

Supporting Information

Structural and Magnetic Investigations of the Novel Pyrophosphate $\text{Na}_7\text{Ni}_3\text{Fe}(\text{P}_2\text{O}_7)_4$

Sirine El Arni ¹, Mohammed Hadouchi ^{1,*}, Abderrazzak Assani ¹, Mohamed Saadi ¹, Mimoun El Marssi ², Abdelilah Lahmar ² and Lahcen El Ammari ¹

¹ Laboratoire de Chimie Appliquée des Matériaux, Centre des Sciences des Matériaux, Faculty of Science, Mohammed V University in Rabat, Avenue Ibn Battouta, BP 1014, Rabat, Morocco

² Laboratoire de Physique de la Matière Condensée, 33 Rue saint-Leu, 80033 Amiens, France

* Correspondence: m.hadouchi@um5r.ac.ma

Table S1. Crystal data, data collection and structure refinement for $\text{Na}_7\text{Ni}_3\text{Fe}(\text{P}_2\text{O}_7)_4$.

Crystal data

Chemical formula	$\text{Na}_7\text{Ni}_3\text{Fe}(\text{P}_2\text{O}_7)_4$
M_r (g/mol)	1088.67
Crystal system	Triclinic, $P\bar{1}$
T (K)	293
a, b, c (Å)	6.3677 (2), 9.3316 (4), 10.8478 (4)
α, β, γ (°)	65.191 (1), 80.533 (1), 73.042 (1)
V (Å ³)	559.00 (4)
Z	1
Radiation type	Mo $K\alpha$ ($\lambda=0.71073$ Å)
μ (mm ⁻¹)	3.97
Crystal size (mm)	0.30 x 0.15 x 0.14

Data collection

Diffractometer	Bruker D8 VENTURE Super DUO
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{\min}, T_{\max}	0.626, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	42169, 5143, 4998
R_{int}	0.027
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.820

Refinement

$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.026, 0.066, 1.09
No. of reflections	5143
No. of parameters	215
$\Delta_{\max}, \Delta_{\min}$ (e Å ⁻³)	2.38, -1.69

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (Å²) for Na₇Ni₃Fe(P₂O₇)₄ obtained by Single-Crystal X-ray Diffraction.

	Wyck.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}	Occ.	<i>BVS</i>
Fe1	2i	0.22223 (3)	0.61147 (2)	0.28234 (2)	0.00448 (5)	0.5	2.713 (4)
Ni1	2i	0.22223 (3)	0.61147 (2)	0.28234 (2)	0.00448 (5)	0.5	2.043 (3)
Ni2	2i	0.14175 (3)	0.26340 (2)	0.23645 (2)	0.00637 (5)	1	2.016 (3)
Na1	2i	0.2927 (2)	0.56726 (17)	0.59144 (14)	0.0397 (3)	1	0.994 (3)
Na2	1b	0.000000	0.000000	0.500000	0.0546 (7)	1	1.179 (2)
Na3	2i	0.52797 (13)	0.79372 (10)	0.02690 (9)	0.01583 (14)	1	1.099 (2)
Na4	2i	0.09325 (18)	0.01580 (13)	0.83235 (11)	0.0291 (2)	1	0.793 (2)
P1	2i	0.07773 (6)	0.65494 (4)	0.04535 (4)	0.00490 (6)	1	4.950 (9)
P2	2i	0.21340 (6)	0.27266 (4)	0.53391 (4)	0.00518 (6)	1	4.993 (10)
P3	2i	0.61900 (6)	0.35858 (5)	0.18618 (4)	0.00511 (6)	1	4.984 (10)
P4	2i	0.42506 (6)	-0.10553 (5)	0.28986 (4)	0.00584 (6)	1	4.910 (9)
O1	2i	-0.11617 (19)	0.71780 (16)	-0.04183 (12)	0.01057 (19)	1	1.967 (5)
O2	2i	0.05928 (19)	0.51600 (14)	0.18447 (11)	0.00767 (17)	1	1.871 (4)
O3	2i	0.28341 (19)	0.57847 (15)	-0.03157 (11)	0.00913 (18)	1	2.110 (5)
O4	2i	0.1385 (2)	0.78680 (15)	0.07123 (13)	0.01042 (19)	1	1.959 (6)
O5	2i	0.1134 (2)	0.23347 (15)	0.43815 (12)	0.01020 (19)	1	2.007 (6)
O6	2i	0.2885 (2)	0.42897 (15)	0.46155 (12)	0.0121 (2)	1	2.174 (5)
O7	2i	0.0658 (2)	0.27239 (16)	0.65837 (12)	0.0129 (2)	1	2.032 (5)
O8	2i	0.42623 (18)	0.12570 (14)	0.59182 (12)	0.00817 (17)	1	1.978 (5)
O9	2i	0.51786 (19)	0.51523 (15)	0.20739 (12)	0.00967 (18)	1	2.088 (6)
O10	2i	0.81476 (19)	0.25328 (15)	0.27411 (12)	0.01009 (19)	1	1.827 (4)
O11	2i	0.4611 (2)	0.26153 (15)	0.19464 (13)	0.0115 (2)	1	1.835 (6)
O12	2i	0.21158 (19)	0.01771 (14)	0.29969 (12)	0.00961 (18)	1	1.965 (4)
O13	2i	0.5511 (2)	-0.05351 (16)	0.15549 (12)	0.0127 (2)	1	1.957 (5)
O14	2i	0.3835 (2)	-0.27306 (15)	0.33606 (14)	0.0131 (2)	1	1.972 (6)

Table S3. Anisotropic atomic displacement parameters (Å²) for Na₇Ni₃Fe(P₂O₇)₄.

	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Fe1	0.00432 (8)	0.00490 (8)	0.00421 (8)	-0.00073 (6)	-0.00033 (5)	-0.00200 (6)
Ni1	0.00432 (8)	0.00490 (8)	0.00421 (8)	-0.00073 (6)	-0.00033 (5)	-0.00200 (6)

Ni2	0.00570 (8)	0.00671 (8)	0.00646 (8)	-0.00132 (6)	-0.00068 (5)	-0.00237 (6)
Na1	0.0416 (6)	0.0509 (7)	0.0422 (7)	0.0031 (5)	-0.0188 (5)	-0.0366 (6)
Na2	0.1007 (17)	0.0480 (10)	0.0445 (10)	-0.0621 (12)	0.0554 (11)	-0.0386 (9)
Na3	0.0102 (3)	0.0169 (3)	0.0186 (3)	-0.0027 (3)	0.0014 (2)	-0.0065 (3)
Na4	0.0272 (5)	0.0191 (4)	0.0269 (5)	-0.0046 (4)	-0.0018 (4)	0.0037 (3)
P1	0.00456 (13)	0.00553 (13)	0.00402 (13)	-0.00069 (10)	-0.00038 (10)	-0.00162 (11)
P2	0.00574 (13)	0.00533 (14)	0.00425 (13)	-0.00089 (11)	-0.00095 (10)	-0.00173 (11)
P3	0.00341 (13)	0.00659 (14)	0.00562 (13)	-0.00078 (10)	-0.00018 (10)	-0.00299 (11)
P4	0.00555 (14)	0.00555 (14)	0.00636 (14)	-0.00004 (11)	-0.00108 (10)	-0.00290 (11)
O1	0.0058 (4)	0.0162 (5)	0.0074 (4)	0.0009 (4)	-0.0021 (3)	-0.0043 (4)
O2	0.0096 (4)	0.0065 (4)	0.0054 (4)	-0.0022 (3)	0.0004 (3)	-0.0010 (3)
O3	0.0063 (4)	0.0119 (5)	0.0056 (4)	0.0016 (3)	0.0008 (3)	-0.0030 (3)
O4	0.0118 (5)	0.0092 (4)	0.0126 (5)	-0.0045 (4)	0.0011 (4)	-0.0058 (4)
O5	0.0135 (5)	0.0113 (5)	0.0077 (4)	-0.0047 (4)	-0.0037 (4)	-0.0033 (4)
O6	0.0185 (5)	0.0073 (4)	0.0097 (5)	-0.0061 (4)	-0.0052 (4)	0.0009 (4)
O7	0.0097 (5)	0.0168 (5)	0.0081 (4)	0.0013 (4)	0.0018 (4)	-0.0051 (4)
O8	0.0077 (4)	0.0075 (4)	0.0094 (4)	0.0013 (3)	-0.0036 (3)	-0.0044 (3)
O9	0.0078 (4)	0.0107 (5)	0.0126 (5)	-0.0005 (3)	0.0010 (3)	-0.0083 (4)
O10	0.0056 (4)	0.0132 (5)	0.0084 (4)	-0.0004 (4)	-0.0024 (3)	-0.0019 (4)
O11	0.0080 (4)	0.0109 (5)	0.0169 (5)	-0.0047 (4)	-0.0013 (4)	-0.0049 (4)
O12	0.0068 (4)	0.0075 (4)	0.0118 (5)	0.0012 (3)	-0.0007 (3)	-0.0031 (4)
O13	0.0126 (5)	0.0160 (5)	0.0073 (4)	-0.0016 (4)	0.0014 (4)	-0.0045 (4)
O14	0.0141 (5)	0.0083 (5)	0.0198 (6)	-0.0033 (4)	-0.0049 (4)	-0.0064 (4)

Table S4. Selected interatomic distances (Å) and angles (°) for Na₇Ni₃Fe(P₂O₇)₄.

Distances (Å)

(Fe(1)/Ni(1))O₆

Fe1/Ni1—O14 ⁱ	1.9811 (12)
Fe1/Ni1—O6	1.9825 (12)
Fe1/Ni1—O7 ⁱⁱ	1.9975 (12)
Fe1/Ni1—O9	2.0333 (12)
Fe1/Ni1—O2	2.1663 (12)
Fe1/Ni1—O4	2.2258 (13)

Ni(2)O₆

Ni2—O11	2.0061 (12)
Ni2—O12	2.0275 (12)
Ni2—O5	2.0699 (12)
Ni2—O1 ⁱⁱⁱ	2.0737 (12)
Ni2—O10 ^{iv}	2.0769 (12)
Ni2—O2	2.0999 (11)

P(1)O ₄		P(2)O ₄	
P1—O1	1.5030 (12)	P2—O7	1.5123 (13)
P1—O4	1.5316 (12)	P2—O5	1.5134 (12)
P1—O2	1.5365 (12)	P2—O6	1.5151 (12)
P1—O3	1.5861 (12)	P2—O8	1.6078 (12)
P(3)O ₄		P(4)O ₄	
P3—O11	1.5067 (12)	P4—O13	1.5010 (13)
P3—O9	1.5129 (12)	P4—O14	1.5183 (13)
P3—O10	1.5229 (12)	P4—O12	1.5248 (12)
P3—O3 ^{ix}	1.6085 (12)	P4—O8 ^{vi}	1.6348 (12)
Na(1)O ₇		Na(2)O ₆	
Na1—O6	2.2824 (16)	Na2—O5	2.2912 (12)
Na1—O9 ^v	2.3926 (16)	Na2—O5 ^{vii}	2.2912 (12)
Na1—O10 ^v	2.5402 (17)	Na2—O12	2.3302 (12)
Na1—O14 ⁱ	2.596 (2)	Na2—O12 ^{vii}	2.3302 (12)
Na1—O6 ^v	2.641 (2)	Na2—O10 ^{vi}	2.7288 (11)
Na1—O5 ⁱⁱ	2.6861 (18)	Na2—O10 ^{iv}	2.7288 (11)
Na1—O14 ^{vi}	2.7976 (18)		
Distortion (×10⁻⁴)	40.393		65.137
Na(3)O ₆		Na(4)O ₅	
Na3—O1 ^{viii}	2.2680 (14)	Na4—O7	2.3232 (16)
Na3—O13 ^{ix}	2.3739 (15)	Na4—O13 ^{vi}	2.4232 (18)
Na3—O13 ⁱ	2.4205 (16)	Na4—O4 ⁱⁱ	2.4875 (17)
Na3—O4	2.4621 (14)	Na4—O4 ^x	2.5698 (16)
Na3—O9	2.5253 (15)	Na4—O12 ^{vii}	2.7499 (17)
Na3—O11 ^{ix}	2.6476 (16)		
Distortion (×10⁻⁴)	23.521		32.990
Angles (°)			
O14 ⁱ —Fe1/Ni1—O6	87.29 (5)	O5—Ni2—O2	87.64 (5)
O14 ⁱ —Fe1/Ni1—O7 ⁱⁱ	91.51 (6)	O1 ⁱⁱⁱ —Ni2—O2	95.03 (5)
O6—Fe1/Ni1—O7 ⁱⁱ	96.42 (5)	O10 ^{iv} —Ni2—O2	92.53 (5)
O14 ⁱ —Fe1/Ni1—O9	86.15 (5)	O1—P1—O4	113.95 (7)

O6—Fe1/Ni1—O9	88.70 (5)	O1—P1—O2	115.61 (7)
O7 ⁱⁱ —Fe1/Ni1—O9	174.28 (5)	O4—P1—O2	107.01 (7)
O14 ⁱ —Fe1/Ni1—O2	169.08 (5)	O1—P1—O3	107.63 (7)
O6—Fe1/Ni1—O2	102.81 (5)	O4—P1—O3	107.33 (7)
O7 ⁱⁱ —Fe1/Ni1—O2	91.45 (5)	O2—P1—O3	104.63 (6)
O9—Fe1/Ni1—O2	89.91 (5)	O7—P2—O5	112.87 (7)
O14 ⁱ —Fe1/Ni1—O4	101.38 (5)	O7—P2—O6	112.00 (8)
O6—Fe1/Ni1—O4	170.79 (5)	O5—P2—O6	112.01 (7)
O7 ⁱⁱ —Fe1/Ni1—O4	86.53 (5)	O7—P2—O8	104.79 (7)
O9—Fe1/Ni1—O4	88.82 (5)	O5—P2—O8	106.71 (7)
O2—Fe1/Ni1—O4	68.31 (4)	O6—P2—O8	107.91 (7)
O11—Ni2—O12	91.43 (5)	O11—P3—O9	115.82 (7)
O11—Ni2—O5	100.22 (5)	O11—P3—O10	111.90 (7)
O12—Ni2—O5	88.64 (5)	O9—P3—O10	112.11 (7)
O11—Ni2—O1 ⁱⁱⁱ	89.78 (5)	O11—P3—O3 ^{ix}	106.80 (7)
O12—Ni2—O1 ⁱⁱⁱ	88.40 (5)	O9—P3—O3 ^{ix}	102.91 (7)
O5—Ni2—O1 ⁱⁱⁱ	169.64 (5)	O10—P3—O3 ^{ix}	106.28 (6)
O11—Ni2—O10 ^{iv}	176.03 (5)	O13—P4—O14	113.74 (8)
O12—Ni2—O10 ^{iv}	85.56 (5)	O13—P4—O12	114.61 (7)
O5—Ni2—O10 ^{iv}	82.32 (5)	O14—P4—O12	110.17 (7)
O1 ⁱⁱⁱ —Ni2—O10 ^{iv}	87.55 (5)	O13—P4—O8 ^{vi}	108.86 (7)
O11—Ni2—O2	90.63 (5)	O14—P4—O8 ^{vi}	103.74 (7)
O12—Ni2—O2	176.01 (5)	O12—P4—O8 ^{vi}	104.74 (6)
P1—O3—P3 ^{ix}	132.97 (8)	P2—O8—P4 ^{vi}	124.54 (7)

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

Table S5. Rietveld refined parameters of Na₇Ni₃Fe(P₂O₇)₄ powder.

Crystal data	
Chemical formula	Na ₇ Ni ₃ Fe(P ₂ O ₇) ₄
Crystal system, space group	Triclinic, P $\bar{1}$
a, b, c (Å)	6.3645 (2), 9.3342 (3), 10.8488 (4)
α, β, γ (°)	65.1546 (19), 80.522 (2), 73.1005 (19)
V (Å ³)	558.92 (3)

Z	1
Data collection	
Diffractometer	Shimadzu 6100
Temperature (K)	298
Radiation type	X-ray, Cu K α (λ = 1.5406 Å)
2 Θ values (°)	2 Θ_{\min} = 10.0, 2 Θ_{\max} = 100.0, 2 Θ_{step} = 0.02
Refinement	
No. data points	4501
No. of fitted parameters	148
Profile function	Pseudo-Voigt
Background	Linear interpolation
Rietveld R-factors	
R _p	9.285
R _{wp}	12.141
R _{exp}	10.074
R _F	3.274
R _B	4.686
Goodness of fit χ^2	1.453

Table S6. Atomic positions, isotropic displacement parameters for Na₇Ni₃Fe(P₂O₇)₄ obtained by Rietveld refinement.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} (Å ²)	Occ.
Fe1	0.2254 (9)	0.6118 (7)	0.2847 (6)	0.00025	0.5
Ni1	0.2254 (9)	0.6118 (7)	0.2847 (6)	0.00025	0.5
Ni2	0.1443 (9)	0.2626 (8)	0.2374 (6)	0.003 (2)	1
Na1	0.287 (3)	0.5667 (17)	0.6009 (15)	0.031 (6)	1
Na2	0.00000	0.00000	0.50000	0.057 (9)	1
Na3	0.530 (2)	0.7950 (15)	0.0284 (12)	0.004 (4)	1
Na4	0.088 (2)	0.0175 (15)	0.8379 (12)	0.00389	1
P1	0.0788 (16)	0.6626 (13)	0.0413 (11)	0.00541	1
P2	0.2153 (16)	0.2724 (12)	0.5320 (11)	0.00550	1

P3	0.6198 (17)	0.3571 (13)	0.1872 (12)	0.00549	1
P4	0.4300 (18)	-0.0992 (13)	0.2827 (11)	0.00794	1
O1	-0.118 (3)	0.722 (2)	-0.0374 (18)	0.00134	1
O2	0.046 (3)	0.539 (3)	0.183 (2)	0.00971	1
O3	0.277 (3)	0.582 (2)	-0.033 (2)	0.01156	1
O4	0.139 (3)	0.793 (2)	0.070 (2)	0.00132	1
O5	0.117 (3)	0.219 (2)	0.444 (2)	0.00129	1
O6	0.295 (3)	0.427 (2)	0.467 (2)	0.00153	1
O7	0.078 (3)	0.260 (2)	0.657 (2)	0.00163	1
O8	0.438 (3)	0.118 (2)	0.5907 (19)	0.00230	1
O9	0.524 (3)	0.514 (3)	0.203 (2)	0.00249	1
O10	0.827 (3)	0.236 (3)	0.277 (2)	0.00128	1
O11	0.470 (3)	0.242 (2)	0.1949 (19)	0.00146	1
O12	0.217 (3)	0.001 (2)	0.3057 (19)	0.00122	1
O13	0.567 (4)	-0.048 (3)	0.145 (2)	0.00161	1
O14	0.388 (3)	-0.254 (2)	0.333 (2)	0.00166	1

Table S7. Selected interatomic distances (Å) and angles (°) for Na₇Ni₃Fe(P₂O₇)₄ obtained by Rietveld refinement.

Distances (Å)			
(Fe(1)/Ni(1))O₆		Ni(2)O₆	
Fe1/Ni1—O14 ⁱⁱ	2.10 (3)	Ni2—O11	2.019 (19)
Fe1/Ni1—O6	2.015 (17)	Ni2—O12	2.159 (19)
Fe1/Ni1—O7 ⁱ	2.110 (19)	Ni2—O5	2.09 (2)
Fe1/Ni1—O9	2.08 (2)	Ni2—O1 ⁱⁱⁱ	2.14 (2)
Fe1/Ni1—O2	2.12 (3)	Ni2—O10 ^{iv}	2.06 (2)
Fe1/Ni1—O4	2.271 (18)	Ni2—O2	2.30 (3)
P(1)O₄		P(2)O₄	
P1—O1	1.47 (2)	P2—O7	1.47 (2)
P1—O4	1.53 (3)	P2—O5	1.53 (3)
P1—O2	1.51 (2)	P2—O6	1.51 (2)
P1—O3	1.56 (2)	P2—O8	1.682 (18)
P(3)O₄		P(4)O₄	

P3—O11	1.60 (3)	P4—O13	1.56 (2)
P3—O9	1.48 (3)	P4—O14	1.40 (2)
P3—O10	1.61 (2)	P4—O12	1.46 (2)
P3—O3 ^{ix}	1.62 (2)	P4—O8 ^{vi}	1.65 (3)
Na(1)O₇		Na(2)O₆	
Na1—O6	2.31 (3)	Na2—O5	2.19 (2)
Na1—O9 ^v	2.35 (3)	Na2—O5 ^{vii}	2.19 (2)
Na1—O10 ^v	2.57 (3)	Na2—O12	2.320 (19)
Na1—O14 ⁱⁱ	2.75 (2)	Na2—O12 ^{vii}	2.320 (19)
Na1—O6 ^v	2.65 (3)	Na2—O10 ^{vi}	2.628 (18)
Na1—O5 ⁱ	2.73 (2)	Na2—O10 ^{iv}	2.628 (18)
Na1—O14 ^{vi}	2.92 (2)		
Na(3)O₆		Na(4)O₅	
Na3—O1 ^{viii}	2.23 (2)	Na4—O7	2.281 (19)
Na3—O13 ^{ix}	2.30 (2)	Na4—O13 ^{vi}	2.34 (3)
Na3—O13 ⁱⁱ	2.38 (4)	Na4—O4 ⁱ	2.40 (2)
Na3—O4	2.46 (2)	Na4—O4 ^x	2.505 (19)
Na3—O9	2.52 (2)	Na4—O12 ^{vii}	2.76 (3)
Na3—O11 ^{ix}	2.59 (3)		
Angles (°)			
O14 ⁱⁱ —Fe1/Ni1—O6	89.8 (13)	O5—Ni2—O2	90.0 (13)
O14 ⁱⁱ —Fe1/Ni1—O7 ⁱ	89.7 (14)	O1 ⁱⁱⁱ —Ni2—O2	95.03 (5)
O6—Fe1/Ni1—O7 ⁱ	98.0 (11)	O10 ^{iv} —Ni2—O2	95.1 (18)
O14 ⁱⁱ —Fe1/Ni1—O9	88.4 (17)	O1—P1—O4	115 (3)
O6—Fe1/Ni1—O9	89.6 (13)	O1—P1—O2	112 (2)
O7 ⁱ —Fe1/Ni1—O9	172.2 (16)	O4—P1—O2	102 (2)
O14 ⁱⁱ —Fe1/Ni1—O2	163 (2)	O1—P1—O3	109.4 (19)
O6—Fe1/Ni1—O2	107.0 (17)	O4—P1—O3	110 (2)
O7 ⁱ —Fe1/Ni1—O2	87.8 (17)	O2—P1—O3	109 (2)
O9—Fe1/Ni1—O2	91.9 (15)	O7—P2—O5	110 (3)
O14 ⁱⁱ —Fe1/Ni1—O4	98.0 (16)	O7—P2—O6	113 (2)
O6—Fe1/Ni1—O4	171.7 (14)	O5—P2—O6	120 (3)
O7 ⁱ —Fe1/Ni1—O4	84.8 (12)	O7—P2—O8	102.1 (18)

O9—Fe1/Ni1—O4	87.9 (11)	O5—P2—O8	103 (2)
O2—Fe1/Ni1—O4	65.2 (13)	O6—P2—O8	106.6 (16)
O11—Ni2—O12	87.1 (13)	O11—P3—O9	122 (3)
O11—Ni2—O5	102.0 (14)	O11—P3—O10	105 (2)
O12—Ni2—O5	85.3 (14)	O9—P3—O10	117 (2)
O11—Ni2—O1 ⁱⁱⁱ	88.1 (14)	O11—P3—O3 ^{ix}	105.5 (19)
O12—Ni2—O1 ⁱⁱⁱ	87.7 (11)	O9—P3—O3 ^{ix}	101 (2)
O5—Ni2—O1 ⁱⁱⁱ	167.4 (18)	O10—P3—O3 ^{ix}	104.1 (18)
O11—Ni2—O10 ^{iv}	167.6 (17)	O13—P4—O14	117 (2)
O12—Ni2—O10 ^{iv}	81.5 (12)	O13—P4—O12	123 (2)
O5—Ni2—O10 ^{iv}	82.0 (15)	O14—P4—O12	102 (2)
O1 ⁱⁱⁱ —Ni2—O10 ^{iv}	86.6 (13)	O13—P4—O8 ^{vi}	112 (2)
O11—Ni2—O2	96.6 (14)	O14—P4—O8 ^{vi}	100 (2)

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