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# *N*,*N*′-Dicyclopentyl-*N*″,*N*″-dimethylphosphoric triamide

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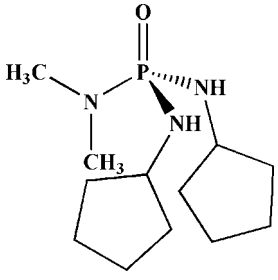
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.056; $wR$ factor = 0.108; data-to-parameter ratio = 17.0.

The P atom in the title molecule, $C_{12}H_{26}N_3OP$, has a distorted tetrahedral configuration: its bond angles lie in the range 101.1 (2)–119.1 (2)°. The P—N bonds to the two cyclopentylamido moieties are significantly different [1.619 (4) and 1.643 (4) Å], with the shorter bond related to an *anti* orientation of the lone electron pair of the corresponding N atom relative to the P═O bond. The O atom of the P═O group acts as a double hydrogen-bond acceptor and is involved in two different intermolecular N—H···O(P) hydrogen bonds, building $R_2^2(8)$ rings that are further linked into chains along [001].

## Related literature

For background to phosphoric triamide compounds, see: Pourayoubi & Tarahhomi *et al.* (2011). For applications of phosphoric triamides as oxygen-donor ligands, see: Pourayoubi & Golen *et al.* (2011). For bond lengths and angles in compounds having a [(N)P(O)(N)$_2$] skeleton, see: Sabbaghi *et al.* (2011). For double hydrogen-bond acceptors, see: Steiner (2002).




## Experimental

*Crystal data*

$C_{12}H_{26}N_3OP$
$M_r$ = 259.33
Orthorhombic, $Pca2_1$
$a$ = 10.962 (5) Å
$b$ = 16.663 (5) Å
$c$ = 8.079 (5) Å
$V$ = 1475.7 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 291 K
0.35 × 0.11 × 0.05 mm

*Data collection*

Stoe IPDS 2T Image Plate diffractometer
Absorption correction: multi-scan [*MULABS* (Blessing, 1995) and *PLATON* (Spek, 2009)]
$T_{min}$ = 0.961, $T_{max}$ = 1.000
7303 measured reflections
2573 independent reflections
1482 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.095

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.108
$S$ = 0.88
2573 reflections
151 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$
Absolute structure: Flack (1983), 1093 Friedel pairs
Flack parameter: −0.20 (18)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.85 | 2.13 | 2.960 (5) | 167 |
| N2—H2···O1$^{ii}$ | 0.85 | 2.33 | 3.131 (5) | 158 |

Symmetry codes: (i) $-x+\frac{3}{2}, y, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y, z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PLATON* (Spek, 2009) and *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2034).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o3401 [ **doi:10.1107/S1600536811048549** ]

# *N*,*N*'-Dicyclopentyl-*N*'',*N*''-dimethylphosphoric triamide

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## Comment

The structure determination of the title molecule was done as part of a project on the synthesis of new phosphoric triamide compounds (Pourayoubi & Tarahhomi *et al.*, 2011) and their application as oxygen donor ligands (Pourayoubi & Golen *et al.*, 2011).

The P═O and P—N bond lengths and the C—N—P bond angles match those found for the other compounds having a [(N)P(O)$(N)_2$] skeleton (Sabbaghi *et al.*, 2011).

The tetrahedral configuration of phosphorus atom (Fig. 1) is significantly distorted as it has also been noted for other phosphoric triamides: the bond angles at the P atom vary in the range from 101.1 (2) [N1—P1—N3] to 119.1 (2)° [O1—P1—N1].

The O atom of the P═O group acts as a double hydrogen-bond acceptor (Steiner, 2002); so, in the crystal structure, each molecule is hydrogen-bonded to two adjacent molecules by forming the $[N—H]_2$···O(P) grouping within a 1-D hydrogen-bonded arrangement parallel to the *c* axis (Fig. 2, Table 1).

## Experimental

Synthesis of $((CH_3)_2N)P(O)Cl_2$: $[(CH_3)_2NH_2]Cl$ (0.184 mol) and $P(O)Cl_3$ (0.552 mol) were refluxed for 8 h and afterwards the excess of $P(O)Cl_3$ was removed in vacuum.

Synthesis of title compound: a solution of cyclopentylamine (14.8 mmol) in $CH_3CN$ (25 ml) was added to a solution of $((CH_3)_2N)P(O)Cl_2$ (3.7 mmol) in $CH_3CN$ (15 ml) at 273 K. After stirring for 4 h, the solvent was removed and the product was washed with deionized water and recrystallized from $CH_3CN$ at room temperature.

## Refinement

The N-bound H atoms were found in difference Fourier map and then constrained to refine with the parent atoms with $U_{iso}$(H) equal to $1.2U_{eq}$(N). The remaining H atoms were positioned geometrically and constrained to refine in a riding-model approximation with $U_{iso}$(H) = $1.2U_{eq}$(C), or $1.5U_{eq}$(methyl). A rotating group model was applied to the methyl groups.

### Figures

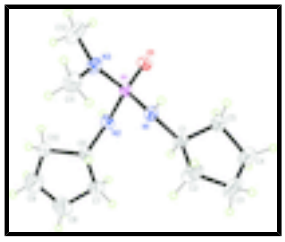

Fig. 1. The molecular structure of the title compound with ellipsoids shown at the 50% probability level.

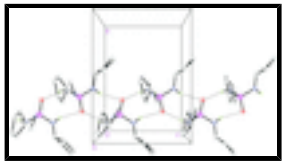

Fig. 2. A view of the crystal packing showing the formation of 1-D arrangement through N—H···O hydrogen bonds (shown as dashed lines). Carbon bound H atoms have been omitted for clarity.

### *N*,*N*'-Dicyclopentyl-*N*'',*N*''-dimethylphosphoric triamide

*Crystal data*

| | |
|---|---|
| $C_{12}H_{26}N_3OP$ | $F(000) = 568$ |
| $M_r = 259.33$ | $D_x = 1.167$ Mg m$^{-3}$ |
| Orthorhombic, $Pca2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å |
| Hall symbol: P 2c -2ac | Cell parameters from 2536 reflections |
| $a = 10.962$ (5) Å | $\theta = 2.0–27.5°$ |
| $b = 16.663$ (5) Å | $\mu = 0.18$ mm$^{-1}$ |
| $c = 8.079$ (5) Å | $T = 291$ K |
| $V = 1475.7$ (12) Å$^3$ | Needle, colourless |
| $Z = 4$ | 0.35 × 0.11 × 0.05 mm |

*Data collection*

| | |
|---|---|
| Stoe IPDS 2T Image Plate diffractometer | 2573 independent reflections |
| Radiation source: fine-focus sealed tube | 1482 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.095$ |
| Detector resolution: 0.15 pixels mm$^{-1}$ | $\theta_{max} = 25.5°$, $\theta_{min} = 2.2°$ |
| ω scans | $h = -11\rightarrow13$ |
| Absorption correction: multi-scan [*MULABS* (Blessing, 1995) and *PLATON* (Spek, 2009)] | $k = -20\rightarrow20$ |
| $T_{min} = 0.961$, $T_{max} = 1.000$ | $l = -8\rightarrow9$ |
| 7303 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | H-atom parameters constrained |
| $wR(F^2) = 0.108$ | $w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.88$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2573 reflections | $\Delta\rho_{max} = 0.16$ e Å$^{-3}$ |
| 151 parameters | $\Delta\rho_{min} = -0.23$ e Å$^{-3}$ |
| 1 restraint | Absolute structure: Flack (1983), 1093 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: −0.20 (18) |

*Special details*

**Experimental**. IR (KBr, cm$^{-1}$): 3290, 3151, 2955, 2866, 2835, 2794, 1459, 1291, 1197, 1159, 1107, 1090, 1030, 993, 932, 889, 762, 703, 555, 496, 464.

**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 | 0.83134 (10) | 1.79029 (6) | 0.70933 (17) | 0.0402 (3) |
| O1 | 0.6995 (2) | 1.78019 (14) | 0.7413 (4) | 0.0476 (9) |
| N1 | 0.8963 (4) | 1.73464 (16) | 0.5707 (5) | 0.0418 (10) |
| H1 | 0.8771 | 1.7422 | 0.4700 | 0.050* |
| N2 | 0.9056 (3) | 1.77094 (19) | 0.8814 (5) | 0.0452 (10) |
| H2 | 0.8616 | 1.7816 | 0.9651 | 0.054* |
| N3 | 0.8558 (4) | 1.8809 (2) | 0.6328 (4) | 0.0545 (12) |
| C1 | 0.9062 (4) | 1.6462 (2) | 0.5936 (6) | 0.0458 (12) |
| H1A | 0.9222 | 1.6352 | 0.7108 | 0.055* |
| C2 | 1.0064 (5) | 1.6094 (3) | 0.4926 (9) | 0.088 (2) |
| H2A | 1.0841 | 1.6147 | 0.5489 | 0.106* |
| H2B | 1.0121 | 1.6354 | 0.3854 | 0.106* |
| C3 | 0.9725 (6) | 1.5223 (3) | 0.4730 (10) | 0.100 (2) |
| H3A | 0.9884 | 1.5046 | 0.3606 | 0.121* |
| H3B | 1.0201 | 1.4894 | 0.5481 | 0.121* |
| C4 | 0.8410 (6) | 1.5149 (3) | 0.5115 (10) | 0.096 (2) |
| H4A | 0.8291 | 1.4821 | 0.6093 | 0.115* |
| H4B | 0.7979 | 1.4903 | 0.4197 | 0.115* |
| C5 | 0.7943 (5) | 1.5994 (2) | 0.5411 (7) | 0.0678 (17) |
| H5A | 0.7594 | 1.6216 | 0.4408 | 0.081* |

| | | | | |
|---|---|---|---|---|
| H5B | 0.7328 | 1.5999 | 0.6275 | 0.081* |
| C6 | 1.0370 (4) | 1.7749 (2) | 0.9067 (6) | 0.0480 (12) |
| H6A | 1.0773 | 1.7747 | 0.7984 | 0.058* |
| C7 | 1.0855 (5) | 1.7061 (3) | 1.0069 (7) | 0.0700 (15) |
| H7A | 1.0208 | 1.6825 | 1.0729 | 0.084* |
| H7B | 1.1188 | 1.6650 | 0.9348 | 0.084* |
| C8 | 1.1810 (7) | 1.7386 (4) | 1.1141 (11) | 0.139 (2) |
| H8A | 1.1771 | 1.7136 | 1.2224 | 0.167* |
| H8B | 1.2607 | 1.7279 | 1.0669 | 0.167* |
| C9 | 1.1626 (7) | 1.8212 (4) | 1.1282 (9) | 0.139 (2) |
| H9A | 1.2401 | 1.8488 | 1.1166 | 0.167* |
| H9B | 1.1302 | 1.8334 | 1.2371 | 0.167* |
| C10 | 1.0791 (5) | 1.8495 (2) | 1.0034 (8) | 0.0702 (17) |
| H10A | 1.1195 | 1.8872 | 0.9301 | 0.084* |
| H10B | 1.0099 | 1.8761 | 1.0544 | 0.084* |
| C11 | 0.9700 (5) | 1.9066 (3) | 0.5626 (8) | 0.0808 (19) |
| H11A | 0.9552 | 1.9478 | 0.4820 | 0.121* |
| H11B | 1.0094 | 1.8619 | 0.5103 | 0.121* |
| H11C | 1.0215 | 1.9274 | 0.6487 | 0.121* |
| C12 | 0.7793 (6) | 1.9460 (2) | 0.6916 (10) | 0.093 (2) |
| H12A | 0.7768 | 1.9877 | 0.6098 | 0.139* |
| H12B | 0.8122 | 1.9669 | 0.7929 | 0.139* |
| H12C | 0.6982 | 1.9263 | 0.7109 | 0.139* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0424 (6) | 0.0398 (4) | 0.0385 (6) | −0.0033 (5) | −0.0014 (9) | 0.0013 (7) |
| O1 | 0.0381 (18) | 0.0585 (16) | 0.046 (3) | −0.0026 (13) | −0.0026 (18) | 0.0068 (16) |
| N1 | 0.054 (3) | 0.0364 (17) | 0.035 (2) | −0.0031 (17) | 0.000 (2) | 0.0055 (17) |
| N2 | 0.039 (3) | 0.057 (2) | 0.039 (2) | −0.0055 (19) | 0.006 (2) | −0.0082 (19) |
| N3 | 0.060 (3) | 0.0419 (19) | 0.061 (3) | −0.0004 (19) | 0.010 (2) | 0.0020 (16) |
| C1 | 0.058 (3) | 0.042 (2) | 0.037 (3) | 0.010 (2) | −0.002 (3) | 0.001 (2) |
| C2 | 0.073 (4) | 0.060 (3) | 0.131 (6) | 0.006 (3) | 0.038 (5) | 0.004 (4) |
| C3 | 0.112 (6) | 0.067 (4) | 0.122 (6) | 0.022 (3) | 0.016 (6) | −0.035 (4) |
| C4 | 0.098 (5) | 0.051 (3) | 0.140 (7) | 0.007 (3) | −0.010 (6) | −0.012 (3) |
| C5 | 0.057 (4) | 0.052 (3) | 0.095 (5) | −0.002 (2) | −0.006 (3) | −0.002 (3) |
| C6 | 0.038 (3) | 0.050 (3) | 0.056 (3) | 0.000 (2) | −0.004 (3) | 0.001 (2) |
| C7 | 0.068 (4) | 0.058 (3) | 0.085 (4) | 0.005 (3) | −0.017 (4) | 0.007 (3) |
| C8 | 0.158 (6) | 0.107 (3) | 0.154 (5) | 0.012 (4) | −0.095 (5) | −0.004 (3) |
| C9 | 0.158 (6) | 0.107 (3) | 0.154 (5) | 0.012 (4) | −0.095 (5) | −0.004 (3) |
| C10 | 0.064 (4) | 0.047 (3) | 0.099 (5) | −0.007 (2) | −0.017 (4) | −0.016 (3) |
| C11 | 0.086 (5) | 0.059 (3) | 0.097 (5) | −0.016 (3) | 0.005 (4) | 0.025 (3) |
| C12 | 0.129 (5) | 0.052 (3) | 0.098 (6) | 0.015 (3) | 0.034 (6) | −0.001 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| P1—O1 | 1.478 (3) | C5—H5A | 0.9700 |
| P1—N1 | 1.619 (4) | C5—H5B | 0.9700 |

| | | | |
|---|---|---|---|
| P1—N2 | 1.643 (4) | C6—C7 | 1.500 (6) |
| P1—N3 | 1.653 (4) | C6—C10 | 1.539 (6) |
| N1—C1 | 1.489 (4) | C6—H6A | 0.9800 |
| N1—H1 | 0.8499 | C7—C8 | 1.463 (8) |
| N2—C6 | 1.456 (5) | C7—H7A | 0.9700 |
| N2—H2 | 0.8489 | C7—H7B | 0.9700 |
| N3—C11 | 1.440 (6) | C8—C9 | 1.395 (8) |
| N3—C12 | 1.451 (6) | C8—H8A | 0.9700 |
| C1—C2 | 1.499 (7) | C8—H8B | 0.9700 |
| C1—C5 | 1.515 (6) | C9—C10 | 1.441 (7) |
| C1—H1A | 0.9800 | C9—H9A | 0.9700 |
| C2—C3 | 1.508 (6) | C9—H9B | 0.9700 |
| C2—H2A | 0.9700 | C10—H10A | 0.9700 |
| C2—H2B | 0.9700 | C10—H10B | 0.9700 |
| C3—C4 | 1.480 (8) | C11—H11A | 0.9600 |
| C3—H3A | 0.9700 | C11—H11B | 0.9600 |
| C3—H3B | 0.9700 | C11—H11C | 0.9600 |
| C4—C5 | 1.516 (6) | C12—H12A | 0.9600 |
| C4—H4A | 0.9700 | C12—H12B | 0.9600 |
| C4—H4B | 0.9700 | C12—H12C | 0.9600 |

| | | | |
|---|---|---|---|
| O1—P1—N1 | 119.06 (19) | H5A—C5—H5B | 108.9 |
| O1—P1—N2 | 108.3 (2) | N2—C6—C7 | 113.0 (4) |
| N1—P1—N2 | 104.78 (19) | N2—C6—C10 | 113.9 (4) |
| O1—P1—N3 | 109.13 (18) | C7—C6—C10 | 103.7 (4) |
| N1—P1—N3 | 101.13 (19) | N2—C6—H6A | 108.7 |
| N2—P1—N3 | 114.55 (18) | C7—C6—H6A | 108.7 |
| C1—N1—P1 | 120.9 (3) | C10—C6—H6A | 108.7 |
| C1—N1—H1 | 106.5 | C8—C7—C6 | 106.9 (4) |
| P1—N1—H1 | 117.9 | C8—C7—H7A | 110.3 |
| C6—N2—P1 | 126.8 (3) | C6—C7—H7A | 110.3 |
| C6—N2—H2 | 116.2 | C8—C7—H7B | 110.3 |
| P1—N2—H2 | 110.6 | C6—C7—H7B | 110.3 |
| C11—N3—C12 | 114.1 (4) | H7A—C7—H7B | 108.6 |
| C11—N3—P1 | 124.1 (3) | C9—C8—C7 | 108.1 (6) |
| C12—N3—P1 | 117.8 (3) | C9—C8—H8A | 110.1 |
| N1—C1—C2 | 113.0 (4) | C7—C8—H8A | 110.1 |
| N1—C1—C5 | 114.6 (4) | C9—C8—H8B | 110.1 |
| C2—C1—C5 | 103.3 (4) | C7—C8—H8B | 110.1 |
| N1—C1—H1A | 108.6 | H8A—C8—H8B | 108.4 |
| C2—C1—H1A | 108.6 | C8—C9—C10 | 110.9 (6) |
| C5—C1—H1A | 108.6 | C8—C9—H9A | 109.5 |
| C1—C2—C3 | 105.7 (4) | C10—C9—H9A | 109.5 |
| C1—C2—H2A | 110.6 | C8—C9—H9B | 109.5 |
| C3—C2—H2A | 110.6 | C10—C9—H9B | 109.5 |
| C1—C2—H2B | 110.6 | H9A—C9—H9B | 108.0 |
| C3—C2—H2B | 110.6 | C9—C10—C6 | 106.4 (4) |
| H2A—C2—H2B | 108.7 | C9—C10—H10A | 110.5 |
| C4—C3—C2 | 107.3 (4) | C6—C10—H10A | 110.5 |
| C4—C3—H3A | 110.3 | C9—C10—H10B | 110.5 |

| | | | |
|---|---|---|---|
| C2—C3—H3A | 110.3 | C6—C10—H10B | 110.5 |
| C4—C3—H3B | 110.3 | H10A—C10—H10B | 108.6 |
| C2—C3—H3B | 110.3 | N3—C11—H11A | 109.5 |
| H3A—C3—H3B | 108.5 | N3—C11—H11B | 109.5 |
| C3—C4—C5 | 106.6 (4) | H11A—C11—H11B | 109.5 |
| C3—C4—H4A | 110.4 | N3—C11—H11C | 109.5 |
| C5—C4—H4A | 110.4 | H11A—C11—H11C | 109.5 |
| C3—C4—H4B | 110.4 | H11B—C11—H11C | 109.5 |
| C5—C4—H4B | 110.4 | N3—C12—H12A | 109.5 |
| H4A—C4—H4B | 108.6 | N3—C12—H12B | 109.5 |
| C1—C5—C4 | 104.4 (4) | H12A—C12—H12B | 109.5 |
| C1—C5—H5A | 110.9 | N3—C12—H12C | 109.5 |
| C4—C5—H5A | 110.9 | H12A—C12—H12C | 109.5 |
| C1—C5—H5B | 110.9 | H12B—C12—H12C | 109.5 |
| C4—C5—H5B | 110.9 | | |

| | | | |
|---|---|---|---|
| O1—P1—N1—C1 | −65.4 (4) | C5—C1—C2—C3 | −32.8 (6) |
| N2—P1—N1—C1 | 55.8 (4) | C1—C2—C3—C4 | 17.9 (8) |
| N3—P1—N1—C1 | 175.1 (3) | C2—C3—C4—C5 | 4.3 (8) |
| O1—P1—N2—C6 | −178.9 (3) | N1—C1—C5—C4 | 158.6 (5) |
| N1—P1—N2—C6 | 53.0 (4) | C2—C1—C5—C4 | 35.2 (6) |
| N3—P1—N2—C6 | −56.8 (4) | C3—C4—C5—C1 | −24.6 (7) |
| O1—P1—N3—C11 | −169.5 (4) | P1—N2—C6—C7 | −138.0 (4) |
| N1—P1—N3—C11 | −43.2 (4) | P1—N2—C6—C10 | 104.0 (5) |
| N2—P1—N3—C11 | 68.9 (4) | N2—C6—C7—C8 | −142.0 (5) |
| O1—P1—N3—C12 | 34.3 (5) | C10—C6—C7—C8 | −18.2 (6) |
| N1—P1—N3—C12 | 160.6 (4) | C6—C7—C8—C9 | 20.8 (8) |
| N2—P1—N3—C12 | −87.3 (4) | C7—C8—C9—C10 | −14.8 (9) |
| P1—N1—C1—C2 | −158.0 (4) | C8—C9—C10—C6 | 2.8 (8) |
| P1—N1—C1—C5 | 84.1 (5) | N2—C6—C10—C9 | 132.9 (5) |
| N1—C1—C2—C3 | −157.2 (5) | C7—C6—C10—C9 | 9.7 (6) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.85 | 2.13 | 2.960 (5) | 167 |
| N2—H2···O1$^{ii}$ | 0.85 | 2.33 | 3.131 (5) | 158 |
| C11—H11B···N1 | 0.96 | 2.50 | 2.978 (6) | 110 |
| C12—H12C···O1 | 0.96 | 2.45 | 2.926 (5) | 111 |

Symmetry codes: (i) −*x*+3/2, *y*, *z*−1/2; (ii) −*x*+3/2, *y*, *z*+1/2.

**Fig. 1**

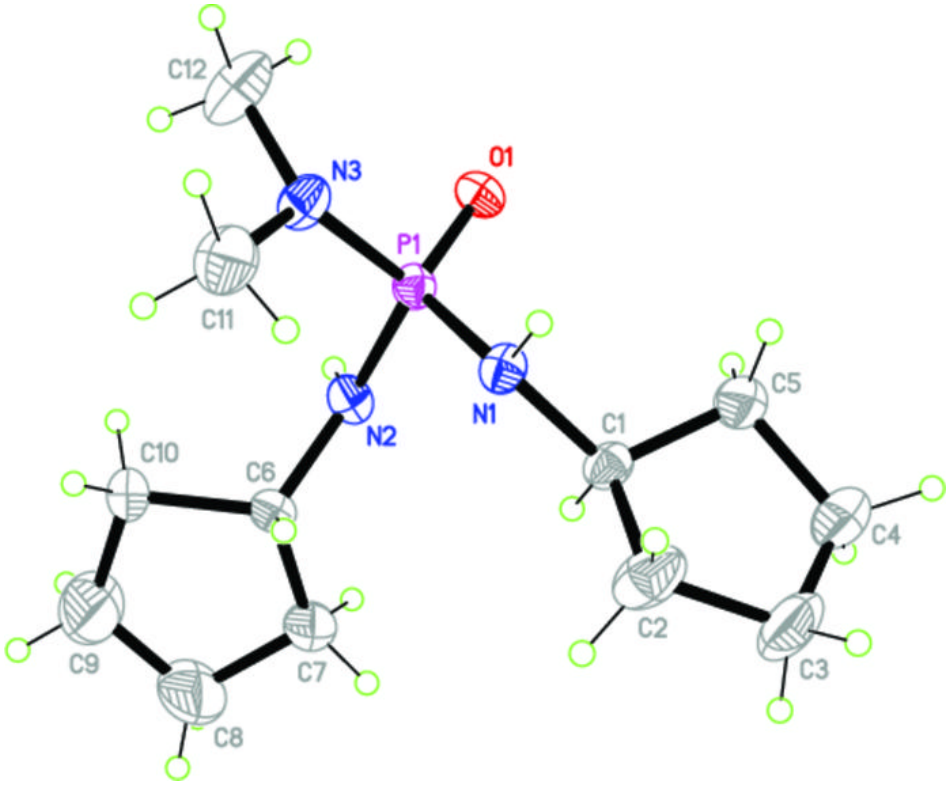

**Fig. 2**