Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3-Bis(6-methylpyridin-2-yl)-1*H*-imidazol-3-ium hexafluorophosphate

Hoyeon Bae,[a] Minyoung Yoon,[b] Ho-Jung Sun,[c] Dong-Heon Lee[d]* and Gyungse Park[e]*

[a]Department of Chemistry, Chonbuk National University, Jeonju, Chonbuk 561-756, Republic of Korea, [b]Center for Smart Supramolecules, Department of Chemistry and Division of Advanced Materials Science, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea, [c]Department of Material Science & Engineering, Kunsan National University, Jeonbuk 573-701, Republic of Korea, [d]Department of Chemistry and Research Institute of Physics and Chemistry, Chonbuk National University, Jeonju 561-756, Republic of Korea, and [e]Department of Chemistry, Kunsan National University, Kunsan, Chonbuk 573-701, Republic of Korea
Correspondence e-mail: dhl@jbnu.ac.kr, parkg@kunsan.ac.kr

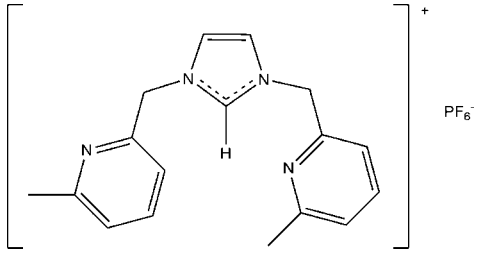
Received 25 February 2013; accepted 13 March 2013

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.133; data-to-parameter ratio = 13.8.

In the title salt, $C_{17}H_{19}N_4^+\cdot PF_6^-$, the two pyridine rings of the cation are inclined to one another by 15.89 (8)°, and inclined to the imidazole ring by 65.05 (10) and 64.07 (10)°. In the crystal, the cations and anions are linked *via* a series of C—H···N and C—H···F hydrogen bonds, forming two-dimensional networks lying parallel to (001).

Related literature

For the isolation of an *N*-heterocyclic carbene, see: Arduengo *et al.* (1991). For related structures, see: Huang *et al.* (2011); Grieco *et al.* (2011); Kim *et al.* (2009). For applications of *N*-heterocyclic carbenes in catalytic processes, see: Enders *et al.* (1996); Frenzel *et al.* (1999); Scholl *et al.* (1999).



Experimental

Crystal data

$C_{17}H_{19}N_4^+\cdot PF_6^-$
M_r = 424.33
Triclinic, $P\overline{1}$
a = 6.3839 (3) Å
b = 12.0353 (5) Å
c = 12.8006 (5) Å
α = 108.039 (2)°
β = 96.091 (2)°
γ = 100.593 (2)°
V = 905.12 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 K
0.16 × 0.07 × 0.07 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.986
19206 measured reflections
3700 independent reflections
2898 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.133
S = 0.97
3700 reflections
269 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F3^{i}	0.95	2.45	3.263 (2)	144
C7—H7A···N2^{ii}	0.99	2.59	3.567 (2)	170
C7—H7B···F6^{iii}	0.99	2.28	3.264 (2)	172
C10—H10···F2^{iv}	0.95	2.53	3.373 (2)	148
C11—H11B···F4^{iv}	0.99	2.44	3.355 (2)	154
C13—H13···F4^{iv}	0.95	2.34	3.193 (2)	149

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

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

This work was supported by the "Human Resource Development (project name: Advanced track for Si-based solar cell materials and devices, project No. 201040100660)" of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korean Government Ministry of Knowledge Economy.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5317).

References

Arduengo, A. J. III, Harlow, R. L. & Kline, M. (1991). *J. Am. Chem. Soc.* **113**, 361–363.
Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Enders, D., Gielen, H., Raabe, G., Runsink, J. & Teles, J. H. (1996). *Chem. Ber.* **129**, 1483–1488.
Frenzel, U., Weskamp, T., Kohl, F. J., Schattenmann, W. C., Nuyken, O. & Herrmann, W. A. (1999). *J. Organomet. Chem.* **586**, 263–265.
Grieco, G., Blacque, O. & Berke, H. (2011). *Acta Cryst.* E**67**, o2066–o2067.
Huang, K., Du, B.-X. & Liu, C.-L. (2011). *Acta Cryst.* E**67**, o2062.
Kim, G. Y., Park, S.-K., Lee, D.-H. & Park, G. (2009). *Acta Cryst.* E**65**, o637.
Scholl, M., Ding, S., Lee, C. W. & Grubbs, R. H. (1999). *Org. Lett.* **1**, 953–956.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, o549 [doi:10.1107/S1600536813006971]

1,3-Bis(6-methylpyridin-2-yl)-1*H*-imidazol-3-ium hexafluorophosphate

Hoyeon Bae, Minyoung Yoon, Ho-Jung Sun, Dong-Heon Lee and Gyungse Park

S1. Comment

N,*N*′-Disubstituted imidazolium salts are of importance because stable and isolable *N*-heterocyclic carbenes (NHCs) can be easily prepared by deprotonation of the imidazolium salts with a strong base. *N*-Heterocyclic carbenes (NHCs) have been a topic of extensive research due to their practical applications in many catalytic processes, *e.g.*, Pd–catalysed Heck–, Suzuki–coupling and Ru-based Grubbs catalyses (Frenzel *et al.*, 1999; Enders *et al.*, 1996; Scholl *et al.*, 1999). We previously synthesized an *N*,*N*′-disubstituted imidazolium salt, 1,3-bis[(6-methyl-2-pyridinyl)methyl]imidazolium bromide, and reported its crystal structure (Kim *et al.*, 2009)). The title compound was obtained by the anion exchange of the $C_{17}H_{19}N_4^+$ Br^- with NH_4PF_6. Here we report the crystal structure of the title compound,1,3-bis[(6-methyl-2-pyridinyl)methyl]imidazolium hexafluorophosphate (Fig. 1).

The asymmetric unit of the title compound consists the $C_{17}H_9N_4$ cation and PF_6 anion. Each of two 6–methylpyridine rings is rotated out of the imidazole plane, with dihedral angle of N1/C2–C6 of 55.83 (9)° and N4/C12–C16 of 11.32 (9)°. The molecular packing is stabilized by four different intermolecular C—H···F hydrogen bonds in the structure. (Table 1 & Fig. 2).

S2. Experimental

Synthesis of 1,3-Bis[(6-methylpyridin-2-yl)-1*H*-imidazolium hexafluorophosphate: A mixture of 1,3-Bis[(6-methyl-pyridin-2-yl)-1*H*-imidazolium bromide (Kim *et al.*, 2009). (2.16 g, 6.01 *x* 10^{-3} mol) and NH_4PF_6 (0.980 g, 6.01 *x* 10^{-3} mol) were dissolved in acetonitrile (35 ml) and the reaction mixture was stirred at room temperature for 19 h. After the solution was filtered the solvent were removed by high-vacuum rotary evaporation. The filtrate was dried under the reduced pressure to afford a brown solid in 95% yield. Single crystals were obtained by Et_2O diffusion into a $CHCl_3$ solution of the compound.

Spectroscopic analysis: 1H NMR ($CDCl_3$, 400 MHz): δ8.95 (s, H, CH), 7.62 (t, 2H, J =7.8 Hz, CH), 7.47 (d, 2H, J = 2 Hz, CH), 7.31 (s, 2H, CH), 7.28(d, 2H J = 10 Hz, CH), 7.14 (d, 2H, J = 7.8 Hz, CH), 5.35 (s, 4H, CH_2), 2.50 (s, 6H, CH_3). 13 C NMR ($CDCl_3$, 100 MHz): δ159.0 (s, C), 150.9 (s, C), 137.9 (s, CH), 136.1 (s, CH), 123.7 (s, CH), 122.4 (s, CH), 120.5 (s, CH), 54.5 (s, CH2), 24.4 (s, CH_3).

S3. Refinement

Hydrogen atoms were treated as riding on their parent carbon atoms, with U_{iso}(H) = 1.2 to .5 U_{eq}(C).

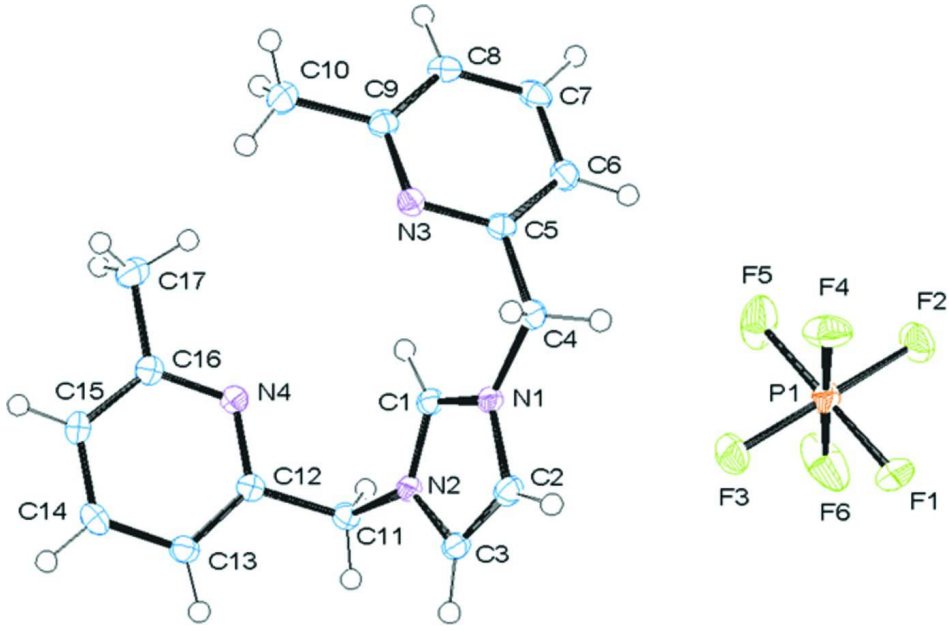


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

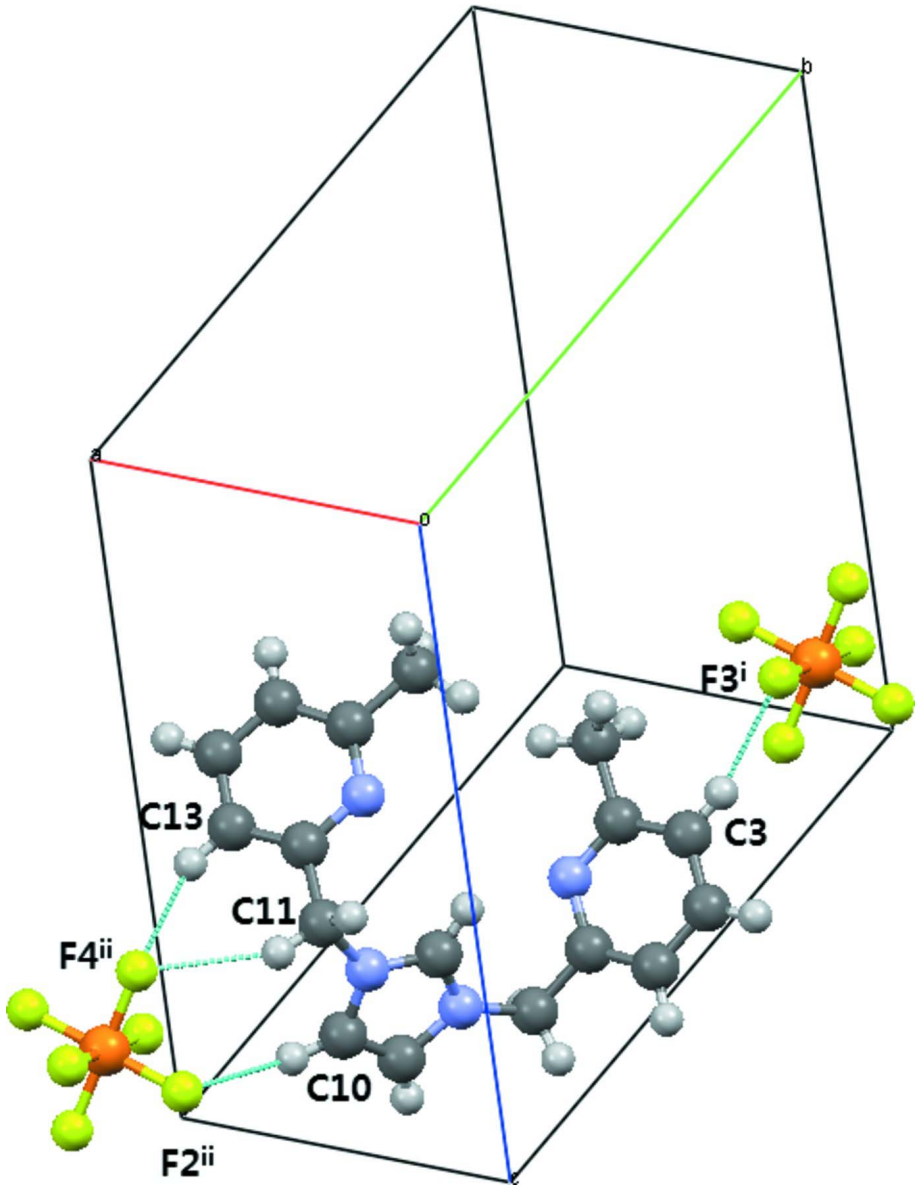


Figure 2

C—H···F interactions (dotted lines) in the title compound. [Symmetry code: (i) -*x*, -*y* + 1, -*z* + 1; (ii) -*x* + 1, -*y*, -*z* + 1]

1,3-Bis(6-methylpyridin-2-yl)-1*H*-imidazol-3-ium hexafluorophosphate

Crystal data

$C_{17}H_{19}N_4^+ \cdot PF_6^-$
M_r = 424.33
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.3839 (3) Å
b = 12.0353 (5) Å
c = 12.8006 (5) Å
α = 108.039 (2)°
β = 96.091 (2)°
γ = 100.593 (2)°
V = 905.12 (7) Å^3
Z = 2
$F(000)$ = 436
D_x = 1.557 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3700 reflections
θ = 1.7–26.5°
μ = 0.22 mm^{-1}

T = 100 K
Block, colorless

0.16 × 0.07 × 0.07 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\theta/2\pi$hi scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.986
19206 measured reflections

3700 independent reflections
2898 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.5°, θ_{min} = 1.7°
h = −8→7
k = −15→15
l = −16→16
4 standard reflections every 10 min
intensity decay: 0.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.133
S = 0.97
3700 reflections
269 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 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}
P1	0.02678 (7)	0.17116 (4)	0.22243 (4)	0.02100 (17)
F1	−0.20955 (18)	0.16206 (10)	0.25487 (10)	0.0319 (3)
F2	0.26436 (17)	0.18066 (10)	0.18965 (10)	0.0307 (3)
F3	0.09571 (18)	0.30854 (9)	0.30069 (11)	0.0335 (3)
F4	0.1109 (2)	0.13509 (11)	0.32678 (10)	0.0383 (3)
F5	−0.0381 (2)	0.03350 (11)	0.14681 (12)	0.0517 (4)
F6	−0.05468 (19)	0.21073 (14)	0.12030 (11)	0.0472 (4)
N1	0.4837 (2)	0.09220 (12)	0.78766 (12)	0.0161 (3)
N2	0.2781 (2)	0.42854 (12)	0.85867 (12)	0.0172 (3)
N3	0.5463 (2)	0.18196 (13)	0.59095 (12)	0.0178 (3)
N4	0.3855 (2)	0.21935 (12)	0.92229 (12)	0.0159 (3)
C1	0.3009 (3)	0.54548 (17)	0.73429 (16)	0.0246 (4)
H1A	0.3075	0.6315	0.7669	0.037*

H1B	0.2319	0.5167	0.6557	0.037*
H1C	0.4478	0.5319	0.7397	0.037*
C2	0.1717 (3)	0.47883 (15)	0.79610 (14)	0.0181 (4)
C3	−0.0512 (3)	0.46979 (15)	0.78953 (15)	0.0201 (4)
H3	−0.1230	0.5075	0.7462	0.025 (5)*
C4	−0.1665 (3)	0.40628 (16)	0.84576 (16)	0.0218 (4)
H4	−0.3181	0.3993	0.8416	0.027 (5)*
C5	−0.0567 (3)	0.35243 (15)	0.90892 (15)	0.0205 (4)
H5	−0.1320	0.3067	0.9477	0.023 (5)*
C6	0.1643 (3)	0.36706 (15)	0.91398 (14)	0.0173 (4)
C7	0.2937 (3)	0.31832 (16)	0.98693 (14)	0.0199 (4)
H7A	0.4132	0.3841	1.0371	0.032 (6)*
H7B	0.1998	0.2888	1.0340	0.023 (5)*
C8	0.3746 (3)	0.17802 (15)	0.81261 (14)	0.0162 (4)
H8	0.3008	0.2054	0.7604	0.017 (5)*
C9	0.5053 (3)	0.15701 (16)	0.96936 (15)	0.0194 (4)
H9	0.5382	0.1678	1.0465	0.033 (6)*
C10	0.5668 (3)	0.07800 (15)	0.88527 (15)	0.0189 (4)
H10	0.6517	0.0227	0.8920	0.030 (5)*
C11	0.5118 (3)	0.02583 (15)	0.67421 (14)	0.0187 (4)
H11A	0.3680	−0.0104	0.6259	0.028 (5)*
H11B	0.5827	−0.0401	0.6767	0.043 (7)*
C12	0.6464 (3)	0.10626 (15)	0.62463 (14)	0.0164 (4)
C13	0.8589 (3)	0.10113 (16)	0.61417 (15)	0.0198 (4)
H13	0.9250	0.0475	0.6396	0.021 (5)*
C14	0.9729 (3)	0.17597 (16)	0.56576 (15)	0.0210 (4)
H14	1.1185	0.1743	0.5573	0.020 (5)*
C15	0.8716 (3)	0.25257 (16)	0.53018 (15)	0.0199 (4)
H15	0.9460	0.3038	0.4960	0.022 (5)*
C16	0.6582 (3)	0.25440 (15)	0.54479 (14)	0.0185 (4)
C17	0.5434 (3)	0.33675 (18)	0.50650 (18)	0.0277 (4)
H17A	0.5198	0.3113	0.4248	0.042*
H17B	0.6318	0.4190	0.5378	0.042*
H17C	0.4035	0.3337	0.5319	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0187 (3)	0.0230 (3)	0.0248 (3)	0.0041 (2)	0.0065 (2)	0.0125 (2)
F1	0.0232 (6)	0.0308 (6)	0.0450 (7)	0.0050 (5)	0.0158 (5)	0.0147 (5)
F2	0.0196 (6)	0.0401 (7)	0.0371 (7)	0.0072 (5)	0.0100 (5)	0.0176 (5)
F3	0.0274 (6)	0.0206 (6)	0.0519 (8)	0.0073 (5)	0.0026 (5)	0.0117 (5)
F4	0.0493 (8)	0.0459 (8)	0.0417 (8)	0.0283 (6)	0.0193 (6)	0.0317 (6)
F5	0.0393 (8)	0.0334 (8)	0.0601 (10)	−0.0049 (6)	0.0220 (7)	−0.0123 (6)
F6	0.0257 (7)	0.0908 (11)	0.0386 (8)	0.0116 (7)	0.0034 (6)	0.0427 (8)
N1	0.0154 (7)	0.0146 (7)	0.0194 (8)	0.0032 (6)	0.0042 (6)	0.0073 (6)
N2	0.0157 (8)	0.0177 (7)	0.0187 (8)	0.0043 (6)	0.0038 (6)	0.0062 (6)
N3	0.0169 (8)	0.0183 (8)	0.0181 (8)	0.0037 (6)	0.0024 (6)	0.0062 (6)

N4	0.0135 (7)	0.0172 (7)	0.0188 (7)	0.0036 (6)	0.0030 (6)	0.0086 (6)
C1	0.0240 (10)	0.0272 (10)	0.0275 (10)	0.0082 (8)	0.0058 (8)	0.0142 (8)
C2	0.0203 (9)	0.0157 (8)	0.0171 (9)	0.0050 (7)	0.0031 (7)	0.0035 (7)
C3	0.0178 (9)	0.0170 (9)	0.0239 (9)	0.0054 (7)	0.0004 (7)	0.0047 (7)
C4	0.0139 (9)	0.0185 (9)	0.0292 (10)	0.0027 (7)	0.0031 (7)	0.0036 (8)
C5	0.0192 (9)	0.0164 (9)	0.0249 (10)	0.0027 (7)	0.0070 (7)	0.0052 (7)
C6	0.0185 (9)	0.0151 (8)	0.0182 (9)	0.0049 (7)	0.0044 (7)	0.0041 (7)
C7	0.0225 (10)	0.0211 (9)	0.0177 (9)	0.0076 (7)	0.0061 (7)	0.0066 (7)
C8	0.0133 (8)	0.0170 (8)	0.0190 (9)	0.0024 (7)	0.0016 (7)	0.0081 (7)
C9	0.0172 (9)	0.0235 (9)	0.0207 (9)	0.0045 (7)	0.0021 (7)	0.0124 (7)
C10	0.0158 (9)	0.0203 (9)	0.0246 (10)	0.0046 (7)	0.0032 (7)	0.0130 (8)
C11	0.0193 (9)	0.0177 (9)	0.0197 (9)	0.0062 (7)	0.0064 (7)	0.0048 (7)
C12	0.0169 (9)	0.0158 (8)	0.0141 (8)	0.0041 (7)	0.0007 (7)	0.0025 (7)
C13	0.0172 (9)	0.0211 (9)	0.0213 (9)	0.0054 (7)	0.0021 (7)	0.0075 (7)
C14	0.0147 (9)	0.0239 (9)	0.0229 (10)	0.0047 (7)	0.0037 (7)	0.0055 (8)
C15	0.0190 (9)	0.0220 (9)	0.0178 (9)	0.0013 (7)	0.0052 (7)	0.0067 (7)
C16	0.0188 (9)	0.0204 (9)	0.0151 (9)	0.0040 (7)	0.0024 (7)	0.0051 (7)
C17	0.0272 (11)	0.0284 (10)	0.0345 (11)	0.0087 (8)	0.0067 (9)	0.0186 (9)

Geometric parameters (Å, º)

P1—F5	1.5883 (13)	C4—H4	0.9500
P1—F6	1.5933 (12)	C5—C6	1.381 (2)
P1—F3	1.5951 (12)	C5—H5	0.9500
P1—F4	1.5980 (12)	C6—C7	1.501 (2)
P1—F1	1.6003 (12)	C7—H7A	0.9900
P1—F2	1.6095 (12)	C7—H7B	0.9900
N1—C8	1.327 (2)	C8—H8	0.9500
N1—C10	1.377 (2)	C9—C10	1.345 (3)
N1—C11	1.473 (2)	C9—H9	0.9500
N2—C2	1.343 (2)	C10—H10	0.9500
N2—C6	1.346 (2)	C11—C12	1.506 (3)
N3—C16	1.341 (2)	C11—H11A	0.9900
N3—C12	1.350 (2)	C11—H11B	0.9900
N4—C8	1.326 (2)	C12—C13	1.388 (2)
N4—C9	1.380 (2)	C13—C14	1.388 (3)
N4—C7	1.482 (2)	C13—H13	0.9500
C1—C2	1.496 (3)	C14—C15	1.376 (2)
C1—H1A	0.9800	C14—H14	0.9500
C1—H1B	0.9800	C15—C16	1.398 (2)
C1—H1C	0.9800	C15—H15	0.9500
C2—C3	1.399 (2)	C16—C17	1.501 (2)
C3—C4	1.375 (3)	C17—H17A	0.9800
C3—H3	0.9500	C17—H17B	0.9800
C4—C5	1.391 (2)	C17—H17C	0.9800
F5—P1—F6	91.57 (8)	C5—C6—C7	120.87 (16)
F5—P1—F3	178.51 (7)	N4—C7—C6	112.82 (14)

F6—P1—F3	89.86 (7)	N4—C7—H7A	109.0
F5—P1—F4	89.92 (8)	C6—C7—H7A	109.0
F6—P1—F4	178.50 (8)	N4—C7—H7B	109.0
F3—P1—F4	88.65 (7)	C6—C7—H7B	109.0
F5—P1—F1	90.45 (7)	H7A—C7—H7B	107.8
F6—P1—F1	89.57 (6)	N4—C8—N1	108.81 (14)
F3—P1—F1	89.98 (6)	N4—C8—H8	125.6
F4—P1—F1	90.59 (7)	N1—C8—H8	125.6
F5—P1—F2	89.65 (7)	C10—C9—N4	106.99 (15)
F6—P1—F2	90.28 (6)	C10—C9—H9	126.5
F3—P1—F2	89.92 (6)	N4—C9—H9	126.5
F4—P1—F2	89.57 (6)	C9—C10—N1	107.26 (15)
F1—P1—F2	179.82 (6)	C9—C10—H10	126.4
C8—N1—C10	108.43 (15)	N1—C10—H10	126.4
C8—N1—C11	124.97 (14)	N1—C11—C12	111.69 (14)
C10—N1—C11	126.59 (14)	N1—C11—H11A	109.3
C2—N2—C6	118.40 (15)	C12—C11—H11A	109.3
C16—N3—C12	118.01 (15)	N1—C11—H11B	109.3
C8—N4—C9	108.50 (14)	C12—C11—H11B	109.3
C8—N4—C7	127.20 (14)	H11A—C11—H11B	107.9
C9—N4—C7	124.26 (15)	N3—C12—C13	122.89 (16)
C2—C1—H1A	109.5	N3—C12—C11	115.65 (15)
C2—C1—H1B	109.5	C13—C12—C11	121.46 (15)
H1A—C1—H1B	109.5	C14—C13—C12	118.66 (16)
C2—C1—H1C	109.5	C14—C13—H13	120.7
H1A—C1—H1C	109.5	C12—C13—H13	120.7
H1B—C1—H1C	109.5	C15—C14—C13	118.86 (17)
N2—C2—C3	121.23 (17)	C15—C14—H14	120.6
N2—C2—C1	117.52 (16)	C13—C14—H14	120.6
C3—C2—C1	121.25 (16)	C14—C15—C16	119.50 (17)
C4—C3—C2	120.01 (17)	C14—C15—H15	120.2
C4—C3—H3	120.0	C16—C15—H15	120.2
C2—C3—H3	120.0	N3—C16—C15	122.06 (16)
C3—C4—C5	118.67 (17)	N3—C16—C17	117.27 (16)
C3—C4—H4	120.7	C15—C16—C17	120.66 (16)
C5—C4—H4	120.7	C16—C17—H17A	109.5
C6—C5—C4	118.44 (17)	C16—C17—H17B	109.5
C6—C5—H5	120.8	H17A—C17—H17B	109.5
C4—C5—H5	120.8	C16—C17—H17C	109.5
N2—C6—C5	123.21 (16)	H17A—C17—H17C	109.5
N2—C6—C7	115.87 (15)	H17B—C17—H17C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F3^{i}	0.95	2.45	3.263 (2)	144
C7—H7*A*···N2^{ii}	0.99	2.59	3.567 (2)	170
C7—H7*B*···F6^{iii}	0.99	2.28	3.264 (2)	172

C10—H10···F2^{iv}	0.95	2.53	3.373 (2)	148
C11—H11*B*···F4^{iv}	0.99	2.44	3.355 (2)	154
C13—H13···F4^{iv}	0.95	2.34	3.193 (2)	149

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) *x*, *y*, *z*+1; (iv) −*x*+1, −*y*, −*z*+1.