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Methyltriphenylphosphonium bromide chloroform hemisolvate

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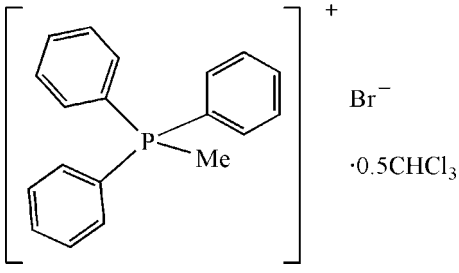
Key indicators: single-crystal X-ray study; T = 96 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.105; data-to-parameter ratio = 25.4.

The title compound, $C_{19}H_{18}P^+\cdot Br^-\cdot 0.5CHCl_3$, was obtained by recrystallization from wet chloroform/diethyl ether and was found to crystallize as the chloroform hemisolvate. There are two independent cations and anions in the asymmetric unit along with one chloroform solvent molecule. The phenyl rings adopt a propellor conformation in both independent cations, but with opposite directions of rotation.

Related literature

For related examples, see: Butchard *et al.* (2006); Bowmaker *et al.* (1990); El Essawi *et al.* (1996); Wermer *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{18}P^+\cdot Br^-\cdot 0.5CHCl_3$
M_r = 416.90
Triclinic, $P\overline{1}$
a = 11.7690 (4) Å
b = 11.9057 (4) Å
c = 15.0898 (7) Å
α = 66.769 (1)°
β = 73.304 (2)°
γ = 82.380 (1)°
V = 1860.57 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.51 mm^{-1}
T = 96 K
0.65 × 0.37 × 0.13 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.35, T_{max} = 0.722
16377 measured reflections
10610 independent reflections
8893 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.105
S = 0.80
10610 reflections
417 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2343).

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supplementary materials

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Methyltriphenylphosphonium bromide chloroform hemisolvate

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Comment

Crystals of the title compound (I) were grown as part of an ongoing project on halide hydrates (Butchard *et al.* 2006). In this case, the compound crystallized from wet chloroform/diethylether with only chloroform solvate. The stucture of (I) is shown below (Fig. 1). The asymmetric unit consists of two phosphonium cations, two bromide anions, and one chloroform solvate molecule. The unit cell is shown in Fig. 2.

Experimental

Crystals of the title compound were obtained by recrystallization of a commercial sample from wet chloroform/diethylether at −35 °C.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic 0.98 Å, U_{iso} = 1.2U_{eq} (C) for CH and 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3 atoms.

Figures

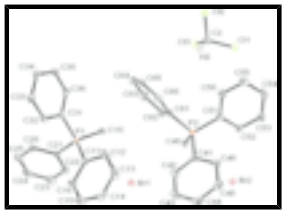

Fig. 1. The molecular structure of (I) showing both of the independent cations and anions with 50% probability ellipsoids. For clarity, all H atoms, other than the chloroform proton, have been omitted.

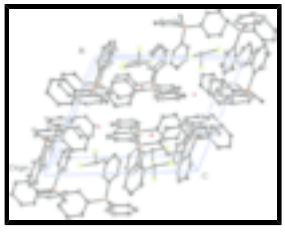

Fig. 2. The unit cell of (I) viewed down the *a* axis. For clarity, all H atoms, other than the chloroform proton, have been omitted.

Methyltriphenylphosphonium bromide chloroform hemisolvate

Crystal data

$C_{19}H_{18}P^{+}\cdot Br^{-}\cdot 0.5CHCl_3$	$Z = 4$
$M_r = 416.90$	$F_{000} = 844$

Triclinic, $P\bar{1}$	D_x = 1.488 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.7690 (4) Å	Cell parameters from 8506 reflections
b = 11.9057 (4) Å	θ = 2.6–31.6º
c = 15.0898 (7) Å	μ = 2.51 mm^{-1}
α = 66.769 (1)º	T = 96 K
β = 73.304 (2)º	Plate, colourless
γ = 82.380 (1)º	0.65 × 0.37 × 0.13 mm
V = 1860.57 (12) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	10610 independent reflections
Radiation source: fine-focus sealed tube	8893 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 96 K	θ_{max} = 31.8º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −17→16
T_{min} = 0.35, T_{max} = 0.722	k = −17→17
16377 measured reflections	l = −19→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.028	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.80	$(\Delta/\sigma)_{max}$ = 0.002
10610 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
417 parameters	$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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}
C2	0.93549 (17)	0.95322 (18)	0.30581 (15)	0.0201 (4)
H2	0.8835	0.8844	0.3504	0.024*
Cl1	1.02829 (5)	0.91593 (6)	0.20549 (5)	0.03299 (13)
Cl2	1.02403 (4)	0.97762 (5)	0.37316 (4)	0.02613 (11)
Cl3	0.84695 (4)	1.08401 (5)	0.26217 (4)	0.02483 (10)
Br1	0.264156 (16)	0.300222 (17)	0.597334 (13)	0.01906 (6)
Br2	0.639404 (16)	0.339708 (15)	0.215697 (13)	0.01670 (6)
P1	0.25469 (4)	0.25808 (4)	0.91409 (3)	0.01210 (9)
P2	0.69318 (4)	0.28499 (4)	0.52675 (3)	0.01364 (9)
C10	0.34736 (16)	0.34979 (16)	0.79770 (13)	0.0163 (3)
H10A	0.3415	0.4333	0.7925	0.024*
H10B	0.3225	0.3446	0.7442	0.024*
H10C	0.4281	0.3210	0.7937	0.024*
C11	0.26895 (16)	0.10230 (16)	0.92330 (13)	0.0150 (3)
C12	0.38227 (19)	0.0536 (2)	0.8979 (2)	0.0384 (6)
H12	0.4484	0.1009	0.8787	0.046*
C13	0.3966 (2)	−0.0660 (2)	0.9013 (2)	0.0377 (6)
H13	0.4723	−0.0985	0.8840	0.045*
C14	0.2983 (2)	−0.13634 (17)	0.93043 (14)	0.0223 (4)
H14	0.3075	−0.2154	0.9310	0.027*
C15	0.18653 (19)	−0.08909 (18)	0.95866 (17)	0.0253 (4)
H15	0.1207	−0.1378	0.9810	0.030*
C16	0.17138 (17)	0.03087 (16)	0.95403 (15)	0.0199 (4)
H16	0.0955	0.0628	0.9716	0.024*
C21	0.10393 (15)	0.31162 (15)	0.92090 (13)	0.0150 (3)
C22	0.05877 (17)	0.33463 (17)	0.83930 (15)	0.0198 (4)
H22	0.1056	0.3201	0.7835	0.024*
C23	−0.05653 (18)	0.37937 (19)	0.84201 (17)	0.0259 (4)
H23	−0.0878	0.3937	0.7884	0.031*
C24	−0.12584 (18)	0.40291 (18)	0.92529 (18)	0.0276 (5)
H24	−0.2025	0.4348	0.9261	0.033*
C25	−0.08197 (18)	0.37942 (18)	1.00572 (17)	0.0257 (4)
H25	−0.1292	0.3941	1.0613	0.031*
C26	0.03339 (17)	0.33354 (17)	1.00444 (15)	0.0205 (4)
H26	0.0633	0.3176	1.0591	0.025*
C31	0.29869 (15)	0.26401 (15)	1.01631 (12)	0.0132 (3)
C32	0.26180 (17)	0.17271 (17)	1.11113 (14)	0.0179 (3)
H32	0.2158	0.1093	1.1204	0.022*
C33	0.29380 (17)	0.17690 (17)	1.19120 (13)	0.0190 (4)
H33	0.2677	0.1175	1.2546	0.023*
C34	0.36508 (16)	0.27013 (17)	1.17661 (13)	0.0176 (3)
H34	0.3884	0.2717	1.2300	0.021*

C35	0.40145 (17)	0.36068 (17)	1.08285 (14)	0.0196 (4)
H35	0.4493	0.4226	1.0737	0.023*
C36	0.36723 (16)	0.36007 (16)	1.00226 (13)	0.0166 (3)
H36	0.3895	0.4225	0.9399	0.020*
C40	0.59777 (16)	0.38815 (17)	0.45664 (14)	0.0176 (3)
H40A	0.6074	0.3748	0.3961	0.026*
H40B	0.6177	0.4707	0.4406	0.026*
H40C	0.5169	0.3744	0.4954	0.026*
C41	0.65468 (16)	0.13170 (16)	0.55482 (13)	0.0149 (3)
C42	0.53788 (17)	0.09560 (19)	0.60718 (15)	0.0215 (4)
H42	0.4833	0.1491	0.6293	0.026*
C43	0.50442 (19)	−0.02113 (19)	0.62582 (15)	0.0260 (4)
H43	0.4274	−0.0462	0.6615	0.031*
C44	0.5846 (2)	−0.09958 (18)	0.59181 (15)	0.0253 (4)
H44	0.5608	−0.1765	0.6029	0.030*
C45	0.7000 (2)	−0.06500 (18)	0.54136 (14)	0.0235 (4)
H45	0.7540	−0.1192	0.5197	0.028*
C46	0.73617 (17)	0.05074 (17)	0.52268 (14)	0.0184 (3)
H46	0.8141	0.0738	0.4890	0.022*
C51	0.84459 (15)	0.31220 (16)	0.45611 (13)	0.0150 (3)
C52	0.87672 (17)	0.31023 (18)	0.36024 (14)	0.0193 (4)
H52	0.8198	0.2997	0.3325	0.023*
C53	0.99547 (19)	0.3242 (2)	0.30674 (16)	0.0261 (4)
H53	1.0183	0.3214	0.2433	0.031*
C54	1.07978 (18)	0.34229 (19)	0.34737 (16)	0.0268 (4)
H54	1.1590	0.3505	0.3113	0.032*
C55	1.04735 (18)	0.3482 (2)	0.44120 (17)	0.0256 (4)
H55	1.1041	0.3626	0.4673	0.031*
C56	0.92945 (17)	0.33249 (18)	0.49621 (15)	0.0209 (4)
H56	0.9072	0.3355	0.5596	0.025*
C61	0.67462 (15)	0.30612 (17)	0.64188 (13)	0.0161 (3)
C62	0.68264 (17)	0.20571 (19)	0.72775 (14)	0.0208 (4)
H62	0.6945	0.1276	0.7262	0.025*
C63	0.67281 (18)	0.2224 (2)	0.81604 (15)	0.0249 (4)
H63	0.6791	0.1557	0.8734	0.030*
C64	0.65364 (18)	0.3391 (2)	0.81809 (16)	0.0260 (4)
H64	0.6458	0.3499	0.8774	0.031*
C65	0.64605 (18)	0.4400 (2)	0.73253 (16)	0.0251 (4)
H65	0.6335	0.5179	0.7345	0.030*
C66	0.65737 (17)	0.42387 (18)	0.64352 (15)	0.0205 (4)
H66	0.6534	0.4910	0.5857	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0161 (8)	0.0215 (9)	0.0230 (9)	−0.0017 (7)	−0.0031 (7)	−0.0096 (7)
Cl1	0.0220 (2)	0.0450 (3)	0.0414 (3)	0.0012 (2)	−0.0020 (2)	−0.0309 (3)
Cl2	0.0238 (2)	0.0294 (2)	0.0297 (3)	0.00343 (19)	−0.0133 (2)	−0.0125 (2)

Cl3	0.0243 (2)	0.0284 (2)	0.0240 (2)	0.00488 (19)	−0.01051 (19)	−0.01082 (19)
Br1	0.01849 (10)	0.02193 (10)	0.01833 (10)	−0.00370 (7)	−0.00503 (7)	−0.00796 (7)
Br2	0.01863 (10)	0.01593 (9)	0.01646 (9)	−0.00120 (6)	−0.00405 (7)	−0.00711 (7)
P1	0.0116 (2)	0.01229 (19)	0.0129 (2)	−0.00235 (15)	−0.00212 (16)	−0.00527 (16)
P2	0.0129 (2)	0.0168 (2)	0.0111 (2)	0.00001 (16)	−0.00274 (16)	−0.00542 (16)
C10	0.0173 (8)	0.0184 (8)	0.0130 (8)	−0.0062 (6)	−0.0015 (6)	−0.0055 (6)
C11	0.0148 (8)	0.0149 (7)	0.0156 (8)	−0.0013 (6)	−0.0020 (6)	−0.0073 (6)
C12	0.0162 (10)	0.0212 (10)	0.0640 (17)	−0.0031 (8)	0.0115 (10)	−0.0163 (11)
C13	0.0269 (11)	0.0217 (10)	0.0492 (15)	0.0034 (9)	0.0144 (10)	−0.0158 (10)
C14	0.0362 (11)	0.0164 (8)	0.0169 (9)	0.0033 (8)	−0.0081 (8)	−0.0093 (7)
C15	0.0247 (10)	0.0163 (8)	0.0394 (12)	−0.0022 (7)	−0.0160 (9)	−0.0091 (8)
C16	0.0155 (8)	0.0156 (8)	0.0305 (10)	0.0006 (6)	−0.0074 (7)	−0.0099 (7)
C21	0.0136 (8)	0.0122 (7)	0.0198 (8)	−0.0014 (6)	−0.0034 (6)	−0.0069 (6)
C22	0.0181 (9)	0.0200 (8)	0.0216 (9)	−0.0008 (7)	−0.0061 (7)	−0.0074 (7)
C23	0.0227 (10)	0.0221 (9)	0.0327 (11)	0.0010 (8)	−0.0142 (8)	−0.0056 (8)
C24	0.0146 (9)	0.0169 (8)	0.0520 (14)	0.0021 (7)	−0.0094 (9)	−0.0137 (9)
C25	0.0172 (9)	0.0214 (9)	0.0394 (12)	−0.0030 (7)	0.0016 (8)	−0.0177 (9)
C26	0.0172 (9)	0.0205 (8)	0.0259 (10)	−0.0029 (7)	−0.0017 (7)	−0.0128 (7)
C31	0.0123 (7)	0.0149 (7)	0.0127 (8)	−0.0014 (6)	−0.0025 (6)	−0.0056 (6)
C32	0.0189 (8)	0.0169 (8)	0.0160 (8)	−0.0061 (7)	−0.0019 (7)	−0.0042 (7)
C33	0.0222 (9)	0.0200 (8)	0.0115 (8)	−0.0027 (7)	−0.0027 (7)	−0.0028 (7)
C34	0.0198 (9)	0.0205 (8)	0.0144 (8)	0.0013 (7)	−0.0058 (7)	−0.0079 (7)
C35	0.0233 (9)	0.0192 (8)	0.0184 (9)	−0.0063 (7)	−0.0065 (7)	−0.0066 (7)
C36	0.0201 (9)	0.0158 (8)	0.0129 (8)	−0.0050 (7)	−0.0030 (7)	−0.0037 (6)
C40	0.0166 (8)	0.0207 (8)	0.0167 (8)	0.0036 (7)	−0.0063 (7)	−0.0082 (7)
C41	0.0149 (8)	0.0163 (8)	0.0139 (8)	−0.0015 (6)	−0.0056 (6)	−0.0045 (6)
C42	0.0151 (8)	0.0249 (9)	0.0208 (9)	−0.0030 (7)	−0.0034 (7)	−0.0049 (7)
C43	0.0250 (10)	0.0259 (10)	0.0221 (10)	−0.0106 (8)	−0.0094 (8)	0.0015 (8)
C44	0.0397 (12)	0.0203 (9)	0.0178 (9)	−0.0097 (8)	−0.0141 (8)	−0.0016 (7)
C45	0.0370 (11)	0.0178 (9)	0.0150 (8)	−0.0028 (8)	−0.0064 (8)	−0.0049 (7)
C46	0.0205 (9)	0.0182 (8)	0.0151 (8)	−0.0016 (7)	−0.0033 (7)	−0.0053 (7)
C51	0.0133 (8)	0.0149 (7)	0.0153 (8)	−0.0012 (6)	−0.0030 (6)	−0.0042 (6)
C52	0.0193 (9)	0.0212 (8)	0.0182 (9)	−0.0032 (7)	−0.0017 (7)	−0.0095 (7)
C53	0.0224 (10)	0.0300 (10)	0.0225 (10)	−0.0054 (8)	0.0048 (8)	−0.0123 (8)
C54	0.0163 (9)	0.0265 (10)	0.0303 (11)	−0.0037 (8)	0.0034 (8)	−0.0086 (8)
C55	0.0173 (9)	0.0277 (10)	0.0309 (11)	−0.0015 (8)	−0.0096 (8)	−0.0074 (8)
C56	0.0172 (9)	0.0254 (9)	0.0187 (9)	−0.0007 (7)	−0.0055 (7)	−0.0062 (7)
C61	0.0120 (8)	0.0237 (9)	0.0138 (8)	−0.0011 (6)	−0.0026 (6)	−0.0085 (7)
C62	0.0205 (9)	0.0260 (9)	0.0156 (8)	0.0034 (7)	−0.0052 (7)	−0.0084 (7)
C63	0.0214 (10)	0.0378 (11)	0.0159 (9)	0.0010 (8)	−0.0063 (7)	−0.0099 (8)
C64	0.0173 (9)	0.0457 (12)	0.0230 (10)	−0.0022 (8)	−0.0045 (8)	−0.0212 (9)
C65	0.0204 (9)	0.0331 (11)	0.0290 (11)	−0.0042 (8)	−0.0032 (8)	−0.0201 (9)
C66	0.0177 (9)	0.0236 (9)	0.0218 (9)	−0.0033 (7)	−0.0032 (7)	−0.0104 (7)

Geometric parameters (Å, °)

C2—Cl3	1.761 (2)	C33—H33	0.9300
C2—Cl2	1.768 (2)	C34—C35	1.385 (3)
C2—Cl1	1.770 (2)	C34—H34	0.9300

C2—H2	0.9800	C35—C36	1.389 (3)
P1—C10	1.7801 (17)	C35—H35	0.9300
P1—C31	1.7908 (17)	C36—H36	0.9300
P1—C21	1.7922 (18)	C40—H40A	0.9600
P1—C11	1.7930 (18)	C40—H40B	0.9600
P2—C40	1.7834 (18)	C40—H40C	0.9600
P2—C41	1.7930 (18)	C41—C46	1.393 (3)
P2—C51	1.7905 (18)	C41—C42	1.401 (2)
P2—C61	1.8003 (18)	C42—C43	1.392 (3)
C10—H10A	0.9600	C42—H42	0.9300
C10—H10B	0.9600	C43—C44	1.376 (3)
C10—H10C	0.9600	C43—H43	0.9300
C11—C16	1.378 (2)	C44—C45	1.379 (3)
C11—C12	1.392 (3)	C44—H44	0.9300
C12—C13	1.394 (3)	C45—C46	1.393 (3)
C12—H12	0.9300	C45—H45	0.9300
C13—C14	1.380 (3)	C46—H46	0.9300
C13—H13	0.9300	C51—C56	1.396 (3)
C14—C15	1.378 (3)	C51—C52	1.395 (3)
C14—H14	0.9300	C52—C53	1.393 (3)
C15—C16	1.392 (3)	C52—H52	0.9300
C15—H15	0.9300	C53—C54	1.384 (3)
C16—H16	0.9300	C53—H53	0.9300
C21—C26	1.395 (3)	C54—C55	1.384 (3)
C21—C22	1.395 (3)	C54—H54	0.9300
C22—C23	1.386 (3)	C55—C56	1.391 (3)
C22—H22	0.9300	C55—H55	0.9300
C23—C24	1.397 (3)	C56—H56	0.9300
C23—H23	0.9300	C61—C62	1.391 (3)
C24—C25	1.368 (3)	C61—C66	1.399 (3)
C24—H24	0.9300	C62—C63	1.394 (3)
C25—C26	1.392 (3)	C62—H62	0.9300
C25—H25	0.9300	C63—C64	1.389 (3)
C26—H26	0.9300	C63—H63	0.9300
C31—C36	1.400 (2)	C64—C65	1.390 (3)
C31—C32	1.399 (2)	C64—H64	0.9300
C32—C33	1.385 (3)	C65—C66	1.398 (3)
C32—H32	0.9300	C65—H65	0.9300
C33—C34	1.390 (3)	C66—H66	0.9300
Cl3—C2—Cl2	110.31 (11)	C35—C34—C33	120.22 (17)
Cl3—C2—Cl1	110.94 (11)	C35—C34—H34	119.9
Cl2—C2—Cl1	109.30 (10)	C33—C34—H34	119.9
Cl3—C2—H2	108.7	C34—C35—C36	120.74 (17)
Cl2—C2—H2	108.7	C34—C35—H35	119.6
Cl1—C2—H2	108.7	C36—C35—H35	119.6
C10—P1—C31	111.05 (8)	C31—C36—C35	118.99 (16)
C10—P1—C21	109.29 (9)	C31—C36—H36	120.5
C31—P1—C21	109.44 (8)	C35—C36—H36	120.5
C10—P1—C11	108.76 (8)	P2—C40—H40A	109.5

C31—P1—C11	107.86 (8)	P2—C40—H40B	109.5
C21—P1—C11	110.42 (8)	H40A—C40—H40B	109.5
C40—P2—C41	108.51 (9)	P2—C40—H40C	109.5
C40—P2—C51	109.82 (8)	H40A—C40—H40C	109.5
C41—P2—C51	110.49 (8)	H40B—C40—H40C	109.5
C40—P2—C61	110.31 (9)	C46—C41—C42	119.97 (17)
C41—P2—C61	108.94 (8)	C46—C41—P2	121.72 (14)
C51—P2—C61	108.77 (8)	C42—C41—P2	118.26 (14)
P1—C10—H10A	109.5	C43—C42—C41	119.32 (19)
P1—C10—H10B	109.5	C43—C42—H42	120.3
H10A—C10—H10B	109.5	C41—C42—H42	120.3
P1—C10—H10C	109.5	C44—C43—C42	120.37 (19)
H10A—C10—H10C	109.5	C44—C43—H43	119.8
H10B—C10—H10C	109.5	C42—C43—H43	119.8
C16—C11—C12	119.74 (17)	C45—C44—C43	120.48 (19)
C16—C11—P1	121.83 (14)	C45—C44—H44	119.8
C12—C11—P1	118.43 (14)	C43—C44—H44	119.8
C13—C12—C11	120.0 (2)	C44—C45—C46	120.3 (2)
C13—C12—H12	120.0	C44—C45—H45	119.9
C11—C12—H12	120.0	C46—C45—H45	119.9
C14—C13—C12	119.9 (2)	C45—C46—C41	119.53 (18)
C14—C13—H13	120.0	C45—C46—H46	120.2
C12—C13—H13	120.0	C41—C46—H46	120.2
C15—C14—C13	119.85 (18)	C56—C51—C52	120.46 (17)
C15—C14—H14	120.1	C56—C51—P2	121.14 (14)
C13—C14—H14	120.1	C52—C51—P2	118.38 (14)
C14—C15—C16	120.54 (18)	C53—C52—C51	118.93 (18)
C14—C15—H15	119.7	C53—C52—H52	120.5
C16—C15—H15	119.7	C51—C52—H52	120.5
C11—C16—C15	119.89 (18)	C52—C53—C54	120.46 (19)
C11—C16—H16	120.1	C52—C53—H53	119.8
C15—C16—H16	120.1	C54—C53—H53	119.8
C26—C21—C22	120.15 (17)	C55—C54—C53	120.62 (19)
C26—C21—P1	121.26 (14)	C55—C54—H54	119.7
C22—C21—P1	118.57 (14)	C53—C54—H54	119.7
C23—C22—C21	119.42 (19)	C54—C55—C56	119.62 (19)
C23—C22—H22	120.3	C54—C55—H55	120.2
C21—C22—H22	120.3	C56—C55—H55	120.2
C24—C23—C22	120.0 (2)	C55—C56—C51	119.86 (19)
C24—C23—H23	120.0	C55—C56—H56	120.1
C22—C23—H23	120.0	C51—C56—H56	120.1
C25—C24—C23	120.59 (19)	C62—C61—C66	120.36 (18)
C25—C24—H24	119.7	C62—C61—P2	119.75 (15)
C23—C24—H24	119.7	C66—C61—P2	119.83 (14)
C24—C25—C26	120.0 (2)	C61—C62—C63	119.84 (19)
C24—C25—H25	120.0	C61—C62—H62	120.1
C26—C25—H25	120.0	C63—C62—H62	120.1
C21—C26—C25	119.75 (19)	C64—C63—C62	119.8 (2)
C21—C26—H26	120.1	C64—C63—H63	120.1

C25—C26—H26	120.1	C62—C63—H63	120.1
C36—C31—C32	120.17 (16)	C63—C64—C65	120.75 (19)
C36—C31—P1	120.53 (13)	C63—C64—H64	119.6
C32—C31—P1	119.28 (13)	C65—C64—H64	119.6
C33—C32—C31	119.97 (17)	C64—C65—C66	119.6 (2)
C33—C32—H32	120.0	C64—C65—H65	120.2
C31—C32—H32	120.0	C66—C65—H65	120.2
C34—C33—C32	119.85 (17)	C61—C66—C65	119.60 (19)
C34—C33—H33	120.1	C61—C66—H66	120.2
C32—C33—H33	120.1	C65—C66—H66	120.2

Fig. 1

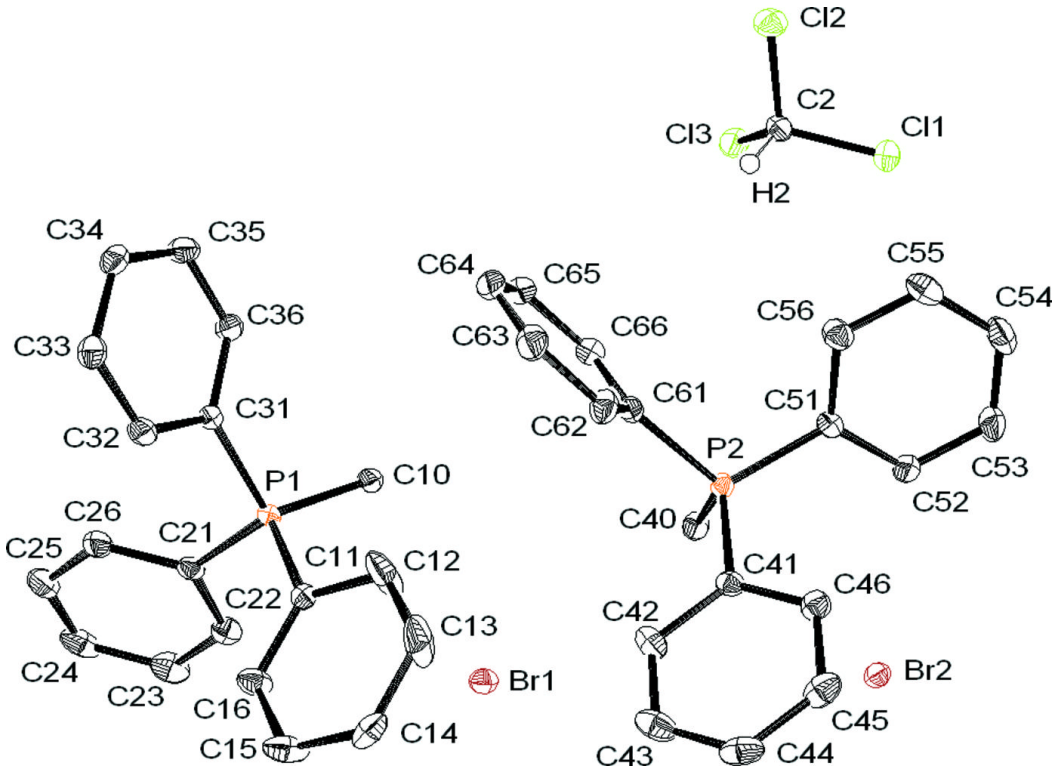
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Fig. 2