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Synthesis and crystal structures of $[Ph_3PCH_2PPh_3]I_2$ dichloromethane disolvate and $[Ph_3PCH_2PPh_3](BI_4)_2$

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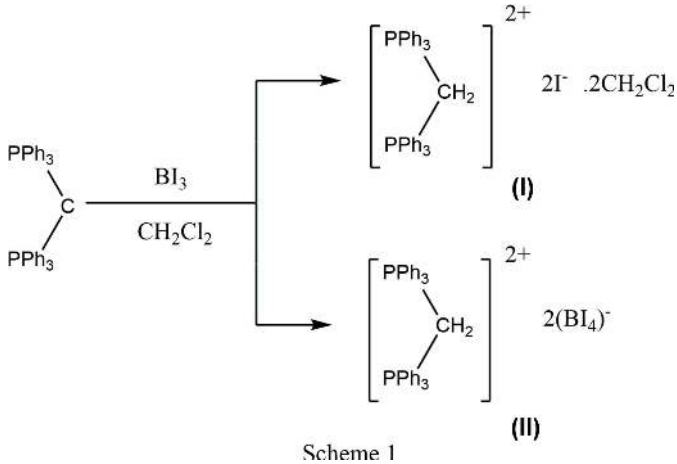
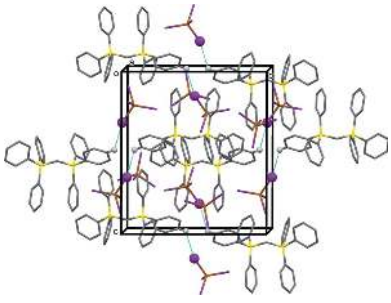
Reaction of BI_3 with carbodiphosphorane, $C(PPh_3)_2$, gives a mixture of the dicationic compounds, methylenebis(triphenylphosphonium) diiodide dichloromethane disolvate, $C_{37}H_{32}P_2^{2+}\cdot 2I^-\cdot 2CH_2Cl_2$ or $[Ph_3PCH_2PPh_3]I_2\cdot 2CH_2Cl_2$ (**I**), methylenebis(triphenylphosphonium) bis(tetraiodoborate), $C_{37}H_{32}P_2^{2+}\cdot 2BI_4^-$ or $[Ph_3PCH_2PPh_3](BI_4)_2$ (**II**). Solvents are the source of the protons at the ylidic C atom. The P—C—P angle is 124.1 (2)° for (**I**) and 121.7 (3)° for (**II**), while the two P—C bond lengths are 1.804 (4) and 1.807 (5) Å in (**I**), and 1.817 (5) and 1.829 (5) Å in (**II**). In the crystal of (**I**), the protons of the central $P—CH_2—P$ C atom exhibit weak C—H···I hydrogen bonds with the respective anions. The anions in turn are linked to the dichloromethane solvent molecules by C—H···I hydrogen bonds. In the crystal of (**II**), one of the BI_4^- anions is linked to a phenyl H atom *via* a weak C—H···I hydrogen bond.

1. Chemical context

Carbodiphosphoranes, $C(PH_3)_2$, have been known since the early 1960s (Ramirez *et al.*, 1961), but recent theoretical and experimental investigations has revived interest in these compounds (Tay *et al.*, 2016; Dordevic *et al.*, 2016). Theoretical studies (Frenking & Tonner, 2009) show the presence of two lone pairs of electrons, σ and π, which can act both as σ- and π-donor substituents (Tay *et al.*, 2013). Herein, we report on the crystal structures of two dicationic carbodiphophorane species, *viz.* $[Ph_3PCH_2PPh_3]I_2\cdot 2CH_2Cl_2$, (**I**), and $[Ph_3PCH_2PPh_3](BI_4)_2$, (**II**).



Scheme 1



2. Structural commentary

Compound $[Ph_3PCH_2PPh_3]I_2$, (**I**), crystallizes as a dichloromethane disolvate (Fig. 1), whereas compound (**II**) is not

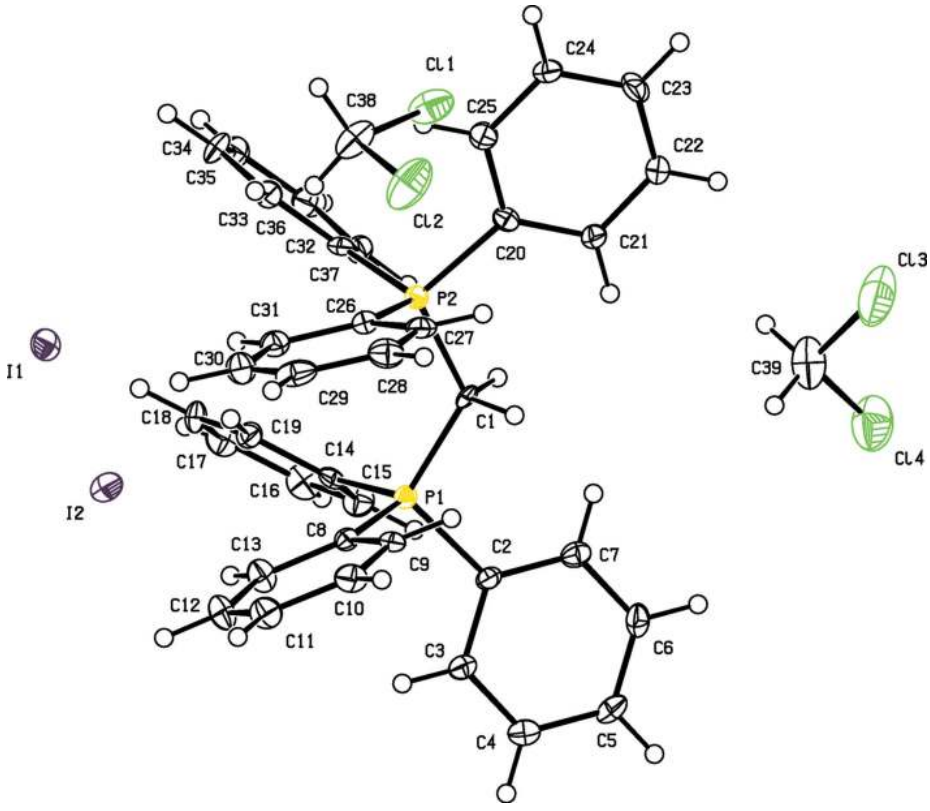


Figure 1
The molecular structure of compound (**I**), showing the atom labelling and 40% probability displacement ellipsoids.

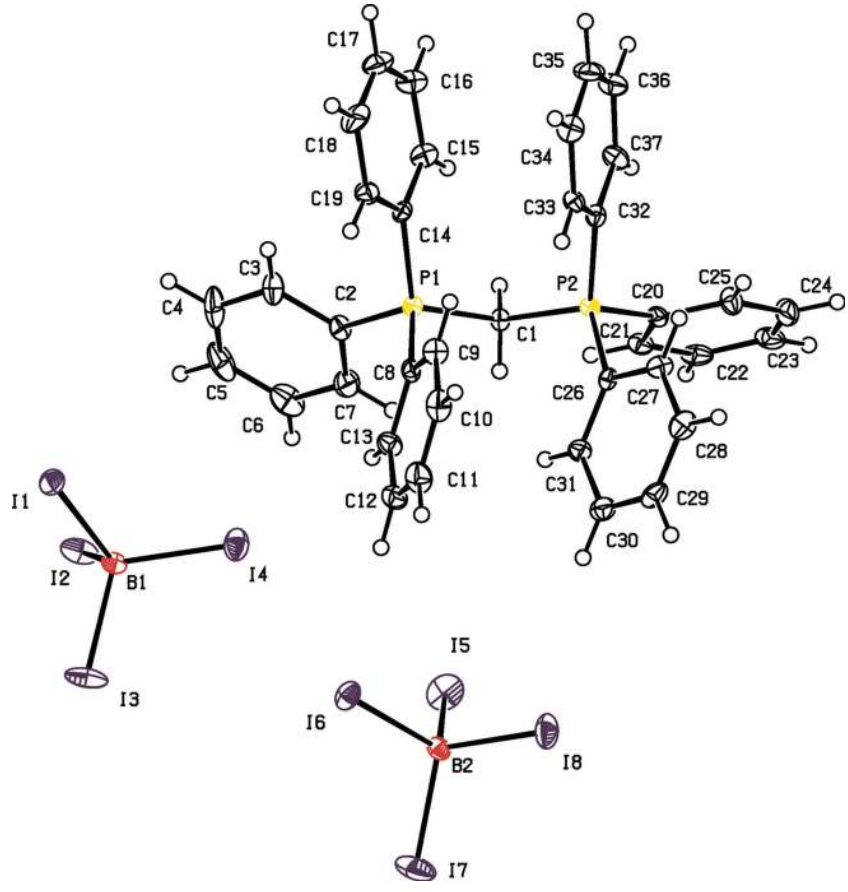


Figure 2
The molecular structure of compound (**II**), showing the atom labelling and 40% probability displacement ellipsoids.

Table 1
Selected geometric parameters (Å, °) for (**I**).

C1—P2	1.804 (4)	C1—P1	1.807 (5)
P1—C1—P2	124.1 (2)		

Table 2
Selected geometric parameters (Å, °) for (**II**).

C1—P2	1.817 (5)	C1—P1	1.829 (5)
P1—C1—P2	121.7 (3)		

Table 3
Hydrogen-bond geometry (Å, °) for (**I**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···I1^{i}	0.99	2.81	3.802 (4)	175
C39—H39*A*···I1^{i}	0.99	3.05	3.986 (7)	159
C1—H1*B*···I2^{i}	0.99	2.83	3.813 (4)	175
C38—H38*B*···I2^{ii}	0.99	2.88	3.848 (6)	166

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

solvated (Fig. 2). For both compounds, the C2/P1/C1/P2/C20 fragment lies in a plane, as shown in Figs. 1 and 2, respectively, with the P1—C1—P2 angle being 124.1 (2)° for (**I**) and 121.7 (3)° for (**II**); see Tables 1 and 2. Such a conformation avoids any significant steric repulsion between the phenyl groups on the adjacent P atoms. The smaller value in compound (**II**) is attributed to decreased steric repulsion and/or an absence of electrostatic repulsion (Walker & Poli, 1989). The P—C bond lengths in compound (**I**) are slightly shorter than those in compound (**II**); see Tables 1 and 2. In (**II**), the BI_4^- anions display regular tetrahedral geometry, with I—B—I angles ranging from 108.1 (3) to 110.9 (3)°.

3. Supramolecular features

In the crystal of (**I**), the iodide anion I1 forms weak hydrogen bonds with atoms H1*A* and H39*A*, while iodide anion I2 forms another pair of weak hydrogen bonds with atoms H1*B* and H38*B*, as shown in Table 3 and Fig. 3. In the crystal of (**II**), a single C—H···I hydrogen bond is observed linking an anion to the $[Ph_3PCH_2PPh_3]^{2+}$ unit (Table 4 and Fig. 4).

4. Database survey

A search of the Cambridge Structural Database (Version 5.38, last update May 2016; Groom *et al.*, 2016) revealed eight

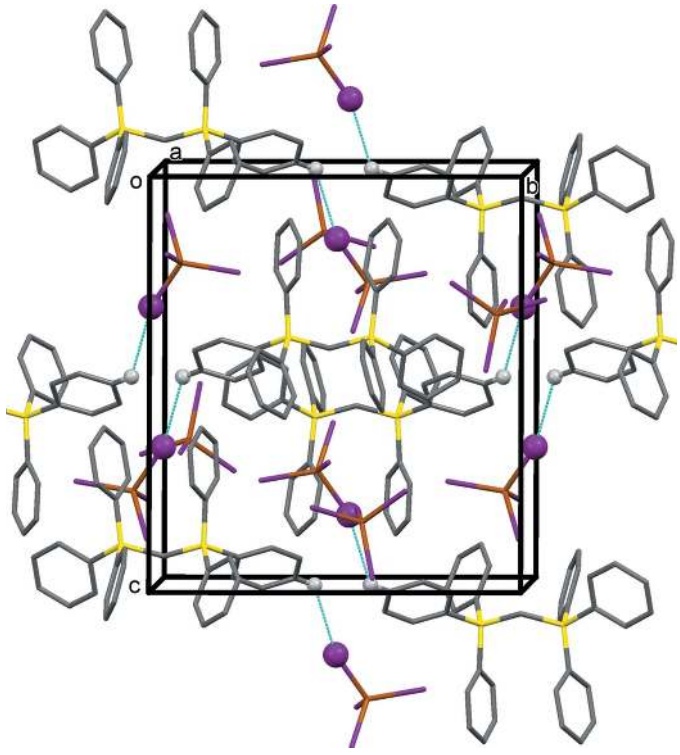


Figure 4
A view along the *a* axis of the crystal packing of compound (**II**). Only the H atom (grey ball) participating in hydrogen bonding (dashed lines) has been included (see Table 4).

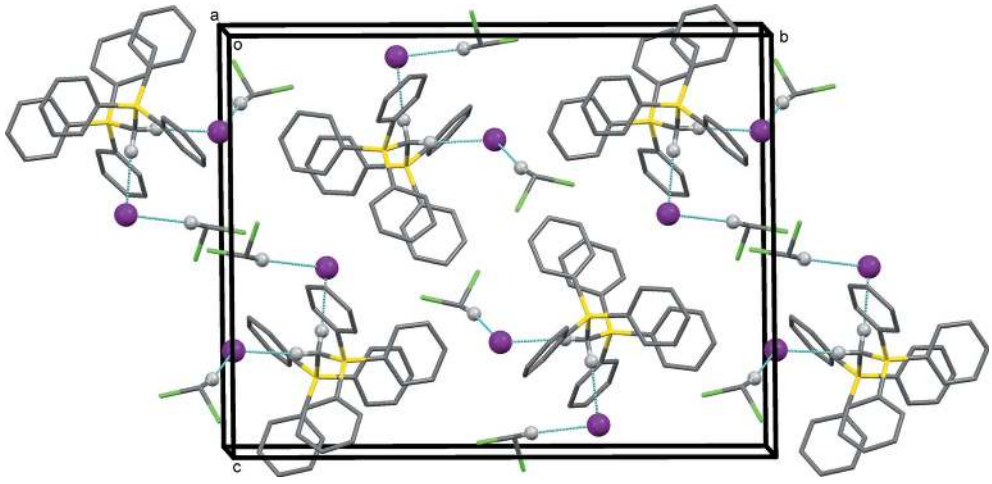


Figure 3
A view along the *a* axis of the crystal packing of compound (**I**). Only the H atoms (grey balls) participating in hydrogen bonding (dashed lines) have been included (see Table 3).

Table 4
Hydrogen-bond geometry (Å, °) for (**II**).

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···I1^{i}	0.95	3.02	3.730 (7)	132

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

reported structures of the dicationic species, which all show similar conformations. In these eight structures, the P—C—P angle varies from *ca* 120.89 to 123.35°, while the P—C bond lengths vary from *ca* 1.802 to 1.833 Å. The smallest P—C—P angle and the shortest P—C bond length, *ca* 120.89° and 1.802 Å, respectively, are observed in methylenebis(triphenylphosphonium) dichloride 1,2-dimethoxyethane monosolvate (CSD refcode CADZUE; Petz *et al.*, 2011). While one of the largest P—C—P angles (*ca* 123.11°) and longest P—C bond lengths (*ca* 1.825 Å) were observed for methylenebis(triphenylphosphonium) bis(tetrachloroindium) dichloromethane monosolvate (CIYGIB; Petz *et al.*, 2008). Interestingly, in compound (**I**), the P—C bond lengths are short [1.804 (4) and 1.807 (5) Å], while the P—C—P angle [124.1 (2)°] is one of the largest observed to date.

5. Synthesis and crystallization

$(Ph_3)_2C$ (0.1 g, 0.19 mmol) and 1 equivalent of BI_3 were mixed in *ca* 10 ml of DCM and left to stir overnight under inert conditions. The volume of the resulting solution was reduced to *ca* 3 ml and layered with *ca* 5 ml of hexane. A crop of crystals formed in a few days [yield 0.02 g, 4% based on $(PPh_3)_2C$, for (**I**) and 0.015 g, 5% based on $(PPh_3)_2C$, for (**II**)].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. The H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C). For both compounds, a small number of reflections were affected by the beam stop and were omitted from the final cycles of refinement.

Acknowledgements

RG thanks the CBC, Nanyang Technological University, for the instrument facilities.

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Table 5
Experimental details.

	(**I**)	(**II**)
Crystal data		
Chemical formula	$C_{37}H_{32}P_2^{2+}\cdot 2I^-\cdot 2CH_2Cl_2$	$C_{37}H_{32}P_2^{2+}\cdot 2BI_4^-$
M_r	962.22	1575.38
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	153	153
a, b, c (Å)	9.7510 (13), 22.914 (3), 18.204 (2)	19.7878 (6), 14.3122 (3), 16.0646 (4)
β (°)	104.629 (2)	96.230 (1)
V (Å^3)	3935.5 (9)	4522.7 (2)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.98	5.58
Crystal size (mm)	0.14 × 0.12 × 0.06	0.14 × 0.12 × 0.08
Data collection		
Diffractometer	Bruker CCD area detector	Bruker CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.74, 0.89	0.51, 0.66
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18605, 7318, 5579	52611, 14486, 9439
R_{int}	0.050	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.607	0.727
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.083, 1.05	0.045, 0.124, 0.92
No. of reflections	7318	14486
No. of parameters	424	442
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.71	2.32, −2.11

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2017). E**73**, 1259-1263 [https://doi.org/10.1107/S2056989017010295]

Synthesis and crystal structures of $[Ph_3PCH_2PPh_3]I_2$ dichloromethane disolvate and $[Ph_3PCH_2PPh_3](BI_4)_2$

Rakesh Ganguly and Violeta Jevtovic

Computing details

For both structures, data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Methylenebis(triphenylphosphonium) diiodide dichloromethane disolvate (I)

Crystal data

$C_{37}H_{32}P_2^{2+}\cdot 2I^-\cdot 2CH_2Cl_2$
M_r = 962.22
Monoclinic, $P2_1/c$
a = 9.7510 (13) Å
b = 22.914 (3) Å
c = 18.204 (2) Å
β = 104.629 (2)°
V = 3935.5 (9) Å^3
Z = 4
$F(000)$ = 1896
D_x = 1.624 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3861 reflections
θ = 2.8–24.4°
μ = 1.98 mm^{-1}
T = 153 K
Plate, colourless
0.14 × 0.12 × 0.06 mm

Data collection

CCD area detector diffractometer
Radiation source: fine-focus sealed tube, Bruker KappaCCD
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.74, T_{max} = 0.89
18605 measured reflections
7318 independent reflections
5579 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.5°, θ_{min} = 2.7°
h = −11→11
k = −27→27
l = −22→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.083
S = 1.05
7318 reflections
424 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0157P)^2 + 9.1897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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.

Refinement. (**I**: reflections 0 0 2, 1 0 0, 0 2 1, 1 1 0, -1 1 1, 0 2 0, 1 1 1, -1 2 4, -1 2 1 and 0 1 1, were affected by the beam stop and omitted from the final cycles of refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5915 (5)	0.66498 (19)	0.7366 (2)	0.0139 (10)
H1A	0.5834	0.6725	0.7889	0.017*
H1B	0.6265	0.6245	0.7362	0.017*
C2	0.3140 (5)	0.6175 (2)	0.7224 (3)	0.0179 (11)
C3	0.1671 (5)	0.6199 (2)	0.6984 (3)	0.0233 (12)
H3	0.1225	0.6458	0.6588	0.028*
C4	0.0859 (6)	0.5846 (2)	0.7323 (3)	0.0278 (13)
H4	−0.0146	0.5861	0.716	0.033*
C5	0.1509 (6)	0.5470 (2)	0.7900 (3)	0.0262 (13)
H5	0.095	0.5231	0.8137	0.031*
C6	0.2969 (6)	0.5441 (2)	0.8133 (3)	0.0247 (12)
H6	0.3414	0.5181	0.8528	0.03*
C7	0.3787 (6)	0.5791 (2)	0.7789 (3)	0.0221 (12)
H7	0.4791	0.5767	0.7943	0.026*
C8	0.3361 (5)	0.73662 (19)	0.6724 (3)	0.0160 (11)
C9	0.3560 (5)	0.7676 (2)	0.7407 (3)	0.0196 (11)
H9	0.4129	0.7519	0.7866	0.024*
C10	0.2921 (5)	0.8211 (2)	0.7402 (3)	0.0243 (12)
H10	0.3057	0.8423	0.7863	0.029*
C11	0.2087 (6)	0.8445 (2)	0.6744 (3)	0.0273 (13)
H11	0.1668	0.8819	0.6749	0.033*
C12	0.1868 (6)	0.8138 (2)	0.6085 (3)	0.0297 (13)
H12	0.1274	0.8295	0.5632	0.036*
C13	0.2501 (6)	0.7597 (2)	0.6065 (3)	0.0249 (12)
H13	0.2344	0.7387	0.5602	0.03*
C14	0.4079 (5)	0.6383 (2)	0.5839 (3)	0.0178 (11)
C15	0.3739 (6)	0.5799 (2)	0.5665 (3)	0.0265 (13)
H15	0.3481	0.5552	0.6028	0.032*
C16	0.3778 (6)	0.5583 (2)	0.4965 (3)	0.0296 (13)
H16	0.354	0.5186	0.4845	0.036*
C17	0.4160 (6)	0.5938 (2)	0.4434 (3)	0.0292 (13)
H17	0.4191	0.5784	0.3954	0.035*
C18	0.4496 (6)	0.6514 (2)	0.4606 (3)	0.0262 (13)
H18	0.475	0.6757	0.4238	0.031*
C19	0.4469 (5)	0.6746 (2)	0.5305 (3)	0.0202 (11)
H19	0.471	0.7143	0.5421	0.024*
C20	0.8846 (5)	0.6956 (2)	0.7980 (3)	0.0176 (11)

C21	0.8860 (5)	0.6523 (2)	0.8515 (3)	0.0212 (11)
H21	0.8018	0.6315	0.8516	0.025*
C22	1.0114 (6)	0.6397 (2)	0.9046 (3)	0.0249 (12)
H22	1.0131	0.6097	0.9408	0.03*
C23	1.1341 (6)	0.6703 (2)	0.9056 (3)	0.0269 (13)
H23	1.2197	0.6613	0.9423	0.032*
C24	1.1314 (6)	0.7142 (2)	0.8528 (3)	0.0264 (12)
H24	1.215	0.7357	0.8538	0.032*
C25	1.0084 (6)	0.7266 (2)	0.7991 (3)	0.0256 (12)
H25	1.0074	0.7564	0.7626	0.031*
C26	0.6846 (5)	0.7867 (2)	0.7281 (3)	0.0172 (11)
C27	0.7029 (5)	0.8101 (2)	0.8007 (3)	0.0226 (12)
H27	0.7453	0.7875	0.8442	0.027*
C28	0.6589 (6)	0.8667 (2)	0.8089 (3)	0.0292 (13)
H28	0.6709	0.883	0.8581	0.035*
C29	0.5976 (6)	0.8995 (2)	0.7454 (3)	0.0318 (14)
H29	0.5678	0.9383	0.751	0.038*
C30	0.5794 (6)	0.8761 (2)	0.6738 (3)	0.0315 (14)
H30	0.5378	0.8992	0.6306	0.038*
C31	0.6212 (5)	0.8193 (2)	0.6641 (3)	0.0238 (12)
H31	0.6067	0.803	0.6147	0.029*
C32	0.7769 (5)	0.6952 (2)	0.6357 (3)	0.0195 (11)
C33	0.8345 (5)	0.7377 (2)	0.5967 (3)	0.0235 (12)
H33	0.8408	0.7771	0.6132	0.028*
C34	0.8822 (6)	0.7217 (2)	0.5340 (3)	0.0309 (14)
H34	0.9199	0.7505	0.5071	0.037*
C35	0.8754 (6)	0.6651 (2)	0.5106 (3)	0.0281 (13)
H35	0.9083	0.6548	0.4675	0.034*
C36	0.8204 (6)	0.6220 (2)	0.5494 (3)	0.0294 (13)
H36	0.8179	0.5824	0.5336	0.035*
C37	0.7700 (5)	0.6376 (2)	0.6108 (3)	0.0210 (11)
H37	0.73	0.6087	0.6364	0.025*
C38	0.9861 (7)	0.9392 (3)	0.8330 (3)	0.0417 (16)
H38A	0.899	0.9367	0.791	0.05*
H38B	1.0557	0.9634	0.8154	0.05*
C39	0.7581 (8)	0.5313 (3)	0.9713 (3)	0.0547 (19)
H39A	0.6844	0.562	0.9607	0.066*
H39B	0.7995	0.5288	0.927	0.066*
Cl1	1.05582 (17)	0.86895 (7)	0.85465 (9)	0.0467 (4)
Cl2	0.9455 (2)	0.97306 (7)	0.91165 (10)	0.0580 (5)
Cl3	0.8912 (3)	0.55037 (10)	1.05242 (10)	0.0822 (7)
Cl4	0.6801 (2)	0.46429 (8)	0.98340 (10)	0.0677 (6)
I1	0.44524 (4)	0.31630 (2)	0.06172 (2)	0.02704 (10)
I2	0.28004 (4)	0.49269 (2)	0.25393 (2)	0.02568 (10)
P1	0.41286 (14)	0.66527 (5)	0.67665 (7)	0.0155 (3)
P2	0.73153 (14)	0.71173 (5)	0.72243 (7)	0.0155 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.018 (3)	0.015 (2)	0.012 (2)	0.000 (2)	0.011 (2)	−0.0007 (18)
C2	0.016 (3)	0.021 (3)	0.018 (3)	−0.003 (2)	0.007 (2)	0.000 (2)
C3	0.019 (3)	0.027 (3)	0.026 (3)	0.001 (2)	0.010 (3)	0.004 (2)
C4	0.020 (3)	0.033 (3)	0.032 (3)	−0.004 (2)	0.007 (3)	0.002 (2)
C5	0.028 (3)	0.025 (3)	0.031 (3)	−0.006 (2)	0.016 (3)	0.003 (2)
C6	0.033 (3)	0.027 (3)	0.016 (3)	0.004 (2)	0.007 (3)	0.004 (2)
C7	0.021 (3)	0.025 (3)	0.023 (3)	0.000 (2)	0.010 (3)	−0.003 (2)
C8	0.015 (3)	0.014 (2)	0.019 (3)	−0.003 (2)	0.004 (2)	0.0011 (19)
C9	0.011 (3)	0.027 (3)	0.020 (3)	0.000 (2)	0.003 (2)	0.002 (2)
C10	0.023 (3)	0.029 (3)	0.022 (3)	0.000 (2)	0.007 (3)	−0.009 (2)
C11	0.029 (3)	0.020 (3)	0.034 (3)	0.006 (2)	0.010 (3)	0.000 (2)
C12	0.031 (3)	0.027 (3)	0.028 (3)	0.007 (3)	0.001 (3)	0.007 (2)
C13	0.030 (3)	0.026 (3)	0.017 (3)	0.006 (2)	0.004 (3)	−0.006 (2)
C14	0.011 (3)	0.022 (3)	0.017 (3)	−0.001 (2)	−0.002 (2)	−0.001 (2)
C15	0.028 (3)	0.023 (3)	0.028 (3)	−0.005 (2)	0.006 (3)	−0.002 (2)
C16	0.035 (4)	0.021 (3)	0.031 (3)	−0.002 (2)	0.004 (3)	−0.008 (2)
C17	0.031 (3)	0.037 (3)	0.019 (3)	0.002 (3)	0.004 (3)	−0.010 (2)
C18	0.029 (3)	0.040 (3)	0.010 (2)	0.000 (3)	0.005 (2)	0.005 (2)
C19	0.020 (3)	0.022 (3)	0.019 (3)	−0.003 (2)	0.005 (2)	0.001 (2)
C20	0.016 (3)	0.018 (2)	0.019 (3)	0.002 (2)	0.003 (2)	−0.002 (2)
C21	0.017 (3)	0.027 (3)	0.019 (3)	−0.004 (2)	0.004 (2)	0.003 (2)
C22	0.023 (3)	0.030 (3)	0.021 (3)	0.000 (2)	0.005 (3)	0.008 (2)
C23	0.021 (3)	0.038 (3)	0.018 (3)	0.003 (3)	−0.003 (2)	0.001 (2)
C24	0.016 (3)	0.039 (3)	0.025 (3)	−0.004 (2)	0.006 (3)	0.004 (2)
C25	0.021 (3)	0.032 (3)	0.022 (3)	−0.006 (2)	0.002 (3)	0.002 (2)
C26	0.016 (3)	0.017 (2)	0.019 (3)	−0.001 (2)	0.006 (2)	−0.001 (2)
C27	0.013 (3)	0.027 (3)	0.029 (3)	−0.002 (2)	0.006 (2)	0.001 (2)
C28	0.025 (3)	0.030 (3)	0.032 (3)	−0.004 (3)	0.006 (3)	−0.007 (2)
C29	0.025 (3)	0.020 (3)	0.056 (4)	−0.003 (2)	0.020 (3)	−0.004 (3)
C30	0.029 (3)	0.026 (3)	0.039 (3)	0.005 (3)	0.009 (3)	0.011 (3)
C31	0.020 (3)	0.024 (3)	0.027 (3)	−0.003 (2)	0.006 (3)	0.001 (2)
C32	0.009 (3)	0.028 (3)	0.021 (3)	−0.001 (2)	0.003 (2)	0.002 (2)
C33	0.021 (3)	0.028 (3)	0.021 (3)	−0.002 (2)	0.004 (2)	0.002 (2)
C34	0.031 (3)	0.043 (3)	0.024 (3)	−0.002 (3)	0.017 (3)	0.011 (3)
C35	0.026 (3)	0.045 (3)	0.015 (3)	0.008 (3)	0.008 (3)	0.003 (2)
C36	0.027 (3)	0.038 (3)	0.024 (3)	0.002 (3)	0.008 (3)	−0.007 (2)
C37	0.023 (3)	0.024 (3)	0.018 (3)	0.003 (2)	0.008 (2)	0.000 (2)
C38	0.050 (4)	0.043 (4)	0.042 (4)	−0.011 (3)	0.027 (4)	−0.002 (3)
C39	0.077 (6)	0.049 (4)	0.036 (4)	0.004 (4)	0.008 (4)	0.007 (3)
Cl1	0.0424 (10)	0.0460 (9)	0.0603 (10)	−0.0025 (8)	0.0290 (9)	−0.0043 (8)
Cl2	0.0904 (15)	0.0384 (9)	0.0600 (11)	−0.0085 (9)	0.0462 (11)	−0.0062 (8)
Cl3	0.1066 (18)	0.0915 (15)	0.0420 (10)	−0.0446 (14)	0.0070 (12)	0.0157 (10)
Cl4	0.0869 (16)	0.0624 (12)	0.0483 (10)	−0.0130 (11)	0.0067 (11)	0.0028 (9)
I1	0.0287 (2)	0.0339 (2)	0.01825 (17)	0.00212 (16)	0.00550 (16)	−0.00344 (15)
I2	0.0279 (2)	0.01925 (17)	0.0337 (2)	0.00037 (15)	0.01483 (17)	0.00000 (14)

P1	0.0156 (7)	0.0181 (6)	0.0130 (6)	−0.0011 (5)	0.0041 (6)	−0.0004 (5)
P2	0.0150 (7)	0.0172 (6)	0.0143 (6)	0.0007 (5)	0.0037 (6)	−0.0001 (5)

Geometric parameters (Å, º)

C1—P2	1.804 (4)	C20—C25	1.396 (7)
C1—P1	1.807 (5)	C20—P2	1.794 (5)
C2—C7	1.380 (7)	C21—C22	1.384 (7)
C2—C3	1.389 (7)	C22—C23	1.383 (7)
C2—P1	1.795 (5)	C23—C24	1.387 (7)
C3—C4	1.383 (7)	C24—C25	1.372 (7)
C4—C5	1.381 (7)	C26—C31	1.391 (7)
C5—C6	1.381 (7)	C26—C27	1.396 (6)
C6—C7	1.387 (7)	C26—P2	1.787 (5)
C8—C13	1.383 (7)	C27—C28	1.385 (7)
C8—C9	1.402 (6)	C28—C29	1.382 (7)
C8—P1	1.792 (5)	C29—C30	1.377 (7)
C9—C10	1.373 (7)	C30—C31	1.390 (7)
C10—C11	1.376 (7)	C32—C37	1.391 (7)
C11—C12	1.360 (7)	C32—C33	1.403 (7)
C12—C13	1.388 (7)	C32—P2	1.786 (5)
C14—C15	1.396 (6)	C33—C34	1.385 (7)
C14—C19	1.403 (6)	C34—C35	1.361 (7)
C14—P1	1.787 (5)	C35—C36	1.397 (7)
C15—C16	1.377 (7)	C36—C37	1.376 (7)
C16—C17	1.384 (7)	C38—Cl1	1.754 (6)
C17—C18	1.377 (7)	C38—Cl2	1.760 (6)
C18—C19	1.387 (6)	C39—Cl4	1.752 (7)
C20—C21	1.388 (6)	C39—Cl3	1.758 (7)
P1—C1—P2	124.1 (2)	C24—C25—C20	120.1 (5)
C7—C2—C3	120.0 (5)	C31—C26—C27	120.6 (4)
C7—C2—P1	122.4 (4)	C31—C26—P2	122.3 (4)
C3—C2—P1	117.5 (4)	C27—C26—P2	116.9 (4)
C4—C3—C2	119.9 (5)	C28—C27—C26	119.6 (5)
C5—C4—C3	120.0 (5)	C29—C28—C27	119.9 (5)
C6—C5—C4	120.2 (5)	C30—C29—C28	120.4 (5)
C5—C6—C7	119.9 (5)	C29—C30—C31	120.9 (5)
C2—C7—C6	119.9 (5)	C30—C31—C26	118.7 (5)
C13—C8—C9	119.5 (4)	C37—C32—C33	119.1 (4)
C13—C8—P1	122.8 (4)	C37—C32—P2	119.2 (4)
C9—C8—P1	117.5 (4)	C33—C32—P2	121.4 (4)
C10—C9—C8	119.1 (5)	C34—C33—C32	119.6 (5)
C9—C10—C11	121.3 (5)	C35—C34—C33	120.6 (5)
C12—C11—C10	119.6 (5)	C34—C35—C36	120.6 (5)
C11—C12—C13	120.8 (5)	C37—C36—C35	119.2 (5)
C8—C13—C12	119.7 (4)	C36—C37—C32	120.8 (5)
C15—C14—C19	120.2 (4)	Cl1—C38—Cl2	112.1 (3)

C15—C14—P1	119.6 (4)	Cl4—C39—Cl3	111.4 (3)
C19—C14—P1	120.1 (4)	C14—P1—C8	111.3 (2)
C16—C15—C14	119.6 (5)	C14—P1—C2	109.7 (2)
C15—C16—C17	120.7 (5)	C8—P1—C2	107.9 (2)
C18—C17—C16	119.7 (5)	C14—P1—C1	111.2 (2)
C17—C18—C19	121.1 (5)	C8—P1—C1	111.0 (2)
C18—C19—C14	118.7 (5)	C2—P1—C1	105.5 (2)
C21—C20—C25	119.9 (5)	C32—P2—C26	112.3 (2)
C21—C20—P2	123.0 (4)	C32—P2—C20	106.8 (2)
C25—C20—P2	117.1 (4)	C26—P2—C20	109.2 (2)
C22—C21—C20	119.3 (5)	C32—P2—C1	111.5 (2)
C23—C22—C21	120.8 (5)	C26—P2—C1	110.4 (2)
C22—C23—C24	119.5 (5)	C20—P2—C1	106.3 (2)
C25—C24—C23	120.3 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···I1^{i}	0.99	2.81	3.802 (4)	175
C39—H39*A*···I1^{i}	0.99	3.05	3.986 (7)	159
C1—H1*B*···I2^{i}	0.99	2.83	3.813 (4)	175
C38—H38*B*···I2^{ii}	0.99	2.88	3.848 (6)	166

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1, −*y*+3/2, *z*+1/2.

Methylenebis(triphenylphosphonium) bis(tetraiodoborate) (II)

Crystal data

$C_{37}H_{32}P_2^{2+}\cdot 2BI_4^-$
M_r = 1575.38
Monoclinic, $P2_1/c$
a = 19.7878 (6) Å
b = 14.3122 (3) Å
c = 16.0646 (4) Å
β = 96.230 (1)°
V = 4522.7 (2) Å^3
Z = 4
$F(000)$ = 2872
D_x = 2.314 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7264 reflections
θ = 2.5–25.5°
μ = 5.58 mm^{-1}
T = 153 K
Block, colourless
0.14 × 0.12 × 0.08 mm

Data collection

CCD area detector diffractometer
Radiation source: fine-focus sealed tube, Bruker KappaCCD
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.51, T_{max} = 0.66
52611 measured reflections
14486 independent reflections
9439 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 31.1°, θ_{min} = 1.8°
h = −28→27
k = −20→20
l = −23→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.124$
$S = 0.92$
14486 reflections
442 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 4.3616P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.32$ e Å^{-3}
$\Delta\rho_{min} = -2.11$ e Å^{-3}

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.

Refinement. **II**: reflections 0 0 2, 2 0 0, 1 1 1, 2 1 0, -1 0 2, -2 1 1, -1 1 1 and 0 1 2, were affected by the beam stop and omitted from the final cycles of refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.4572 (3)	0.0659 (4)	0.2238 (4)	0.0196 (12)
B2	0.9220 (3)	0.4312 (4)	0.1661 (4)	0.0209 (12)
C1	0.6997 (3)	0.5283 (3)	0.5764 (3)	0.0163 (10)
H1A	0.689	0.5285	0.5148	0.02*
H1B	0.6557	0.5311	0.6003	0.02*
C2	0.6780 (3)	0.3291 (3)	0.5616 (4)	0.0194 (11)
C3	0.6740 (3)	0.2450 (4)	0.6055 (4)	0.0336 (15)
H3	0.6999	0.236	0.6582	0.04*
C4	0.6314 (4)	0.1752 (4)	0.5707 (6)	0.046 (2)
H4	0.6286	0.1177	0.5996	0.056*
C5	0.5937 (3)	0.1876 (5)	0.4963 (5)	0.0428 (19)
H5	0.5651	0.1385	0.4736	0.051*
C6	0.5958 (3)	0.2702 (5)	0.4526 (5)	0.0398 (16)
H6	0.5683	0.2788	0.401	0.048*
C7	0.6390 (3)	0.3410 (4)	0.4857 (4)	0.0321 (14)
H7	0.6417	0.3979	0.4558	0.039*
C8	0.8151 (3)	0.4054 (3)	0.5583 (4)	0.0186 (10)
C9	0.8776 (3)	0.4303 (4)	0.6004 (4)	0.0238 (12)
H9	0.8806	0.448	0.6576	0.029*
C10	0.9357 (3)	0.4292 (4)	0.5589 (4)	0.0298 (14)
H10	0.9785	0.4454	0.5879	0.036*
C11	0.9310 (3)	0.4046 (4)	0.4758 (5)	0.0333 (15)
H11	0.9707	0.4045	0.4474	0.04*
C12	0.8694 (3)	0.3799 (4)	0.4332 (4)	0.0287 (13)
H12	0.8668	0.3633	0.3757	0.034*
C13	0.8110 (3)	0.3791 (4)	0.4739 (4)	0.0241 (12)
H13	0.7687	0.361	0.4448	0.029*
C14	0.7477 (3)	0.4003 (3)	0.7157 (3)	0.0183 (10)

C15	0.6960 (3)	0.4326 (4)	0.7618 (4)	0.0249 (12)
H15	0.6581	0.4654	0.7347	0.03*
C16	0.7009 (3)	0.4160 (4)	0.8470 (4)	0.0309 (13)
H16	0.666	0.4374	0.8785	0.037*
C17	0.7562 (4)	0.3684 (4)	0.8869 (4)	0.0336 (14)
H17	0.7594	0.3582	0.9456	0.04*
C18	0.8066 (3)	0.3357 (4)	0.8414 (4)	0.0331 (14)
H18	0.8443	0.3029	0.869	0.04*
C19	0.8024 (3)	0.3507 (4)	0.7556 (4)	0.0237 (11)
H19	0.8367	0.3271	0.7243	0.028*
C20	0.6845 (3)	0.7276 (3)	0.5731 (3)	0.0177 (10)
C21	0.6246 (3)	0.7120 (4)	0.5224 (3)	0.0209 (11)
H21	0.6117	0.6502	0.5061	0.025*
C22	0.5832 (3)	0.7867 (4)	0.4954 (4)	0.0282 (13)
H22	0.542	0.7764	0.4604	0.034*
C23	0.6024 (4)	0.8767 (4)	0.5201 (4)	0.0342 (15)
H23	0.5738	0.9279	0.5026	0.041*
C24	0.6626 (3)	0.8924 (4)	0.5695 (4)	0.0311 (14)
H24	0.6757	0.9544	0.585	0.037*
C25	0.7040 (3)	0.8184 (4)	0.5966 (4)	0.0258 (12)
H25	0.7454	0.8292	0.6311	0.031*
C26	0.8159 (2)	0.6531 (3)	0.5470 (3)	0.0156 (10)
C27	0.8679 (3)	0.7133 (4)	0.5778 (4)	0.0222 (11)
H27	0.8692	0.7374	0.6331	0.027*
C28	0.9174 (3)	0.7379 (4)	0.5279 (4)	0.0294 (13)
H28	0.9526	0.7796	0.5485	0.035*
C29	0.9159 (3)	0.7025 (4)	0.4487 (4)	0.0264 (13)
H29	0.9504	0.7199	0.415	0.032*
C30	0.8655 (3)	0.6422 (4)	0.4165 (4)	0.0268 (13)
H30	0.8655	0.6175	0.3617	0.032*
C31	0.8144 (3)	0.6179 (4)	0.4658 (4)	0.0215 (11)
H31	0.7786	0.5776	0.4442	0.026*
C32	0.7668 (3)	0.6419 (3)	0.7154 (3)	0.0177 (10)
C33	0.8287 (3)	0.6088 (3)	0.7527 (3)	0.0182 (10)
H33	0.863	0.5903	0.719	0.022*
C34	0.8404 (3)	0.6030 (4)	0.8390 (4)	0.0273 (12)
H34	0.8825	0.5797	0.8647	0.033*
C35	0.7913 (4)	0.6309 (4)	0.8873 (4)	0.0335 (14)
H35	0.7993	0.6254	0.9465	0.04*
C36	0.7303 (3)	0.6667 (4)	0.8515 (4)	0.0311 (14)
H36	0.6974	0.6881	0.886	0.037*
C37	0.7170 (3)	0.6715 (4)	0.7645 (4)	0.0254 (12)
H37	0.6747	0.6946	0.7392	0.03*
I1	0.50473 (2)	−0.01702 (3)	0.33197 (3)	0.02907 (10)
I2	0.34522 (2)	0.03252 (3)	0.19998 (3)	0.03574 (11)
I3	0.50580 (2)	0.02646 (4)	0.11044 (3)	0.03911 (12)
I4	0.47021 (2)	0.21823 (3)	0.24780 (3)	0.03478 (11)
I5	0.81419 (2)	0.44916 (3)	0.19353 (3)	0.04437 (13)

I6	0.97031 (2)	0.31216 (3)	0.24298 (3)	0.02826 (10)
I7	0.92629 (3)	0.40188 (4)	0.03197 (3)	0.04945 (14)
I8	0.97951 (3)	0.56167 (3)	0.20371 (3)	0.04060 (12)
P1	0.73738 (7)	0.41452 (9)	0.60508 (9)	0.0155 (3)
P2	0.74413 (6)	0.63678 (8)	0.60451 (8)	0.0139 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.014 (3)	0.027 (3)	0.017 (3)	−0.003 (2)	−0.002 (2)	−0.004 (2)
B2	0.020 (3)	0.022 (3)	0.020 (3)	0.001 (2)	−0.001 (2)	−0.004 (2)
C1	0.013 (2)	0.015 (2)	0.020 (3)	0.0006 (18)	0.001 (2)	0.0000 (18)
C2	0.012 (2)	0.020 (2)	0.026 (3)	−0.0061 (18)	0.001 (2)	−0.004 (2)
C3	0.036 (4)	0.019 (3)	0.045 (4)	−0.006 (2)	0.002 (3)	−0.002 (3)
C4	0.047 (4)	0.017 (3)	0.076 (6)	−0.009 (3)	0.008 (4)	−0.006 (3)
C5	0.026 (3)	0.035 (3)	0.068 (5)	−0.011 (3)	0.009 (3)	−0.026 (3)
C6	0.028 (3)	0.050 (4)	0.039 (4)	−0.007 (3)	−0.007 (3)	−0.016 (3)
C7	0.036 (4)	0.029 (3)	0.030 (3)	−0.009 (3)	0.000 (3)	−0.002 (2)
C8	0.019 (3)	0.014 (2)	0.025 (3)	−0.0005 (19)	0.008 (2)	−0.0023 (19)
C9	0.018 (3)	0.026 (3)	0.028 (3)	0.000 (2)	0.000 (2)	0.000 (2)
C10	0.019 (3)	0.026 (3)	0.045 (4)	0.002 (2)	0.004 (3)	0.000 (3)
C11	0.026 (3)	0.029 (3)	0.047 (4)	0.003 (2)	0.013 (3)	−0.003 (3)
C12	0.033 (3)	0.027 (3)	0.028 (3)	0.000 (2)	0.012 (3)	−0.005 (2)
C13	0.022 (3)	0.026 (3)	0.024 (3)	−0.003 (2)	0.002 (2)	−0.005 (2)
C14	0.022 (3)	0.016 (2)	0.016 (3)	−0.0050 (19)	−0.001 (2)	0.0026 (18)
C15	0.021 (3)	0.031 (3)	0.023 (3)	−0.001 (2)	0.001 (2)	0.003 (2)
C16	0.029 (3)	0.042 (3)	0.023 (3)	−0.003 (3)	0.005 (3)	0.001 (3)
C17	0.041 (4)	0.040 (3)	0.020 (3)	−0.001 (3)	0.003 (3)	0.009 (3)
C18	0.036 (4)	0.034 (3)	0.027 (3)	0.003 (3)	−0.010 (3)	0.015 (3)
C19	0.027 (3)	0.024 (3)	0.019 (3)	0.002 (2)	−0.001 (2)	0.000 (2)
C20	0.019 (3)	0.017 (2)	0.018 (3)	0.0048 (18)	0.004 (2)	−0.0011 (19)
C21	0.019 (3)	0.026 (3)	0.017 (3)	0.004 (2)	−0.001 (2)	−0.001 (2)
C22	0.026 (3)	0.042 (3)	0.015 (3)	0.012 (3)	−0.001 (2)	0.003 (2)
C23	0.048 (4)	0.035 (3)	0.020 (3)	0.023 (3)	0.007 (3)	0.002 (2)
C24	0.044 (4)	0.021 (3)	0.027 (3)	0.011 (3)	−0.002 (3)	0.001 (2)
C25	0.027 (3)	0.020 (2)	0.029 (3)	0.004 (2)	−0.002 (2)	−0.002 (2)
C26	0.012 (2)	0.014 (2)	0.021 (3)	−0.0003 (17)	0.0027 (19)	0.0021 (18)
C27	0.017 (3)	0.030 (3)	0.019 (3)	−0.006 (2)	−0.001 (2)	0.001 (2)
C28	0.020 (3)	0.032 (3)	0.036 (4)	−0.006 (2)	0.004 (3)	0.004 (3)
C29	0.020 (3)	0.029 (3)	0.032 (3)	0.002 (2)	0.012 (2)	0.010 (2)
C30	0.030 (3)	0.026 (3)	0.025 (3)	0.008 (2)	0.008 (3)	0.005 (2)
C31	0.023 (3)	0.022 (2)	0.021 (3)	0.002 (2)	0.006 (2)	0.000 (2)
C32	0.017 (2)	0.017 (2)	0.019 (3)	−0.0017 (18)	−0.001 (2)	−0.0002 (19)
C33	0.017 (3)	0.019 (2)	0.018 (3)	−0.0006 (19)	−0.001 (2)	−0.0029 (19)
C34	0.022 (3)	0.031 (3)	0.026 (3)	−0.002 (2)	−0.009 (2)	0.001 (2)
C35	0.045 (4)	0.042 (3)	0.014 (3)	−0.008 (3)	0.005 (3)	−0.004 (2)
C36	0.036 (4)	0.036 (3)	0.023 (3)	0.001 (3)	0.010 (3)	−0.004 (2)
C37	0.022 (3)	0.028 (3)	0.026 (3)	0.004 (2)	0.006 (2)	−0.005 (2)

I1	0.0364 (2)	0.02556 (18)	0.0242 (2)	0.00250 (15)	−0.00166 (16)	0.00448 (15)
I2	0.01692 (19)	0.0617 (3)	0.0287 (2)	−0.00711 (17)	0.00315 (16)	−0.01338 (19)
I3	0.0213 (2)	0.0782 (3)	0.0185 (2)	0.0046 (2)	0.00497 (16)	−0.0110 (2)
I4	0.0394 (2)	0.02487 (18)	0.0370 (2)	−0.00048 (16)	−0.00956 (19)	0.00293 (16)
I5	0.0205 (2)	0.0557 (3)	0.0576 (3)	0.01384 (19)	0.0074 (2)	0.0110 (2)
I6	0.02340 (19)	0.02538 (17)	0.0370 (2)	0.00730 (14)	0.00765 (16)	0.00962 (15)
I7	0.0586 (3)	0.0673 (3)	0.0207 (2)	0.0183 (3)	−0.0038 (2)	−0.0119 (2)
I8	0.0512 (3)	0.02285 (19)	0.0443 (3)	−0.00971 (18)	−0.0105 (2)	−0.00049 (17)
P1	0.0129 (6)	0.0158 (6)	0.0175 (7)	−0.0006 (5)	−0.0006 (5)	0.0012 (5)
P2	0.0108 (6)	0.0163 (6)	0.0143 (6)	0.0015 (4)	0.0001 (5)	−0.0008 (5)

Geometric parameters (Å, º)

B1—I3	2.224 (6)	C14—P1	1.779 (5)
B1—I4	2.224 (6)	C15—C16	1.382 (8)
B1—I1	2.226 (6)	C16—C17	1.386 (9)
B1—I2	2.258 (6)	C17—C18	1.380 (9)
B2—I7	2.206 (6)	C18—C19	1.389 (8)
B2—I8	2.236 (6)	C20—C21	1.382 (8)
B2—I5	2.241 (6)	C20—C25	1.396 (7)
B2—I6	2.255 (6)	C20—P2	1.791 (5)
C1—P2	1.817 (5)	C21—C22	1.388 (7)
C1—P1	1.829 (5)	C22—C23	1.388 (9)
C2—C7	1.382 (8)	C23—C24	1.376 (10)
C2—C3	1.402 (8)	C24—C25	1.381 (8)
C2—P1	1.784 (5)	C26—C27	1.390 (7)
C3—C4	1.385 (9)	C26—C31	1.395 (7)
C4—C5	1.350 (11)	C26—P2	1.792 (5)
C5—C6	1.377 (10)	C27—C28	1.378 (8)
C6—C7	1.394 (8)	C28—C29	1.368 (9)
C8—C9	1.390 (8)	C29—C30	1.376 (8)
C8—C13	1.400 (8)	C30—C31	1.394 (8)
C8—P1	1.788 (5)	C32—C33	1.389 (7)
C9—C10	1.389 (8)	C32—C37	1.392 (7)
C10—C11	1.374 (9)	C32—P2	1.791 (5)
C11—C12	1.379 (9)	C33—C34	1.384 (8)
C12—C13	1.387 (8)	C34—C35	1.367 (9)
C14—C19	1.391 (8)	C35—C36	1.377 (9)
C14—C15	1.405 (8)	C36—C37	1.396 (9)
I3—B1—I4	109.8 (3)	C21—C20—C25	120.3 (5)
I3—B1—I1	108.7 (3)	C21—C20—P2	123.1 (4)
I4—B1—I1	110.9 (3)	C25—C20—P2	116.5 (4)
I3—B1—I2	108.1 (3)	C20—C21—C22	120.0 (5)
I4—B1—I2	109.3 (3)	C23—C22—C21	119.4 (6)
I1—B1—I2	110.1 (3)	C24—C23—C22	120.7 (5)
I7—B2—I8	110.5 (3)	C23—C24—C25	120.2 (6)
I7—B2—I5	110.6 (3)	C24—C25—C20	119.4 (6)

I8—B2—I5	108.6 (2)	C27—C26—C31	119.8 (5)
I7—B2—I6	109.4 (2)	C27—C26—P2	119.6 (4)
I8—B2—I6	108.1 (3)	C31—C26—P2	119.8 (4)
I5—B2—I6	109.6 (3)	C28—C27—C26	119.7 (5)
P1—C1—P2	121.7 (3)	C29—C28—C27	120.2 (6)
C7—C2—C3	119.5 (5)	C28—C29—C30	121.6 (5)
C7—C2—P1	122.8 (4)	C29—C30—C31	118.9 (6)
C3—C2—P1	117.6 (5)	C30—C31—C26	119.8 (5)
C4—C3—C2	118.8 (7)	C33—C32—C37	120.3 (5)
C5—C4—C3	121.1 (7)	C33—C32—P2	121.9 (4)
C4—C5—C6	121.3 (6)	C37—C32—P2	117.4 (4)
C5—C6—C7	118.8 (7)	C34—C33—C32	119.7 (5)
C2—C7—C6	120.5 (6)	C35—C34—C33	120.0 (6)
C9—C8—C13	119.6 (5)	C34—C35—C36	121.0 (6)
C9—C8—P1	122.5 (4)	C35—C36—C37	119.9 (6)
C13—C8—P1	117.7 (4)	C32—C37—C36	119.0 (6)
C10—C9—C8	120.2 (6)	C14—P1—C2	108.2 (3)
C11—C10—C9	119.8 (6)	C14—P1—C8	113.6 (3)
C10—C11—C12	120.7 (6)	C2—P1—C8	110.2 (2)
C11—C12—C13	120.3 (6)	C14—P1—C1	110.7 (2)
C12—C13—C8	119.4 (5)	C2—P1—C1	106.2 (2)
C19—C14—C15	120.0 (5)	C8—P1—C1	107.8 (2)
C19—C14—P1	121.2 (4)	C32—P2—C20	109.7 (2)
C15—C14—P1	118.5 (4)	C32—P2—C26	112.4 (2)
C16—C15—C14	119.3 (6)	C20—P2—C26	107.2 (2)
C15—C16—C17	120.5 (6)	C32—P2—C1	110.1 (2)
C18—C17—C16	120.2 (6)	C20—P2—C1	105.3 (2)
C17—C18—C19	120.3 (6)	C26—P2—C1	111.9 (2)
C18—C19—C14	119.7 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···I1^{i}	0.95	3.02	3.730 (7)	132

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