# organic compounds

# Bis(triphenyl-λ5-phosphanylidene)ammonium hydrogen dichloride

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In the title compound, $[(Ph_3P)_2N]^+\cdot[Cl\text{-}H\text{-}Cl]^-$ or $C_{36}H_{30}NP_2^+\cdot Cl_2H^-$, the H atom of the $[Cl—H—Cl]^-$ anion and the N atom of the $[(Ph_3P)_2N]^+$ cation are located on a twofold axis, yielding overall symmetry 2 for both the cation and the anion. The central P—N—P angle $[144.12\,(13)°]$ of the cation is in the expected range and indicates only weak cation–anion interactions. The almost linear $[Cl—H—Cl]^-$ anion is a rare example of a symmetric hydrogen bridge in a hydrogen dichloride anion. The Cl···Cl distance and two equal Cl—H bonds are typical of such a symmetric hydrogen dichloride anion.

## Related literature

For selected examples containing the $[Cl—H—Cl]^-$ anion, see: Atwood *et al.* (1990); Mootz *et al.* (1981); Habtemariam *et al.* (2001); Swann *et al.* (1984); Neumüller *et al.* (2005). For other bis(triphenyl-λ5-phosphanylidene)ammonium halide structures, see: Knapp & Uzun (2010a,b); Beckett *et al.* (2010). For a discussion of the $[(Ph_3P)_2N]^+$ cation, see: Lewis & Dance (2000). For a description of the Cambridge Structural Database, see: Allen (2002). For the synthesis of $[(Ph_3P)_2N]Cl$, see: Ruff & Schlientz (1974).
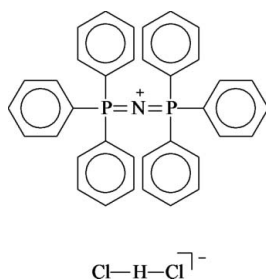


## Experimental

### Crystal data

$C_{36}H_{30}NP_2^+\cdot Cl_2H^-$

$M_r = 610.46$

Orthorhombic, $Pbcn$
$a = 11.6467\,(3)$ Å
$b = 16.5474\,(4)$ Å
$c = 15.7584\,(3)$ Å
$V = 3037.00\,(12)$ Å$^3$

$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.35$ mm$^{-1}$
$T = 100$ K
$0.18 \times 0.14 \times 0.09$ mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.940$, $T_{max} = 0.970$

28633 measured reflections
2994 independent reflections
2671 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.085$
$S = 1.08$
2994 reflections
189 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.61$ e Å$^{-3}$
$\Delta\rho_{min} = -0.79$ e Å$^{-3}$

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

| $D—H\cdots A$ | $D—H$ | $H\cdots A$ | $D\cdots A$ | $D—H\cdots A$ |
|---|---|---|---|---|
| Cl1—H1···Cl1$^i$ | 1.56 (1) | 1.56 (1) | 3.1045 (9) | 173 (3) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2011); software used to prepare material for publication: *SHELXL97*.

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# supporting information

## Bis(triphenyl-$\lambda^5$-phosphanylidene)ammonium hydrogen dichloride

### Jorit Gellhaar and Carsten Knapp

### S1. Comment

The Cambridge Structural Database (Allen, 2002) currently contains more than 1200 structures containing the $[(Ph_3P)_2N]^+$ cation ($[(Ph_3P)_2N]^+ = [PNP]^+$). Usually this cation is partnered by a bulky anion, while crystal structures containing small anions and especially halides are rare. The crystal structures of some solvate-free halides, $[(Ph_3P)_2N]I$ (Beckett *et al.*, 2010) and $[(Ph_3P)_2N]Cl$ (Knapp & Uzun, 2010*a*), and the acetontrile solvate $[(Ph_3P)_2N]Br \cdot CH_3CN$ (Knapp & Uzun, 2010*b*), were published only very recently.

Bis(triphenyl-$\lambda^5$-phosphanylidene)ammonium chloride $[(Ph_3P)_2N]Cl$ was synthesized according to a published method (Ruff *et al.*, 1974). Solvate-free single crystals suitable for X-ray diffraction of the title compound were obtained as a by-product by layering a $CH_3CN$ solution with diethyl ether. The H atom of the $[Cl—H—Cl]^-$ anion and the N atom of the $[(Ph_3P)_2N]^+$ cation are located on a twofold axis, yielding overall symmetry 2 for the cation. The central P—N—P angle [144.12 (13)°] and the P—N [1.5762 (7) Å] and P—C distances [1.7940 (16)–1.8028 (15) Å] are in the expected range for the $[(Ph_3P)_2N]^+$ cation (Lewis & Dance, 2000).

The number of structurally characterized hydrogen dichloride anions is still limited. Often disorder or low crystal quality does not allow to establish unequivically the position of the H atom. The Cl···Cl distances in all hydrogen dichloride anions deviate only slightly from an averaged distance of 3.10 Å. The anion in the title compound contains a symmetric hydrogen bridge with H—Cl distances of 1.56 (1) Å and a Cl···Cl distance of 3.1045 (9) Å. The anion is almost linear and a Cl—H—Cl angle of 173 (3)° is observed. A very similar hydrogen dichloride anion was found in the the crystal structure of [K(18 C-6)][Cl—H—Cl], where H—Cl is 1.56 Å and Cl···Cl 3.117 (1) Å (Atwood *et al.*, 1990).

### S2. Experimental

Single crystals of the title compound, suitable for X-ray diffraction analysis, were obtained as a by-product by layering a $CH_3CN$ solution of $[(Ph_3P)_2N]Cl$ with diethyl ether.

### S3. Refinement

The carbon-bonded hydrogen atoms were positioned geometrically and refined using a riding model. The same $U_{iso}$ value was used for all H atoms, which refined to 0.0226 (13) Å². The coordinates for the hydrogen atom in the $[Cl—H—Cl]^-$ anion were taken from the Fourier map and the atom was refined isotropically.
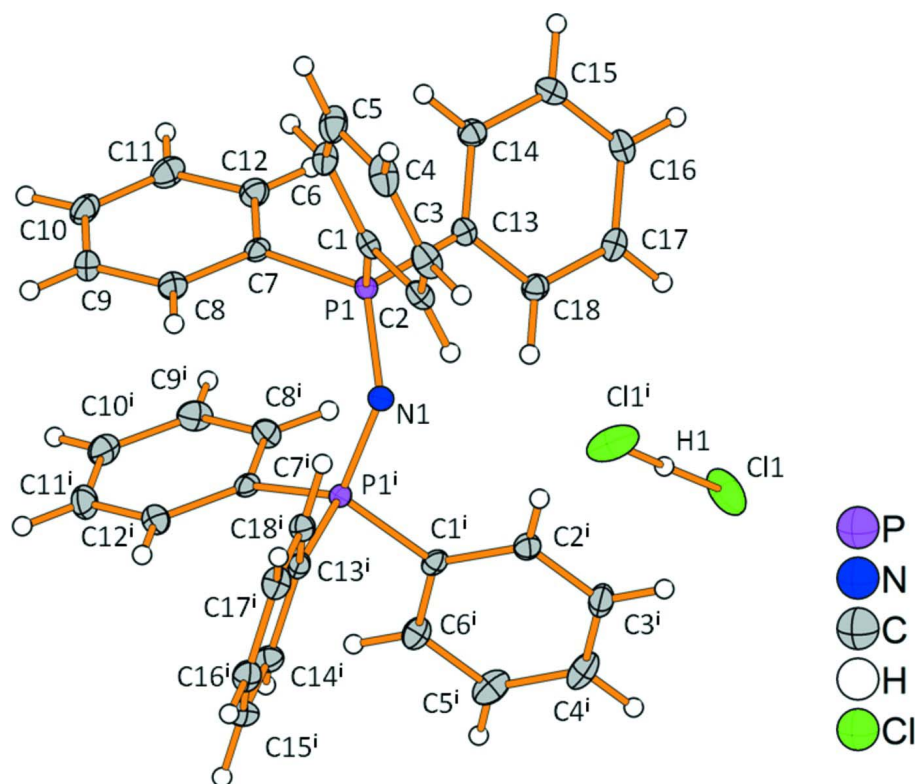
**Figure 1**

A view of the ionic unit of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level. H atoms are drawn with arbitrary radii. [Symmetry code: (i) -x+1, y, -z+0.5.]

**Bis(triphenylphosphanylidene)ammonium hydrogen dichloride**

*Crystal data*

| | |
|---|---|
| $C_{36}H_{30}NP_2{}^+ \cdot Cl_2H^-$ | $F(000) = 1272$ |
| $M_r = 610.46$ | $D_x = 1.335$ Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2n 2ab | Cell parameters from 9956 reflections |
| $a = 11.6467$ (3) Å | $\theta = 2.5$–30.8° |
| $b = 16.5474$ (4) Å | $\mu = 0.35$ mm$^{-1}$ |
| $c = 15.7584$ (3) Å | $T = 100$ K |
| $V = 3037.00$ (12) Å$^3$ | Block, colourless |
| $Z = 4$ | $0.18 \times 0.14 \times 0.09$ mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 28633 measured reflections |
| | 2994 independent reflections |
| Radiation source: microfocus sealed tube | 2671 reflections with $I > 2\sigma(I)$ |
| Multilayer mirro optics monochromator | $R_{int} = 0.030$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$ |
| Absorption correction: multi-scan | $h = -14 \rightarrow 14$ |
| (*SADABS*; Bruker, 2001) | $k = -19 \rightarrow 20$ |
| $T_{min} = 0.940$, $T_{max} = 0.970$ | $l = -19 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.085$ | |
| $S = 1.08$ | H atoms treated by a mixture of independent and constrained refinement |
| 2994 reflections | |
| 189 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 2.5322P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} < 0.001$ |
| | $\Delta\rho_{max} = 0.61$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.79$ e Å$^{-3}$ |

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| P1 | 0.37492 (3) | 0.47726 (2) | 0.22743 (2) | 0.01086 (11) |
| N1 | 0.5000 | 0.44792 (11) | 0.2500 | 0.0142 (4) |
| C1 | 0.32847 (13) | 0.42600 (9) | 0.13289 (10) | 0.0136 (3) |
| C2 | 0.37451 (13) | 0.35003 (10) | 0.11482 (10) | 0.0163 (3) |
| H2 | 0.4320 | 0.3275 | 0.1505 | 0.0226 (13)* |
| C3 | 0.33594 (15) | 0.30750 (10) | 0.04441 (11) | 0.0203 (4) |
| H3 | 0.3678 | 0.2561 | 0.0315 | 0.0226 (13)* |
| C4 | 0.25109 (16) | 0.33988 (10) | −0.00703 (11) | 0.0227 (4) |
| H4 | 0.2247 | 0.3104 | −0.0549 | 0.0226 (13)* |
| C5 | 0.20431 (15) | 0.41512 (11) | 0.01091 (11) | 0.0224 (4) |
| H5 | 0.1460 | 0.4369 | −0.0245 | 0.0226 (13)* |
| C6 | 0.24288 (14) | 0.45863 (10) | 0.08092 (10) | 0.0173 (3) |
| H6 | 0.2112 | 0.5102 | 0.0933 | 0.0226 (13)* |
| C7 | 0.36204 (12) | 0.58392 (9) | 0.20936 (10) | 0.0126 (3) |
| C8 | 0.43189 (13) | 0.61829 (10) | 0.14660 (10) | 0.0171 (3) |
| H8 | 0.4784 | 0.5847 | 0.1118 | 0.0226 (13)* |
| C9 | 0.43306 (14) | 0.70100 (10) | 0.13533 (11) | 0.0203 (4) |
| H9 | 0.4809 | 0.7243 | 0.0931 | 0.0226 (13)* |
| C10 | 0.36455 (14) | 0.75028 (10) | 0.18551 (11) | 0.0204 (4) |
| H10 | 0.3661 | 0.8072 | 0.1778 | 0.0226 (13)* |
| C11 | 0.29393 (15) | 0.71670 (10) | 0.24675 (11) | 0.0210 (4) |
| H11 | 0.2462 | 0.7505 | 0.2803 | 0.0226 (13)* |
| C12 | 0.29273 (14) | 0.63361 (10) | 0.25912 (10) | 0.0169 (3) |
| H12 | 0.2447 | 0.6107 | 0.3015 | 0.0226 (13)* |

| C13 | 0.27637 (13) | 0.44720 (9) | 0.30980 (10) | 0.0128 (3) |
| C14 | 0.15825 (13) | 0.45901 (10) | 0.30003 (10) | 0.0162 (3) |
| H14 | 0.1295 | 0.4861 | 0.2513 | 0.0226 (13)* |
| C15 | 0.08307 (14) | 0.43109 (10) | 0.36169 (11) | 0.0189 (3) |
| H15 | 0.0028 | 0.4391 | 0.3550 | 0.0226 (13)* |
| C16 | 0.12438 (14) | 0.39159 (10) | 0.43294 (10) | 0.0179 (3) |
| H16 | 0.0724 | 0.3723 | 0.4748 | 0.0226 (13)* |
| C17 | 0.24172 (14) | 0.38023 (10) | 0.44327 (10) | 0.0174 (3) |
| H17 | 0.2700 | 0.3534 | 0.4923 | 0.0226 (13)* |
| C18 | 0.31776 (13) | 0.40806 (9) | 0.38184 (10) | 0.0149 (3) |
| H18 | 0.3980 | 0.4004 | 0.3890 | 0.0226 (13)* |
| Cl1 | 0.49306 (4) | 0.14372 (3) | 0.15163 (3) | 0.03665 (15) |
| H1 | 0.5000 | 0.149 (3) | 0.2500 | 0.087 (15)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| --- | --- | --- | --- | --- | --- | --- |
| P1 | 0.0108 (2) | 0.0097 (2) | 0.0120 (2) | −0.00044 (14) | −0.00017 (14) | −0.00049 (14) |
| N1 | 0.0123 (9) | 0.0108 (9) | 0.0196 (10) | 0.000 | −0.0001 (7) | 0.000 |
| C1 | 0.0144 (7) | 0.0138 (8) | 0.0127 (7) | −0.0053 (6) | 0.0026 (6) | −0.0011 (6) |
| C2 | 0.0148 (7) | 0.0154 (8) | 0.0188 (8) | −0.0027 (6) | 0.0026 (6) | −0.0021 (6) |
| C3 | 0.0231 (8) | 0.0158 (8) | 0.0219 (9) | −0.0040 (7) | 0.0065 (7) | −0.0059 (7) |
| C4 | 0.0334 (9) | 0.0200 (9) | 0.0146 (8) | −0.0099 (7) | 0.0004 (7) | −0.0030 (7) |
| C5 | 0.0300 (9) | 0.0212 (9) | 0.0160 (8) | −0.0063 (7) | −0.0066 (7) | 0.0041 (7) |
| C6 | 0.0229 (8) | 0.0135 (8) | 0.0155 (8) | −0.0021 (6) | −0.0011 (6) | 0.0015 (6) |
| C7 | 0.0126 (7) | 0.0118 (7) | 0.0134 (7) | 0.0000 (6) | −0.0044 (6) | −0.0001 (6) |
| C8 | 0.0160 (7) | 0.0169 (8) | 0.0184 (8) | 0.0015 (6) | 0.0007 (6) | 0.0006 (6) |
| C9 | 0.0187 (8) | 0.0174 (9) | 0.0247 (9) | −0.0021 (7) | −0.0007 (7) | 0.0067 (7) |
| C10 | 0.0218 (8) | 0.0118 (8) | 0.0276 (9) | 0.0007 (6) | −0.0076 (7) | 0.0019 (7) |
| C11 | 0.0231 (8) | 0.0158 (8) | 0.0240 (9) | 0.0054 (7) | −0.0021 (7) | −0.0027 (7) |
| C12 | 0.0173 (8) | 0.0166 (8) | 0.0169 (8) | 0.0019 (6) | 0.0003 (6) | 0.0001 (6) |
| C13 | 0.0148 (7) | 0.0106 (7) | 0.0130 (8) | −0.0014 (6) | 0.0006 (6) | −0.0023 (6) |
| C14 | 0.0155 (7) | 0.0185 (8) | 0.0147 (8) | −0.0014 (6) | −0.0018 (6) | 0.0002 (6) |
| C15 | 0.0133 (7) | 0.0214 (9) | 0.0219 (9) | −0.0024 (6) | 0.0001 (6) | −0.0006 (7) |
| C16 | 0.0202 (8) | 0.0153 (8) | 0.0180 (8) | −0.0039 (6) | 0.0047 (6) | 0.0001 (6) |
| C17 | 0.0230 (8) | 0.0142 (8) | 0.0149 (8) | 0.0002 (6) | −0.0009 (6) | 0.0022 (6) |
| C18 | 0.0151 (7) | 0.0127 (8) | 0.0168 (8) | 0.0008 (6) | −0.0009 (6) | −0.0005 (6) |
| Cl1 | 0.0363 (3) | 0.0556 (3) | 0.0181 (2) | 0.0236 (2) | −0.00128 (18) | −0.0032 (2) |

*Geometric parameters (Å, º)*

| | | | |
| --- | --- | --- | --- |
| P1—N1 | 1.5762 (7) | C9—C10 | 1.388 (2) |
| P1—C7 | 1.7940 (16) | C9—H9 | 0.9500 |
| P1—C1 | 1.7976 (16) | C10—C11 | 1.384 (2) |
| P1—C13 | 1.8028 (15) | C10—H10 | 0.9500 |
| N1—P1[i] | 1.5761 (7) | C11—C12 | 1.389 (2) |
| C1—C2 | 1.396 (2) | C11—H11 | 0.9500 |
| C1—C6 | 1.399 (2) | C12—H12 | 0.9500 |

| | | | |
|---|---|---|---|
| C2—C3 | 1.389 (2) | C13—C18 | 1.393 (2) |
| C2—H2 | 0.9500 | C13—C14 | 1.398 (2) |
| C3—C4 | 1.386 (3) | C14—C15 | 1.387 (2) |
| C3—H3 | 0.9500 | C14—H14 | 0.9500 |
| C4—C5 | 1.388 (3) | C15—C16 | 1.386 (2) |
| C4—H4 | 0.9500 | C15—H15 | 0.9500 |
| C5—C6 | 1.392 (2) | C16—C17 | 1.389 (2) |
| C5—H5 | 0.9500 | C16—H16 | 0.9500 |
| C6—H6 | 0.9500 | C17—C18 | 1.390 (2) |
| C7—C12 | 1.394 (2) | C17—H17 | 0.9500 |
| C7—C8 | 1.401 (2) | C18—H18 | 0.9500 |
| C8—C9 | 1.380 (2) | Cl1—H1 | 1.555 (3) |
| C8—H8 | 0.9500 | | |
| | | | |
| N1—P1—C7 | 114.59 (8) | C8—C9—C10 | 120.24 (16) |
| N1—P1—C1 | 108.65 (7) | C8—C9—H9 | 119.9 |
| C7—P1—C1 | 107.91 (7) | C10—C9—H9 | 119.9 |
| N1—P1—C13 | 109.93 (6) | C11—C10—C9 | 120.19 (15) |
| C7—P1—C13 | 109.42 (7) | C11—C10—H10 | 119.9 |
| C1—P1—C13 | 105.96 (7) | C9—C10—H10 | 119.9 |
| P1<sup>i</sup>—N1—P1 | 144.12 (13) | C10—C11—C12 | 120.08 (16) |
| C2—C1—C6 | 120.13 (14) | C10—C11—H11 | 120.0 |
| C2—C1—P1 | 118.58 (12) | C12—C11—H11 | 120.0 |
| C6—C1—P1 | 121.17 (12) | C11—C12—C7 | 119.95 (16) |
| C3—C2—C1 | 119.67 (15) | C11—C12—H12 | 120.0 |
| C3—C2—H2 | 120.2 | C7—C12—H12 | 120.0 |
| C1—C2—H2 | 120.2 | C18—C13—C14 | 119.68 (14) |
| C4—C3—C2 | 120.14 (16) | C18—C13—P1 | 119.66 (11) |
| C4—C3—H3 | 119.9 | C14—C13—P1 | 120.57 (12) |
| C2—C3—H3 | 119.9 | C15—C14—C13 | 119.84 (15) |
| C3—C4—C5 | 120.49 (16) | C15—C14—H14 | 120.1 |
| C3—C4—H4 | 119.8 | C13—C14—H14 | 120.1 |
| C5—C4—H4 | 119.8 | C16—C15—C14 | 120.37 (15) |
| C4—C5—C6 | 119.92 (16) | C16—C15—H15 | 119.8 |
| C4—C5—H5 | 120.0 | C14—C15—H15 | 119.8 |
| C6—C5—H5 | 120.0 | C15—C16—C17 | 120.03 (15) |
| C5—C6—C1 | 119.63 (16) | C15—C16—H16 | 120.0 |
| C5—C6—H6 | 120.2 | C17—C16—H16 | 120.0 |
| C1—C6—H6 | 120.2 | C16—C17—C18 | 120.02 (15) |
| C12—C7—C8 | 119.59 (15) | C16—C17—H17 | 120.0 |
| C12—C7—P1 | 122.65 (12) | C18—C17—H17 | 120.0 |
| C8—C7—P1 | 117.57 (12) | C17—C18—C13 | 120.06 (14) |
| C9—C8—C7 | 119.94 (15) | C17—C18—H18 | 120.0 |
| C9—C8—H8 | 120.0 | C13—C18—H18 | 120.0 |
| C7—C8—H8 | 120.0 | | |
| | | | |
| C7—P1—N1—P1<sup>i</sup> | 8.50 (6) | C12—C7—C8—C9 | 1.0 (2) |
| C1—P1—N1—P1<sup>i</sup> | 129.26 (6) | P1—C7—C8—C9 | −174.15 (13) |

| | | | |
|---|---|---|---|
| C13—P1—N1—P1ⁱ | −115.21 (6) | C7—C8—C9—C10 | −0.5 (2) |
| N1—P1—C1—C2 | 27.31 (14) | C8—C9—C10—C11 | −0.5 (3) |
| C7—P1—C1—C2 | 152.11 (12) | C9—C10—C11—C12 | 1.0 (3) |
| C13—P1—C1—C2 | −90.78 (13) | C10—C11—C12—C7 | −0.5 (2) |
| N1—P1—C1—C6 | −156.65 (13) | C8—C7—C12—C11 | −0.5 (2) |
| C7—P1—C1—C6 | −31.85 (15) | P1—C7—C12—C11 | 174.41 (13) |
| C13—P1—C1—C6 | 85.26 (14) | N1—P1—C13—C18 | 3.27 (15) |
| C6—C1—C2—C3 | 0.8 (2) | C7—P1—C13—C18 | −123.40 (13) |
| P1—C1—C2—C3 | 176.89 (12) | C1—P1—C13—C18 | 120.50 (13) |
| C1—C2—C3—C4 | −0.8 (2) | N1—P1—C13—C14 | −173.36 (13) |
| C2—C3—C4—C5 | 0.4 (3) | C7—P1—C13—C14 | 59.97 (14) |
| C3—C4—C5—C6 | 0.2 (3) | C1—P1—C13—C14 | −56.13 (14) |
| C4—C5—C6—C1 | −0.2 (2) | C18—C13—C14—C15 | −0.6 (2) |
| C2—C1—C6—C5 | −0.3 (2) | P1—C13—C14—C15 | 176.07 (12) |
| P1—C1—C6—C5 | −176.29 (12) | C13—C14—C15—C16 | 0.0 (2) |
| N1—P1—C7—C12 | −118.52 (12) | C14—C15—C16—C17 | 0.4 (3) |
| C1—P1—C7—C12 | 120.31 (13) | C15—C16—C17—C18 | −0.4 (2) |
| C13—P1—C7—C12 | 5.46 (15) | C16—C17—C18—C13 | −0.1 (2) |
| N1—P1—C7—C8 | 56.51 (13) | C14—C13—C18—C17 | 0.6 (2) |
| C1—P1—C7—C8 | −64.66 (13) | P1—C13—C18—C17 | −176.05 (12) |
| C13—P1—C7—C8 | −179.52 (12) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| Cl1—H1···Cl1ⁱ | 1.56 (1) | 1.56 (1) | 3.1045 (9) | 173 (3) |

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