# r-2,c-6-Bis(4-bromophenyl)-t-3,t-5-dimethyltetrahydropyran-4-one

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In the title compound, $C_{19}H_{18}Br_2O_2$, the tetrahydropyran ring has a chair conformation with an equatorial disposition of all the methyl and *p*-bromophenyl groups. The structure is stabilized by intermolecular C—H···O, C—H···$\pi$ and Br···Br interactions [Br···Br = 3.4756 (9) Å], forming a zigzag layer arrangement.

## Related literature

For related literature, see: Baliah & Mangalam (1978); Belakhov *et al.* (2002); Eliel (1962); Japp & Maitland (1904); Jose Kavitha *et al.* (2003); Krishnamoorthy *et al.* (2003); Kumar *et al.* (1999); Noller (1966); Ray *et al.* (1998); Usman *et al.* (2002).
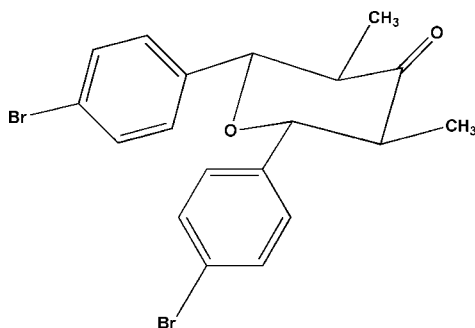


## Experimental

### Crystal data

| | |
|---|---|
| $C_{19}H_{18}Br_2O_2$ | $V = 3626.6$ (12) Å$^3$ |
| $M_r = 438.15$ | $Z = 8$ |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a = 15.146$ (3) Å | $\mu = 4.48$ mm$^{-1}$ |
| $b = 9.1460$ (18) Å | $T = 297$ (2) K |
| $c = 26.180$ (5) Å | $0.22 \times 0.20 \times 0.19$ mm |

### Data collection

| | |
|---|---|
| Bruker Kappa-APEXII CCD area-detector diffractometer | 38553 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 1999) | 3450 independent reflections |
| $T_{min} = 0.439$, $T_{max} = 0.483$ | 2171 reflections with $I > 2\sigma(I)$ |
| (expected range = 0.388–0.427) | $R_{int} = 0.047$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | 210 parameters |
| $wR(F^2) = 0.094$ | H-atom parameters constrained |
| $S = 1.05$ | $\Delta\rho_{max} = 0.62$ e Å$^{-3}$ |
| 3450 reflections | $\Delta\rho_{min} = -0.41$ e Å$^{-3}$ |

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

*Cg* is the centroid of the C12–C17 ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|---|---|---|---|
| C4—H4···$Cg$[i] | 0.98 | 2.77 | 3.687 | 156 |
| C14—H14···O1[ii] | 0.93 | 2.68 | 3.403 (5) | 136 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2166).

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**supplementary materials**

## *r*-2,*c*-6-Bis(4-bromophenyl)-*t*-3,*t*-5-dimethyltetrahydropyran-4-one

### P. Parthiban, S. Umamatheswari, A. Doddi, V. Ramkumar and S. Kabilan

### Comment

Pyran-4-one derivatives are very important, naturally available and biologically active six-membered heterocyclic compounds (Noller, 1966). Japp and Maitland were the first to report the synthesis of several substituted tetrahydropyran derivatives (Japp & Maitland, 1904). While reviewing the literature, depending upon the number and nature of the substituents and the level of unsaturation, different conformations are reported for the six-membered heterocyclic ring, namely, sofa (Ray *et al.*, 1998), planar (Kumar *et al.*, 1999), chair (Belakhov *et al.*, 2002; Krishnamoorthy *et al.*, 2003; Jose Kavitha *et al.*, 2003) or twist boat (Usman *et al.*, 2002). Moreover, the synthesized compound contains two pairs of chiral carbons with identical groups on each. According to Eliel, there can be four racemic and two *meso* forms (Eliel, 1962).

In the title compound $C_{19}H_{18}Br_2O_2$, as shown in Fig. 1, the tetrahydropyran ring adopts a chair conformation. Both the methyl groups and *p*-Br phenyl rings occupy equatorial positions. Similar kinds of compounds with *p*-Cl or *p*-CH$_3$ substituents reported earlier exist in the chair conformation with equatorial orientations of all the phenyl and methyl groups. The absolute configuration of the chiral atoms C1, C2, C4 and C5 are *S*, *R*, *S* and *R*, respectively.

The crystal structure is stabilized by intermolecular C—H⋯O, C—H⋯π and Br⋯Br interactions. These contacts facilitate the formation of a zigzag network extendend over the *ac* plane. In the crystal structure the adjacent layers are linked through C—H⋯π interactions, *viz*. C4—H4⋯$Cg^i$ with H4⋯$Cg^i$ = 2.766 Å, C4⋯$Cg^i$ = 3.687 Å and C4—H4⋯$Cg^i$ = 156°, where $Cg^i$ denotes the centroid of the C12–C17 aryl ring of the molecule (symmetry code: i = 2 − *x*, 1/2 + *y*, 3/2 − *z*).

The molecules are also held together by C—H⋯O interactions between C14 and O1$^{ii}$ of 3.403 (5) Å, C14—H14⋯O1$^{ii}$ = 136°, symmetry code: ii = 1/2 + *x*, *y*, 3/2 − *z*. A short contact is also seen between Br1⋯Br2$^{iii}$ (3.4756 (9) Å, symmetry code: iii = 5/2 − *x*,-*y*,-1/2 + *z*).

### Experimental

The title compound was obtained by the condensation of pentan-3-one and *p*-bromo benzaldehyde in a 1:2 molar ratio in ethanol by adopting the literature procedure for similar types of compounds (Baliah & Mangalam, 1978). Diffraction quality crystals were obtained by recrystallization of the obtained compound in ethanol.

### Refinement

All the hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms, with aromatic C—H = 0.93 Å, aliphatic C—H = 0.98 Å and methyl C—H = 0.96 Å. The displacement parameters were set for phenyl and aliphatic H atoms at $U_{iso}(H) = 1.2U_{eq}(C)$ and for methyl H atoms at $1.5U_{eq}(C)$.

# supplementary materials

**Figures**
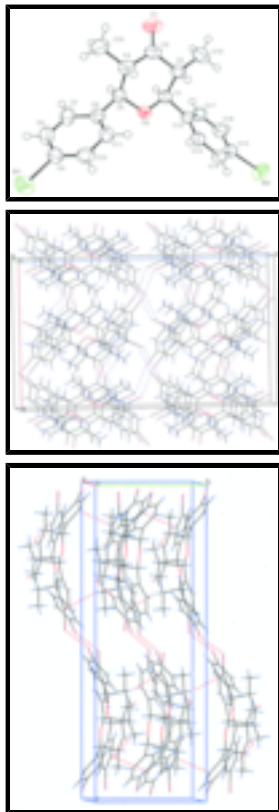




Fig. 1. *ORTEP* of the molecule with atoms represented as 50% probability ellipsoids.



**r-2,c-6-Bis(4-bromophenyl)-t-3,t-5-dimethyltetrahydropyran-4-one**

*Crystal data*

| | |
|---|---|
| $C_{19}H_{18}Br_2O_2$ | $F_{000} = 1744$ |
| $M_r = 438.15$ | $D_x = 1.605$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 5214 reflections |
| $a = 15.146$ (3) Å | $\theta = 2.1–26.0º$ |
| $b = 9.1460$ (18) Å | $\mu = 4.48$ mm$^{-1}$ |
| $c = 26.180$ (5) Å | $T = 297$ (2) K |
| $V = 3626.6$ (12) Å$^3$ | Rectangular, colourless |
| $Z = 8$ | $0.22 \times 0.20 \times 0.19$ mm |

*Data collection*

| | |
|---|---|
| Bruker Kappa-APEXII CCD area-detector diffractometer | 3450 independent reflections |
| Radiation source: fine-focus sealed tube | 2171 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.047$ |

| | |
|---|---|
| $T = 297(2)$ K | $\theta_{max} = 26.0°$ |
| $\varphi$ and $\omega$ scans | $\theta_{min} = 2.1°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 1999) | $h = -17 \rightarrow 17$ |
| $T_{min} = 0.439$, $T_{max} = 0.483$ | $k = -10 \rightarrow 10$ |
| 38553 measured reflections | $l = -32 \rightarrow 29$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | H-atom parameters constrained |
| $wR(F^2) = 0.094$ | $w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 4.4775P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 3450 reflections | $\Delta\rho_{max} = 0.62$ e Å$^{-3}$ |
| 210 parameters | $\Delta\rho_{min} = -0.41$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Br1 | 1.23772 (3) | 0.02246 (7) | 0.981200 (17) | 0.0872 (2) |
| Br2 | 1.08186 (3) | 0.16048 (6) | 0.532667 (17) | 0.08003 (19) |
| C1 | 0.9071 (2) | 0.1921 (4) | 0.74443 (12) | 0.0387 (8) |
| H1 | 0.8595 | 0.1200 | 0.7473 | 0.046* |
| C2 | 0.8682 (2) | 0.3470 (4) | 0.75042 (13) | 0.0460 (9) |
| H2 | 0.9174 | 0.4165 | 0.7488 | 0.055* |
| C3 | 0.8285 (2) | 0.3578 (4) | 0.80309 (14) | 0.0484 (9) |
| C4 | 0.8888 (2) | 0.3119 (4) | 0.84640 (13) | 0.0459 (9) |
| H4 | 0.9356 | 0.3856 | 0.8489 | 0.055* |
| C5 | 0.9333 (2) | 0.1659 (4) | 0.83367 (12) | 0.0402 (8) |
| H5 | 0.8891 | 0.0879 | 0.8357 | 0.048* |
| C6 | 1.0073 (2) | 0.1311 (4) | 0.86997 (12) | 0.0407 (8) |

| | | | | |
|------|--------------|--------------|--------------|--------------|
| C7 | 0.9971 (3) | 0.0304 (4) | 0.90867 (13) | 0.0518 (10) |
| H7 | 0.9431 | −0.0168 | 0.9125 | 0.062* |
| C8 | 1.0649 (3) | −0.0019 (4) | 0.94173 (14) | 0.0592 (11) |
| H8 | 1.0572 | −0.0709 | 0.9675 | 0.071* |
| C9 | 1.1438 (3) | 0.0689 (5) | 0.93619 (13) | 0.0532 (10) |
| C10 | 1.1559 (2) | 0.1721 (4) | 0.89904 (14) | 0.0550 (10) |
| H10 | 1.2094 | 0.2212 | 0.8962 | 0.066* |
| C11 | 1.0871 (2) | 0.2026 (4) | 0.86575 (14) | 0.0496 (9) |
| H11 | 1.0950 | 0.2722 | 0.8402 | 0.059* |
| C12 | 0.9531 (2) | 0.1727 (4) | 0.69389 (12) | 0.0384 (8) |
| C13 | 1.0388 (2) | 0.2201 (4) | 0.68676 (14) | 0.0463 (9) |
| H13 | 1.0703 | 0.2579 | 0.7143 | 0.056* |
| C14 | 1.0784 (2) | 0.2121 (4) | 0.63948 (15) | 0.0512 (10) |
| H14 | 1.1362 | 0.2437 | 0.6350 | 0.061* |
| C15 | 1.0313 (3) | 0.1570 (4) | 0.59899 (14) | 0.0502 (10) |
| C16 | 0.9471 (3) | 0.1062 (4) | 0.60490 (14) | 0.0509 (10) |
| H16 | 0.9163 | 0.0677 | 0.5773 | 0.061* |
| C17 | 0.9086 (2) | 0.1129 (4) | 0.65277 (13) | 0.0458 (9) |
| H17 | 0.8518 | 0.0766 | 0.6574 | 0.055* |
| C18 | 0.8418 (3) | 0.3087 (5) | 0.89754 (15) | 0.0745 (13) |
| H18A | 0.8107 | 0.3990 | 0.9025 | 0.112* |
| H18B | 0.8843 | 0.2960 | 0.9244 | 0.112* |
| H18C | 0.8006 | 0.2289 | 0.8981 | 0.112* |
| C19 | 0.8032 (3) | 0.3881 (5) | 0.70866 (16) | 0.0738 (13) |
| H19A | 0.7555 | 0.3189 | 0.7082 | 0.111* |
| H19B | 0.8327 | 0.3873 | 0.6762 | 0.111* |
| H19C | 0.7802 | 0.4841 | 0.7152 | 0.111* |
| O1 | 0.75334 (19) | 0.3972 (4) | 0.81016 (11) | 0.0765 (9) |
| O2 | 0.97028 (14) | 0.1662 (2) | 0.78362 (8) | 0.0409 (6) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| Br1 | 0.0670 (3) | 0.1321 (5) | 0.0623 (3) | 0.0304 (3) | −0.0187 (2) | 0.0014 (3) |
| Br2 | 0.0892 (4) | 0.0904 (4) | 0.0605 (3) | 0.0113 (3) | 0.0319 (2) | 0.0005 (2) |
| C1 | 0.0311 (19) | 0.043 (2) | 0.0426 (19) | −0.0031 (16) | −0.0013 (15) | 0.0015 (16) |
| C2 | 0.036 (2) | 0.047 (2) | 0.055 (2) | 0.0024 (17) | 0.0000 (17) | 0.0033 (19) |
| C3 | 0.034 (2) | 0.049 (2) | 0.062 (2) | 0.0027 (18) | 0.0028 (17) | −0.0037 (18) |
| C4 | 0.039 (2) | 0.050 (2) | 0.050 (2) | 0.0006 (18) | 0.0024 (16) | −0.0097 (17) |
| C5 | 0.036 (2) | 0.044 (2) | 0.0406 (19) | −0.0080 (17) | 0.0015 (15) | 0.0008 (16) |
| C6 | 0.045 (2) | 0.039 (2) | 0.0380 (18) | −0.0010 (17) | −0.0004 (16) | −0.0036 (17) |
| C7 | 0.054 (2) | 0.054 (2) | 0.048 (2) | −0.013 (2) | −0.0010 (18) | 0.0052 (19) |
| C8 | 0.069 (3) | 0.066 (3) | 0.043 (2) | 0.004 (2) | −0.001 (2) | 0.0091 (19) |
| C9 | 0.054 (3) | 0.068 (3) | 0.037 (2) | 0.015 (2) | −0.0064 (18) | −0.008 (2) |
| C10 | 0.036 (2) | 0.068 (3) | 0.062 (2) | −0.001 (2) | −0.0012 (18) | −0.001 (2) |
| C11 | 0.043 (2) | 0.055 (2) | 0.050 (2) | −0.003 (2) | 0.0003 (18) | 0.0107 (18) |
| C12 | 0.0322 (19) | 0.038 (2) | 0.0447 (19) | 0.0023 (16) | −0.0010 (15) | 0.0031 (16) |
| C13 | 0.035 (2) | 0.054 (2) | 0.050 (2) | −0.0040 (18) | −0.0035 (17) | 0.0031 (18) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C14 | 0.033 (2) | 0.058 (2) | 0.063 (3) | −0.0003 (19) | 0.0070 (19) | 0.007 (2) |
| C15 | 0.049 (2) | 0.050 (2) | 0.051 (2) | 0.011 (2) | 0.0112 (18) | 0.0035 (19) |
| C16 | 0.054 (3) | 0.053 (2) | 0.046 (2) | 0.003 (2) | −0.0053 (18) | −0.0061 (18) |
| C17 | 0.036 (2) | 0.053 (2) | 0.048 (2) | −0.0065 (18) | 0.0000 (16) | −0.0035 (18) |
| C18 | 0.061 (3) | 0.107 (4) | 0.055 (2) | 0.019 (3) | 0.010 (2) | −0.011 (2) |
| C19 | 0.068 (3) | 0.087 (3) | 0.066 (3) | 0.032 (3) | −0.006 (2) | 0.008 (2) |
| O1 | 0.0427 (17) | 0.108 (3) | 0.0783 (19) | 0.0243 (17) | 0.0096 (15) | 0.0015 (18) |
| O2 | 0.0334 (13) | 0.0489 (15) | 0.0403 (12) | 0.0071 (11) | −0.0021 (10) | −0.0006 (11) |

*Geometric parameters (Å, °)*

| | | | |
|-----------|-----------|-------------|-----------|
| Br1—C9 | 1.895 (4) | C8—H8 | 0.9300 |
| Br2—C15 | 1.898 (3) | C9—C10 | 1.368 (5) |
| C1—O2 | 1.422 (4) | C10—C11 | 1.386 (5) |
| C1—C12 | 1.505 (5) | C10—H10 | 0.9300 |
| C1—C2 | 1.543 (5) | C11—H11 | 0.9300 |
| C1—H1 | 0.9800 | C12—C13 | 1.382 (5) |
| C2—C3 | 1.508 (5) | C12—C17 | 1.382 (5) |
| C2—C19 | 1.519 (5) | C13—C14 | 1.377 (5) |
| C2—H2 | 0.9800 | C13—H13 | 0.9300 |
| C3—O1 | 1.208 (4) | C14—C15 | 1.373 (5) |
| C3—C4 | 1.515 (5) | C14—H14 | 0.9300 |
| C4—C18 | 1.516 (5) | C15—C16 | 1.366 (5) |
| C4—C5 | 1.533 (5) | C16—C17 | 1.384 (5) |
| C4—H4 | 0.9800 | C16—H16 | 0.9300 |
| C5—O2 | 1.425 (4) | C17—H17 | 0.9300 |
| C5—C6 | 1.503 (5) | C18—H18A | 0.9600 |
| C5—H5 | 0.9800 | C18—H18B | 0.9600 |
| C6—C7 | 1.378 (5) | C18—H18C | 0.9600 |
| C6—C11 | 1.379 (5) | C19—H19A | 0.9600 |
| C7—C8 | 1.375 (5) | C19—H19B | 0.9600 |
| C7—H7 | 0.9300 | C19—H19C | 0.9600 |
| C8—C9 | 1.368 (6) | | |
| O2—C1—C12 | 107.7 (3) | C8—C9—Br1 | 118.9 (3) |
| O2—C1—C2 | 109.7 (3) | C9—C10—C11 | 119.1 (4) |
| C12—C1—C2 | 112.0 (3) | C9—C10—H10 | 120.5 |
| O2—C1—H1 | 109.2 | C11—C10—H10 | 120.5 |
| C12—C1—H1 | 109.2 | C6—C11—C10 | 120.8 (3) |
| C2—C1—H1 | 109.2 | C6—C11—H11 | 119.6 |
| C3—C2—C19 | 112.6 (3) | C10—C11—H11 | 119.6 |
| C3—C2—C1 | 107.8 (3) | C13—C12—C17 | 118.5 (3) |
| C19—C2—C1 | 113.7 (3) | C13—C12—C1 | 121.1 (3) |
| C3—C2—H2 | 107.5 | C17—C12—C1 | 120.4 (3) |
| C19—C2—H2 | 107.5 | C14—C13—C12 | 120.9 (3) |
| C1—C2—H2 | 107.5 | C14—C13—H13 | 119.5 |
| O1—C3—C2 | 122.4 (3) | C12—C13—H13 | 119.5 |
| O1—C3—C4 | 122.4 (3) | C15—C14—C13 | 119.2 (3) |
| C2—C3—C4 | 115.2 (3) | C15—C14—H14 | 120.4 |
| C3—C4—C18 | 112.6 (3) | C13—C14—H14 | 120.4 |

| | | | |
|---|---|---|---|
| C3—C4—C5 | 110.1 (3) | C16—C15—C14 | 121.5 (3) |
| C18—C4—C5 | 112.4 (3) | C16—C15—Br2 | 119.1 (3) |
| C3—C4—H4 | 107.1 | C14—C15—Br2 | 119.4 (3) |
| C18—C4—H4 | 107.1 | C15—C16—C17 | 118.7 (3) |
| C5—C4—H4 | 107.1 | C15—C16—H16 | 120.6 |
| O2—C5—C6 | 106.8 (3) | C17—C16—H16 | 120.6 |
| O2—C5—C4 | 111.8 (3) | C12—C17—C16 | 121.2 (3) |
| C6—C5—C4 | 112.0 (3) | C12—C17—H17 | 119.4 |
| O2—C5—H5 | 108.7 | C16—C17—H17 | 119.4 |
| C6—C5—H5 | 108.7 | C4—C18—H18A | 109.5 |
| C4—C5—H5 | 108.7 | C4—C18—H18B | 109.5 |
| C7—C6—C11 | 118.3 (3) | H18A—C18—H18B | 109.5 |
| C7—C6—C5 | 121.5 (3) | C4—C18—H18C | 109.5 |
| C11—C6—C5 | 120.2 (3) | H18A—C18—H18C | 109.5 |
| C8—C7—C6 | 121.5 (4) | H18B—C18—H18C | 109.5 |
| C8—C7—H7 | 119.3 | C2—C19—H19A | 109.5 |
| C6—C7—H7 | 119.3 | C2—C19—H19B | 109.5 |
| C9—C8—C7 | 119.0 (4) | H19A—C19—H19B | 109.5 |
| C9—C8—H8 | 120.5 | C2—C19—H19C | 109.5 |
| C7—C8—H8 | 120.5 | H19A—C19—H19C | 109.5 |
| C10—C9—C8 | 121.3 (3) | H19B—C19—H19C | 109.5 |
| C10—C9—Br1 | 119.8 (3) | C1—O2—C5 | 113.6 (2) |
| | | | |
| O2—C1—C2—C3 | −57.3 (3) | C7—C8—C9—Br1 | −179.2 (3) |
| C12—C1—C2—C3 | −176.8 (3) | C8—C9—C10—C11 | −1.5 (6) |
| O2—C1—C2—C19 | 177.1 (3) | Br1—C9—C10—C11 | 178.7 (3) |
| C12—C1—C2—C19 | 57.7 (4) | C7—C6—C11—C10 | 1.1 (5) |
| C19—C2—C3—O1 | −0.9 (5) | C5—C6—C11—C10 | 179.8 (3) |
| C1—C2—C3—O1 | −127.2 (4) | C9—C10—C11—C6 | 0.5 (6) |
| C19—C2—C3—C4 | 177.5 (3) | O2—C1—C12—C13 | −38.4 (4) |
| C1—C2—C3—C4 | 51.3 (4) | C2—C1—C12—C13 | 82.2 (4) |
| O1—C3—C4—C18 | 5.0 (5) | O2—C1—C12—C17 | 144.6 (3) |
| C2—C3—C4—C18 | −173.4 (3) | C2—C1—C12—C17 | −94.8 (4) |
| O1—C3—C4—C5 | 131.3 (4) | C17—C12—C13—C14 | 1.9 (5) |
| C2—C3—C4—C5 | −47.1 (4) | C1—C12—C13—C14 | −175.1 (3) |
| C3—C4—C5—O2 | 48.3 (4) | C12—C13—C14—C15 | 0.4 (6) |
| C18—C4—C5—O2 | 174.7 (3) | C13—C14—C15—C16 | −1.9 (6) |
| C3—C4—C5—C6 | 168.1 (3) | C13—C14—C15—Br2 | 174.9 (3) |
| C18—C4—C5—C6 | −65.5 (4) | C14—C15—C16—C17 | 1.0 (6) |
| O2—C5—C6—C7 | −134.4 (3) | Br2—C15—C16—C17 | −175.8 (3) |
| C4—C5—C6—C7 | 103.0 (4) | C13—C12—C17—C16 | −2.8 (5) |
| O2—C5—C6—C11 | 47.0 (4) | C1—C12—C17—C16 | 174.2 (3) |
| C4—C5—C6—C11 | −75.7 (4) | C15—C16—C17—C12 | 1.4 (6) |
| C11—C6—C7—C8 | −1.7 (6) | C12—C1—O2—C5 | −173.8 (3) |
| C5—C6—C7—C8 | 179.7 (3) | C2—C1—O2—C5 | 64.2 (3) |
| C6—C7—C8—C9 | 0.7 (6) | C6—C5—O2—C1 | 177.7 (3) |
| C7—C8—C9—C10 | 1.0 (6) | C4—C5—O2—C1 | −59.5 (3) |

*Hydrogen-bond geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
| --- | --- | --- | --- | --- |
| C4—H4···Cg[i] | 0.98 | 2.77 | 3.687 | 156 |
| C14—H14···O1[ii] | 0.93 | 2.68 | 3.403 (5) | 136 |

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

**Fig. 1**

**Fig. 2**

**Fig. 3**