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# 1,3,5-Triaza-7-phosphaadamantan-1-ium nitrate

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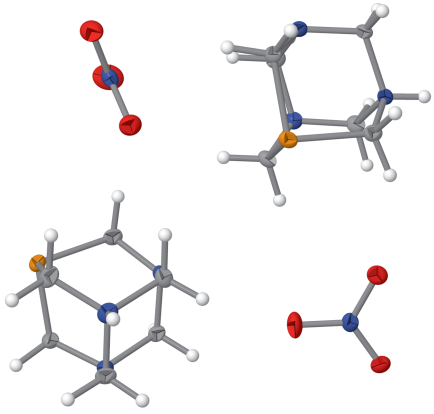
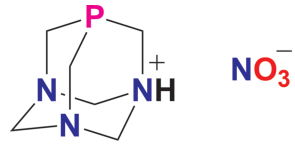
**Structural data:** full structural data are available from iucrdata.iucr.org

The title salt, $C_6H_{13}N_3P^+\cdot NO_3^-$ or [PTAH][$NO_3$], crystallizes in the triclinic space group $P\overline{1}$ with two independent $PTAH^+$ cations and two nitrate anions in the asymmetric unit. In the crystal, N—H···O and C—H···O hydrogen bonds link the $PTAH^+$ and oxygen atoms of the nitrate anion, forming a three-dimensional supramolecular structure.

3D view



Chemical scheme




## Structure description

1,3,5-Triaza-7-phosphaadamantane (PTA) is a well established water-soluble cage-type phosphine that incorporates a soft phosphorus donor atom at the bridgehead position 7 and three nitrogen atoms at positions 1, 3, and 5 of an adamantane-like bicyclic framework (Daigle *et al.*, 1998). Protonation at one of these nitrogen atoms readily yields the $PTAH^+$ ($C_6H_{13}N_3P^+$) cation, which is commonly encountered during the synthesis of PTA-based metal–phosphine complexes (Kirillov *et al.*, 2007; Tu *et al.*, 2008).

The title compound shows solid-state structural features for a N– protonated $PTAH^+$ cage in the absence of metal coordination. The asymmetric unit of the title compound contains two independent $PTAH^+$ cations together with two nitrate anions (Fig. 1). The P—C bond distances in the PTA moieties are between 1.847 (4) and 1.856 (3) Å with C—P—C bond angles between 96.7 (1) and 96.8 (2)°. The N—C bond distances of the non-protonated nitrogen atoms of both PTA moieties are between 1.434 (5)–1.482 (5) Å, while the N—C distances at the protonation nitrogen centres are observed between 1.501 (4) and 1.524 (5) Å. The N—C distances at the protonated N atoms are notably longer than N—C distances of the non-protonated nitrogen atoms of the PTA moieties, which are consistent with the expected weakening of N—C bonds upon quaternization of the nitrogen atom. All distances and angles are in good agreement with those reported for structurally related PTA-based compounds (Akbayeva *et al.*, 2005; Kirillov *et al.*, 2007; Tu *et al.*, 2008). In the crystal, N—H···O, N—H···(O,O) and C—H···O hydrogen bonds

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.88 (3) | 1.89 (3) | 2.7576 (18) | 166 |
| N4—H4···O2$^{ii}$ | 0.90 (3) | 2.09 (3) | 2.9076 (19) | 151 |
| N4—H4···O3$^{ii}$ | 0.90 (3) | 2.16 (3) | 2.9448 (19) | 145 |
| C2—H2$B$···O4 | 0.99 | 2.30 | 3.202 (2) | 151 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+2$.

(Table 1) link the $PTAH^+$ NH groupings and oxygen atoms of the nitrate anion, forming a three-dimensional supramolecular structure as depicted in Fig. 2.

## Synthesis and crystallization

PTA was prepared according to the literature method (Daigle *et al.*, 1998). In an attempt to synthesize a PTA–$Zn^{II}$ complex, an aqueous solution of $Zn(NO_3)_2{\cdot}6H_2O$ (0.297 g, 1.0 mmol) in distilled water (5 ml) was added to a solution of PTA (0.312 g, 2.0 mmol) in distilled water (10 ml) and the mixture was stirred at room temperature for 30 minutes. The colourless solution was filtered and the filtrate was transferred to an open vial and allowed to evaporate slowly at ambient temperature. After several days, colourless block-shaped crystals of the title compound, $[PTAH]_2[NO_3]_2$, were isolated and identified by single-crystal X-ray diffraction analysis. The formation of the protonated phosphine salt rather than the intended $Zn^{II}$ complex can be attributed to N-protonation of PTA in the weakly acidic nitrate medium, which is consistent with a related literature report (Akbayeva *et al.*, 2005).

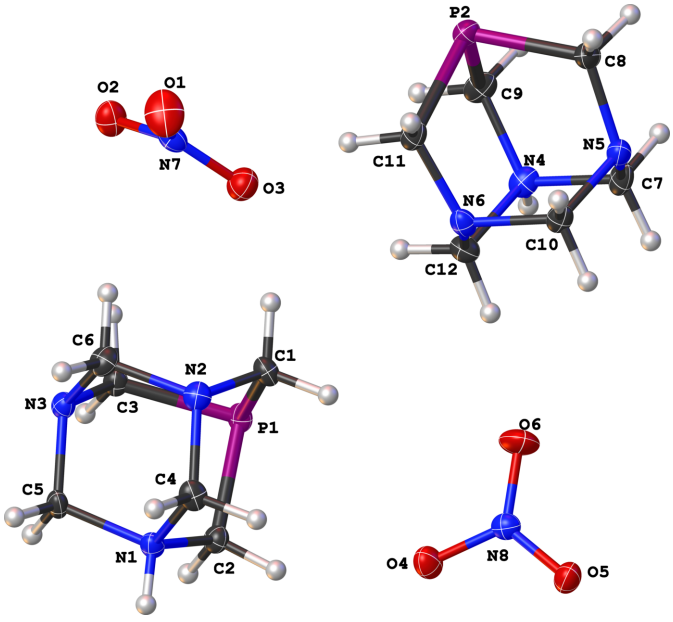



**Figure 1**
The molecular structure of (**I**) shown with displacement ellipsoids at the 50% probability level. All C-bound hydrogen atoms are omitted for clarity.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_6H_{13}N_3P^+{\cdot}NO_3^-$ |
| $M_r$ | 220.17 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 100 |
| $a, b, c$ (Å) | 7.0750 (3), 9.8950 (4), 13.6434 (5) |
| $\alpha, \beta, \gamma$ (°) | 102.614 (2), 90.123 (2), 90.613 (2) |
| $V$ (Å$^3$) | 932.02 (6) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.29 |
| Crystal size (mm) | 0.34 × 0.31 × 0.23 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.892, 0.937 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 14497, 4661, 4486 |
| $R_{int}$ | 0.024 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.676 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.034, 0.100, 1.12 |
| No. of reflections | 4661 |
| No. of parameters | 262 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.58, −0.42 |

Computer programs: *APEX2*, *SAINT*, *SAINT-Plus* and *XPREP* (Bruker, 2008), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015\bb007) and *OLEX2* (Dolomanov *et al.*, 2009).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal chosen for data collection was found to be twinned and was modelled using twin law (1 0 0) with a BASF value of 0.0628 (6).

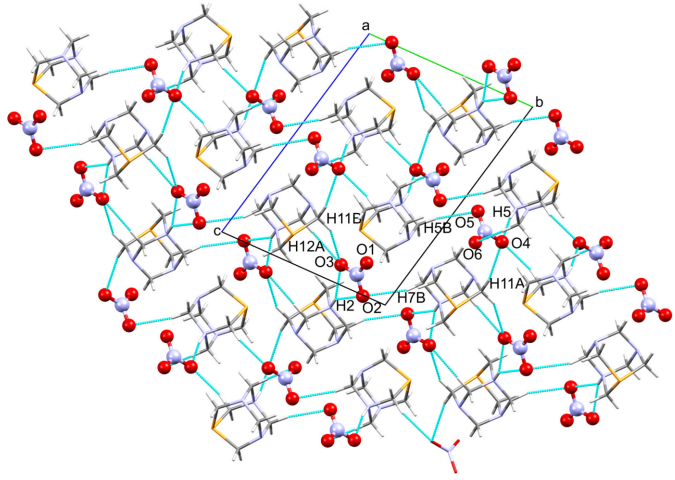



**Figure 2**
Representation of N—H···O and C—H···O hydrogen bonds in the crystal structure of (**I**) (cyan dotted bonds).

## Acknowledgements

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# full crystallographic data

*IUCrData* (2026). **11**, x260929 [https://doi.org/10.1107/S2414314626009296]

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### 1,3,5-Triaza-7-phosphaadamantan-1-ium nitrate

*Crystal data*

$C_6H_{13}N_3P^+\cdot NO_3^-$
$M_r$ = 220.17
Triclinic, $P\overline{1}$
$a$ = 7.0750 (3) Å
$b$ = 9.8950 (4) Å
$c$ = 13.6434 (5) Å
$\alpha$ = 102.614 (2)°
$\beta$ = 90.123 (2)°
$\gamma$ = 90.613 (2)°
$V$ = 932.02 (6) Å$^3$
$Z$ = 4
$F(000)$ = 464
$D_x$ = 1.569 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9920 reflections
$\theta$ = 2.9–28.7°
$\mu$ = 0.28 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.34 × 0.31 × 0.23 mm

*Data collection*

Bruker APEXII CCD diffractometer
Graphite monochromator
Detector resolution: 8 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min}$ = 0.892, $T_{max}$ = 0.937
14497 measured reflections
4661 independent reflections
4486 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 28.7°, $\theta_{min}$ = 1.5°
$h$ = −9→9
$k$ = −13→11
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
$S$ = 1.12
4661 reflections
262 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.5707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

*Special details*

**Experimental**. School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Private Bag X54001, Durban, 4000, South Africa

**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**. Refined as a 2-component twin.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5452 (2) | 0.58160 (17) | 0.67349 (12) | 0.0177 (3) |
| H1A | 0.559898 | 0.484998 | 0.635389 | 0.021* |
| H1B | 0.430137 | 0.584724 | 0.715039 | 0.021* |
| C2 | 0.9257 (2) | 0.64444 (17) | 0.65902 (11) | 0.0159 (3) |
| H2A | 1.043130 | 0.688530 | 0.691149 | 0.019* |
| H2B | 0.957663 | 0.550475 | 0.620874 | 0.019* |
| C3 | 0.7049 (2) | 0.81794 (16) | 0.79430 (11) | 0.0151 (3) |
| H3A | 0.598675 | 0.832972 | 0.842440 | 0.018* |
| H3B | 0.817625 | 0.865805 | 0.829325 | 0.018* |
| C4 | 0.6744 (2) | 0.66343 (17) | 0.53348 (11) | 0.0171 (3) |
| H4A | 0.642100 | 0.712138 | 0.479655 | 0.020* |
| H4B | 0.697789 | 0.565164 | 0.501755 | 0.020* |
| C5 | 0.8137 (2) | 0.87607 (16) | 0.64080 (11) | 0.0159 (3) |
| H5A | 0.928007 | 0.916872 | 0.678346 | 0.019* |
| H5B | 0.783790 | 0.931556 | 0.590665 | 0.019* |
| C6 | 0.4904 (2) | 0.81704 (18) | 0.65371 (12) | 0.0186 (3) |
| H6A | 0.455189 | 0.871198 | 0.603550 | 0.022* |
| H6B | 0.383885 | 0.821402 | 0.701167 | 0.022* |
| C7 | 0.3115 (3) | 0.09677 (17) | 0.85258 (12) | 0.0202 (3) |
| H7A | 0.422824 | 0.046099 | 0.820145 | 0.024* |
| H7B | 0.267050 | 0.050265 | 0.905718 | 0.024* |
| C8 | −0.0136 (2) | 0.14861 (17) | 0.82629 (13) | 0.0208 (3) |
| H8A | −0.051385 | 0.095291 | 0.876739 | 0.025* |
| H8B | −0.113529 | 0.134999 | 0.774059 | 0.025* |
| C9 | 0.2147 (3) | 0.32251 (19) | 0.96221 (12) | 0.0209 (3) |
| H9A | 0.260870 | 0.416957 | 0.993355 | 0.025* |
| H9B | 0.182965 | 0.275116 | 1.016978 | 0.025* |
| C10 | 0.2283 (2) | 0.16418 (17) | 0.70205 (11) | 0.0166 (3) |
| H10A | 0.126133 | 0.160151 | 0.651774 | 0.020* |
| H10B | 0.338778 | 0.115395 | 0.667117 | 0.020* |
| C11 | 0.1177 (2) | 0.39337 (17) | 0.78380 (12) | 0.0186 (3) |
| H11A | 0.024661 | 0.390929 | 0.729145 | 0.022* |
| H11B | 0.159792 | 0.490778 | 0.807723 | 0.022* |
| C12 | 0.4297 (2) | 0.31706 (18) | 0.81655 (12) | 0.0187 (3) |
| H12A | 0.461679 | 0.415170 | 0.846099 | 0.022* |
| H12B | 0.544255 | 0.272155 | 0.783434 | 0.022* |
| N5 | 0.1644 (2) | 0.09148 (14) | 0.77929 (10) | 0.0167 (3) |
| N4 | 0.3693 (2) | 0.24516 (15) | 0.89982 (10) | 0.0181 (3) |
| N6 | 0.2811 (2) | 0.31048 (14) | 0.74263 (9) | 0.0161 (3) |
| N2 | 0.51768 (19) | 0.67146 (15) | 0.60160 (10) | 0.0169 (3) |
| N1 | 0.85319 (19) | 0.72773 (14) | 0.58714 (10) | 0.0144 (2) |
| N3 | 0.65804 (19) | 0.88163 (14) | 0.70931 (10) | 0.0148 (3) |
| N7 | 0.2859 (2) | 0.76573 (15) | 0.93218 (10) | 0.0174 (3) |
| N8 | 0.78748 (19) | 0.20712 (15) | 0.55432 (10) | 0.0164 (3) |
| O1 | 0.1566 (2) | 0.77076 (17) | 0.87169 (11) | 0.0342 (3) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.31980 (19) | 0.86667 (14) | 1.00409 (9) | 0.0235 (3) |
| O3 | 0.38752 (19) | 0.65990 (14) | 0.92249 (10) | 0.0240 (3) |
| O4 | 0.87968 (18) | 0.32028 (13) | 0.56299 (9) | 0.0223 (3) |
| O5 | 0.83586 (18) | 0.10535 (13) | 0.48843 (9) | 0.0217 (3) |
| O6 | 0.6530 (2) | 0.19967 (16) | 0.61060 (11) | 0.0323 (3) |
| P1 | 0.75278 (6) | 0.62929 (4) | 0.75817 (3) | 0.01556 (10) |
| P2 | −0.00150 (6) | 0.33549 (4) | 0.88862 (3) | 0.01797 (10) |
| H1 | 0.941 (4) | 0.728 (3) | 0.5413 (18) | 0.029 (6)* |
| H4 | 0.471 (4) | 0.243 (3) | 0.9390 (19) | 0.034 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0194 (7) | 0.0160 (7) | 0.0186 (7) | −0.0037 (6) | −0.0006 (6) | 0.0059 (6) |
| C2 | 0.0172 (7) | 0.0147 (7) | 0.0165 (7) | 0.0023 (5) | −0.0009 (5) | 0.0051 (5) |
| C3 | 0.0196 (7) | 0.0144 (7) | 0.0115 (6) | 0.0003 (5) | 0.0004 (5) | 0.0032 (5) |
| C4 | 0.0208 (7) | 0.0183 (8) | 0.0120 (6) | −0.0022 (6) | −0.0039 (5) | 0.0033 (5) |
| C5 | 0.0219 (7) | 0.0111 (7) | 0.0154 (6) | −0.0009 (5) | 0.0022 (6) | 0.0040 (5) |
| C6 | 0.0169 (7) | 0.0191 (8) | 0.0200 (7) | 0.0036 (6) | −0.0029 (6) | 0.0048 (6) |
| C7 | 0.0282 (8) | 0.0148 (7) | 0.0193 (7) | 0.0062 (6) | 0.0012 (6) | 0.0072 (6) |
| C8 | 0.0197 (7) | 0.0151 (7) | 0.0257 (8) | −0.0020 (6) | 0.0059 (6) | 0.0002 (6) |
| C9 | 0.0258 (8) | 0.0244 (8) | 0.0118 (6) | 0.0045 (7) | 0.0010 (6) | 0.0019 (6) |
| C10 | 0.0218 (7) | 0.0163 (7) | 0.0114 (6) | 0.0026 (6) | 0.0008 (5) | 0.0023 (5) |
| C11 | 0.0215 (7) | 0.0160 (7) | 0.0193 (7) | 0.0044 (6) | −0.0001 (6) | 0.0057 (6) |
| C12 | 0.0167 (7) | 0.0207 (8) | 0.0194 (7) | −0.0014 (6) | 0.0004 (6) | 0.0060 (6) |
| N5 | 0.0193 (6) | 0.0136 (6) | 0.0174 (6) | 0.0012 (5) | 0.0029 (5) | 0.0036 (5) |
| N4 | 0.0202 (7) | 0.0209 (7) | 0.0135 (6) | 0.0041 (5) | −0.0034 (5) | 0.0045 (5) |
| N6 | 0.0204 (6) | 0.0162 (6) | 0.0121 (5) | −0.0024 (5) | 0.0010 (5) | 0.0043 (5) |
| N2 | 0.0169 (6) | 0.0179 (7) | 0.0159 (6) | 0.0002 (5) | −0.0032 (5) | 0.0037 (5) |
| N1 | 0.0178 (6) | 0.0137 (6) | 0.0120 (5) | −0.0006 (5) | 0.0017 (5) | 0.0033 (5) |
| N3 | 0.0173 (6) | 0.0133 (6) | 0.0146 (6) | 0.0019 (5) | 0.0006 (5) | 0.0049 (5) |
| N7 | 0.0176 (6) | 0.0206 (7) | 0.0158 (6) | −0.0032 (5) | −0.0009 (5) | 0.0079 (5) |
| N8 | 0.0166 (6) | 0.0200 (7) | 0.0139 (6) | 0.0022 (5) | −0.0001 (5) | 0.0067 (5) |
| O1 | 0.0320 (7) | 0.0357 (8) | 0.0363 (8) | −0.0024 (6) | −0.0197 (6) | 0.0108 (6) |
| O2 | 0.0307 (7) | 0.0216 (6) | 0.0174 (5) | −0.0017 (5) | −0.0020 (5) | 0.0028 (5) |
| O3 | 0.0247 (6) | 0.0220 (6) | 0.0256 (6) | 0.0031 (5) | 0.0005 (5) | 0.0057 (5) |
| O4 | 0.0259 (6) | 0.0189 (6) | 0.0207 (6) | −0.0038 (5) | 0.0005 (5) | 0.0014 (5) |
| O5 | 0.0263 (6) | 0.0163 (6) | 0.0219 (6) | 0.0030 (5) | 0.0035 (5) | 0.0029 (5) |
| O6 | 0.0290 (7) | 0.0378 (8) | 0.0317 (7) | 0.0015 (6) | 0.0165 (6) | 0.0113 (6) |
| P1 | 0.0199 (2) | 0.01446 (19) | 0.01372 (17) | 0.00056 (15) | −0.00136 (14) | 0.00611 (14) |
| P2 | 0.0180 (2) | 0.0162 (2) | 0.01841 (19) | 0.00172 (15) | 0.00339 (15) | 0.00101 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—H1A | 0.9900 | C8—H8A | 0.9900 |
| C1—H1B | 0.9900 | C8—H8B | 0.9900 |
| C1—N2 | 1.475 (2) | C8—N5 | 1.475 (2) |
| C1—P1 | 1.8583 (17) | C8—P2 | 1.8599 (17) |

| | | | |
|---|---|---|---|
| C2—H2A | 0.9900 | C9—H9A | 0.9900 |
| C2—H2B | 0.9900 | C9—H9B | 0.9900 |
| C2—N1 | 1.5046 (19) | C9—N4 | 1.498 (2) |
| C2—P1 | 1.8550 (16) | C9—P2 | 1.8488 (18) |
| C3—H3A | 0.9900 | C10—H10A | 0.9900 |
| C3—H3B | 0.9900 | C10—H10B | 0.9900 |
| C3—N3 | 1.4744 (19) | C10—N5 | 1.469 (2) |
| C3—P1 | 1.8587 (16) | C10—N6 | 1.476 (2) |
| C4—H4A | 0.9900 | C11—H11A | 0.9900 |
| C4—H4B | 0.9900 | C11—H11B | 0.9900 |
| C4—N2 | 1.440 (2) | C11—N6 | 1.465 (2) |
| C4—N1 | 1.522 (2) | C11—P2 | 1.8539 (17) |
| C5—H5A | 0.9900 | C12—H12A | 0.9900 |
| C5—H5B | 0.9900 | C12—H12B | 0.9900 |
| C5—N1 | 1.519 (2) | C12—N4 | 1.526 (2) |
| C5—N3 | 1.440 (2) | C12—N6 | 1.447 (2) |
| C6—H6A | 0.9900 | N4—H4 | 0.90 (3) |
| C6—H6B | 0.9900 | N1—H1 | 0.88 (3) |
| C6—N2 | 1.475 (2) | N7—O1 | 1.2395 (19) |
| C6—N3 | 1.469 (2) | N7—O2 | 1.2583 (19) |
| C7—H7A | 0.9900 | N7—O3 | 1.2598 (19) |
| C7—H7B | 0.9900 | N8—O4 | 1.2726 (19) |
| C7—N5 | 1.434 (2) | N8—O5 | 1.2461 (18) |
| C7—N4 | 1.520 (2) | N8—O6 | 1.2358 (18) |

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| H1A—C1—H1B | 107.6 | H10A—C10—H10B | 107.7 |
| N2—C1—H1A | 108.7 | N5—C10—H10A | 108.9 |
| N2—C1—H1B | 108.7 | N5—C10—H10B | 108.9 |
| N2—C1—P1 | 114.41 (11) | N5—C10—N6 | 113.46 (12) |
| P1—C1—H1A | 108.7 | N6—C10—H10A | 108.9 |
| P1—C1—H1B | 108.7 | N6—C10—H10B | 108.9 |
| H2A—C2—H2B | 107.8 | H11A—C11—H11B | 107.6 |
| N1—C2—H2A | 109.0 | N6—C11—H11A | 108.6 |
| N1—C2—H2B | 109.0 | N6—C11—H11B | 108.6 |
| N1—C2—P1 | 112.97 (10) | N6—C11—P2 | 114.53 (11) |
| P1—C2—H2A | 109.0 | P2—C11—H11A | 108.6 |
| P1—C2—H2B | 109.0 | P2—C11—H11B | 108.6 |
| H3A—C3—H3B | 107.6 | H12A—C12—H12B | 108.0 |
| N3—C3—H3A | 108.7 | N4—C12—H12A | 109.4 |
| N3—C3—H3B | 108.7 | N4—C12—H12B | 109.4 |
| N3—C3—P1 | 114.36 (10) | N6—C12—H12A | 109.4 |
| P1—C3—H3A | 108.7 | N6—C12—H12B | 109.4 |
| P1—C3—H3B | 108.7 | N6—C12—N4 | 111.18 (13) |
| H4A—C4—H4B | 108.0 | C7—N5—C8 | 111.48 (13) |
| N2—C4—H4A | 109.3 | C7—N5—C10 | 109.32 (13) |
| N2—C4—H4B | 109.3 | C10—N5—C8 | 111.82 (13) |
| N2—C4—N1 | 111.63 (12) | C7—N4—C12 | 108.65 (12) |
| N1—C4—H4A | 109.3 | C7—N4—H4 | 108.4 (17) |

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| N1—C4—H4B | 109.3 | C9—N4—C7 | 112.16 (14) |
| H5A—C5—H5B | 108.0 | C9—N4—C12 | 111.31 (13) |
| N1—C5—H5A | 109.4 | C9—N4—H4 | 108.9 (17) |
| N1—C5—H5B | 109.4 | C12—N4—H4 | 107.3 (17) |
| N3—C5—H5A | 109.4 | C11—N6—C10 | 111.89 (13) |
| N3—C5—H5B | 109.4 | C12—N6—C10 | 109.13 (13) |
| N3—C5—N1 | 111.00 (12) | C12—N6—C11 | 111.92 (12) |
| H6A—C6—H6B | 107.7 | C1—N2—C6 | 111.46 (12) |
| N2—C6—H6A | 108.8 | C4—N2—C1 | 111.54 (13) |
| N2—C6—H6B | 108.8 | C4—N2—C6 | 109.34 (13) |
| N3—C6—H6A | 108.8 | C2—N1—C4 | 111.58 (12) |
| N3—C6—H6B | 108.8 | C2—N1—C5 | 111.25 (12) |
| N3—C6—N2 | 113.82 (13) | C2—N1—H1 | 107.7 (16) |
| H7A—C7—H7B | 108.0 | C4—N1—H1 | 107.9 (16) |
| N5—C7—H7A | 109.3 | C5—N1—C4 | 109.21 (12) |
| N5—C7—H7B | 109.3 | C5—N1—H1 | 109.1 (17) |
| N5—C7—N4 | 111.52 (13) | C5—N3—C3 | 111.94 (12) |
| N4—C7—H7A | 109.3 | C5—N3—C6 | 109.19 (12) |
| N4—C7—H7B | 109.3 | C6—N3—C3 | 112.10 (13) |
| H8A—C8—H8B | 107.6 | O1—N7—O2 | 120.77 (15) |
| N5—C8—H8A | 108.6 | O1—N7—O3 | 120.72 (15) |
| N5—C8—H8B | 108.6 | O2—N7—O3 | 118.50 (14) |
| N5—C8—P2 | 114.68 (11) | O5—N8—O4 | 118.67 (13) |
| P2—C8—H8A | 108.6 | O6—N8—O4 | 120.04 (15) |
| P2—C8—H8B | 108.6 | O6—N8—O5 | 121.29 (15) |
| H9A—C9—H9B | 107.8 | C1—P1—C3 | 96.70 (7) |
| N4—C9—H9A | 109.0 | C2—P1—C1 | 96.64 (7) |
| N4—C9—H9B | 109.0 | C2—P1—C3 | 94.86 (7) |
| N4—C9—P2 | 112.85 (10) | C9—P2—C8 | 95.54 (8) |
| P2—C9—H9A | 109.0 | C9—P2—C11 | 96.54 (8) |
| P2—C9—H9B | 109.0 | C11—P2—C8 | 96.12 (8) |

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| N5—C7—N4—C9 | 66.80 (17) | N1—C2—P1—C1 | 47.23 (12) |
| N5—C7—N4—C12 | −56.67 (17) | N1—C2—P1—C3 | −50.11 (12) |
| N5—C8—P2—C9 | −50.15 (14) | N1—C4—N2—C1 | −68.34 (17) |
| N5—C8—P2—C11 | 47.06 (14) | N1—C4—N2—C6 | 55.40 (16) |
| N5—C10—N6—C11 | −66.12 (17) | N1—C5—N3—C3 | 67.37 (16) |
| N5—C10—N6—C12 | 58.29 (17) | N1—C5—N3—C6 | −57.35 (16) |
| N4—C7—N5—C8 | −66.85 (17) | N3—C3—P1—C1 | −46.57 (12) |
| N4—C7—N5—C10 | 57.29 (16) | N3—C3—P1—C2 | 50.72 (12) |
| N4—C9—P2—C8 | 48.69 (14) | N3—C5—N1—C2 | −67.05 (16) |
| N4—C9—P2—C11 | −48.14 (14) | N3—C5—N1—C4 | 56.55 (16) |
| N4—C12—N6—C10 | −56.64 (16) | N3—C6—N2—C1 | 66.20 (17) |
| N4—C12—N6—C11 | 67.76 (17) | N3—C6—N2—C4 | −57.59 (17) |
| N6—C10—N5—C7 | −58.57 (17) | P1—C1—N2—C4 | 62.84 (15) |
| N6—C10—N5—C8 | 65.37 (17) | P1—C1—N2—C6 | −59.69 (15) |
| N6—C11—P2—C8 | −47.61 (13) | P1—C2—N1—C4 | −59.88 (14) |
| N6—C11—P2—C9 | 48.71 (13) | P1—C2—N1—C5 | 62.35 (15) |

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| N6—C12—N4—C7 | 56.30 (17) | P1—C3—N3—C5 | −64.15 (15) |
| N6—C12—N4—C9 | −67.68 (17) | P1—C3—N3—C6 | 58.94 (15) |
| N2—C1—P1—C2 | −48.54 (13) | P2—C8—N5—C7 | 63.47 (17) |
| N2—C1—P1—C3 | 47.17 (12) | P2—C8—N5—C10 | −59.25 (16) |
| N2—C4—N1—C2 | 67.66 (16) | P2—C9—N4—C7 | −60.94 (16) |
| N2—C4—N1—C5 | −55.74 (16) | P2—C9—N4—C12 | 61.03 (16) |
| N2—C6—N3—C3 | −65.97 (17) | P2—C11—N6—C10 | 60.33 (15) |
| N2—C6—N3—C5 | 58.66 (17) | P2—C11—N6—C12 | −62.51 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.88 (3) | 1.89 (3) | 2.7576 (18) | 166 |
| N4—H4···O2$^{ii}$ | 0.90 (3) | 2.09 (3) | 2.9076 (19) | 151 |
| N4—H4···O3$^{ii}$ | 0.90 (3) | 2.16 (3) | 2.9448 (19) | 145 |
| C2—H2*B*···O4 | 0.99 | 2.30 | 3.202 (2) | 151 |

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