Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,3′-Dibromo-6,6′-dimethoxybiphenyl-2,2′-dicarboxylic acid ethanol monosolvate

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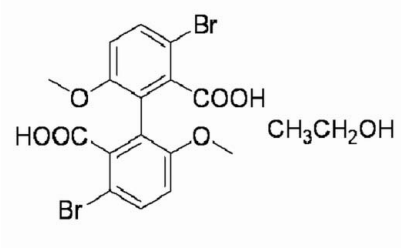
Received 5 April 2010; accepted 10 April 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 14.4.

In the title compound, $C_{16}H_{12}Br_2O_6\cdot C_2H_5OH$, the two benzene rings are twisted by 80.64 (5)° and the carboxyl groups form dihedral angles of 72.48 (3) and 89.41 (2)° with the corresponding benzene rings. In the crystal structure, the biphenyl molecules are connected by intermolecular O—H···O and O—H···Br hydrogen bonds, resulting in a chain along the b axis.

Related literature

For complexes containing diphenic acids, see: Wang *et al.* (2007); Yang *et al.* (2007). For the synthesis of the title compound, see: Choi *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{12}Br_2O_6\cdot C_2H_6O$
M_r = 506.14
Monoclinic, $P2_1/c$
a = 9.9872 (9) Å
b = 23.230 (2) Å
c = 8.3967 (7) Å
β = 90.143 (1)°
V = 1948.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.20 mm^{-1}
T = 296 K
0.41 × 0.34 × 0.32 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.278, T_{max} = 0.347
14693 measured reflections
3606 independent reflections
2825 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.02
3606 reflections
250 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O7	0.82	1.79	2.594 (3)	165
O6—H6···O3^{i}	0.82	1.89	2.711 (3)	174
O7—H7···O5^{ii}	0.82	2.07	2.879 (3)	167
O7—H7···Br1^{ii}	0.82	3.04	3.445 (2)	113

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

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: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

We are grateful to the National Natural Sciences Foundation of China (grant No. 20872057) and the Natural Science Foundation of Henan Province (No. 082300420040) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2670).

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supporting information

Acta Cryst. (2010). E**66**, o1144 [https://doi.org/10.1107/S1600536810013279]

3,3′-Dibromo-6,6′-dimethoxybiphenyl-2,2′-dicarboxylic acid ethanol monosolvate

Xiao Zhang, Long Li, Le Zhou and Baoming Ji

S1. Comment

Diphenic acid and its derivatives have been proved to be a kind of multifunctional and flexible ligand in the construction of complexes possessing novel and interesting topological structures (Choi *et al.* 2007). Our interest in these compounds has led us to prepare the title compound according to the literature methods (Choi *et al.* 2007). In this contribution, we report the synthesis and crystal structure of the title compound.

The molecule of the title compound (Fig. 1.), is built up form one benzene ring connected to the other benzene ring through the 2 and 2′ carbon atoms, in which the bond lengths and angles are within ranges as reported by Wang *et al.*. (2007). In the crystal structure, except the carboxyl group, both methoxyl group and bromino group lie in the corresponding benzene ring plane, with an r.m.s. deviation of 0.0180 (1) Å and 0.0124 (1) Å.respectively. And, the dihedral angle between the two benzene rings is 80.64 (5)°. It must be pointed out that the striking feature of the title compound is the interesting arrangement of the tilte molecules, which connected each other by the formation of intermolecular O—H···O hydrogen bonds to form one-dimensional chain along the *b* axis (Fig.2.). Interestingly, the solvent molecules interact with the carboxylate oxygen atoms and bromine atoms from the chains via O—H···O and O—H···Br hydrogen bonds respectively, resulting in the formation of a 2D supramolecular network with 1D channels along the *c* axis. Detail hydrogen bonds are given in Table 1.

S2. Experimental

2,2′-Dimethoxy-6,6′-Diacetylbiphenyl (0.298 mg, 1 mmol) was suspended and stirred in 1,4-dioxane (24 ml). NaOH (1.76 g, 30.1 mmol) was dissolved in 11.8 ml of water. At 0 °C, bromine (0.80 ml) was added to the NaOH solution which was stirred for 15 min. The NaOBr solution was added gradually to the 1,4-dioxane solution at room temperature, then was stirred at 60 °C for 2 h and cooled to room temperature. The mixture was acidified with *conc*. HCl (pH < 2) and filtered, washed with water (5 × 100 ml). The products were dried under vacuum, gave the title compounds as white solid (0.253 g, yield 84%).

S3. Refinement

All H atoms were placed in calculated positions (C—H 0.93 ~0.97 Å, O—H 0.82 Å) and were included in the refinement in the riding model approximation, with *U*ĩso~(H) set to 1.2 ~1.5Ueq (C, O)

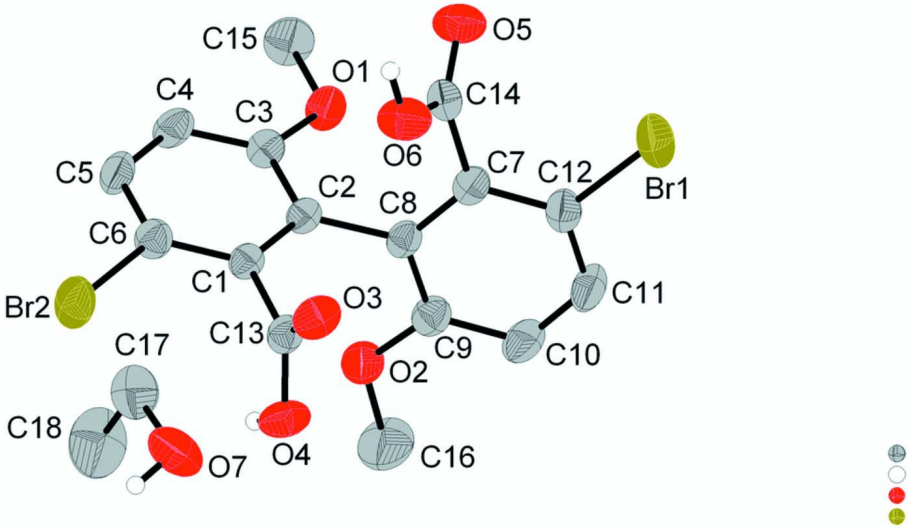

Figure 1

View of the title molecule with the atom numbering scheme and 30% probability displacement ellipsoids for non-hydrogen atoms.

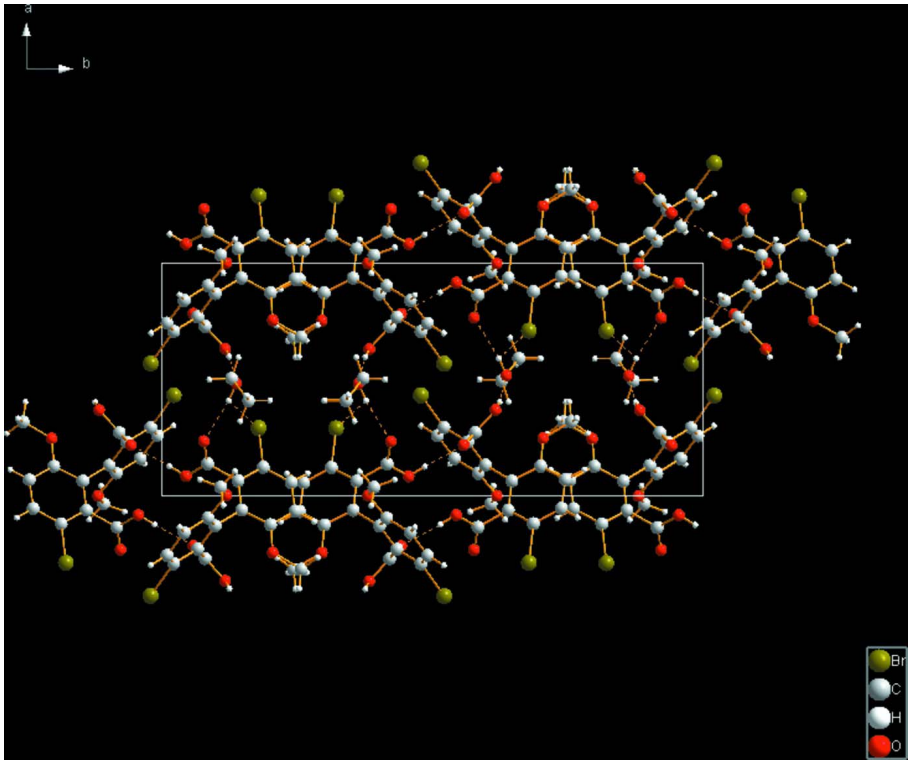

Figure 2

View of a 2D supramolecular network with 1D channels along the *c* axis. (O—H···O and O—H···Br hydrogen bonds are indicated as broken lines).

3,3′-Dibromo-6,6′-dimethoxybiphenyl-2,2′-dicarboxylic acid ethanol monosolvate

Crystal data

$C_{16}H_{12}Br_2O_6 \cdot C_2H_6O$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.9872\ (9)$ Å
$b = 23.230\ (2)$ Å
$c = 8.3967\ (7)$ Å
$\beta = 90.143\ (1)°$
$V = 1948.1\ (3)$ Å^3
$Z = 4$
$F(000) = 1008$
$D_x = 1.726$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4208 reflections
$\theta = 2.6–24.1°$
$\mu = 4.20$ mm^{-1}
$T = 296$ K
Block, colourless
0.41 × 0.34 × 0.32 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.278$, $T_{max} = 0.347$
14693 measured reflections
3606 independent reflections
2825 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.6°$
$h = -12 \rightarrow 12$
$k = -28 \rightarrow 27$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.069$
$S = 1.02$
3606 reflections
250 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
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 1.1811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	1.29076 (3)	0.321685 (15)	0.54701 (4)	0.05407 (12)
Br2	0.56847 (4)	0.521511 (14)	0.30185 (4)	0.05610 (12)
C1	0.7693 (3)	0.43425 (10)	0.2858 (3)	0.0278 (6)
C2	0.8694 (3)	0.40203 (10)	0.2113 (3)	0.0274 (6)
C3	0.9035 (3)	0.41516 (11)	0.0534 (3)	0.0305 (6)
C4	0.8397 (3)	0.45929 (12)	−0.0261 (3)	0.0370 (7)
H4	0.8629	0.4676	−0.1307	0.044*
C5	0.7418 (3)	0.49106 (12)	0.0482 (3)	0.0385 (7)
H5	0.6992	0.5208	−0.0061	0.046*
C6	0.7069 (3)	0.47879 (11)	0.2029 (3)	0.0344 (6)
C7	1.0635 (3)	0.35965 (11)	0.3670 (3)	0.0308 (6)
C8	0.9375 (3)	0.35320 (11)	0.2973 (3)	0.0293 (6)
C9	0.8739 (3)	0.29955 (11)	0.3056 (3)	0.0354 (6)
C10	0.9326 (3)	0.25405 (12)	0.3876 (4)	0.0448 (7)
H10	0.8887	0.2189	0.3952	0.054*
C11	1.0562 (3)	0.26145 (12)	0.4574 (4)	0.0460 (8)
H11	1.0956	0.2312	0.5128	0.055*
C12	1.1220 (3)	0.31319 (12)	0.4460 (3)	0.0360 (6)
C13	0.7292 (3)	0.42070 (11)	0.4544 (3)	0.0327 (6)
C14	1.1369 (3)	0.41600 (11)	0.3540 (3)	0.0330 (6)
C15	1.0350 (3)	0.39177 (14)	−0.1754 (3)	0.0502 (8)
H15A	0.9570	0.3871	−0.2412	0.075*
H15B	1.1028	0.3650	−0.2082	0.075*
H15C	1.0682	0.4304	−0.1859	0.075*
C16	0.6822 (4)	0.24274 (15)	0.2386 (5)	0.0773 (12)
H16A	0.7326	0.2127	0.1882	0.116*
H16B	0.5972	0.2468	0.1862	0.116*
H16C	0.6682	0.2331	0.3485	0.116*
C17	0.5058 (3)	0.37183 (15)	0.0619 (4)	0.0576 (9)
H17A	0.5957	0.3592	0.0357	0.069*
H17B	0.4998	0.4126	0.0382	0.069*
C18	0.4087 (4)	0.34029 (17)	−0.0378 (5)	0.0830 (13)
H18A	0.4097	0.3003	−0.0093	0.124*
H18B	0.4325	0.3444	−0.1479	0.124*
H18C	0.3206	0.3557	−0.0211	0.124*
O1	1.0004 (2)	0.38108 (8)	−0.0119 (2)	0.0405 (5)
O2	0.7542 (2)	0.29550 (8)	0.2283 (2)	0.0470 (5)
O3	0.7835 (2)	0.44226 (8)	0.5689 (2)	0.0435 (5)
O4	0.6324 (2)	0.38329 (9)	0.4742 (2)	0.0465 (5)
H4A	0.5983	0.3758	0.3877	0.070*
O5	1.2337 (2)	0.42307 (9)	0.2715 (3)	0.0525 (6)
O6	1.0841 (2)	0.45596 (8)	0.4443 (3)	0.0506 (6)
H6	1.1260	0.4860	0.4336	0.076*
O7	0.4832 (2)	0.36322 (12)	0.2271 (3)	0.0622 (6)
H7	0.4102	0.3767	0.2514	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04607 (19)	0.0635 (2)	0.0526 (2)	0.01334 (16)	−0.01252 (15)	0.00325 (16)
Br2	0.0602 (2)	0.0550 (2)	0.0532 (2)	0.02797 (17)	0.01663 (16)	0.00940 (16)
C1	0.0313 (14)	0.0268 (13)	0.0251 (13)	−0.0016 (11)	−0.0020 (11)	0.0003 (11)
C2	0.0319 (14)	0.0245 (13)	0.0258 (13)	−0.0013 (11)	−0.0011 (11)	0.0006 (10)
C3	0.0353 (15)	0.0269 (14)	0.0292 (14)	0.0011 (11)	0.0018 (11)	−0.0029 (11)
C4	0.0467 (17)	0.0395 (16)	0.0248 (14)	0.0004 (13)	0.0050 (12)	0.0071 (12)
C5	0.0448 (17)	0.0353 (16)	0.0353 (16)	0.0063 (13)	−0.0009 (13)	0.0113 (12)
C6	0.0364 (15)	0.0330 (14)	0.0339 (15)	0.0040 (12)	0.0024 (12)	0.0006 (12)
C7	0.0381 (15)	0.0279 (14)	0.0265 (13)	0.0058 (12)	0.0064 (11)	−0.0004 (11)
C8	0.0351 (15)	0.0276 (14)	0.0251 (13)	0.0049 (11)	0.0045 (11)	0.0019 (11)
C9	0.0402 (16)	0.0306 (15)	0.0354 (15)	0.0016 (12)	0.0022 (12)	0.0006 (12)
C10	0.0538 (19)	0.0277 (15)	0.0529 (19)	−0.0013 (14)	0.0013 (15)	0.0080 (13)
C11	0.054 (2)	0.0341 (16)	0.0502 (19)	0.0091 (14)	−0.0031 (15)	0.0140 (14)
C12	0.0378 (16)	0.0400 (16)	0.0300 (14)	0.0096 (13)	0.0005 (12)	0.0025 (12)
C13	0.0358 (16)	0.0307 (14)	0.0316 (15)	0.0058 (12)	0.0043 (12)	0.0029 (12)
C14	0.0305 (15)	0.0353 (15)	0.0332 (15)	0.0045 (12)	−0.0038 (12)	0.0000 (12)
C15	0.058 (2)	0.059 (2)	0.0339 (16)	0.0082 (16)	0.0147 (14)	−0.0030 (14)
C16	0.072 (3)	0.055 (2)	0.105 (3)	−0.029 (2)	−0.025 (2)	0.018 (2)
C17	0.057 (2)	0.059 (2)	0.057 (2)	0.0043 (18)	−0.0069 (17)	0.0004 (17)
C18	0.098 (3)	0.069 (3)	0.081 (3)	−0.006 (2)	−0.036 (3)	−0.012 (2)
O1	0.0503 (12)	0.0419 (11)	0.0293 (10)	0.0118 (9)	0.0104 (9)	0.0007 (8)
O2	0.0429 (12)	0.0363 (11)	0.0619 (13)	−0.0087 (9)	−0.0098 (10)	0.0050 (10)
O3	0.0576 (13)	0.0463 (12)	0.0267 (10)	−0.0083 (10)	−0.0016 (9)	−0.0019 (9)
O4	0.0519 (13)	0.0543 (13)	0.0333 (11)	−0.0164 (11)	0.0048 (9)	0.0042 (10)
O5	0.0485 (13)	0.0472 (13)	0.0618 (14)	−0.0043 (10)	0.0195 (11)	−0.0020 (11)
O6	0.0546 (14)	0.0331 (11)	0.0641 (14)	−0.0054 (10)	0.0152 (11)	−0.0127 (10)
O7	0.0397 (13)	0.0960 (19)	0.0508 (14)	0.0005 (13)	0.0022 (10)	−0.0063 (13)

Geometric parameters (Å, º)

Br1—C12	1.896 (3)	C13—O3	1.212 (3)
Br2—C6	1.895 (3)	C13—O4	1.310 (3)
C1—C6	1.393 (3)	C14—O5	1.202 (3)
C1—C2	1.398 (4)	C14—O6	1.311 (3)
C1—C13	1.506 (4)	C15—O1	1.438 (3)
C2—C3	1.403 (3)	C15—H15A	0.9600
C2—C8	1.506 (3)	C15—H15B	0.9600
C3—O1	1.366 (3)	C15—H15C	0.9600
C3—C4	1.379 (4)	C16—O2	1.424 (4)
C4—C5	1.376 (4)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.375 (4)	C16—H16C	0.9600
C5—H5	0.9300	C17—O7	1.420 (4)
C7—C12	1.394 (4)	C17—C18	1.475 (5)
C7—C8	1.395 (4)	C17—H17A	0.9700

C7—C14	1.505 (4)	C17—H17B	0.9700
C8—C9	1.401 (4)	C18—H18A	0.9600
C9—O2	1.362 (3)	C18—H18B	0.9600
C9—C10	1.390 (4)	C18—H18C	0.9600
C10—C11	1.376 (4)	O4—H4A	0.8200
C10—H10	0.9300	O6—H6	0.8200
C11—C12	1.373 (4)	O7—H7	0.8200
C11—H11	0.9300		

C6—C1—C2	119.6 (2)	O3—C13—O4	120.2 (2)
C6—C1—C13	120.3 (2)	O3—C13—C1	122.7 (2)
C2—C1—C13	120.1 (2)	O4—C13—C1	117.1 (2)
C1—C2—C3	118.8 (2)	O5—C14—O6	124.2 (3)
C1—C2—C8	120.7 (2)	O5—C14—C7	123.6 (2)
C3—C2—C8	120.4 (2)	O6—C14—C7	112.2 (2)
O1—C3—C4	124.3 (2)	O1—C15—H15A	109.5
O1—C3—C2	115.3 (2)	O1—C15—H15B	109.5
C4—C3—C2	120.4 (2)	H15A—C15—H15B	109.5
C5—C4—C3	120.5 (2)	O1—C15—H15C	109.5
C5—C4—H4	119.8	H15A—C15—H15C	109.5
C3—C4—H4	119.8	H15B—C15—H15C	109.5
C6—C5—C4	119.9 (3)	O2—C16—H16A	109.5
C6—C5—H5	120.0	O2—C16—H16B	109.5
C4—C5—H5	120.0	H16A—C16—H16B	109.5
C5—C6—C1	120.8 (2)	O2—C16—H16C	109.5
C5—C6—Br2	119.5 (2)	H16A—C16—H16C	109.5
C1—C6—Br2	119.73 (19)	H16B—C16—H16C	109.5
C12—C7—C8	119.5 (2)	O7—C17—C18	112.2 (3)
C12—C7—C14	120.3 (2)	O7—C17—H17A	109.2
C8—C7—C14	120.2 (2)	C18—C17—H17A	109.2
C7—C8—C9	118.9 (2)	O7—C17—H17B	109.2
C7—C8—C2	121.7 (2)	C18—C17—H17B	109.2
C9—C8—C2	119.3 (2)	H17A—C17—H17B	107.9
O2—C9—C10	123.5 (2)	C17—C18—H18A	109.5
O2—C9—C8	115.8 (2)	C17—C18—H18B	109.5
C10—C9—C8	120.7 (3)	H18A—C18—H18B	109.5
C11—C10—C9	119.5 (3)	C17—C18—H18C	109.5
C11—C10—H10	120.2	H18A—C18—H18C	109.5
C9—C10—H10	120.2	H18B—C18—H18C	109.5
C12—C11—C10	120.5 (3)	C3—O1—C15	117.1 (2)
C12—C11—H11	119.7	C9—O2—C16	118.3 (2)
C10—C11—H11	119.7	C13—O4—H4A	109.5
C11—C12—C7	120.7 (3)	C14—O6—H6	109.5
C11—C12—Br1	119.0 (2)	C17—O7—H7	109.5
C7—C12—Br1	120.2 (2)		

C6—C1—C2—C3	−0.7 (4)	C7—C8—C9—O2	−176.9 (2)
C13—C1—C2—C3	179.2 (2)	C2—C8—C9—O2	2.1 (4)

C6—C1—C2—C8	−179.3 (2)	C7—C8—C9—C10	2.6 (4)
C13—C1—C2—C8	0.6 (4)	C2—C8—C9—C10	−178.4 (2)
C1—C2—C3—O1	−178.8 (2)	O2—C9—C10—C11	177.7 (3)
C8—C2—C3—O1	−0.2 (3)	C8—C9—C10—C11	−1.8 (4)
C1—C2—C3—C4	0.4 (4)	C9—C10—C11—C12	−0.3 (5)
C8—C2—C3—C4	179.0 (2)	C10—C11—C12—C7	1.7 (4)
O1—C3—C4—C5	179.2 (3)	C10—C11—C12—Br1	179.0 (2)
C2—C3—C4—C5	0.0 (4)	C8—C7—C12—C11	−0.8 (4)
C3—C4—C5—C6	−0.1 (4)	C14—C7—C12—C11	−179.5 (3)
C4—C5—C6—C1	−0.2 (4)	C8—C7—C12—Br1	−178.13 (19)
C4—C5—C6—Br2	−178.3 (2)	C14—C7—C12—Br1	3.2 (3)
C2—C1—C6—C5	0.7 (4)	C6—C1—C13—O3	−91.2 (3)
C13—C1—C6—C5	−179.2 (3)	C2—C1—C13—O3	88.9 (3)
C2—C1—C6—Br2	178.67 (19)	C6—C1—C13—O4	89.8 (3)
C13—C1—C6—Br2	−1.2 (3)	C2—C1—C13—O4	−90.1 (3)
C12—C7—C8—C9	−1.3 (4)	C12—C7—C14—O5	70.9 (4)
C14—C7—C8—C9	177.4 (2)	C8—C7—C14—O5	−107.8 (3)
C12—C7—C8—C2	179.7 (2)	C12—C7—C14—O6	−108.4 (3)
C14—C7—C8—C2	−1.6 (4)	C8—C7—C14—O6	73.0 (3)
C1—C2—C8—C7	−100.4 (3)	C4—C3—O1—C15	−1.3 (4)
C3—C2—C8—C7	81.1 (3)	C2—C3—O1—C15	177.9 (2)
C1—C2—C8—C9	80.6 (3)	C10—C9—O2—C16	3.2 (4)
C3—C2—C8—C9	−97.9 (3)	C8—C9—O2—C16	−177.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O7	0.82	1.79	2.594 (3)	165
O6—H6···O3^{i}	0.82	1.89	2.711 (3)	174
O7—H7···O5^{ii}	0.82	2.07	2.879 (3)	167
O7—H7···Br1^{ii}	0.82	3.04	3.445 (2)	113

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