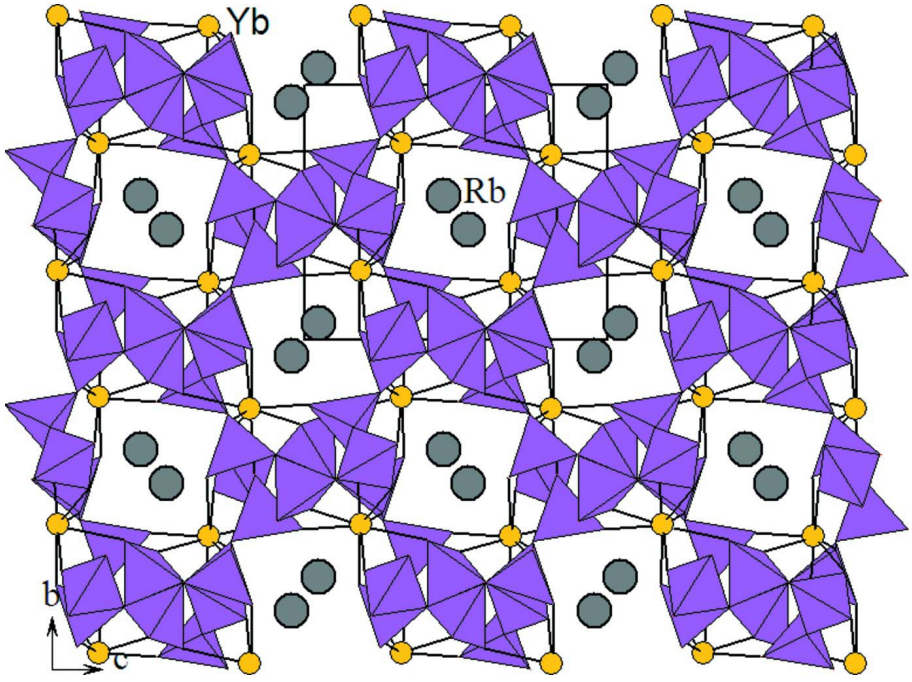

Figure 2

The packing of the structure of $RbYb(PO_3)_4$, viewed along the *a* axis. Polyhedra represents PO_4 tetrahedra.

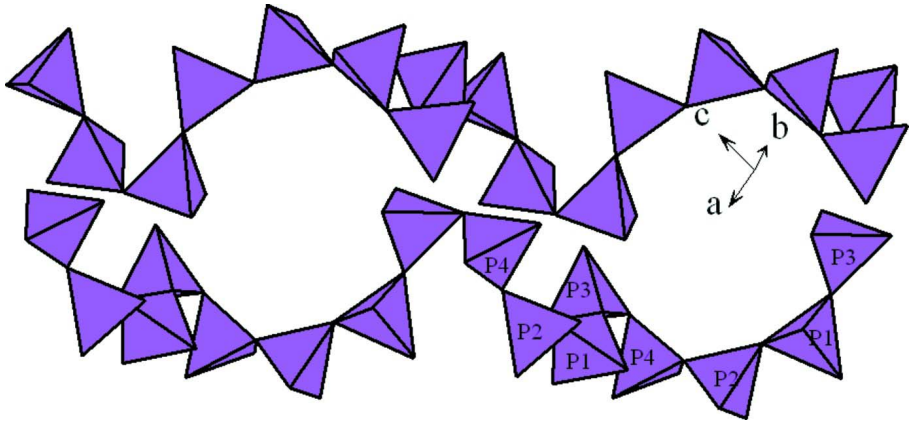

Figure 3

The polyphosphate double spiral chains

Rubidium ytterbium(III) tetrakis(polyphosphate)

Crystal data

$RbYb(PO_3)_4$
$M_r = 574.40$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.2022\ (15)$ Å
$b = 8.7975\ (13)$ Å
$c = 10.9300\ (16)$ Å
$\beta = 106.323\ (2)°$
$V = 941.5\ (2)$ Å^3
$Z = 4$
$F(000) = 1049$
$D_x = 4.052$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2802 reflections
$\theta = 2.4–29.5°$
$\mu = 15.80$ mm^{-1}

T = 296 K
Block, colorless

0.10 × 0.07 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.725, T_{max} = 0.854

9912 measured reflections
2676 independent reflections
2024 reflections with $I > 2\sigma(I)$
R_{int} = 0.143
θ_{max} = 30.1°, θ_{min} = 2.4°
h = −14→14
k = −12→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.078
S = 1.00
2676 reflections
163 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.95 e Å^{-3}
$\Delta\rho_{min}$ = −2.99 e Å^{-3}

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}
Yb	0.49845 (3)	0.22753 (3)	0.68227 (3)	0.00898 (9)
Rb	0.68841 (9)	−0.06519 (10)	0.95773 (7)	0.02424 (19)
P1	0.45844 (18)	−0.1715 (2)	0.63271 (16)	0.0088 (3)
P2	0.85263 (18)	0.0916 (2)	0.74217 (16)	0.0093 (3)
P3	0.75504 (18)	0.0245 (2)	1.27947 (15)	0.0088 (3)
P4	0.67393 (18)	0.3877 (2)	0.97599 (16)	0.0091 (3)
O1	0.4366 (5)	−0.2434 (6)	0.5063 (4)	0.0135 (11)
O2	0.5242 (5)	−0.2914 (6)	0.7444 (5)	0.0141 (10)
O3	0.5348 (5)	−0.0274 (6)	0.6642 (5)	0.0144 (10)
O4	0.8988 (5)	−0.0414 (6)	0.8251 (5)	0.0137 (10)
O5	0.7325 (5)	0.1773 (6)	0.7555 (5)	0.0142 (10)
O6	0.6458 (5)	−0.0858 (6)	1.2179 (4)	0.0112 (10)
O7	0.6895 (5)	0.1572 (6)	1.3448 (5)	0.0122 (10)
O8	0.8156 (5)	0.3283 (6)	1.0176 (5)	0.0140 (11)
O9	0.5637 (5)	0.2853 (6)	0.9024 (4)	0.0118 (10)

O10	0.6370 (5)	0.4504 (6)	1.1006 (4)	0.0100 (10)
O11	0.3317 (5)	0.4059 (6)	0.6976 (4)	0.0125 (10)
O12	0.6715 (5)	−0.4534 (6)	0.9034 (4)	0.0134 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb	0.00774 (14)	0.01101 (15)	0.00853 (13)	−0.00035 (12)	0.00286 (9)	−0.00056 (12)
Rb	0.0245 (4)	0.0340 (5)	0.0145 (4)	0.0045 (3)	0.0060 (3)	−0.0013 (3)
P1	0.0063 (8)	0.0108 (8)	0.0098 (8)	0.0007 (6)	0.0029 (6)	0.0001 (7)
P2	0.0078 (8)	0.0108 (9)	0.0089 (8)	−0.0006 (6)	0.0018 (6)	−0.0012 (6)
P3	0.0074 (8)	0.0117 (9)	0.0076 (8)	−0.0011 (6)	0.0024 (7)	0.0015 (6)
P4	0.0076 (8)	0.0127 (9)	0.0066 (7)	−0.0003 (6)	0.0015 (6)	0.0006 (6)
O1	0.013 (2)	0.020 (3)	0.009 (2)	−0.001 (2)	0.0051 (18)	−0.0006 (19)
O2	0.012 (2)	0.018 (3)	0.011 (2)	0.006 (2)	0.0026 (19)	0.006 (2)
O3	0.006 (2)	0.016 (3)	0.022 (3)	−0.005 (2)	0.005 (2)	−0.002 (2)
O4	0.014 (3)	0.013 (3)	0.014 (2)	0.001 (2)	0.005 (2)	−0.002 (2)
O5	0.006 (2)	0.021 (3)	0.015 (2)	0.002 (2)	0.0018 (19)	−0.005 (2)
O6	0.010 (2)	0.013 (3)	0.011 (2)	−0.0024 (19)	0.0025 (19)	−0.0004 (19)
O7	0.011 (2)	0.012 (3)	0.015 (2)	−0.002 (2)	0.006 (2)	−0.0038 (19)
O8	0.010 (2)	0.020 (3)	0.013 (2)	0.004 (2)	0.0054 (19)	0.002 (2)
O9	0.007 (2)	0.015 (2)	0.011 (2)	−0.004 (2)	0.0002 (18)	−0.003 (2)
O10	0.005 (2)	0.019 (3)	0.007 (2)	−0.0004 (19)	0.0035 (18)	−0.0024 (19)
O11	0.014 (3)	0.017 (3)	0.010 (2)	0.001 (2)	0.010 (2)	0.001 (2)
O12	0.019 (3)	0.013 (3)	0.007 (2)	−0.002 (2)	0.002 (2)	0.0045 (19)

Geometric parameters (Å, º)

Yb—O8^{i}	2.253 (5)	P2—O4	1.474 (5)
Yb—O3	2.291 (5)	P2—O5	1.480 (5)
Yb—O4^{ii}	2.300 (5)	P2—O12^{ii}	1.590 (5)
Yb—O1^{iii}	2.339 (5)	P2—O2^{ii}	1.599 (5)
Yb—O5	2.337 (5)	P2—Rb^{ii}	3.681 (2)
Yb—O11	2.355 (5)	P3—O11^{vi}	1.477 (5)
Yb—O9	2.364 (5)	P3—O6	1.488 (5)
Yb—O6^{iv}	2.412 (5)	P3—O10^{vii}	1.595 (5)
Yb—P4	3.5025 (18)	P3—O7	1.609 (5)
Yb—P3^{iv}	3.5196 (18)	P3—Yb^{iv}	3.5196 (18)
Yb—Rb	4.0215 (9)	P4—O8	1.483 (5)
Yb—Rb^{ii}	4.3152 (10)	P4—O9	1.489 (5)
Rb—O4	2.915 (5)	P4—O12^{x}	1.604 (5)
Rb—O1^{v}	2.962 (5)	P4—O10	1.609 (5)
Rb—O11^{vi}	2.970 (5)	O1—Yb^{iii}	2.339 (5)
Rb—O6	3.000 (5)	O1—Rb^{ix}	2.962 (5)
Rb—O2	3.164 (5)	O2—P2^{viii}	1.599 (5)
Rb—O3	3.168 (5)	O4—Yb^{viii}	2.300 (5)
Rb—O5	3.193 (5)	O5—Rb^{ii}	3.504 (5)
Rb—O7^{vii}	3.265 (5)	O6—Yb^{iv}	2.412 (5)

Rb—O9	3.326 (5)	O7—P1^{iv}	1.601 (5)
Rb—O12	3.463 (5)	O7—Rb^{xi}	3.265 (5)
Rb—P3	3.4796 (19)	O8—Yb^{vi}	2.253 (5)
Rb—O5^{viii}	3.504 (5)	O10—P3^{xi}	1.595 (5)
P1—O3	1.477 (5)	O11—P3^{i}	1.477 (5)
P1—O1	1.479 (5)	O11—Rb^{i}	2.970 (5)
P1—O7^{iv}	1.601 (5)	O12—P2^{viii}	1.590 (5)
P1—O2	1.610 (5)	O12—P4^{xii}	1.604 (5)
P1—Rb^{ix}	3.695 (2)		

O8^{i}—Yb—O3	80.51 (18)	O6—Rb—P3	25.18 (10)
O8^{i}—Yb—O4^{ii}	116.63 (18)	O2—Rb—P3	143.14 (10)
O3—Yb—O4^{ii}	140.91 (18)	O3—Rb—P3	154.20 (11)
O8^{i}—Yb—O1^{iii}	71.65 (18)	O5—Rb—P3	121.50 (10)
O3—Yb—O1^{iii}	83.67 (18)	O7^{vii}—Rb—P3	64.64 (9)
O4^{ii}—Yb—O1^{iii}	70.81 (17)	O9—Rb—P3	85.96 (9)
O8^{i}—Yb—O5	140.30 (18)	O12—Rb—P3	112.54 (9)
O3—Yb—O5	70.73 (18)	O4—Rb—O5^{viii}	51.42 (13)
O4^{ii}—Yb—O5	75.36 (18)	O1^{v}—Rb—O5^{viii}	53.59 (12)
O1^{iii}—Yb—O5	78.36 (18)	O11^{vi}—Rb—O5^{viii}	138.09 (13)
O8^{i}—Yb—O11	75.48 (18)	O6—Rb—O5^{viii}	135.50 (13)
O3—Yb—O11	142.76 (18)	O2—Rb—O5^{viii}	43.63 (12)
O4^{ii}—Yb—O11	76.06 (17)	O3—Rb—O5^{viii}	62.28 (13)
O1^{iii}—Yb—O11	114.32 (16)	O5—Rb—O5^{viii}	82.41 (2)
O5—Yb—O11	142.25 (18)	O7^{vii}—Rb—O5^{viii}	80.78 (12)
O8^{i}—Yb—O9	142.46 (17)	O9—Rb—O5^{viii}	128.79 (12)
O3—Yb—O9	107.00 (18)	O12—Rb—O5^{viii}	42.07 (12)
O4^{ii}—Yb—O9	81.08 (17)	P3—Rb—O5^{viii}	143.41 (9)
O1^{iii}—Yb—O9	144.61 (17)	O3—P1—O1	121.0 (3)
O5—Yb—O9	73.97 (17)	O3—P1—O7^{iv}	110.8 (3)
O11—Yb—O9	77.69 (17)	O1—P1—O7^{iv}	106.0 (3)
O8^{i}—Yb—O6^{iv}	77.00 (17)	O3—P1—O2	107.8 (3)
O3—Yb—O6^{iv}	70.55 (17)	O1—P1—O2	110.4 (3)
O4^{ii}—Yb—O6^{iv}	144.63 (17)	O7^{iv}—P1—O2	98.3 (3)
O1^{iii}—Yb—O6^{iv}	142.15 (17)	O3—P1—Rb^{ix}	157.9 (2)
O5—Yb—O6^{iv}	116.22 (17)	O1—P1—Rb^{ix}	49.7 (2)
O11—Yb—O6^{iv}	76.54 (17)	O7^{iv}—P1—Rb^{ix}	62.01 (18)
O9—Yb—O6^{iv}	71.55 (16)	O2—P1—Rb^{ix}	94.2 (2)
O8^{i}—Yb—P4	156.26 (13)	O3—P1—Rb	54.7 (2)
O3—Yb—P4	114.82 (13)	O1—P1—Rb	150.9 (2)
O4^{ii}—Yb—P4	63.63 (12)	O7^{iv}—P1—Rb	101.48 (18)
O1^{iii}—Yb—P4	125.81 (12)	O2—P1—Rb	55.5 (2)
O5—Yb—P4	63.41 (13)	Rb^{ix}—P1—Rb	144.73 (6)
O11—Yb—P4	81.96 (12)	O4—P2—O5	118.2 (3)
O9—Yb—P4	19.19 (12)	O4—P2—O12^{ii}	110.5 (3)
O6^{iv}—Yb—P4	90.74 (11)	O5—P2—O12^{ii}	109.0 (3)
O8^{i}—Yb—P3^{iv}	59.09 (13)	O4—P2—O2^{ii}	110.3 (3)
O3—Yb—P3^{iv}	62.33 (13)	O5—P2—O2^{ii}	108.4 (3)

O4^{ii}—Yb—P3^{iv}	156.75 (13)	O12^{ii}—P2—O2^{ii}	98.6 (3)
O1^{iii}—Yb—P3^{iv}	122.81 (12)	O4—P2—Rb	53.8 (2)
O5—Yb—P3^{iv}	123.65 (14)	O5—P2—Rb	64.7 (2)
O11—Yb—P3^{iv}	80.89 (13)	O12^{ii}—P2—Rb	126.9 (2)
O9—Yb—P3^{iv}	91.18 (12)	O2^{ii}—P2—Rb	134.3 (2)
O6^{iv}—Yb—P3^{iv}	19.64 (11)	O4—P2—Rb^{ii}	168.4 (2)
P4—Yb—P3^{iv}	110.36 (4)	O5—P2—Rb^{ii}	71.5 (2)
O8^{i}—Yb—Rb	125.11 (14)	O12^{ii}—P2—Rb^{ii}	69.6 (2)
O3—Yb—Rb	51.84 (13)	O2^{ii}—P2—Rb^{ii}	58.8 (2)
O4^{ii}—Yb—Rb	117.65 (12)	Rb—P2—Rb^{ii}	136.06 (6)
O1^{iii}—Yb—Rb	120.11 (13)	O11^{vi}—P3—O6	116.9 (3)
O5—Yb—Rb	52.52 (13)	O11^{vi}—P3—O10^{vii}	107.9 (3)
O11—Yb—Rb	125.40 (11)	O6—P3—O10^{vii}	111.2 (3)
O9—Yb—Rb	55.76 (13)	O11^{vi}—P3—O7	109.0 (3)
O6^{iv}—Yb—Rb	63.71 (11)	O6—P3—O7	108.8 (3)
P4—Yb—Rb	63.69 (3)	O10^{vii}—P3—O7	102.0 (3)
P3^{iv}—Yb—Rb	73.93 (3)	O11^{vi}—P3—Rb	57.8 (2)
O8^{i}—Yb—Rb^{ii}	109.77 (13)	O6—P3—Rb	59.07 (19)
O3—Yb—Rb^{ii}	103.25 (13)	O10^{vii}—P3—Rb	129.2 (2)
O4^{ii}—Yb—Rb^{ii}	39.06 (13)	O7—P3—Rb	128.73 (19)
O1^{iii}—Yb—Rb^{ii}	40.64 (12)	O11^{vi}—P3—Yb^{iv}	149.9 (2)
O5—Yb—Rb^{ii}	54.17 (13)	O6—P3—Yb^{iv}	33.00 (19)
O11—Yb—Rb^{ii}	111.43 (12)	O10^{vii}—P3—Yb^{iv}	90.31 (19)
O9—Yb—Rb^{ii}	104.20 (12)	O7—P3—Yb^{iv}	89.63 (19)
O6^{iv}—Yb—Rb^{ii}	170.36 (11)	Rb—P3—Yb^{iv}	92.05 (4)
P4—Yb—Rb^{ii}	85.20 (3)	O8—P4—O9	118.4 (3)
P3^{iv}—Yb—Rb^{ii}	161.86 (3)	O8—P4—O12^{x}	109.7 (3)
Rb—Yb—Rb^{ii}	106.683 (15)	O9—P4—O12^{x}	110.8 (3)
O4—Rb—O1^{v}	54.42 (14)	O8—P4—O10	107.5 (3)
O4—Rb—O11^{vi}	99.00 (14)	O9—P4—O10	110.1 (3)
O1^{v}—Rb—O11^{vi}	85.77 (14)	O12^{x}—P4—O10	98.4 (3)
O4—Rb—O6	142.98 (13)	O8—P4—Yb	110.0 (2)
O1^{v}—Rb—O6	98.05 (13)	O9—P4—Yb	31.48 (19)
O11^{vi}—Rb—O6	50.08 (14)	O12^{x}—P4—Yb	87.94 (19)
O4—Rb—O2	89.44 (14)	O10—P4—Yb	137.13 (18)
O1^{v}—Rb—O2	91.34 (13)	O8—P4—Rb	67.5 (2)
O11^{vi}—Rb—O2	167.11 (13)	O9—P4—Rb	53.3 (2)
O6—Rb—O2	118.21 (14)	O12^{x}—P4—Rb	147.1 (2)
O4—Rb—O3	73.31 (13)	O10—P4—Rb	113.9 (2)
O1^{v}—Rb—O3	113.31 (13)	Yb—P4—Rb	64.49 (3)
O11^{vi}—Rb—O3	145.61 (14)	P1—O1—Yb^{iii}	142.4 (3)
O6—Rb—O3	143.52 (13)	P1—O1—Rb^{ix}	107.9 (2)
O2—Rb—O3	46.43 (13)	Yb^{iii}—O1—Rb^{ix}	108.41 (17)
O4—Rb—O5	48.79 (13)	P2^{viii}—O2—P1	129.8 (3)
O1^{v}—Rb—O5	102.94 (13)	P2^{viii}—O2—Rb	95.6 (2)
O11^{vi}—Rb—O5	99.53 (14)	P1—O2—Rb	99.7 (2)
O6—Rb—O5	141.49 (14)	P1—O3—Yb	140.6 (3)
O2—Rb—O5	93.36 (13)	P1—O3—Rb	102.9 (3)

O3—Rb—O5	49.81 (13)	Yb—O3—Rb	93.51 (16)
O4—Rb—O7^{vii}	100.66 (14)	P2—O4—Yb^{viii}	138.6 (3)
O1^{v}—Rb—O7^{vii}	46.25 (13)	P2—O4—Rb	102.2 (2)
O11^{vi}—Rb—O7^{vii}	76.57 (13)	Yb^{viii}—O4—Rb	111.14 (19)
O6—Rb—O7^{vii}	57.20 (13)	P2—O5—Yb	149.0 (3)
O2—Rb—O7^{vii}	92.37 (13)	P2—O5—Rb	90.6 (2)
O3—Rb—O7^{vii}	137.41 (14)	Yb—O5—Rb	91.97 (16)
O5—Rb—O7^{vii}	148.80 (13)	P2—O5—Rb^{ii}	84.9 (2)
O4—Rb—O9	98.07 (14)	Yb—O5—Rb^{ii}	93.09 (16)
O1^{v}—Rb—O9	145.46 (13)	Rb—O5—Rb^{ii}	174.93 (17)
O11^{vi}—Rb—O9	77.95 (13)	P3—O6—Yb^{iv}	127.4 (3)
O6—Rb—O9	94.50 (13)	P3—O6—Rb	95.7 (2)
O2—Rb—O9	110.67 (12)	Yb^{iv}—O6—Rb	136.85 (19)
O3—Rb—O9	70.33 (13)	P1^{iv}—O7—P3	130.7 (3)
O5—Rb—O9	51.39 (12)	P1^{iv}—O7—Rb^{xi}	92.3 (2)
O7^{vii}—Rb—O9	150.34 (12)	P3—O7—Rb^{xi}	135.0 (2)
O4—Rb—O12	89.65 (13)	P4—O8—Yb^{vi}	147.0 (3)
O1^{v}—Rb—O12	57.93 (13)	P4—O9—Yb	129.3 (3)
O11^{vi}—Rb—O12	127.26 (12)	P4—O9—Rb	105.7 (2)
O6—Rb—O12	95.14 (13)	Yb—O9—Rb	88.25 (15)
O2—Rb—O12	42.48 (12)	P3^{xi}—O10—P4	124.3 (3)
O3—Rb—O12	86.74 (13)	P3^{i}—O11—Yb	146.7 (3)
O5—Rb—O12	123.37 (12)	P3^{i}—O11—Rb^{i}	97.3 (2)
O7^{vii}—Rb—O12	50.74 (12)	Yb—O11—Rb^{i}	115.97 (17)
O9—Rb—O12	152.28 (12)	P2^{viii}—O12—P4^{xii}	133.6 (3)
O4—Rb—P3	121.61 (10)	P2^{viii}—O12—Rb	84.9 (2)
O1^{v}—Rb—P3	91.92 (10)	P4^{xii}—O12—Rb	141.4 (2)
O11^{vi}—Rb—P3	24.90 (10)		

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