Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-[(Diphenylphosphoryl)(hydroxy)-methyl]-5-methoxyphenol

**Yutian Shao, Chao Yang* and Wujiong Xia**

State Key Laboratory of Urban Water Resource and Environment (SKLUWRE) & Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin, Heilongjiang 150090, People's Republic of China
Correspondence e-mail: xyyang@hit.edu.cn

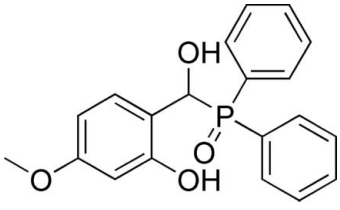
Received 28 April 2012; accepted 8 May 2012

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.044; $wR$ factor = 0.114; data-to-parameter ratio = 13.2.

In the title compound, $C_{20}H_{19}O_4P$, the dihedral angle between the phenyl rings is 73.3 (4)° and the dihedral angles between the benzene ring and the two phenyl rings are 43.0 (3) and 54.3 (1)°. In the crystal, O—H···O hydrogen bonds and weak O—H···O interactions are observed, which form a supramolecular sheet parallel to (010).

## Related literature

For α-hydroxylphosphine oxides, see: Marmor & Seyferth (1969); Toyota *et al.* (1993); Kazankova *et al.* (2003); For substrates used in the preparation of α-carboxylphosphine oxides, see: Fischer *et al.* (1993) and for substrates used in the preparation of unsymmetrical phosphine oxides, see: Miller *et al.* (1957).




## Experimental

### Crystal data

$C_{20}H_{19}O_4P$
$M_r$ = 354.32
Monoclinic, $P2_1/n$
$a$ = 8.349 (7) Å
$b$ = 17.406 (14) Å
$c$ = 12.639 (10) Å
$\beta$ = 107.863 (9)°
$V$ = 1748 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 296 K
0.20 × 0.15 × 0.10 mm

### Data collection

Bruker SMART CCD APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.965, $T_{max}$ = 0.982
8150 measured reflections
3017 independent reflections
2124 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
$S$ = 1.04
3017 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O1$^{i}$ | 0.82 | 1.81 | 2.613 (2) | 168 |
| O4—H4···O3$^{ii}$ | 0.82 | 2.28 | 3.046 (3) | 156 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

The work is supported by the National Natural Science Foundation (Nos 21002018 and 21072038), the Fundamental Research Funds for the Central Universities (No. HIT.BRET2.2010001), WZSTP (No. G20100056), ZJSTP (No. 2011-C23116).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2135).

## References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fischer, M., Hickmann, E., Kropp, R., Schroeder, J. & Trentmann, B. (1993). US Patent 5504236.
Kazankova, M. A., Shulyupin, M. O. & Beletskaya, I. P. (2003). *Synlett*, pp. 2155–2158.
Marmor, R. S. & Seyferth, D. (1969). *J. Org. Chem.* **34**, 748–749.
Miller, R. C., Miller, C. D., Rogers, W. Jr & Hamilton, L. A. (1957). *J. Am. Chem. Soc.* **79**, 424–427.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Toyota, M., Seishi, T. & Fukumoto, K. (1993). *Tetrahedron Lett.* **34**, 5947–5950.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1708 [doi:10.1107/S1600536812020685]

## 2-[(Diphenylphosphoryl)(hydroxy)methyl]-5-methoxyphenol

**Yutian Shao, Chao Yang and Wujiong Xia**

### Comment

*α*-hydroxylphosphine oxides are molecules (Marmor *et al.*, 1969; Toyota, *et al.*, 1993; Kazankova *et al..*, 2003) that are used as substrates for the preparation of *α*-carboxylphosphine oxides (Fischer, *et al.*, 1993) and unsymmetrical phosphine oxides (Miller *et al.*, 1957). We present herin, the preparation and crystal structure of the title compound, $C_{20}H_{19}O_4P$, (I).

In the title compound (I), the dihedral angle between the two mono-substituted benzene rings is 73.3 (4)° (Fig. 1). The dihedral angle between the tri- substituted benzene ring and two mono-substituted benzene rings is 43. 0(3)° and 54.3 (0)°, respectively. O—H···O hydrogen bonds and weak O—H···O intermolecular interactions (Table 1) are observed which form a two-dimensional supramolecular sheet and influence crystal packing (Fig. 2).

### Experimental

The title compound was obtained from the following procedure. To a flame dried round-bottomed flask, 2-hydroxy-4-methoxy-benzaldehyde (1.0equiv), potassiumtert-butoxide (1.5equiv) and anhydrous DMF were added under $N_2$ protection. After the addition of chlorodiphenylphosphine (1.5 equiv. in anhydrous DMF) and stirred overnight at room temperature, water was added to quench the reaction. The product was extracted with $CH_2Cl_2$, dried with $Na_2SO_4$ and concentrated under pressure to give an oil residue, which was purified through a silica gel column to yield the title compound.

### Refinement

All H atoms were placed in calculated positions and then refined using the riding model, with atom–H lengths of 0.93Å (CH), 0.98Å or 0.82Å (OH) Isotropic displacement parameters were set to 1.2 (CH) or 1.5 ($CH_3$) times $U_{eq}$ of the parent atom.

### Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

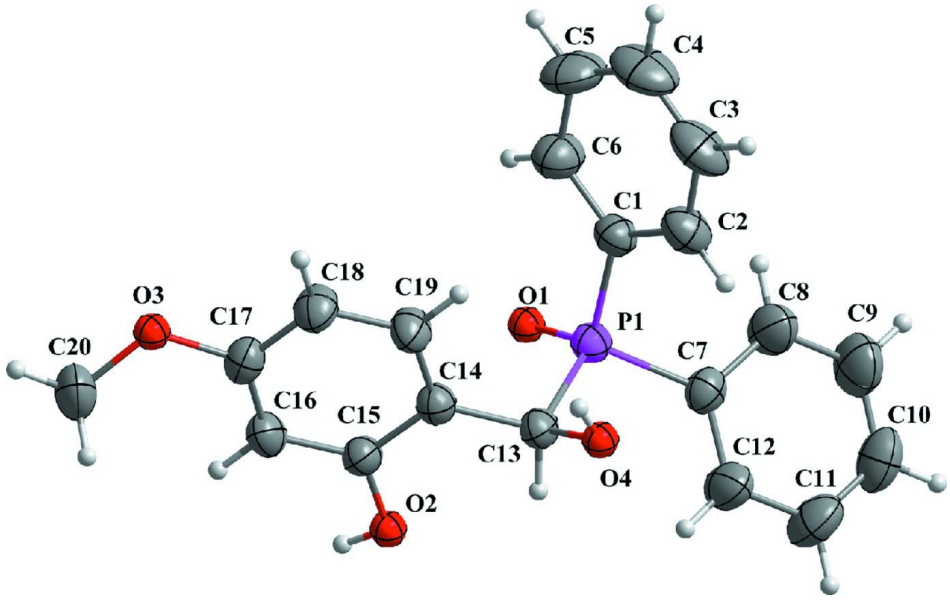



**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

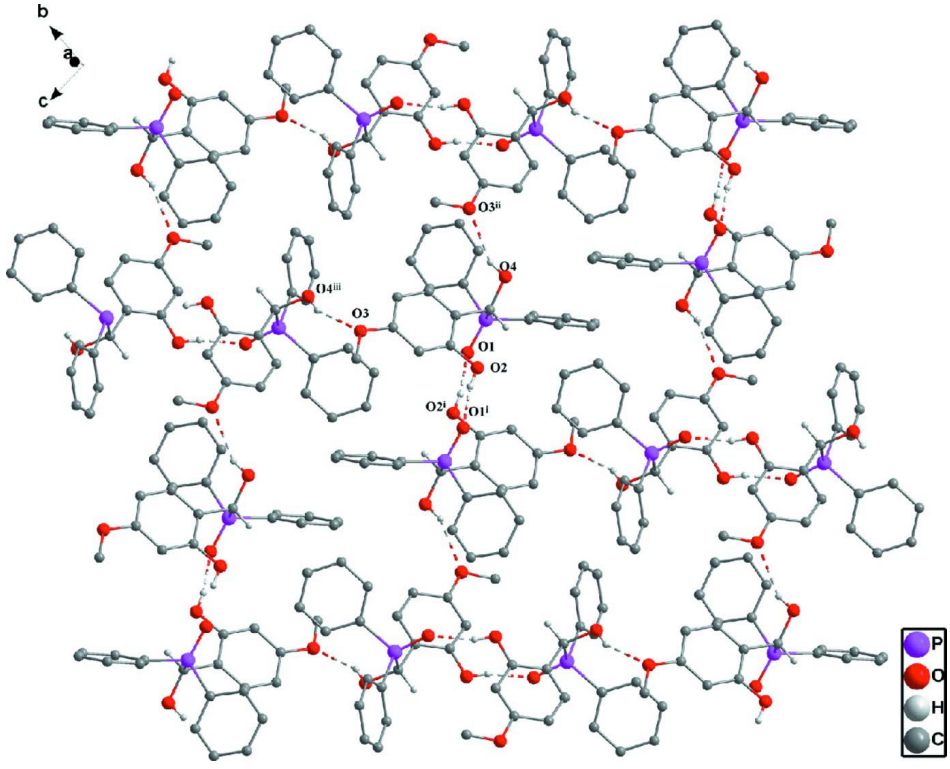



**Figure 2**

Packing diagram of the title compound viewed aloing the a axis. Dashed lines represent O—H···O hydrogen bonds and weak O—H···O intermolecular interactions. H atoms not involved in hydrogen bonding are omitted for clarity. [symmetry codes: (i) 1 - *x*, - *y*, 2 -*z*; (ii) *x* - 1/2, 0.5 - *y*, *z* - 0.5; (iii) *x* + 1/2, 0.5 - *y*, 0.5 + *z*].

**2-[(Diphenylphosphoryl)(hydroxy)methyl]-5-methoxyphenol**

*Crystal data*

$C_{20}H_{19}O_4P$
$M_r = 354.32$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.349$ (7) Å
$b = 17.406$ (14) Å
$c = 12.639$ (10) Å
$\beta = 107.863$ (9)°
$V = 1748$ (2) Å$^3$
$Z = 4$
$F(000) = 744$
$D_x = 1.346$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 255 reflections
$\theta = 25.6$–$3.1°$
$\mu = 0.18$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.20 × 0.15 × 0.10 mm

*Data collection*

Bruker SMART CCD APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.965$, $T_{max} = 0.982$
8150 measured reflections
3017 independent reflections
2124 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow7$
$k = -20\rightarrow20$
$l = -15\rightarrow12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.114$
$S = 1.04$
3017 reflections
229 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.1885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å$^{-3}$
$\Delta\rho_{min} = -0.25$ e Å$^{-3}$

*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 | 0.18172 (8) | 0.11354 (3) | 0.82003 (5) | 0.0358 (2) |
| O1 | 0.2141 (2) | 0.08777 (9) | 0.93707 (13) | 0.0448 (5) |
| O2 | 0.6011 (2) | 0.00424 (8) | 0.91075 (14) | 0.0510 (5) |
| H2 | 0.6570 | −0.0200 | 0.9652 | 0.077* |

| | | | | |
|---|---|---|---|---|
| O3 | 0.9492 (2) | 0.21531 (10) | 1.09662 (15) | 0.0536 (5) |
| O4 | 0.3359 (2) | 0.13072 (10) | 0.66335 (14) | 0.0510 (5) |
| H4 | 0.3793 | 0.1733 | 0.6665 | 0.077* |
| C1 | 0.1266 (3) | 0.21306 (13) | 0.8032 (2) | 0.0380 (6) |
| C2 | 0.0631 (3) | 0.24707 (15) | 0.6995 (2) | 0.0497 (7) |
| H2A | 0.0431 | 0.2171 | 0.6359 | 0.060* |
| C3 | 0.0295 (4) | 0.32424 (16) | 0.6896 (3) | 0.0639 (9) |
| H3 | −0.0112 | 0.3466 | 0.6196 | 0.077* |
| C4 | 0.0560 (4) | 0.36781 (16) | 0.7825 (3) | 0.0725 (10) |
| H4A | 0.0307 | 0.4200 | 0.7757 | 0.087* |
| C5 | 0.1198 (5) | 0.33591 (16) | 0.8866 (3) | 0.0749 (10) |
| H5 | 0.1385 | 0.3665 | 0.9495 | 0.090* |
| C6 | 0.1560 (4) | 0.25804 (15) | 0.8973 (2) | 0.0551 (8) |
| H6 | 0.1998 | 0.2362 | 0.9675 | 0.066* |
| C7 | 0.0125 (3) | 0.06133 (13) | 0.7244 (2) | 0.0389 (6) |
| C8 | −0.1523 (4) | 0.07782 (17) | 0.7203 (2) | 0.0587 (8) |
| H8 | −0.1737 | 0.1176 | 0.7632 | 0.070* |
| C9 | −0.2837 (4) | 0.03577 (19) | 0.6533 (3) | 0.0698 (9) |
| H9 | −0.3933 | 0.0477 | 0.6511 | 0.084* |
| C10 | −0.2562 (4) | −0.02306 (18) | 0.5903 (3) | 0.0629 (9) |
| H10 | −0.3460 | −0.0517 | 0.5462 | 0.076* |
| C11 | −0.0960 (4) | −0.03961 (17) | 0.5925 (3) | 0.0651 (9) |
| H11 | −0.0764 | −0.0792 | 0.5486 | 0.078* |
| C12 | 0.0377 (4) | 0.00201 (15) | 0.6594 (2) | 0.0572 (8) |
| H12 | 0.1466 | −0.0103 | 0.6605 | 0.069* |
| C13 | 0.3672 (3) | 0.10114 (13) | 0.77302 (19) | 0.0368 (6) |
| H13 | 0.3831 | 0.0456 | 0.7680 | 0.044* |
| C14 | 0.5235 (3) | 0.13105 (13) | 0.85807 (19) | 0.0363 (6) |
| C15 | 0.6364 (3) | 0.07990 (12) | 0.92673 (19) | 0.0363 (6) |
| C16 | 0.7810 (3) | 0.10582 (13) | 1.0067 (2) | 0.0404 (6) |
| H16 | 0.8560 | 0.0710 | 1.0519 | 0.048* |
| C17 | 0.8119 (3) | 0.18334 (14) | 1.0182 (2) | 0.0412 (6) |
| C18 | 0.7035 (3) | 0.23562 (14) | 0.9503 (2) | 0.0465 (7) |
| H18 | 0.7269 | 0.2879 | 0.9575 | 0.056* |
| C19 | 0.5600 (3) | 0.20922 (13) | 0.8717 (2) | 0.0438 (7) |
| H19 | 0.4860 | 0.2444 | 0.8268 | 0.053* |
| C20 | 1.0787 (4) | 0.16408 (17) | 1.1566 (2) | 0.0635 (9) |
| H20A | 1.0368 | 0.1320 | 1.2040 | 0.095* |
| H20B | 1.1732 | 0.1932 | 1.2009 | 0.095* |
| H20C | 1.1132 | 0.1326 | 1.1051 | 0.095* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0395 (4) | 0.0306 (3) | 0.0328 (4) | 0.0029 (3) | 0.0043 (3) | 0.0020 (3) |
| O1 | 0.0551 (12) | 0.0408 (9) | 0.0339 (10) | 0.0076 (8) | 0.0070 (8) | 0.0076 (8) |
| O2 | 0.0608 (13) | 0.0318 (9) | 0.0454 (12) | 0.0020 (8) | −0.0059 (9) | 0.0032 (8) |
| O3 | 0.0452 (11) | 0.0561 (11) | 0.0473 (11) | −0.0069 (9) | −0.0035 (9) | −0.0058 (9) |
| O4 | 0.0523 (12) | 0.0566 (12) | 0.0382 (11) | −0.0021 (9) | 0.0052 (9) | −0.0001 (8) |
| C1 | 0.0376 (15) | 0.0336 (12) | 0.0420 (15) | 0.0032 (10) | 0.0113 (12) | 0.0028 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0507 (17) | 0.0484 (15) | 0.0498 (17) | 0.0114 (13) | 0.0153 (14) | 0.0107 (13) |
| C3 | 0.061 (2) | 0.0520 (18) | 0.082 (2) | 0.0177 (15) | 0.0261 (18) | 0.0295 (17) |
| C4 | 0.077 (2) | 0.0345 (16) | 0.111 (3) | 0.0128 (15) | 0.036 (2) | 0.0162 (19) |
| C5 | 0.098 (3) | 0.0414 (17) | 0.084 (3) | 0.0054 (17) | 0.027 (2) | −0.0193 (16) |
| C6 | 0.067 (2) | 0.0413 (15) | 0.0536 (19) | 0.0057 (14) | 0.0141 (16) | −0.0002 (13) |
| C7 | 0.0437 (16) | 0.0392 (13) | 0.0317 (14) | −0.0021 (11) | 0.0083 (12) | 0.0027 (11) |
| C8 | 0.0465 (18) | 0.0670 (19) | 0.064 (2) | −0.0067 (14) | 0.0193 (15) | −0.0151 (15) |
| C9 | 0.0446 (19) | 0.085 (2) | 0.076 (2) | −0.0130 (17) | 0.0135 (17) | −0.0075 (19) |
| C10 | 0.055 (2) | 0.073 (2) | 0.054 (2) | −0.0242 (16) | 0.0065 (16) | −0.0039 (16) |
| C11 | 0.072 (2) | 0.0586 (18) | 0.063 (2) | −0.0190 (17) | 0.0185 (18) | −0.0223 (15) |
| C12 | 0.0478 (18) | 0.0513 (17) | 0.070 (2) | −0.0069 (13) | 0.0144 (16) | −0.0182 (15) |
| C13 | 0.0390 (15) | 0.0327 (12) | 0.0340 (14) | 0.0028 (10) | 0.0042 (11) | −0.0002 (10) |
| C14 | 0.0371 (14) | 0.0358 (13) | 0.0336 (14) | 0.0011 (10) | 0.0074 (11) | 0.0002 (10) |
| C15 | 0.0399 (15) | 0.0327 (13) | 0.0337 (14) | 0.0010 (11) | 0.0073 (12) | −0.0022 (10) |
| C16 | 0.0407 (15) | 0.0416 (14) | 0.0355 (15) | 0.0064 (11) | 0.0065 (12) | 0.0040 (11) |
| C17 | 0.0399 (15) | 0.0464 (14) | 0.0342 (15) | −0.0054 (12) | 0.0070 (12) | −0.0039 (11) |
| C18 | 0.0501 (17) | 0.0331 (13) | 0.0487 (17) | −0.0054 (12) | 0.0038 (14) | 0.0000 (12) |
| C19 | 0.0463 (16) | 0.0347 (13) | 0.0420 (16) | 0.0039 (11) | 0.0012 (13) | 0.0045 (11) |
| C20 | 0.0416 (18) | 0.080 (2) | 0.057 (2) | 0.0037 (15) | −0.0022 (15) | −0.0090 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P1—O1 | 1.489 (2) | C8—C9 | 1.373 (4) |
| P1—C1 | 1.788 (3) | C8—H8 | 0.9300 |
| P1—C7 | 1.799 (3) | C9—C10 | 1.359 (4) |
| P1—C13 | 1.833 (3) | C9—H9 | 0.9300 |
| O2—C15 | 1.351 (3) | C10—C11 | 1.360 (4) |
| O2—H2 | 0.8200 | C10—H10 | 0.9300 |
| O3—C17 | 1.382 (3) | C11—C12 | 1.381 (4) |
| O3—C20 | 1.426 (3) | C11—H11 | 0.9300 |
| O4—C13 | 1.426 (3) | C12—H12 | 0.9300 |
| O4—H4 | 0.8200 | C13—C14 | 1.507 (3) |
| C1—C6 | 1.382 (3) | C13—H13 | 0.9800 |
| C1—C2 | 1.386 (3) | C14—C15 | 1.390 (3) |
| C2—C3 | 1.370 (4) | C14—C19 | 1.394 (3) |
| C2—H2A | 0.9300 | C15—C16 | 1.391 (3) |
| C3—C4 | 1.358 (4) | C16—C17 | 1.373 (3) |
| C3—H3 | 0.9300 | C16—H16 | 0.9300 |
| C4—C5 | 1.375 (4) | C17—C18 | 1.381 (3) |
| C4—H4A | 0.9300 | C18—C19 | 1.379 (3) |
| C5—C6 | 1.386 (4) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—H19 | 0.9300 |
| C6—H6 | 0.9300 | C20—H20A | 0.9600 |
| C7—C12 | 1.375 (4) | C20—H20B | 0.9600 |
| C7—C8 | 1.391 (4) | C20—H20C | 0.9600 |
| | | | |
| O1—P1—C1 | 111.82 (11) | C11—C10—H10 | 120.3 |
| O1—P1—C7 | 112.41 (11) | C10—C11—C12 | 120.4 (3) |
| C1—P1—C7 | 106.81 (12) | C10—C11—H11 | 119.8 |
| O1—P1—C13 | 111.88 (11) | C12—C11—H11 | 119.8 |

| | | | |
|---|---|---|---|
| C1—P1—C13 | 106.70 (11) | C7—C12—C11 | 121.1 (3) |
| C7—P1—C13 | 106.86 (13) | C7—C12—H12 | 119.4 |
| C15—O2—H2 | 109.5 | C11—C12—H12 | 119.4 |
| C17—O3—C20 | 117.1 (2) | O4—C13—C14 | 115.4 (2) |
| C13—O4—H4 | 109.5 | O4—C13—P1 | 110.58 (16) |
| C6—C1—C2 | 119.2 (2) | C14—C13—P1 | 111.17 (17) |
| C6—C1—P1 | 118.36 (19) | O4—C13—H13 | 106.4 |
| C2—C1—P1 | 122.41 (19) | C14—C13—H13 | 106.4 |
| C3—C2—C1 | 120.9 (3) | P1—C13—H13 | 106.4 |
| C3—C2—H2A | 119.6 | C15—C14—C19 | 117.9 (2) |
| C1—C2—H2A | 119.6 | C15—C14—C13 | 119.8 (2) |
| C4—C3—C2 | 119.6 (3) | C19—C14—C13 | 122.3 (2) |
| C4—C3—H3 | 120.2 | O2—C15—C14 | 117.1 (2) |
| C2—C3—H3 | 120.2 | O2—C15—C16 | 121.7 (2) |
| C3—C4—C5 | 120.9 (3) | C14—C15—C16 | 121.1 (2) |
| C3—C4—H4A | 119.5 | C17—C16—C15 | 119.3 (2) |
| C5—C4—H4A | 119.5 | C17—C16—H16 | 120.4 |
| C4—C5—C6 | 119.8 (3) | C15—C16—H16 | 120.4 |
| C4—C5—H5 | 120.1 | C16—C17—C18 | 121.0 (2) |
| C6—C5—H5 | 120.1 | C16—C17—O3 | 124.0 (2) |
| C1—C6—C5 | 119.6 (3) | C18—C17—O3 | 114.9 (2) |
| C1—C6—H6 | 120.2 | C19—C18—C17 | 119.1 (2) |
| C5—C6—H6 | 120.2 | C19—C18—H18 | 120.4 |
| C12—C7—C8 | 117.6 (2) | C17—C18—H18 | 120.4 |
| C12—C7—P1 | 123.2 (2) | C18—C19—C14 | 121.5 (2) |
| C8—C7—P1 | 119.0 (2) | C18—C19—H19 | 119.2 |
| C9—C8—C7 | 120.4 (3) | C14—C19—H19 | 119.2 |
| C9—C8—H8 | 119.8 | O3—C20—H20A | 109.5 |
| C7—C8—H8 | 119.8 | O3—C20—H20B | 109.5 |
| C10—C9—C8 | 121.1 (3) | H20A—C20—H20B | 109.5 |
| C10—C9—H9 | 119.5 | O3—C20—H20C | 109.5 |
| C8—C9—H9 | 119.5 | H20A—C20—H20C | 109.5 |
| C9—C10—C11 | 119.3 (3) | H20B—C20—H20C | 109.5 |
| C9—C10—H10 | 120.3 | | |

| | | | |
|---|---|---|---|
| O1—P1—C1—C6 | 14.3 (3) | C10—C11—C12—C7 | −0.6 (5) |
| C7—P1—C1—C6 | 137.7 (2) | O1—P1—C13—O4 | −176.33 (14) |
| C13—P1—C1—C6 | −108.3 (2) | C1—P1—C13—O4 | −53.73 (18) |
| O1—P1—C1—C2 | −168.7 (2) | C7—P1—C13—O4 | 60.24 (18) |
| C7—P1—C1—C2 | −45.3 (2) | O1—P1—C13—C14 | −46.77 (19) |
| C13—P1—C1—C2 | 68.7 (2) | C1—P1—C13—C14 | 75.83 (18) |
| C6—C1—C2—C3 | 0.0 (4) | C7—P1—C13—C14 | −170.20 (15) |
| P1—C1—C2—C3 | −177.0 (2) | O4—C13—C14—C15 | −130.8 (2) |
| C1—C2—C3—C4 | −1.1 (4) | P1—C13—C14—C15 | 102.3 (2) |
| C2—C3—C4—C5 | 1.5 (5) | O4—C13—C14—C19 | 49.7 (3) |
| C3—C4—C5—C6 | −0.7 (5) | P1—C13—C14—C19 | −77.3 (3) |
| C2—C1—C6—C5 | 0.7 (4) | C19—C14—C15—O2 | −178.5 (2) |
| P1—C1—C6—C5 | 177.8 (2) | C13—C14—C15—O2 | 1.9 (3) |
| C4—C5—C6—C1 | −0.4 (5) | C19—C14—C15—C16 | 0.1 (4) |

| | | | |
|---|---|---|---|
| O1—P1—C7—C12 | −100.7 (2) | C13—C14—C15—C16 | −179.4 (2) |
| C1—P1—C7—C12 | 136.3 (2) | O2—C15—C16—C17 | 179.0 (2) |
| C13—P1—C7—C12 | 22.4 (3) | C14—C15—C16—C17 | 0.4 (4) |
| O1—P1—C7—C8 | 74.9 (2) | C15—C16—C17—C18 | −1.3 (4) |
| C1—P1—C7—C8 | −48.0 (2) | C15—C16—C17—O3 | 178.4 (2) |
| C13—P1—C7—C8 | −161.9 (2) | C20—O3—C17—C16 | 10.2 (4) |
| C12—C7—C8—C9 | 0.0 (4) | C20—O3—C17—C18 | −170.1 (2) |
| P1—C7—C8—C9 | −175.9 (2) | C16—C17—C18—C19 | 1.7 (4) |
| C7—C8—C9—C10 | 0.5 (5) | O3—C17—C18—C19 | −178.1 (2) |
| C8—C9—C10—C11 | −1.0 (5) | C17—C18—C19—C14 | −1.1 (4) |
| C9—C10—C11—C12 | 1.1 (5) | C15—C14—C19—C18 | 0.2 (4) |
| C8—C7—C12—C11 | 0.0 (4) | C13—C14—C19—C18 | 179.7 (2) |
| P1—C7—C12—C11 | 175.8 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O1$^{i}$ | 0.82 | 1.81 | 2.613 (2) | 168 |
| O4—H4···O3$^{ii}$ | 0.82 | 2.28 | 3.046 (3) | 156 |

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