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# Isopropyltriphenylphosphonium bromide monohydrate

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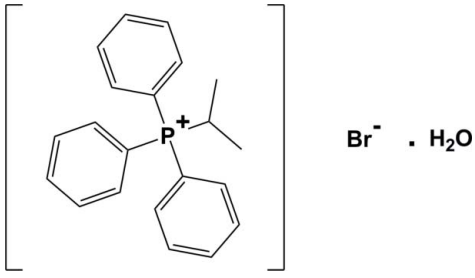
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.007 Å; disorder in solvent or counterion; $R$ factor = 0.049; $wR$ factor = 0.140; data-to-parameter ratio = 18.6.

In the title water-solvated salt, $C_{21}H_{22}P^+\cdot Br^-\cdot H_2O$, the ionic components are linked by short C—H···Br contacts along the $a$-axis direction. The two half occupied water molecules are connected to each other by strong O—H···O hydrogen bonds and they are also linked to the bromide anion by short O—H···Br contacts.

## Related literature

For information on phase-transfer catalysts, see: Asai *et al.* (1994). For the crystal structure of tetraphenylphosphoniuum bromide, see: Alcock *et al.* (1985). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{21}H_{22}P^+\cdot Br^-\cdot H_2O$
$M_r$ = 403.28
Orthorhombic, $P2_12_12_1$
$a$ = 9.078 (5) Å
$b$ = 13.043 (5) Å
$c$ = 17.755 (5) Å
$V$ = 2102.3 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.04 mm$^{-1}$
$T$ = 293 K
0.20 × 0.15 × 0.13 mm

### Data collection

Brucker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.668, $T_{max}$ = 0.688
12177 measured reflections
4250 independent reflections
3331 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.140
$S$ = 1.03
4250 reflections
228 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$
Absolute structure: Flack (1983), 1799 Friedel pairs
Flack parameter: 0.014 (13)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*O1*···Br1$^{i}$ | 0.85 | 2.86 | 3.701 (8) | 169 |
| O1—H2*O1*···O2 | 0.85 | 2.20 | 2.960 (11) | 149 |
| O2—H1*O2*···Br1$^{ii}$ | 0.85 | 2.68 | 3.526 (7) | 175 |
| O2—H2*O2*···Br1$^{iii}$ | 0.85 | 2.81 | 3.598 (8) | 154 |
| C19—H19···Br1$^{iv}$ | 0.98 | 2.76 | 3.723 (4) | 169 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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: SU2327).

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# supporting information

*Acta Cryst.* (2011). E**67**, o3149 [https://doi.org/10.1107/S1600536811044849]

## Isopropyltriphenylphosphonium bromide monohydrate

**Hai Wang, Xi-Man Zhang, Ping Li and Hong-Yu Chen**

### S1. Comment

The title compound belongs to a family of phase transfer catalysts, which usually contain large alkyl or aryl ions, such as $R_4N^+$,$R_4P^+$,$R_4B^-$ *etc*. Because of their ease of dissolution in water, such salts have a conveninient to satisfactory hydrophobic hydration(Asai, *et al.*, 1994).

The asymmetry unit of the title structure consists of one isopropyltriphenylphosphonium cation, one bromide anion and two half occupied water molecules (Fig. 1). In contrast with tetraphenylphosphonium salts, the major character of the cation of the title compound is that one phenyl group has been substituted by an isopropyl group. The fluctuation of the $C_{phenyl}$—P1 bond lengths in the title compound [from 1.789 (4)–1.806 (4) Å] is similar to that in the crystal structure of tetraphenylphosphonium bromide [1.801 (3)Å; Alcock, *et al.*, 1985]. The bonds between P1 and the C atoms of phenyl rings are C$sp^2$—Psp$^3$ bonds, but the connection between P1 and isopropyl group is typically an C$sp^3$—Psp$^3$ bond (Allen, *et al.*, 1987). The bond length of C19—P1 [1.818 (3) Å] associated with the isopropyl group is longer than that involving the phenyl groups, which vary from 1.789 (4) - 1.806 (4) Å.

In the crystal the water molecules are linked to the Br anion by short O—H···Br contacts, and the two half occupied water molecules are connected to one another by strong O-H···O hydrogen bonds (Table 1 and Fig. 2). The large cations and bromide anions are linked by short C19—H19···Br1 contacts (Table 1 and Fig. 2). These weak interactions also that play an important role in the stabilization of the crystal structure.

### S2. Experimental

Triphenyl phosphine (10.5 g) and 2-bromopropane (4.2 mL) were placed in a teflon lined tube. The sealed tube was placed in an autoclave and heated to 433 K for 48 h, then cooled at a rate of 10 K/min. Colourless block-like crystals of the title compound were obtained.

### S3. Refinement

The water H atoms were located in difference Fourier maps and were subsequently treated as riding atoms: O—H = 0.85 Å with $U_{iso}$(H) = 1.5$U_{eq}$(O). The C-bound H-atoms were included in calculated positions and treated as riding atoms: C-H = 0.93, 0.96, and 0.98 Å for CH(aromatic), $CH_3$, and CH(methine) H-atoms, respectively, with = k × $U_{eq}$(parent C-atom), where k = 1.5 for $CH_3$ H-atoms and k = 1.2 for all other H-atoms.

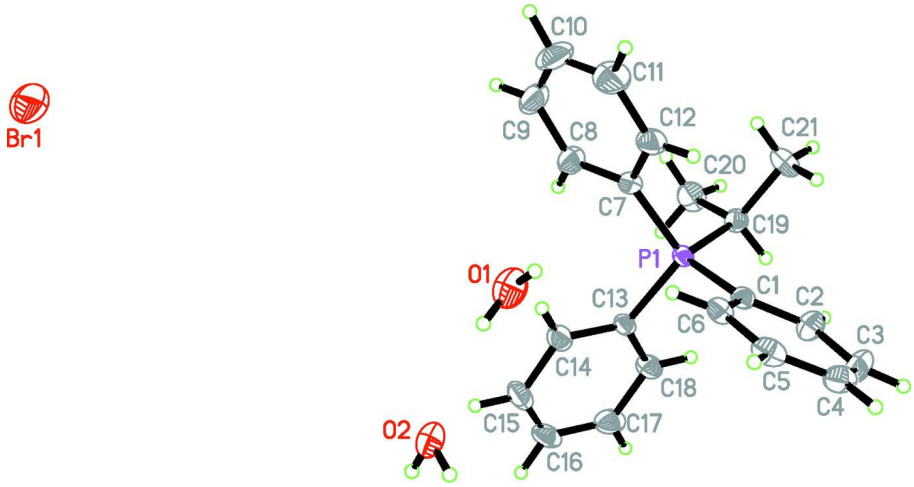


**Figure 1**

A view of the molecular structure of the title compound, with the numbering scheme and thermal ellipsoids drawn at the 30%probability level.

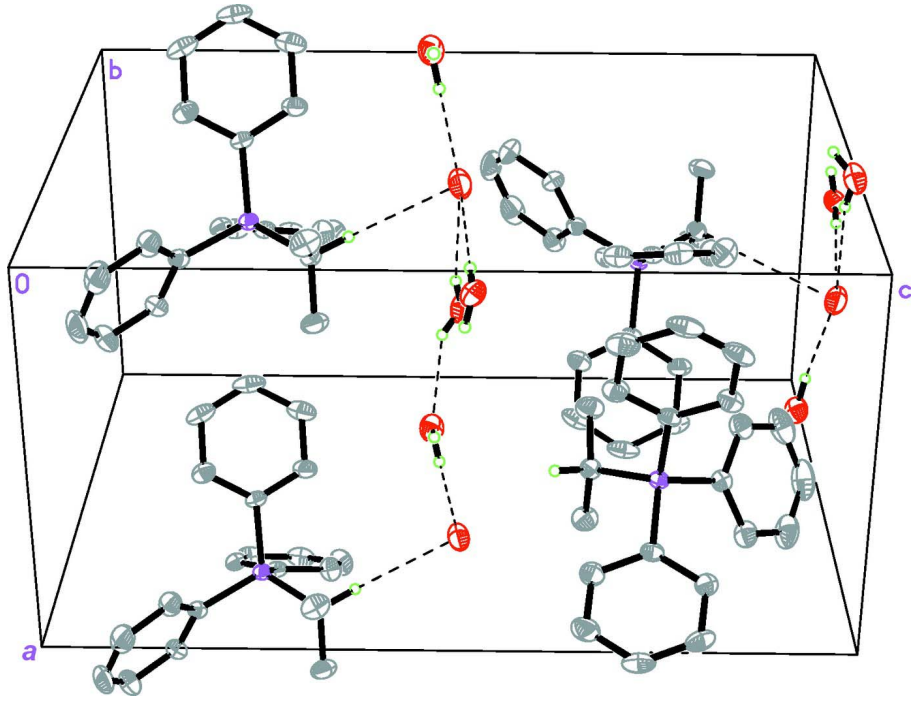


**Figure 2**

A view of the crystal packing of the title compound, showing the O-H···Br and O-H···O hydrogen bonds, and the C-H···Br contacts as dashed lines [H atoms not involved in these contacts have been omitted for calrity].

## Isopropyltriphenylphosphonium bromide monohydrate

*Crystal data*

$C_{21}H_{22}P^{+}\cdot Br^{-}\cdot H_2O$
$M_r$ = 403.28
Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab
$a$ = 9.078 (5) Å
$b$ = 13.043 (5) Å

$c$ = 17.755 (5) Å
$V$ = 2102.3 (15) Å$^3$
$Z$ = 4
$F$(000) = 832
$D_x$ = 1.274 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71069 Å

Cell parameters from 3565 reflections
$\theta$ = 2.5–23.5°
$\mu$ = 2.04 mm$^{-1}$
$T$ = 293 K
ROD, colourless
0.20 × 0.15 × 0.13 mm

*Data collection*

Brucker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.668, $T_{max}$ = 0.688

12177 measured reflections
4250 independent reflections
3331 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 26.4°, $\theta_{min}$ = 1.9°
$h$ = −7→11
$k$ = −16→15
$l$ = −21→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.140
$S$ = 1.03
4250 reflections
228 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$
Absolute structure: Flack (1983), 1799 Friedel pairs
Absolute structure parameter: 0.014 (13)

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Br1 | 0.46181 (8) | 0.58731 (5) | 0.00805 (3) | 0.0720 (2) | |
| C1 | 0.2804 (4) | 0.5002 (3) | 0.7564 (2) | 0.0320 (8) | |
| C2 | 0.2503 (5) | 0.4645 (3) | 0.8289 (3) | 0.0468 (11) | |
| H2 | 0.2722 | 0.5050 | 0.8705 | 0.056* | |
| C3 | 0.1873 (6) | 0.3679 (4) | 0.8386 (3) | 0.0570 (13) | |
| H3 | 0.1690 | 0.3433 | 0.8868 | 0.068* | |
| C4 | 0.1527 (5) | 0.3098 (3) | 0.7778 (3) | 0.0502 (13) | |
| H4 | 0.1075 | 0.2466 | 0.7850 | 0.060* | |
| C5 | 0.1833 (5) | 0.3426 (3) | 0.7054 (3) | 0.0463 (12) | |

| | | | | | |
|---|---|---|---|---|---|
| H5 | 0.1607 | 0.3011 | 0.6644 | 0.056* | |
| C6 | 0.2478 (4) | 0.4378 (3) | 0.6943 (2) | 0.0371 (9) | |
| H6 | 0.2694 | 0.4602 | 0.6458 | 0.045* | |
| C7 | 0.3207 (5) | 0.6876 (3) | 0.6626 (2) | 0.0340 (9) | |
| C8 | 0.4105 (6) | 0.7668 (3) | 0.6355 (3) | 0.0493 (12) | |
| H8 | 0.5032 | 0.7770 | 0.6564 | 0.059* | |
| C9 | 0.3631 (8) | 0.8296 (4) | 0.5783 (3) | 0.0737 (18) | |
| H9 | 0.4228 | 0.8822 | 0.5604 | 0.088* | |
| C10 | 0.2238 (10) | 0.8130 (5) | 0.5476 (3) | 0.082 (2) | |
| H10 | 0.1893 | 0.8561 | 0.5098 | 0.098* | |
| C11 | 0.1386 (7) | 0.7354 (6) | 0.5719 (3) | 0.0754 (18) | |
| H11 | 0.0478 | 0.7239 | 0.5491 | 0.090* | |
| C12 | 0.1835 (5) | 0.6726 (4) | 0.6299 (3) | 0.0498 (12) | |
| H12 | 0.1223 | 0.6205 | 0.6471 | 0.060* | |
| C13 | 0.5706 (4) | 0.5878 (3) | 0.7380 (2) | 0.0312 (8) | |
| C14 | 0.6312 (5) | 0.5673 (3) | 0.6682 (3) | 0.0430 (10) | |
| H14 | 0.5765 | 0.5766 | 0.6245 | 0.052* | |
| C15 | 0.7767 (5) | 0.5321 (3) | 0.6648 (3) | 0.0538 (14) | |
| H15 | 0.8199 | 0.5187 | 0.6183 | 0.065* | |
| C16 | 0.8552 (5) | 0.5173 (3) | 0.7293 (4) | 0.0567 (14) | |
| H16 | 0.9514 | 0.4930 | 0.7264 | 0.068* | |
| C17 | 0.7943 (5) | 0.5379 (4) | 0.7989 (3) | 0.0569 (14) | |
| H17 | 0.8493 | 0.5277 | 0.8425 | 0.068* | |
| C18 | 0.6508 (4) | 0.5737 (3) | 0.8037 (3) | 0.0446 (11) | |
| H18 | 0.6089 | 0.5880 | 0.8503 | 0.054* | |
| C19 | 0.3403 (5) | 0.7009 (3) | 0.8260 (2) | 0.0352 (9) | |
| H19 | 0.3655 | 0.6618 | 0.8713 | 0.042* | |
| C20 | 0.4348 (6) | 0.7974 (3) | 0.8257 (3) | 0.0538 (13) | |
| H20A | 0.4054 | 0.8408 | 0.7847 | 0.081* | |
| H20B | 0.5365 | 0.7789 | 0.8198 | 0.081* | |
| H20C | 0.4220 | 0.8334 | 0.8724 | 0.081* | |
| C21 | 0.1779 (5) | 0.7266 (4) | 0.8303 (3) | 0.0530 (12) | |
| H21A | 0.1593 | 0.7669 | 0.8745 | 0.079* | |
| H21B | 0.1216 | 0.6644 | 0.8327 | 0.079* | |
| H21C | 0.1498 | 0.7648 | 0.7864 | 0.079* | |
| O1 | 0.4288 (9) | 0.4940 (6) | 0.5103 (4) | 0.0650 (19) | 0.50 |
| H1O1 | 0.3405 | 0.4745 | 0.5027 | 0.097* | 0.50 |
| H2O1 | 0.4722 | 0.4469 | 0.4855 | 0.097* | 0.50 |
| O2 | 0.6608 (8) | 0.3426 (5) | 0.4736 (4) | 0.0566 (18) | 0.50 |
| H1O2 | 0.6370 | 0.2797 | 0.4777 | 0.085* | 0.50 |
| H2O2 | 0.7522 | 0.3365 | 0.4835 | 0.085* | 0.50 |
| P1 | 0.37744 (10) | 0.61951 (7) | 0.74506 (6) | 0.0269 (2) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0904 (5) | 0.0823 (4) | 0.0433 (3) | 0.0170 (3) | −0.0098 (3) | 0.0009 (3) |
| C1 | 0.0245 (18) | 0.0290 (17) | 0.042 (2) | 0.0013 (15) | 0.0014 (18) | 0.0014 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.054 (3) | 0.039 (2) | 0.047 (3) | −0.008 (2) | 0.000 (2) | 0.005 (2) |
| C3 | 0.062 (3) | 0.048 (3) | 0.061 (3) | −0.016 (3) | 0.000 (3) | 0.019 (2) |
| C4 | 0.035 (3) | 0.032 (2) | 0.084 (4) | −0.0057 (18) | −0.004 (2) | 0.004 (2) |
| C5 | 0.035 (2) | 0.035 (2) | 0.068 (3) | −0.001 (2) | −0.006 (2) | −0.018 (2) |
| C6 | 0.033 (2) | 0.037 (2) | 0.041 (2) | 0.0025 (18) | 0.0034 (18) | −0.0061 (18) |
| C7 | 0.033 (2) | 0.032 (2) | 0.036 (2) | 0.0060 (17) | 0.0020 (18) | 0.0009 (17) |
| C8 | 0.059 (3) | 0.040 (2) | 0.049 (3) | 0.000 (2) | 0.006 (2) | 0.006 (2) |
| C9 | 0.111 (5) | 0.050 (3) | 0.061 (4) | 0.020 (3) | 0.026 (4) | 0.021 (3) |
| C10 | 0.125 (6) | 0.077 (4) | 0.042 (3) | 0.043 (4) | −0.001 (4) | 0.021 (3) |
| C11 | 0.071 (4) | 0.110 (5) | 0.045 (3) | 0.026 (4) | −0.017 (3) | 0.006 (3) |
| C12 | 0.043 (3) | 0.064 (3) | 0.043 (3) | 0.014 (2) | −0.006 (2) | 0.005 (2) |
| C13 | 0.0247 (17) | 0.0274 (17) | 0.042 (2) | 0.0007 (14) | 0.0065 (16) | −0.0011 (17) |
| C14 | 0.041 (2) | 0.036 (2) | 0.053 (3) | 0.000 (2) | 0.009 (2) | −0.0011 (19) |
| C15 | 0.041 (3) | 0.042 (3) | 0.079 (4) | 0.000 (2) | 0.028 (3) | −0.007 (3) |
| C16 | 0.029 (2) | 0.038 (2) | 0.104 (5) | 0.0034 (19) | 0.016 (3) | 0.006 (3) |
| C17 | 0.035 (3) | 0.053 (3) | 0.083 (4) | 0.003 (2) | −0.007 (3) | 0.016 (3) |
| C18 | 0.030 (2) | 0.049 (3) | 0.055 (3) | 0.006 (2) | 0.0002 (19) | 0.004 (2) |
| C19 | 0.037 (2) | 0.032 (2) | 0.036 (2) | 0.0005 (17) | 0.0023 (18) | −0.0023 (16) |
| C20 | 0.053 (3) | 0.037 (2) | 0.071 (3) | −0.009 (2) | 0.008 (3) | −0.010 (2) |
| C21 | 0.036 (2) | 0.061 (3) | 0.061 (3) | 0.009 (2) | 0.006 (2) | −0.012 (2) |
| O1 | 0.072 (5) | 0.077 (5) | 0.045 (4) | −0.015 (4) | −0.011 (4) | 0.001 (3) |
| O2 | 0.062 (4) | 0.059 (4) | 0.049 (4) | −0.009 (3) | 0.008 (3) | 0.013 (3) |
| P1 | 0.0222 (4) | 0.0273 (4) | 0.0313 (5) | 0.0001 (4) | 0.0016 (4) | 0.0009 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.395 (6) | C13—C18 | 1.387 (6) |
| C1—C6 | 1.402 (6) | C13—P1 | 1.806 (4) |
| C1—P1 | 1.800 (4) | C14—C15 | 1.400 (6) |
| C2—C3 | 1.394 (6) | C14—H14 | 0.9300 |
| C2—H2 | 0.9300 | C15—C16 | 1.363 (8) |
| C3—C4 | 1.355 (7) | C15—H15 | 0.9300 |
| C3—H3 | 0.9300 | C16—C17 | 1.381 (8) |
| C4—C5 | 1.384 (7) | C16—H16 | 0.9300 |
| C4—H4 | 0.9300 | C17—C18 | 1.386 (6) |
| C5—C6 | 1.387 (6) | C17—H17 | 0.9300 |
| C5—H5 | 0.9300 | C18—H18 | 0.9300 |
| C6—H6 | 0.9300 | C19—C21 | 1.514 (6) |
| C7—C12 | 1.388 (6) | C19—C20 | 1.523 (6) |
| C7—C8 | 1.400 (6) | C19—P1 | 1.818 (4) |
| C7—P1 | 1.789 (4) | C19—H19 | 0.9800 |
| C8—C9 | 1.374 (7) | C20—H20A | 0.9600 |
| C8—H8 | 0.9300 | C20—H20B | 0.9600 |
| C9—C10 | 1.394 (10) | C20—H20C | 0.9600 |
| C9—H9 | 0.9300 | C21—H21A | 0.9600 |
| C10—C11 | 1.345 (10) | C21—H21B | 0.9600 |
| C10—H10 | 0.9300 | C21—H21C | 0.9600 |
| C11—C12 | 1.377 (7) | O1—H1O1 | 0.8522 |

| | | | |
|---|---|---|---|
| C11—H11 | 0.9300 | O1—H2O1 | 0.8527 |
| C12—H12 | 0.9300 | O2—H1O2 | 0.8515 |
| C13—C14 | 1.382 (6) | O2—H2O2 | 0.8512 |
| | | | |
| C2—C1—C6 | 119.4 (4) | C13—C14—H14 | 120.7 |
| C2—C1—P1 | 119.2 (3) | C15—C14—H14 | 120.7 |
| C6—C1—P1 | 121.1 (3) | C16—C15—C14 | 120.2 (5) |
| C3—C2—C1 | 119.7 (5) | C16—C15—H15 | 119.9 |
| C3—C2—H2 | 120.2 | C14—C15—H15 | 119.9 |
| C1—C2—H2 | 120.2 | C15—C16—C17 | 121.1 (4) |
| C4—C3—C2 | 120.2 (5) | C15—C16—H16 | 119.5 |
| C4—C3—H3 | 119.9 | C17—C16—H16 | 119.5 |
| C2—C3—H3 | 119.9 | C16—C17—C18 | 119.7 (5) |
| C3—C4—C5 | 121.4 (4) | C16—C17—H17 | 120.1 |
| C3—C4—H4 | 119.3 | C18—C17—H17 | 120.1 |
| C5—C4—H4 | 119.3 | C17—C18—C13 | 119.2 (5) |
| C4—C5—C6 | 119.5 (4) | C17—C18—H18 | 120.4 |
| C4—C5—H5 | 120.2 | C13—C18—H18 | 120.4 |
| C6—C5—H5 | 120.2 | C21—C19—C20 | 111.4 (4) |
| C5—C6—C1 | 119.8 (4) | C21—C19—P1 | 110.5 (3) |
| C5—C6—H6 | 120.1 | C20—C19—P1 | 112.1 (3) |
| C1—C6—H6 | 120.1 | C21—C19—H19 | 107.6 |
| C12—C7—C8 | 118.9 (4) | C20—C19—H19 | 107.6 |
| C12—C7—P1 | 122.0 (3) | P1—C19—H19 | 107.6 |
| C8—C7—P1 | 118.7 (3) | C19—C20—H20A | 109.5 |
| C9—C8—C7 | 120.8 (5) | C19—C20—H20B | 109.5 |
| C9—C8—H8 | 119.6 | H20A—C20—H20B | 109.5 |
| C7—C8—H8 | 119.6 | C19—C20—H20C | 109.5 |
| C8—C9—C10 | 118.7 (6) | H20A—C20—H20C | 109.5 |
| C8—C9—H9 | 120.7 | H20B—C20—H20C | 109.5 |
| C10—C9—H9 | 120.7 | C19—C21—H21A | 109.5 |
| C11—C10—C9 | 120.9 (5) | C19—C21—H21B | 109.5 |
| C11—C10—H10 | 119.6 | H21A—C21—H21B | 109.5 |
| C9—C10—H10 | 119.6 | C19—C21—H21C | 109.5 |
| C10—C11—C12 | 121.1 (6) | H21A—C21—H21C | 109.5 |
| C10—C11—H11 | 119.4 | H21B—C21—H21C | 109.5 |
| C12—C11—H11 | 119.4 | H1O1—O1—H2O1 | 98.0 |
| C11—C12—C7 | 119.6 (5) | H1O2—O2—H2O2 | 98.0 |
| C11—C12—H12 | 120.2 | C7—P1—C1 | 112.38 (19) |
| C7—C12—H12 | 120.2 | C7—P1—C13 | 109.67 (19) |
| C14—C13—C18 | 121.2 (4) | C1—P1—C13 | 106.56 (17) |
| C14—C13—P1 | 119.5 (3) | C7—P1—C19 | 107.68 (18) |
| C18—C13—P1 | 118.8 (3) | C1—P1—C19 | 108.99 (19) |
| C13—C14—C15 | 118.6 (5) | C13—P1—C19 | 111.62 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*O*1···Br1$^{i}$ | 0.85 | 2.86 | 3.701 (8) | 169 |
| O1—H2*O*1···O2 | 0.85 | 2.20 | 2.960 (11) | 149 |
| O2—H1*O*2···Br1$^{ii}$ | 0.85 | 2.68 | 3.526 (7) | 175 |
| O2—H2*O*2···Br1$^{iii}$ | 0.85 | 2.81 | 3.598 (8) | 154 |
| C19—H19···Br1$^{iv}$ | 0.98 | 2.76 | 3.723 (4) | 169 |

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