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# *N-tert*-Butyl *O*-2-isopropyl-5-methylcyclohexyl phenylphosphonamidate

**Li-Juan Liu, Fan-Jie Meng, Hao Xu, Daqi Wang and Chang-Qiu Zhao***

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: literabc@hotmail.com

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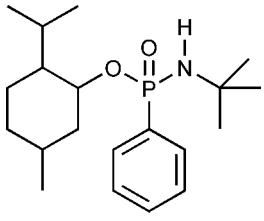
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.053; $wR$ factor = 0.130; data-to-parameter ratio = 16.2.

In the title compound, $C_{20}H_{34}NO_2P$, the P atom has an irregular tetrahedral environment and exhibits $S_p$ chirality. In the crystal, weak intermolecular N—H···O and C—H···O hydrogen bonds link the molecules into chains extending in [010].

## Related literature

For the crystal structures of related P-chiral compounds, see: Chaloner *et al.* (1991); Meng *et al.* (2010).



## Experimental

### *Crystal data*

$C_{20}H_{34}NO_2P$
$M_r$ = 351.45
Orthorhombic, $P2_12_12_1$
$a$ = 8.305 (3) Å
$b$ = 11.064 (4) Å
$c$ = 22.557 (9) Å
$V$ = 2072.8 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.14 mm$^{-1}$
$T$ = 298 K
0.45 × 0.40 × 0.37 mm

### *Data collection*

Bruker SMART-1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.938, $T_{max}$ = 0.949
10336 measured reflections
3610 independent reflections
1993 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.075

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.130
$S$ = 1.02
3610 reflections
223 parameters
114 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$
Absolute structure: Flack (1983), 2085 Friedel pairs
Flack parameter: 0.06 (17)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.52 | 3.326 (4) | 156 |
| C13—H13···O2$^{i}$ | 0.93 | 2.51 | 3.391 (5) | 157 |

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

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 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: CV5071).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o1244 [ **doi:10.1107/S1600536811012864** ]

# *N-tert*-Butyl *O*-2-isopropyl-5-methylcyclohexyl phenylphosphonamidate

**L.-J. Liu, F.-J. Meng, H. Xu, D. Wang and C.-Q. Zhao**

## Comment

We recently reported the crystal stucture of 2-isopropyl-5-methylcyclohexyl *N*-cyclohexyl-*P*- phenylphosphonamidate synthesized by the reaction of ($R_p$)-*O*-menthyl phenylphosphinate with cyclohexylamine (Meng *et al.*, 2010). Herein we report the title compound (I) obtained by the reaction of the same phosphinate with *tert*-butylamine.

In (I) (Fig.1), the configuration of the central P atom was detemined as *S* and the four groups around the P atom form an irregular tetrahedron. A stable chair conformation was observed for the 2-isopropyl-5-methylcyclohexyloxy, in which the isopropyl, methyl and oxygen atom locate at equatorial bond. The absolute configuration of $C_4$, $C_7$, and $C_{11}$ are *S*, *R*, and *R*, respectively. The bond angle around the P atom are normal and comparable with those observed in the related compounds (Meng *et al.*, 2010; Chaloner *et al.* 1991).

In the crystal structure, the molecules are linked by weak intermolecular N1—H1···O2 and C13—H13···O2 hodrogen bonds (Tabel 1) into chains extended in [010].

## Experimental

Carbon tetrachloride was added to a solution of ($R_p$)-*O*-menthyl-phenylphosphonothioate dissolved in dry ether and *tert*-butylamine.The reaction mixture was stirred for 30 h at room temperature. The crystal suitable for X-ray diffraction was obtained by recrystallization with dichloromethane/hexane.

## Refinement

All H atoms were fixed geometrically (C—H = 0.93 - 0.98 Å; N—H = 0.86 Å), and treated as riding, with $U_{iso}$(H) = 1.2-1.5 $U_{eq}$of the parent atom.

## Figures

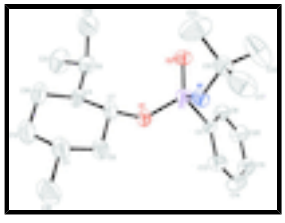


Fig. 1. The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

### *N-tert*-Butyl *O*-2-isopropyl-5-methylcyclohexyl phenylphosphonamidate

*Crystal data*

| | |
|---|---|
| $C_{20}H_{34}NO_2P$ | $F(000) = 768$ |
| $M_r = 351.45$ | $D_x = 1.126$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 1474 reflections |
| $a = 8.305$ (3) Å | $\theta = 2.6$–$18.0°$ |
| $b = 11.064$ (4) Å | $\mu = 0.14$ mm$^{-1}$ |
| $c = 22.557$ (9) Å | $T = 298$ K |
| $V = 2072.8$ (15) Å$^3$ | Block, colourless |
| $Z = 4$ | 0.45 × 0.40 × 0.37 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART-1000 CCD area-detector diffractometer | 3610 independent reflections |
| Radiation source: fine-focus sealed tube | 1993 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.075$ |
| φ and ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -9\rightarrow9$ |
| $T_{min} = 0.938$, $T_{max} = 0.949$ | $k = -10\rightarrow13$ |
| 10336 measured reflections | $l = -26\rightarrow25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | H-atom parameters constrained |
| $wR(F^2) = 0.130$ | $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3610 reflections | $\Delta\rho_{max} = 0.27$ e Å$^{-3}$ |
| 223 parameters | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |
| 114 restraints | Absolute structure: Flack (1983), 2085 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.06 (17) |

*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 | 0.54415 (14) | 0.34918 (10) | 0.23972 (5) | 0.0462 (3) |
| O1 | 0.6726 (3) | 0.2945 (3) | 0.19552 (12) | 0.0503 (8) |
| O2 | 0.5009 (3) | 0.4756 (2) | 0.23040 (13) | 0.0578 (9) |
| N1 | 0.3903 (4) | 0.2570 (3) | 0.23664 (16) | 0.0521 (9) |
| H1 | 0.4139 | 0.1816 | 0.2332 | 0.063* |
| C4 | 0.7421 (5) | 0.3383 (5) | 0.09282 (17) | 0.0586 (13) |
| H4 | 0.8542 | 0.3192 | 0.1027 | 0.070* |
| C5 | 0.6512 (5) | 0.3284 (4) | 0.30808 (17) | 0.0418 (11) |
| C6 | 0.7238 (7) | 0.4734 (5) | 0.1000 (2) | 0.0679 (14) |
| H6 | 0.7301 | 0.4912 | 0.1425 | 0.082* |
| C7 | 0.6383 (5) | 0.2641 (4) | 0.13399 (18) | 0.0511 (12) |
| H7 | 0.5247 | 0.2806 | 0.1256 | 0.061* |
| C8 | 0.6923 (6) | 0.4277 (4) | 0.3410 (2) | 0.0624 (14) |
| H8 | 0.6632 | 0.5044 | 0.3281 | 0.075* |
| C9 | 0.6699 (6) | 0.1301 (4) | 0.1270 (2) | 0.0636 (14) |
| H9A | 0.7795 | 0.1132 | 0.1394 | 0.076* |
| H9B | 0.5983 | 0.0861 | 0.1533 | 0.076* |
| C10 | 0.2175 (5) | 0.2851 (4) | 0.2390 (2) | 0.0605 (12) |
| C11 | 0.6471 (7) | 0.0842 (5) | 0.0651 (2) | 0.0708 (15) |
| H11 | 0.5336 | 0.0970 | 0.0551 | 0.085* |
| C12 | 0.7434 (7) | 0.1585 (6) | 0.0229 (2) | 0.0831 (17) |
| H12A | 0.7165 | 0.1348 | −0.0173 | 0.100* |
| H12B | 0.8568 | 0.1418 | 0.0291 | 0.100* |
| C13 | 0.6942 (6) | 0.2165 (4) | 0.3286 (2) | 0.0627 (14) |
| H13 | 0.6688 | 0.1482 | 0.3065 | 0.075* |
| C14 | 0.7741 (6) | 0.2041 (5) | 0.3811 (2) | 0.0750 (16) |
| H14 | 0.7992 | 0.1275 | 0.3952 | 0.090* |
| C15 | 0.8169 (6) | 0.3034 (6) | 0.4129 (2) | 0.0723 (16) |
| H15 | 0.8739 | 0.2941 | 0.4481 | 0.087* |
| C16 | 0.7145 (6) | 0.2930 (5) | 0.0299 (2) | 0.0732 (16) |
| H16A | 0.6046 | 0.3111 | 0.0183 | 0.088* |
| H16B | 0.7856 | 0.3362 | 0.0032 | 0.088* |
| C17 | 0.1234 (6) | 0.1719 (5) | 0.2447 (3) | 0.1004 (18) |
| H17A | 0.1550 | 0.1304 | 0.2802 | 0.151* |
| H17B | 0.1435 | 0.1211 | 0.2110 | 0.151* |
| H17C | 0.0107 | 0.1908 | 0.2467 | 0.151* |
| C18 | 0.6792 (8) | −0.0509 (5) | 0.0587 (2) | 0.103 (2) |
| H18A | 0.6648 | −0.0744 | 0.0181 | 0.154* |

| | | | | |
|---|---|---|---|---|
| H18B | 0.6054 | −0.0951 | 0.0833 | 0.154* |
| H18C | 0.7876 | −0.0683 | 0.0708 | 0.154* |
| C19 | 0.5637 (7) | 0.5245 (5) | 0.0774 (2) | 0.0915 (19) |
| H19A | 0.5523 | 0.5065 | 0.0360 | 0.137* |
| H19B | 0.5621 | 0.6105 | 0.0830 | 0.137* |
| H19C | 0.4764 | 0.4885 | 0.0990 | 0.137* |
| C20 | 0.7781 (7) | 0.4143 (5) | 0.3941 (2) | 0.0723 (16) |
| H20 | 0.8077 | 0.4819 | 0.4160 | 0.087* |
| C21 | 0.8611 (8) | 0.5424 (6) | 0.0696 (3) | 0.109 (2) |
| H21A | 0.9626 | 0.5089 | 0.0817 | 0.163* |
| H21B | 0.8566 | 0.6261 | 0.0807 | 0.163* |
| H21C | 0.8502 | 0.5354 | 0.0274 | 0.163* |
| C22 | 0.1788 (8) | 0.3622 (6) | 0.2900 (3) | 0.136 (2) |
| H22A | 0.0641 | 0.3665 | 0.2948 | 0.204* |
| H22B | 0.2210 | 0.4419 | 0.2835 | 0.204* |
| H22C | 0.2260 | 0.3286 | 0.3252 | 0.204* |
| C23 | 0.1671 (8) | 0.3533 (7) | 0.1851 (3) | 0.137 (2) |
| H23A | 0.0565 | 0.3770 | 0.1890 | 0.206* |
| H23B | 0.1793 | 0.3028 | 0.1508 | 0.206* |
| H23C | 0.2332 | 0.4240 | 0.1809 | 0.206* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0430 (6) | 0.0520 (7) | 0.0436 (7) | −0.0011 (6) | −0.0006 (6) | 0.0021 (6) |
| O1 | 0.0398 (17) | 0.071 (2) | 0.0398 (17) | −0.0001 (16) | −0.0011 (14) | −0.0013 (14) |
| O2 | 0.054 (2) | 0.0493 (18) | 0.070 (2) | −0.0005 (15) | −0.0028 (16) | 0.0074 (15) |
| N1 | 0.037 (2) | 0.052 (2) | 0.068 (2) | −0.0012 (17) | 0.0005 (19) | −0.0009 (19) |
| C4 | 0.042 (3) | 0.093 (4) | 0.041 (3) | 0.000 (3) | −0.004 (2) | 0.006 (3) |
| C5 | 0.040 (3) | 0.051 (3) | 0.035 (2) | −0.003 (2) | −0.0010 (19) | 0.005 (2) |
| C6 | 0.067 (4) | 0.075 (4) | 0.062 (3) | −0.014 (3) | 0.004 (3) | 0.001 (3) |
| C7 | 0.040 (3) | 0.076 (4) | 0.038 (3) | −0.002 (3) | 0.003 (2) | −0.009 (2) |
| C8 | 0.077 (4) | 0.057 (3) | 0.053 (3) | 0.008 (3) | −0.009 (3) | −0.005 (3) |
| C9 | 0.053 (3) | 0.080 (4) | 0.058 (3) | 0.005 (3) | 0.003 (2) | −0.005 (3) |
| C10 | 0.042 (3) | 0.065 (3) | 0.074 (3) | −0.004 (2) | 0.001 (3) | −0.003 (3) |
| C11 | 0.065 (4) | 0.090 (4) | 0.057 (3) | 0.004 (3) | 0.001 (3) | −0.011 (3) |
| C12 | 0.078 (4) | 0.115 (5) | 0.056 (3) | 0.008 (4) | 0.008 (3) | −0.014 (3) |
| C13 | 0.074 (4) | 0.050 (3) | 0.064 (3) | 0.001 (3) | −0.017 (3) | −0.002 (2) |
| C14 | 0.076 (4) | 0.076 (4) | 0.073 (4) | −0.001 (3) | −0.028 (3) | 0.010 (3) |
| C15 | 0.067 (4) | 0.101 (5) | 0.048 (3) | 0.004 (3) | −0.019 (3) | 0.002 (3) |
| C16 | 0.072 (4) | 0.104 (5) | 0.044 (3) | −0.003 (3) | 0.002 (3) | 0.001 (3) |
| C17 | 0.055 (3) | 0.079 (4) | 0.168 (5) | −0.013 (3) | 0.010 (4) | −0.014 (4) |
| C18 | 0.120 (6) | 0.098 (5) | 0.090 (4) | 0.020 (4) | −0.006 (4) | −0.037 (3) |
| C19 | 0.097 (5) | 0.084 (4) | 0.093 (4) | −0.006 (4) | 0.017 (4) | 0.014 (3) |
| C20 | 0.093 (5) | 0.064 (4) | 0.059 (4) | −0.002 (4) | −0.018 (3) | −0.016 (3) |
| C21 | 0.098 (5) | 0.118 (5) | 0.110 (5) | −0.046 (4) | 0.018 (4) | 0.020 (4) |
| C22 | 0.081 (4) | 0.143 (5) | 0.183 (6) | −0.013 (4) | 0.033 (4) | −0.072 (5) |
| C23 | 0.074 (4) | 0.166 (6) | 0.172 (6) | −0.017 (4) | −0.036 (4) | 0.072 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| P1—O2 | 1.459 (3) | C12—H12A | 0.9700 |
| P1—O1 | 1.581 (3) | C12—H12B | 0.9700 |
| P1—N1 | 1.636 (3) | C13—C14 | 1.365 (6) |
| P1—C5 | 1.794 (4) | C13—H13 | 0.9300 |
| O1—C7 | 1.456 (5) | C14—C15 | 1.359 (6) |
| N1—C10 | 1.470 (5) | C14—H14 | 0.9300 |
| N1—H1 | 0.8600 | C15—C20 | 1.338 (6) |
| C4—C7 | 1.510 (6) | C15—H15 | 0.9300 |
| C4—C6 | 1.512 (6) | C16—H16A | 0.9700 |
| C4—C16 | 1.524 (6) | C16—H16B | 0.9700 |
| C4—H4 | 0.9800 | C17—H17A | 0.9600 |
| C5—C13 | 1.369 (6) | C17—H17B | 0.9600 |
| C5—C8 | 1.370 (6) | C17—H17C | 0.9600 |
| C6—C19 | 1.533 (7) | C18—H18A | 0.9600 |
| C6—C21 | 1.534 (7) | C18—H18B | 0.9600 |
| C6—H6 | 0.9800 | C18—H18C | 0.9600 |
| C7—C9 | 1.514 (6) | C19—H19A | 0.9600 |
| C7—H7 | 0.9800 | C19—H19B | 0.9600 |
| C8—C20 | 1.400 (6) | C19—H19C | 0.9600 |
| C8—H8 | 0.9300 | C20—H20 | 0.9300 |
| C9—C11 | 1.497 (6) | C21—H21A | 0.9600 |
| C9—H9A | 0.9700 | C21—H21B | 0.9600 |
| C9—H9B | 0.9700 | C21—H21C | 0.9600 |
| C10—C22 | 1.469 (7) | C22—H22A | 0.9600 |
| C10—C17 | 1.483 (6) | C22—H22B | 0.9600 |
| C10—C23 | 1.490 (7) | C22—H22C | 0.9600 |
| C11—C12 | 1.490 (7) | C23—H23A | 0.9600 |
| C11—C18 | 1.525 (7) | C23—H23B | 0.9600 |
| C11—H11 | 0.9800 | C23—H23C | 0.9600 |
| C12—C16 | 1.516 (7) | | |
| O2—P1—O1 | 116.25 (17) | C16—C12—H12B | 109.0 |
| O2—P1—N1 | 113.53 (18) | H12A—C12—H12B | 107.8 |
| O1—P1—N1 | 105.14 (17) | C5—C13—C14 | 120.7 (4) |
| O2—P1—C5 | 111.6 (2) | C5—C13—H13 | 119.6 |
| O1—P1—C5 | 99.14 (18) | C14—C13—H13 | 119.6 |
| N1—P1—C5 | 110.08 (19) | C15—C14—C13 | 120.3 (5) |
| C7—O1—P1 | 123.9 (3) | C15—C14—H14 | 119.9 |
| C10—N1—P1 | 129.0 (3) | C13—C14—H14 | 119.9 |
| C10—N1—H1 | 115.5 | C20—C15—C14 | 120.7 (5) |
| P1—N1—H1 | 115.5 | C20—C15—H15 | 119.7 |
| C7—C4—C6 | 114.5 (4) | C14—C15—H15 | 119.7 |
| C7—C4—C16 | 108.0 (4) | C12—C16—C4 | 113.3 (4) |
| C6—C4—C16 | 114.2 (4) | C12—C16—H16A | 108.9 |
| C7—C4—H4 | 106.5 | C4—C16—H16A | 108.9 |
| C6—C4—H4 | 106.5 | C12—C16—H16B | 108.9 |
| C16—C4—H4 | 106.5 | C4—C16—H16B | 108.9 |

| | | | |
|---|---|---|---|
| C13—C5—C8 | 118.5 (4) | H16A—C16—H16B | 107.7 |
| C13—C5—P1 | 122.4 (4) | C10—C17—H17A | 109.5 |
| C8—C5—P1 | 119.2 (4) | C10—C17—H17B | 109.5 |
| C4—C6—C19 | 114.6 (4) | H17A—C17—H17B | 109.5 |
| C4—C6—C21 | 111.6 (5) | C10—C17—H17C | 109.5 |
| C19—C6—C21 | 108.2 (4) | H17A—C17—H17C | 109.5 |
| C4—C6—H6 | 107.4 | H17B—C17—H17C | 109.5 |
| C19—C6—H6 | 107.4 | C11—C18—H18A | 109.5 |
| C21—C6—H6 | 107.4 | C11—C18—H18B | 109.5 |
| O1—C7—C4 | 110.4 (4) | H18A—C18—H18B | 109.5 |
| O1—C7—C9 | 107.0 (3) | C11—C18—H18C | 109.5 |
| C4—C7—C9 | 111.7 (4) | H18A—C18—H18C | 109.5 |
| O1—C7—H7 | 109.2 | H18B—C18—H18C | 109.5 |
| C4—C7—H7 | 109.2 | C6—C19—H19A | 109.5 |
| C9—C7—H7 | 109.2 | C6—C19—H19B | 109.5 |
| C5—C8—C20 | 120.4 (5) | H19A—C19—H19B | 109.5 |
| C5—C8—H8 | 119.8 | C6—C19—H19C | 109.5 |
| C20—C8—H8 | 119.8 | H19A—C19—H19C | 109.5 |
| C11—C9—C7 | 114.0 (4) | H19B—C19—H19C | 109.5 |
| C11—C9—H9A | 108.7 | C15—C20—C8 | 119.4 (5) |
| C7—C9—H9A | 108.7 | C15—C20—H20 | 120.3 |
| C11—C9—H9B | 108.7 | C8—C20—H20 | 120.3 |
| C7—C9—H9B | 108.7 | C6—C21—H21A | 109.5 |
| H9A—C9—H9B | 107.6 | C6—C21—H21B | 109.5 |
| N1—C10—C22 | 111.4 (4) | H21A—C21—H21B | 109.5 |
| N1—C10—C17 | 109.8 (4) | C6—C21—H21C | 109.5 |
| C22—C10—C17 | 107.8 (5) | H21A—C21—H21C | 109.5 |
| N1—C10—C23 | 110.6 (4) | H21B—C21—H21C | 109.5 |
| C22—C10—C23 | 106.5 (5) | C10—C22—H22A | 109.5 |
| C17—C10—C23 | 110.6 (5) | C10—C22—H22B | 109.5 |
| C12—C11—C9 | 109.9 (4) | H22A—C22—H22B | 109.5 |
| C12—C11—C18 | 112.7 (5) | C10—C22—H22C | 109.5 |
| C9—C11—C18 | 113.5 (4) | H22A—C22—H22C | 109.5 |
| C12—C11—H11 | 106.8 | H22B—C22—H22C | 109.5 |
| C9—C11—H11 | 106.8 | C10—C23—H23A | 109.5 |
| C18—C11—H11 | 106.8 | C10—C23—H23B | 109.5 |
| C11—C12—C16 | 113.0 (4) | H23A—C23—H23B | 109.5 |
| C11—C12—H12A | 109.0 | C10—C23—H23C | 109.5 |
| C16—C12—H12A | 109.0 | H23A—C23—H23C | 109.5 |
| C11—C12—H12B | 109.0 | H23B—C23—H23C | 109.5 |
| O2—P1—O1—C7 | −73.5 (3) | C16—C4—C7—C9 | 55.0 (5) |
| N1—P1—O1—C7 | 52.9 (3) | C13—C5—C8—C20 | 0.7 (7) |
| C5—P1—O1—C7 | 166.8 (3) | P1—C5—C8—C20 | −179.0 (4) |
| O2—P1—N1—C10 | −14.7 (5) | O1—C7—C9—C11 | −177.5 (4) |
| O1—P1—N1—C10 | −142.9 (4) | C4—C7—C9—C11 | −56.6 (5) |
| C5—P1—N1—C10 | 111.2 (4) | P1—N1—C10—C22 | −51.2 (6) |
| O2—P1—C5—C13 | 175.2 (4) | P1—N1—C10—C17 | −170.6 (4) |
| O1—P1—C5—C13 | −61.8 (4) | P1—N1—C10—C23 | 67.1 (6) |
| N1—P1—C5—C13 | 48.1 (4) | C7—C9—C11—C12 | 52.8 (6) |

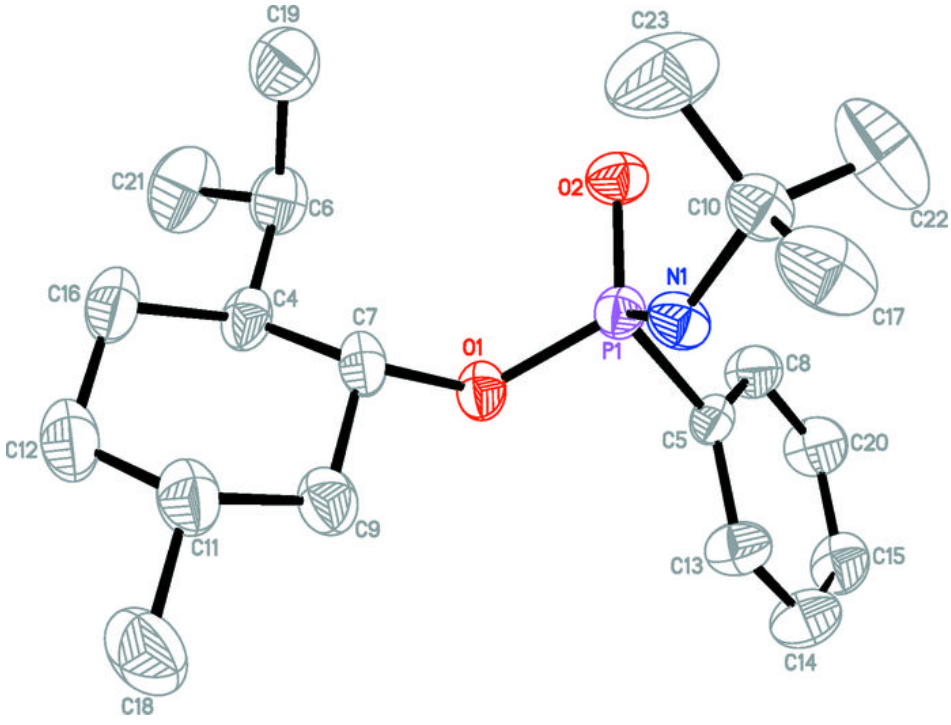
| | | | |
|---|---|---|---|
| O2—P1—C5—C8 | −5.2 (4) | C7—C9—C11—C18 | −180.0 (5) |
| O1—P1—C5—C8 | 117.9 (4) | C9—C11—C12—C16 | −51.2 (6) |
| N1—P1—C5—C8 | −132.2 (3) | C18—C11—C12—C16 | −178.9 (4) |
| C7—C4—C6—C19 | −71.5 (5) | C8—C5—C13—C14 | 1.0 (7) |
| C16—C4—C6—C19 | 53.6 (6) | P1—C5—C13—C14 | −179.3 (4) |
| C7—C4—C6—C21 | 165.0 (4) | C5—C13—C14—C15 | −2.3 (8) |
| C16—C4—C6—C21 | −69.8 (6) | C13—C14—C15—C20 | 1.7 (9) |
| P1—O1—C7—C4 | 118.4 (4) | C11—C12—C16—C4 | 54.8 (6) |
| P1—O1—C7—C9 | −119.8 (3) | C7—C4—C16—C12 | −54.9 (6) |
| C6—C4—C7—O1 | −57.7 (5) | C6—C4—C16—C12 | 176.5 (4) |
| C16—C4—C7—O1 | 173.9 (4) | C14—C15—C20—C8 | 0.0 (9) |
| C6—C4—C7—C9 | −176.6 (4) | C5—C8—C20—C15 | −1.2 (8) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.52 | 3.326 (4) | 156 |
| C13—H13···O2$^{i}$ | 0.93 | 2.51 | 3.391 (5) | 157 |

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

**Fig. 1**


C19
C23
C21
C6
O2
C10
C22
N1
C16
C4
C7
C17
O1
P1
C8
C12
C5
C20
C9
C13
C15
C11
C14
C18