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5,5′,7,7′-Tetramethoxy-2,2′-ethano-1,1′-spirobiindane

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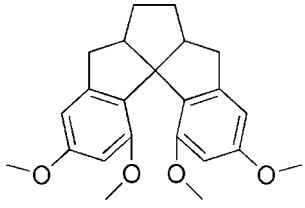
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.101; data-to-parameter ratio = 14.4.

In the title compound, $C_{23}H_{26}O_4$, there is a dihedral angle of 83.7 (6)° between the two benzene rings. The five-membered rings have chair conformations.

Related literature

For related literature, see: Bandin *et al.* (2000); Birman *et al.* (1999); Lan *et al.* (2006); Zhu *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{26}O_4$
M_r = 366.44
Monoclinic, $P2_1/c$
a = 12.7089 (11) Å
b = 10.0905 (8) Å
c = 16.1664 (13) Å
β = 104.306 (2)°
V = 2008.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.33 × 0.21 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.974, T_{max} = 0.988
9884 measured reflections
3576 independent reflections
2013 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.08
3576 reflections
249 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2064).

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supplementary materials

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5,5',7,7'-Tetramethoxy-2,2'-ethano-1,1'-spirobiindane

W.-X. Hu, J.-F. Wei and X.-Y. Shi

Comment

The symmetric chiral ligands, such as BINOL (1,1'-binaphthalene-2,2'-diol), BINAP [2,2'-bis(diphenylphosphino)-1,1'-binaphthyl], SPINOL (1,1'-spirobiindane-7,7'-diol), *etc*, are widely used in catalytic asymmetric synthesis (Lan *et al.*, 2006; Birman *et al.*, 1999; Zhu *et al.*, 2005). Even minor modifications of the chiral ligands were found to enhance manifold functional capability of these ligands in asymmetric catalysis (Bandin *et al.*, 2000). We also report the synthesis of the title compound here.

The title compound (Fig. 1) was obtained in three steps (experimental section). The molecule has an approximate C_2 symmetry. Two phenyl groups make a dihedral angle of 83.7 (6)°.

Experimental

A solution of 3,5-dimethoxybenzaldehyde (7.9 g, 47.6 mmol) and cyclopentanone (2 g, 23.8 mmol) in 20 ml of ethanol was added to a solution of 0.8 g of NaOH in 30 ml 50% aqueous ethanol over a period of 30 min and stirred for 8 h at room temperature. The yellow solid obtained was filtered and washed with water and the product vacuum dried (7.2 g, 85%). The yellow product is 2,6-bis(3,5-dimethoxybenzylidene)cyclopentanone, which was dissolveed in 30 ml of acetone and then stirred with Raney nickel (3 g) under hydrogen atmosphere at room temperature and the reaction progress monitored by TLC. Upon disappearance of the starting material in TLC (*ca* 12 h, rotary evaporator), the reaction mixture was carefully filtered off without allowing the Raney nickel to become dry by washing with acetone and the filtrate was concentrated in a rotary evaporator. The crude product was crystallized from 95% ethanol to yield 2,6-bis(3,5-dimethoxybenzyl)cyclopentanone (2.8 g, 92.4%). This compound (2 g, 5.56 mmol) and $H_3PW_{12}O_{40}$ (2.57 g, 0.834 mmol) in 20 ml toluene were charged in a 50 ml flask with water segregator and reflux condenser, followed by reflux and dehydration until no water was separated for 12 h when the solution turned red slowly, then cooled, filtered and washed with $CHCl_3$. The organic phase was combined, evaporated and the residue was recrystallized from a hexane–ethyl acetate (3:1) mixture to give 1.8 g of the title compound (88.7% yield).

$_1$H NMR: ($CDCl_3$) 1.23–1.29 (m, 2H), 1.96–2.00 (m, 2H), 2.61–2.66 (m, 4H), 3.36–3.44 (m, 2H), 3.55 (s, 6H), 3.77 (s, 6H), 6.20 (s, 2H), 6.34 (s,2*H*).

Refinement

The H atoms (pyridine ring) were placed in calculated positions [Csp^2—H = 0.93 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

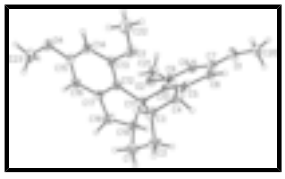


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.

5,5',7,7'-Tetramethoxy-2,2'-ethano-1,1'-spirobiindane

Crystal data

$C_{23}H_{26}O_4$	F_{000} = 784
M_r = 366.44	D_x = 1.212 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3576 reflections
a = 12.7089 (11) Å	θ = 1.7–25.1º
b = 10.0905 (8) Å	μ = 0.08 mm^{-1}
c = 16.1664 (13) Å	T = 298 (2) K
β = 104.306 (2)º	Block, colourless
V = 2008.9 (3) Å^3	0.33 × 0.21 × 0.15 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	3576 independent reflections
Radiation source: fine-focus sealed tube	2013 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 298(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −15→15
T_{min} = 0.974, T_{max} = 0.988	k = −12→11
9884 measured reflections	l = −11→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.101	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
3576 reflections	$\Delta\rho_{min}$ = −0.10 e Å^{-3}

249 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0095 (8)

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}
O1	0.01787 (11)	0.00651 (13)	0.11905 (9)	0.0934 (5)
O2	0.11557 (9)	0.45860 (11)	0.10743 (7)	0.0615 (3)
O3	0.26734 (10)	0.31122 (11)	−0.09967 (7)	0.0720 (4)
O4	0.21271 (10)	0.76096 (12)	−0.18685 (8)	0.0753 (4)
C1	0.48840 (15)	0.4601 (2)	0.18491 (13)	0.0857 (6)
H1A	0.5280	0.5093	0.1508	0.103*
H1B	0.5161	0.4837	0.2445	0.103*
C2	0.49705 (15)	0.3121 (2)	0.17181 (13)	0.0844 (6)
H2A	0.4716	0.2625	0.2145	0.101*
H2B	0.5713	0.2865	0.1743	0.101*
C3	0.42396 (14)	0.28916 (18)	0.08308 (11)	0.0666 (5)
H3	0.4621	0.3118	0.0392	0.080*
C4	0.37550 (15)	0.14983 (17)	0.06805 (12)	0.0730 (6)
H4A	0.3700	0.1214	0.0098	0.088*
H4B	0.4198	0.0866	0.1068	0.088*
C5	0.26458 (14)	0.16203 (17)	0.08514 (10)	0.0574 (5)
C6	0.19459 (17)	0.06072 (17)	0.09508 (11)	0.0671 (5)
H6	0.2143	−0.0277	0.0930	0.081*
C7	0.09506 (15)	0.09546 (18)	0.10816 (11)	0.0641 (5)
C8	0.06579 (14)	0.22698 (17)	0.11182 (10)	0.0597 (5)
H8	−0.0019	0.2483	0.1204	0.072*
C9	0.13625 (13)	0.32636 (15)	0.10281 (10)	0.0505 (4)
C10	0.23758 (13)	0.29369 (15)	0.08937 (9)	0.0496 (4)
C11	0.32709 (12)	0.38749 (16)	0.07973 (9)	0.0514 (4)
C12	0.29743 (12)	0.47861 (16)	0.00341 (10)	0.0503 (4)
C13	0.26767 (13)	0.44407 (16)	−0.08266 (10)	0.0517 (4)
C14	0.24065 (13)	0.54127 (17)	−0.14428 (10)	0.0566 (5)
H14	0.2207	0.5184	−0.2018	0.068*

C15	0.24339 (13)	0.67340 (17)	−0.11997 (11)	0.0571 (5)
C16	0.27449 (13)	0.71002 (16)	−0.03510 (12)	0.0604 (5)
H16	0.2774	0.7988	−0.0192	0.072*
C17	0.30128 (13)	0.61047 (17)	0.02569 (10)	0.0543 (4)
C18	0.33526 (15)	0.62685 (17)	0.12096 (11)	0.0685 (5)
H18A	0.2758	0.6610	0.1425	0.082*
H18B	0.3964	0.6870	0.1373	0.082*
C19	0.36713 (14)	0.48682 (17)	0.15539 (10)	0.0619 (5)
H19	0.3321	0.4665	0.2015	0.074*
C20	0.03804 (18)	−0.13115 (18)	0.11287 (13)	0.0989 (7)
H20A	0.0585	−0.1485	0.0606	0.148*
H20B	−0.0265	−0.1801	0.1135	0.148*
H20C	0.0957	−0.1578	0.1604	0.148*
C21	0.01061 (14)	0.49516 (17)	0.11711 (13)	0.0794 (6)
H21A	−0.0442	0.4600	0.0704	0.119*
H21B	0.0049	0.5900	0.1176	0.119*
H21C	0.0006	0.4600	0.1698	0.119*
C22	0.2423 (2)	0.27137 (19)	−0.18592 (13)	0.1168 (9)
H22A	0.1692	0.2970	−0.2132	0.175*
H22B	0.2491	0.1769	−0.1890	0.175*
H22C	0.2915	0.3131	−0.2143	0.175*
C23	0.22177 (17)	0.89829 (17)	−0.16809 (13)	0.0850 (6)
H23A	0.1752	0.9208	−0.1316	0.127*
H23B	0.2006	0.9480	−0.2202	0.127*
H23C	0.2956	0.9190	−0.1398	0.127*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0960 (11)	0.0534 (9)	0.1336 (13)	−0.0154 (7)	0.0338 (9)	−0.0010 (8)
O2	0.0575 (8)	0.0496 (8)	0.0802 (8)	0.0036 (6)	0.0222 (6)	−0.0009 (6)
O3	0.1176 (11)	0.0527 (8)	0.0469 (8)	0.0052 (7)	0.0223 (7)	−0.0020 (6)
O4	0.0980 (10)	0.0589 (9)	0.0687 (9)	0.0035 (7)	0.0202 (7)	0.0151 (7)
C1	0.0645 (14)	0.1059 (18)	0.0789 (15)	−0.0058 (12)	0.0033 (11)	−0.0021 (12)
C2	0.0551 (12)	0.1137 (18)	0.0815 (15)	0.0141 (11)	0.0117 (11)	0.0149 (13)
C3	0.0684 (13)	0.0810 (14)	0.0559 (12)	0.0144 (10)	0.0260 (10)	0.0110 (10)
C4	0.0853 (15)	0.0739 (14)	0.0629 (12)	0.0268 (11)	0.0244 (10)	0.0095 (10)
C5	0.0708 (13)	0.0570 (12)	0.0452 (10)	0.0114 (10)	0.0158 (9)	0.0050 (8)
C6	0.0936 (15)	0.0490 (11)	0.0570 (12)	0.0103 (11)	0.0150 (10)	0.0018 (9)
C7	0.0725 (14)	0.0558 (13)	0.0621 (12)	−0.0061 (10)	0.0130 (10)	0.0008 (9)
C8	0.0612 (12)	0.0526 (12)	0.0639 (12)	0.0025 (9)	0.0129 (9)	0.0014 (9)
C9	0.0619 (12)	0.0422 (11)	0.0453 (10)	0.0049 (9)	0.0093 (8)	0.0016 (8)
C10	0.0590 (11)	0.0530 (11)	0.0365 (9)	0.0064 (8)	0.0114 (8)	0.0041 (7)
C11	0.0552 (10)	0.0601 (11)	0.0411 (10)	0.0052 (9)	0.0160 (8)	0.0031 (8)
C12	0.0525 (10)	0.0556 (11)	0.0446 (10)	−0.0001 (8)	0.0152 (8)	0.0001 (8)
C13	0.0617 (11)	0.0474 (11)	0.0487 (11)	0.0002 (8)	0.0188 (8)	−0.0004 (8)
C14	0.0679 (12)	0.0579 (12)	0.0459 (10)	−0.0014 (9)	0.0178 (8)	0.0029 (9)
C15	0.0644 (12)	0.0541 (12)	0.0558 (12)	0.0005 (9)	0.0208 (9)	0.0129 (10)

C16	0.0721 (12)	0.0498 (11)	0.0639 (13)	−0.0045 (9)	0.0256 (10)	−0.0033 (10)
C17	0.0582 (11)	0.0578 (12)	0.0496 (11)	−0.0054 (8)	0.0183 (9)	−0.0032 (9)
C18	0.0790 (13)	0.0717 (13)	0.0561 (12)	−0.0113 (10)	0.0190 (10)	−0.0101 (9)
C19	0.0584 (12)	0.0783 (13)	0.0483 (10)	−0.0052 (10)	0.0119 (9)	−0.0031 (9)
C20	0.1240 (19)	0.0513 (14)	0.1129 (18)	−0.0128 (12)	0.0132 (15)	0.0006 (11)
C21	0.0659 (13)	0.0621 (13)	0.1158 (17)	0.0110 (10)	0.0329 (12)	−0.0006 (11)
C22	0.235 (3)	0.0622 (14)	0.0548 (14)	−0.0128 (15)	0.0381 (16)	−0.0153 (10)
C23	0.1083 (17)	0.0570 (14)	0.0975 (16)	0.0083 (11)	0.0403 (13)	0.0200 (11)

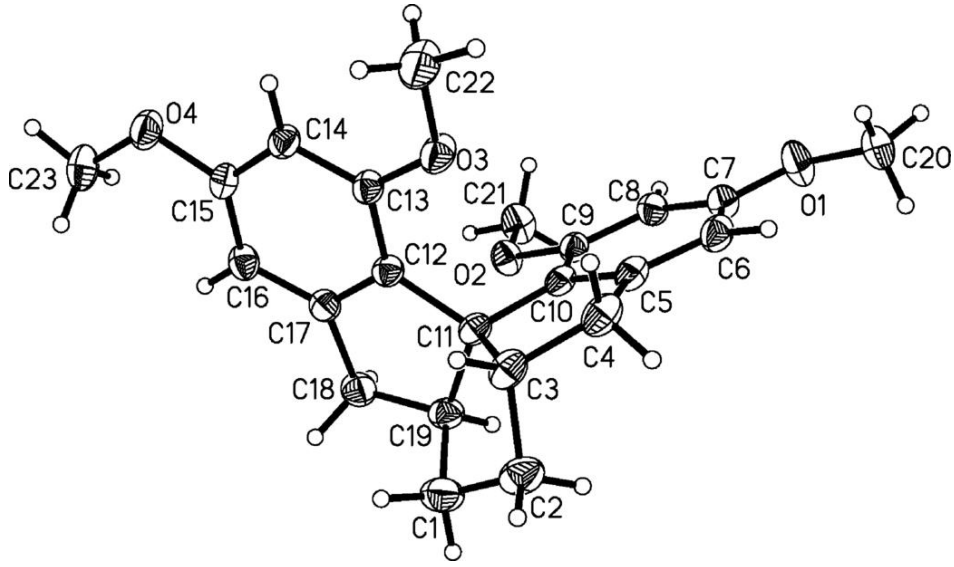
Geometric parameters (Å, °)

O1—C7	1.373 (2)	C10—C11	1.517 (2)
O1—C20	1.420 (2)	C11—C12	1.510 (2)
O2—C9	1.3656 (17)	C11—C19	1.566 (2)
O2—C21	1.4294 (18)	C12—C17	1.376 (2)
O3—C13	1.3682 (18)	C12—C13	1.393 (2)
O3—C22	1.410 (2)	C13—C14	1.380 (2)
O4—C15	1.3759 (19)	C14—C15	1.388 (2)
O4—C23	1.4171 (19)	C14—H14	0.9300
C1—C2	1.516 (3)	C15—C16	1.381 (2)
C1—C19	1.521 (2)	C16—C17	1.388 (2)
C1—H1A	0.9700	C16—H16	0.9300
C1—H1B	0.9700	C17—C18	1.502 (2)
C2—C3	1.522 (2)	C18—C19	1.536 (2)
C2—H2A	0.9700	C18—H18A	0.9700
C2—H2B	0.9700	C18—H18B	0.9700
C3—C4	1.530 (2)	C19—H19	0.9800
C3—C11	1.572 (2)	C20—H20A	0.9600
C3—H3	0.9800	C20—H20B	0.9600
C4—C5	1.507 (2)	C20—H20C	0.9600
C4—H4A	0.9700	C21—H21A	0.9600
C4—H4B	0.9700	C21—H21B	0.9600
C5—C10	1.378 (2)	C21—H21C	0.9600
C5—C6	1.390 (2)	C22—H22A	0.9600
C6—C7	1.378 (2)	C22—H22B	0.9600
C6—H6	0.9300	C22—H22C	0.9600
C7—C8	1.383 (2)	C23—H23A	0.9600
C8—C9	1.376 (2)	C23—H23B	0.9600
C8—H8	0.9300	C23—H23C	0.9600
C9—C10	1.397 (2)		
C7—O1—C20	118.91 (16)	C17—C12—C11	112.92 (14)
C9—O2—C21	117.11 (13)	C13—C12—C11	127.96 (15)
C13—O3—C22	117.84 (13)	O3—C13—C14	124.30 (15)
C15—O4—C23	117.87 (15)	O3—C13—C12	115.63 (14)
C2—C1—C19	103.52 (16)	C14—C13—C12	120.07 (15)
C2—C1—H1A	111.1	C13—C14—C15	119.61 (15)
C19—C1—H1A	111.1	C13—C14—H14	120.2
C2—C1—H1B	111.1	C15—C14—H14	120.2
C19—C1—H1B	111.1	O4—C15—C16	124.39 (16)

H1A—C1—H1B	109.0	O4—C15—C14	114.33 (16)
C1—C2—C3	103.46 (15)	C16—C15—C14	121.29 (15)
C1—C2—H2A	111.1	C15—C16—C17	118.02 (15)
C3—C2—H2A	111.1	C15—C16—H16	121.0
C1—C2—H2B	111.1	C17—C16—H16	121.0
C3—C2—H2B	111.1	C12—C17—C16	121.87 (15)
H2A—C2—H2B	109.0	C12—C17—C18	110.93 (15)
C2—C3—C4	114.65 (15)	C16—C17—C18	127.19 (16)
C2—C3—C11	103.13 (14)	C17—C18—C19	104.68 (14)
C4—C3—C11	107.07 (14)	C17—C18—H18A	110.8
C2—C3—H3	110.6	C19—C18—H18A	110.8
C4—C3—H3	110.6	C17—C18—H18B	110.8
C11—C3—H3	110.6	C19—C18—H18B	110.8
C5—C4—C3	104.71 (14)	H18A—C18—H18B	108.9
C5—C4—H4A	110.8	C1—C19—C18	115.66 (15)
C3—C4—H4A	110.8	C1—C19—C11	103.89 (14)
C5—C4—H4B	110.8	C18—C19—C11	107.47 (13)
C3—C4—H4B	110.8	C1—C19—H19	109.9
H4A—C4—H4B	108.9	C18—C19—H19	109.9
C10—C5—C6	121.93 (16)	C11—C19—H19	109.9
C10—C5—C4	110.09 (16)	O1—C20—H20A	109.5
C6—C5—C4	127.97 (16)	O1—C20—H20B	109.5
C7—C6—C5	117.93 (16)	H20A—C20—H20B	109.5
C7—C6—H6	121.0	O1—C20—H20C	109.5
C5—C6—H6	121.0	H20A—C20—H20C	109.5
O1—C7—C6	124.43 (17)	H20B—C20—H20C	109.5
O1—C7—C8	114.43 (17)	O2—C21—H21A	109.5
C6—C7—C8	121.14 (17)	O2—C21—H21B	109.5
C9—C8—C7	120.37 (16)	H21A—C21—H21B	109.5
C9—C8—H8	119.8	O2—C21—H21C	109.5
C7—C8—H8	119.8	H21A—C21—H21C	109.5
O2—C9—C8	124.55 (15)	H21B—C21—H21C	109.5
O2—C9—C10	115.87 (14)	O3—C22—H22A	109.5
C8—C9—C10	119.57 (15)	O3—C22—H22B	109.5
C5—C10—C9	119.04 (15)	H22A—C22—H22B	109.5
C5—C10—C11	113.21 (14)	O3—C22—H22C	109.5
C9—C10—C11	127.74 (14)	H22A—C22—H22C	109.5
C12—C11—C10	114.94 (13)	H22B—C22—H22C	109.5
C12—C11—C19	102.46 (13)	O4—C23—H23A	109.5
C10—C11—C19	115.23 (12)	O4—C23—H23B	109.5
C12—C11—C3	116.61 (12)	H23A—C23—H23B	109.5
C10—C11—C3	101.74 (13)	O4—C23—H23C	109.5
C19—C11—C3	106.06 (13)	H23A—C23—H23C	109.5
C17—C12—C13	119.12 (14)	H23B—C23—H23C	109.5
C19—C1—C2—C3	45.85 (18)	C10—C11—C12—C17	117.93 (15)
C1—C2—C3—C4	−153.35 (15)	C19—C11—C12—C17	−7.82 (17)
C1—C2—C3—C11	−37.33 (18)	C3—C11—C12—C17	−123.13 (16)
C2—C3—C4—C5	95.86 (17)	C10—C11—C12—C13	−61.8 (2)
C11—C3—C4—C5	−17.87 (17)	C19—C11—C12—C13	172.49 (15)

C3—C4—C5—C10	12.87 (18)	C3—C11—C12—C13	57.2 (2)
C3—C4—C5—C6	−167.74 (16)	C22—O3—C13—C14	2.9 (2)
C10—C5—C6—C7	1.0 (2)	C22—O3—C13—C12	−177.36 (17)
C4—C5—C6—C7	−178.31 (17)	C17—C12—C13—O3	179.06 (14)
C20—O1—C7—C6	−3.0 (3)	C11—C12—C13—O3	−1.3 (2)
C20—O1—C7—C8	177.41 (15)	C17—C12—C13—C14	−1.2 (2)
C5—C6—C7—O1	−179.96 (16)	C11—C12—C13—C14	178.52 (15)
C5—C6—C7—C8	−0.4 (3)	O3—C13—C14—C15	179.81 (15)
O1—C7—C8—C9	179.30 (14)	C12—C13—C14—C15	0.0 (2)
C6—C7—C8—C9	−0.3 (3)	C23—O4—C15—C16	5.2 (2)
C21—O2—C9—C8	−4.0 (2)	C23—O4—C15—C14	−174.92 (14)
C21—O2—C9—C10	177.12 (14)	C13—C14—C15—O4	−178.73 (14)
C7—C8—C9—O2	−178.43 (15)	C13—C14—C15—C16	1.1 (2)
C7—C8—C9—C10	0.4 (2)	O4—C15—C16—C17	178.73 (15)
C6—C5—C10—C9	−0.9 (2)	C14—C15—C16—C17	−1.1 (2)
C4—C5—C10—C9	178.50 (14)	C13—C12—C17—C16	1.2 (2)
C6—C5—C10—C11	178.08 (14)	C11—C12—C17—C16	−178.55 (14)
C4—C5—C10—C11	−2.48 (18)	C13—C12—C17—C18	−179.81 (14)
O2—C9—C10—C5	179.15 (13)	C11—C12—C17—C18	0.47 (19)
C8—C9—C10—C5	0.2 (2)	C15—C16—C17—C12	−0.1 (2)
O2—C9—C10—C11	0.3 (2)	C15—C16—C17—C18	−178.90 (16)
C8—C9—C10—C11	−178.65 (14)	C12—C17—C18—C19	7.32 (19)
C5—C10—C11—C12	118.32 (15)	C16—C17—C18—C19	−173.73 (16)
C9—C10—C11—C12	−62.8 (2)	C2—C1—C19—C18	−152.31 (15)
C5—C10—C11—C19	−122.85 (14)	C2—C1—C19—C11	−34.81 (18)
C9—C10—C11—C19	56.1 (2)	C17—C18—C19—C1	103.58 (17)
C5—C10—C11—C3	−8.63 (16)	C17—C18—C19—C11	−11.91 (17)
C9—C10—C11—C3	170.29 (15)	C12—C11—C19—C1	−111.14 (14)
C2—C3—C11—C12	128.93 (16)	C10—C11—C19—C1	123.31 (15)
C4—C3—C11—C12	−109.76 (16)	C3—C11—C19—C1	11.61 (17)
C2—C3—C11—C10	−105.22 (15)	C12—C11—C19—C18	11.92 (16)
C4—C3—C11—C10	16.09 (16)	C10—C11—C19—C18	−113.63 (15)
C2—C3—C11—C19	15.64 (17)	C3—C11—C19—C18	134.67 (14)
C4—C3—C11—C19	136.95 (13)		

Fig. 1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