Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9,10-Bis{2-[1-(2-pyridylmethyl)-imidazolium-3-yl]ethoxy}anthracene bis(hexafluoridophosphate)

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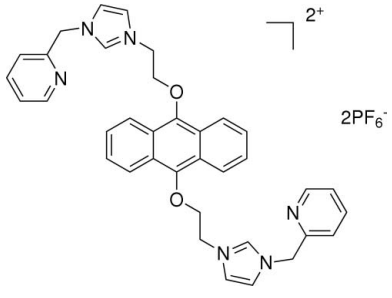
Received 13 November 2007; accepted 27 November 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in solvent or counterion; R factor = 0.055; wR factor = 0.159; data-to-parameter ratio = 8.9.

The cation of the title compound, $C_{36}H_{34}N_6O_2^{2+}\cdot 2PF_6^-$, lies across a crystallographic inversion centre. The imidazole and pyridine rings form dihedral angles of 82.28 (5)° and 11.87 (7)°, respectively, with the anthracene ring system. The crystal packing is stabilized by π–π interactions between the pyridine ring and the central ring of anthracene, with a ring centroid–centroid distance of 3.684 (3) Å. The PF_6^- anion is disordered over three different positions with occupancies of 0.284 (6), 0.354 (8) and 0.362 (9).

Related literature

For the synthesis, see: Liu *et al.* (2003). For related structures, see: Liu *et al.* (2007); Pei *et al.* (2005); Qin *et al.* (2006).



Experimental

Crystal data

$C_{36}H_{34}N_6O_2^{2+}\cdot 2PF_6^-$
M_r = 872.63
Triclinic, $P\overline{1}$
a = 8.829 (4) Å
b = 9.811 (4) Å
c = 12.586 (5) Å
α = 72.382 (7)°
β = 78.759 (7)°
γ = 65.598 (7)°
V = 943.2 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.950, T_{max} = 0.962
4911 measured reflections
3307 independent reflections
1792 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.159
S = 1.01
3307 reflections
373 parameters
319 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

The authors thank the Scientific Research Fund Projects of China West Normal University (grant No. 06B003) and the Youth Fund Projects of Sichuan Educational Department (grant No. 2006B039).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2523).

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supporting information

Acta Cryst. (2008). E**64**, o189 [https://doi.org/10.1107/S1600536807063842]

9,10-Bis{2-[1-(2-pyridylmethyl)imidazolium-3-yl]ethoxy}anthracene bis(hexafluoridophosphate)

Li-Hui Guo, Da-Bin Qin, Shao-Jin Gu, Gui-Yu Wang and Jie-Wei Luo

S1. Comment

Imidazolium salts or its derivatives or analogs are used as ionic liquids, and as catalysts in many organic transformation processes. They are also used to obtain N-heterocyclic carbene complexes. We report here the crystal structure of the title compound.

The asymmetric unit of the title compound contains one-half of the organic cation and a PF_6 counter ion. The cation lies on a crystallographic inversion center. Bond lengths and angles in the title molecule (Fig. 1) are within normal ranges. The imidazole ring is almost perpendicular to the anthracene ring system, with a dihedral angle of 82.28 (5)°, and the pyridine ring is almost parallel to the anthracene ring system, with a dihedral angle of 11.87 (7)°. The crystal packing is stabilized by π-π interactions between pyridine ring and central ring of anthracene [centroid-centroid distance is 3.684 (3) %A.

S2. Experimental

The title compound was prepared according to the reported procedure of Liu *et al.* (2003). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from acetonitrile.

S3. Refinement

The PF_6 group is disordered over three different positions with refined occupancies of 0.284 (6), 0.354 (8) and 0.362 (9). The P—F distances were restrained to 1.56 (1) Å, and the displacement parameters of disordered F atoms were restrained to an approximate isotropic behaviour, and also restrained to have the same U^{ij} components. H atoms were placed in calculated positions with C—H = 0.93–0.97 Å, and refined using a riding model approximation, with U_{iso}(H) = 1.2$_{eq}$(C).

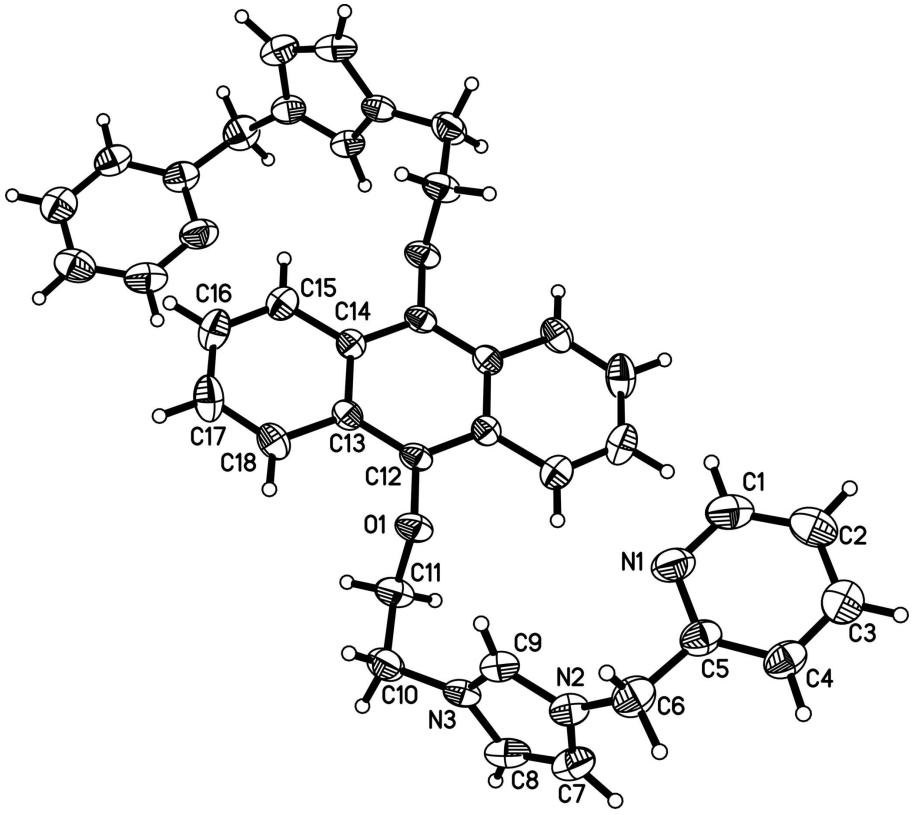

Figure 1

View of the cationic unit in the title compound. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - *x*, 1 - *y*, 2 - *z*).

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Crystal data

$C_{36}H_{34}N_6O_2^{2+}\cdot 2PF_6^-$
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$a = 8.829\ (4)$ Å
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$c = 12.586\ (5)$ Å
$\alpha = 72.382\ (7)°$
$\beta = 78.759\ (7)°$
$\gamma = 65.598\ (7)°$
$V = 943.2\ (7)$ Å^3
$Z = 1$
$F(000) = 446$
$D_x = 1.536$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1209 reflections
$\theta = 2.7–21.5°$
$\mu = 0.22$ mm^{-1}
$T = 294$ K
Block, yellow
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.950$, $T_{max} = 0.962$
4911 measured reflections
3307 independent reflections
1792 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -10\rightarrow10$
$k = -11\rightarrow6$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.159$
$S = 1.01$
3307 reflections
373 parameters
319 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
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.3109P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.015$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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}	Occ. (<1)
O1	0.3505 (3)	0.6951 (3)	0.80589 (19)	0.0542 (7)	
N1	−0.1667 (4)	1.0465 (4)	0.9161 (3)	0.0759 (11)	
N2	−0.1181 (4)	1.0404 (4)	0.6845 (3)	0.0594 (9)	
N3	0.0945 (4)	0.8468 (4)	0.6444 (2)	0.0537 (9)	
C1	−0.2180 (7)	1.0165 (6)	1.0243 (4)	0.0824 (14)	
H1	−0.1385	0.9512	1.0749	0.099*	
C2	−0.3809 (7)	1.0760 (6)	1.0655 (4)	0.0786 (14)	
H2	−0.4105	1.0523	1.1420	0.094*	
C3	−0.4988 (6)	1.1708 (5)	0.9918 (5)	0.0741 (13)	
H3	−0.6107	1.2126	1.0168	0.089*	
C4	−0.4483 (5)	1.2030 (5)	0.8795 (4)	0.0665 (12)	
H4	−0.5260	1.2661	0.8273	0.080*	
C5	−0.2824 (5)	1.1410 (5)	0.8457 (4)	0.0623 (11)	
C6	−0.2179 (5)	1.1793 (5)	0.7253 (4)	0.0747 (13)	
H6A	−0.3115	1.2428	0.6799	0.090*	
H6B	−0.1501	1.2389	0.7172	0.090*	
C7	−0.1765 (6)	0.9587 (6)	0.6444 (4)	0.0714 (13)	
H7	−0.2876	0.9820	0.6362	0.086*	
C8	−0.0454 (6)	0.8389 (6)	0.6192 (3)	0.0690 (13)	
H8	−0.0484	0.7637	0.5899	0.083*	
C9	0.0470 (5)	0.9692 (5)	0.6840 (3)	0.0571 (11)	
H9	0.1176	1.0009	0.7079	0.069*	
C10	0.2667 (5)	0.7415 (5)	0.6272 (3)	0.0697 (13)	
H10A	0.3375	0.8007	0.6007	0.084*	
H10B	0.2736	0.6916	0.5697	0.084*	

C11	0.3307 (5)	0.6199 (5)	0.7318 (3)	0.0616 (11)	
H11A	0.2521	0.5702	0.7660	0.074*	
H11B	0.4368	0.5418	0.7143	0.074*	
C12	0.4252 (4)	0.5939 (4)	0.9027 (3)	0.0440 (9)	
C13	0.5991 (4)	0.5322 (4)	0.9005 (3)	0.0449 (9)	
C14	0.6758 (4)	0.4338 (4)	1.0009 (3)	0.0438 (9)	
C15	0.8534 (4)	0.3686 (5)	0.9977 (4)	0.0590 (11)	
H15	0.9055	0.3045	1.0623	0.071*	
C16	0.9462 (5)	0.3990 (5)	0.9021 (4)	0.0722 (13)	
H16	1.0620	0.3538	0.9010	0.087*	
C17	0.8715 (5)	0.4974 (5)	0.8043 (4)	0.0749 (14)	
H17	0.9382	0.5187	0.7396	0.090*	
C18	0.7031 (5)	0.5624 (5)	0.8023 (3)	0.0592 (11)	
H18	0.6555	0.6269	0.7363	0.071*	
P1	0.71210 (13)	0.71357 (15)	0.41845 (9)	0.0645 (4)	
F1	0.551 (2)	0.702 (3)	0.3935 (19)	0.114 (6)	0.284 (6)
F2	0.789 (2)	0.5628 (17)	0.3757 (17)	0.092 (4)	0.284 (6)
F3	0.758 (2)	0.811 (2)	0.3001 (11)	0.111 (4)	0.284 (6)
F4	0.6560 (19)	0.8681 (17)	0.4551 (19)	0.134 (5)	0.284 (6)
F5	0.662 (2)	0.615 (2)	0.5320 (11)	0.130 (5)	0.284 (6)
F6	0.8857 (15)	0.655 (2)	0.4618 (15)	0.115 (5)	0.284 (6)
F1A	0.5497 (16)	0.672 (2)	0.4454 (14)	0.119 (5)	0.354 (8)
F2A	0.7523 (17)	0.631 (2)	0.3229 (13)	0.093 (4)	0.354 (8)
F3A	0.590 (2)	0.8701 (16)	0.3574 (15)	0.144 (5)	0.354 (8)
F4A	0.6405 (16)	0.7923 (18)	0.5218 (10)	0.097 (4)	0.354 (8)
F5A	0.761 (2)	0.5581 (15)	0.5135 (13)	0.130 (4)	0.354 (8)
F6A	0.8703 (15)	0.7530 (19)	0.3841 (15)	0.114 (5)	0.354 (8)
F1B	0.5218 (10)	0.776 (2)	0.4093 (15)	0.112 (4)	0.362 (9)
F2B	0.7395 (16)	0.722 (2)	0.2880 (7)	0.101 (4)	0.362 (9)
F3B	0.661 (2)	0.8926 (11)	0.3589 (17)	0.123 (4)	0.362 (9)
F4B	0.6951 (19)	0.712 (2)	0.5411 (7)	0.108 (4)	0.362 (9)
F5B	0.8139 (15)	0.5346 (9)	0.4402 (17)	0.109 (4)	0.362 (9)
F6B	0.8931 (11)	0.7078 (15)	0.4201 (10)	0.066 (3)	0.362 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0699 (16)	0.0451 (16)	0.0411 (14)	−0.0139 (13)	−0.0158 (12)	−0.0056 (12)
N1	0.070 (2)	0.078 (3)	0.075 (3)	−0.015 (2)	−0.029 (2)	−0.016 (2)
N2	0.062 (2)	0.056 (2)	0.057 (2)	−0.0193 (19)	−0.0174 (16)	−0.0072 (18)
N3	0.066 (2)	0.055 (2)	0.0356 (17)	−0.0213 (18)	−0.0148 (15)	−0.0023 (16)
C1	0.093 (4)	0.076 (3)	0.079 (4)	−0.022 (3)	−0.036 (3)	−0.016 (3)
C2	0.112 (4)	0.070 (3)	0.071 (3)	−0.047 (3)	−0.011 (3)	−0.023 (3)
C3	0.078 (3)	0.061 (3)	0.097 (4)	−0.032 (3)	−0.008 (3)	−0.032 (3)
C4	0.064 (3)	0.051 (3)	0.086 (3)	−0.015 (2)	−0.024 (2)	−0.017 (2)
C5	0.064 (3)	0.046 (3)	0.073 (3)	−0.013 (2)	−0.021 (2)	−0.012 (2)
C6	0.071 (3)	0.058 (3)	0.084 (3)	−0.014 (2)	−0.019 (2)	−0.009 (3)
C7	0.068 (3)	0.077 (3)	0.075 (3)	−0.032 (3)	−0.027 (2)	−0.006 (3)

C8	0.090 (3)	0.068 (3)	0.060 (3)	−0.038 (3)	−0.032 (2)	−0.004 (2)
C9	0.061 (3)	0.059 (3)	0.053 (2)	−0.022 (2)	−0.0181 (19)	−0.008 (2)
C10	0.076 (3)	0.076 (3)	0.045 (2)	−0.015 (2)	−0.008 (2)	−0.014 (2)
C11	0.078 (3)	0.052 (3)	0.047 (2)	−0.011 (2)	−0.018 (2)	−0.014 (2)
C12	0.057 (2)	0.035 (2)	0.035 (2)	−0.0121 (18)	−0.0091 (17)	−0.0064 (17)
C13	0.053 (2)	0.042 (2)	0.040 (2)	−0.0203 (18)	−0.0008 (17)	−0.0102 (18)
C14	0.047 (2)	0.038 (2)	0.045 (2)	−0.0141 (17)	−0.0026 (17)	−0.0126 (18)
C15	0.051 (2)	0.058 (3)	0.065 (3)	−0.017 (2)	−0.007 (2)	−0.015 (2)
C16	0.046 (2)	0.070 (3)	0.090 (4)	−0.015 (2)	0.001 (2)	−0.018 (3)
C17	0.065 (3)	0.068 (3)	0.077 (3)	−0.027 (2)	0.022 (2)	−0.012 (3)
C18	0.070 (3)	0.058 (3)	0.045 (2)	−0.029 (2)	0.006 (2)	−0.007 (2)
P1	0.0483 (6)	0.0874 (10)	0.0528 (7)	−0.0162 (6)	−0.0078 (5)	−0.0219 (7)
F1	0.084 (7)	0.149 (10)	0.128 (9)	−0.048 (6)	−0.055 (6)	−0.025 (8)
F2	0.114 (7)	0.086 (7)	0.091 (8)	−0.042 (5)	−0.007 (6)	−0.036 (6)
F3	0.134 (7)	0.097 (7)	0.092 (7)	−0.060 (6)	0.002 (6)	0.003 (6)
F4	0.158 (7)	0.100 (7)	0.110 (7)	−0.007 (6)	0.006 (7)	−0.051 (6)
F5	0.126 (7)	0.137 (7)	0.084 (6)	−0.032 (6)	0.017 (6)	−0.008 (6)
F6	0.098 (6)	0.126 (8)	0.114 (8)	−0.037 (6)	−0.050 (6)	−0.003 (6)
F1A	0.070 (5)	0.154 (8)	0.126 (8)	−0.060 (5)	0.011 (5)	−0.010 (7)
F2A	0.109 (6)	0.085 (7)	0.090 (7)	−0.026 (6)	−0.001 (5)	−0.048 (6)
F3A	0.118 (8)	0.121 (7)	0.146 (7)	−0.023 (6)	−0.030 (7)	0.010 (6)
F4A	0.116 (6)	0.101 (7)	0.050 (5)	−0.015 (5)	−0.001 (5)	−0.026 (5)
F5A	0.128 (7)	0.110 (6)	0.099 (6)	−0.020 (5)	−0.011 (6)	0.011 (5)
F6A	0.106 (6)	0.113 (8)	0.127 (9)	−0.072 (6)	−0.002 (6)	0.005 (6)
F1B	0.051 (4)	0.129 (8)	0.128 (7)	−0.016 (5)	−0.009 (4)	−0.019 (7)
F2B	0.122 (6)	0.108 (8)	0.069 (5)	−0.030 (6)	−0.003 (4)	−0.037 (5)
F3B	0.108 (7)	0.093 (6)	0.132 (7)	−0.032 (5)	−0.023 (6)	0.022 (6)
F4B	0.142 (7)	0.131 (8)	0.047 (4)	−0.040 (6)	−0.019 (4)	−0.024 (5)
F5B	0.126 (6)	0.077 (5)	0.113 (7)	−0.029 (4)	−0.015 (6)	−0.020 (5)
F6B	0.061 (4)	0.075 (7)	0.060 (6)	−0.040 (4)	−0.023 (4)	0.019 (5)

Geometric parameters (Å, º)

O1—C12	1.395 (4)	C11—H11A	0.97
O1—C11	1.425 (4)	C11—H11B	0.97
N1—C5	1.327 (5)	C12—C14^{i}	1.385 (5)
N1—C1	1.332 (6)	C12—C13	1.397 (5)
N2—C9	1.330 (5)	C13—C18	1.421 (5)
N2—C7	1.361 (5)	C13—C14	1.429 (5)
N2—C6	1.467 (5)	C14—C12^{i}	1.385 (5)
N3—C9	1.316 (5)	C14—C15	1.425 (5)
N3—C8	1.370 (5)	C15—C16	1.345 (5)
N3—C10	1.461 (5)	C15—H15	0.93
C1—C2	1.370 (6)	C16—C17	1.398 (6)
C1—H1	0.93	C16—H16	0.93
C2—C3	1.366 (6)	C17—C18	1.356 (5)
C2—H2	0.93	C17—H17	0.93
C3—C4	1.377 (6)	C18—H18	0.93

C3—H3	0.93	P1—F4B	1.518 (8)
C4—C5	1.369 (5)	P1—F3A	1.533 (9)
C4—H4	0.93	P1—F6	1.544 (9)
C5—C6	1.502 (6)	P1—F1B	1.547 (8)
C6—H6A	0.97	P1—F6A	1.548 (9)
C6—H6B	0.97	P1—F2A	1.554 (8)
C7—C8	1.335 (5)	P1—F5	1.562 (9)
C7—H7	0.93	P1—F2	1.565 (9)
C8—H8	0.93	P1—F1	1.566 (10)
C9—H9	0.93	P1—F5B	1.571 (8)
C10—C11	1.503 (5)	P1—F4	1.572 (9)
C10—H10A	0.97	P1—F6B	1.579 (8)
C10—H10B	0.97		

C12—O1—C11	113.8 (3)	O1—C11—H11A	110.3
C5—N1—C1	116.9 (4)	C10—C11—H11A	110.3
C9—N2—C7	107.9 (4)	O1—C11—H11B	110.3
C9—N2—C6	125.3 (4)	C10—C11—H11B	110.3
C7—N2—C6	126.7 (4)	H11A—C11—H11B	108.5
C9—N3—C8	107.9 (4)	C14^{i}—C12—O1	118.8 (3)
C9—N3—C10	125.7 (4)	C14^{i}—C12—C13	122.5 (3)
C8—N3—C10	126.4 (4)	O1—C12—C13	118.6 (3)
N1—C1—C2	123.9 (4)	C12—C13—C18	122.7 (3)
N1—C1—H1	118.0	C12—C13—C14	118.7 (3)
C2—C1—H1	118.0	C18—C13—C14	118.6 (3)
C3—C2—C1	118.5 (5)	C12^{i}—C14—C15	122.7 (3)
C3—C2—H2	120.8	C12^{i}—C14—C13	118.8 (3)
C1—C2—H2	120.8	C15—C14—C13	118.5 (3)
C2—C3—C4	118.5 (5)	C16—C15—C14	120.6 (4)
C2—C3—H3	120.8	C16—C15—H15	119.7
C4—C3—H3	120.8	C14—C15—H15	119.7
C5—C4—C3	119.3 (4)	C15—C16—C17	121.0 (4)
C5—C4—H4	120.4	C15—C16—H16	119.5
C3—C4—H4	120.4	C17—C16—H16	119.5
N1—C5—C4	123.0 (4)	C18—C17—C16	121.0 (4)
N1—C5—C6	115.1 (4)	C18—C17—H17	119.5
C4—C5—C6	121.9 (4)	C16—C17—H17	119.5
N2—C6—C5	112.2 (3)	C17—C18—C13	120.3 (4)
N2—C6—H6A	109.2	C17—C18—H18	119.9
C5—C6—H6A	109.2	C13—C18—H18	119.9
N2—C6—H6B	109.2	F4B—P1—F1B	94.3 (8)
C5—C6—H6B	109.2	F3A—P1—F6A	96.6 (10)
H6A—C6—H6B	107.9	F3A—P1—F2A	97.0 (10)
C8—C7—N2	107.5 (4)	F6A—P1—F2A	92.4 (9)
C8—C7—H7	126.3	F6—P1—F5	87.0 (10)
N2—C7—H7	126.3	F6—P1—F2	83.7 (10)
C7—C8—N3	107.5 (4)	F5—P1—F2	87.4 (10)
C7—C8—H8	126.2	F6—P1—F1	156.8 (13)

N3—C8—H8	126.2	F5—P1—F1	77.1 (11)
N3—C9—N2	109.1 (4)	F2—P1—F1	78.9 (12)
N3—C9—H9	125.4	F4B—P1—F5B	93.5 (8)
N2—C9—H9	125.4	F1B—P1—F5B	118.9 (9)
N3—C10—C11	112.8 (3)	F6—P1—F4	91.2 (10)
N3—C10—H10A	109.0	F5—P1—F4	97.5 (10)
C11—C10—H10A	109.0	F2—P1—F4	172.8 (9)
N3—C10—H10B	109.0	F1—P1—F4	107.3 (11)
C11—C10—H10B	109.0	F4B—P1—F6B	84.2 (7)
H10A—C10—H10B	107.8	F1B—P1—F6B	161.1 (9)
O1—C11—C10	107.3 (3)	F5B—P1—F6B	79.9 (7)
C5—N1—C1—C2	0.5 (7)	C9—N3—C10—C11	83.6 (5)
N1—C1—C2—C3	0.6 (8)	C8—N3—C10—C11	−98.5 (4)
C1—C2—C3—C4	−0.4 (7)	C12—O1—C11—C10	−174.0 (3)
C2—C3—C4—C5	−0.8 (6)	N3—C10—C11—O1	−70.3 (4)
C1—N1—C5—C4	−1.9 (7)	C11—O1—C12—C14^{i}	−96.3 (4)
C1—N1—C5—C6	176.5 (4)	C11—O1—C12—C13	87.7 (4)
C3—C4—C5—N1	2.1 (7)	C14^{i}—C12—C13—C18	−179.0 (3)
C3—C4—C5—C6	−176.2 (4)	O1—C12—C13—C18	−3.1 (5)
C9—N2—C6—C5	−93.4 (5)	C14^{i}—C12—C13—C14	1.5 (6)
C7—N2—C6—C5	84.1 (5)	O1—C12—C13—C14	177.3 (3)
N1—C5—C6—N2	55.0 (5)	C12—C13—C14—C12^{i}	−1.4 (6)
C4—C5—C6—N2	−126.6 (4)	C18—C13—C14—C12^{i}	179.0 (3)
C9—N2—C7—C8	−0.5 (5)	C12—C13—C14—C15	178.7 (3)
C6—N2—C7—C8	−178.3 (4)	C18—C13—C14—C15	−0.8 (5)
N2—C7—C8—N3	0.3 (5)	C12^{i}—C14—C15—C16	−180.0 (4)
C9—N3—C8—C7	0.1 (4)	C13—C14—C15—C16	−0.1 (6)
C10—N3—C8—C7	−178.1 (3)	C14—C15—C16—C17	1.3 (7)
C8—N3—C9—N2	−0.4 (4)	C15—C16—C17—C18	−1.5 (7)
C10—N3—C9—N2	177.8 (3)	C16—C17—C18—C13	0.5 (7)
C7—N2—C9—N3	0.5 (4)	C12—C13—C18—C17	−178.9 (4)
C6—N2—C9—N3	178.4 (3)	C14—C13—C18—C17	0.6 (6)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.