

Tetrakis(benzylamino)phosphonium chloride

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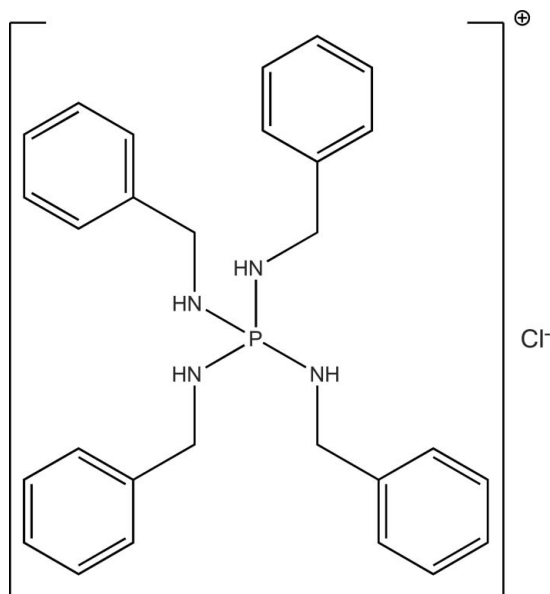
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Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 20.1.

The title salt, $[\text{P}(\text{NHCH}_2\text{C}_6\text{H}_5)_4]^+\text{Cl}^-$, crystallizes with the P atom and Cl^- anion lying on a twofold rotation axis. The P atom has a slightly distorted tetrahedral geometry with two classes of N–P–N angles [101.15 (10) and 100.55 (11)° and 113.07 (9) and 114.83 (8)°] and the environments of sp^2 -hybridized N atoms are essentially planar (sum of angles = 359.9 and 360.1°). In the crystal, the phosphonium ion interacts with each neighboring chloride ion *via* two approximately equal N–H...Cl interactions, forming parallel chains along the c axis.

Related literature

For background information on phosphonium salts, see: Hart & Sisler (1964); Levason *et al.* (2006); Schiemenz *et al.* (2003). For related structures, see: Bickley *et al.* (2004); Horstmann & Schnick (1996)



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $\text{C}_{28}\text{H}_{32}\text{N}_4\text{P}^+\text{Cl}^-$ | $V = 1283.1$ (6) Å ³ |
| $M_r = 491.00$ | $Z = 2$ |
| Orthorhombic, $P2_12_12$ | Mo $K\alpha$ radiation |
| $a = 11.359$ (3) Å | $\mu = 0.24$ mm ⁻¹ |
| $b = 14.258$ (4) Å | $T = 193$ K |
| $c = 7.923$ (3) Å | $0.50 \times 0.40 \times 0.25$ mm |

Data collection

| | |
|--|---|
| Rebuilt Syntex P21/Siemens P3 four-circle diffractometer | $R_{\text{int}} = 0.024$ |
| 6760 measured reflections | 2 standard reflections every 98 reflections |
| 3122 independent reflections | intensity decay: 2% |
| 2677 reflections with $I > 2\sigma(I)$ | |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | $\Delta\rho_{\text{max}} = 0.35$ e Å ⁻³ |
| $wR(F^2) = 0.094$ | $\Delta\rho_{\text{min}} = -0.33$ e Å ⁻³ |
| $S = 1.01$ | Absolute structure: Flack (1983), 1321 Friedel pairs |
| 3122 reflections | Flack parameter: 0.08 (8) |
| 155 parameters | |
| H-atom parameters constrained | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1C}\cdots\text{Cl1}^{\dagger}$ | 0.86 | 2.35 | 3.1848 (17) | 163 |
| $\text{N2}-\text{H2A}\cdots\text{Cl1}$ | 0.86 | 2.35 | 3.1855 (18) | 165 |

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

Data collection: *P3/PC* (Siemens, 1989); cell refinement: *P3/PC*; data reduction: *P3/PC*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2077).

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supporting information

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S1. Comment

Phosphonium salts, $[\text{PR}_4]^+$, are widely used as large cations to stabilize a variety of anionic species and to phase-transfer anions into low polarity organic media (Levason *et al.*, 2006). A few examples of tetraamino phosphonium salts exist in the literature (Hart & Sisler, 1964) and some of them are used as catalysis for preparing fluorine-containing compounds by a halogen/fluorine exchange reaction (Schiemenz *et al.*, 2003). Also, the crystal structure of $\text{P}(\text{NH}_2)_4\text{Cl}$ (Horstmann & Schnick, 1996) and $[\text{P}(\text{NHPh})_4]\text{Cl}$ (Bickley *et al.*, 2004) have been reported. In an effort to further investigation into these types of compounds, the crystal structure of $[\text{P}(\text{NHCH}_2\text{C}_6\text{H}_5)_4]^+\text{Cl}^-$ is presented.

The title salt, $[\text{P}(\text{NHCH}_2\text{C}_6\text{H}_5)_4]^+\text{Cl}^-$, crystallizes with the P atom and Cl^- anion lying on a two-fold rotation axis in the space group $P2_12_12$. The supramolecular structure of compound exhibits a polymeric chain of alternating phosphonium and chloride ions in the solid state (Fig. 2) with $\text{P}\cdots\text{P}$ distances of 7.923 Å. The phosphonium ion interacts with each neighboring chloride ion *via* two equal $\text{N}\cdots\text{H}\cdots\text{Cl}$ interactions and six-membered rings around each phosphorus atom are formed. The centroid-centroid distance between adjacent phenyl rings is 4.009 Å, indicating no strong π - π stacking interactions exist in compound.

The four P-N bonds are of almost equal lengths 1.6166 (14) and 1.6184 (14) Å and are similar to those found in $[\text{P}(\text{NHPh})_4]\text{Cl}$ (Bickley *et al.*, 2004) and $\text{P}(\text{NH}_2)_4\text{Cl}$ (Horstmann & Schnick, 1996). These P-N bonds are shorter than the typical P-N single bond length (1.77 Å). As observed in $[\text{P}(\text{NHPh})_4]\text{Cl}$, there are two classes of N-P-N angles resulting in a distorted tetrahedral environment for P1. More acute angles of 101.15 (10) and 100.55° are observed within the hydrogen bonding chelates of the N1-P1-N1^i and N2-P1-N2^i (*i*: -*x*, -*y*, *z*) units respectively, whereas the remaining four N-P-N angles are 113.07 (9) and 114.83 (8)°. Although the main cause for the distortion from the ideal tetrahedral geometry is unclear, it seems to be partly controlled by hydrogen bonding. The sum of angles around nitrogen atoms are exactly 360° and these atoms are sp^2 hybridized.

S2. Experimental

All the reagents and solvents were used as obtained without further purification. Phosphorus pentachloride (2 mmol) was added drop wise with constant stirring to a toluene solution (30 ml) of benzylamine (8 mmol) at 0°C. After an hour stirring, the reaction mixture was refluxed for 3 h. The solid formed during the reaction was filtered and then washed with distilled water, toluene, chloroform and dried. Single crystals suitable for single-crystal X-ray diffraction analysis were obtained from the mixture of MeOH and CH_3CN solution.

S3. Refinement

The hydrogen atoms of NH groups were found in difference Fourier synthesis, the H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with with the $U_{\text{iso}}(\text{H})$ parameters equal to 1.2 $U_{\text{eq}}(\text{X})$, where $U(\text{X})$ are the equivalent thermal parameters of the atoms to which corresponding H atoms are bonded.

The absolute structure parameter (Flack, 1983) is refined based on 1321 Friedel pairs.

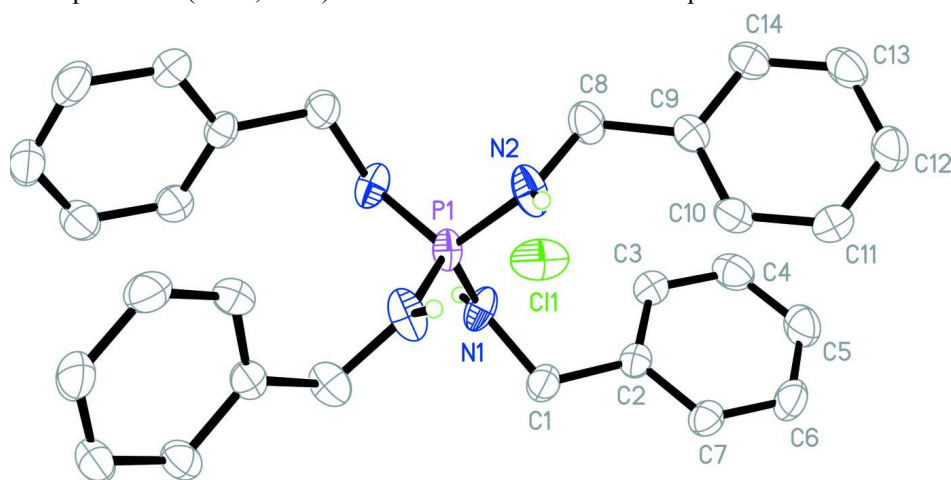


Figure 1

The structure of the title compound with 50% displacement ellipsoids and C-bound H atoms omitted. Unlabeled atoms are related to labeled atoms by a two-fold rotation.

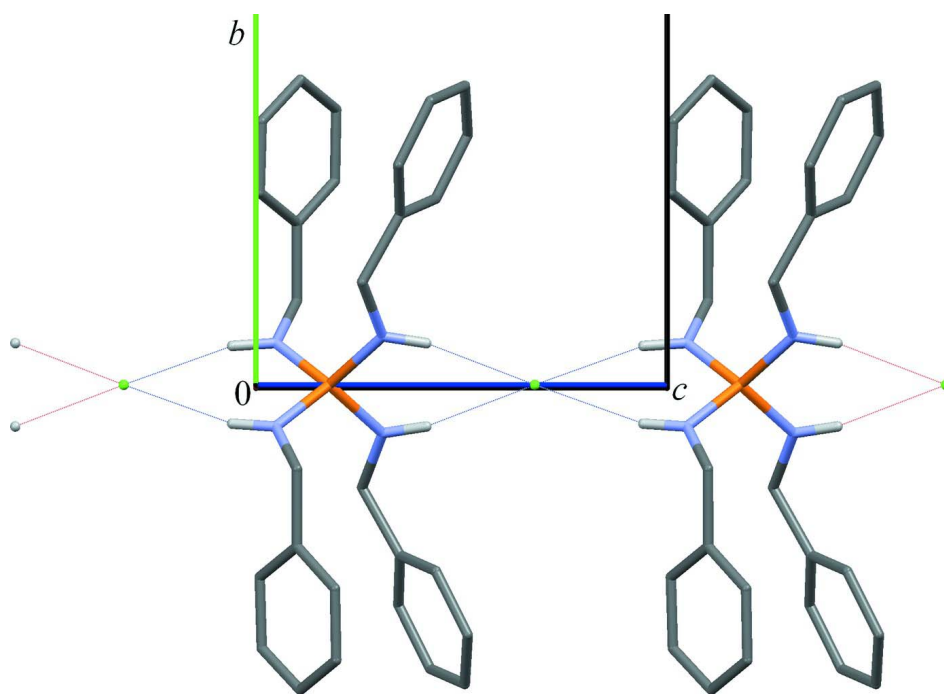


Figure 2

An *a*-axis projection showing hydrogen bonding dotted lines. The long *b* axis is truncated.

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Crystal data

$C_{28}H_{32}N_4P^+ \cdot Cl^-$
 $M_r = 491.00$
 Orthorhombic, $P2_12_12$
 Hall symbol: $P\ 2\ 2ab$

$a = 11.359\ (3)\ \text{\AA}$
 $b = 14.258\ (4)\ \text{\AA}$
 $c = 7.923\ (3)\ \text{\AA}$
 $V = 1283.1\ (6)\ \text{\AA}^3$

$Z = 2$
 $F(000) = 520$
 $D_x = 1.271 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 24 reflections
 $\theta = 10\text{--}11^\circ$
 $\mu = 0.24 \text{ mm}^{-1}$
 $T = 193 \text{ K}$
 Plate, colourless
 $0.50 \times 0.40 \times 0.25 \text{ mm}$

Data collection

Rebuilt Syntex P2₁/Siemens P3 four-circle diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $\theta/2\theta$ scans
 6760 measured reflections
 3122 independent reflections
 2677 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 28.1^\circ$, $\theta_{\text{min}} = 2.3^\circ$
 $h = -15 \rightarrow 15$
 $k = -18 \rightarrow 18$
 $l = -10 \rightarrow 10$
 2 standard reflections every 98 reflections
 intensity decay: 2%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.094$
 $S = 1.01$
 3122 reflections
 155 parameters
 0 restraints
 Primary atom site location: structure-invariant direct methods
 Secondary atom site location: difference Fourier map
 Hydrogen site location: difference Fourier map
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.1221P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983), 1321 Friedel pairs
 Absolute structure parameter: 0.08 (8)

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| C11 | 0.0000 | 0.0000 | 0.67845 (6) | 0.03585 (15) |
| P1 | 0.0000 | 0.0000 | 0.17782 (6) | 0.02407 (13) |
| N1 | 0.08364 (13) | 0.05683 (9) | 0.04823 (17) | 0.0305 (3) |
| H1C | 0.0684 | 0.0528 | -0.0578 | 0.037* |
| N2 | -0.07306 (14) | 0.06507 (10) | 0.30836 (17) | 0.0347 (3) |
| H2A | -0.0623 | 0.0560 | 0.4146 | 0.042* |
| C1 | 0.18316 (15) | 0.11449 (11) | 0.0998 (2) | 0.0327 (4) |
| H1A | 0.2487 | 0.1016 | 0.0248 | 0.039* |
| H1B | 0.2067 | 0.0958 | 0.2125 | 0.039* |
| C2 | 0.16072 (13) | 0.21915 (10) | 0.1000 (2) | 0.0255 (3) |

| | | | | |
|------|---------------|--------------|------------|------------|
| C3 | 0.06933 (14) | 0.25994 (12) | 0.0093 (2) | 0.0309 (3) |
| H3A | 0.0193 | 0.2226 | -0.0548 | 0.037* |
| C4 | 0.05265 (16) | 0.35639 (13) | 0.0142 (3) | 0.0396 (4) |
| H4A | -0.0090 | 0.3832 | -0.0461 | 0.047* |
| C5 | 0.12664 (17) | 0.41274 (12) | 0.1078 (3) | 0.0435 (5) |
| H5A | 0.1142 | 0.4772 | 0.1120 | 0.052* |
| C6 | 0.21920 (16) | 0.37315 (12) | 0.1953 (3) | 0.0394 (4) |
| H6A | 0.2703 | 0.4111 | 0.2564 | 0.047* |
| C7 | 0.23623 (14) | 0.27655 (11) | 0.1922 (2) | 0.0301 (3) |
| H7A | 0.2984 | 0.2502 | 0.2520 | 0.036* |
| C8 | -0.15598 (16) | 0.13807 (12) | 0.2581 (2) | 0.0342 (4) |
| H8A | -0.2355 | 0.1160 | 0.2787 | 0.041* |
| H8B | -0.1480 | 0.1491 | 0.1379 | 0.041* |
| C9 | -0.13829 (14) | 0.22969 (11) | 0.3506 (2) | 0.0265 (3) |
| C10 | -0.03555 (14) | 0.25145 (12) | 0.4376 (2) | 0.0311 (3) |
| H10A | 0.0248 | 0.2075 | 0.4437 | 0.037* |
| C11 | -0.02213 (15) | 0.33760 (13) | 0.5152 (3) | 0.0392 (4) |
| H11A | 0.0472 | 0.3514 | 0.5725 | 0.047* |
| C12 | -0.11172 (17) | 0.40365 (12) | 0.5081 (3) | 0.0419 (4) |
| H12A | -0.1024 | 0.4617 | 0.5597 | 0.050* |
| C13 | -0.21480 (16) | 0.38267 (12) | 0.4238 (3) | 0.0374 (4) |
| H13A | -0.2752 | 0.4266 | 0.4191 | 0.045* |
| C14 | -0.22821 (14) | 0.29623 (12) | 0.3465 (2) | 0.0317 (3) |
| H14A | -0.2982 | 0.2824 | 0.2909 | 0.038* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|------------|-------------|-------------|-------------|-------------|
| C11 | 0.0282 (3) | 0.0634 (4) | 0.0159 (2) | -0.0003 (3) | 0.000 | 0.000 |
| P1 | 0.0382 (3) | 0.0190 (2) | 0.0151 (2) | 0.0001 (2) | 0.000 | 0.000 |
| N1 | 0.0447 (8) | 0.0280 (6) | 0.0188 (6) | -0.0127 (6) | -0.0030 (6) | -0.0009 (5) |
| N2 | 0.0570 (9) | 0.0301 (6) | 0.0169 (6) | 0.0133 (7) | 0.0002 (6) | -0.0021 (5) |
| C1 | 0.0334 (8) | 0.0262 (7) | 0.0387 (9) | -0.0025 (6) | -0.0071 (7) | -0.0007 (7) |
| C2 | 0.0281 (7) | 0.0251 (7) | 0.0234 (7) | -0.0037 (6) | 0.0038 (6) | -0.0003 (6) |
| C3 | 0.0296 (7) | 0.0322 (8) | 0.0309 (8) | -0.0019 (6) | -0.0011 (6) | -0.0003 (7) |
| C4 | 0.0343 (8) | 0.0371 (9) | 0.0473 (11) | 0.0062 (7) | 0.0032 (8) | 0.0078 (8) |
| C5 | 0.0431 (10) | 0.0251 (8) | 0.0624 (13) | -0.0012 (7) | 0.0105 (9) | 0.0014 (8) |
| C6 | 0.0394 (9) | 0.0304 (8) | 0.0483 (11) | -0.0120 (7) | 0.0038 (9) | -0.0070 (8) |
| C7 | 0.0288 (7) | 0.0311 (8) | 0.0305 (8) | -0.0046 (6) | 0.0020 (7) | -0.0007 (7) |
| C8 | 0.0399 (9) | 0.0340 (8) | 0.0288 (8) | 0.0069 (7) | -0.0046 (7) | -0.0056 (7) |
| C9 | 0.0297 (7) | 0.0273 (7) | 0.0225 (8) | 0.0029 (6) | 0.0037 (6) | 0.0023 (6) |
| C10 | 0.0258 (7) | 0.0320 (7) | 0.0354 (8) | 0.0049 (6) | 0.0031 (7) | -0.0015 (7) |
| C11 | 0.0277 (8) | 0.0379 (9) | 0.0520 (11) | -0.0061 (7) | 0.0008 (8) | -0.0068 (8) |
| C12 | 0.0424 (10) | 0.0238 (8) | 0.0595 (12) | -0.0031 (7) | 0.0106 (9) | -0.0052 (8) |
| C13 | 0.0357 (9) | 0.0284 (8) | 0.0481 (11) | 0.0093 (7) | 0.0061 (8) | 0.0055 (7) |
| C14 | 0.0299 (7) | 0.0330 (8) | 0.0323 (9) | 0.0064 (6) | -0.0019 (7) | 0.0041 (7) |

Geometric parameters (Å, °)

| | | | |
|-------------------------------------|-------------|--------------|-------------|
| P1—N1 ⁱ | 1.6166 (14) | C5—H5A | 0.9300 |
| P1—N1 | 1.6166 (14) | C6—C7 | 1.391 (2) |
| P1—N2 ⁱ | 1.6184 (14) | C6—H6A | 0.9300 |
| P1—N2 | 1.6184 (14) | C7—H7A | 0.9300 |
| N1—C1 | 1.456 (2) | C8—C9 | 1.511 (2) |
| N1—H1C | 0.8600 | C8—H8A | 0.9700 |
| N2—C8 | 1.459 (2) | C8—H8B | 0.9700 |
| N2—H2A | 0.8600 | C9—C10 | 1.391 (2) |
| C1—C2 | 1.514 (2) | C9—C14 | 1.395 (2) |
| C1—H1A | 0.9700 | C10—C11 | 1.382 (3) |
| C1—H1B | 0.9700 | C10—H10A | 0.9300 |
| C2—C3 | 1.390 (2) | C11—C12 | 1.388 (3) |
| C2—C7 | 1.393 (2) | C11—H11A | 0.9300 |
| C3—C4 | 1.389 (3) | C12—C13 | 1.380 (3) |
| C3—H3A | 0.9300 | C12—H12A | 0.9300 |
| C4—C5 | 1.379 (3) | C13—C14 | 1.385 (2) |
| C4—H4A | 0.9300 | C13—H13A | 0.9300 |
| C5—C6 | 1.380 (3) | C14—H14A | 0.9300 |
| | | | |
| N1 ⁱ —P1—N1 | 101.15 (10) | C5—C6—C7 | 120.14 (17) |
| N1 ⁱ —P1—N2 ⁱ | 114.83 (8) | C5—C6—H6A | 119.9 |
| N1—P1—N2 ⁱ | 113.07 (9) | C7—C6—H6A | 119.9 |
| N1 ⁱ —P1—N2 | 113.07 (9) | C6—C7—C2 | 120.37 (17) |
| N1—P1—N2 | 114.83 (8) | C6—C7—H7A | 119.8 |
| N2 ⁱ —P1—N2 | 100.55 (11) | C2—C7—H7A | 119.8 |
| C1—N1—P1 | 124.13 (12) | N2—C8—C9 | 113.49 (14) |
| C1—N1—H1C | 117.9 | N2—C8—H8A | 108.9 |
| P1—N1—H1C | 117.9 | C9—C8—H8A | 108.9 |
| C8—N2—P1 | 124.45 (12) | N2—C8—H8B | 108.9 |
| C8—N2—H2A | 117.8 | C9—C8—H8B | 108.9 |
| P1—N2—H2A | 117.8 | H8A—C8—H8B | 107.7 |
| N1—C1—C2 | 115.22 (14) | C10—C9—C14 | 118.34 (15) |
| N1—C1—H1A | 108.5 | C10—C9—C8 | 123.02 (14) |
| C2—C1—H1A | 108.5 | C14—C9—C8 | 118.64 (15) |
| N1—C1—H1B | 108.5 | C11—C10—C9 | 120.76 (15) |
| C2—C1—H1B | 108.5 | C11—C10—H10A | 119.6 |
| H1A—C1—H1B | 107.5 | C9—C10—H10A | 119.6 |
| C3—C2—C7 | 119.02 (14) | C10—C11—C12 | 120.27 (17) |
| C3—C2—C1 | 122.52 (14) | C10—C11—H11A | 119.9 |
| C7—C2—C1 | 118.45 (15) | C12—C11—H11A | 119.9 |
| C4—C3—C2 | 120.11 (16) | C13—C12—C11 | 119.65 (16) |
| C4—C3—H3A | 119.9 | C13—C12—H12A | 120.2 |
| C2—C3—H3A | 119.9 | C11—C12—H12A | 120.2 |
| C5—C4—C3 | 120.59 (17) | C12—C13—C14 | 120.01 (16) |
| C5—C4—H4A | 119.7 | C12—C13—H13A | 120.0 |
| C3—C4—H4A | 119.7 | C14—C13—H13A | 120.0 |

| | | | |
|---------------------------|--------------|-----------------|--------------|
| C4—C5—C6 | 119.74 (16) | C13—C14—C9 | 120.96 (16) |
| C4—C5—H5A | 120.1 | C13—C14—H14A | 119.5 |
| C6—C5—H5A | 120.1 | C9—C14—H14A | 119.5 |
| N1 ⁱ —P1—N1—C1 | -174.86 (17) | C5—C6—C7—C2 | 0.5 (3) |
| N2 ⁱ —P1—N1—C1 | -51.55 (15) | C3—C2—C7—C6 | 1.0 (2) |
| N2—P1—N1—C1 | 63.05 (15) | C1—C2—C7—C6 | 179.71 (17) |
| N1 ⁱ —P1—N2—C8 | -56.69 (16) | P1—N2—C8—C9 | -132.58 (14) |
| N1—P1—N2—C8 | 58.69 (17) | N2—C8—C9—C10 | 17.1 (2) |
| N2 ⁱ —P1—N2—C8 | -179.61 (19) | N2—C8—C9—C14 | -163.97 (15) |
| P1—N1—C1—C2 | -101.97 (17) | C14—C9—C10—C11 | -1.2 (3) |
| N1—C1—C2—C3 | -19.8 (2) | C8—C9—C10—C11 | 177.70 (17) |
| N1—C1—C2—C7 | 161.45 (15) | C9—C10—C11—C12 | 0.4 (3) |
| C7—C2—C3—C4 | -1.4 (2) | C10—C11—C12—C13 | 0.4 (3) |
| C1—C2—C3—C4 | 179.90 (17) | C11—C12—C13—C14 | -0.3 (3) |
| C2—C3—C4—C5 | 0.4 (3) | C12—C13—C14—C9 | -0.6 (3) |
| C3—C4—C5—C6 | 1.0 (3) | C10—C9—C14—C13 | 1.4 (2) |
| C4—C5—C6—C7 | -1.5 (3) | C8—C9—C14—C13 | -177.61 (16) |

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

Hydrogen-bond geometry (Å, °)

| <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> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1C...C11 ⁱⁱ | 0.86 | 2.35 | 3.1848 (17) | 163 |
| N2—H2A...C11 | 0.86 | 2.35 | 3.1855 (18) | 165 |

Symmetry code: (ii) $x, y, z-1$.