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Diethyl 4,4′-[(1,3-dioxolane-2,2-diyl)-bis(propylideneoxy)]dibenzoate

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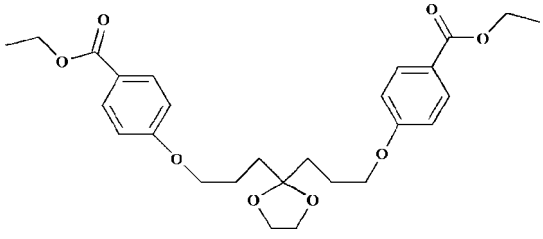
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.138; data-to-parameter ratio = 19.3.

The title ester, $C_{27}H_{34}O_8$, was synthesized by reacting 1,7-dichloro-4-oxoheptane, sodium hydroxide and ethyl *p*-hydroxybenzoate at 333 K in dimethyl sulfoxide. The 1,3-dioxolane ring is planar [largest deviation from the mean plane = 0.080 (1) Å] and makes dihedral angles of 59.83 (6) and 86.01 (6)° with the benzene rings. The angle between the mean planes of the two benzene rings is 36.05 (8)°.

Related literature

For related literature, see: Gonzàlez-Duarte *et al.* (1996); Ping *et al.* (2007); Ríos-Moreno *et al.* (2003).



Experimental

Crystal data

$C_{27}H_{34}O_8$
M_r = 486.54
Monoclinic, $P2_1/c$
a = 20.445 (3) Å
b = 7.1533 (9) Å
c = 18.828 (3) Å
β = 111.178 (2)°
V = 2567.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.980
15083 measured reflections
6146 independent reflections
4195 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.138
S = 1.04
6146 reflections
318 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2261).

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supplementary materials

Acta Cryst. (2007). E**63**, o4674 [**doi:10.1107/S1600536807057200**]

Diethyl 4,4'-[(1,3-dioxolane-2,2-diyl)bis(propylideneoxy)]dibenzoate

L.-P. Zhang, Z.-F. Jia, G.-H. Wei and Y.-Y. Liu

Comment

Dicarboxylic ester is a precursor for the synthesis

of dicarboxylate found as bridging ligand. In this

paper, the structure of the title compound, (I), is

described.

In the title compound (I), the 1,3-dioxolane is planar with the largest deviation from the mean plane being 0.080 (1) Å. It makes dihedral angles of 59.83 (6)° and 86.01 (6) respectively with the benzene rings (Fig. 1). The angle between the mean planes of the two benzene rings is 36.05 (8)°.

Both the C3—O1 (1.203 (2) Å) and the C25—O7 (1.197 (2) Å) distances are similar to those of coordinated ester molecules (Gonzàlez-Duarte *et al.*, 1996; Ríos-Moreno *et al.*, 2003). The C3—O2 and the C25—O8 distances are shorter than that of the reported ester molecule (Ping *et al.*, 2007). The O1—C3—O2 and O7—C25—O8 angles are 122.7 (2)° and 123.3 (2)° respectively.

Experimental

To a solution of 1,7-dichloro-4-oxoheptane (5.3 g, 3.0 mmol) and ethylene glycol (1.9 g, 3.0 mmol) in cyclohexane (22.5 ml) was added 0.015 g sodium bisulfate. The reaction mixture was refluxed for 3 h with azeotropic removal of water *via* a Dean–Stark trap, until there was no water created. The resulting clear solution was cooled down, washed with water twice, and then distilled. Collected the distillation between 447 K and 453 K.

A mixture of ethyl *p*-hydroxybenzoate (8.3 g, 50 mmol) and NaOH (2.0 g, 50 mmol) in DMSO (10 ml) was stirred at 333 K for 1 h, and then the collected distillation (5.5 g, 25 mmol) in the last step was added. The mixture was cooled to room temperature after stirring at 333 K for 2 h, then poured into 200 ml of water and a white solid formed immediately. The obtained precipitate (0.20 g) was dissolved in 15 ml me thanol, and colorless single crystals of (I) were obtained after several days at room temperature.

Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic), 0.97 Å (methylene) or 0.96Å (methyl) with U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$, $C_{methylene}$) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

Figures

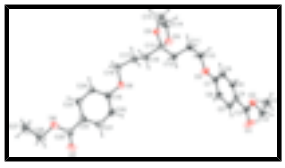


Fig. 1. Molecular view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as smal spheres of arbitrary radii.

Diethyl 4,4'-[(1,3-dioxolane-2,2-diyl)bis(propylideneoxy)]dibenzoate

Crystal data

$C_{27}H_{34}O_8$	F_{000} = 1040
M_r = 486.54	D_x = 1.259 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6146 reflections
a = 20.445 (3) Å	θ = 2.1–28.4º
b = 7.1533 (9) Å	μ = 0.09 mm^{-1}
c = 18.828 (3) Å	T = 273 (2) K
β = 111.178 (2)º	Block, colorless
V = 2567.6 (6) Å^3	0.40 × 0.30 × 0.25 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	6146 independent reflections
Radiation source: fine-focus sealed tube	4195 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 273(2) K	θ_{max} = 28.4º
ω scans	θ_{min} = 2.1º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	h = −26→22
T_{min} = 0.970, T_{max} = 0.980	k = −7→9
15083 measured reflections	l = −23→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.138	$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.323P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$

6146 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
318 parameters	$\Delta\rho_{min} = -0.20$ 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}
C1	0.02684 (12)	−0.3465 (3)	0.84609 (13)	0.0823 (6)
H1A	0.0708	−0.3324	0.8876	0.123*
H1B	−0.0016	−0.4364	0.8596	0.123*
H1C	0.0030	−0.2284	0.8355	0.123*
C2	0.03974 (11)	−0.4122 (3)	0.77711 (12)	0.0746 (5)
H2A	0.0619	−0.5343	0.7864	0.090*
H2B	−0.0043	−0.4223	0.7343	0.090*
C3	0.10844 (9)	−0.3230 (2)	0.70460 (10)	0.0607 (4)
C4	0.15387 (8)	−0.1780 (2)	0.69055 (9)	0.0518 (4)
C5	0.17838 (9)	−0.2043 (2)	0.63103 (10)	0.0586 (4)
H5	0.1656	−0.3113	0.6012	0.070*
C6	0.22105 (9)	−0.0743 (2)	0.61594 (9)	0.0577 (4)
H6	0.2371	−0.0938	0.5762	0.069*
C7	0.24012 (8)	0.0860 (2)	0.66001 (8)	0.0490 (3)
C8	0.21656 (8)	0.1141 (2)	0.72001 (9)	0.0534 (4)
H8	0.2297	0.2209	0.7501	0.064*
C9	0.17343 (8)	−0.0179 (2)	0.73460 (9)	0.0534 (4)
H9	0.1574	0.0011	0.7744	0.064*
C10	0.30664 (9)	0.3697 (2)	0.68653 (10)	0.0552 (4)
H10A	0.3370	0.3332	0.7374	0.066*
H10B	0.2674	0.4396	0.6905	0.066*
C11	0.34663 (8)	0.4888 (2)	0.64991 (9)	0.0525 (4)
H11A	0.3615	0.6027	0.6793	0.063*
H11B	0.3154	0.5238	0.5992	0.063*
C12	0.41081 (7)	0.3922 (2)	0.64395 (8)	0.0462 (3)
H12A	0.4380	0.3384	0.6931	0.055*
H12B	0.3954	0.2906	0.6076	0.055*
C13	0.45780 (7)	0.52163 (19)	0.61951 (7)	0.0414 (3)

C14	0.42956 (14)	0.8031 (3)	0.55640 (12)	0.0881 (7)
H14A	0.3858	0.8718	0.5365	0.106*
H14B	0.4590	0.8399	0.5283	0.106*
C15	0.46497 (11)	0.8422 (2)	0.63740 (10)	0.0681 (5)
H15A	0.5066	0.9171	0.6457	0.082*
H15B	0.4340	0.9098	0.6571	0.082*
C16	0.51950 (7)	0.4206 (2)	0.60861 (8)	0.0464 (3)
H16A	0.5020	0.3088	0.5786	0.056*
H16B	0.5389	0.5011	0.5797	0.056*
C17	0.57797 (8)	0.3653 (2)	0.68199 (8)	0.0509 (4)
H17A	0.5929	0.4749	0.7141	0.061*
H17B	0.5599	0.2753	0.7088	0.061*
C18	0.64087 (8)	0.2817 (2)	0.66954 (9)	0.0521 (4)
H18A	0.6545	0.3597	0.6350	0.063*
H18B	0.6802	0.2741	0.7176	0.063*
C19	0.67059 (7)	0.0015 (2)	0.61767 (8)	0.0454 (3)
C20	0.65193 (8)	−0.1792 (2)	0.59131 (9)	0.0543 (4)
H20	0.6090	−0.2270	0.5891	0.065*
C21	0.69578 (8)	−0.2883 (2)	0.56840 (9)	0.0537 (4)
H21	0.6823	−0.4090	0.5508	0.064*
C22	0.76018 (8)	−0.2196 (2)	0.57126 (8)	0.0511 (4)
C23	0.77802 (8)	−0.0381 (2)	0.59612 (10)	0.0610 (4)
H23	0.8204	0.0107	0.5967	0.073*
C24	0.73444 (8)	0.0730 (2)	0.62020 (10)	0.0569 (4)
H24	0.7478	0.1938	0.6378	0.068*
C25	0.80624 (9)	−0.3425 (3)	0.54606 (10)	0.0633 (4)
C26	0.90744 (14)	−0.3554 (3)	0.51253 (19)	0.1142 (10)
H26A	0.9328	−0.4491	0.5495	0.137*
H26B	0.8797	−0.4190	0.4659	0.137*
C27	0.95507 (16)	−0.2345 (4)	0.49826 (19)	0.1164 (9)
H27A	0.9298	−0.1401	0.4626	0.175*
H27B	0.9840	−0.3041	0.4774	0.175*
H27C	0.9840	−0.1763	0.5450	0.175*
O1	0.09351 (9)	−0.4681 (2)	0.67015 (9)	0.1014 (5)
O2	0.08523 (6)	−0.27723 (16)	0.76033 (7)	0.0661 (3)
O3	0.28179 (6)	0.20775 (16)	0.64019 (6)	0.0605 (3)
O4	0.41679 (5)	0.61061 (14)	0.54943 (5)	0.0524 (3)
O5	0.48317 (5)	0.66843 (14)	0.67395 (5)	0.0501 (3)
O6	0.62232 (5)	0.09811 (14)	0.63770 (6)	0.0526 (3)
O7	0.79521 (8)	−0.50437 (19)	0.53014 (10)	0.0900 (4)
O8	0.86127 (7)	−0.25069 (19)	0.54170 (9)	0.0838 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0864 (14)	0.0771 (13)	0.1029 (15)	0.0097 (11)	0.0576 (12)	0.0188 (11)
C2	0.0739 (11)	0.0675 (11)	0.0927 (14)	−0.0166 (9)	0.0424 (10)	0.0046 (10)
C3	0.0622 (9)	0.0556 (9)	0.0676 (10)	−0.0103 (8)	0.0274 (8)	−0.0040 (8)

C4	0.0486 (8)	0.0490 (8)	0.0586 (9)	−0.0037 (7)	0.0201 (7)	−0.0008 (7)
C5	0.0665 (10)	0.0512 (9)	0.0601 (10)	−0.0099 (7)	0.0252 (8)	−0.0129 (7)
C6	0.0660 (10)	0.0589 (9)	0.0555 (9)	−0.0062 (8)	0.0309 (8)	−0.0097 (7)
C7	0.0472 (8)	0.0518 (8)	0.0509 (8)	−0.0057 (6)	0.0211 (6)	−0.0026 (7)
C8	0.0574 (9)	0.0512 (8)	0.0578 (9)	−0.0099 (7)	0.0282 (7)	−0.0109 (7)
C9	0.0537 (8)	0.0534 (9)	0.0601 (9)	−0.0047 (7)	0.0291 (7)	−0.0048 (7)
C10	0.0575 (9)	0.0540 (9)	0.0636 (9)	−0.0105 (7)	0.0336 (8)	−0.0116 (7)
C11	0.0556 (9)	0.0497 (8)	0.0589 (9)	−0.0058 (7)	0.0288 (7)	−0.0044 (7)
C12	0.0499 (8)	0.0450 (8)	0.0472 (8)	−0.0030 (6)	0.0218 (6)	0.0016 (6)
C13	0.0471 (7)	0.0426 (7)	0.0338 (6)	−0.0021 (6)	0.0139 (5)	0.0003 (5)
C14	0.1272 (19)	0.0538 (11)	0.0686 (12)	0.0055 (11)	0.0177 (12)	0.0171 (9)
C15	0.1049 (14)	0.0425 (8)	0.0639 (10)	−0.0050 (9)	0.0390 (10)	0.0012 (7)
C16	0.0520 (8)	0.0498 (8)	0.0432 (7)	−0.0041 (6)	0.0241 (6)	0.0000 (6)
C17	0.0528 (8)	0.0552 (9)	0.0493 (8)	0.0013 (7)	0.0241 (7)	0.0014 (7)
C18	0.0498 (8)	0.0512 (8)	0.0591 (9)	−0.0029 (7)	0.0241 (7)	0.0005 (7)
C19	0.0429 (7)	0.0476 (8)	0.0463 (8)	−0.0009 (6)	0.0170 (6)	0.0048 (6)
C20	0.0496 (8)	0.0513 (8)	0.0639 (9)	−0.0106 (7)	0.0227 (7)	0.0041 (7)
C21	0.0607 (9)	0.0449 (8)	0.0544 (9)	−0.0065 (7)	0.0195 (7)	−0.0006 (7)
C22	0.0515 (8)	0.0535 (8)	0.0484 (8)	−0.0013 (7)	0.0180 (7)	−0.0056 (6)
C23	0.0463 (8)	0.0659 (10)	0.0759 (11)	−0.0128 (8)	0.0282 (8)	−0.0181 (8)
C24	0.0483 (8)	0.0540 (9)	0.0723 (10)	−0.0124 (7)	0.0264 (7)	−0.0167 (8)
C25	0.0612 (10)	0.0609 (10)	0.0694 (11)	−0.0005 (8)	0.0256 (8)	−0.0096 (8)
C26	0.1107 (19)	0.0841 (15)	0.186 (3)	−0.0003 (14)	0.099 (2)	−0.0398 (17)
C27	0.126 (2)	0.1080 (19)	0.157 (3)	0.0088 (16)	0.102 (2)	−0.0145 (18)
O1	0.1405 (14)	0.0758 (9)	0.1170 (12)	−0.0527 (9)	0.0816 (11)	−0.0353 (9)
O2	0.0699 (7)	0.0577 (7)	0.0833 (8)	−0.0126 (6)	0.0429 (7)	−0.0037 (6)
O3	0.0704 (7)	0.0621 (7)	0.0611 (7)	−0.0204 (6)	0.0382 (6)	−0.0136 (5)
O4	0.0580 (6)	0.0573 (6)	0.0379 (5)	−0.0015 (5)	0.0124 (4)	0.0065 (4)
O5	0.0602 (6)	0.0420 (5)	0.0434 (5)	−0.0025 (4)	0.0132 (5)	−0.0037 (4)
O6	0.0459 (5)	0.0482 (6)	0.0698 (7)	−0.0037 (4)	0.0280 (5)	0.0013 (5)
O7	0.0909 (10)	0.0598 (8)	0.1276 (13)	−0.0012 (7)	0.0495 (9)	−0.0207 (8)
O8	0.0768 (8)	0.0726 (8)	0.1228 (12)	−0.0071 (7)	0.0609 (8)	−0.0309 (8)

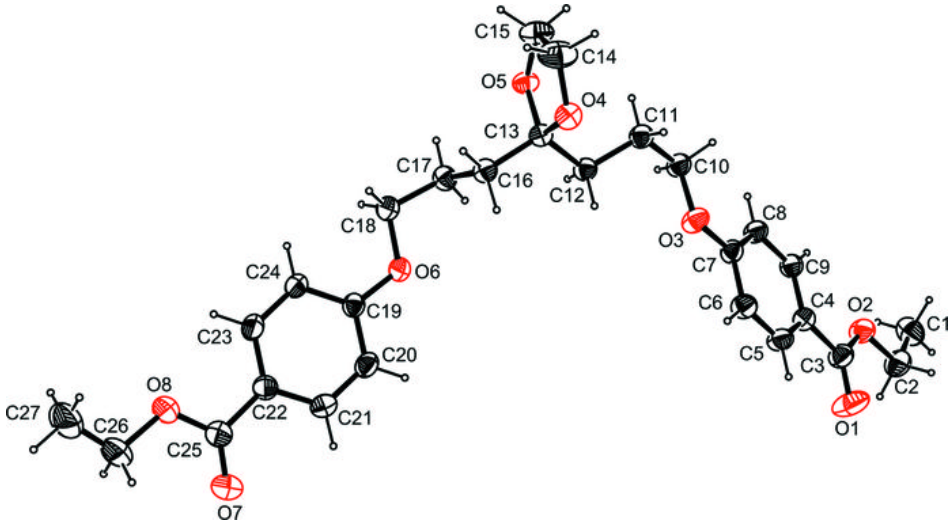
Geometric parameters (Å, °)

C1—C2	1.491 (3)	C14—H14A	0.9700
C1—H1A	0.9600	C14—H14B	0.9700
C1—H1B	0.9600	C15—O5	1.4041 (19)
C1—H1C	0.9600	C15—H15A	0.9700
C2—O2	1.452 (2)	C15—H15B	0.9700
C2—H2A	0.9700	C16—C17	1.517 (2)
C2—H2B	0.9700	C16—H16A	0.9700
C3—O1	1.204 (2)	C16—H16B	0.9700
C3—O2	1.339 (2)	C17—C18	1.511 (2)
C3—C4	1.479 (2)	C17—H17A	0.9700
C4—C9	1.385 (2)	C17—H17B	0.9700
C4—C5	1.396 (2)	C18—O6	1.4368 (18)
C5—C6	1.373 (2)	C18—H18A	0.9700
C5—H5	0.9300	C18—H18B	0.9700

C6—C7	1.386 (2)	C19—O6	1.3647 (17)
C6—H6	0.9300	C19—C24	1.387 (2)
C7—O3	1.3613 (17)	C19—C20	1.388 (2)
C7—C8	1.394 (2)	C20—C21	1.371 (2)
C8—C9	1.386 (2)	C20—H20	0.9300
C8—H8	0.9300	C21—C22	1.388 (2)
C9—H9	0.9300	C21—H21	0.9300
C10—O3	1.4289 (18)	C22—C23	1.384 (2)
C10—C11	1.509 (2)	C22—C25	1.486 (2)
C10—H10A	0.9700	C23—C24	1.387 (2)
C10—H10B	0.9700	C23—H23	0.9300
C11—C12	1.523 (2)	C24—H24	0.9300
C11—H11A	0.9700	C25—O7	1.197 (2)
C11—H11B	0.9700	C25—O8	1.331 (2)
C12—C13	1.5204 (18)	C26—C27	1.399 (3)
C12—H12A	0.9700	C26—O8	1.459 (2)
C12—H12B	0.9700	C26—H26A	0.9700
C13—O5	1.4277 (16)	C26—H26B	0.9700
C13—O4	1.4316 (16)	C27—H27A	0.9600
C13—C16	1.5305 (19)	C27—H27B	0.9600
C14—O4	1.399 (2)	C27—H27C	0.9600
C14—C15	1.459 (3)		
C2—C1—H1A	109.5	O5—C15—C14	106.64 (14)
C2—C1—H1B	109.5	O5—C15—H15A	110.4
H1A—C1—H1B	109.5	C14—C15—H15A	110.4
C2—C1—H1C	109.5	O5—C15—H15B	110.4
H1A—C1—H1C	109.5	C14—C15—H15B	110.4
H1B—C1—H1C	109.5	H15A—C15—H15B	108.6
O2—C2—C1	107.97 (16)	C17—C16—C13	114.68 (11)
O2—C2—H2A	110.1	C17—C16—H16A	108.6
C1—C2—H2A	110.1	C13—C16—H16A	108.6
O2—C2—H2B	110.1	C17—C16—H16B	108.6
C1—C2—H2B	110.1	C13—C16—H16B	108.6
H2A—C2—H2B	108.4	H16A—C16—H16B	107.6
O1—C3—O2	122.72 (15)	C18—C17—C16	113.37 (12)
O1—C3—C4	124.21 (16)	C18—C17—H17A	108.9
O2—C3—C4	113.07 (14)	C16—C17—H17A	108.9
C9—C4—C5	118.85 (14)	C18—C17—H17B	108.9
C9—C4—C3	122.47 (14)	C16—C17—H17B	108.9
C5—C4—C3	118.68 (14)	H17A—C17—H17B	107.7
C6—C5—C4	120.93 (15)	O6—C18—C17	108.38 (12)
C6—C5—H5	119.5	O6—C18—H18A	110.0
C4—C5—H5	119.5	C17—C18—H18A	110.0
C5—C6—C7	119.91 (14)	O6—C18—H18B	110.0
C5—C6—H6	120.0	C17—C18—H18B	110.0
C7—C6—H6	120.0	H18A—C18—H18B	108.4
O3—C7—C6	115.69 (13)	O6—C19—C24	124.70 (13)
O3—C7—C8	124.32 (13)	O6—C19—C20	115.96 (12)
C6—C7—C8	119.99 (14)	C24—C19—C20	119.32 (14)

C9—C8—C7	119.56 (14)	C21—C20—C19	121.10 (14)
C9—C8—H8	120.2	C21—C20—H20	119.4
C7—C8—H8	120.2	C19—C20—H20	119.4
C4—C9—C8	120.76 (14)	C20—C21—C22	120.34 (14)
C4—C9—H9	119.6	C20—C21—H21	119.8
C8—C9—H9	119.6	C22—C21—H21	119.8
O3—C10—C11	108.09 (12)	C23—C22—C21	118.41 (14)
O3—C10—H10A	110.1	C23—C22—C25	122.90 (14)
C11—C10—H10A	110.1	C21—C22—C25	118.67 (14)
O3—C10—H10B	110.1	C22—C23—C24	121.76 (14)
C11—C10—H10B	110.1	C22—C23—H23	119.1
H10A—C10—H10B	108.4	C24—C23—H23	119.1
C10—C11—C12	113.66 (13)	C23—C24—C19	119.03 (14)
C10—C11—H11A	108.8	C23—C24—H24	120.5
C12—C11—H11A	108.8	C19—C24—H24	120.5
C10—C11—H11B	108.8	O7—C25—O8	123.31 (16)
C12—C11—H11B	108.8	O7—C25—C22	124.65 (16)
H11A—C11—H11B	107.7	O8—C25—C22	112.04 (14)
C13—C12—C11	113.68 (12)	C27—C26—O8	110.2 (2)
C13—C12—H12A	108.8	C27—C26—H26A	109.6
C11—C12—H12A	108.8	O8—C26—H26A	109.6
C13—C12—H12B	108.8	C27—C26—H26B	109.6
C11—C12—H12B	108.8	O8—C26—H26B	109.6
H12A—C12—H12B	107.7	H26A—C26—H26B	108.1
O5—C13—O4	105.94 (10)	C26—C27—H27A	109.5
O5—C13—C12	109.64 (11)	C26—C27—H27B	109.5
O4—C13—C12	109.03 (11)	H27A—C27—H27B	109.5
O5—C13—C16	109.88 (11)	C26—C27—H27C	109.5
O4—C13—C16	108.84 (10)	H27A—C27—H27C	109.5
C12—C13—C16	113.24 (11)	H27B—C27—H27C	109.5
O4—C14—C15	106.96 (14)	C3—O2—C2	116.36 (14)
O4—C14—H14A	110.3	C7—O3—C10	118.10 (11)
C15—C14—H14A	110.3	C14—O4—C13	108.90 (12)
O4—C14—H14B	110.3	C15—O5—C13	109.63 (11)
C15—C14—H14B	110.3	C19—O6—C18	118.04 (11)
H14A—C14—H14B	108.6	C25—O8—C26	116.51 (16)

Fig. 1


C15
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