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Synthesis and crystal structure of dipotassium nickel polyphosphate

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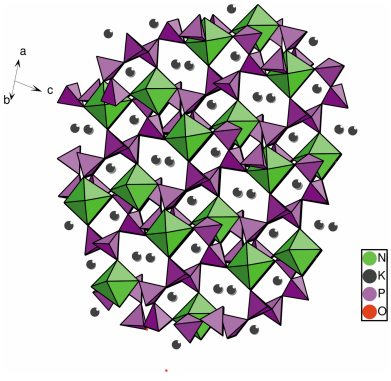
Single crystals of $K_2Ni(PO_3)_4$ were obtained by solid-state reaction. The structure consists of infinite zigzag polyphosphate chains, running along the *c*-axis direction, linked by Ni^{2+} ions and delimiting large tunnels in which the K^+ ions are located. Ni^{2+} ions form slightly distorted NiO_6 octahedra and the coordination numbers of the independent potassium cations are 8 and 10.

1. Chemical context

Transition-metal oxides (Fe, Co, or Ni) in melted phosphate systems of alkali metals (M_2O–P_2O_5, M = Li, Na, or K) are widely studied (Pontchara & Durif, 1974; Litvin & Masloboev, 1989; Panahandeh & Jung, 2003; Moutataouia *et al.*, 2014; Ouaatta *et al.*, 2019). These materials present various and interesting properties and applications, such as catalysts (Moffat, 1978), ferroelectric and/or magnetic materials (Lazoryak *et al.*, 2004; Hatert *et al.*, 2004; Essehli *et al.*, 2015) and ion-conduction properties (La Parola *et al.*, 2018; Orikasa *et al.*, 2016; Daidouh *et al.*, 1999). Some of these specific properties, such as catalytic activity, are similar to those found in the phosphate systems themselves (Kapshuk *et al.*, 2000). These compounds have been characterized by several physico-chemical and structural methods. Among these studies, some have been devoted to nickel-based phosphates associated with alkali metals, such as the polyphosphates $MNi(PO_3)_3$ (M = Li, Na, or K; Kapshuk *et al.*, 2000) and $NiCs_4(PO_3)_6$ (Sbai *et al.*, 2004). For all these samples, the study of their structural characteristics is essential for understanding most of the physical properties (Fischer *et al.*, 1994). The title polyphosphate, $K_2Ni(PO_3)_4$, designated as (**1**), was obtained in the quest to synthesize new condensed phosphates appearing in the A_2O–MO–LnO_3–P_2O_5 quaternary system (A: an alkali metal, M: transition metal divalent cation, Ln: lanthanide or Y metal). This compound has been observed in the diagram $Ni(PO_3)_2$–KPO_3 (Pontchara & Durif, 1974) but, to our knowledge, its crystal structure has not yet been reported. We report herein on its synthesis and structural characterization by single crystal X-ray diffraction.



2. Structural commentary

The title compound, (**1**), crystallizes in the non-centrosymmetric monoclinic space group *Cc*. The asymmetric unit contains 19 atoms corresponding to the chemical formula

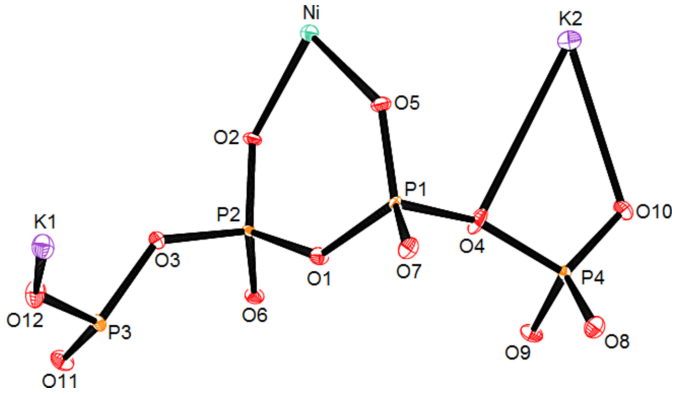


Figure 1
The asymmetric unit of $K_2Ni(PO_3)_4$.

$K_2Ni(PO_3)_4$, as shown in Fig. 1. The structure is based on infinite zigzag polyphosphate chains running almost along the *c*-axis direction and linked by NiO_6 octahedra (Fig. 2). Each NiO_6 octahedron shares corners with six different PO_4 tetrahedra belonging to three polyphosphate chains. All the terminal O atoms of the PO_4 tetrahedra in the polyphosphate chains interact with the Ni and K atoms. Such an arrangement creates a three-dimensional framework that delimits large hexagonal and pentagonal tunnels in which the K^+ ions are located (Fig. 3). The NiO_6 octahedra are slightly distorted, with Ni—O distances ranging from 2.017 (2) to 2.167 (2) Å and the O—Ni—O angles from 82.52 (6)° to 173.51 (6)°. In the four PO_4 tetrahedra, the equatorial and apical distances P—OE and P—OL, respectively, range from 1.469 (2) to 1.493 (2) Å for P—OE and 1.578 (1) to 1.602 (1)Å for P—OL and the O—P—O angles range from 100.37 (10) to 120.76 (10)°. The unit cell contains two crystallographically non-equivalent K atoms (K1 and K2) both located in large hexagonal and pentagonal tunnels (Fig. 3). The coordination

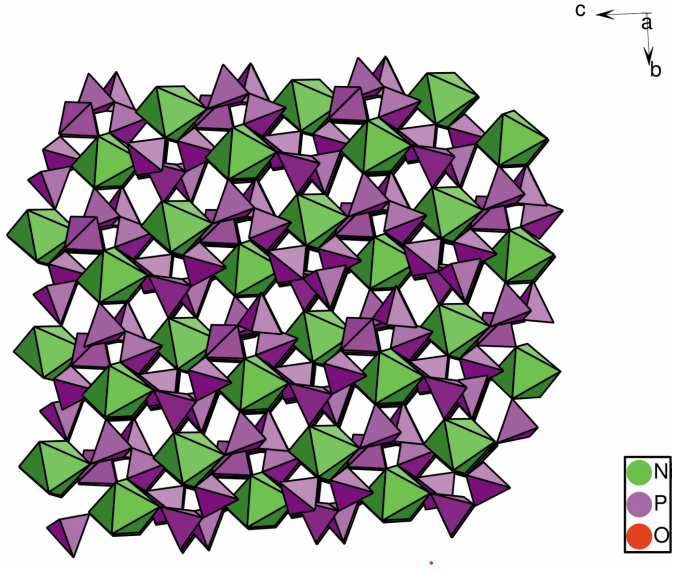


Figure 2
Projection of the $K_2Ni(PO_3)_4$ structure along [100].

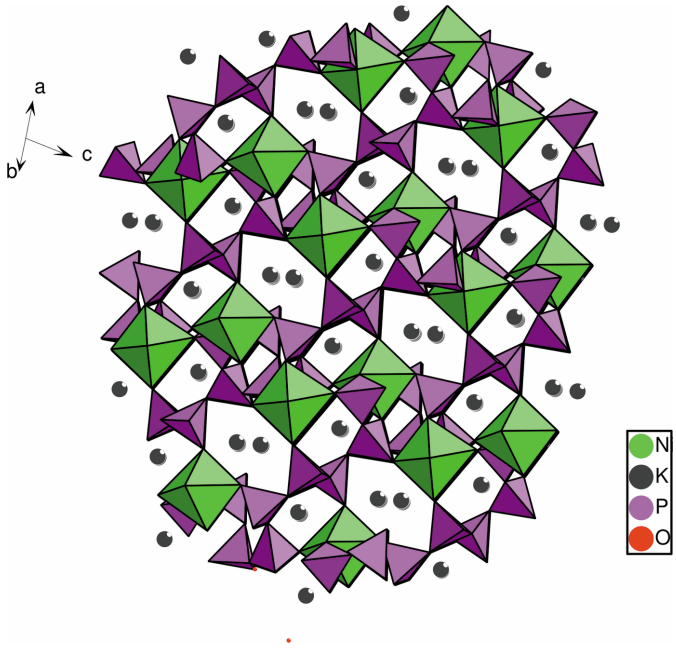


Figure 3
Polyhedral representation of the structure of $K_2Ni(PO_3)_4$ showing the tunnels in which the K^+ cations are located.

number (CN) is 8 for K1 and 10 for K2. The K—O interactions range from 2.582 (2) and 3.111 (2) Å for K1 (mean distance: 2.841 Å) and 2.761 (2) to 3.414 (2) Å for K2 (mean distance: 3.041 Å)

3. Database survey

A search in the Cambridge Structural Database (Version 5.43, November 2021; Groom *et al.*, 2016) revealed about a dozen alkaline nickel-based phosphates: $TlNi_4(PO_4)_3$, $Tl_4Ni_7(PO_4)_6$ and $Tl_2Ni_4(P_2O_7)(PO_4)_2$ (Panahandeh & Jung, 2003), $KNi_3(PO_4)P_2O_7$ (Moutataouia *et al.*, 2014), $K_2Ni_4(PO_4)_2$-(P_2O_7) (Palkina *et al.*, 1980), $K_2NiP_2O_7$ (El Maadi *et al.*, 1995), $AM_4(PO_4)_3$ (*A* = Na, K, Rb; *M* = Ni, Mn) (Daidouh *et al.*, 1999), $MNi(PO_3)_3$ (*M* = Na or K) (Kapshuk *et al.*, 2000), $KNiPO_4$ (Fischer *et al.*, 1994), $NiCs_4(PO_3)_6$ and $NiK_4(P_3O_9)_2$ (Sbai *et al.*, 2004). As in the case of the title compound, the structures of $MNi(PO_3)_3$ (*M* = Na or K) polyphosphates are based on infinite zigzag polyphosphate chains, linked by Ni^{2+} ions in octahedral coordination and delimiting tunnels in which the alkali ions are located (Fig. 3). The metal atoms (*M*) and nickel atoms form infinite ···Ni–*M*–Ni–*M*··· columns of polyhedra sharing edges and alternating with the polyphosphate chains. In the $NaNi(PO_3)_3$ structure (Kapshuk *et al.*, 2000), the polyphosphate chains run along the *a*-axis direction, and the Na atom exhibits a distorted octahedral environment whereas in $KNi(PO_3)_3$, the polyphosphate chains are run in the same direction as in the title polyphosphate (*c*-axis) and the coordination polyhedron of the K atom is a distorted tricapped trigonal prism (CN = 9), unlike in the title polyphosphate where the K atoms exhibit two different coordination numbers (8 and 10). In the other alkaline nickel-based

phosphates $TlNi_4(PO_4)_3$, $Tl_4Ni_7(PO_4)_6$, $Tl_2Ni_4(P_2O_7)(PO_4)_2$, $KNi_3(PO_4)P_2O_7$, $K_2Ni_4(PO_4)_2(P_2O_7)$, $K_2NiP_2O_7$, $AM_4(PO_4)_3$ (A = Na, K, Rb; M = Ni, Mn); the structural arrangements are markedly different from that of the title compound being based on alkali and Ni polyhedra sharing edges and forming chains that are linked together by isolated PO_4 and/or diphosphate (P_2O_7) groups. In addition, the coordination polyhedron of the Ni atom is not always octahedral. For instance, it is 7-coordinated in $TlNi_4(PO_4)_3$, 5-coordinated in $KNi_4(PO_4)_3$ and has an unusual coordination of only four oxygen atoms in a distorted tetrahedron in $Tl_2Ni_4(P_2O_7)(PO_4)_2$. The coordination numbers of the metal atoms (Tl and K) in these phosphates range from 6 to 12. Thallium nickel phosphate, $Tl_2Ni_4(P_2O_7)(PO_4)_2$, adopts the $K_2Ni_4(PO_4)_2(P_2O_7)$ structure, and the environments of the alkali and nickel atoms are nearly identical.

4. Synthesis and crystallization

Single crystals of $K_2Ni(PO_3)_4$ were prepared by solid-state reaction. A mixture of the reagents K_2CO_3, $NiCl_2{\cdot}6H_2O$, $NH_4H_2PO_4$ and La_2O_3 in a molar ratio of K:Ni:P:La of 0.4:0.05:1:0.02 was placed in a porcelain crucible. The reaction mixture was then calcined at 623 K for 1 h and gradually heated to 823 K. Maintained at this temperature for 72 h, the reaction mixture then underwent slow cooling at a rate of 1 K h^{-1} to 773 K and then to room temperature with furnace inertia. The crystals obtained were recovered after washing with boiling water.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Solving and refinement tests of the structure were carried out in both the centrosymmetric and non-centrosymmetric space groups $C2/c$ and Cc. Better results with a much convergent refinement were obtained with the non-centrosymmetric model. The use of the TWIN refinement mode made the refinement results significantly improved. No Extinction correction was applied. The residual maximum and minimum electron density peaks are located 0.13 Å from P1 and 0.36 Å from Ni1, respectively. However, the minimum density observed in the vicinity of a nickel atom is rather largely negative (−2.6 e $Å^{-3}$) indicating probably that the absorption correction applied was not optimal.

Acknowledgements

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Table 1
Experimental details.

Crystal data	
Chemical formula	$K_2Ni(PO_3)_4$
M_r	452.79
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	293
a, *b*, *c* (Å)	11.07179 (16), 12.50386 (16), 7.53969 (11)
β (°)	103.2349 (14)
V (Å^3)	1016.07 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.43
Crystal size (mm)	0.12 × 0.08 × 0.07
Data collection	
Diffractometer	SuperNova
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.509, 0.710
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33158, 8076, 7869
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.999
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.088, 1.07
No. of reflections	8076
No. of parameters	173
No. of restraints	2
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.83, −2.85
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.539 (9)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

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Computing details

Dipotassium nickel polyphosphate

Crystal data

$K_2Ni(PO_3)_4$
M_r = 452.79
Monoclinic, *Cc*
a = 11.07179 (16) Å
b = 12.50386 (16) Å
c = 7.53969 (11) Å
β = 103.2349 (14)°
V = 1016.07 (3) Å^3
Z = 4
F(000) = 888
D_x = 2.960 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5641 reflections
θ = 2.5–45.2°
μ = 3.43 mm^{-1}
T = 293 K
Block, metallic reddish red
0.12 × 0.08 × 0.07 mm

Data collection

SuperNova diffractometer
θ/2*θ* scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.509, T_{max} = 0.710
33158 measured reflections
8076 independent reflections
7869 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 45.2°, θ_{min} = 2.5°
h = −22→21
k = −24→24
l = −14→14
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.088
S = 1.07
8076 reflections
173 parameters
2 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 1.2215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −2.85 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.539 (9)

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 2-component inversion twin.
Data were collected on a SuperNova diffractometer equipped with a (Mo)X-ray Source and an Atlas CCD detector. Cell refinement and data reduction were performed with CrysAlisPro 1.171.42.49 (Rigaku, 2022) and adsorption correction withSCALE3 ABSPACK scaling algorithm (Rigaku Oxford Diffraction, 2022). Using the SHELX software package, the structure was solved by the direct method with the SHELXS program (Sheldrick, 2015a) and refined by the full-matrix least-squares method using SHELXL program (Sheldrick, 2015b). The programs *Ortep-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006) were used for molecular graphics and the software *publCIF* (Westrip, 2010) to prepare material for publication.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.94642 (3)	0.34669 (2)	0.79387 (4)	0.00586 (5)
K1	0.61359 (4)	0.63341 (3)	0.12530 (6)	0.00747 (6)
K2	1.31600 (5)	0.37393 (4)	0.96892 (7)	0.01014 (7)
P1	1.05470 (5)	0.57511 (4)	0.70758 (7)	0.00330 (7)
P2	0.83590 (5)	0.57688 (4)	0.86578 (7)	0.00340 (7)
P3	0.62807 (5)	0.68963 (4)	0.62381 (7)	0.00407 (7)
P4	1.28454 (5)	0.66069 (4)	0.97345 (7)	0.00384 (7)
O1	0.94041 (16)	0.62429 (12)	0.7749 (2)	0.0065 (2)
O2	0.84766 (14)	0.45926 (12)	0.8902 (2)	0.00540 (19)
O3	0.71177 (15)	0.58966 (12)	0.7095 (2)	0.0066 (2)
O4	1.16650 (16)	0.59314 (15)	0.8769 (2)	0.0088 (2)
O5	1.04508 (15)	0.45704 (12)	0.6879 (2)	0.0058 (2)
O6	0.82806 (16)	0.64783 (12)	1.0220 (2)	0.0059 (2)
O7	1.07218 (15)	0.64267 (13)	0.5525 (2)	0.0059 (2)
O8	1.31674 (15)	0.73723 (13)	0.8407 (2)	0.0074 (2)
O9	1.23326 (16)	0.72198 (13)	1.1278 (2)	0.0070 (2)
O10	1.37679 (15)	0.58280 (13)	1.0701 (2)	0.0085 (2)
O11	0.55585 (16)	0.72302 (13)	0.7586 (2)	0.0076 (2)
O12	0.56100 (16)	0.66049 (14)	0.4387 (2)	0.0085 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.00581 (9)	0.00526 (8)	0.00660 (8)	0.00012 (7)	0.00160 (7)	0.00007 (7)
K1	0.00615 (13)	0.00922 (13)	0.00764 (13)	−0.00002 (12)	0.00283 (10)	−0.00036 (12)
K2	0.00994 (16)	0.00745 (14)	0.01295 (17)	−0.00041 (12)	0.00245 (13)	−0.00230 (12)
P1	0.00303 (16)	0.00325 (16)	0.00364 (15)	−0.00080 (12)	0.00081 (12)	−0.00030 (12)
P2	0.00332 (16)	0.00287 (15)	0.00425 (15)	0.00051 (12)	0.00139 (12)	−0.00014 (12)
P3	0.00380 (16)	0.00497 (16)	0.00343 (15)	0.00063 (12)	0.00079 (12)	0.00020 (13)
P4	0.00303 (16)	0.00393 (17)	0.00437 (16)	−0.00011 (12)	0.00048 (13)	−0.00040 (12)
O1	0.0059 (5)	0.0051 (4)	0.0101 (6)	0.0000 (4)	0.0052 (4)	0.0001 (4)
O2	0.0059 (5)	0.0030 (4)	0.0075 (5)	0.0009 (3)	0.0020 (4)	0.0005 (3)
O3	0.0050 (5)	0.0051 (4)	0.0085 (5)	0.0007 (4)	−0.0008 (4)	0.0003 (4)
O4	0.0073 (5)	0.0110 (6)	0.0063 (5)	−0.0048 (4)	−0.0023 (4)	0.0003 (4)
O5	0.0065 (5)	0.0037 (4)	0.0076 (5)	−0.0006 (4)	0.0026 (4)	−0.0007 (4)
O6	0.0069 (5)	0.0053 (5)	0.0057 (5)	0.0009 (4)	0.0019 (4)	−0.0014 (4)
O7	0.0065 (5)	0.0067 (5)	0.0048 (5)	−0.0015 (4)	0.0017 (4)	0.0008 (4)

O8	0.0073 (5)	0.0075 (5)	0.0082 (5)	−0.0011 (4)	0.0035 (4)	0.0013 (4)
O9	0.0087 (5)	0.0064 (5)	0.0064 (5)	0.0020 (4)	0.0029 (4)	−0.0011 (4)
O10	0.0060 (5)	0.0068 (5)	0.0112 (6)	0.0023 (4)	−0.0007 (4)	0.0016 (4)
O11	0.0085 (5)	0.0078 (5)	0.0078 (5)	0.0023 (4)	0.0043 (4)	0.0005 (4)
O12	0.0074 (5)	0.0129 (6)	0.0044 (5)	−0.0006 (4)	−0.0004 (4)	−0.0008 (4)

Geometric parameters (Å, º)

Ni1—K1^{i}	3.6212 (6)	K2—O6^{vi}	2.8540 (16)
Ni1—K1^{ii}	3.8294 (5)	K2—O7^{i}	2.9168 (18)
Ni1—K2^{iii}	3.7520 (6)	K2—O8^{i}	3.1274 (18)
Ni1—K2	4.0161 (6)	K2—O9^{iv}	2.7951 (17)
Ni1—O2	2.0168 (15)	K2—O10^{iv}	3.273 (2)
Ni1—O5	2.0335 (16)	K2—O10	2.7605 (18)
Ni1—O6^{iv}	2.1666 (16)	K2—O11^{x}	3.2612 (18)
Ni1—O7^{i}	2.1253 (16)	K2—O12^{x}	2.8069 (19)
Ni1—O8^{v}	2.0717 (16)	P1—O1	1.5910 (17)
Ni1—O11^{vi}	2.0194 (16)	P1—O4	1.5779 (16)
K1—P2^{vii}	3.5486 (7)	P1—O5	1.4852 (16)
K1—P2^{iv}	3.7705 (7)	P1—O7	1.4903 (16)
K1—P4^{viii}	3.5763 (7)	P2—O1	1.5882 (17)
K1—O2^{iv}	3.1108 (16)	P2—O2	1.4842 (16)
K1—O3^{iv}	3.0080 (16)	P2—O3	1.6002 (16)
K1—O6^{vii}	2.6693 (18)	P2—O6	1.4928 (16)
K1—O7^{ix}	2.8697 (16)	P3—O3	1.6016 (16)
K1—O8^{ix}	2.9396 (17)	P3—O9^{ix}	1.6009 (17)
K1—O10^{viii}	2.6358 (18)	P3—O11	1.4893 (17)
K1—O11^{vii}	2.9154 (17)	P3—O12	1.4691 (17)
K1—O12	2.5817 (18)	P4—O4	1.5860 (17)
K2—P3^{x}	3.4765 (7)	P4—O8	1.4858 (17)
K2—P4	3.6034 (7)	P4—O9	1.6022 (17)
K2—O4	3.195 (2)	P4—O10	1.4771 (16)
K2—O5	3.4141 (17)		

K1^{i}—Ni1—K1^{ii}	125.300 (12)	O10—K2—O5	90.43 (4)
K1^{i}—Ni1—K2^{iii}	67.218 (12)	O10—K2—O6^{vi}	153.87 (5)
K1^{ii}—Ni1—K2	62.662 (11)	O10—K2—O7^{i}	100.77 (5)
K1^{i}—Ni1—K2	171.099 (12)	O10—K2—O8^{i}	102.85 (5)
K2^{iii}—Ni1—K1^{ii}	88.300 (11)	O10—K2—O9^{iv}	131.91 (5)
K2^{iii}—Ni1—K2	119.195 (13)	O10—K2—O10^{iv}	90.52 (4)
O2—Ni1—K1^{ii}	118.16 (5)	O10—K2—O11^{x}	93.26 (5)
O2—Ni1—K1^{i}	59.09 (5)	O10—K2—O12^{x}	89.34 (5)
O2—Ni1—K2^{iii}	126.08 (5)	O11^{x}—K2—P3^{x}	25.28 (3)
O2—Ni1—K2	114.71 (5)	O11^{x}—K2—P4	115.41 (3)
O2—Ni1—O5	92.99 (6)	O11^{x}—K2—O5	173.59 (4)
O2—Ni1—O6^{iv}	93.34 (6)	O11^{x}—K2—O10^{iv}	111.68 (4)
O2—Ni1—O7^{i}	85.48 (6)	O12^{x}—K2—P3^{x}	24.16 (3)
O2—Ni1—O8^{v}	86.88 (7)	O12^{x}—K2—P4	104.51 (4)

O2—Ni1—O11^{vi}	166.65 (7)	O12^{x}—K2—O4	125.18 (5)
O5—Ni1—K1^{ii}	120.40 (5)	O12^{x}—K2—O5	136.41 (5)
O5—Ni1—K1^{i}	114.24 (5)	O12^{x}—K2—O6^{vi}	81.05 (5)
O5—Ni1—K2	58.20 (5)	O12^{x}—K2—O7^{i}	165.05 (5)
O5—Ni1—K2^{iii}	113.79 (5)	O12^{x}—K2—O8^{i}	101.57 (5)
O5—Ni1—O6^{iv}	82.52 (6)	O12^{x}—K2—O10^{iv}	62.93 (5)
O5—Ni1—O7^{i}	91.15 (6)	O12^{x}—K2—O11^{x}	48.97 (4)
O5—Ni1—O8^{v}	166.15 (7)	K1^{xi}—P1—K2^{iv}	65.244 (13)
O6^{iv}—Ni1—K1^{i}	47.10 (5)	O1—P1—K1^{xi}	81.92 (6)
O6^{iv}—Ni1—K1^{ii}	137.45 (4)	O1—P1—K2^{iv}	146.61 (6)
O6^{iv}—Ni1—K2	131.17 (5)	O4—P1—K1^{xi}	82.08 (7)
O6^{iv}—Ni1—K2^{iii}	49.19 (4)	O4—P1—K2^{iv}	79.50 (7)
O7^{i}—Ni1—K1^{ii}	47.74 (4)	O4—P1—O1	102.73 (10)
O7^{i}—Ni1—K1^{i}	135.89 (5)	O5—P1—K1^{xi}	162.46 (7)
O7^{i}—Ni1—K2^{iii}	135.94 (4)	O5—P1—K2^{iv}	99.47 (7)
O7^{i}—Ni1—K2	44.68 (5)	O5—P1—O1	111.84 (9)
O7^{i}—Ni1—O6^{iv}	173.50 (6)	O5—P1—O4	104.35 (10)
O8^{v}—Ni1—K1^{i}	54.26 (5)	O5—P1—O7	120.29 (9)
O8^{v}—Ni1—K1^{ii}	71.27 (5)	O7—P1—K1^{xi}	42.80 (6)
O8^{v}—Ni1—K2^{iii}	56.46 (5)	O7—P1—K2^{iv}	44.18 (7)
O8^{v}—Ni1—K2	133.93 (5)	O7—P1—O1	106.67 (9)
O8^{v}—Ni1—O6^{iv}	83.66 (6)	O7—P1—O4	109.57 (10)
O8^{v}—Ni1—O7^{i}	102.64 (7)	K1^{xii}—P2—K1^{i}	86.856 (17)
O11^{vi}—Ni1—K1^{ii}	48.53 (5)	K1^{xii}—P2—K2^{xiii}	67.271 (14)
O11^{vi}—Ni1—K1^{i}	126.83 (5)	K1^{i}—P2—K2^{xiii}	135.710 (18)
O11^{vi}—Ni1—K2^{iii}	60.25 (5)	O1—P2—K1^{xii}	146.03 (6)
O11^{vi}—Ni1—K2	60.75 (5)	O1—P2—K1^{i}	120.85 (7)
O11^{vi}—Ni1—O5	94.32 (7)	O1—P2—K2^{xiii}	78.82 (6)
O11^{vi}—Ni1—O6^{iv}	98.67 (7)	O1—P2—O3	103.48 (9)
O11^{vi}—Ni1—O7^{i}	83.22 (7)	O2—P2—K1^{xii}	100.44 (7)
O11^{vi}—Ni1—O8^{v}	88.67 (7)	O2—P2—K1^{i}	52.96 (6)
Ni1^{iv}—K1—P2^{iv}	51.633 (11)	O2—P2—K2^{xiii}	161.42 (7)
P2^{vii}—K1—Ni1^{iv}	55.151 (12)	O2—P2—O1	111.80 (9)
P2^{vii}—K1—P2^{iv}	70.573 (13)	O2—P2—O3	103.08 (9)
P2^{vii}—K1—P4^{viii}	128.817 (18)	O2—P2—O6	120.69 (9)
P4^{viii}—K1—Ni1^{iv}	170.418 (17)	O3—P2—K1^{i}	50.17 (6)
P4^{viii}—K1—P2^{iv}	136.511 (17)	O3—P2—K1^{xii}	78.39 (7)
O2^{iv}—K1—Ni1^{iv}	33.80 (3)	O3—P2—K2^{xiii}	88.45 (6)
O2^{iv}—K1—P2^{iv}	22.39 (3)	O6—P2—K1^{i}	130.12 (7)
O2^{iv}—K1—P2^{vii}	72.46 (3)	O6—P2—K1^{xii}	43.42 (7)
O2^{iv}—K1—P4^{viii}	151.52 (3)	O6—P2—K2^{xiii}	40.83 (6)
O3^{iv}—K1—Ni1^{iv}	72.55 (3)	O6—P2—O1	107.34 (9)
O3^{iv}—K1—P2^{vii}	70.67 (4)	O6—P2—O3	109.04 (9)
O3^{iv}—K1—P2^{iv}	24.11 (3)	K2^{xiii}—P3—K1	134.104 (18)
O3^{iv}—K1—P4^{viii}	116.65 (3)	K2^{xiv}—P3—K1	79.126 (15)
O3^{iv}—K1—O2^{iv}	46.48 (4)	K2^{xiv}—P3—K2^{xiii}	136.71 (2)
O6^{vii}—K1—Ni1^{iv}	36.48 (4)	O3—P3—K1	98.32 (7)
O6^{vii}—K1—P2^{iv}	70.19 (4)	O3—P3—K2^{xiv}	113.32 (6)

O6^{vii}—K1—P2^{vii}	22.61 (3)	O3—P3—K2^{xiii}	91.25 (6)
O6^{vii}—K1—P4^{viii}	144.02 (4)	O9^{ix}—P3—K1	90.70 (6)
O6^{vii}—K1—O2^{iv}	63.03 (5)	O9^{ix}—P3—K2^{xiii}	43.41 (6)
O6^{vii}—K1—O3^{iv}	79.73 (5)	O9^{ix}—P3—K2^{xiv}	145.79 (6)
O6^{vii}—K1—O7^{ix}	89.55 (5)	O9^{ix}—P3—O3	100.37 (9)
O6^{vii}—K1—O8^{ix}	60.32 (5)	O11—P3—K1	145.19 (7)
O6^{vii}—K1—O11^{vii}	73.37 (5)	O11—P3—K2^{xiii}	69.63 (7)
O7^{ix}—K1—Ni1^{iv}	96.04 (4)	O11—P3—K2^{xiv}	69.25 (7)
O7^{ix}—K1—P2^{iv}	146.15 (4)	O11—P3—O3	107.15 (10)
O7^{ix}—K1—P2^{vii}	100.93 (4)	O11—P3—O9^{ix}	107.19 (10)
O7^{ix}—K1—P4^{viii}	74.89 (4)	O12—P3—K1	27.68 (7)
O7^{ix}—K1—O2^{iv}	124.00 (4)	O12—P3—K2^{xiv}	51.45 (8)
O7^{ix}—K1—O3^{iv}	168.30 (5)	O12—P3—K2^{xiii}	153.56 (7)
O7^{ix}—K1—O8^{ix}	68.73 (5)	O12—P3—O3	108.05 (9)
O7^{ix}—K1—O11^{vii}	56.84 (5)	O12—P3—O9^{ix}	113.35 (10)
O8^{ix}—K1—Ni1^{iv}	34.89 (3)	O12—P3—O11	118.97 (11)
O8^{ix}—K1—P2^{iv}	77.60 (3)	K1^{xv}—P4—K1^{xi}	126.000 (18)
O8^{ix}—K1—P2^{vii}	82.80 (3)	K1^{xv}—P4—K2^{i}	79.159 (15)
O8^{ix}—K1—P4^{viii}	135.97 (4)	K1^{xv}—P4—K2	79.311 (16)
O8^{ix}—K1—O2^{iv}	55.29 (4)	K2—P4—K1^{xi}	133.819 (19)
O8^{ix}—K1—O3^{iv}	101.52 (5)	K2^{i}—P4—K1^{xi}	133.235 (18)
O10^{viii}—K1—Ni1^{iv}	165.34 (4)	K2—P4—K2^{i}	84.614 (14)
O10^{viii}—K1—P2^{iv}	115.13 (4)	O4—P4—K1^{xi}	79.54 (7)
O10^{viii}—K1—P2^{vii}	130.96 (4)	O4—P4—K1^{xv}	140.19 (8)
O10^{viii}—K1—P4^{viii}	21.38 (4)	O4—P4—K2	62.42 (7)
O10^{viii}—K1—O2^{iv}	131.63 (5)	O4—P4—K2^{i}	106.16 (7)
O10^{viii}—K1—O3^{iv}	96.26 (5)	O4—P4—O9	101.31 (10)
O10^{viii}—K1—O6^{vii}	152.78 (6)	O8—P4—K1^{xi}	42.82 (7)
O10^{viii}—K1—O7^{ix}	95.42 (5)	O8—P4—K1^{xv}	83.87 (7)
O10^{viii}—K1—O8^{ix}	145.79 (5)	O8—P4—K2	126.58 (7)
O10^{viii}—K1—O11^{vii}	87.03 (5)	O8—P4—K2^{i}	140.74 (7)
O11^{vii}—K1—Ni1^{iv}	106.92 (4)	O8—P4—O4	109.49 (10)
O11^{vii}—K1—P2^{iv}	134.53 (4)	O8—P4—O9	111.14 (9)
O11^{vii}—K1—P2^{vii}	65.34 (3)	O9—P4—K1^{xi}	88.55 (6)
O11^{vii}—K1—P4^{viii}	70.95 (4)	O9—P4—K1^{xv}	108.51 (6)
O11^{vii}—K1—O2^{iv}	136.18 (5)	O9—P4—K2^{i}	44.69 (6)
O11^{vii}—K1—O3^{iv}	123.15 (5)	O9—P4—K2	122.27 (6)
O11^{vii}—K1—O8^{ix}	106.65 (5)	O10—P4—K1^{xv}	40.58 (7)
O12—K1—Ni1^{iv}	95.42 (4)	O10—P4—K1^{xi}	162.48 (8)
O12—K1—P2^{vii}	149.42 (4)	O10—P4—K2^{i}	61.96 (8)
O12—K1—P2^{iv}	84.87 (4)	O10—P4—K2	44.86 (7)
O12—K1—P4^{viii}	81.60 (4)	O10—P4—O4	106.22 (10)
O12—K1—O2^{iv}	77.92 (5)	O10—P4—O8	120.76 (10)
O12—K1—O3^{iv}	94.28 (5)	O10—P4—O9	106.09 (10)
O12—K1—O6^{vii}	131.32 (5)	P2—O1—P1	134.80 (10)
O12—K1—O7^{ix}	89.27 (5)	Ni1—O2—K1^{i}	87.11 (5)
O12—K1—O8^{ix}	74.13 (5)	P2—O2—Ni1	133.34 (10)
O12—K1—O10^{viii}	75.61 (6)	P2—O2—K1^{i}	104.66 (7)

O12—K1—O11^{vii}	140.45 (5)	P2—O3—K1^{i}	105.71 (7)
P3^{x}—K2—P4	108.365 (18)	P2—O3—P3	134.04 (11)
O4—K2—P3^{x}	134.00 (3)	P3—O3—K1^{i}	119.39 (8)
O4—K2—P4	26.10 (3)	P1—O4—K2	108.94 (9)
O4—K2—O5	42.80 (4)	P1—O4—P4	149.18 (13)
O4—K2—O10^{iv}	82.19 (5)	P4—O4—K2	91.47 (8)
O4—K2—O11^{x}	140.01 (4)	Ni1—O5—K2	91.39 (5)
O5—K2—P3^{x}	160.47 (3)	P1—O5—Ni1	131.91 (10)
O5—K2—P4	68.28 (3)	P1—O5—K2	102.00 (7)
O6^{vi}—K2—P3^{x}	73.47 (4)	Ni1^{i}—O6—K1^{xii}	96.42 (6)
O6^{vi}—K2—P4	170.35 (4)	Ni1^{i}—O6—K2^{xiii}	95.74 (5)
O6^{vi}—K2—O4	152.31 (5)	K1^{xii}—O6—K2^{xiii}	95.26 (5)
O6^{vi}—K2—O5	113.25 (4)	P2—O6—Ni1^{i}	129.30 (10)
O6^{vi}—K2—O7^{i}	85.13 (5)	P2—O6—K1^{xii}	113.98 (9)
O6^{vi}—K2—O8^{i}	56.20 (5)	P2—O6—K2^{xiii}	119.17 (9)
O6^{vi}—K2—O10^{iv}	106.24 (5)	Ni1^{iv}—O7—K1^{xi}	99.02 (6)
O6^{vi}—K2—O11^{x}	62.17 (5)	Ni1^{iv}—O7—K2^{iv}	104.50 (6)
O7^{i}—K2—P3^{x}	143.99 (4)	K1^{xi}—O7—K2^{iv}	89.74 (5)
O7^{i}—K2—P4	88.43 (3)	P1—O7—Ni1^{iv}	125.44 (10)
O7^{i}—K2—O4	69.44 (5)	P1—O7—K1^{xi}	116.54 (8)
O7^{i}—K2—O5	55.30 (4)	P1—O7—K2^{iv}	114.96 (9)
O7^{i}—K2—O8^{i}	65.62 (5)	Ni1^{xvi}—O8—K1^{xi}	90.84 (6)
O7^{i}—K2—O10^{iv}	127.26 (5)	Ni1^{xvi}—O8—K2^{iv}	90.02 (6)
O7^{i}—K2—O11^{x}	118.74 (5)	K1^{xi}—O8—K2^{iv}	84.52 (4)
O8^{i}—K2—P3^{x}	78.40 (3)	P4—O8—Ni1^{xvi}	145.38 (11)
O8^{i}—K2—P4	114.47 (3)	P4—O8—K1^{xi}	117.09 (9)
O8^{i}—K2—O4	118.08 (5)	P4—O8—K2^{iv}	111.44 (8)
O8^{i}—K2—O5	120.88 (4)	P3^{xi}—O9—K2^{i}	113.41 (8)
O8^{i}—K2—O10^{iv}	159.73 (5)	P3^{xi}—O9—P4	133.93 (11)
O8^{i}—K2—O11^{x}	53.12 (4)	P4—O9—K2^{i}	111.54 (8)
O9^{iv}—K2—P3^{x}	107.59 (4)	K1^{xv}—O10—K2	116.20 (6)
O9^{iv}—K2—P4	115.06 (4)	K1^{xv}—O10—K2^{i}	102.79 (5)
O9^{iv}—K2—O4	97.12 (5)	K2—O10—K2^{i}	108.77 (6)
O9^{iv}—K2—O5	60.22 (4)	P4—O10—K1^{xv}	118.04 (9)
O9^{iv}—K2—O6^{vi}	72.48 (5)	P4—O10—K2^{i}	94.57 (8)
O9^{iv}—K2—O7^{i}	92.51 (5)	P4—O10—K2	112.97 (9)
O9^{iv}—K2—O8^{i}	124.55 (5)	Ni1^{xiii}—O11—K1^{xii}	100.21 (6)
O9^{iv}—K2—O10^{iv}	47.05 (4)	Ni1^{xiii}—O11—K2^{xiv}	87.23 (6)
O9^{iv}—K2—O11^{x}	120.12 (5)	K1^{xii}—O11—K2^{xiv}	117.41 (6)
O9^{iv}—K2—O12^{x}	88.78 (5)	P3—O11—Ni1^{xiii}	137.44 (11)
O10^{iv}—K2—P3^{x}	87.07 (3)	P3—O11—K1^{xii}	120.26 (9)
O10—K2—P3^{x}	87.87 (4)	P3—O11—K2^{xiv}	85.46 (7)
O10^{iv}—K2—P4	83.39 (3)	K1—O12—K2^{xiv}	118.61 (6)
O10—K2—P4	22.17 (3)	P3—O12—K1	136.99 (11)
O10—K2—O4	47.91 (4)	P3—O12—K2^{xiv}	104.38 (9)
O10^{iv}—K2—O5	73.49 (4)		
K1^{xi}—P1—O1—P2	−175.17 (16)	O1—P2—O2—Ni1	−12.87 (16)

K1^{xi}—P1—O4—K2	−149.54 (7)	O1—P2—O2—K1^{i}	−112.96 (8)
K1^{xi}—P1—O4—P4	−20.6 (3)	O1—P2—O3—K1^{i}	119.13 (8)
K1^{xi}—P1—O5—Ni1	−159.81 (12)	O1—P2—O3—P3	−72.00 (17)
K1^{xi}—P1—O5—K2	97.2 (2)	O1—P2—O6—Ni1^{i}	−79.45 (13)
K1^{xi}—P1—O7—Ni1^{iv}	−124.79 (16)	O1—P2—O6—K1^{xii}	159.07 (8)
K1^{xi}—P1—O7—K2^{iv}	103.12 (10)	O1—P2—O6—K2^{xiii}	47.77 (11)
K1^{i}—P2—O1—P1	−59.95 (18)	O2—P2—O1—P1	−1.07 (19)
K1^{xii}—P2—O1—P1	159.50 (8)	O2—P2—O3—K1^{i}	2.53 (10)
K1^{xii}—P2—O2—Ni1	178.03 (11)	O2—P2—O3—P3	171.40 (15)
K1^{i}—P2—O2—Ni1	100.09 (14)	O2—P2—O6—Ni1^{i}	50.18 (16)
K1^{xii}—P2—O2—K1^{i}	77.94 (5)	O2—P2—O6—K1^{xii}	−71.30 (12)
K1^{xii}—P2—O3—K1^{i}	−95.65 (6)	O2—P2—O6—K2^{xiii}	177.41 (8)
K1^{i}—P2—O3—P3	168.9 (2)	O3—P2—O1—P1	−111.34 (16)
K1^{xii}—P2—O3—P3	73.22 (15)	O3—P2—O2—Ni1	97.66 (13)
K1^{xii}—P2—O6—Ni1^{i}	121.48 (15)	O3—P2—O2—K1^{i}	−2.43 (10)
K1^{i}—P2—O6—Ni1^{i}	115.61 (10)	O3—P2—O6—Ni1^{i}	169.07 (11)
K1^{i}—P2—O6—K1^{xii}	−5.87 (12)	O3—P2—O6—K1^{xii}	47.60 (11)
K1^{xii}—P2—O6—K2^{xiii}	−111.29 (12)	O3—P2—O6—K2^{xiii}	−63.70 (11)
K1^{i}—P2—O6—K2^{xiii}	−117.17 (7)	O3—P3—O11—Ni1^{xiii}	170.05 (14)
K1—P3—O3—K1^{i}	−63.59 (8)	O3—P3—O11—K1^{xii}	10.20 (12)
K1—P3—O3—P2	128.73 (15)	O3—P3—O11—K2^{xiv}	−109.04 (7)
K1—P3—O11—Ni1^{xiii}	−54.8 (2)	O3—P3—O12—K1	−72.92 (16)
K1—P3—O11—K1^{xii}	145.33 (7)	O3—P3—O12—K2^{xiv}	105.83 (9)
K1—P3—O11—K2^{xiv}	26.10 (12)	O4—P1—O1—P2	−95.24 (17)
K1—P3—O12—K2^{xiv}	178.75 (19)	O4—P1—O5—Ni1	90.47 (14)
K1^{xi}—P4—O4—K2	152.97 (5)	O4—P1—O5—K2	−12.48 (10)
K1^{xv}—P4—O4—K2	17.57 (12)	O4—P1—O7—Ni1^{iv}	−177.97 (11)
K1^{xv}—P4—O4—P1	−115.0 (2)	O4—P1—O7—K1^{xi}	−53.18 (12)
K1^{xi}—P4—O4—P1	20.4 (3)	O4—P1—O7—K2^{iv}	49.94 (12)
K1^{xi}—P4—O8—Ni1^{xvi}	140.4 (2)	O4—P4—O8—Ni1^{xvi}	−171.34 (17)
K1^{xv}—P4—O8—Ni1^{xvi}	−29.95 (18)	O4—P4—O8—K1^{xi}	48.30 (12)
K1^{xv}—P4—O8—K1^{xi}	−170.31 (8)	O4—P4—O8—K2^{iv}	−46.62 (12)
K1^{xi}—P4—O8—K2^{iv}	−94.92 (10)	O4—P4—O9—K2^{i}	101.62 (9)
K1^{xv}—P4—O8—K2^{iv}	94.78 (6)	O4—P4—O9—P3^{xi}	−65.16 (17)
K1^{xi}—P4—O9—K2^{i}	−179.35 (6)	O4—P4—O10—K1^{xv}	152.89 (10)
K1^{xv}—P4—O9—K2^{i}	−51.64 (8)	O4—P4—O10—K2	12.62 (13)
K1^{xv}—P4—O9—P3^{xi}	141.58 (13)	O4—P4—O10—K2^{i}	−99.99 (9)
K1^{xi}—P4—O9—P3^{xi}	13.87 (15)	O5—P1—O1—P2	16.13 (19)
K1^{xi}—P4—O10—K1^{xv}	45.8 (3)	O5—P1—O4—K2	13.82 (11)
K1^{xi}—P4—O10—K2^{i}	153.0 (2)	O5—P1—O4—P4	142.7 (3)
K1^{xv}—P4—O10—K2	−140.27 (15)	O5—P1—O7—Ni1^{iv}	61.21 (15)
K1^{xi}—P4—O10—K2	−94.4 (2)	O5—P1—O7—K1^{xi}	−174.00 (8)
K1^{xv}—P4—O10—K2^{i}	107.12 (10)	O5—P1—O7—K2^{iv}	−70.88 (11)
K2^{iv}—P1—O1—P2	174.58 (7)	O6—P2—O1—P1	133.43 (16)
K2^{iv}—P1—O4—K2	−83.38 (6)	O6—P2—O2—Ni1	−140.52 (12)
K2^{iv}—P1—O4—P4	45.5 (3)	O6—P2—O2—K1^{i}	119.39 (9)
K2^{iv}—P1—O5—Ni1	171.95 (10)	O6—P2—O3—K1^{i}	−126.86 (8)
K2^{iv}—P1—O5—K2	69.00 (5)	O6—P2—O3—P3	42.01 (19)

K2^{iv}—P1—O7—Ni1^{iv}	132.09 (15)	O7—P1—O1—P2	149.54 (15)
K2^{iv}—P1—O7—K1^{xi}	−103.12 (10)	O7—P1—O4—K2	−116.23 (9)
K2^{xiii}—P2—O1—P1	163.00 (16)	O7—P1—O4—P4	12.7 (3)
K2^{xiii}—P2—O2—Ni1	−135.19 (15)	O7—P1—O5—Ni1	−146.17 (12)
K2^{xiii}—P2—O2—K1^{i}	124.72 (18)	O7—P1—O5—K2	110.88 (9)
K2^{xiii}—P2—O3—K1^{i}	−162.76 (6)	O8—P4—O4—K2	121.90 (8)
K2^{xiii}—P2—O3—P3	6.11 (15)	O8—P4—O4—P1	−10.7 (3)
K2^{xiii}—P2—O6—Ni1^{i}	−127.23 (17)	O8—P4—O9—K2^{i}	−142.14 (9)
K2^{xiii}—P2—O6—K1^{xii}	111.29 (12)	O8—P4—O9—P3^{xi}	51.08 (18)
K2^{xiii}—P3—O3—K1^{i}	161.44 (8)	O8—P4—O10—K1^{xv}	27.62 (15)
K2^{xiv}—P3—O3—K1^{i}	18.10 (11)	O8—P4—O10—K2	−112.65 (11)
K2^{xiii}—P3—O3—P2	−6.24 (16)	O8—P4—O10—K2^{i}	134.73 (9)
K2^{xiv}—P3—O3—P2	−149.58 (13)	O9^{ix}—P3—O3—K1^{i}	−155.84 (9)
K2^{xiii}—P3—O11—Ni1^{xiii}	85.23 (15)	O9^{ix}—P3—O3—P2	36.48 (18)
K2^{xiv}—P3—O11—Ni1^{xiii}	−80.91 (15)	O9^{ix}—P3—O11—Ni1^{xiii}	63.04 (18)
K2^{xiii}—P3—O11—K1^{xii}	−74.63 (8)	O9^{ix}—P3—O11—K1^{xii}	−96.82 (10)
K2^{xiv}—P3—O11—K1^{xii}	119.23 (10)	O9^{ix}—P3—O11—K2^{xiv}	143.95 (7)
K2^{xiii}—P3—O11—K2^{xiv}	166.14 (5)	O9^{ix}—P3—O12—K1	37.38 (18)
K2^{xiii}—P3—O12—K1	62.0 (2)	O9^{ix}—P3—O12—K2^{xiv}	−143.87 (8)
K2^{xiv}—P3—O12—K1	−178.75 (19)	O9—P4—O4—K2	−120.65 (7)
K2^{xiii}—P3—O12—K2^{xiv}	−119.20 (14)	O9—P4—O4—P1	106.8 (3)
K2^{i}—P4—O4—K2	−74.83 (5)	O9—P4—O8—Ni1^{xvi}	77.6 (2)
K2—P4—O4—P1	−132.6 (3)	O9—P4—O8—K1^{xi}	−62.80 (11)
K2^{i}—P4—O4—P1	152.6 (3)	O9—P4—O8—K2^{iv}	−157.72 (8)
K2^{i}—P4—O8—Ni1^{xvi}	34.6 (3)	O9—P4—O10—K1^{xv}	−99.86 (11)
K2—P4—O8—Ni1^{xvi}	−101.76 (18)	O9—P4—O10—K2	119.87 (9)
K2—P4—O8—K1^{xi}	117.88 (7)	O9—P4—O10—K2^{i}	7.26 (9)
K2^{i}—P4—O8—K1^{xi}	−105.80 (10)	O10—P4—O4—K2	−10.01 (10)
K2—P4—O8—K2^{iv}	22.96 (11)	O10—P4—O4—P1	−142.6 (3)
K2^{i}—P4—O8—K2^{iv}	159.29 (5)	O10—P4—O8—Ni1^{xvi}	−47.6 (2)
K2—P4—O9—K2^{i}	37.22 (10)	O10—P4—O8—K1^{xi}	172.04 (9)
K2—P4—O9—P3^{xi}	−129.56 (12)	O10—P4—O8—K2^{iv}	77.12 (12)
K2^{i}—P4—O9—P3^{xi}	−166.8 (2)	O10—P4—O9—K2^{i}	−9.12 (11)
K2^{i}—P4—O10—K1^{xv}	−107.12 (10)	O10—P4—O9—P3^{xi}	−175.90 (14)
K2—P4—O10—K1^{xv}	140.27 (15)	O11—P3—O3—K1^{i}	92.39 (11)
K2—P4—O10—K2^{i}	−112.61 (10)	O11—P3—O3—P2	−75.29 (18)
K2^{i}—P4—O10—K2	112.61 (10)	O11—P3—O12—K1	164.75 (12)
O1—P1—O4—K2	130.66 (8)	O11—P3—O12—K2^{xiv}	−16.50 (12)
O1—P1—O4—P4	−100.4 (3)	O12—P3—O3—K1^{i}	−36.92 (13)
O1—P1—O5—Ni1	−19.87 (16)	O12—P3—O3—P2	155.39 (15)
O1—P1—O5—K2	−122.82 (8)	O12—P3—O11—Ni1^{xiii}	−67.17 (19)
O1—P1—O7—Ni1^{iv}	−67.44 (13)	O12—P3—O11—K1^{xii}	132.98 (10)
O1—P1—O7—K1^{xi}	57.35 (10)	O12—P3—O11—K2^{xiv}	13.74 (10)
O1—P1—O7—K2^{iv}	160.47 (8)		

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