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# Crystal structure of the diglycidyl ether of eugenol

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The diepoxy monomer, $C_{13}H_{16}O_4$ {**DGE-Eu**; systematic name: 2-[3-methoxy-4-(oxiran-2-ylmethoxy)benzyl]oxirane}, was synthesized from eugenol by a three-step reaction. It consists of a 1,2,4-trisubstituted benzene ring substituted by diglycidyl ether, a methoxy group and a methyloxirane group. The three-membered oxirane rings are inclined to the benzene ring by 61.0 (3) and 27.9 (3)°. The methylene C atom of one of the two terminal epoxide rings is positionally disordered [refined occupancy ratio = 0.69 (1):0.31 (1)]. In the crystal, molecules are linked by C—H⋯O hydrogen bonds, forming layers parallel to the *ab* plane. The layers are linked by C—H⋯π interactions, forming a three-dimensional network.

1. Chemical context

The past two decades have witnessed an increasing interest in the environmental quest for the replacement of petroleum-based chemicals by monomers from renewable resources. Advances in particular in the catalytic conversion of biomass have led to a wide range of useful platform molecules (Besson *et al.*, 2014). This sustainable approach is also strongly considered in the field of polymer synthesis (Gandini *et al.*, 2016). In the specific domain of epoxy thermosets, numerous studies have been conducted in order to find alternatives to the diglycidyl ether of bisphenol A (BADGE), which is the main building-block used for formulation resins (Auvergne *et al.*, 2014). Classically, the synthetic approach is based on the functionalization of bio-sourced molecules by the grafting of glycidyl ether groups. In this context and in our ongoing studies on the chemical modification of bio-based building blocks for material applications (Mhanna *et al.*, 2014; Bigot *et al.*, 2016; François *et al.*, 2016), we report herein on the synthesis and crystal structure of the diglycidyl ether of eugenol (**DGE-Eu**), prepared from eugenol in a three-step synthesis (Qin *et al.*, 2014).
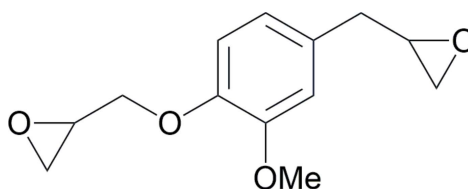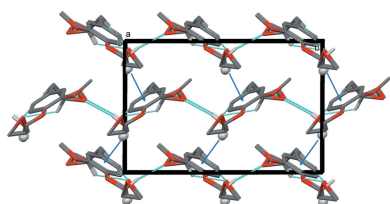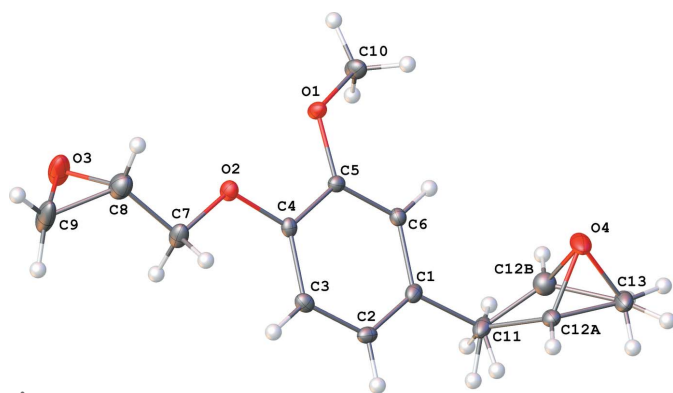
Figure 1
A view of the molecular structure of the title compound (**DGE-Eu**), with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The major and minor components of atom C12 (C12*A*/C12*B*) are shown.

2. Structural commentary

The title compound (**DGE-EU**), has an asymmetrical structure, which is depicted in Fig. 1. It is composed of a benzene ring with three oxygenated functional groups: (i) 2-[(λ^1-oxidanyl)methyl]oxirane, (ii) methoxy and (iii) 2-methyl-oxirane. While atoms O1, O2 and C11 lie in the plane of the benzene ring, the methoxy group (O1/C5/C10) is inclined to the benzene ring by 11.2 (3)°. The two oxirane rings (O3/C8/C9 and O4/C12*A*/C13) are inclined to the benzene ring by 61.0 (3) and 27.9 (3)°, respectively. The molecule shows disorder with an occupation factor equal to 0.69 (1) for the major component of the methylene group (C12*A*) of the oxirane ring (C11/C12/O3). Such disorder is commonly observed for diglycidyl ether derivatives (CSD; Groom *et al.*, 2016).

3. Supramolecular features

The crystal packing of **DGE-Eu** viewed along the *c*-axis is depicted in Fig. 2. All oxygen atoms of **DGE-Eu** are involved
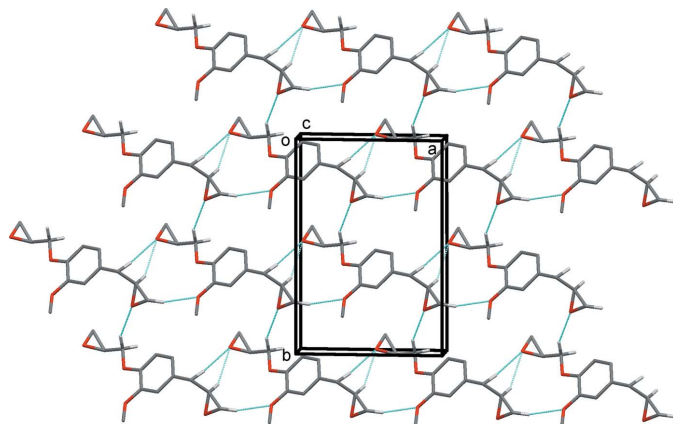
Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the benzene ring (C1–C6).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7*B*$\cdots$O4[i]	0.99	2.53	3.452 (4)	155
C11—H11*C*$\cdots$O3[ii]	0.99	2.43	3.413 (4)	170
C13—H13*B*$\cdots$O1[ii]	0.99	2.57	3.358 (4)	136
C12*A*—H12*A*$\cdots$O3[ii]	1.00	2.45	3.177 (5)	129
C7—H7*A*$\cdots$*Cg*[iii]	0.99	2.57	3.465 (4)	150

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

in C—H$\cdots$O hydrogen bonds with surrounding molecules, forming layers lying parallel to the *ab* plane (Fig. 2 and Table 1). In addition, the layers are linked C—H$\cdots\pi$ interactions, with the C7—H7*A* group positioned almost orthogonally to the benzene ring, so forming a three-dimensional network (Table 1 and Fig. 3).

4. Database survey

To date, and to the best of our knowledge, only nine crystallographic structures comprising diglycidyl ether-substituted benzene ring moieties have been deposited in the Cambridge Structural Database (WebCSD v1.1.2, update 2017-04-05; Groom *et al.*, 2016). They include 2,2-bis(3,5-dibromo-4-hydroxybenzene)propane diglycidyl ether (COMNEX: Saf'yanov *et al.*, 1984), 2,2-bis[4-(oxiran-2-ylmethoxy)-3,5-dibromophenyl]propane (COMNEY: Cheban *et al.*, 1985), diglycidyl ether of bisphenol A (DGEBPA: Flippen-Anderson & Gilardi, 1980; DGEBPA01: Heinemann *et al.*, 1993; DGEBPA10: Flippen-Anderson & Gilardi, 1981), *p*-di(2,3-epoxypropyloxy)benzene (EOXHQE: Saf'yanov *et al.*, 1977), 2,2′-[1,3-phenylene-bis(oxymethylene)]bis(oxirane) (FITWOU: Bocelli & Grenier-Loustalot, 1987), 2-(4-{4-[4-(oxiran-2-ylmethoxy)phenoxy]phenyl}phenoxymethyl)-oxirane (LAQTII: Song *et al.*, 2012) and 10-[2,5-bis(2,3-epoxy-1-propoxy)phenyl]-9-oxa-10-phosphaphenanthren-10-one

Figure 2
Crystal packing of **DGE-Eu** viewed along the *c* axis, showing the layer-like C—H$\cdots$O hydrogen-bonded network (dashed lines; see Table 1). Only the major component of atom C12 (C12*A*) is shown. For clarity, only H atoms H7*B*, H11*C*, H12*A*, H13*B* and H7*A* have been included.

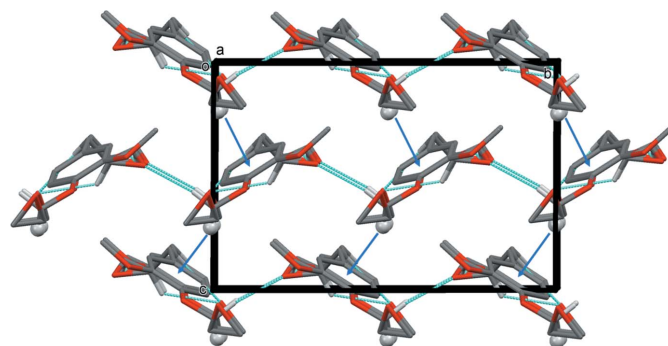**Figure 3**
Crystal packing of **DGE-Eu**, viewed along the *a* axis, showing the layer-like C—H$\cdots$O hydrogen-bonded networks linked by C—H$\cdots\pi$ interactions (dashed lines and blue arrows, respectively; see Table 1). For clarity, only H atoms H7*B*, H11*C*, H12*A*, H13*B* and H7*A* (grey ball) have been included. Only the major component of atom C12 (C12*A*) is shown.

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(LIPSOS: Cho *et al.*, 1999). In some of these compounds, an epoxy ring is disordered, which is also observed for the title compound **DGE-Eu**. In terms of application, these compounds are used as precursors of thermosetting resins. The polymerization process involving the epoxy rings occurs in the presence of amines and acid anhydrides and leads to cross-linked rigid materials.

5. Synthesis and crystallization

The title compound was prepared from a commercial source of eugenol (Sigma–Aldrich), according to a three-step procedure previously reported in the literature (Qin *et al.*, 2014). The details of the synthesis of the title compound are summarized in Fig. 4. Following purification by silica gel column chromatography, colourless prismatic crystals were obtained by slow evaporation of an ethyl acetate solution, and were finally characterized as **DGE-Eu**.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were placed at calculated positions and refined using a riding model: C—H = 0.95–1.00 Å with $U_{iso}(H) = 1.5U_{eq}$(C-methyl) and $1.2U_{eq}$(C) for other H atoms. Atom C12 atom of the epoxypropane (oxirane) group (C11/C12/O3) was found to be disordered over two positions with a refined occupancy ratio of 0.69 (1): 0.31 (1) for atoms C12A:C12B.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{16}O_4$
M_r	236.26
Crystal system, space group	Monoclinic, Cc
Temperature (K)	115
a, b, c (Å)	9.8262 (5), 13.4434 (7), 9.4251 (8)
β (°)	109.897 (2)
V (Å^3)	1170.71 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	$0.4 \times 0.35 \times 0.3$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.700, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18897, 2680, 2586
R_{int}	0.021
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.121, 1.07
No. of reflections	2680
No. of parameters	160
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.69, −0.28
Absolute structure	Flack x determined using 1234 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.20 (18)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2015* (Sheldrick, 2015a), *SHELXL2015* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008).

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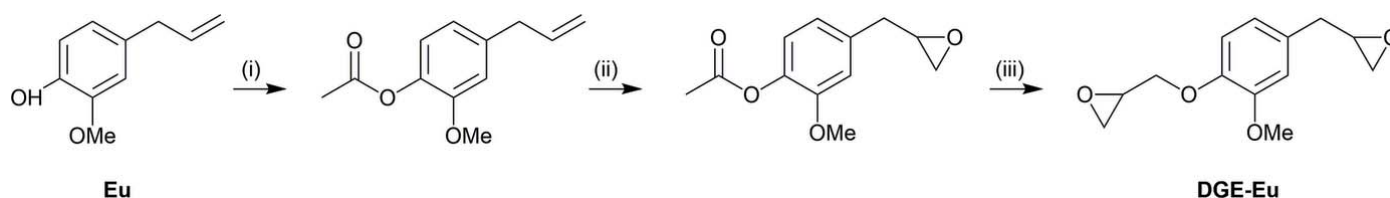
Figure 4
Reagents and conditions for the synthesis of **DGE-Eu** from eugenol (Qin *et al.*, 2014): (i) acetic anhydride, 358 K; (ii) *m*-chloroperoxybenzoic acid, CH_2Cl_2, room temperature; (iii) epichlorohydrin, NaOH, C_2H_5OH, 358 K.

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supporting information

Crystal structure of the diglycidyl ether of eugenol

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT2015 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2015* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2-[3-Methoxy-4-(oxiran-2-ylmethoxy)benzyl]oxirane

Crystal data

$C_{13}H_{16}O_4$	$F(000) = 504$
$M_r = 236.26$	$D_x = 1.340$ Mg m^{-3}
Monoclinic, Cc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: C -2yc	Cell parameters from 9992 reflections
$a = 9.8262$ (5) Å	$\theta = 2.7$–33.0°
$b = 13.4434$ (7) Å	$\mu = 0.10$ mm^{-1}
$c = 9.4251$ (8) Å	$T = 115$ K
$\beta = 109.897$ (2)°	Prism, colourless
$V = 1170.71$ (13) Å^3	0.4 × 0.35 × 0.3 mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	18897 measured reflections
Radiation source: X-ray tube, Siemens KFF Mo 2K-180	2680 independent reflections
	2586 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.021$
φ and ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$h = -12 \rightarrow 12$
	$k = -17 \rightarrow 17$
$T_{min} = 0.700$, $T_{max} = 0.747$	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	
$wR(F^2) = 0.121$	Hydrogen site location: inferred from neighbouring sites
$S = 1.07$	
2680 reflections	H-atom parameters constrained
160 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 1.3035P]$
2 restraints	where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.69$ e Å⁻³
$\Delta\rho_{min} = -0.28$ e Å⁻³

Absolute structure: Flack x determined using
1234 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.20 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.3186 (2)	0.75130 (14)	0.4046 (2)	0.0215 (4)	
O2	0.3043 (2)	0.59282 (15)	0.5548 (2)	0.0221 (4)	
O3	0.0296 (3)	0.4884 (2)	0.5717 (4)	0.0511 (9)	
O4	0.8644 (3)	0.79876 (18)	0.4484 (3)	0.0406 (7)	
C1	0.6472 (3)	0.6219 (2)	0.3926 (3)	0.0204 (6)	
C2	0.6394 (3)	0.5387 (2)	0.4744 (3)	0.0203 (5)	
H2	0.7121	0.4890	0.4925	0.024*	
C3	0.5262 (3)	0.5260 (2)	0.5313 (3)	0.0204 (6)	
H3	0.5220	0.4677	0.5867	0.025*	
C4	0.4203 (3)	0.5984 (2)	0.5068 (3)	0.0169 (5)	
C5	0.4272 (3)	0.6842 (2)	0.4242 (3)	0.0171 (5)	
C6	0.5397 (3)	0.6949 (2)	0.3680 (3)	0.0187 (5)	
H6	0.5441	0.7527	0.3119	0.022*	
C7	0.2935 (3)	0.5033 (3)	0.6333 (4)	0.0287 (7)	
H7A	0.3828	0.4935	0.7213	0.034*	
H7B	0.2807	0.4452	0.5655	0.034*	
C8	0.1678 (4)	0.5132 (3)	0.6838 (5)	0.0382 (8)	
H8	0.1691	0.5701	0.7526	0.046*	
C9	0.0890 (4)	0.4237 (4)	0.6998 (5)	0.0522 (12)	
H9A	0.1274	0.3584	0.6826	0.063*	
H9B	0.0428	0.4238	0.7782	0.063*	
C10	0.3084 (3)	0.8287 (2)	0.2985 (4)	0.0269 (6)	
H10A	0.3053	0.7997	0.2020	0.040*	
H10B	0.3929	0.8724	0.3366	0.040*	
H10C	0.2201	0.8674	0.2839	0.040*	
C11	0.7701 (3)	0.6367 (3)	0.3324 (4)	0.0278 (7)	
H11A	0.8071	0.5708	0.3159	0.033*	0.690 (11)
H11B	0.7323	0.6706	0.2334	0.033*	0.690 (11)
H11C	0.8536	0.5974	0.3965	0.033*	0.310 (11)
H11D	0.7401	0.6074	0.2299	0.033*	0.310 (11)
C13	0.9712 (4)	0.7691 (2)	0.3826 (4)	0.0324 (7)	
H13A	0.9471	0.7781	0.2725	0.039*	0.690 (11)
H13B	1.0745	0.7788	0.4434	0.039*	0.690 (11)
H13C	1.0477	0.7222	0.4401	0.039*	0.310 (11)
H13D	1.0014	0.8187	0.3216	0.039*	0.310 (11)

C12A	0.8911 (4)	0.6954 (3)	0.4331 (5)	0.0203 (11)	0.690 (11)
H12A	0.9476	0.6614	0.5295	0.024*	0.690 (11)
C12B	0.8184 (12)	0.7317 (8)	0.3230 (12)	0.032 (3)*	0.310 (11)
H12B	0.7600	0.7658	0.2274	0.038*	0.310 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0200 (9)	0.0204 (9)	0.0264 (10)	0.0043 (7)	0.0107 (7)	0.0072 (8)
O2	0.0216 (10)	0.0238 (10)	0.0222 (9)	−0.0004 (8)	0.0089 (8)	0.0056 (8)
O3	0.0229 (12)	0.0500 (17)	0.070 (2)	−0.0009 (11)	0.0028 (12)	0.0306 (16)
O4	0.0437 (14)	0.0246 (12)	0.0679 (18)	−0.0074 (10)	0.0379 (13)	−0.0174 (12)
C1	0.0174 (12)	0.0230 (13)	0.0210 (13)	−0.0033 (11)	0.0067 (10)	−0.0078 (11)
C2	0.0186 (12)	0.0202 (12)	0.0194 (12)	0.0029 (10)	0.0029 (10)	−0.0036 (10)
C3	0.0226 (13)	0.0187 (12)	0.0168 (12)	−0.0001 (10)	0.0026 (10)	0.0014 (9)
C4	0.0165 (12)	0.0195 (13)	0.0129 (11)	−0.0036 (9)	0.0026 (10)	0.0003 (9)
C5	0.0160 (11)	0.0170 (12)	0.0167 (11)	0.0005 (9)	0.0035 (9)	−0.0010 (9)
C6	0.0191 (12)	0.0175 (12)	0.0198 (12)	−0.0019 (9)	0.0068 (10)	−0.0008 (9)
C7	0.0218 (14)	0.0326 (16)	0.0299 (15)	0.0008 (12)	0.0067 (11)	0.0146 (13)
C8	0.0330 (17)	0.042 (2)	0.0429 (19)	0.0016 (15)	0.0170 (15)	0.0098 (16)
C9	0.0247 (16)	0.056 (2)	0.075 (3)	0.0001 (16)	0.0159 (18)	0.040 (2)
C10	0.0292 (15)	0.0234 (14)	0.0304 (15)	0.0051 (12)	0.0133 (12)	0.0108 (12)
C11	0.0215 (13)	0.0314 (16)	0.0346 (16)	−0.0047 (12)	0.0146 (12)	−0.0140 (12)
C13	0.0323 (16)	0.0259 (14)	0.049 (2)	−0.0044 (13)	0.0267 (15)	−0.0069 (14)
C12A	0.021 (2)	0.020 (2)	0.023 (2)	0.0008 (15)	0.0118 (16)	−0.0013 (15)

Geometric parameters (Å, º)

O1—C5	1.361 (3)	C8—H8	1.0000
O1—C10	1.423 (3)	C8—C9	1.467 (5)
O2—C4	1.364 (3)	C9—H9A	0.9900
O2—C7	1.435 (3)	C9—H9B	0.9900
O3—C8	1.447 (5)	C10—H10A	0.9800
O3—C9	1.441 (4)	C10—H10B	0.9800
O4—C13	1.444 (4)	C10—H10C	0.9800
O4—C12A	1.430 (4)	C11—H11A	0.9900
O4—C12B	1.432 (11)	C11—H11B	0.9900
C1—C2	1.374 (4)	C11—H11C	0.9900
C1—C6	1.402 (4)	C11—H11D	0.9900
C1—C11	1.513 (4)	C11—C12A	1.473 (5)
C2—H2	0.9500	C11—C12B	1.375 (12)
C2—C3	1.400 (4)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C3—C4	1.386 (4)	C13—H13C	0.9900
C4—C5	1.406 (4)	C13—H13D	0.9900
C5—C6	1.386 (4)	C13—C12A	1.443 (5)
C6—H6	0.9500	C13—C12B	1.499 (12)
C7—H7A	0.9900	C12A—H12A	1.0000

C7—H7B	0.9900	C12B—H12B	1.0000
C7—C8	1.473 (5)		
C5—O1—C10	116.4 (2)	O1—C10—H10B	109.5
C4—O2—C7	115.7 (2)	O1—C10—H10C	109.5
C9—O3—C8	61.1 (2)	H10A—C10—H10B	109.5
C12A—O4—C13	60.3 (2)	H10A—C10—H10C	109.5
C12B—O4—C13	62.8 (5)	H10B—C10—H10C	109.5
C2—C1—C6	118.7 (3)	C1—C11—H11A	108.8
C2—C1—C11	121.4 (3)	C1—C11—H11B	108.8
C6—C1—C11	119.9 (3)	C1—C11—H11C	107.6
C1—C2—H2	119.4	C1—C11—H11D	107.6
C1—C2—C3	121.1 (3)	H11A—C11—H11B	107.7
C3—C2—H2	119.4	H11C—C11—H11D	107.0
C2—C3—H3	120.0	C12A—C11—C1	113.6 (3)
C4—C3—C2	120.0 (2)	C12A—C11—H11A	108.8
C4—C3—H3	120.0	C12A—C11—H11B	108.8
O2—C4—C3	124.8 (2)	C12B—C11—C1	118.9 (5)
O2—C4—C5	115.6 (2)	C12B—C11—H11C	107.6
C3—C4—C5	119.6 (2)	C12B—C11—H11D	107.6
O1—C5—C4	115.8 (2)	O4—C13—H13A	117.8
O1—C5—C6	124.7 (2)	O4—C13—H13B	117.8
C6—C5—C4	119.5 (2)	O4—C13—H13C	118.0
C1—C6—H6	119.4	O4—C13—H13D	118.0
C5—C6—C1	121.2 (2)	O4—C13—C12B	58.2 (5)
C5—C6—H6	119.4	H13A—C13—H13B	115.0
O2—C7—H7A	110.1	H13C—C13—H13D	115.1
O2—C7—H7B	110.1	C12A—C13—O4	59.4 (2)
O2—C7—C8	108.0 (3)	C12A—C13—H13A	117.8
H7A—C7—H7B	108.4	C12A—C13—H13B	117.8
C8—C7—H7A	110.1	C12B—C13—H13C	118.0
C8—C7—H7B	110.1	C12B—C13—H13D	118.0
O3—C8—C7	115.2 (3)	O4—C12A—C11	116.8 (3)
O3—C8—H8	116.8	O4—C12A—C13	60.4 (2)
O3—C8—C9	59.3 (2)	O4—C12A—H12A	114.7
C7—C8—H8	116.8	C11—C12A—H12A	114.7
C9—C8—C7	119.3 (4)	C13—C12A—C11	124.5 (4)
C9—C8—H8	116.8	C13—C12A—H12A	114.7
O3—C9—C8	59.7 (2)	O4—C12B—C13	59.0 (5)
O3—C9—H9A	117.8	O4—C12B—H12B	112.2
O3—C9—H9B	117.8	C11—C12B—O4	123.4 (8)
C8—C9—H9A	117.8	C11—C12B—C13	127.6 (8)
C8—C9—H9B	117.8	C11—C12B—H12B	112.2
H9A—C9—H9B	114.9	C13—C12B—H12B	112.2
O1—C10—H10A	109.5		
O1—C5—C6—C1	−179.6 (3)	C3—C4—C5—O1	179.6 (2)
O2—C4—C5—O1	0.9 (3)	C3—C4—C5—C6	0.2 (4)

O2—C4—C5—C6	−178.5 (2)	C4—O2—C7—C8	176.7 (3)
O2—C7—C8—O3	83.5 (4)	C4—C5—C6—C1	−0.2 (4)
O2—C7—C8—C9	150.9 (4)	C6—C1—C2—C3	0.6 (4)
O4—C13—C12A—C11	103.8 (4)	C6—C1—C11—C12A	84.8 (4)
O4—C13—C12B—C11	−110.4 (10)	C6—C1—C11—C12B	31.8 (7)
C1—C2—C3—C4	−0.7 (4)	C7—O2—C4—C3	−1.3 (4)
C1—C11—C12A—O4	−69.5 (4)	C7—O2—C4—C5	177.3 (2)
C1—C11—C12A—C13	−140.5 (3)	C7—C8—C9—O3	−103.5 (4)
C1—C11—C12B—O4	54.5 (11)	C9—O3—C8—C7	110.4 (4)
C1—C11—C12B—C13	128.8 (8)	C10—O1—C5—C4	−168.6 (2)
C2—C1—C6—C5	−0.1 (4)	C10—O1—C5—C6	10.8 (4)
C2—C1—C11—C12A	−93.8 (4)	C11—C1—C2—C3	179.3 (2)
C2—C1—C11—C12B	−146.8 (6)	C11—C1—C6—C5	−178.8 (2)
C2—C3—C4—O2	178.8 (2)	C13—O4—C12A—C11	−116.3 (4)
C2—C3—C4—C5	0.3 (4)	C13—O4—C12B—C11	117.2 (10)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the benzene ring (C1–C6).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C7—H7*B*⋯O4[i]	0.99	2.53	3.452 (4)	155
C11—H11*C*⋯O3[ii]	0.99	2.43	3.413 (4)	170
C13—H13*B*⋯O1[ii]	0.99	2.57	3.358 (4)	136
C12*A*—H12*A*⋯O3[ii]	1.00	2.45	3.177 (5)	129
C7—H7*A*⋯Cg[iii]	0.99	2.57	3.465 (4)	150

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