

Crystal structure of triphenylphosphoniummethyl-
enetrifluoroborateChristopher M. Bateman,^a Lev N. Zakharov^b and Eric R. Abbey^{a*}^aDept. of Chemistry, Biochemistry, and Physics, Eastern Washington University, Cheney, WA 99004, USA, and^bDepartment of Chemistry and Biochemistry, CAMCOR, University of Oregon, Eugene, OR 97403, USA.

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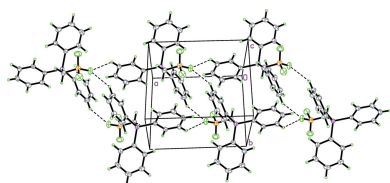
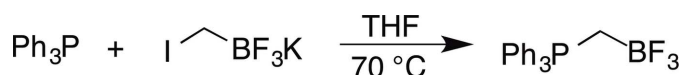
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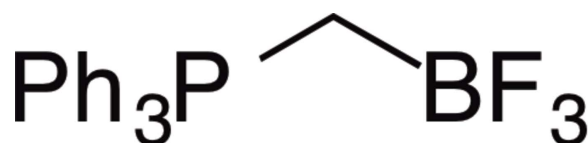
The title compound, C₁₉H₁₇BF₃P {alternative name: triphenyl[(trifluoroboranyl)methyl]phosphonium}, was formed by the reaction of triphenylphosphine with potassium iodomethyltrifluoroborate. The molecule features a nearly staggered conformation along the P–C bond and a less than staggered conformation along the C–B bond. In the crystal, weak C–H···F hydrogen bonds between the *meta*-phenyl C–H groups and the trifluoroborate B–F groups form chains of R₂²(16) rings along [100]. These chains are further stabilized by weak C–H···π interactions. A weak intramolecular C–H···F hydrogen bond is also observed.

1. Chemical context

Alkyltriphenylphosphonium (Ph₃PRX) salts are widely used as precursors in the preparation of phosphorus ylides for Wittig-type olefination (Julia, 1985). Such olefination reactions continue to be one of the most important means of alkene generation. Potassium organotrifluoroborates (KRBF₃) are common substrates used in Suzuki–Miyaura coupling as stable boronic acid precursors. Additionally, they may be used to produce organodihaloboranes (RBX₂) (Darses & Genet, 2008). Seyferth & Grim (1961) showed that reaction of triphenylphosphinemethylene ylide (Ph₃PCH₂[−]) with boron trifluoride diethyletherate (BF₃·OEt₂) yields triphenyl[(trifluoroboranyl)methyl]phosphonium (Ph₃PCH₂BF₃). We have synthesized Ph₃PCH₂BF₃ *via* an alternate route, by reacting triphenylphosphine (PPh₃) with potassium iodomethyltrifluoroborate (ICH₂BF₃K) in 45% yield.



There are many examples of zwitterionic organotrifluoroborates containing ammonium moieties, but very few containing phosphonium groups have been reported (see *Database survey*). Phosphonium trifluoroborates have been shown to enhance the hydrolytic stability of the RBF₃ moiety (Wade *et al.*, 2010.) In this context we synthesized Ph₃PCH₂BF₃ and report herein its crystal structure.



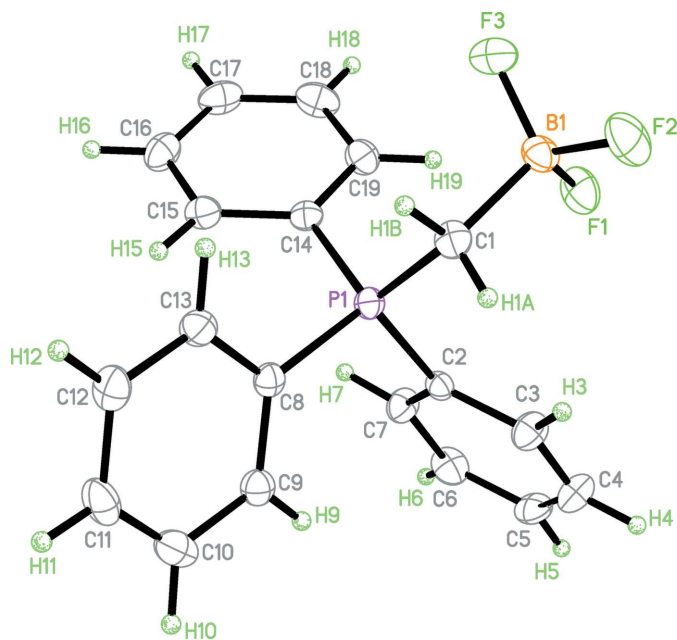


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. A weak intramolecular C—H...F hydrogen bond forms an *S*(7) ring (Table 1). The molecule features a nearly *anti* conformation along the P1—C1 bond [B1—C1—P1—C8 torsion angle = 172.4 (2)°] and a less staggered conformation along the C1—B1 bond [F2—B1—C1—P1 torsion angle = 158.3 (2)°].

The B—F bond lengths fall within normal ranges for organotrifluoroborate compounds. The methylene C—P bond length [1.787 (4) Å] and the C—B bond length [1.636 (4) Å] also fall within the normal range for similar compounds (Allen *et al.*, 1987). In terms of the surrounding angles, the B and P atoms appear to be *sp*³ hybridized. The methylene carbon is predominantly *sp*³ hybridized, but has a distorted tetrahedral geometry with a P1—C1—B1 angle of 119.7 (2)°.

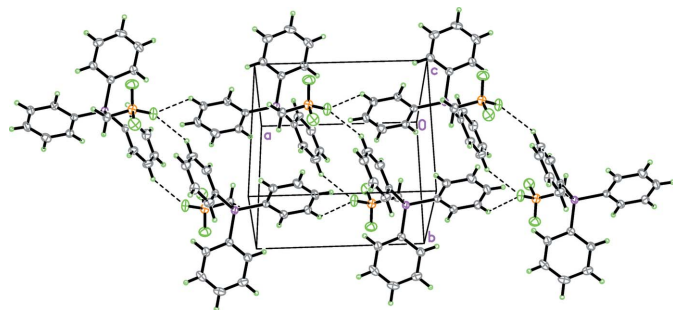


Figure 2
Part of the crystal structure, showing weak C—H...F hydrogen bonds as dashed lines.

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

Cg1 is the centroid of the C2—C7 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...F1 ⁱ	0.95 (3)	2.44 (2)	3.293 (4)	149.7 (17)
C12—H12...F1 ⁱⁱ	0.96 (3)	2.37 (3)	3.084 (3)	131 (2)
C19—H19...F1	0.97 (2)	2.43 (2)	3.263 (3)	143.9 (18)
C11—H11...Cg1 ⁱⁱ	0.89 (3)	2.77 (3)	3.639 (3)	165 (2)

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

3. Supramolecular features

In the crystal, two weak C—H...F hydrogen bonds between the *meta* hydrogen atoms on the triphenylphosphonium rings and the trifluoroborate moiety (Table 1) fall within the range of distances observed in other triphenylphosphonium trifluoroborates (Wade *et al.*, 2010) and form chains of *R*₂²(16) rings along the [100] axis (Fig. 2). These chains are further stabilized by herringbone edge-to-face weak C—H... π interactions (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update February 2017; Groom *et al.*, 2016) for phosphonium-containing trifluoroborates yielded only five structures: FUYDIN (Wade *et al.*, 2010), OZOJOD (Gott *et al.*, 2011), PUXWEL (Piskunov *et al.*, 2010), ZEKLEI (Li *et al.*, 2012) and ZEKLOS (Zibo *et al.*, 2012).

5. Synthesis and crystallization

Potassium iodomethyltrifluoroborate (1.00 g, 4.04 mmol) and triphenylphosphine (1.11 g, 4.23 mmol) were combined in a pressure flask containing a stir bar under nitrogen, and anhydrous THF (25.0 mL) was added. The flask was sealed and heated to 343 K for 18 h. The reaction was cooled to room temperature and the solvent was removed *in vacuo*. The residue was washed with Et₂O (3 x 10 mL) and the resulting solid was dissolved in a minimal amount of acetone and the product was precipitated with water and collected by filtration, to afford a white solid (0.63 g, 1.82 mmol, 45%). X-ray quality crystals were grown by slow diffusion of pentane into a solution of the title compound dissolved in dichloromethane.

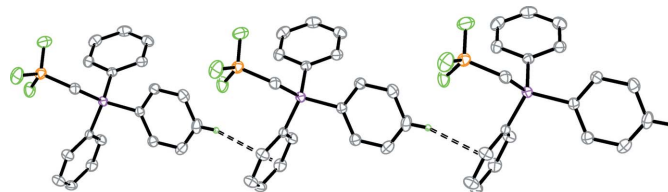


Figure 3
Part of the crystal structure, showing weak C—H... π interactions along [100] as dashed lines. Only the H atoms involved in these interactions are shown.

^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.66 (*m*, 9H), 7.56 (*m*, 6H), 2.07 (*br d*, 2H, $J = 15$ Hz). ^{13}C NMR (126 MHz, CDCl_3) δ (ppm): 133.7 (*d*, $J = 3$ Hz), 133.5 (*d*, $J = 10$ Hz), 129.6 (*d*, $J = 12$ Hz) 123.2 (*d*, $J = 87$ Hz) (C–B *not* observed). ^{11}B NMR (160 MHz, CDCl_3) δ (ppm): 2.49 (*q*, $J = 47$ Hz). ^{19}F NMR (470 MHz, CDCl_3) δ (ppm): -138.9 (*q*, $J = 37$ Hz). FTIR (ATR, cm^{-1}): 3070, 2960, 1587, 1484, 1438, 1146, 1104, 1025, 994, 969, 824, 754, 725, 691, 511, 497.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were refined independently with isotropic displacement parameters.

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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. & Orpen, A. G. (1987). *J. Chem. Soc. Perkin Trans 2*, pp. S1–S19.
- Bruker (2012). *APEX2*, *SAINT*, *SADABS* and *SHELXS97*. Bruker AXS inc., Madison, Wisconsin, USA.
- Darses, S. & Genet, J.-P. (2008). *Chem. Rev.* **108**, 288–325.
- Gott, A. L., Piers, W. E., Dutton, J. L., McDonald, R. & Parvez, M. (2011). *Organometallics*, **30**, 4236–4249.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Julia, M. (1985). *Pure Appl. Chem.* **57**, 763–768.
- Li, Z., Chansaenpak, K., Liu, S., Wade, C. R., Conti, P. S. & Gabbai, F. P. (2012). *Med. Chem. Commun.* **3**, 1305–1308.
- Piskunov, A. V., Mescheryakova, I. N., Fukin, G. K., Cherkasov, V. K. & Abakumov, G. A. (2010). *New J. Chem.* **34**, 1746–1750.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{19}\text{H}_{17}\text{BF}_3\text{P}$
M_r	344.10
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, b, c (Å)	9.514 (2), 9.870 (3), 9.883 (3)
α, β, γ (°)	64.609 (6), 87.539 (7), 86.660 (7)
V (Å ³)	836.8 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.19
Crystal size (mm)	0.13 × 0.07 × 0.01
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2012)
T_{\min} , T_{\max}	0.925, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11811, 2953, 2090
R_{int}	0.061
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.094, 1.02
No. of reflections	2953
No. of parameters	285
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.26, -0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* and *SHELXTL* (Sheldrick 2008) and *SHELXL2013* (Sheldrick 2015).

- Seyferth, D. & Grim, S. O. (1961). *J. Am. Chem. Soc.* **83**, 1613–1616.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Wade, C. R., Zhao, H. & Gabbai, F. (2010). *Chem. Commun.* **46**, 6830–6831.

supporting information

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Crystal structure of triphenylphosphoniummethylenetrifluoroborate

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Triphenylphosphoniummethylenetrifluoroborate

Crystal data

$C_{19}H_{17}BF_3P$	$Z = 2$
$M_r = 344.10$	$F(000) = 356$
Triclinic, $P\bar{1}$	$D_x = 1.366 \text{ Mg m}^{-3}$
$a = 9.514 (2) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 9.870 (3) \text{ \AA}$	Cell parameters from 2126 reflections
$c = 9.883 (3) \text{ \AA}$	$\theta = 2.3\text{--}23.9^\circ$
$\alpha = 64.609 (6)^\circ$	$\mu = 0.19 \text{ mm}^{-1}$
$\beta = 87.539 (7)^\circ$	$T = 173 \text{ K}$
$\gamma = 86.660 (7)^\circ$	Plate, colorless
$V = 836.8 (4) \text{ \AA}^3$	$0.13 \times 0.07 \times 0.01 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	2953 independent reflections
Radiation source: sealed tube	2090 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.061$
Absorption correction: multi-scan (SADABS; Bruker, 2012)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.925$, $T_{\text{max}} = 1.000$	$h = -11 \rightarrow 11$
11811 measured reflections	$k = -10 \rightarrow 11$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2]$
$wR(F^2) = 0.094$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2953 reflections	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
285 parameters	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
0 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.88100 (6)	0.18041 (7)	0.68950 (7)	0.01697 (18)
B1	0.6884 (3)	0.2752 (3)	0.8793 (3)	0.0230 (7)
F1	0.58103 (14)	0.26765 (16)	0.79007 (15)	0.0321 (4)
F2	0.66153 (16)	0.40289 (16)	0.90564 (16)	0.0385 (4)
F3	0.68558 (16)	0.14803 (16)	1.01567 (15)	0.0381 (4)
C1	0.8421 (3)	0.2870 (3)	0.7950 (3)	0.0208 (6)
C2	0.7769 (2)	0.2468 (2)	0.5241 (2)	0.0159 (5)
C3	0.7246 (3)	0.3952 (3)	0.4576 (3)	0.0244 (6)
C4	0.6496 (3)	0.4457 (3)	0.3269 (3)	0.0290 (6)
C5	0.6268 (3)	0.3508 (3)	0.2611 (3)	0.0260 (6)
C6	0.6785 (3)	0.2042 (3)	0.3260 (3)	0.0270 (6)
C7	0.7526 (3)	0.1511 (3)	0.4578 (3)	0.0227 (6)
C8	1.0645 (2)	0.1992 (2)	0.6332 (2)	0.0177 (5)
C9	1.1081 (3)	0.2542 (3)	0.4834 (3)	0.0208 (6)
C10	1.2509 (3)	0.2685 (3)	0.4467 (3)	0.0271 (6)
C11	1.3487 (3)	0.2274 (3)	0.5571 (3)	0.0282 (6)
C12	1.3064 (3)	0.1730 (3)	0.7066 (3)	0.0249 (6)
C13	1.1648 (2)	0.1596 (3)	0.7452 (3)	0.0224 (6)
C14	0.8521 (2)	-0.0170 (3)	0.7952 (2)	0.0175 (5)
C15	0.9617 (3)	-0.1247 (3)	0.8201 (3)	0.0221 (6)
C16	0.9361 (3)	-0.2760 (3)	0.8966 (3)	0.0276 (6)
C17	0.8011 (3)	-0.3208 (3)	0.9478 (3)	0.0296 (6)
C18	0.6919 (3)	-0.2144 (3)	0.9237 (3)	0.0293 (6)
C19	0.7161 (3)	-0.0636 (3)	0.8475 (3)	0.0234 (6)
H1A	0.860 (3)	0.389 (3)	0.727 (3)	0.034 (8)*
H1B	0.913 (3)	0.256 (3)	0.864 (3)	0.036 (8)*
H3	0.736 (3)	0.457 (3)	0.510 (3)	0.048 (8)*
H4	0.616 (2)	0.547 (3)	0.282 (2)	0.024 (7)*
H5	0.578 (2)	0.385 (3)	0.171 (3)	0.029 (7)*
H6	0.662 (3)	0.139 (3)	0.281 (3)	0.032 (7)*
H7	0.785 (2)	0.043 (3)	0.508 (2)	0.022 (6)*
H9	1.043 (2)	0.282 (2)	0.404 (2)	0.019 (6)*
H10	1.279 (2)	0.310 (3)	0.342 (3)	0.030 (7)*
H11	1.441 (3)	0.233 (3)	0.535 (3)	0.028 (7)*
H12	1.374 (3)	0.148 (3)	0.784 (3)	0.039 (8)*
H13	1.135 (2)	0.119 (2)	0.851 (3)	0.024 (6)*
H15	1.055 (2)	-0.099 (2)	0.789 (2)	0.020 (6)*
H16	1.014 (3)	-0.352 (3)	0.915 (3)	0.036 (7)*
H17	0.785 (3)	-0.429 (3)	1.000 (3)	0.042 (8)*

H18	0.603 (3)	-0.246 (3)	0.958 (3)	0.032 (7)*
H19	0.639 (2)	0.011 (3)	0.829 (2)	0.023 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0150 (3)	0.0181 (4)	0.0176 (3)	-0.0004 (2)	-0.0011 (2)	-0.0073 (3)
B1	0.0240 (16)	0.0278 (18)	0.0209 (15)	0.0002 (13)	-0.0003 (12)	-0.0141 (13)
F1	0.0175 (7)	0.0438 (10)	0.0395 (9)	0.0008 (6)	-0.0033 (6)	-0.0220 (8)
F2	0.0425 (9)	0.0369 (10)	0.0466 (10)	-0.0011 (7)	0.0079 (7)	-0.0287 (8)
F3	0.0475 (10)	0.0350 (9)	0.0237 (8)	0.0007 (7)	0.0056 (7)	-0.0058 (7)
C1	0.0199 (13)	0.0252 (16)	0.0203 (13)	-0.0003 (11)	-0.0050 (11)	-0.0123 (12)
C2	0.0132 (12)	0.0185 (14)	0.0163 (12)	-0.0006 (10)	0.0006 (9)	-0.0078 (10)
C3	0.0286 (14)	0.0200 (15)	0.0252 (13)	-0.0005 (11)	-0.0048 (11)	-0.0100 (12)
C4	0.0344 (16)	0.0198 (16)	0.0270 (14)	0.0022 (12)	-0.0058 (12)	-0.0044 (12)
C5	0.0255 (14)	0.0309 (17)	0.0167 (13)	-0.0010 (12)	-0.0047 (11)	-0.0051 (12)
C6	0.0273 (14)	0.0368 (17)	0.0250 (14)	-0.0013 (12)	-0.0035 (11)	-0.0205 (13)
C7	0.0283 (14)	0.0198 (15)	0.0220 (13)	0.0021 (11)	-0.0040 (11)	-0.0108 (12)
C8	0.0173 (12)	0.0140 (13)	0.0212 (12)	-0.0012 (10)	-0.0003 (10)	-0.0069 (10)
C9	0.0215 (13)	0.0191 (14)	0.0224 (13)	-0.0003 (10)	-0.0006 (11)	-0.0093 (11)
C10	0.0301 (15)	0.0254 (16)	0.0269 (15)	-0.0053 (12)	0.0085 (12)	-0.0124 (12)
C11	0.0174 (14)	0.0246 (16)	0.0433 (17)	-0.0053 (11)	0.0070 (13)	-0.0153 (13)
C12	0.0182 (14)	0.0222 (15)	0.0332 (15)	-0.0034 (11)	-0.0032 (12)	-0.0102 (12)
C13	0.0190 (13)	0.0228 (14)	0.0221 (13)	-0.0027 (10)	0.0001 (11)	-0.0063 (11)
C14	0.0188 (12)	0.0195 (14)	0.0152 (12)	-0.0023 (10)	-0.0021 (9)	-0.0081 (10)
C15	0.0210 (14)	0.0238 (15)	0.0205 (13)	-0.0042 (11)	-0.0007 (11)	-0.0082 (11)
C16	0.0343 (16)	0.0196 (15)	0.0277 (14)	0.0022 (12)	-0.0050 (12)	-0.0091 (12)
C17	0.0448 (18)	0.0187 (16)	0.0238 (14)	-0.0086 (13)	0.0007 (12)	-0.0070 (12)
C18	0.0292 (16)	0.0316 (17)	0.0293 (15)	-0.0142 (13)	0.0073 (12)	-0.0145 (13)
C19	0.0192 (13)	0.0257 (15)	0.0264 (14)	-0.0030 (12)	0.0012 (11)	-0.0120 (12)

Geometric parameters (Å, °)

P1—C1	1.787 (2)	C8—C13	1.401 (3)
P1—C2	1.796 (2)	C9—C10	1.390 (3)
P1—C8	1.805 (2)	C9—H9	0.96 (2)
P1—C14	1.804 (2)	C10—C11	1.373 (4)
B1—F3	1.394 (3)	C10—H10	0.96 (2)
B1—F2	1.400 (3)	C11—C12	1.388 (4)
B1—F1	1.404 (3)	C11—H11	0.89 (2)
B1—C1	1.636 (4)	C12—C13	1.383 (3)
C1—H1A	0.96 (3)	C12—H12	0.95 (3)
C1—H1B	0.92 (3)	C13—H13	0.99 (2)
C2—C3	1.394 (3)	C14—C15	1.395 (3)
C2—C7	1.395 (3)	C14—C19	1.401 (3)
C3—C4	1.383 (3)	C15—C16	1.385 (3)
C3—H3	0.97 (3)	C15—H15	0.94 (2)
C4—C5	1.380 (4)	C16—C17	1.385 (4)

C4—H4	0.95 (2)	C16—H16	0.99 (3)
C5—C6	1.377 (4)	C17—C18	1.385 (4)
C5—H5	0.94 (2)	C17—H17	0.99 (3)
C6—C7	1.385 (3)	C18—C19	1.378 (3)
C6—H6	0.95 (2)	C18—H18	0.92 (3)
C7—H7	1.00 (2)	C19—H19	0.97 (2)
C8—C9	1.394 (3)		
C1—P1—C2	111.67 (12)	C9—C8—C13	119.8 (2)
C1—P1—C8	108.25 (11)	C9—C8—P1	122.17 (18)
C2—P1—C8	108.48 (10)	C13—C8—P1	118.04 (17)
C1—P1—C14	113.04 (12)	C10—C9—C8	119.6 (2)
C2—P1—C14	107.54 (10)	C10—C9—H9	117.9 (13)
C8—P1—C14	107.70 (11)	C8—C9—H9	122.5 (13)
F3—B1—F2	109.0 (2)	C11—C10—C9	120.4 (2)
F3—B1—F1	108.4 (2)	C11—C10—H10	121.1 (14)
F2—B1—F1	108.5 (2)	C9—C10—H10	118.5 (14)
F3—B1—C1	110.9 (2)	C10—C11—C12	120.6 (2)
F2—B1—C1	109.1 (2)	C10—C11—H11	121.3 (15)
F1—B1—C1	110.84 (19)	C12—C11—H11	118.1 (15)
B1—C1—P1	119.66 (17)	C13—C12—C11	119.9 (2)
B1—C1—H1A	111.2 (15)	C13—C12—H12	119.0 (15)
P1—C1—H1A	105.1 (15)	C11—C12—H12	121.1 (15)
B1—C1—H1B	110.3 (16)	C12—C13—C8	119.8 (2)
P1—C1—H1B	103.3 (16)	C12—C13—H13	120.1 (13)
H1A—C1—H1B	106 (2)	C8—C13—H13	120.1 (13)
C3—C2—C7	119.4 (2)	C15—C14—C19	119.2 (2)
C3—C2—P1	120.63 (17)	C15—C14—P1	121.19 (17)
C7—C2—P1	119.90 (17)	C19—C14—P1	119.50 (18)
C4—C3—C2	119.7 (2)	C16—C15—C14	120.3 (2)
C4—C3—H3	122.1 (16)	C16—C15—H15	117.2 (14)
C2—C3—H3	118.0 (16)	C14—C15—H15	122.5 (14)
C5—C4—C3	120.6 (3)	C17—C16—C15	120.0 (3)
C5—C4—H4	120.7 (14)	C17—C16—H16	120.0 (15)
C3—C4—H4	118.7 (14)	C15—C16—H16	120.0 (15)
C6—C5—C4	120.0 (2)	C16—C17—C18	120.1 (3)
C6—C5—H5	118.9 (15)	C16—C17—H17	118.8 (15)
C4—C5—H5	121.1 (15)	C18—C17—H17	121.2 (15)
C5—C6—C7	120.3 (2)	C19—C18—C17	120.4 (3)
C5—C6—H6	119.8 (15)	C19—C18—H18	120.3 (16)
C7—C6—H6	119.9 (15)	C17—C18—H18	119.2 (16)
C6—C7—C2	120.0 (2)	C18—C19—C14	120.0 (2)
C6—C7—H7	120.3 (13)	C18—C19—H19	120.6 (13)
C2—C7—H7	119.6 (13)	C14—C19—H19	119.4 (13)
F3—B1—C1—P1	81.6 (2)	C2—P1—C8—C13	177.28 (18)
F2—B1—C1—P1	-158.33 (17)	C14—P1—C8—C13	-66.6 (2)
F1—B1—C1—P1	-38.9 (3)	C13—C8—C9—C10	0.4 (3)

C2—P1—C1—B1	68.2 (2)	P1—C8—C9—C10	178.94 (18)
C8—P1—C1—B1	-172.42 (19)	C8—C9—C10—C11	0.6 (4)
C14—P1—C1—B1	-53.2 (2)	C9—C10—C11—C12	-0.8 (4)
C1—P1—C2—C3	25.8 (2)	C10—C11—C12—C13	0.1 (4)
C8—P1—C2—C3	-93.4 (2)	C11—C12—C13—C8	0.8 (4)
C14—P1—C2—C3	150.38 (18)	C9—C8—C13—C12	-1.1 (3)
C1—P1—C2—C7	-156.73 (19)	P1—C8—C13—C12	-179.71 (19)
C8—P1—C2—C7	84.1 (2)	C1—P1—C14—C15	-119.9 (2)
C14—P1—C2—C7	-32.2 (2)	C2—P1—C14—C15	116.40 (19)
C7—C2—C3—C4	-0.1 (4)	C8—P1—C14—C15	-0.3 (2)
P1—C2—C3—C4	177.32 (19)	C1—P1—C14—C19	63.0 (2)
C2—C3—C4—C5	-0.3 (4)	C2—P1—C14—C19	-60.7 (2)
C3—C4—C5—C6	0.2 (4)	C8—P1—C14—C19	-177.42 (18)
C4—C5—C6—C7	0.5 (4)	C19—C14—C15—C16	-0.4 (3)
C5—C6—C7—C2	-1.0 (4)	P1—C14—C15—C16	-177.49 (18)
C3—C2—C7—C6	0.8 (4)	C14—C15—C16—C17	0.4 (4)
P1—C2—C7—C6	-176.70 (18)	C15—C16—C17—C18	-0.5 (4)
C1—P1—C8—C9	-122.6 (2)	C16—C17—C18—C19	0.6 (4)
C2—P1—C8—C9	-1.3 (2)	C17—C18—C19—C14	-0.6 (4)
C14—P1—C8—C9	114.8 (2)	C15—C14—C19—C18	0.5 (3)
C1—P1—C8—C13	55.9 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the centroid of the C2–C7 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 \cdots F1 ⁱ	0.95 (3)	2.44 (2)	3.293 (4)	149.7 (17)
C12—H12 \cdots F1 ⁱⁱ	0.96 (3)	2.37 (3)	3.084 (3)	131 (2)
C19—H19 \cdots F1	0.97 (2)	2.43 (2)	3.263 (3)	143.9 (18)
C11—H11 \cdots Cg ⁱⁱ	0.89 (3)	2.77 (3)	3.639 (3)	165 (2)

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