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Tris(1,10-phenanthroline-κ^2N,N')nickel(II) bis(hexafluoridophosphate)

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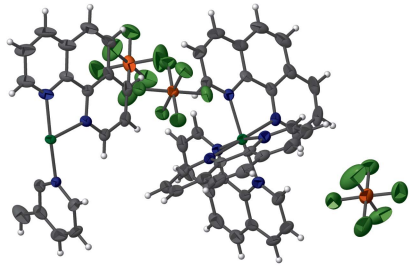
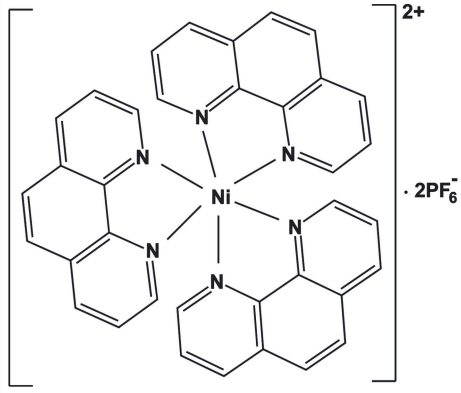
The asymmetric unit of the title compound, $[Ni(C_{36}H_{24}N_6)_3](PF_6)_2$, contains one and a half nickel(II) complex dications and three hexafluoridophosphate anions, one of the dications having crystallographic twofold rotational symmetry. Each Ni^{II} atom displays a distorted octahedral coordination geometry provided by the six N atoms of three bidentate 1,10-phenanthroline ligands with bite angles of 79.68 (11)–80.76 (12)°. In the crystal, C—H···F hydrogen bonds link the anions and dications into a three-dimensional supramolecular framework. Within the framework complex dications with twofold rotational symmetry are linked by weak π–π stacking interactions [centroid-to-centroid distances = 3.712 (2) Å].

3D view



Chemical scheme



Structure description

Cationic complexes of general formula $[M(L)_3]^{n+}$ (where L is a chelate ligand such as 1,10-phenanthroline, bipyridine and their derivatives) are important agents for developing novel diagnostic and therapeutic compounds that can recognize and cleave DNA (Zaworotko *et al.*, 2007; Zelenko *et al.*, 1997; Naing *et al.*, 1995; Barton, 1986; Liu *et al.*, 2004; Sammes & Yahioglu, 1994; Sigman *et al.*, 1979), and show the ability to form outer-sphere complexes with anions, neutral molecules or a combination of them (Zaworotko *et al.*, 2007; Johansson, 1976). Herein, the synthesis and crystal structure of tris(1,10-phenanthroline-κ^2N,N')nickel(II) bis(hexafluoridophosphate) are reported. The crystal structure of the hemihydrate of the title compound has been reported at least twice (Brewer *et al.*, 2003; Bouzaid *et al.*, 2012).

The bond lengths and angles in the title complex are very similar to those reported for the hemihydrate form (Brewer *et al.*, 2003; Bouzaid *et al.*, 2012). The asymmetric unit of the title compound is illustrated in Fig. 1. It consists of one and a half nickel(II) complex

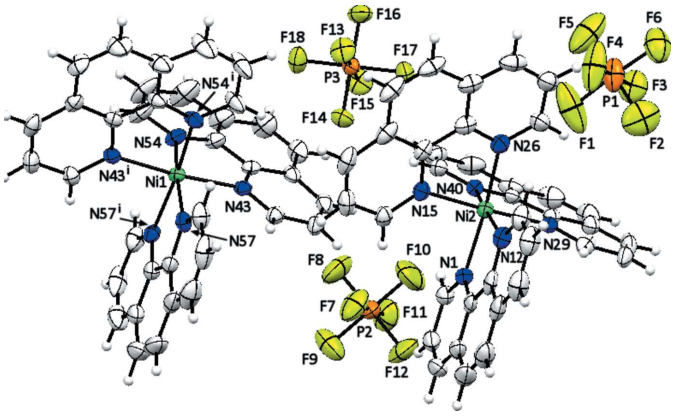


Figure 1
The expanded asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level. C-atom labels have been omitted for clarity. [Symmetry code: (i) $1-x, y, \frac{3}{2}-z$.]

dications and three anions. One dication has crystallographic imposed twofold rotational symmetry, the twofold axis passing through the Ni1 atom and bisecting the C62—C62^{i} and C63—C63^{i} bonds [symmetry code: (i) $1-x, y, \frac{3}{2}-z$]. Both nickel(II) cations are coordinated in a distorted octahedral geometry by six N atoms from three 1,10-phenanthroline ligands. The Ni—N bond lengths are similar and fall in a narrow range [2.077 (3)–2.108 (3) Å; mean value 2.091 (4) Å]. The 1,10-phenanthroline ligands adopt the expected chelating coordination mode with chelating angles in the range 79.68 (11)–80.76 (12)°. The P—F bond lengths in the hexafluoridophosphate anions are unexceptional, and range from 1.559 (5) to 1.606 (2) Å (mean value 1.593 Å).

In the crystal, C—H···F hydrogen bonds link the anions and dications into a three-dimensional framework (Table 1 and Fig. 2). Within the framework, inversion-related six-membered rings of 1,10-phenanthroline ligands belonging to complex dications with twofold rotational symmetry are connected through π–π stacking interactions [$Cg\cdots Cg^{i}$ = 3.712 Å; Cg is the centroid of the N57/C58–C63 ring; symmetry code: (i) $1-x, 1-y, 2-z$].

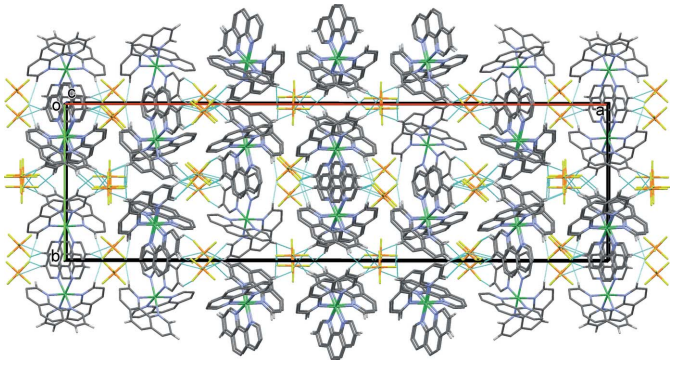


Figure 2
A view along the c axis of the crystal packing of the title compound. The hydrogen bonds (Table 1) are shown as dashed lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H91···F6^{i}	0.93	2.53	3.385 (6)	152
C10—H101···F2^{i}	0.94	2.43	3.226 (6)	143
C16—H161···F12^{ii}	0.95	2.36	3.126 (5)	137
C20—H201···F16^{iii}	0.94	2.46	3.385 (5)	171
C24—H241···F4^{iv}	0.93	2.42	3.271 (6)	152
C25—H251···F5^{iv}	0.94	2.50	3.266 (6)	139
C44—H441···F9^{ii}	0.95	2.50	3.173 (5)	129
C51—H511···F18^{v}	0.94	2.41	3.253 (6)	149
C52—H521···F13^{vi}	0.94	2.48	3.209 (6)	134
C59—H591···F9^{vii}	0.94	2.50	3.417 (6)	167

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $x, -y, z+\frac{1}{2}$; (iv) $x, -y, z-\frac{1}{2}$; (v) $-x+1, -y, -z+1$; (vi) $-x+1, y, -z+\frac{3}{2}$; (vii) $x, y, z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{12}H_8N_2)_3](PF_6P)_2$
M_r	889.26
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	180
a, b, c (Å)	55.058 (8), 15.8074 (9), 12.0688 (7)
β (°)	95.088 (9)
V (Å^3)	10462.4 (17)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.75
Crystal size (mm)	0.30 × 0.15 × 0.15
Data collection	
Diffractometer	Oxford Diffraction Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min}, T_{max}	0.76, 0.89
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	174626, 13212, 8649
R_{int}	0.105
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.683
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.071, 0.063, 1.11
No. of reflections	8015
No. of parameters	771
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, −0.56

Computer programs: *Gemini* (Oxford Diffraction, 2006), *CrysAlis PRO* (Agilent, 2011), *SUPERFLIP* (Palatinus & Chapuis, 2007), *CRYSTALS* (Betteridge *et al.*, 2003) and *CAMERON* (Watkin *et al.*, 1996). Weighting scheme: Prince (1982); Watkin (1994).

Synthesis and crystallization

1,10-Phenanthroline hydrochloride (3 mmol, 0.702 g) and potassium hexafluoridophosphate (2 mmol, 0.368 g) were dissolved separately in 10 ml of ethanol, and $NiCl_2$ (1 mmol, 0,125 g) was dissolved in 5 ml of water. The 1,10-phenanthroline hydrochloride solution was added dropwise to the metal salt solution while stirring at room temperature. The potassium hexafluoridophosphate solution was then added dropwise to the reaction mixture while stirring at room temperature. The solution was kept at room temperature to evaporate slowly. After two months, crystals suitable for X-ray analysis were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
Barton, J. K. (1986). *Science*, **233**, 727–734.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Bouzaid, J., Schultz, M., Lao, Z., Bartley, J., Bostrom, T. & McMurtrie, J. (2012). *Cryst. Growth Des.* **12**, 3906–3916.
Brewer, B., Brooks, N. R., Abdul-Halim, S. & Sykes, A. G. (2003). *J. Chem. Crystallogr.* **33**, 651–662.
Johansson, L. (1976). *Chem. Scr.* **10**, 72.
Liu, F., Wang, K., Bai, G., Zhang, Y. & Gao, L. (2004). *Inorg. Chem.* **43**, 1799–1806.
Naing, K., Takahashi, M., Taniguchi, M. & Yamagishi, A. (1995). *Inorg. Chem.* **34**, 350–356.
Oxford Diffraction (2006). *Gemini User Manual*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Prince, E. (1982). in *Mathematical Techniques in Crystallography and Materials Science*. New York: Springer-Verlag.
Sammes, P. G. & Yahioglu, G. (1994). *Chem. Soc. Rev.* **23**, 327–334.
Sigman, D. S., Graham, D. R., D'Aurora, V. & Stern, A. M. (1979). *J. Biol. Chem.* **254**, 12269–12272.
Watkin, D. (1994). *Acta Cryst.* A**50**, 411–437.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, Oxford, England.
Zaworotko, M. J., Hammud, H. H. & Kravtsov, V. Ch. (2007). *J. Chem. Crystallogr.* **37**, 219–231.
Zelenko, O., Gallagher, J. & Sigman, D. S. (1997). *Angew. Chem. Int. Ed. Engl.* **36**, 2776–2778.

full crystallographic data

IUCrData (2018). **3**, x180709 [https://doi.org/10.1107/S2414314618007095]

Tris(1,10-phenanthroline-κ^2N,N')nickel(II) bis(hexafluoridophosphate)

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Tris(1,10-phenanthroline-κ^2N,N')nickel(II) bis(hexafluoridophosphate)

Crystal data

$[Ni(C_{12}H_8N_2)_3](PF_6P)_2$
M_r = 889.26
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 55.058 (8) Å
b = 15.8074 (9) Å
c = 12.0688 (7) Å
β = 95.088 (9)°
V = 10462.4 (17) Å^3
Z = 12
F(000) = 5376
D_x = 1.694 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 13382 reflections
θ = 3–25°
μ = 0.75 mm^{-1}
T = 180 K
Rod, colourless
0.30 × 0.15 × 0.15 mm

Data collection

Oxford Diffraction Gemini diffractometer
Graphite monochromator
φ & ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2011)
T_{min} = 0.76, T_{max} = 0.89
174626 measured reflections
13212 independent reflections
8649 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.105
θ_{max} = 29.0°, θ_{min} = 2.9°
h = −74→73
k = −21→21
l = −16→16

Refinement

Refinement on *F*
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.063
S = 1.11
8015 reflections
771 parameters
0 restraints
Primary atom site location: other
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
Method, part 1, Chebychev polynomial (Watkin, 1994; *P*rince, 1982) *w*ith the coefficients 18.5, 18.7, 17.2, 6.67
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1 K.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.28702 (4)	0.7500	0.0225
Ni2	0.335001 (8)	0.26714 (3)	0.58164 (3)	0.0256
C2	0.35684 (7)	0.4148 (2)	0.4524 (3)	0.0340
C3	0.36127 (7)	0.4999 (3)	0.4323 (4)	0.0436
C4	0.35140 (8)	0.5601 (3)	0.4966 (4)	0.0470
C5	0.33704 (7)	0.5355 (2)	0.5815 (4)	0.0401
C6	0.32584 (9)	0.5945 (3)	0.6538 (5)	0.0580
C7	0.31233 (8)	0.5660 (3)	0.7344 (5)	0.0569
C8	0.30842 (7)	0.4789 (3)	0.7512 (4)	0.0442
C9	0.29420 (8)	0.4457 (3)	0.8335 (4)	0.0508
C10	0.29149 (8)	0.3615 (3)	0.8442 (4)	0.0508
C11	0.30293 (7)	0.3074 (3)	0.7732 (3)	0.0441
C13	0.31907 (6)	0.4199 (3)	0.6826 (3)	0.0360
C14	0.33340 (6)	0.4484 (2)	0.5959 (3)	0.0317
C16	0.38217 (6)	0.3227 (2)	0.7271 (3)	0.0342
C17	0.39874 (7)	0.3189 (3)	0.8206 (4)	0.0446
C18	0.39795 (7)	0.2522 (3)	0.8933 (4)	0.0466
C19	0.37986 (7)	0.1890 (3)	0.8712 (3)	0.0413
C20	0.37686 (9)	0.1177 (3)	0.9420 (3)	0.0508
C21	0.35819 (9)	0.0636 (3)	0.9215 (3)	0.0483
C22	0.34057 (7)	0.0734 (2)	0.8269 (3)	0.0388
C23	0.32040 (9)	0.0215 (3)	0.8037 (4)	0.0494
C24	0.30482 (8)	0.0351 (3)	0.7091 (4)	0.0467
C25	0.30947 (7)	0.1018 (2)	0.6396 (4)	0.0396
C27	0.34385 (7)	0.1399 (2)	0.7524 (3)	0.0318
C28	0.36362 (6)	0.1988 (2)	0.7752 (3)	0.0302
C30	0.28248 (7)	0.2968 (3)	0.4666 (3)	0.0398
C31	0.26463 (7)	0.2946 (3)	0.3759 (4)	0.0503
C32	0.26997 (8)	0.2581 (3)	0.2784 (4)	0.0505
C33	0.29363 (7)	0.2256 (2)	0.2685 (3)	0.0405
C34	0.30145 (10)	0.1915 (3)	0.1673 (4)	0.0528
C35	0.32438 (10)	0.1635 (3)	0.1615 (4)	0.0502
C36	0.34196 (8)	0.1669 (2)	0.2572 (3)	0.0398
C37	0.36599 (9)	0.1341 (3)	0.2595 (4)	0.0461
C38	0.38097 (7)	0.1374 (2)	0.3562 (3)	0.0398
C39	0.37276 (7)	0.1760 (2)	0.4500 (3)	0.0325
C41	0.33495 (7)	0.2013 (2)	0.3571 (3)	0.0294
C42	0.31047 (6)	0.2314 (2)	0.3624 (3)	0.0313
C44	0.44804 (6)	0.3264 (2)	0.6375 (3)	0.0303
C45	0.42959 (7)	0.3218 (3)	0.5502 (3)	0.0384
C46	0.43194 (7)	0.2672 (3)	0.4646 (3)	0.0369
C47	0.45302 (6)	0.2177 (2)	0.4638 (3)	0.0299
C48	0.45713 (8)	0.1594 (3)	0.3752 (3)	0.0409
C49	0.47815 (9)	0.1160 (3)	0.3771 (4)	0.0534
C50	0.49742 (9)	0.1271 (3)	0.4647 (3)	0.0468

C51	0.52012 (10)	0.0859 (3)	0.4673 (4)	0.0639
C52	0.53742 (10)	0.1013 (3)	0.5540 (4)	0.0605
C53	0.53241 (8)	0.1582 (3)	0.6377 (3)	0.0453
C55	0.49376 (7)	0.1827 (2)	0.5520 (3)	0.0318
C56	0.47110 (6)	0.2271 (2)	0.5517 (3)	0.0268
C58	0.47251 (7)	0.3882 (3)	0.9230 (3)	0.0437
C59	0.46412 (8)	0.4631 (4)	0.9695 (4)	0.0575
C60	0.47035 (9)	0.5380 (4)	0.9277 (5)	0.0623
C61	0.48501 (8)	0.5421 (3)	0.8395 (4)	0.0472
C62	0.49283 (9)	0.6192 (3)	0.7922 (5)	0.0636
C63	0.49248 (6)	0.4643 (2)	0.7966 (3)	0.0334
N1	0.34328 (5)	0.38920 (18)	0.5323 (2)	0.0286
N12	0.31617 (6)	0.3355 (2)	0.6940 (3)	0.0350
N15	0.36507 (5)	0.26401 (19)	0.7026 (2)	0.0298
N26	0.32829 (5)	0.1537 (2)	0.6601 (3)	0.0330
N29	0.30495 (5)	0.26429 (18)	0.4606 (2)	0.0287
N40	0.35058 (5)	0.20718 (17)	0.4516 (2)	0.0265
N43	0.46863 (5)	0.28123 (17)	0.6385 (2)	0.0256
N54	0.51094 (6)	0.19813 (19)	0.6374 (2)	0.0328
N57	0.48651 (5)	0.38841 (19)	0.8375 (2)	0.0293
F1	0.27673 (8)	0.1148 (4)	0.9191 (3)	0.1264
F2	0.23623 (8)	0.1238 (3)	0.9320 (3)	0.0994
F3	0.25131 (6)	0.0441 (2)	0.8016 (2)	0.0695
F4	0.25927 (6)	0.0566 (4)	1.0635 (3)	0.1113
F5	0.27424 (8)	−0.0263 (4)	0.9308 (4)	0.1228
F6	0.23327 (6)	−0.0145 (3)	0.9432 (3)	0.0852
F7	0.41325 (6)	0.4319 (3)	0.3368 (3)	0.0777
F8	0.43308 (6)	0.3495 (2)	0.2241 (3)	0.0839
F9	0.43158 (7)	0.4876 (2)	0.1956 (3)	0.0841
F10	0.39201 (7)	0.3460 (3)	0.2180 (5)	0.1143
F11	0.41023 (6)	0.4020 (2)	0.0740 (3)	0.0743
F12	0.39042 (6)	0.4841 (2)	0.1897 (3)	0.0765
F13	0.41694 (5)	0.02840 (17)	0.79123 (19)	0.0506
F14	0.41810 (4)	0.13614 (14)	0.6696 (2)	0.0425
F15	0.42032 (5)	0.04235 (17)	0.53008 (19)	0.0509
F16	0.41912 (5)	−0.06609 (15)	0.6520 (2)	0.0530
F17	0.38947 (4)	0.03366 (15)	0.6404 (2)	0.0438
F18	0.44786 (4)	0.03646 (17)	0.6804 (2)	0.0506
P1	0.25548 (2)	0.04758 (11)	0.93193 (10)	0.0602
P2	0.411657 (19)	0.41582 (7)	0.20514 (10)	0.0426
P3	0.418689 (17)	0.03522 (6)	0.66055 (7)	0.0290
H21	0.3637	0.3732	0.4096	0.0425*
H31	0.3709	0.5158	0.3758	0.0554*
H41	0.3541	0.6181	0.4845	0.0571*
H61	0.3281	0.6521	0.6441	0.0804*
H71	0.3051	0.6055	0.7796	0.0782*
H91	0.2865	0.4826	0.8797	0.0673*
H101	0.2823	0.3392	0.8993	0.0725*

H111	0.3011	0.2486	0.7810	0.0561*
H161	0.3831	0.3687	0.6776	0.0513*
H171	0.4102	0.3621	0.8352	0.0561*
H181	0.4094	0.2473	0.9552	0.0571*
H201	0.3881	0.1089	1.0038	0.0604*
H211	0.3565	0.0183	0.9702	0.0603*
H231	0.3178	−0.0240	0.8520	0.0605*
H241	0.2911	0.0012	0.6923	0.0594*
H251	0.2988	0.1110	0.5755	0.0502*
H301	0.2789	0.3223	0.5338	0.0515*
H311	0.2493	0.3181	0.3817	0.0623*
H321	0.2580	0.2535	0.2182	0.0592*
H341	0.2899	0.1874	0.1052	0.0690*
H351	0.3289	0.1420	0.0935	0.0633*
H371	0.3714	0.1106	0.1950	0.0584*
H381	0.3966	0.1145	0.3594	0.0505*
H391	0.3833	0.1802	0.5149	0.0402*
H441	0.4459	0.3624	0.6984	0.0363*
H451	0.4158	0.3563	0.5516	0.0454*
H461	0.4196	0.2636	0.4065	0.0441*
H481	0.4450	0.1508	0.3166	0.0531*
H491	0.4804	0.0782	0.3196	0.0652*
H511	0.5233	0.0475	0.4106	0.0761*
H521	0.5528	0.0759	0.5565	0.0701*
H531	0.5441	0.1673	0.6978	0.0612*
H581	0.4684	0.3351	0.9510	0.0593*
H591	0.4544	0.4602	1.0293	0.0762*
H601	0.4648	0.5881	0.9585	0.0804*
H621	0.4884	0.6716	0.8221	0.0803*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0293 (3)	0.0199 (3)	0.0181 (3)	0.0000	0.0016 (2)	0.0000
Ni2	0.0252 (2)	0.0287 (2)	0.0231 (2)	−0.00003 (17)	0.00271 (16)	0.00161 (16)
C2	0.0325 (18)	0.034 (2)	0.0347 (19)	−0.0019 (15)	−0.0002 (15)	0.0009 (15)
C3	0.0311 (19)	0.047 (2)	0.051 (2)	−0.0088 (17)	−0.0065 (17)	0.0110 (19)
C4	0.045 (2)	0.0289 (19)	0.064 (3)	−0.0077 (17)	−0.014 (2)	0.0034 (18)
C5	0.0298 (18)	0.0312 (18)	0.056 (2)	0.0010 (16)	−0.0116 (17)	−0.0058 (18)
C6	0.046 (2)	0.038 (2)	0.087 (4)	0.0071 (19)	−0.011 (2)	−0.020 (2)
C7	0.039 (2)	0.055 (3)	0.074 (3)	0.009 (2)	−0.006 (2)	−0.027 (2)
C8	0.0262 (18)	0.058 (3)	0.046 (2)	0.0092 (17)	−0.0100 (16)	−0.0224 (19)
C9	0.036 (2)	0.079 (3)	0.038 (2)	0.010 (2)	0.0066 (18)	−0.026 (2)
C10	0.036 (2)	0.078 (3)	0.039 (2)	0.005 (2)	0.0090 (18)	−0.010 (2)
C11	0.033 (2)	0.062 (3)	0.038 (2)	0.0031 (18)	0.0076 (17)	−0.0010 (18)
C13	0.0210 (16)	0.055 (2)	0.0300 (18)	0.0057 (15)	−0.0080 (14)	−0.0121 (16)
C14	0.0199 (15)	0.0365 (18)	0.0365 (19)	0.0014 (13)	−0.0099 (14)	−0.0079 (15)
C16	0.0272 (17)	0.0363 (19)	0.039 (2)	0.0031 (14)	0.0045 (15)	−0.0058 (15)

C17	0.0303 (19)	0.060 (3)	0.043 (2)	−0.0023 (18)	−0.0017 (17)	−0.0157 (19)
C18	0.0331 (19)	0.069 (3)	0.036 (2)	0.0152 (19)	−0.0058 (16)	−0.0176 (19)
C19	0.039 (2)	0.054 (2)	0.0315 (19)	0.0184 (18)	0.0041 (16)	−0.0003 (17)
C20	0.050 (2)	0.073 (3)	0.030 (2)	0.029 (2)	0.0047 (18)	0.0082 (19)
C21	0.059 (3)	0.052 (3)	0.035 (2)	0.023 (2)	0.012 (2)	0.0153 (18)
C22	0.048 (2)	0.037 (2)	0.0338 (19)	0.0126 (17)	0.0156 (17)	0.0048 (15)
C23	0.058 (3)	0.033 (2)	0.062 (3)	0.0076 (19)	0.031 (2)	0.0113 (19)
C24	0.042 (2)	0.035 (2)	0.066 (3)	0.0005 (17)	0.017 (2)	0.0022 (19)
C25	0.038 (2)	0.0309 (19)	0.050 (2)	−0.0028 (15)	0.0037 (18)	−0.0021 (16)
C27	0.0349 (18)	0.0332 (18)	0.0293 (17)	0.0076 (14)	0.0145 (14)	0.0000 (14)
C28	0.0290 (17)	0.039 (2)	0.0226 (16)	0.0080 (14)	0.0027 (13)	−0.0017 (14)
C30	0.0307 (18)	0.046 (2)	0.044 (2)	0.0018 (16)	0.0090 (16)	0.0170 (17)
C31	0.0216 (17)	0.064 (3)	0.065 (3)	−0.0012 (17)	0.0002 (18)	0.026 (2)
C32	0.036 (2)	0.059 (3)	0.052 (3)	−0.0152 (19)	−0.0194 (19)	0.016 (2)
C33	0.042 (2)	0.035 (2)	0.042 (2)	−0.0069 (16)	−0.0113 (17)	0.0057 (16)
C34	0.069 (3)	0.047 (2)	0.038 (2)	−0.012 (2)	−0.016 (2)	−0.0018 (18)
C35	0.077 (3)	0.041 (2)	0.031 (2)	−0.002 (2)	−0.001 (2)	−0.0073 (17)
C36	0.061 (3)	0.0271 (18)	0.0315 (19)	−0.0017 (17)	0.0056 (18)	−0.0027 (14)
C37	0.068 (3)	0.032 (2)	0.040 (2)	0.0089 (19)	0.015 (2)	−0.0072 (16)
C38	0.039 (2)	0.034 (2)	0.048 (2)	0.0083 (16)	0.0120 (18)	0.0018 (16)
C39	0.0301 (18)	0.0254 (17)	0.042 (2)	−0.0002 (13)	0.0032 (15)	0.0009 (14)
C41	0.0374 (18)	0.0167 (15)	0.0333 (17)	−0.0021 (13)	−0.0010 (14)	−0.0016 (12)
C42	0.0343 (18)	0.0237 (16)	0.0343 (18)	−0.0050 (14)	−0.0061 (14)	0.0073 (14)
C44	0.0270 (17)	0.0326 (18)	0.0316 (18)	0.0017 (13)	0.0041 (14)	0.0028 (14)
C45	0.0244 (18)	0.048 (2)	0.043 (2)	0.0009 (15)	0.0021 (16)	0.0085 (17)
C46	0.0299 (17)	0.043 (2)	0.038 (2)	−0.0122 (16)	−0.0022 (15)	0.0128 (16)
C47	0.0325 (17)	0.0290 (18)	0.0270 (16)	−0.0088 (14)	−0.0041 (14)	0.0078 (13)
C48	0.049 (2)	0.048 (2)	0.0238 (18)	−0.0070 (18)	−0.0090 (16)	−0.0031 (15)
C49	0.066 (3)	0.053 (3)	0.039 (2)	0.005 (2)	−0.007 (2)	−0.0198 (19)
C50	0.063 (3)	0.041 (2)	0.034 (2)	0.0134 (19)	−0.0036 (19)	−0.0102 (17)
C51	0.083 (4)	0.066 (3)	0.039 (2)	0.037 (3)	−0.011 (2)	−0.025 (2)
C52	0.067 (3)	0.067 (3)	0.046 (3)	0.045 (3)	−0.006 (2)	−0.015 (2)
C53	0.054 (3)	0.045 (2)	0.034 (2)	0.0253 (19)	−0.0130 (18)	−0.0061 (17)
C55	0.042 (2)	0.0263 (17)	0.0255 (17)	0.0073 (14)	−0.0033 (15)	−0.0013 (13)
C56	0.0321 (17)	0.0219 (16)	0.0265 (16)	0.0001 (13)	0.0035 (13)	0.0058 (12)
C58	0.0308 (19)	0.063 (3)	0.038 (2)	−0.0032 (18)	0.0089 (16)	−0.0095 (19)
C59	0.028 (2)	0.105 (4)	0.041 (2)	0.007 (2)	0.0085 (18)	−0.029 (3)
C60	0.045 (3)	0.074 (4)	0.066 (3)	0.020 (2)	−0.004 (2)	−0.032 (3)
C61	0.034 (2)	0.042 (2)	0.062 (3)	0.0089 (17)	−0.0152 (19)	−0.016 (2)
C62	0.064 (3)	0.030 (2)	0.091 (4)	0.0090 (19)	−0.027 (3)	−0.006 (2)
C63	0.0248 (16)	0.0336 (19)	0.041 (2)	0.0025 (14)	−0.0038 (15)	−0.0050 (15)
N1	0.0286 (14)	0.0260 (14)	0.0311 (15)	0.0006 (11)	0.0023 (12)	0.0001 (11)
N12	0.0323 (16)	0.0427 (19)	0.0297 (16)	0.0035 (13)	0.0013 (13)	−0.0046 (13)
N15	0.0263 (14)	0.0354 (16)	0.0277 (14)	0.0027 (12)	0.0033 (11)	−0.0018 (12)
N26	0.0311 (15)	0.0352 (16)	0.0329 (16)	0.0039 (12)	0.0043 (13)	0.0017 (12)
N29	0.0247 (13)	0.0279 (15)	0.0333 (15)	−0.0008 (11)	0.0014 (11)	0.0079 (12)
N40	0.0251 (14)	0.0247 (14)	0.0297 (14)	−0.0014 (11)	0.0015 (11)	0.0011 (11)
N43	0.0315 (14)	0.0217 (14)	0.0230 (13)	−0.0001 (11)	−0.0005 (11)	0.0032 (10)

N54	0.0434 (17)	0.0278 (15)	0.0258 (15)	0.0125 (13)	−0.0052 (13)	−0.0029 (11)
N57	0.0233 (13)	0.0358 (16)	0.0291 (14)	−0.0030 (11)	0.0042 (11)	−0.0078 (12)
F1	0.100 (3)	0.200 (5)	0.087 (3)	−0.081 (3)	0.051 (2)	−0.069 (3)
F2	0.113 (3)	0.119 (3)	0.073 (2)	0.023 (3)	0.047 (2)	−0.001 (2)
F3	0.075 (2)	0.097 (2)	0.0379 (14)	0.0023 (17)	0.0082 (14)	−0.0026 (14)
F4	0.0544 (19)	0.243 (6)	0.0360 (16)	−0.002 (3)	0.0008 (14)	−0.009 (2)
F5	0.099 (3)	0.191 (5)	0.081 (3)	0.068 (3)	0.020 (2)	0.049 (3)
F6	0.069 (2)	0.119 (3)	0.068 (2)	−0.024 (2)	0.0075 (17)	0.016 (2)
F7	0.0672 (19)	0.113 (3)	0.0529 (17)	0.0268 (18)	0.0049 (15)	0.0250 (17)
F8	0.0631 (19)	0.093 (2)	0.097 (3)	0.0404 (18)	0.0115 (18)	0.027 (2)
F9	0.099 (3)	0.083 (2)	0.069 (2)	−0.050 (2)	0.0048 (18)	0.0007 (17)
F10	0.075 (2)	0.074 (2)	0.198 (5)	−0.033 (2)	0.034 (3)	0.008 (3)
F11	0.075 (2)	0.086 (2)	0.0576 (18)	0.0052 (17)	−0.0161 (16)	−0.0223 (16)
F12	0.087 (2)	0.0665 (19)	0.070 (2)	0.0381 (17)	−0.0264 (17)	−0.0016 (15)
F13	0.0607 (16)	0.0662 (17)	0.0246 (11)	−0.0020 (13)	0.0021 (10)	0.0049 (10)
F14	0.0478 (13)	0.0289 (12)	0.0505 (13)	−0.0044 (9)	0.0032 (11)	−0.0041 (9)
F15	0.0677 (17)	0.0617 (16)	0.0238 (11)	−0.0035 (13)	0.0061 (11)	−0.0007 (10)
F16	0.0678 (17)	0.0286 (12)	0.0590 (16)	0.0035 (11)	−0.0145 (13)	0.0001 (10)
F17	0.0346 (12)	0.0424 (13)	0.0527 (14)	−0.0079 (9)	−0.0056 (10)	0.0041 (10)
F18	0.0318 (12)	0.0618 (16)	0.0575 (16)	0.0037 (11)	0.0003 (11)	−0.0174 (12)
P1	0.0423 (6)	0.1060 (12)	0.0325 (6)	−0.0096 (7)	0.0043 (5)	−0.0044 (6)
P2	0.0366 (5)	0.0364 (6)	0.0528 (6)	−0.0015 (4)	−0.0071 (5)	0.0107 (5)
P3	0.0318 (4)	0.0301 (5)	0.0246 (4)	−0.0022 (3)	−0.0008 (3)	0.0005 (3)

Geometric parameters (Å, º)

Ni1—N43^{i}	2.096 (3)	C34—H341	0.941
Ni1—N57^{i}	2.092 (3)	C35—C36	1.441 (6)
Ni1—N54^{i}	2.080 (3)	C35—H351	0.943
Ni1—N43	2.096 (3)	C36—C37	1.419 (6)
Ni1—N54	2.080 (3)	C36—C41	1.408 (5)
Ni1—N57	2.092 (3)	C37—C38	1.369 (6)
Ni2—N1	2.082 (3)	C37—H371	0.934
Ni2—N12	2.082 (3)	C38—C39	1.397 (5)
Ni2—N15	2.108 (3)	C38—H381	0.931
Ni2—N26	2.077 (3)	C39—N40	1.318 (4)
Ni2—N29	2.108 (3)	C39—H391	0.936
Ni2—N40	2.082 (3)	C41—C42	1.436 (5)
C2—C3	1.392 (6)	C41—N40	1.369 (4)
C2—N1	1.333 (5)	C42—N29	1.353 (5)
C2—H21	0.938	C44—C45	1.399 (5)
C3—C4	1.371 (7)	C44—N43	1.339 (4)
C3—H31	0.934	C44—H441	0.945
C4—C5	1.403 (7)	C45—C46	1.362 (6)
C4—H41	0.942	C45—H451	0.935
C5—C6	1.452 (6)	C46—C47	1.401 (5)
C5—C14	1.404 (5)	C46—H461	0.933
C6—C7	1.353 (8)	C47—C48	1.444 (5)

C6—H61	0.926	C47—C56	1.397 (5)
C7—C8	1.410 (7)	C48—C49	1.343 (6)
C7—H71	0.940	C48—H481	0.938
C8—C9	1.420 (7)	C49—C50	1.441 (6)
C8—C13	1.409 (5)	C49—H491	0.932
C9—C10	1.347 (7)	C50—C51	1.407 (6)
C9—H91	0.933	C50—C55	1.401 (5)
C10—C11	1.399 (6)	C51—C52	1.373 (7)
C10—H101	0.939	C51—H511	0.942
C11—N12	1.329 (5)	C52—C53	1.399 (6)
C11—H111	0.941	C52—H521	0.933
C13—C14	1.438 (5)	C53—N54	1.340 (5)
C13—N12	1.351 (5)	C53—H531	0.935
C14—N1	1.355 (5)	C55—C56	1.431 (5)
C16—C17	1.388 (6)	C55—N54	1.357 (5)
C16—N15	1.336 (5)	C56—N43	1.369 (4)
C16—H161	0.945	C58—C59	1.405 (7)
C17—C18	1.375 (7)	C58—N57	1.342 (5)
C17—H171	0.937	C58—H581	0.939
C18—C19	1.419 (7)	C59—C60	1.344 (8)
C18—H181	0.936	C59—H591	0.937
C19—C20	1.433 (6)	C60—C61	1.394 (8)
C19—C28	1.408 (5)	C60—H601	0.938
C20—C21	1.343 (7)	C61—C62	1.429 (7)
C20—H201	0.935	C61—C63	1.409 (5)
C21—C22	1.440 (6)	C62—C62^{i}	1.344 (12)
C21—H211	0.936	C62—H621	0.944
C22—C23	1.390 (6)	C63—C63^{i}	1.455 (8)
C22—C27	1.405 (5)	C63—N57	1.349 (5)
C23—C24	1.383 (7)	F1—P1	1.598 (4)
C23—H231	0.944	F2—P1	1.605 (4)
C24—C25	1.385 (6)	F3—P1	1.571 (3)
C24—H241	0.934	F4—P1	1.589 (3)
C25—N26	1.327 (5)	F5—P1	1.559 (5)
C25—H251	0.940	F6—P1	1.583 (4)
C27—C28	1.440 (5)	F7—P2	1.603 (3)
C27—N26	1.361 (5)	F8—P2	1.580 (3)
C28—N15	1.361 (5)	F9—P2	1.590 (3)
C30—C31	1.405 (6)	F10—P2	1.563 (3)
C30—N29	1.348 (5)	F11—P2	1.593 (3)
C30—H301	0.942	F12—P2	1.590 (3)
C31—C32	1.366 (7)	F13—P3	1.592 (2)
C31—H311	0.933	F14—P3	1.599 (2)
C32—C33	1.415 (6)	F15—P3	1.589 (2)
C32—H321	0.940	F16—P3	1.605 (3)
C33—C34	1.436 (6)	F17—P3	1.606 (2)
C33—C42	1.402 (5)	F18—P3	1.603 (2)
C34—C35	1.345 (7)		

N43^{i}—Ni1—N57^{i}	92.77 (11)	C36—C41—C42	119.7 (3)
N43^{i}—Ni1—N54^{i}	79.68 (11)	C36—C41—N40	122.6 (3)
N57^{i}—Ni1—N54^{i}	169.60 (12)	C42—C41—N40	117.7 (3)
N43^{i}—Ni1—N43	175.00 (15)	C41—C42—C33	119.9 (3)
N57^{i}—Ni1—N43	91.07 (11)	C41—C42—N29	116.8 (3)
N54^{i}—Ni1—N43	96.90 (11)	C33—C42—N29	123.3 (3)
N43^{i}—Ni1—N54	96.90 (11)	C45—C44—N43	122.5 (3)
N57^{i}—Ni1—N54	92.94 (12)	C45—C44—H441	119.0
N54^{i}—Ni1—N54	95.04 (18)	N43—C44—H441	118.5
N43—Ni1—N54	79.68 (11)	C44—C45—C46	119.5 (4)
N43^{i}—Ni1—N57	91.07 (11)	C44—C45—H451	119.4
N57^{i}—Ni1—N57	79.97 (16)	C46—C45—H451	121.1
N54^{i}—Ni1—N57	92.94 (12)	C45—C46—C47	119.6 (3)
N43—Ni1—N57	92.77 (11)	C45—C46—H461	119.8
N54—Ni1—N57	169.60 (12)	C47—C46—H461	120.6
N1—Ni2—N12	80.76 (12)	C46—C47—C48	123.1 (3)
N1—Ni2—N15	92.37 (12)	C46—C47—C56	118.0 (3)
N12—Ni2—N15	88.11 (12)	C48—C47—C56	118.9 (3)
N1—Ni2—N26	169.54 (12)	C47—C48—C49	120.3 (4)
N12—Ni2—N26	91.86 (12)	C47—C48—H481	120.2
N15—Ni2—N26	79.91 (12)	C49—C48—H481	119.5
N1—Ni2—N29	90.00 (11)	C48—C49—C50	121.8 (4)
N12—Ni2—N29	93.27 (12)	C48—C49—H491	118.9
N15—Ni2—N29	177.43 (12)	C50—C49—H491	119.2
N26—Ni2—N29	97.87 (12)	C49—C50—C51	123.7 (4)
N1—Ni2—N40	95.21 (11)	C49—C50—C55	118.9 (4)
N12—Ni2—N40	171.81 (12)	C51—C50—C55	117.4 (4)
N15—Ni2—N40	99.23 (11)	C50—C51—C52	119.3 (4)
N26—Ni2—N40	93.00 (11)	C50—C51—H511	120.2
N29—Ni2—N40	79.54 (11)	C52—C51—H511	120.5
C3—C2—N1	122.5 (4)	C51—C52—C53	119.8 (4)
C3—C2—H21	119.7	C51—C52—H521	120.9
N1—C2—H21	117.8	C53—C52—H521	119.3
C2—C3—C4	119.2 (4)	C52—C53—N54	122.1 (4)
C2—C3—H31	120.5	C52—C53—H531	119.6
C4—C3—H31	120.3	N54—C53—H531	118.3
C3—C4—C5	119.9 (4)	C50—C55—C56	119.3 (3)
C3—C4—H41	120.8	C50—C55—N54	123.1 (3)
C5—C4—H41	119.3	C56—C55—N54	117.6 (3)
C4—C5—C6	123.9 (4)	C55—C56—C47	120.8 (3)
C4—C5—C14	117.2 (4)	C55—C56—N43	116.7 (3)
C6—C5—C14	118.9 (4)	C47—C56—N43	122.4 (3)
C5—C6—C7	120.5 (4)	C59—C58—N57	122.4 (4)
C5—C6—H61	119.2	C59—C58—H581	120.6
C7—C6—H61	120.4	N57—C58—H581	117.0
C6—C7—C8	122.0 (4)	C58—C59—C60	119.3 (4)
C6—C7—H71	118.9	C58—C59—H591	119.8

C8—C7—H71	119.1	C60—C59—H591	120.9
C7—C8—C9	124.2 (4)	C59—C60—C61	120.7 (4)
C7—C8—C13	119.0 (4)	C59—C60—H601	119.5
C9—C8—C13	116.7 (4)	C61—C60—H601	119.8
C8—C9—C10	120.4 (4)	C60—C61—C62	124.0 (4)
C8—C9—H91	119.6	C60—C61—C63	116.6 (5)
C10—C9—H91	120.1	C62—C61—C63	119.4 (5)
C9—C10—C11	119.0 (4)	C61—C62—C62^{i}	121.4 (3)
C9—C10—H101	120.7	C61—C62—H621	119.9
C11—C10—H101	120.3	C62^{i}—C62—H621	118.7
C10—C11—N12	122.8 (4)	C63^{i}—C63—C61	119.2 (3)
C10—C11—H111	119.0	C63^{i}—C63—N57	117.2 (2)
N12—C11—H111	118.2	C61—C63—N57	123.6 (4)
C8—C13—C14	120.2 (4)	C14—N1—C2	118.6 (3)
C8—C13—N12	122.3 (4)	C14—N1—Ni2	111.6 (2)
C14—C13—N12	117.4 (3)	C2—N1—Ni2	129.7 (2)
C13—C14—C5	119.4 (3)	C13—N12—C11	118.7 (3)
C13—C14—N1	118.0 (3)	C13—N12—Ni2	112.1 (2)
C5—C14—N1	122.6 (4)	C11—N12—Ni2	129.2 (3)
C17—C16—N15	123.3 (4)	C28—N15—C16	117.7 (3)
C17—C16—H161	118.5	C28—N15—Ni2	112.1 (2)
N15—C16—H161	118.2	C16—N15—Ni2	129.2 (3)
C16—C17—C18	119.7 (4)	C27—N26—C25	118.5 (3)
C16—C17—H171	120.4	C27—N26—Ni2	112.7 (2)
C18—C17—H171	119.8	C25—N26—Ni2	128.1 (3)
C17—C18—C19	118.8 (4)	C42—N29—C30	118.2 (3)
C17—C18—H181	121.1	C42—N29—Ni2	113.1 (2)
C19—C18—H181	120.1	C30—N29—Ni2	128.5 (3)
C18—C19—C20	123.9 (4)	C41—N40—C39	118.5 (3)
C18—C19—C28	117.5 (4)	C41—N40—Ni2	112.8 (2)
C20—C19—C28	118.6 (4)	C39—N40—Ni2	128.7 (3)
C19—C20—C21	121.2 (4)	C56—N43—C44	117.9 (3)
C19—C20—H201	119.3	C56—N43—Ni1	112.7 (2)
C21—C20—H201	119.5	C44—N43—Ni1	129.2 (2)
C20—C21—C22	121.9 (4)	C55—N54—C53	118.2 (3)
C20—C21—H211	119.2	C55—N54—Ni1	113.2 (2)
C22—C21—H211	118.9	C53—N54—Ni1	128.5 (3)
C21—C22—C23	124.5 (4)	C63—N57—C58	117.4 (3)
C21—C22—C27	118.2 (4)	C63—N57—Ni1	112.8 (2)
C23—C22—C27	117.3 (4)	C58—N57—Ni1	129.8 (3)
C22—C23—C24	120.0 (4)	F2—P1—F1	89.4 (3)
C22—C23—H231	119.2	F2—P1—F4	87.7 (2)
C24—C23—H231	120.8	F1—P1—F4	90.3 (2)
C23—C24—C25	119.0 (4)	F2—P1—F6	87.2 (2)
C23—C24—H241	121.4	F1—P1—F6	176.5 (3)
C25—C24—H241	119.6	F4—P1—F6	90.2 (2)
C24—C25—N26	122.7 (4)	F2—P1—F3	89.4 (2)
C24—C25—H251	118.8	F1—P1—F3	88.3 (2)

N26—C25—H251	118.4	F4—P1—F3	176.7 (3)
C22—C27—C28	119.9 (3)	F6—P1—F3	91.06 (19)
C22—C27—N26	122.4 (4)	F2—P1—F5	179.5 (2)
C28—C27—N26	117.6 (3)	F1—P1—F5	90.3 (3)
C27—C28—C19	120.1 (4)	F4—P1—F5	92.7 (3)
C27—C28—N15	116.9 (3)	F6—P1—F5	93.1 (3)
C19—C28—N15	123.0 (4)	F3—P1—F5	90.2 (2)
C31—C30—N29	122.1 (4)	F7—P2—F11	178.8 (2)
C31—C30—H301	119.6	F7—P2—F9	88.9 (2)
N29—C30—H301	118.3	F11—P2—F9	89.98 (19)
C30—C31—C32	119.5 (4)	F7—P2—F12	89.08 (18)
C30—C31—H311	120.6	F11—P2—F12	90.32 (18)
C32—C31—H311	119.9	F9—P2—F12	90.7 (2)
C31—C32—C33	119.7 (4)	F7—P2—F8	89.25 (19)
C31—C32—H321	120.6	F11—P2—F8	91.33 (19)
C33—C32—H321	119.7	F9—P2—F8	88.5 (2)
C32—C33—C34	123.8 (4)	F12—P2—F8	178.1 (2)
C32—C33—C42	117.1 (4)	F7—P2—F10	89.5 (3)
C34—C33—C42	119.0 (4)	F11—P2—F10	91.6 (2)
C33—C34—C35	121.4 (4)	F9—P2—F10	178.4 (3)
C33—C34—H341	118.1	F12—P2—F10	89.0 (2)
C35—C34—H341	120.5	F8—P2—F10	91.8 (2)
C34—C35—C36	120.9 (4)	F17—P3—F16	89.72 (14)
C34—C35—H351	119.1	F17—P3—F18	179.79 (14)
C36—C35—H351	120.0	F16—P3—F18	90.09 (14)
C35—C36—C37	124.1 (4)	F17—P3—F14	89.97 (13)
C35—C36—C41	119.0 (4)	F16—P3—F14	179.57 (15)
C37—C36—C41	116.8 (4)	F18—P3—F14	90.22 (14)
C36—C37—C38	119.6 (4)	F17—P3—F13	90.05 (14)
C36—C37—H371	119.5	F16—P3—F13	89.91 (14)
C38—C37—H371	120.9	F18—P3—F13	90.03 (14)
C37—C38—C39	119.6 (4)	F14—P3—F13	89.79 (14)
C37—C38—H381	120.4	F17—P3—F15	89.73 (14)
C39—C38—H381	120.1	F16—P3—F15	90.27 (15)
C38—C39—N40	122.8 (4)	F18—P3—F15	90.19 (15)
C38—C39—H391	119.1	F14—P3—F15	90.02 (14)
N40—C39—H391	118.1	F13—P3—F15	179.72 (16)

Symmetry code: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H91···F6^{ii}	0.93	2.53	3.385 (6)	152
C10—H101···F2^{ii}	0.94	2.43	3.226 (6)	143
C16—H161···F12^{iii}	0.95	2.36	3.126 (5)	137
C20—H201···F16^{iv}	0.94	2.46	3.385 (5)	171
C24—H241···F4^{v}	0.93	2.42	3.271 (6)	152

C25—H251···F5^{v}	0.94	2.50	3.266 (6)	139
C44—H441···F9^{iii}	0.95	2.50	3.173 (5)	129
C51—H511···F18^{vi}	0.94	2.41	3.253 (6)	149
C52—H521···F13^{i}	0.94	2.48	3.209 (6)	134
C59—H591···F9^{vii}	0.94	2.50	3.417 (6)	167

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