Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2-Hydroxyethyl)triphenylphosphonium chloride

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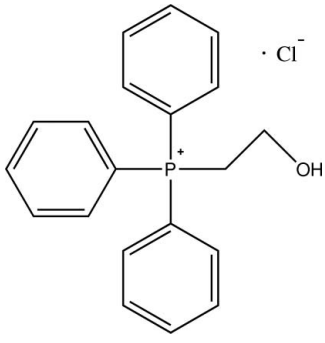
Received 23 January 2011; accepted 8 February 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 16.2.

In the crystal structure of the title compound, $C_{20}H_{20}OP^+\cdot Cl^-$, the cations and anions are linked by intermolecular C—H···Cl and O—H···Cl hydrogen bonds into chains running parallel to the b axis. In the cation, the hydroxyethyl group is disordered over two orientations with site-occupancy factors of 0.554 (4) and 0.446 (4).

Related literature

For general background to the Wittig reaction, see: Wittig & Schöllkopf (1954); Wittig & Haag (1955). For the synthesis, applications and biological activity of triphenylphosphonium compounds, see: Rideout *et al.* (1989); Cooper *et al.* (2001); Dubios & Lin (1978); Lou & Shang (2000); Calderon *et al.* (2008). For related structures, see: Shafiq *et al.* (2008); Wu *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{20}OP^+\cdot Cl^-$
M_r = 342.78
Monoclinic, $C2/c$
a = 14.1988 (4) Å
b = 12.5743 (3) Å
c = 19.7098 (6) Å
β = 92.510 (2)°
V = 3515.61 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 296 K
0.76 × 0.71 × 0.60 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.599, T_{max} = 0.905
26668 measured reflections
3725 independent reflections
3317 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.07
3725 reflections
230 parameters
35 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1	0.93	2.78	3.7009 (19)	171
C19—H19*C*···Cl1	0.97	2.73	3.6325 (18)	154
O1*B*—H1*B*···Cl1^{i}	0.82	2.32	3.115 (4)	162
O1*A*—H1*A*···Cl1^{i}	0.82	2.55	3.314 (4)	155
C19—H19*B*···Cl1^{i}	0.97	2.78	3.5935 (19)	142

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was financially supported by the BAP Selcuk University in Turkey. The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS 2 diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2551).

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supporting information

Acta Cryst. (2011). E**67**, o641 [doi:10.1107/S160053681100482X]

(2-Hydroxyethyl)triphenylphosphonium chloride

Ümit Ceylan, Hasan Tanak, Ercan Türkkan, Ömer Dereli and Orhan Büyükgüngör

S1. Comment

Triphenylphosphonium compounds and their various derivatives are key reagents in the Wittig reactions and are used to convert aldehydes and ketones into alkenes (Wittig & Schöllkopf, 1954; Wittig & Haag, 1955), specifically in applications ranging from the synthesis of simple alkenes to the construction of complex biologically active molecules in the pharmaceutical research (Rideout *et al.*, 1989; Cooper *et al.*, 2001). They are also an important class of isoaromatic compounds and have widespread applications for their antimicrobial and anticancer activities (Dubios & Lin, 1978; Lou & Shang, 2000). In addition, phosphonium compounds enhance flame retardancy mainly in textile industry (Calderon *et al.*, 2008).

The title compound crystallizes with one cation and anion in the asymmetric unit (Fig. 1). In the molecule, the hydroxyethyl group (C19—C20—O1) is disordered over two orientations with site occupancy factors of 0.554 (4) and 0.446 (4), respectively. The dihedral angles between rings A (C1—C6), B (C7—C12) and C (C13—C18) are A/B = 73.79 (1)°, A/C = 67.88 (1)° and B/C = 70.96 (1)°. All the geometric parameters are in agreement with those observed in related compounds (Shafiq *et al.*, 2008; Wu *et al.*, 2007). The minimum separation between the P^+ and Cl^- centres is 4.211 (1)Å. In the crystal structure, intermolecular C—H···Cl and C—H···O hydrogen bonds (Table 1) link the ions to form chains parallel to the *b* axis (Fig. 2).

S2. Experimental

(2-Hydroxyethyl)triphenylphosphonium chloride powder was purchased from Merck. Single crystals suitable for X-ray ananlysis were grown by slow evaporation of a concentrated acetonitrile solution.

S3. Refinement

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.93, 0.97 and 0.82 Å for aromatic CH, CH_2, and OH groups, respectively. The displacement parameters of the H atoms were constrained as U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). In the molecule, the hydroxyethyl group, (C19—C20—O1) is disordered over two orientations with site occupancy factors of 0.554 (4) and 0.446 (4). The disordered atoms were refined using the following restraints: SIMU, DELU and SADI (*SHELXL*; Sheldrick, 2008).

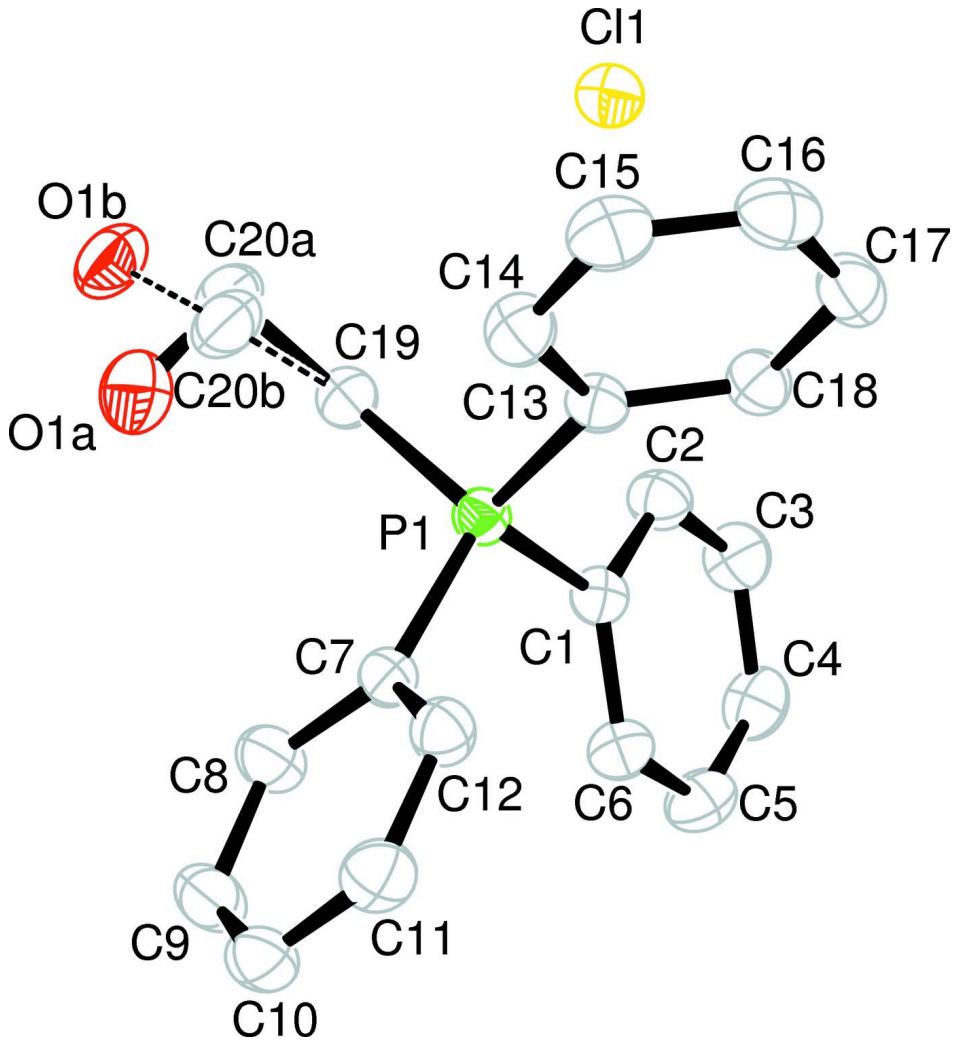

Figure 1

The structure of the title compound, with 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

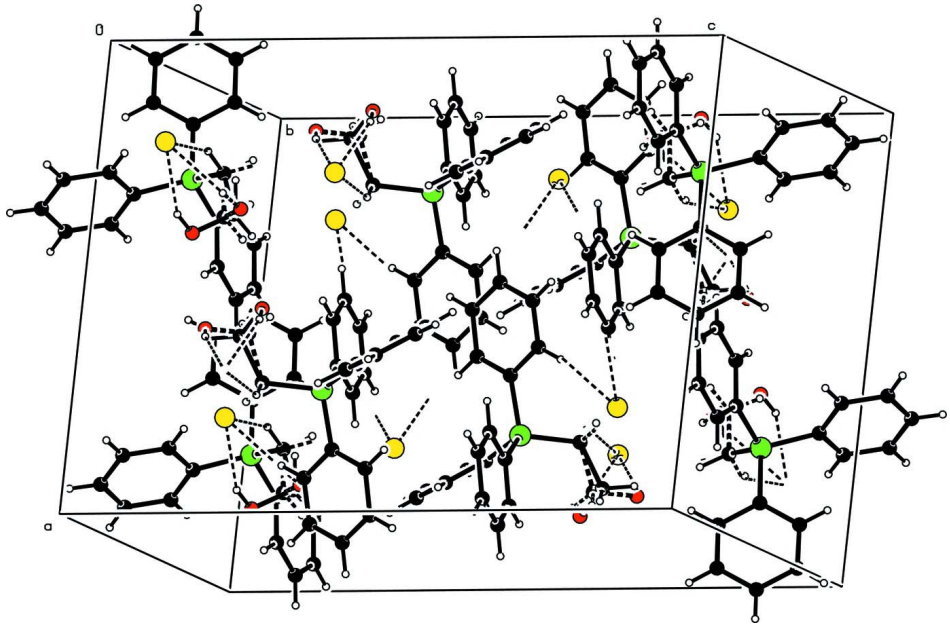

Figure 2

The crystal packing of the title compound. Intermolecular hydrogen bonds are drawn as dashed lines.

(2-Hydroxyethyl)triphenylphosphonium chloride

Crystal data

$C_{20}H_{20}OP^{+}\cdot Cl^{-}$
$M_r = 342.78$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 14.1988\ (4)$ Å
$b = 12.5743\ (3)$ Å
$c = 19.7098\ (6)$ Å
$\beta = 92.510\ (2)°$
$V = 3515.61\ (17)$ Å^3
$Z = 8$
$F(000) = 1440$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 36925 reflections
$\theta = 2.1–27.3°$
$\mu = 0.31$ mm^{-1}
$T = 296$ K
Prism, colorless
0.76 × 0.71 × 0.60 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.599$, $T_{max} = 0.905$
26668 measured reflections
3725 independent reflections
3317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.8°$, $\theta_{min} = 2.1°$
$h = -17\rightarrow17$
$k = -15\rightarrow15$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.101$
$S = 1.07$
3725 reflections
230 parameters
35 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
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 1.6584P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0106 (6)

Special details

Experimental. 360 frames, detector distance = 120 mm

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)
Cl1	0.25807 (3)	0.74387 (4)	0.18184 (2)	0.06015 (16)	
P1	0.22348 (3)	0.60936 (3)	0.37482 (2)	0.04301 (14)	
C1	0.34518 (11)	0.64165 (12)	0.39231 (8)	0.0449 (3)	
C2	0.39771 (12)	0.68183 (14)	0.33985 (9)	0.0545 (4)	
H2	0.3690	0.6949	0.2973	0.065*	
C3	0.49228 (13)	0.70205 (16)	0.35142 (11)	0.0633 (5)	
H3	0.5273	0.7292	0.3166	0.076*	
C4	0.53530 (13)	0.68242 (17)	0.41386 (11)	0.0655 (5)	
H4	0.5994	0.6958	0.4210	0.079*	
C5	0.48442 (14)	0.64332 (17)	0.46574 (10)	0.0652 (5)	
H5	0.5140	0.6305	0.5080	0.078*	
C6	0.38882 (12)	0.62269 (15)	0.45550 (9)	0.0543 (4)	
H6	0.3542	0.5963	0.4908	0.065*	
C7	0.18175 (11)	0.54012 (13)	0.44737 (8)	0.0457 (3)	
C8	0.21070 (14)	0.43627 (15)	0.46028 (9)	0.0606 (5)	
H8	0.2449	0.3994	0.4287	0.073*	
C9	0.18823 (16)	0.38821 (15)	0.52053 (10)	0.0665 (5)	
H9	0.2087	0.3193	0.5298	0.080*	
C10	0.13605 (13)	0.44101 (16)	0.56677 (9)	0.0608 (5)	
H10	0.1221	0.4082	0.6074	0.073*	
C11	0.10449 (13)	0.54206 (17)	0.55326 (9)	0.0617 (5)	
H11	0.0675	0.5769	0.5841	0.074*	
C12	0.12762 (12)	0.59252 (14)	0.49368 (9)	0.0527 (4)	
H12	0.1068	0.6615	0.4848	0.063*	
C13	0.15396 (11)	0.72717 (13)	0.36117 (8)	0.0450 (3)	
C14	0.05633 (12)	0.71654 (16)	0.34952 (10)	0.0581 (4)	
H14	0.0288	0.6494	0.3490	0.070*	
C15	0.00133 (13)	0.80521 (18)	0.33882 (10)	0.0667 (5)	

H15	−0.0634	0.7980	0.3308	0.080*	
C16	0.04150 (15)	0.90428 (17)	0.33992 (10)	0.0677 (5)	
H16	0.0037	0.9640	0.3329	0.081*	
C17	0.13779 (15)	0.91629 (15)	0.35143 (10)	0.0629 (5)	
H17	0.1646	0.9838	0.3522	0.076*	
C18	0.19394 (12)	0.82728 (13)	0.36184 (9)	0.0510 (4)	
H18	0.2587	0.8349	0.3693	0.061*	
C19	0.22152 (13)	0.52738 (14)	0.29984 (8)	0.0548 (4)	
H19A	0.2554	0.5656	0.2658	0.066*	0.554 (4)
H19B	0.2580	0.4641	0.3111	0.066*	0.554 (4)
H19C	0.2453	0.5679	0.2624	0.066*	0.446 (4)
H19D	0.2628	0.4668	0.3078	0.066*	0.446 (4)
O1A	0.0805 (2)	0.4345 (3)	0.31380 (16)	0.0879 (10)	0.554 (4)
H1A	0.1117	0.3827	0.3265	0.132*	0.554 (4)
C20A	0.1293 (4)	0.4906 (5)	0.2660 (4)	0.0667 (14)	0.554 (4)
H20A	0.0926	0.5514	0.2500	0.080*	0.554 (4)
H20B	0.1414	0.4454	0.2275	0.080*	0.554 (4)
O1B	0.1262 (3)	0.4096 (3)	0.23172 (16)	0.0766 (11)	0.446 (4)
H1B	0.1513	0.3564	0.2483	0.115*	0.446 (4)
C20B	0.1230 (4)	0.4883 (6)	0.2807 (6)	0.0672 (17)	0.446 (4)
H20C	0.0940	0.4603	0.3206	0.081*	0.446 (4)
H20D	0.0848	0.5471	0.2634	0.081*	0.446 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0621 (3)	0.0621 (3)	0.0561 (3)	0.0009 (2)	0.0013 (2)	0.00363 (19)
P1	0.0439 (2)	0.0434 (2)	0.0418 (2)	−0.00118 (16)	0.00250 (15)	0.00225 (15)
C1	0.0427 (8)	0.0448 (8)	0.0472 (8)	0.0022 (6)	0.0027 (6)	−0.0008 (6)
C2	0.0510 (9)	0.0598 (10)	0.0529 (9)	−0.0018 (8)	0.0037 (7)	0.0069 (7)
C3	0.0509 (10)	0.0718 (12)	0.0680 (11)	−0.0066 (9)	0.0106 (8)	0.0017 (9)
C4	0.0458 (9)	0.0720 (12)	0.0784 (13)	−0.0019 (8)	0.0006 (9)	−0.0108 (10)
C5	0.0562 (10)	0.0778 (13)	0.0604 (11)	0.0042 (9)	−0.0114 (8)	−0.0055 (9)
C6	0.0543 (9)	0.0613 (10)	0.0471 (8)	0.0014 (8)	0.0019 (7)	−0.0021 (7)
C7	0.0487 (8)	0.0458 (8)	0.0426 (7)	−0.0049 (6)	0.0026 (6)	0.0010 (6)
C8	0.0772 (12)	0.0519 (10)	0.0536 (9)	0.0067 (9)	0.0128 (9)	0.0036 (8)
C9	0.0862 (14)	0.0535 (10)	0.0602 (11)	0.0025 (9)	0.0076 (10)	0.0128 (8)
C10	0.0636 (11)	0.0698 (12)	0.0495 (9)	−0.0113 (9)	0.0074 (8)	0.0110 (8)
C11	0.0621 (10)	0.0727 (12)	0.0513 (9)	−0.0048 (9)	0.0144 (8)	−0.0046 (8)
C12	0.0568 (9)	0.0496 (9)	0.0522 (9)	−0.0016 (7)	0.0067 (7)	−0.0014 (7)
C13	0.0438 (8)	0.0482 (8)	0.0432 (7)	0.0017 (6)	0.0033 (6)	0.0035 (6)
C14	0.0468 (9)	0.0621 (10)	0.0654 (11)	−0.0026 (8)	0.0017 (8)	0.0010 (8)
C15	0.0475 (10)	0.0838 (14)	0.0683 (12)	0.0128 (9)	−0.0026 (8)	−0.0017 (10)
C16	0.0713 (12)	0.0689 (12)	0.0626 (11)	0.0249 (10)	0.0007 (9)	0.0045 (9)
C17	0.0767 (13)	0.0480 (9)	0.0644 (11)	0.0044 (9)	0.0073 (9)	0.0040 (8)
C18	0.0495 (9)	0.0510 (9)	0.0528 (9)	−0.0004 (7)	0.0043 (7)	0.0021 (7)
C19	0.0666 (10)	0.0499 (9)	0.0476 (8)	−0.0022 (8)	0.0013 (7)	−0.0016 (7)
O1A	0.0844 (19)	0.087 (2)	0.091 (2)	−0.0292 (16)	−0.0075 (15)	0.0052 (17)

C20A	0.080 (2)	0.0603 (19)	0.058 (3)	−0.0002 (17)	−0.0162 (18)	−0.0101 (17)
O1B	0.086 (2)	0.075 (2)	0.067 (2)	−0.0013 (17)	−0.0132 (16)	−0.0231 (16)
C20B	0.073 (2)	0.064 (2)	0.063 (4)	0.003 (2)	−0.018 (2)	−0.014 (2)

Geometric parameters (Å, º)

P1—C1	1.7938 (16)	C13—C18	1.381 (2)
P1—C13	1.7939 (16)	C13—C14	1.401 (2)
P1—C7	1.7968 (15)	C14—C15	1.372 (3)
P1—C19	1.8009 (17)	C14—H14	0.9300
C1—C6	1.387 (2)	C15—C16	1.370 (3)
C1—C2	1.396 (2)	C15—H15	0.9300
C2—C3	1.376 (2)	C16—C17	1.384 (3)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.372 (3)	C17—C18	1.384 (2)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.369 (3)	C18—H18	0.9300
C4—H4	0.9300	C19—C20A	1.515 (4)
C5—C6	1.388 (3)	C19—C20B	1.516 (4)
C5—H5	0.9300	C19—H19A	0.9700
C6—H6	0.9300	C19—H19B	0.9700
C7—C12	1.385 (2)	C19—H19C	0.9700
C7—C8	1.389 (2)	C19—H19D	0.9700
C8—C9	1.382 (2)	O1A—C20A	1.386 (8)
C8—H8	0.9300	O1A—H1A	0.8200
C9—C10	1.371 (3)	C20A—H20A	0.9700
C9—H9	0.9300	C20A—H20B	0.9700
C10—C11	1.370 (3)	O1B—C20B	1.383 (8)
C10—H10	0.9300	O1B—H1B	0.8200
C11—C12	1.387 (2)	C20B—H20C	0.9700
C11—H11	0.9300	C20B—H20D	0.9700
C12—H12	0.9300		
C1—P1—C13	111.16 (7)	C15—C14—H14	120.0
C1—P1—C7	107.77 (7)	C13—C14—H14	120.0
C13—P1—C7	108.73 (7)	C16—C15—C14	120.17 (18)
C1—P1—C19	105.51 (8)	C16—C15—H15	119.9
C13—P1—C19	111.16 (8)	C14—C15—H15	119.9
C7—P1—C19	112.45 (8)	C15—C16—C17	120.62 (18)
C6—C1—C2	119.68 (15)	C15—C16—H16	119.7
C6—C1—P1	121.49 (12)	C17—C16—H16	119.7
C2—C1—P1	118.76 (12)	C18—C17—C16	119.63 (18)
C3—C2—C1	119.56 (17)	C18—C17—H17	120.2
C3—C2—H2	120.2	C16—C17—H17	120.2
C1—C2—H2	120.2	C13—C18—C17	120.12 (16)
C4—C3—C2	120.56 (18)	C13—C18—H18	119.9
C4—C3—H3	119.7	C17—C18—H18	119.9
C2—C3—H3	119.7	C20A—C19—P1	121.2 (4)

C5—C4—C3	120.38 (18)	C20B—C19—P1	111.8 (4)
C5—C4—H4	119.8	C20A—C19—H19A	107.0
C3—C4—H4	119.8	C20B—C19—H19A	118.0
C4—C5—C6	120.22 (18)	P1—C19—H19A	107.0
C4—C5—H5	119.9	C20A—C19—H19B	107.0
C6—C5—H5	119.9	C20B—C19—H19B	105.6
C1—C6—C5	119.60 (17)	P1—C19—H19B	107.0
C1—C6—H6	120.2	H19A—C19—H19B	106.8
C5—C6—H6	120.2	C20A—C19—H19C	98.6
C12—C7—C8	119.65 (15)	C20B—C19—H19C	109.3
C12—C7—P1	120.38 (13)	P1—C19—H19C	109.3
C8—C7—P1	119.74 (12)	H19B—C19—H19C	113.9
C9—C8—C7	119.39 (17)	C20A—C19—H19D	109.6
C9—C8—H8	120.3	C20B—C19—H19D	109.3
C7—C8—H8	120.3	P1—C19—H19D	109.3
C10—C9—C8	120.75 (18)	H19A—C19—H19D	100.8
C10—C9—H9	119.6	H19C—C19—H19D	107.9
C8—C9—H9	119.6	O1A—C20A—C19	107.7 (5)
C11—C10—C9	120.12 (16)	O1A—C20A—H20A	110.2
C11—C10—H10	119.9	C19—C20A—H20A	110.2
C9—C10—H10	119.9	O1A—C20A—H20B	110.2
C10—C11—C12	120.10 (17)	C19—C20A—H20B	110.2
C10—C11—H11	120.0	H20A—C20A—H20B	108.5
C12—C11—H11	120.0	C20B—O1B—H1B	109.5
C7—C12—C11	119.94 (17)	O1B—C20B—C19	110.3 (6)
C7—C12—H12	120.0	O1B—C20B—H20C	109.6
C11—C12—H12	120.0	C19—C20B—H20C	109.6
C18—C13—C14	119.46 (16)	O1B—C20B—H20D	109.6
C18—C13—P1	121.88 (12)	C19—C20B—H20D	109.6
C14—C13—P1	118.66 (13)	H20C—C20B—H20D	108.1
C15—C14—C13	120.00 (18)		

C13—P1—C1—C6	112.88 (14)	P1—C7—C12—C11	−172.90 (14)
C7—P1—C1—C6	−6.17 (16)	C10—C11—C12—C7	0.8 (3)
C19—P1—C1—C6	−126.51 (14)	C1—P1—C13—C18	2.53 (16)
C13—P1—C1—C2	−70.32 (15)	C7—P1—C13—C18	121.01 (14)
C7—P1—C1—C2	170.63 (13)	C19—P1—C13—C18	−114.68 (15)
C19—P1—C1—C2	50.29 (15)	C1—P1—C13—C14	−177.47 (13)
C6—C1—C2—C3	0.1 (3)	C7—P1—C13—C14	−58.99 (15)
P1—C1—C2—C3	−176.77 (14)	C19—P1—C13—C14	65.32 (15)
C1—C2—C3—C4	0.4 (3)	C18—C13—C14—C15	0.1 (3)
C2—C3—C4—C5	−0.6 (3)	P1—C13—C14—C15	−179.91 (15)
C3—C4—C5—C6	0.3 (3)	C13—C14—C15—C16	−0.4 (3)
C2—C1—C6—C5	−0.4 (3)	C14—C15—C16—C17	0.3 (3)
P1—C1—C6—C5	176.39 (14)	C15—C16—C17—C18	0.1 (3)
C4—C5—C6—C1	0.2 (3)	C14—C13—C18—C17	0.3 (2)
C1—P1—C7—C12	101.87 (14)	P1—C13—C18—C17	−179.67 (13)
C13—P1—C7—C12	−18.72 (16)	C16—C17—C18—C13	−0.4 (3)

C19—P1—C7—C12	−142.27 (14)	C1—P1—C19—C20A	−175.4 (3)
C1—P1—C7—C8	−72.50 (16)	C13—P1—C19—C20A	−54.8 (3)
C13—P1—C7—C8	166.91 (14)	C7—P1—C19—C20A	67.4 (3)
C19—P1—C7—C8	43.36 (17)	C1—P1—C19—C20B	176.9 (4)
C12—C7—C8—C9	−2.6 (3)	C13—P1—C19—C20B	−62.5 (4)
P1—C7—C8—C9	171.81 (16)	C7—P1—C19—C20B	59.6 (4)
C7—C8—C9—C10	1.5 (3)	C20B—C19—C20A—O1A	−20 (2)
C8—C9—C10—C11	0.8 (3)	P1—C19—C20A—O1A	−57.9 (5)
C9—C10—C11—C12	−2.0 (3)	C20A—C19—C20B—O1B	47 (2)
C8—C7—C12—C11	1.5 (3)	P1—C19—C20B—O1B	−168.2 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1	0.93	2.78	3.7009 (19)	171
C19—H19*C*···Cl1	0.97	2.73	3.6325 (18)	154
O1*B*—H1*B*···Cl1^{i}	0.82	2.32	3.115 (4)	162
O1*A*—H1*A*···Cl1^{i}	0.82	2.55	3.314 (4)	155
C19—H19*B*···Cl1^{i}	0.97	2.78	3.5935 (19)	142

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