# 2-Isopropyl-5-methylcyclohexyl cyclohexyl(phenyl)phosphinate

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

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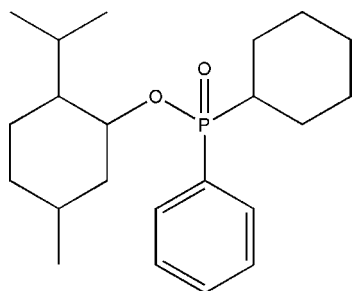Correspondence e-mail: literabc@hotmail.com

In the title molecule, $C_{22}H_{35}O_2P$, the two cyclohexyl rings exhibit chair conformations. In the crystal, molecules related by translation along the $b$ axis are linked by the weak intermolecular C—H···O hydrogen bonds.

## Related literature

For the crystal structure of a related P-chiral compound, see: Fu & Zhao (2010).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{22}H_{35}O_2P$ | $a$ = 11.4892 (13) Å |
| $M_r$ = 362.47 | $b$ = 5.8872 (6) Å |
| Monoclinic, $P2_1$ | $c$ = 16.3531 (17) Å |
| $\beta$ = 94.696 (1)° | $\mu$ = 0.14 mm$^{-1}$ |
| $V$ = 1102.4 (2) Å$^3$ | $T$ = 298 K |
| $Z$ = 2 | 0.45 × 0.11 × 0.08 mm |
| Mo $K\alpha$ radiation | |

### Data collection

| | |
|---|---|
| Bruker SMART-1000 CCD area-detector diffractometer | 5833 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{min}$ = 0.941, $T_{max}$ = 0.989 | 3646 independent reflections |
| | 2125 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.051 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.053 | H-atom parameters constrained |
| $wR(F^2)$ = 0.119 | $\Delta\rho_{max}$ = 0.15 e Å$^{-3}$ |
| $S$ = 0.92 | $\Delta\rho_{min}$ = −0.16 e Å$^{-3}$ |
| 3646 reflections | Absolute structure: Flack (1983), 1493 Friedel pairs |
| 229 parameters | Flack parameter: 0.19 (14) |
| 1 restraint | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C21—H21$A$···O2$^i$ | 0.97 | 2.54 | 3.376 (5) | 145 |
| C17—H17···O2$^i$ | 0.98 | 2.47 | 3.346 (5) | 149 |

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

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*.

## References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Fu, B. & Zhao, C.-Q. (2010). *Acta Cryst.* E**66**, o859.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

## 2-Isopropyl-5-methylcyclohexyl cyclohexyl(phenyl)phosphinate

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### S1. Comment

In continuation of our study of phenylphosphinates (Fu & Zhao, 2010), we present here the title compound (I) prepared from substitution of *O*-menthyl phenylphosphoryl chloride with cyclohexyl magnesium chloride.

In (I) (Fig. 1), the configuration of phosphorus atom was determined as *R*. The compound is comprised of fully extended substituents: cyclohexyl, menthyoxy and phenyl, which form an irregular tetrahedron. The geometric parameters of (I) are usual. The bond angle of C17—P—C11 is 108.65 (18)°, O1—P—C11 is 105.37 (15)°, O1—P—C17 is 102.47 (15)°, O2—P—O1 is 113.94 (16)°, O2—P—C17 is 115.03 (18)° and O2—P—C11 is 110.65 (18) °.

In the crystal structure, the molecules related by translation along *b* axis are linked by the weak intermolecular C—H⋯O hydrogen bonds (Table 1) into chains.

### S2. Experimental

*O*-Menthyl phenylphosphoryl chloride (0.3 mmol) was added to a stirred ether solution of cyclohexyl magnesium chloride (0.6 mmol) under nitrogen and the mixture was stirred for 24 h at room temperature. After washing with water, the resulting solution was purified by preparative TLC on silica gel to afford optically pure product. The crystal suitable for X-ray diffraction was obtained from recrystallization with ethyl ether/hexane.

### S3. Refinement

All H atoms were fixed geometrically and treated as riding, with C—H = 0.93 - 0.98 Å and with $U_{iso}$(H) = 1.2-1.5 $U_{eq}$(C).
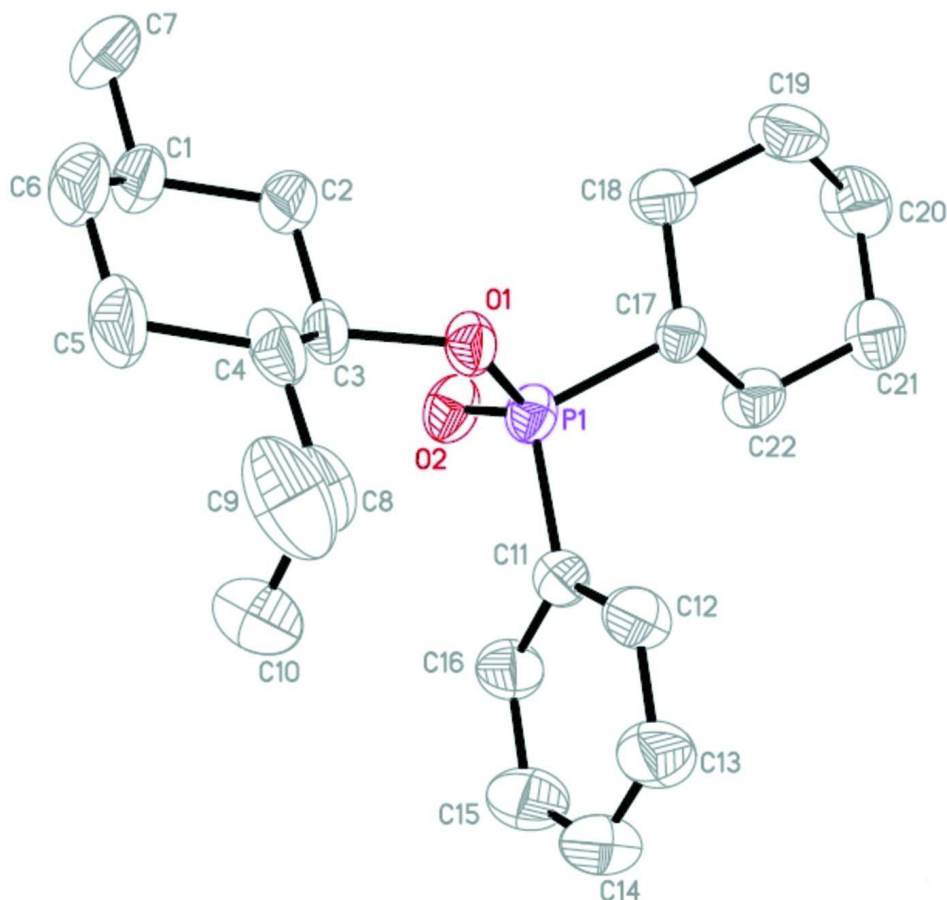
**Figure 1**

The molecular structure of (I) showing the atomic numbering and 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

**2-Isopropyl-5-methylcyclohexyl cyclohexyl(phenyl)phosphinate**

*Crystal data*

| | |
|---|---|
| $C_{22}H_{35}O_2P$ | $F(000) = 396$ |
| $M_r = 362.47$ | $D_x = 1.092$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2yb | Cell parameters from 1233 reflections |
| $a = 11.4892$ (13) Å | $\theta = 2.5–26.0°$ |
| $b = 5.8872$ (6) Å | $\mu = 0.14$ mm$^{-1}$ |
| $c = 16.3531$ (17) Å | $T = 298$ K |
| $\beta = 94.696$ (1)° | Block, colourless |
| $V = 1102.4$ (2) Å$^3$ | $0.45 \times 0.11 \times 0.08$ mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART-1000 CCD area-detector diffractometer | Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) |
| Radiation source: fine-focus sealed tube | $T_{min} = 0.941$, $T_{max} = 0.989$ |
| Graphite monochromator | 5833 measured reflections |
| $\varphi$ and $\omega$ scans | 3646 independent reflections |
| | 2125 reflections with $I > 2\sigma(I)$ |

| | | |
|---|---|---|
| $R_{int} = 0.051$ | | $k = -6\rightarrow6$ |
| $\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$ | | $l = -19\rightarrow19$ |
| $h = -13\rightarrow10$ | | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | H-atom parameters constrained |
| $wR(F^2) = 0.119$ | $w = 1/[\sigma^2(F_o^2) + (0.0454P)^2]$ |
| $S = 0.92$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3646 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 229 parameters | $\Delta\rho_{max} = 0.15$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.16$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 1493 Friedel pairs |
| Secondary atom site location: difference Fourier map | Absolute structure parameter: 0.19 (14) |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.23767 (17) | 0.3099 (5) | 0.23127 (13) | 0.0631 (7) |
| O2 | 0.0655 (2) | 0.5689 (4) | 0.26004 (16) | 0.0743 (8) |
| P1 | 0.11424 (7) | 0.33939 (18) | 0.26861 (5) | 0.0574 (3) |
| C1 | 0.3668 (4) | 0.8147 (10) | 0.1266 (3) | 0.1001 (15) |
| H1 | 0.3503 | 0.9307 | 0.1671 | 0.120* |
| C2 | 0.2885 (3) | 0.6094 (8) | 0.1401 (2) | 0.0784 (13) |
| H2A | 0.2073 | 0.6561 | 0.1330 | 0.094* |
| H2B | 0.3008 | 0.4947 | 0.0991 | 0.094* |
| C3 | 0.3131 (3) | 0.5077 (7) | 0.2245 (2) | 0.0656 (11) |
| H3 | 0.2941 | 0.6204 | 0.2654 | 0.079* |
| C4 | 0.4397 (3) | 0.4344 (8) | 0.2429 (3) | 0.0788 (13) |
| H4 | 0.4556 | 0.3199 | 0.2017 | 0.095* |
| C5 | 0.5175 (4) | 0.6387 (9) | 0.2281 (3) | 0.1134 (18) |
| H5A | 0.5059 | 0.7535 | 0.2692 | 0.136* |
| H5B | 0.5986 | 0.5913 | 0.2351 | 0.136* |
| C6 | 0.4939 (4) | 0.7439 (10) | 0.1434 (3) | 0.118 (2) |
| H6A | 0.5436 | 0.8759 | 0.1392 | 0.141* |
| H6B | 0.5136 | 0.6351 | 0.1022 | 0.141* |
| C7 | 0.3404 (5) | 0.9182 (10) | 0.0410 (3) | 0.141 (2) |
| H7A | 0.3626 | 0.8129 | 0.0003 | 0.211* |

| H7B | 0.3837 | 1.0566 | 0.0371 | 0.211* |
|---|---|---|---|---|
| H7C | 0.2583 | 0.9498 | 0.0322 | 0.211* |
| C8 | 0.4657 (3) | 0.3225 (10) | 0.3271 (3) | 0.0899 (13) |
| H8 | 0.4093 | 0.1986 | 0.3305 | 0.108* |
| C9 | 0.5883 (4) | 0.2143 (10) | 0.3369 (4) | 0.138 (2) |
| H9A | 0.6015 | 0.1294 | 0.2884 | 0.207* |
| H9B | 0.5936 | 0.1145 | 0.3835 | 0.207* |
| H9C | 0.6462 | 0.3316 | 0.3450 | 0.207* |
| C10 | 0.4503 (4) | 0.4809 (11) | 0.4004 (3) | 0.1130 (18) |
| H10A | 0.5076 | 0.5998 | 0.4014 | 0.170* |
| H10B | 0.4603 | 0.3955 | 0.4505 | 0.170* |
| H10C | 0.3735 | 0.5462 | 0.3950 | 0.170* |
| C11 | 0.1394 (3) | 0.2629 (7) | 0.3751 (2) | 0.0579 (11) |
| C12 | 0.1898 (3) | 0.0589 (8) | 0.4006 (3) | 0.0777 (12) |
| H12 | 0.2096 | −0.0463 | 0.3617 | 0.093* |
| C13 | 0.2111 (4) | 0.0089 (9) | 0.4834 (3) | 0.0985 (16) |
| H13 | 0.2465 | −0.1278 | 0.4995 | 0.118* |
| C14 | 0.1804 (5) | 0.1593 (12) | 0.5412 (3) | 0.1094 (18) |
| H14 | 0.1933 | 0.1251 | 0.5967 | 0.131* |
| C15 | 0.1302 (4) | 0.3623 (12) | 0.5164 (3) | 0.1083 (17) |
| H15 | 0.1102 | 0.4666 | 0.5556 | 0.130* |
| C16 | 0.1088 (3) | 0.4143 (8) | 0.4334 (2) | 0.0821 (14) |
| H16 | 0.0738 | 0.5516 | 0.4176 | 0.099* |
| C17 | 0.0280 (3) | 0.1208 (6) | 0.2167 (2) | 0.0535 (9) |
| H17 | 0.0700 | −0.0232 | 0.2254 | 0.064* |
| C18 | 0.0112 (4) | 0.1628 (9) | 0.1254 (2) | 0.0875 (14) |
| H18A | 0.0867 | 0.1661 | 0.1029 | 0.105* |
| H18B | −0.0256 | 0.3095 | 0.1153 | 0.105* |
| C19 | −0.0646 (4) | −0.0220 (11) | 0.0820 (2) | 0.1093 (17) |
| H19A | −0.0772 | 0.0142 | 0.0241 | 0.131* |
| H19B | −0.0238 | −0.1662 | 0.0871 | 0.131* |
| C20 | −0.1814 (4) | −0.0440 (10) | 0.1178 (3) | 0.1077 (17) |
| H20A | −0.2260 | 0.0944 | 0.1077 | 0.129* |
| H20B | −0.2251 | −0.1684 | 0.0913 | 0.129* |
| C21 | −0.1641 (3) | −0.0873 (8) | 0.2087 (3) | 0.0850 (15) |
| H21A | −0.1264 | −0.2334 | 0.2183 | 0.102* |
| H21B | −0.2396 | −0.0931 | 0.2312 | 0.102* |
| C22 | −0.0900 (3) | 0.0966 (8) | 0.2526 (2) | 0.0755 (13) |
| H22A | −0.1313 | 0.2402 | 0.2478 | 0.091* |
| H22B | −0.0776 | 0.0593 | 0.3104 | 0.091* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0564 (13) | 0.0584 (18) | 0.0767 (15) | −0.0131 (15) | 0.0192 (11) | −0.0118 (15) |
| O2 | 0.0739 (17) | 0.055 (2) | 0.096 (2) | 0.0069 (16) | 0.0223 (14) | 0.0092 (15) |
| P1 | 0.0537 (5) | 0.0531 (6) | 0.0667 (6) | −0.0016 (6) | 0.0136 (4) | 0.0013 (6) |
| C1 | 0.118 (4) | 0.091 (4) | 0.098 (3) | −0.049 (4) | 0.050 (3) | −0.018 (3) |

| | | | | | |
|---|---|---|---|---|---|
| C2 | 0.081 (3) | 0.080 (3) | 0.078 (3) | −0.022 (3) | 0.025 (2) | −0.011 (2) |
| C3 | 0.064 (3) | 0.057 (3) | 0.078 (3) | −0.024 (2) | 0.021 (2) | −0.018 (2) |
| C4 | 0.053 (3) | 0.083 (3) | 0.102 (3) | −0.020 (2) | 0.016 (2) | −0.037 (3) |
| C5 | 0.079 (3) | 0.119 (5) | 0.146 (5) | −0.050 (3) | 0.031 (3) | −0.034 (4) |
| C6 | 0.106 (4) | 0.126 (5) | 0.130 (5) | −0.055 (3) | 0.060 (3) | −0.032 (4) |
| C7 | 0.193 (6) | 0.128 (6) | 0.109 (4) | −0.060 (5) | 0.062 (4) | 0.013 (4) |
| C8 | 0.063 (2) | 0.088 (3) | 0.116 (4) | −0.007 (3) | −0.013 (2) | −0.017 (4) |
| C9 | 0.083 (3) | 0.115 (5) | 0.208 (6) | 0.013 (3) | −0.039 (4) | −0.046 (4) |
| C10 | 0.110 (4) | 0.134 (5) | 0.093 (3) | 0.004 (3) | −0.004 (3) | −0.026 (4) |
| C11 | 0.051 (2) | 0.063 (3) | 0.061 (2) | −0.0008 (19) | 0.0085 (18) | −0.005 (2) |
| C12 | 0.088 (3) | 0.076 (3) | 0.068 (3) | 0.005 (3) | −0.003 (2) | −0.007 (2) |
| C13 | 0.112 (4) | 0.099 (4) | 0.080 (3) | 0.007 (3) | −0.024 (3) | 0.011 (3) |
| C14 | 0.129 (4) | 0.132 (6) | 0.065 (3) | −0.011 (4) | −0.003 (3) | −0.001 (4) |
| C15 | 0.131 (4) | 0.125 (6) | 0.072 (3) | 0.005 (4) | 0.028 (3) | −0.023 (4) |
| C16 | 0.090 (3) | 0.088 (4) | 0.071 (3) | 0.001 (3) | 0.021 (2) | −0.014 (3) |
| C17 | 0.047 (2) | 0.053 (2) | 0.062 (2) | −0.0024 (18) | 0.0107 (17) | 0.0018 (19) |
| C18 | 0.085 (3) | 0.116 (4) | 0.061 (3) | −0.025 (3) | 0.007 (2) | 0.000 (3) |
| C19 | 0.104 (4) | 0.156 (5) | 0.067 (3) | −0.027 (3) | −0.001 (3) | −0.023 (3) |
| C20 | 0.074 (3) | 0.140 (5) | 0.104 (4) | −0.027 (3) | −0.019 (3) | −0.012 (3) |
| C21 | 0.053 (2) | 0.096 (4) | 0.106 (3) | −0.017 (2) | 0.003 (2) | −0.003 (3) |
| C22 | 0.052 (2) | 0.101 (4) | 0.074 (3) | −0.011 (3) | 0.0116 (19) | 0.007 (3) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| O1—C3 | 1.461 (4) | C10—H10A | 0.9600 |
| O1—P1 | 1.599 (2) | C10—H10B | 0.9600 |
| O2—P1 | 1.465 (3) | C10—H10C | 0.9600 |
| P1—C17 | 1.794 (4) | C11—C16 | 1.372 (5) |
| P1—C11 | 1.799 (4) | C11—C12 | 1.382 (5) |
| C1—C6 | 1.523 (6) | C12—C13 | 1.388 (5) |
| C1—C2 | 1.533 (6) | C12—H12 | 0.9300 |
| C1—C7 | 1.534 (6) | C13—C14 | 1.362 (7) |
| C1—H1 | 0.9800 | C13—H13 | 0.9300 |
| C2—C3 | 1.510 (5) | C14—C15 | 1.374 (7) |
| C2—H2A | 0.9700 | C14—H14 | 0.9300 |
| C2—H2B | 0.9700 | C15—C16 | 1.393 (6) |
| C3—C4 | 1.523 (5) | C15—H15 | 0.9300 |
| C3—H3 | 0.9800 | C16—H16 | 0.9300 |
| C4—C5 | 1.529 (6) | C17—C18 | 1.511 (4) |
| C4—C8 | 1.535 (6) | C17—C22 | 1.528 (4) |
| C4—H4 | 0.9800 | C17—H17 | 0.9800 |
| C5—C6 | 1.521 (6) | C18—C19 | 1.530 (6) |
| C5—H5A | 0.9700 | C18—H18A | 0.9700 |
| C5—H5B | 0.9700 | C18—H18B | 0.9700 |
| C6—H6A | 0.9700 | C19—C20 | 1.513 (5) |
| C6—H6B | 0.9700 | C19—H19A | 0.9700 |
| C7—H7A | 0.9600 | C19—H19B | 0.9700 |
| C7—H7B | 0.9600 | C20—C21 | 1.506 (5) |

| | | | |
|---|---|---|---|
| C7—H7C | 0.9600 | C20—H20A | 0.9700 |
| C8—C10 | 1.540 (6) | C20—H20B | 0.9700 |
| C8—C9 | 1.542 (6) | C21—C22 | 1.520 (5) |
| C8—H8 | 0.9800 | C21—H21A | 0.9700 |
| C9—H9A | 0.9600 | C21—H21B | 0.9700 |
| C9—H9B | 0.9600 | C22—H22A | 0.9700 |
| C9—H9C | 0.9600 | C22—H22B | 0.9700 |
| | | | |
| C3—O1—P1 | 119.5 (2) | C8—C10—H10A | 109.5 |
| O2—P1—O1 | 114.04 (15) | C8—C10—H10B | 109.5 |
| O2—P1—C17 | 115.11 (17) | H10A—C10—H10B | 109.5 |
| O1—P1—C17 | 102.36 (14) | C8—C10—H10C | 109.5 |
| O2—P1—C11 | 110.69 (17) | H10A—C10—H10C | 109.5 |
| O1—P1—C11 | 105.39 (14) | H10B—C10—H10C | 109.5 |
| C17—P1—C11 | 108.49 (17) | C16—C11—C12 | 118.6 (4) |
| C6—C1—C2 | 108.9 (4) | C16—C11—P1 | 118.7 (3) |
| C6—C1—C7 | 112.8 (4) | C12—C11—P1 | 122.7 (3) |
| C2—C1—C7 | 111.7 (4) | C11—C12—C13 | 121.0 (4) |
| C6—C1—H1 | 107.7 | C11—C12—H12 | 119.5 |
| C2—C1—H1 | 107.7 | C13—C12—H12 | 119.5 |
| C7—C1—H1 | 107.7 | C14—C13—C12 | 120.2 (5) |
| C3—C2—C1 | 112.1 (3) | C14—C13—H13 | 119.9 |
| C3—C2—H2A | 109.2 | C12—C13—H13 | 119.9 |
| C1—C2—H2A | 109.2 | C13—C14—C15 | 119.1 (5) |
| C3—C2—H2B | 109.2 | C13—C14—H14 | 120.4 |
| C1—C2—H2B | 109.2 | C15—C14—H14 | 120.4 |
| H2A—C2—H2B | 107.9 | C14—C15—C16 | 121.0 (5) |
| O1—C3—C2 | 108.5 (3) | C14—C15—H15 | 119.5 |
| O1—C3—C4 | 108.8 (3) | C16—C15—H15 | 119.5 |
| C2—C3—C4 | 113.4 (3) | C11—C16—C15 | 119.9 (4) |
| O1—C3—H3 | 108.7 | C11—C16—H16 | 120.0 |
| C2—C3—H3 | 108.7 | C15—C16—H16 | 120.0 |
| C4—C3—H3 | 108.7 | C18—C17—C22 | 110.4 (3) |
| C3—C4—C5 | 107.9 (4) | C18—C17—P1 | 111.8 (3) |
| C3—C4—C8 | 114.3 (3) | C22—C17—P1 | 111.0 (2) |
| C5—C4—C8 | 114.0 (4) | C18—C17—H17 | 107.8 |
| C3—C4—H4 | 106.7 | C22—C17—H17 | 107.8 |
| C5—C4—H4 | 106.7 | P1—C17—H17 | 107.8 |
| C8—C4—H4 | 106.7 | C17—C18—C19 | 111.3 (4) |
| C6—C5—C4 | 113.7 (4) | C17—C18—H18A | 109.4 |
| C6—C5—H5A | 108.8 | C19—C18—H18A | 109.4 |
| C4—C5—H5A | 108.8 | C17—C18—H18B | 109.4 |
| C6—C5—H5B | 108.8 | C19—C18—H18B | 109.4 |
| C4—C5—H5B | 108.8 | H18A—C18—H18B | 108.0 |
| H5A—C5—H5B | 107.7 | C20—C19—C18 | 111.8 (4) |
| C1—C6—C5 | 111.9 (4) | C20—C19—H19A | 109.3 |
| C1—C6—H6A | 109.2 | C18—C19—H19A | 109.3 |
| C5—C6—H6A | 109.2 | C20—C19—H19B | 109.3 |

| | | | |
|---|---|---|---|
| C1—C6—H6B | 109.2 | C18—C19—H19B | 109.3 |
| C5—C6—H6B | 109.2 | H19A—C19—H19B | 107.9 |
| H6A—C6—H6B | 107.9 | C21—C20—C19 | 110.3 (3) |
| C1—C7—H7A | 109.5 | C21—C20—H20A | 109.6 |
| C1—C7—H7B | 109.5 | C19—C20—H20A | 109.6 |
| H7A—C7—H7B | 109.5 | C21—C20—H20B | 109.6 |
| C1—C7—H7C | 109.5 | C19—C20—H20B | 109.6 |
| H7A—C7—H7C | 109.5 | H20A—C20—H20B | 108.1 |
| H7B—C7—H7C | 109.5 | C20—C21—C22 | 111.7 (4) |
| C4—C8—C10 | 114.4 (4) | C20—C21—H21A | 109.3 |
| C4—C8—C9 | 112.3 (4) | C22—C21—H21A | 109.3 |
| C10—C8—C9 | 109.3 (4) | C20—C21—H21B | 109.3 |
| C4—C8—H8 | 106.8 | C22—C21—H21B | 109.3 |
| C10—C8—H8 | 106.8 | H21A—C21—H21B | 108.0 |
| C9—C8—H8 | 106.8 | C17—C22—C21 | 111.5 (3) |
| C8—C9—H9A | 109.5 | C17—C22—H22A | 109.3 |
| C8—C9—H9B | 109.5 | C21—C22—H22A | 109.3 |
| H9A—C9—H9B | 109.5 | C17—C22—H22B | 109.3 |
| C8—C9—H9C | 109.5 | C21—C22—H22B | 109.3 |
| H9A—C9—H9C | 109.5 | H22A—C22—H22B | 108.0 |
| H9B—C9—H9C | 109.5 | | |
| | | | |
| C3—O1—P1—O2 | 25.3 (3) | O2—P1—C11—C12 | −177.1 (3) |
| C3—O1—P1—C17 | 150.3 (3) | O1—P1—C11—C12 | −53.3 (3) |
| C3—O1—P1—C11 | −96.4 (3) | C17—P1—C11—C12 | 55.7 (3) |
| C6—C1—C2—C3 | 55.2 (5) | C16—C11—C12—C13 | −1.2 (6) |
| C7—C1—C2—C3 | −179.5 (4) | P1—C11—C12—C13 | 178.0 (3) |
| P1—O1—C3—C2 | −93.0 (3) | C11—C12—C13—C14 | 1.3 (7) |
| P1—O1—C3—C4 | 143.1 (3) | C12—C13—C14—C15 | −1.2 (8) |
| C1—C2—C3—O1 | −178.3 (3) | C13—C14—C15—C16 | 1.0 (8) |
| C1—C2—C3—C4 | −57.3 (5) | C12—C11—C16—C15 | 0.9 (6) |
| O1—C3—C4—C5 | 175.1 (3) | P1—C11—C16—C15 | −178.2 (3) |
| C2—C3—C4—C5 | 54.3 (5) | C14—C15—C16—C11 | −0.9 (7) |
| O1—C3—C4—C8 | −57.0 (4) | O2—P1—C17—C18 | 60.0 (3) |
| C2—C3—C4—C8 | −177.9 (4) | O1—P1—C17—C18 | −64.3 (3) |
| C3—C4—C5—C6 | −53.9 (5) | C11—P1—C17—C18 | −175.4 (3) |
| C8—C4—C5—C6 | 178.1 (4) | O2—P1—C17—C22 | −63.8 (3) |
| C2—C1—C6—C5 | −54.5 (5) | O1—P1—C17—C22 | 171.9 (3) |
| C7—C1—C6—C5 | −179.2 (4) | C11—P1—C17—C22 | 60.8 (3) |
| C4—C5—C6—C1 | 56.4 (6) | C22—C17—C18—C19 | −54.7 (5) |
| C3—C4—C8—C10 | −64.6 (5) | P1—C17—C18—C19 | −178.8 (3) |
| C5—C4—C8—C10 | 60.1 (5) | C17—C18—C19—C20 | 55.9 (5) |
| C3—C4—C8—C9 | 170.0 (4) | C18—C19—C20—C21 | −55.8 (6) |
| C5—C4—C8—C9 | −65.3 (5) | C19—C20—C21—C22 | 56.0 (5) |
| O2—P1—C11—C16 | 2.0 (3) | C18—C17—C22—C21 | 55.1 (4) |
| O1—P1—C11—C16 | 125.8 (3) | P1—C17—C22—C21 | 179.7 (3) |
| C17—P1—C11—C16 | −125.2 (3) | C20—C21—C22—C17 | −56.2 (5) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C21—H21*A*···O2ⁱ | 0.97 | 2.54 | 3.376 (5) | 145 |
| C17—H17···O2ⁱ | 0.98 | 2.47 | 3.346 (5) | 149 |

Symmetry code: (i) *x*, *y*−1, *z*.