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1-[Bicyclo[4.2.0]octa-1(6),2,4-trien-3-yl]-3-[bicyclo[4.2.0]octa-1(6),2,4-trien-3-ylmethyl]imidazolium hexafluorophosphate

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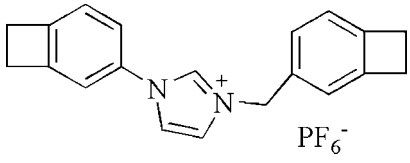
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.075; wR factor = 0.223; data-to-parameter ratio = 11.8.

In the title compound, $C_{20}H_{19}N_2^+\cdot PF_6^-$, the two benzocyclobutene units are essentially planar and they form dihedral angles of 38.0 (2) and 72.7 (2)°, with the central imidazolium ring. In the crystal structure, weak C—H$\cdots\pi$ and π–π stacking interactions [centroid–centroid distance = 3.742 (2) Å] contribute to the stability of the crystal structure. The PF_6^- ion is disordered over two positions with site occupancies of 0.869 (9) and 0.131 (9).

Related literature

For related literature, see: Farona (1996); Kirchhoff & Bruza (1993); Michellys *et al.* (2001); Nemeto & Fukumoto (1998); Zhang *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{19}N_2^+\cdot F_6P^-$
M_r = 432.34
Triclinic, $P\overline{1}$
a = 9.311 (3) Å
b = 10.138 (3) Å
c = 10.562 (3) Å
α = 86.82 (2)°
β = 86.44 (2)°
γ = 73.61 (2)°
V = 953.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 (2) K
0.28 × 0.25 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3558 measured reflections
3522 independent reflections
2238 reflections with $I > 2\sigma(I)$
R_{int} = 0.006
3 standard reflections every 300 reflections
intensity decay: 4.6%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.223
S = 1.15
3522 reflections
299 parameters
81 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

*Cg*1 is the centroid of the C3–C8 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2*B*$\cdots$*Cg*1^{i}	0.97	3.00	3.813 (5)	143

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

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2536).

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supplementary materials

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1-[Bicyclo[4.2.0]octa-1(6),2,4-trien-3-yl]-3-[bicyclo[4.2.0]octa-1(6),2,4-trien-3-ylmethyl]imidazolium hexafluorophosphate

F.-H. Zhu, J.-X. Yang, Z.-H. Mao and R.-G. Xie

Comment

Benzocyclobutenes (BCBs) are important building blocks for new polymers and advanced materials (Nemeto & Fukumoto, 1998; Michellys *et al.*, 2001). Most of the reported benzocyclobutene monomers in the literature are bis-BCB-functionalized compounds owing to their highly crosslinked structure and their excellent properties such as the insolubility, low solvent pickup and good thermal stability (Farona, 1996; Zhang *et al.*, 2006; Kirchhoff & Bruza, 1993). We report here the crystal structure of the title compound, a novel bisbenzocyclobutene-terminated imidazolium which was obtained by an anion metathesis between 1-(4-benzocyclobutenyl)-3-(4-benzocyclobutenylmethyl) imidazolium choloride and hexafluorophosphate ammonium.

The two benzocyclobutene units are essentially planar. The plane of the C1—C8 and C13—C20 benzocyclobutene units form dihedral angles of 38.0 (2) and 72.7 (2)°, respectively, with the central imidazolium ring.

A combination of intermolecular π-π and C—H···π interactions provide packing forces in the crystal structure of the title compound. A π-π interaction between C13—C15/C18—C20 benzene ring and its symmetry- related counterpart at (−*x*, 1 − *y*, −*z*), with their centroids separated by 3.742 (2) Å, plays an important part in the connection of two adjacent molecules. In addition, a weak C—H···π interaction between C2—H2B group and C3—C8 benzene ring at (1 − *x*, −1 − *y*, 1 − *z*) contributes to the crystal packing (Table 1).

Experimental

4-(*N*-imidazolyl)benzocyclobutene (5 mmol, 850 mg) and 4-cholomethylbenzocyclobutene (5 mmol, 760 mg) were placed in a two-necked round-bottomed flask under a nitrogen atmosphere, and the mixture was heated at 353 K for 3 h. After the reaction was completed, the resulting 1-(4-benzocyclobutenyl)-3-(4-benzocyclobutenylmethyl)imidazolium chloride, [BBMI][Cl^-], was obtained in 85% yield (1.381 g). [BBMI][Cl^-] was dissolved in deioned water, and NH_4PF_6 was added to replace Cl^- ions by PF_6^- ions, to obtain the title compound as a white solid (yield 1.331 g). Colourless crystals of the title compound were obtained by recrystallization of the solid from acetone and ethanol (1:1 *v*/*v*). ^{1}H NMR (400 MHz, $CDCl_3$,): δ 8.84 (s, 1H), 7.41 (t, 1H), 7.31 (m, 2H), 7.27 (2 d, 1H), 7.22 (d, 1H), 7.18 (d, J = 8.0 Hz, 1H), 7.15 (s, 1H), 7.09 (d, J = 7.6 Hz, 1H), 5.37 (s, 2H), 3.21 (s, 4H), 3.17 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$,): δ 148.58, 148.04, 7.65, 147.21, 133.71, 133.42, 130.78, 128.20, 124.45, 123.53, 122.77, 121.88, 121.46, 117.09, 54.52, 29.47, 29.32 p.p.m.

Refinement

H atoms were positioned geometrically and refined in the riding model approximation with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). Four F atoms of the PF_6^- ion are disordered over two positions (F3,F4,F5,F6/F3A,F4A,F5A,F6A)

with refined occupancies of 0.869 (9) and 0.131 (9). The disordered F atoms were restrained to be coplanar, with the F···F distances restrained to be equal. The displacement parameters of disordered F atoms were restrained to be approximately isotropic.

Figures

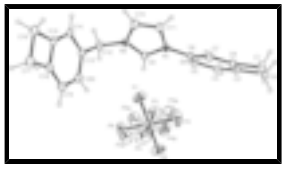


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering.

1-[Bicyclo[4.2.0]octa-1(6),2,4-trien-3-yl]-3-[bicyclo[4.2.0]octa- 1(6),2,4-trien-3-ylmethyl]imidazolium hexafluorophosphate

Crystal data

$C_{20}H_{19}N_2^+ \cdot F_6P^-$	$Z = 2$
$M_r = 432.34$	$F_{000} = 444$
Triclinic, $P\overline{1}$	$D_x = 1.505$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.311$ (3) Å	Cell parameters from 20 reflections
$b = 10.138$ (3) Å	$\theta = 4.9$–9.1°
$c = 10.562$ (3) Å	$\mu = 0.21$ mm^{-1}
$\alpha = 86.82$ (2)°	$T = 296$ (2) K
$\beta = 86.44$ (2)°	Block, colourless
$\gamma = 73.61$ (2)°	0.28 × 0.25 × 0.18 mm
$V = 953.9$ (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.006$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.5^\circ$
Monochromator: graphite	$\theta_{min} = 1.9^\circ$
$T = 296(2)$ K	$h = -10 \rightarrow 11$
$\omega/2\theta$ scans	$k = -2 \rightarrow 12$
Absorption correction: none	$l = -12 \rightarrow 12$
3558 measured reflections	3 standard reflections
3522 independent reflections	every 300 reflections
2238 reflections with $I > 2\sigma(I)$	intensity decay: 4.6%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.075$	H-atom parameters constrained
$wR(F^2) = 0.223$	$w = 1/[\sigma^2(F_o^2) + (0.1349P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	$(\Delta/\sigma)_{max} = 0.001$
3522 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
299 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
81 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.3258 (3)	−0.0608 (3)	0.3056 (3)	0.0388 (7)	
N2	0.1779 (3)	0.1062 (3)	0.1997 (3)	0.0412 (7)	
C1	0.7078 (6)	−0.4108 (5)	0.5742 (4)	0.0654 (13)	
H1A	0.6556	−0.4310	0.6520	0.078*	
H1B	0.7911	−0.3758	0.5917	0.078*	
C2	0.7481 (5)	−0.5286 (5)	0.4784 (4)	0.0658 (13)	
H2A	0.8522	−0.5547	0.4476	0.079*	
H2B	0.7152	−0.6086	0.5066	0.079*	
C3	0.6426 (4)	−0.4283 (4)	0.3899 (4)	0.0486 (10)	
C4	0.5802 (5)	−0.4138 (4)	0.2742 (4)	0.0534 (11)	
H4	0.6062	−0.4838	0.2166	0.064*	
C5	0.4756 (4)	−0.2881 (4)	0.2472 (3)	0.0477 (10)	
H5	0.4297	−0.2731	0.1700	0.057*	
C6	0.4397 (4)	−0.1854 (4)	0.3348 (3)	0.0385 (8)	
C7	0.5044 (4)	−0.2001 (4)	0.4520 (3)	0.0452 (9)	
H7	0.4809	−0.1304	0.5099	0.054*	
C8	0.6057 (5)	−0.3256 (4)	0.4753 (3)	0.0474 (9)	
C9	0.2990 (4)	0.0017 (3)	0.1915 (3)	0.0381 (8)	
H9	0.3572	−0.0247	0.1175	0.046*	
C10	0.1233 (5)	0.1122 (4)	0.3233 (4)	0.0583 (12)	
H10	0.0378	0.1759	0.3552	0.070*	
C11	0.2151 (5)	0.0095 (4)	0.3902 (4)	0.0525 (10)	
H11	0.2059	−0.0104	0.4768	0.063*	

C12	0.1133 (4)	0.2028 (4)	0.0937 (3)	0.0457 (9)	
H12A	0.0101	0.2026	0.0854	0.055*	
H12B	0.1688	0.1715	0.0150	0.055*	
C13	0.1181 (4)	0.3462 (4)	0.1145 (3)	0.0394 (8)	
C14	−0.0027 (4)	0.4358 (4)	0.1797 (3)	0.0414 (9)	
H14	−0.0882	0.4103	0.2072	0.050*	
C15	0.0126 (4)	0.5639 (4)	0.2006 (3)	0.0446 (9)	
C16	−0.0632 (5)	0.7005 (4)	0.2603 (5)	0.0611 (12)	
H16A	−0.0769	0.6945	0.3520	0.073*	
H16B	−0.1550	0.7522	0.2215	0.073*	
C17	0.0771 (5)	0.7460 (4)	0.2122 (4)	0.0613 (12)	
H17A	0.0569	0.8218	0.1496	0.074*	
H17B	0.1360	0.7622	0.2793	0.074*	
C18	0.1361 (4)	0.6058 (4)	0.1564 (3)	0.0448 (9)	
C19	0.2544 (4)	0.5185 (4)	0.0891 (4)	0.0494 (10)	
H19	0.3375	0.5464	0.0583	0.059*	
C20	0.2429 (4)	0.3886 (4)	0.0702 (3)	0.0465 (10)	
H20	0.3209	0.3271	0.0264	0.056*	
P1	0.67915 (11)	0.11989 (10)	0.17994 (9)	0.0466 (4)	
F1	0.5204 (3)	0.1791 (4)	0.2485 (3)	0.0890 (10)	
F2	0.8367 (3)	0.0567 (3)	0.1101 (3)	0.0964 (11)	
F3	0.6267 (4)	0.0006 (4)	0.1205 (3)	0.0908 (17)	0.869 (9)
F4	0.7321 (5)	0.0220 (4)	0.2990 (3)	0.109 (2)	0.869 (9)
F5	0.7340 (4)	0.2334 (4)	0.2388 (5)	0.112 (2)	0.869 (9)
F6	0.6275 (5)	0.2124 (5)	0.0586 (4)	0.120 (2)	0.869 (9)
F3A	0.6793 (7)	−0.018 (2)	0.2185 (12)	0.127 (14)	0.131 (9)
F4A	0.7527 (10)	0.1314 (12)	0.3022 (15)	0.090 (10)	0.131 (9)
F5A	0.6805 (7)	0.260 (2)	0.1369 (12)	0.103 (11)	0.131 (9)
F6A	0.6104 (10)	0.1040 (12)	0.0613 (16)	0.093 (10)	0.131 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0443 (17)	0.0364 (15)	0.0320 (15)	−0.0048 (13)	−0.0036 (12)	−0.0025 (12)
N2	0.0480 (18)	0.0395 (16)	0.0332 (15)	−0.0068 (14)	−0.0038 (13)	−0.0028 (12)
C1	0.075 (3)	0.066 (3)	0.047 (2)	−0.005 (2)	−0.023 (2)	0.011 (2)
C2	0.064 (3)	0.065 (3)	0.056 (3)	0.002 (2)	−0.013 (2)	0.012 (2)
C3	0.046 (2)	0.051 (2)	0.042 (2)	−0.0017 (18)	−0.0069 (16)	0.0010 (17)
C4	0.050 (2)	0.055 (2)	0.046 (2)	0.0046 (18)	−0.0117 (17)	−0.0145 (18)
C5	0.049 (2)	0.055 (2)	0.0348 (19)	−0.0043 (18)	−0.0110 (16)	−0.0087 (17)
C6	0.0361 (18)	0.0414 (19)	0.0340 (17)	−0.0041 (15)	−0.0050 (14)	0.0004 (14)
C7	0.057 (2)	0.048 (2)	0.0287 (17)	−0.0099 (18)	−0.0066 (16)	−0.0024 (15)
C8	0.055 (2)	0.050 (2)	0.0331 (18)	−0.0094 (18)	−0.0107 (16)	0.0070 (16)
C9	0.044 (2)	0.0407 (19)	0.0286 (16)	−0.0088 (16)	−0.0053 (14)	−0.0017 (14)
C10	0.068 (3)	0.049 (2)	0.042 (2)	0.008 (2)	0.0080 (19)	−0.0024 (18)
C11	0.061 (3)	0.050 (2)	0.0356 (19)	0.0015 (19)	0.0081 (18)	−0.0034 (16)
C12	0.052 (2)	0.046 (2)	0.0351 (18)	−0.0040 (17)	−0.0135 (16)	−0.0021 (16)
C13	0.0406 (19)	0.0434 (19)	0.0305 (17)	−0.0041 (15)	−0.0117 (14)	0.0019 (14)

C14	0.0363 (19)	0.043 (2)	0.0417 (19)	−0.0050 (15)	−0.0094 (15)	0.0040 (15)
C15	0.041 (2)	0.043 (2)	0.044 (2)	−0.0004 (16)	−0.0123 (16)	0.0019 (16)
C16	0.058 (3)	0.043 (2)	0.075 (3)	−0.0011 (19)	−0.008 (2)	−0.008 (2)
C17	0.063 (3)	0.050 (2)	0.071 (3)	−0.015 (2)	−0.014 (2)	−0.002 (2)
C18	0.045 (2)	0.047 (2)	0.0414 (19)	−0.0100 (17)	−0.0131 (16)	0.0077 (16)
C19	0.042 (2)	0.064 (3)	0.044 (2)	−0.0179 (19)	−0.0051 (17)	0.0037 (18)
C20	0.040 (2)	0.056 (2)	0.0373 (19)	−0.0024 (17)	−0.0069 (16)	−0.0042 (17)
P1	0.0469 (6)	0.0481 (6)	0.0409 (6)	−0.0061 (5)	−0.0024 (4)	−0.0045 (4)
F1	0.0595 (17)	0.125 (2)	0.0650 (17)	0.0038 (16)	0.0102 (13)	−0.0246 (17)
F2	0.0592 (18)	0.098 (2)	0.127 (3)	−0.0126 (16)	0.0273 (18)	−0.042 (2)
F3	0.093 (3)	0.122 (4)	0.078 (3)	−0.060 (3)	0.027 (2)	−0.048 (3)
F4	0.165 (4)	0.074 (3)	0.054 (2)	0.023 (3)	−0.021 (2)	0.0058 (18)
F5	0.105 (3)	0.082 (3)	0.158 (5)	−0.031 (2)	0.003 (3)	−0.061 (3)
F6	0.151 (4)	0.106 (4)	0.060 (2)	0.024 (3)	0.002 (2)	0.034 (2)
F3A	0.122 (19)	0.094 (16)	0.18 (2)	−0.059 (14)	−0.017 (16)	0.033 (16)
F4A	0.077 (13)	0.105 (19)	0.079 (13)	−0.006 (12)	−0.049 (11)	0.013 (12)
F5A	0.140 (19)	0.086 (15)	0.091 (17)	−0.050 (13)	0.001 (14)	0.004 (13)
F6A	0.145 (18)	0.095 (17)	0.052 (12)	−0.048 (14)	−0.024 (11)	−0.012 (12)

Geometric parameters (Å, °)

N1—C9	1.334 (4)	C12—H12B	0.97
N1—C11	1.382 (4)	C13—C20	1.395 (5)
N1—C6	1.435 (4)	C13—C14	1.400 (5)
N2—C9	1.313 (4)	C14—C15	1.378 (5)
N2—C10	1.370 (5)	C14—H14	0.93
N2—C12	1.484 (4)	C15—C18	1.381 (6)
C1—C8	1.517 (5)	C15—C16	1.518 (5)
C1—C2	1.558 (6)	C16—C17	1.552 (7)
C1—H1A	0.97	C16—H16A	0.97
C1—H1B	0.97	C16—H16B	0.97
C2—C3	1.522 (5)	C17—C18	1.510 (5)
C2—H2A	0.97	C17—H17A	0.97
C2—H2B	0.97	C17—H17B	0.97
C3—C4	1.368 (5)	C18—C19	1.387 (5)
C3—C8	1.371 (5)	C19—C20	1.378 (5)
C4—C5	1.395 (5)	C19—H19	0.93
C4—H4	0.93	C20—H20	0.93
C5—C6	1.386 (5)	P1—F3A	1.43 (3)
C5—H5	0.93	P1—F5A	1.47 (2)
C6—C7	1.393 (5)	P1—F6A	1.48 (2)
C7—C8	1.373 (5)	P1—F4A	1.524 (18)
C7—H7	0.93	P1—F5	1.556 (4)
C9—H9	0.93	P1—F6	1.563 (4)
C10—C11	1.343 (5)	P1—F4	1.572 (4)
C10—H10	0.93	P1—F1	1.576 (3)
C11—H11	0.93	P1—F2	1.579 (3)
C12—C13	1.497 (5)	P1—F3	1.597 (4)
C12—H12A	0.97		

C9—N1—C11	107.5 (3)	C15—C14—H14	122.0
C9—N1—C6	126.8 (3)	C13—C14—H14	122.0
C11—N1—C6	125.4 (3)	C14—C15—C18	123.0 (3)
C9—N2—C10	108.2 (3)	C14—C15—C16	144.1 (4)
C9—N2—C12	125.8 (3)	C18—C15—C16	93.0 (3)
C10—N2—C12	125.9 (3)	C15—C16—C17	86.7 (3)
C8—C1—C2	86.7 (3)	C15—C16—H16A	114.2
C8—C1—H1A	114.2	C17—C16—H16A	114.2
C2—C1—H1A	114.2	C15—C16—H16B	114.2
C8—C1—H1B	114.2	C17—C16—H16B	114.2
C2—C1—H1B	114.2	H16A—C16—H16B	111.4
H1A—C1—H1B	111.4	C18—C17—C16	86.8 (3)
C3—C2—C1	86.3 (3)	C18—C17—H17A	114.2
C3—C2—H2A	114.3	C16—C17—H17A	114.2
C1—C2—H2A	114.3	C18—C17—H17B	114.2
C3—C2—H2B	114.3	C16—C17—H17B	114.2
C1—C2—H2B	114.3	H17A—C17—H17B	111.3
H2A—C2—H2B	111.4	C15—C18—C19	121.1 (4)
C4—C3—C8	122.4 (3)	C15—C18—C17	93.5 (3)
C4—C3—C2	144.0 (4)	C19—C18—C17	145.3 (4)
C8—C3—C2	93.5 (3)	C20—C19—C18	116.7 (4)
C3—C4—C5	116.3 (3)	C20—C19—H19	121.6
C3—C4—H4	121.8	C18—C19—H19	121.6
C5—C4—H4	121.8	C19—C20—C13	122.2 (3)
C6—C5—C4	120.5 (3)	C19—C20—H20	118.9
C6—C5—H5	119.8	C13—C20—H20	118.9
C4—C5—H5	119.8	F3A—P1—F5A	178.4 (5)
C5—C6—C7	123.0 (3)	F3A—P1—F6A	88.8 (6)
C5—C6—N1	118.5 (3)	F5A—P1—F6A	90.0 (6)
C7—C6—N1	118.5 (3)	F3A—P1—F4A	89.6 (6)
C8—C7—C6	114.7 (3)	F5A—P1—F4A	91.5 (6)
C8—C7—H7	122.7	F6A—P1—F4A	178.2 (6)
C6—C7—H7	122.7	F5—P1—F6	92.2 (3)
C3—C8—C7	123.1 (3)	F5—P1—F4	89.7 (3)
C3—C8—C1	93.5 (3)	F6—P1—F4	177.9 (2)
C7—C8—C1	143.4 (3)	F3A—P1—F1	91.1 (2)
N2—C9—N1	109.6 (3)	F5A—P1—F1	90.1 (2)
N2—C9—H9	125.2	F6A—P1—F1	91.5 (2)
N1—C9—H9	125.2	F4A—P1—F1	89.5 (2)
C11—C10—N2	107.8 (3)	F5—P1—F1	89.43 (19)
C11—C10—H10	126.1	F6—P1—F1	90.82 (19)
N2—C10—H10	126.1	F4—P1—F1	90.17 (19)
C10—C11—N1	106.8 (3)	F3A—P1—F2	87.5 (2)
C10—C11—H11	126.6	F5A—P1—F2	91.3 (2)
N1—C11—H11	126.6	F6A—P1—F2	87.4 (2)
N2—C12—C13	111.8 (3)	F4A—P1—F2	91.5 (2)
N2—C12—H12A	109.3	F5—P1—F2	92.30 (19)
C13—C12—H12A	109.3	F6—P1—F2	89.4 (2)
N2—C12—H12B	109.3	F4—P1—F2	89.5 (2)

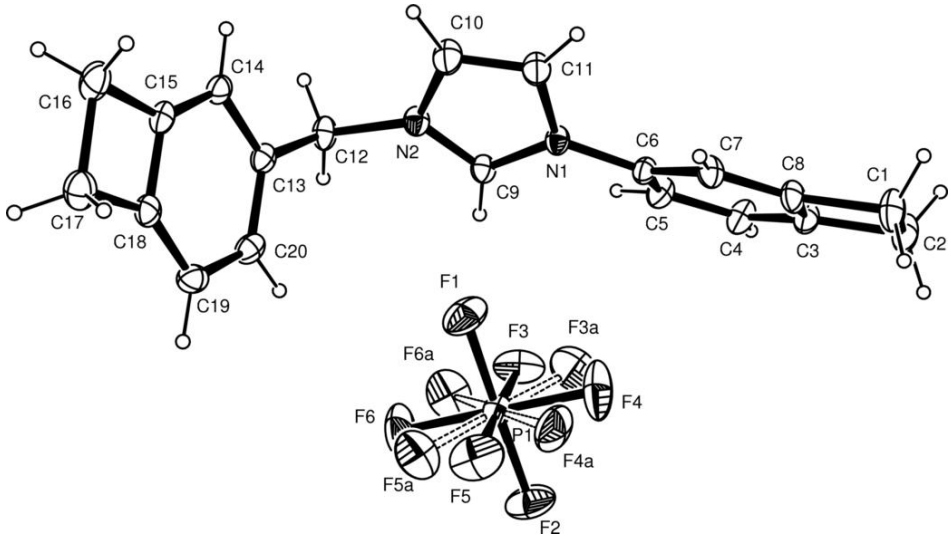
C13—C12—H12B	109.3	F1—P1—F2	178.25 (18)
H12A—C12—H12B	107.9	F5—P1—F3	178.5 (2)
C20—C13—C14	120.9 (3)	F6—P1—F3	88.8 (3)
C20—C13—C12	119.8 (3)	F4—P1—F3	89.3 (2)
C14—C13—C12	119.3 (3)	F1—P1—F3	91.61 (18)
C15—C14—C13	116.0 (4)	F2—P1—F3	86.66 (17)
C8—C1—C2—C3	0.8 (3)	C12—N2—C10—C11	−178.3 (4)
C1—C2—C3—C4	−177.7 (7)	N2—C10—C11—N1	−0.8 (5)
C1—C2—C3—C8	−0.9 (4)	C9—N1—C11—C10	0.7 (5)
C8—C3—C4—C5	−0.3 (7)	C6—N1—C11—C10	−174.1 (4)
C2—C3—C4—C5	176.0 (6)	C9—N2—C12—C13	−115.5 (4)
C3—C4—C5—C6	0.3 (7)	C10—N2—C12—C13	63.2 (5)
C4—C5—C6—C7	0.4 (7)	N2—C12—C13—C20	89.8 (4)
C4—C5—C6—N1	−176.8 (4)	N2—C12—C13—C14	−89.5 (4)
C9—N1—C6—C5	−35.6 (6)	C20—C13—C14—C15	−2.4 (5)
C11—N1—C6—C5	138.2 (4)	C12—C13—C14—C15	177.0 (3)
C9—N1—C6—C7	147.2 (4)	C13—C14—C15—C18	2.5 (5)
C11—N1—C6—C7	−39.0 (5)	C13—C14—C15—C16	−178.8 (5)
C5—C6—C7—C8	−0.9 (6)	C14—C15—C16—C17	−179.7 (5)
N1—C6—C7—C8	176.2 (3)	C18—C15—C16—C17	−0.8 (3)
C4—C3—C8—C7	−0.3 (7)	C15—C16—C17—C18	0.8 (3)
C2—C3—C8—C7	−178.1 (4)	C14—C15—C18—C19	−1.0 (6)
C4—C3—C8—C1	178.7 (4)	C16—C15—C18—C19	179.7 (3)
C2—C3—C8—C1	0.9 (4)	C14—C15—C18—C17	−179.9 (3)
C6—C7—C8—C3	0.9 (6)	C16—C15—C18—C17	0.9 (3)
C6—C7—C8—C1	−177.5 (6)	C16—C17—C18—C15	−0.9 (3)
C2—C1—C8—C3	−0.9 (4)	C16—C17—C18—C19	−179.2 (6)
C2—C1—C8—C7	177.7 (6)	C15—C18—C19—C20	−0.7 (5)
C10—N2—C9—N1	−0.2 (4)	C17—C18—C19—C20	177.3 (5)
C12—N2—C9—N1	178.7 (3)	C18—C19—C20—C13	0.8 (5)
C11—N1—C9—N2	−0.3 (4)	C14—C13—C20—C19	0.8 (5)
C6—N1—C9—N2	174.4 (3)	C12—C13—C20—C19	−178.6 (3)
C9—N2—C10—C11	0.6 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2B···Cg1^{i}	0.97	3.00	3.813 (5)	143

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

Fig. 1


C10
C11
C14
C15
C16
C12
N2
C6
C7
C8
C1
C13
C9
N1
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C4
C3
C2
C17
C18
C20
C19
F1
F3
F3a
F6a
F4
F6
P1
F4a
F5a
F5
F2