# organic compounds

# Bicyclo[2.2.1]hept-7-yl *p*-bromobenzoate

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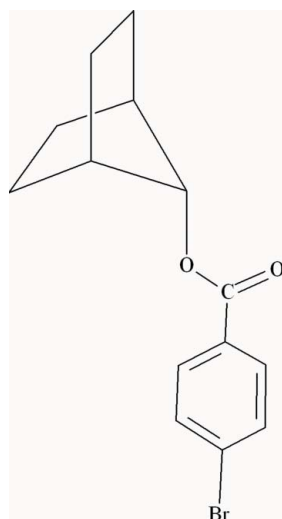Correspondence e-mail: blloyd@weber.edu

The title compound, $C_{14}H_{15}BrO_2$, contains a sterically unencumbered norbornyl group. The dihedral angle between the plane of the carboxylate group and the mean plane of the adjacent benzene ring is 5.3 (2)°. The dihedral angle between the plane of the carboxylate group and the norbornyl methano C—O bond is 4.5 (1)°, the methano C atom deviating by 0.141 (2) Å from this plane. In the crystal, molecules pack as pairs of enantiomers, with a distance of 3.747 (1) Å between the centroids of nearest parallel benzene rings.

## Related literature

For calculated and experimental norbornane and related structures, see: Allinger *et al.* (1989); Pfund *et al.* (1980). For related polycyclic *p*-bromobenzoate structures, see: Lloyd & Arif (2012); Lloyd *et al.* (1995, 2000). For a high resolution low temperature powder synchrotron X-ray diffraction structure of norbornane, see: Fitch & Jobic (1993). For some norbornyl bond lengths and angles, see: Watson *et al.* (1992). For possible C—O bond-length correlation to reactivity in a 7-norbornenyl benzoate, see: Jones *et al.* (1992).



## Experimental

### Crystal data

$C_{14}H_{15}BrO_2$
$M_r = 295.17$
Monoclinic, $P2_1/c$
$a = 11.7401$ (2) Å
$b = 6.3767$ (1) Å
$c = 17.7462$ (3) Å
$\beta = 109.584$ (1)°

$V = 1251.68$ (4) Å$^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.27$ mm$^{-1}$
$T = 150$ K
$0.30 \times 0.25 \times 0.18$ mm

### Data collection

Nonius KappaCCD Diffractometer
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
$T_{min} = 0.440$, $T_{max} = 0.591$

5495 measured reflections
2882 independent reflections
2469 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.055$
$S = 1.03$
2882 reflections

215 parameters
All H-atom parameters refined
$\Delta\rho_{max} = 0.38$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 2012), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

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# supporting information

## Bicyclo[2.2.1]hept-7-yl *p*-bromobenzoate

**Barry A. Lloyd and Atta M. Arif**

### S1. Comment

Many norbornyl structures have been previously determined, but precise bond lengths and angles are derivative dependent (Watson *et al.*, 1992). The Cambridge Crystallographic Database contains only five 7-norbornyl benzoate structures, but these are complicated by additional substituents and their associated steric interactions (for example, see Pfund *et al.*, 1980). An *ORTEP*-3 drawing (Farrugia, 2012) of title compound structure **1** is shown in Fig. 1, and a cell packing diagram is shown in Fig. 2. Structure **1** norbornyl group bond lengths and bond angles agree with reported values, but their precision is about ten times better than geometry averaged values (Watson *et al.*, 1992). Structure **1** was determined so that bond length, bond angle, least-squares plane, and nonbonding contact comparisons could be made with other related *p*-bromobenzoate structures (Lloyd & Arif, 2012, Lloyd *et al.*, 2000 and Lloyd *et al.*, 1995).

No nonhydrogen atom intermolecular contacts exist shorter than van der Waals radii sums, the smallest being O1[i]···C13[ii] at 3.257 (2) Å [symmetry code: (ii) *x*, -1 + *y*, *z*]. Least squares planes are defined as C1—C7—C4 (plane 1), C1—C2—C3—C4 (plane 2), and C1—C6—C5—C4 (plane 3). Interplanar 1:2, 1:3, and 1:4 angles are: 121.2 (1)°, 125.5 (1)°, and 113.3 (1)°, respectively. Angle 1:2 is 1.4° larger than the corresponding 296 K structure **2** (Fig. 3) angle (Lloyd *et al.*, 1995), but smaller than corresponding angles of our other seven norbornenyl structures. Structure **1** angle 1: 3 is larger than analogous angles in all eight norbornenyl structures, and angle 2:3 is smaller for all except structure **3**. Smaller 1:2 and larger 1:3 angles in structure **1** are likely a consequence of a longer C2—C3 norbornyl single bond (*versus* a shorter norbornenyl C2=C3 double bond) which bends C7 toward plane 2. The slightly larger structure **1** 2:3 angle *versus* **3** might result from intramolecular H3B···H5A and H2B···H6A contacts, 2.35 (3) and 2.40 (3) Å, respectively (Lloyd & Arif, 2012). Reactant structural features (such as C7—O2 bond length) that might portend the large norbornenyl: norbornyl solvolytic reactivity ratio are not obvious, and the late transition state idea (Jones *et al.*, 1992) is supported.

### S2. Experimental

7-Norborncyl *p*-bromobenzoate (title compound **1**) was made from commercial bicyclo[2.2.1]heptan-7-ol (7-norborneol, Alfa Products). Under a dry nitrogen atmosphere, 1.06 g freshly distilled (about 300 K, 7 Pa) *p*-bromobenzoyl chloride, 15 ml reagent grade dichloromethane, 0.802 g dry, freshly distilled (from $CaH_2$ under $N_2$) pyridine, and 0.540 g of sublimed (373 K, 7 Pa) 7-norborneol were combined and the mixture was refluxed for 15 min, then stirred for 2 d at 296 K. The reaction mixture was poured into 10 ml of 5% HCl solution, and layers were separated. The dichloromethane layer was washed twice more with 5% HCl solution, the dichloromethane was evaporated, and the residue was dissolved in about 3 ml of ether. The mixture was chromatographed on Florisil (petroleum ether, then ether). Recovered 1.22 g of **1**, 85.3% yield, mp 350–351 K after two recrystallizations from petroleum ether/ether: ¹H NMR ($CDCl_3$, 90 MHz) δ 1.10–1.57 (4 H, m), 1.57–2.09 (4 H, m), 2.31 (2 H, m), 4.99 (1 H, s), 7.57 (2 H, d), 7.88 (2 H, d). Crystals were regrown slowly by dissolving 1.0 g of **1** in 5 ml of anhydrous ether in a 30 ml beaker. The beaker was placed inside a desiccator along with a 20 ml beaker containing 15 ml of petroleum ether (bp 303–333 K), and the desiccator was placed inside a freezer

at 253 K. A one-hole rubber stopper was placed in the desiccator neck with glass wool inserted into the hole, allowing for slow evaporation. Crystals began forming after 3 d and they were filtered out after 5 d. One of these crystals was selected for X-ray analysis.

## S3. Refinement

A colorless prism shaped crystal 0.30 × 0.25 × 0.18 mm in size was mounted on a glass fiber with traces of viscous oil and then transferred to a Nonius KappaCCD diffractometer equipped with Mo K$\alpha$ radiation ($\lambda$ = 0.71073 Å). Ten frames of data were collected at 150 (1) K with an oscillation range of 1 °/frame and an exposure time of 20 sec/frame (Nonius, 1998). Indexing and unit cell refinement based on all observed reflection from those ten frames, indicated a monoclinic **P** lattice. A total of 5495 reflections ($\Theta_{max}$ = 27.48°) were indexed, integrated and corrected for Lorentz, polarization and absorption effects using *DENZO– SMN* and *SCALEPAC* (Otwinowski & Minor, 1997). Post refinement of the unit cell gave a = 11.7401 (2) Å, b = 6.3767 (1) Å, c = 17.7462 (3) Å, $\beta$ =109.584 (1)°, and V = 1251.68 (4) Å$^3$. Axial photographs and systematic absences were consistent with the compound having crystallized in the monoclinic space group **P**2$_1$/c.

The structure was solved by a combination of direct and heavy atom methods using *SIR*97 (Altomare *et al.*, 1999). All of the non-hydrogen atoms were refined with anisotropic displacement coefficients. Hydrogen atoms were located and refined isotropically using *SHELXL97* (Sheldrick, 2008). The weighting scheme employed was w = 1/[$\sigma^2$(F$_o^2$) + (0.0254P)$^2$ + 0.4883P] where P = (F$_o^2$ + 2F$_c^2$) /3. The refinement converged to R1 = 0.0224, wR2 = 0.0527, and S = 1.025 for 2469 reflections with I > 2$\sigma$(I), and R1 = 0.0294, wR2 = 0.0552, and S = 1.025 for 2882 unique reflections and 215 parameters, where R1 = $\Sigma$ (|| F$_o$ | − |F$_c$ ||) / $\Sigma$ |F$_o$|, wR2 = [$\Sigma$($w$(F$_o^2$ − F$_c^2$)2) / $\Sigma$(F$_o^2$)$^2$]$^{1/2}$, and S = Goodness-of-fit on F$^2$ = [$\Sigma$ ($w$(F$_o^2$ − F$_c^2$)$^2$ / (n-p)] $^{1/2}$, n is the number of reflections and p is the number of parameters refined.

The maximum $\Delta/\sigma$ in the final cycle of the least-squares was 0.001, and the residual peaks on the final difference-Fourier map ranged from -0.35 to 0.382 e/Å$^3$. Scattering factors were taken from the International Tables for Crystallography, Volume C, Chapters 4 pp 206–222 and 6 pp 476–516.
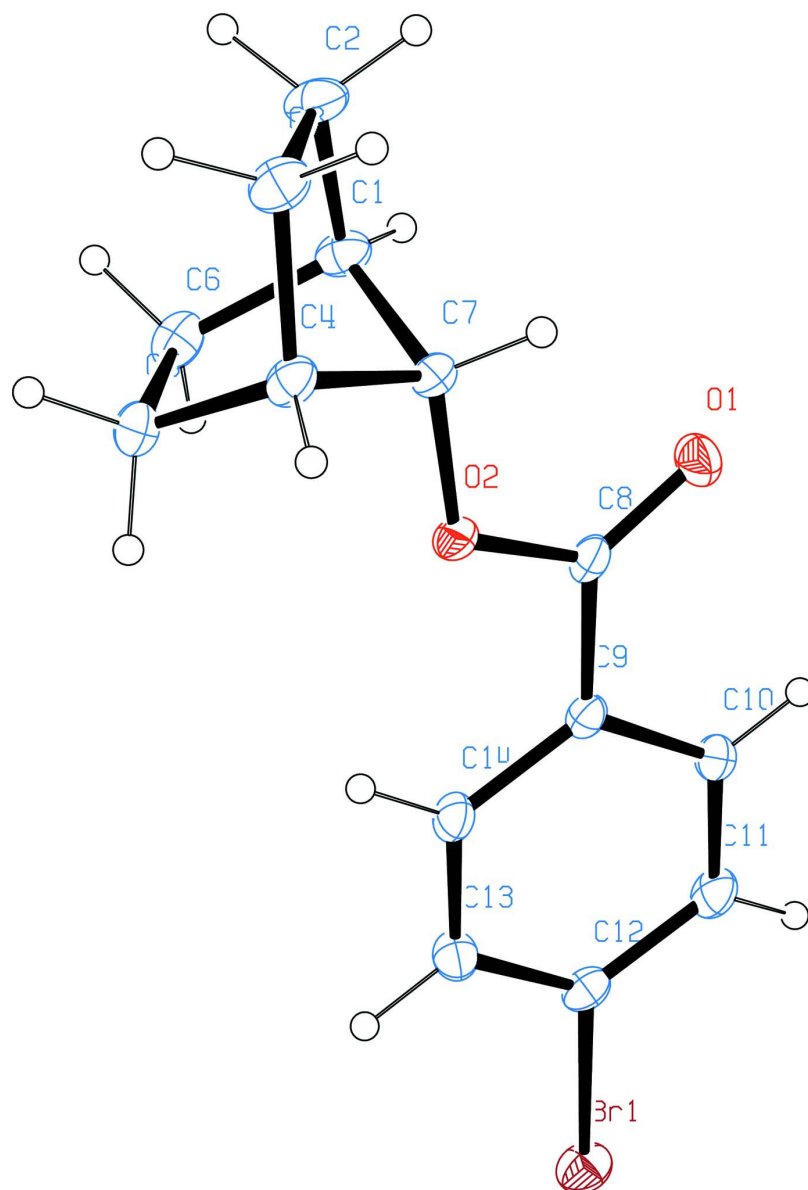
**Figure 1**

*ORTEP-3* drawing of the title compound showing 50% displacement ellipsoids.
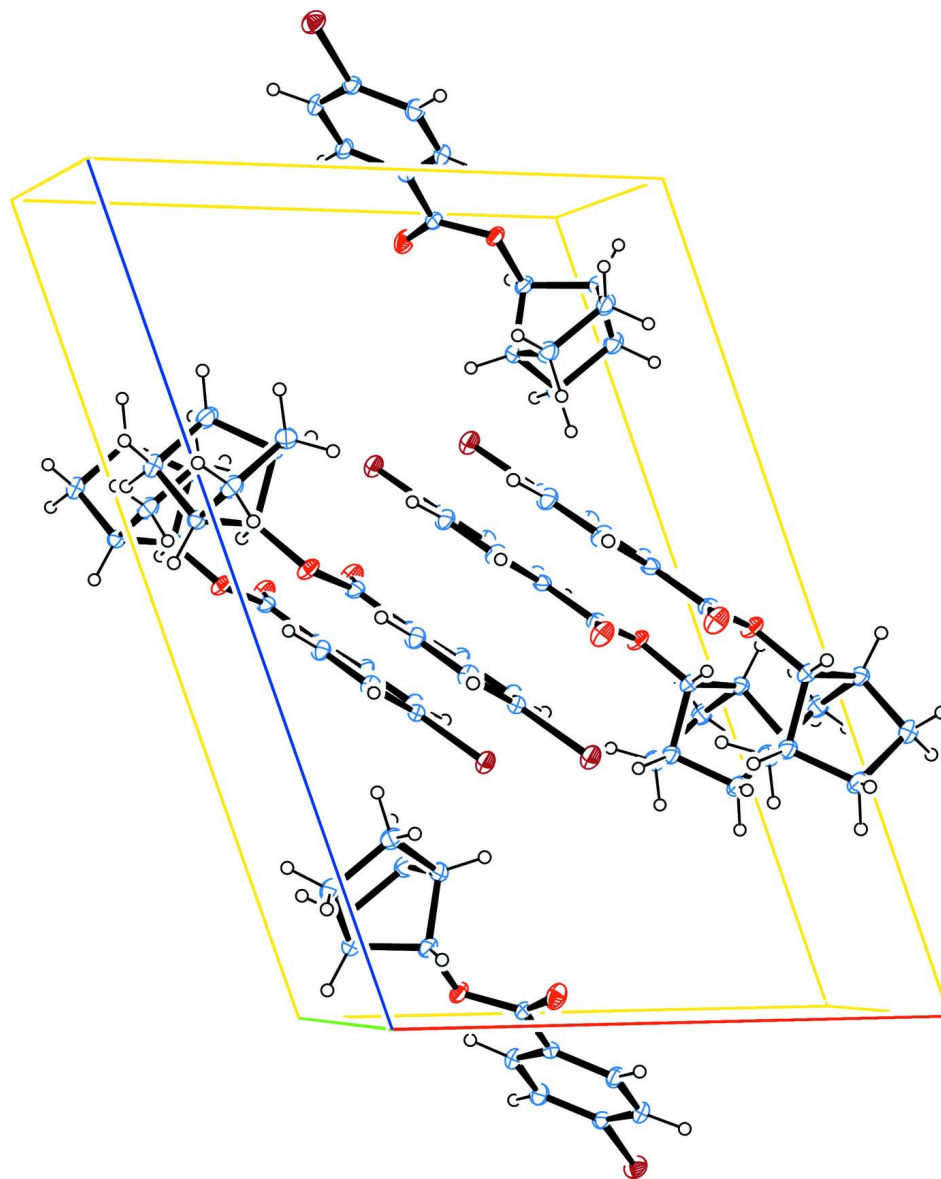
**Figure 2**

Cell packing diagram for the title compound.
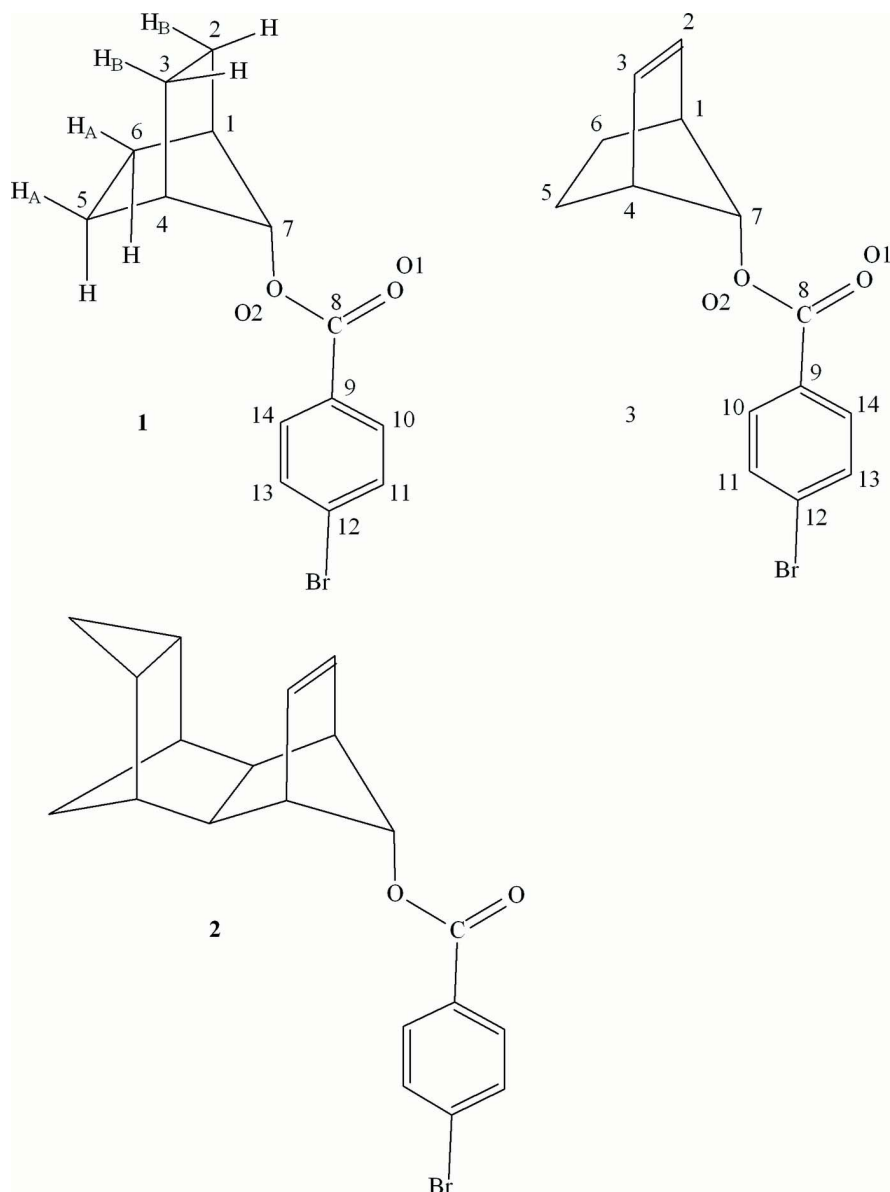
**Figure 3**

Compounds **1**, **2**, and **3**.

## Bicyclo[2.2.1]hept-7-yl *p*-bromobenzoate

*Crystal data*

| | |
|---|---|
| $C_{14}H_{15}BrO_2$ | $F(000) = 600$ |
| $M_r = 295.17$ | $D_x = 1.566$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: 351 K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 11.7401$ (2) Å | Cell parameters from 3135 reflections |
| $b = 6.3767$ (1) Å | $\theta = 1.0–27.5°$ |
| $c = 17.7462$ (3) Å | $\mu = 3.27$ mm$^{-1}$ |
| $\beta = 109.584$ (1)° | $T = 150$ K |
| $V = 1251.68$ (4) Å$^3$ | Prism, colourless |
| $Z = 4$ | $0.30 \times 0.25 \times 0.18$ mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD Diffractometer | 2882 independent reflections |
| Radiation source: fine-focus sealed tube | 2469 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.015$ |
| Phi and $\omega$ scans | $\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan | $h = -15 \rightarrow 15$ |
| (*DENZO-SMN*; Otwinowski & Minor, 1997) | $k = -8 \rightarrow 8$ |
| $T_{min} = 0.440$, $T_{max} = 0.591$ | $l = -22 \rightarrow 23$ |
| 5495 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from |
| Least-squares matrix: full | neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.022$ | All H-atom parameters refined |
| $wR(F^2) = 0.055$ | $w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 0.4883P]$ |
| $S = 1.03$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2882 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 215 parameters | $\Delta\rho_{max} = 0.38$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant | Extinction correction: *SHELXL*, |
| direct methods | $Fc^* = kFc[1 + 0.001 x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ |
| Secondary atom site location: difference Fourier | Extinction coefficient: 0.0091 (7) |
| map | |

*Special details*

**Experimental**. The program *DENZO-SMN* (Otwinowski & Minor, 1997) uses a scaling algorithm which effectively corrects for absorption effects. High redundancy data were used in the scaling program hence the 'multi-scan′ code word was used. No transmission coefficients are available from the program (only scale factors for each frame). The scale factors in the experimental table are calculated from the 'size′ command in the *SHELXL-97* input file.

**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 $F^2 > 2\sigma(F^2)$ 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 | 0.29724 (11) | −0.03809 (19) | 0.03440 (7) | 0.0345 (3) |
| O2 | 0.17768 (10) | 0.23527 (18) | 0.03757 (6) | 0.0275 (2) |
| Br1 | 0.470495 (15) | 0.70360 (3) | −0.187891 (10) | 0.03601 (8) |
| C1 | 0.20441 (14) | 0.1660 (3) | 0.18033 (9) | 0.0284 (3) |
| C2 | 0.12314 (16) | 0.0547 (3) | 0.22003 (10) | 0.0357 (4) |
| C3 | −0.00686 (16) | 0.0964 (3) | 0.16107 (11) | 0.0341 (4) |
| C4 | 0.01573 (14) | 0.2271 (3) | 0.09468 (9) | 0.0268 (3) |
| C5 | 0.05962 (15) | 0.4456 (3) | 0.12780 (10) | 0.0313 (4) |
| C6 | 0.18971 (16) | 0.4036 (3) | 0.18646 (10) | 0.0336 (4) |
| C7 | 0.13181 (14) | 0.1242 (3) | 0.09249 (9) | 0.0253 (3) |
| C8 | 0.26378 (13) | 0.1393 (3) | 0.01604 (8) | 0.0244 (3) |

| | | | |
|---|---|---|---|
| C9 | 0.31177 (13) | 0.2786 (2) | −0.03379 (8) | 0.0224 (3) |
| C10 | 0.39565 (15) | 0.1984 (3) | −0.06648 (9) | 0.0274 (3) |
| C11 | 0.44332 (15) | 0.3225 (3) | −0.11205 (10) | 0.0303 (4) |
| C12 | 0.40660 (13) | 0.5289 (3) | −0.12504 (8) | 0.0257 (3) |
| C13 | 0.32412 (15) | 0.6139 (3) | −0.09307 (10) | 0.0291 (3) |
| C14 | 0.27768 (14) | 0.4878 (3) | −0.04697 (9) | 0.0270 (3) |
| H1 | 0.2846 (17) | 0.116 (3) | 0.1972 (10) | 0.029 (4)* |
| H2A | 0.1403 (19) | −0.093 (4) | 0.2256 (12) | 0.049 (6)* |
| H2B | 0.1354 (16) | 0.109 (3) | 0.2741 (11) | 0.036 (5)* |
| H3A | −0.0457 (17) | −0.037 (3) | 0.1400 (12) | 0.039 (5)* |
| H3B | −0.0543 (18) | 0.179 (3) | 0.1874 (12) | 0.038 (5)* |
| H4 | −0.0512 (17) | 0.230 (3) | 0.0436 (11) | 0.031 (5)* |
| H5A | 0.0057 (17) | 0.507 (3) | 0.1529 (11) | 0.034 (5)* |
| H5B | 0.0597 (17) | 0.540 (3) | 0.0856 (11) | 0.035 (5)* |
| H6A | 0.2006 (18) | 0.443 (3) | 0.2418 (12) | 0.046 (6)* |
| H6B | 0.2501 (18) | 0.476 (3) | 0.1699 (12) | 0.043 (5)* |
| H7 | 0.1235 (16) | −0.023 (3) | 0.0794 (10) | 0.029 (5)* |
| H10 | 0.4167 (17) | 0.061 (3) | −0.0576 (11) | 0.038 (5)* |
| H11 | 0.5023 (19) | 0.270 (3) | −0.1319 (13) | 0.042 (5)* |
| H13 | 0.3001 (19) | 0.760 (3) | −0.1028 (12) | 0.040 (5)* |
| H14 | 0.2213 (17) | 0.543 (3) | −0.0241 (11) | 0.035 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0420 (7) | 0.0262 (6) | 0.0433 (7) | 0.0084 (5) | 0.0250 (5) | 0.0038 (5) |
| O2 | 0.0331 (6) | 0.0299 (6) | 0.0262 (5) | 0.0085 (5) | 0.0190 (5) | 0.0049 (5) |
| Br1 | 0.03629 (11) | 0.04188 (13) | 0.03518 (11) | −0.00802 (7) | 0.01902 (8) | 0.00085 (8) |
| C1 | 0.0223 (7) | 0.0396 (10) | 0.0243 (7) | 0.0034 (7) | 0.0093 (6) | 0.0054 (7) |
| C2 | 0.0356 (9) | 0.0473 (11) | 0.0288 (8) | 0.0035 (8) | 0.0169 (7) | 0.0101 (8) |
| C3 | 0.0299 (8) | 0.0427 (11) | 0.0349 (9) | −0.0027 (8) | 0.0177 (7) | 0.0010 (8) |
| C4 | 0.0227 (7) | 0.0357 (9) | 0.0231 (7) | 0.0029 (6) | 0.0090 (6) | 0.0000 (6) |
| C5 | 0.0347 (9) | 0.0312 (9) | 0.0333 (8) | 0.0059 (7) | 0.0184 (7) | −0.0013 (7) |
| C6 | 0.0326 (9) | 0.0396 (10) | 0.0301 (8) | −0.0049 (7) | 0.0125 (7) | −0.0081 (8) |
| C7 | 0.0294 (8) | 0.0267 (8) | 0.0245 (7) | 0.0020 (6) | 0.0151 (6) | 0.0015 (6) |
| C8 | 0.0244 (7) | 0.0296 (8) | 0.0203 (7) | 0.0036 (6) | 0.0090 (6) | −0.0045 (6) |
| C9 | 0.0214 (7) | 0.0273 (8) | 0.0179 (6) | 0.0016 (6) | 0.0056 (5) | −0.0030 (6) |
| C10 | 0.0304 (8) | 0.0273 (8) | 0.0285 (8) | 0.0068 (7) | 0.0153 (6) | 0.0003 (7) |
| C11 | 0.0269 (8) | 0.0389 (10) | 0.0295 (8) | 0.0053 (7) | 0.0154 (6) | −0.0017 (7) |
| C12 | 0.0221 (7) | 0.0343 (9) | 0.0207 (7) | −0.0046 (6) | 0.0074 (6) | −0.0025 (6) |
| C13 | 0.0300 (8) | 0.0263 (8) | 0.0326 (8) | 0.0009 (7) | 0.0125 (7) | −0.0010 (7) |
| C14 | 0.0266 (7) | 0.0293 (8) | 0.0284 (8) | 0.0046 (6) | 0.0134 (6) | −0.0027 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.206 (2) | C5—C6 | 1.556 (2) |
| O2—C8 | 1.3421 (17) | C5—H5A | 0.971 (19) |
| O2—C7 | 1.4469 (18) | C5—H5B | 0.96 (2) |

| | | | |
|---|---|---|---|
| Br1—C12 | 1.8997 (15) | C6—H6A | 0.98 (2) |
| C1—C7 | 1.529 (2) | C6—H6B | 0.97 (2) |
| C1—C6 | 1.533 (3) | C7—H7 | 0.966 (19) |
| C1—C2 | 1.537 (2) | C8—C9 | 1.491 (2) |
| C1—H1 | 0.944 (18) | C9—C14 | 1.390 (2) |
| C2—C3 | 1.557 (2) | C9—C10 | 1.397 (2) |
| C2—H2A | 0.96 (2) | C10—C11 | 1.377 (2) |
| C2—H2B | 0.984 (19) | C10—H10 | 0.91 (2) |
| C3—C4 | 1.537 (2) | C11—C12 | 1.380 (2) |
| C3—H3A | 0.98 (2) | C11—H11 | 0.94 (2) |
| C3—H3B | 0.99 (2) | C12—C13 | 1.386 (2) |
| C4—C7 | 1.525 (2) | C13—C14 | 1.383 (2) |
| C4—C5 | 1.533 (2) | C13—H13 | 0.97 (2) |
| C4—H4 | 0.981 (19) | C14—H14 | 0.953 (19) |
| | | | |
| C8—O2—C7 | 117.02 (12) | C1—C6—H6A | 110.0 (13) |
| C7—C1—C6 | 101.97 (13) | C5—C6—H6A | 113.4 (12) |
| C7—C1—C2 | 99.62 (13) | C1—C6—H6B | 109.8 (12) |
| C6—C1—C2 | 108.80 (14) | C5—C6—H6B | 111.6 (12) |
| C7—C1—H1 | 114.8 (11) | H6A—C6—H6B | 108.6 (17) |
| C6—C1—H1 | 116.0 (12) | O2—C7—C4 | 110.13 (13) |
| C2—C1—H1 | 113.8 (11) | O2—C7—C1 | 113.28 (13) |
| C1—C2—C3 | 103.42 (13) | C4—C7—C1 | 95.54 (12) |
| C1—C2—H2A | 111.1 (13) | O2—C7—H7 | 110.2 (10) |
| C3—C2—H2A | 111.2 (13) | C4—C7—H7 | 114.0 (11) |
| C1—C2—H2B | 112.1 (12) | C1—C7—H7 | 113.0 (10) |
| C3—C2—H2B | 112.7 (11) | O1—C8—O2 | 124.01 (14) |
| H2A—C2—H2B | 106.5 (17) | O1—C8—C9 | 124.44 (13) |
| C4—C3—C2 | 103.05 (13) | O2—C8—C9 | 111.55 (13) |
| C4—C3—H3A | 110.9 (11) | C14—C9—C10 | 119.00 (14) |
| C2—C3—H3A | 109.6 (12) | C14—C9—C8 | 121.81 (13) |
| C4—C3—H3B | 110.0 (11) | C10—C9—C8 | 119.17 (14) |
| C2—C3—H3B | 110.7 (11) | C11—C10—C9 | 121.02 (15) |
| H3A—C3—H3B | 112.2 (16) | C11—C10—H10 | 121.0 (12) |
| C7—C4—C5 | 102.27 (13) | C9—C10—H10 | 117.9 (12) |
| C7—C4—C3 | 99.88 (13) | C10—C11—C12 | 118.71 (14) |
| C5—C4—C3 | 108.73 (13) | C10—C11—H11 | 120.7 (13) |
| C7—C4—H4 | 115.4 (11) | C12—C11—H11 | 120.5 (13) |
| C5—C4—H4 | 113.6 (11) | C11—C12—C13 | 121.77 (15) |
| C3—C4—H4 | 115.4 (11) | C11—C12—Br1 | 119.64 (11) |
| C4—C5—C6 | 103.21 (13) | C13—C12—Br1 | 118.59 (13) |
| C4—C5—H5A | 110.9 (11) | C14—C13—C12 | 118.87 (16) |
| C6—C5—H5A | 114.0 (11) | C14—C13—H13 | 120.9 (12) |
| C4—C5—H5B | 111.2 (11) | C12—C13—H13 | 120.2 (12) |
| C6—C5—H5B | 111.8 (11) | C13—C14—C9 | 120.61 (14) |
| H5A—C5—H5B | 105.9 (16) | C13—C14—H14 | 120.3 (12) |
| C1—C6—C5 | 103.36 (13) | C9—C14—H14 | 119.1 (12) |

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| C7—C1—C2—C3 | −35.57 (17) | C6—C1—C7—C4 | −54.16 (14) |
| C6—C1—C2—C3 | 70.69 (17) | C2—C1—C7—C4 | 57.56 (15) |
| C1—C2—C3—C4 | −0.06 (19) | C7—O2—C8—O1 | 6.3 (2) |
| C2—C3—C4—C7 | 35.81 (17) | C7—O2—C8—C9 | −174.22 (12) |
| C2—C3—C4—C5 | −70.86 (17) | O1—C8—C9—C14 | −174.03 (15) |
| C7—C4—C5—C6 | −33.78 (15) | O2—C8—C9—C14 | 6.5 (2) |
| C3—C4—C5—C6 | 71.24 (15) | O1—C8—C9—C10 | 4.3 (2) |
| C7—C1—C6—C5 | 34.25 (15) | O2—C8—C9—C10 | −175.22 (13) |
| C2—C1—C6—C5 | −70.38 (16) | C14—C9—C10—C11 | −0.8 (2) |
| C4—C5—C6—C1 | −0.36 (16) | C8—C9—C10—C11 | −179.21 (15) |
| C8—O2—C7—C4 | −166.14 (13) | C9—C10—C11—C12 | 0.0 (2) |
| C8—O2—C7—C1 | 88.22 (16) | C10—C11—C12—C13 | 0.5 (2) |
| C5—C4—C7—O2 | −63.24 (15) | C10—C11—C12—Br1 | −179.84 (12) |
| C3—C4—C7—O2 | −175.05 (13) | C11—C12—C13—C14 | 0.0 (2) |
| C5—C4—C7—C1 | 54.04 (14) | Br1—C12—C13—C14 | −179.71 (12) |
| C3—C4—C7—C1 | −57.76 (15) | C12—C13—C14—C9 | −0.9 (2) |
| C6—C1—C7—O2 | 60.55 (15) | C10—C9—C14—C13 | 1.3 (2) |
| C2—C1—C7—O2 | 172.27 (13) | C8—C9—C14—C13 | 179.63 (14) |