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2-Ethyl-5-triphenylmethyl-1,3-dioxane

Lin Yuan,[a] Jiang-Hua Shi,[a] Min Zhang[a] and Seik Weng Ng[b]*

[a]Department of Biology and Chemistry, Hunan University of Science and Engineering, Yongzhou Hunan 425100, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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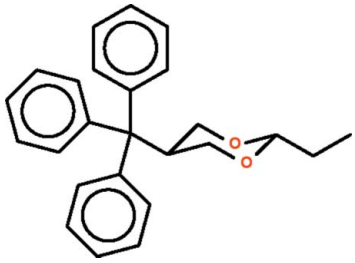
Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.114; data-to-parameter ratio = 17.1.

In the title compound, $C_{25}H_{26}O_2$, the dioxane ring adopts a chair conformation with the two substituent groups occupying equatorial positions.

Related literature

For the crystal structure of 2,2-dimethyl-5-triphenyl-1,3-dioxane, see: Zhang *et al.* (2009).



Experimental

Crystal data

$C_{25}H_{26}O_2$
M_r = 358.46
Monoclinic, $P2_1/c$
a = 10.5401 (6) Å
b = 13.3550 (8) Å
c = 14.6044 (8) Å
β = 110.523 (1)°
V = 1925.28 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 110 K
0.45 × 0.35 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
9493 measured reflections
4174 independent reflections
3047 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.04
4174 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2066).

References

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Zhang, M., Yuan, X.-Y. & Liu, X.-M. (2009). *Acta Cryst.* E**65**, o304.

supporting information

Acta Cryst. (2010). E**66**, o2582 [doi:10.1107/S1600536810036767]

2-Ethyl-5-triphenylmethyl-1,3-dioxane

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S1. Comment

A previous study reported the crystal structure of 2,2-dimethyl-5-triphenylmethyl-1,3-dioxane (Zhang *et al.*, 2009). Such disubstituted 1,3-dioxanes are known from NMR studies to have substituents in equatorial rather than in axial orientations on the six-membered ring. The the title compound, 2-ethyl-5-triphenylmethyl-1,3-dioxane analog (Scheme I, Fig. 1), has similar features for the dioxane part, which adopts a chair conformation. The substitutent groups occupy equatorial positions.

S2. Experimental

2-Triphenylmethyl-1,3-propanediol (0.24 g, 5.0 mmol), propionaldehyde (20 mmol) and *p*-toluenesulfonic acid (0.1 g) were stirred in dichloromethane (20 ml) for a week. The solvent was evaporated and the residue was dissolved in ether (20 ml) after which the solution was washed with water and 5% sodium bicarbonate (20 ml). The organic phase was dried with anhydrous sodium sulfate. The solvent was evaporated and the product was recrystallized from ethyl acetate to give 1.0 g (yield 60%) of colorless crystals.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.95–0.99 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C).

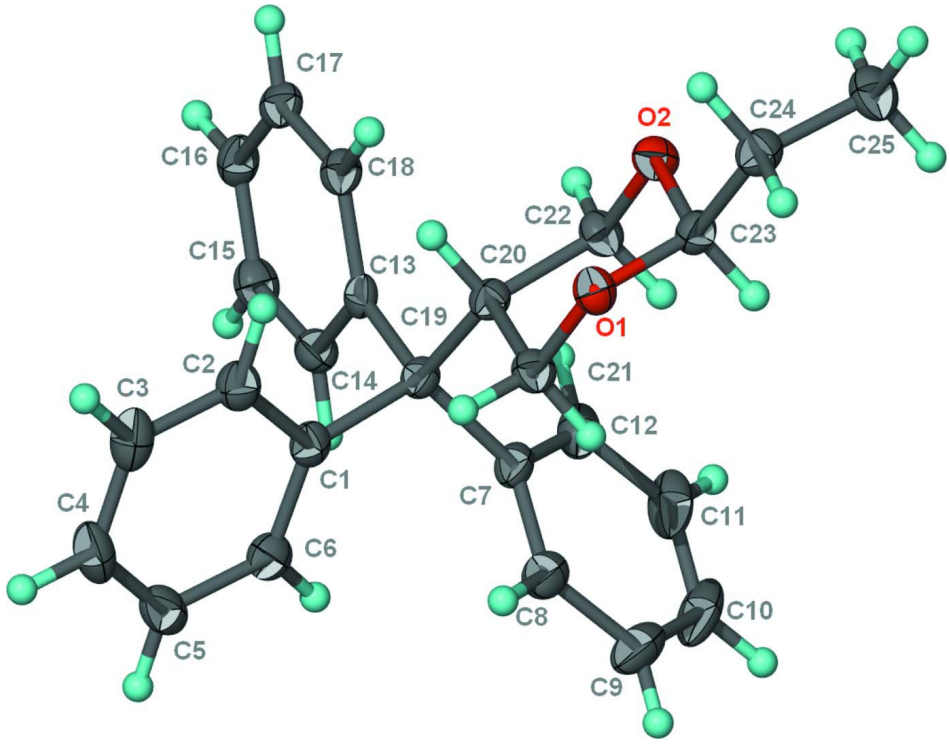

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level.

2-Ethyl-5-triphenylmethyl-1,3-dioxane

Crystal data

$C_{25}H_{26}O_2$
$M_r = 358.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.5401\ (6)$ Å
$b = 13.3550\ (8)$ Å
$c = 14.6044\ (8)$ Å
$\beta = 110.523\ (1)°$
$V = 1925.28\ (19)$ Å^3
$Z = 4$

$F(000) = 768$
$D_x = 1.237$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3994 reflections
$\theta = 2.6–27.0°$
$\mu = 0.08$ mm^{-1}
$T = 110$ K
Block, colorless
0.45 × 0.35 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
9493 measured reflections
4174 independent reflections

3047 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow13$
$k = -17\rightarrow12$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.114$
$S = 1.04$
4174 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.2859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.30810 (9)	0.32447 (7)	0.08575 (6)	0.0188 (2)
O2	0.26796 (9)	0.32596 (7)	0.23220 (7)	0.0191 (2)
C1	0.71880 (14)	0.43893 (10)	0.23149 (9)	0.0179 (3)
C2	0.65864 (15)	0.52062 (11)	0.17152 (10)	0.0212 (3)
H2	0.5682	0.5389	0.1633	0.025*
C3	0.72914 (16)	0.57512 (11)	0.12403 (11)	0.0258 (3)
H3	0.6864	0.6300	0.0835	0.031*
C4	0.86148 (16)	0.55018 (12)	0.13528 (11)	0.0272 (4)
H4	0.9093	0.5872	0.1022	0.033*
C5	0.92283 (15)	0.47091 (12)	0.19517 (11)	0.0249 (3)
H5	1.0137	0.4537	0.2038	0.030*
C6	0.85276 (14)	0.41622 (11)	0.24288 (10)	0.0214 (3)
H6	0.8968	0.3622	0.2841	0.026*
C7	0.69636 (13)	0.27847 (10)	0.32337 (10)	0.0196 (3)
C8	0.72962 (14)	0.21427 (11)	0.25990 (11)	0.0242 (3)
H8	0.7284	0.2387	0.1985	0.029*
C9	0.76470 (15)	0.11462 (12)	0.28526 (13)	0.0325 (4)
H9	0.7870	0.0719	0.2411	0.039*
C10	0.76718 (16)	0.07774 (12)	0.37422 (14)	0.0361 (4)
H10	0.7914	0.0100	0.3915	0.043*
C11	0.73423 (16)	0.13999 (12)	0.43758 (13)	0.0316 (4)
H11	0.7355	0.1150	0.4988	0.038*
C12	0.69899 (14)	0.23933 (11)	0.41254 (11)	0.0239 (3)
H12	0.6763	0.2813	0.4570	0.029*
C13	0.67391 (13)	0.45454 (10)	0.38294 (9)	0.0161 (3)
C14	0.80413 (14)	0.45411 (11)	0.45377 (10)	0.0194 (3)
H14	0.8701	0.4091	0.4470	0.023*
C15	0.83889 (15)	0.51776 (11)	0.53341 (10)	0.0226 (3)
H15	0.9278	0.5156	0.5807	0.027*
C16	0.74504 (15)	0.58467 (11)	0.54476 (10)	0.0214 (3)
H16	0.7689	0.6287	0.5993	0.026*
C17	0.61592 (15)	0.58622 (11)	0.47519 (10)	0.0202 (3)
H17	0.5504	0.6314	0.4824	0.024*
C18	0.58085 (14)	0.52241 (10)	0.39474 (10)	0.0183 (3)

H18	0.4921	0.5253	0.3473	0.022*
C19	0.64436 (13)	0.38587 (10)	0.29220 (9)	0.0162 (3)
C20	0.48869 (13)	0.37838 (10)	0.23326 (9)	0.0163 (3)
H20	0.4528	0.4483	0.2205	0.020*
C21	0.45229 (13)	0.32618 (11)	0.13438 (10)	0.0191 (3)
H21A	0.4950	0.3620	0.0933	0.023*
H21B	0.4876	0.2568	0.1440	0.023*
C22	0.41008 (13)	0.32455 (11)	0.28894 (10)	0.0186 (3)
H22A	0.4418	0.2545	0.3020	0.022*
H22B	0.4263	0.3582	0.3525	0.022*
C23	0.24357 (14)	0.27454 (11)	0.14269 (9)	0.0178 (3)
H23A	0.2791	0.2046	0.1563	0.021*
C24	0.09327 (14)	0.27184 (11)	0.08743 (10)	0.0207 (3)
H24A	0.0758	0.2405	0.0227	0.025*
H24B	0.0578	0.3412	0.0765	0.025*
C25	0.01923 (15)	0.21322 (12)	0.14283 (11)	0.0261 (3)
H25A	−0.0782	0.2131	0.1051	0.039*
H25B	0.0354	0.2447	0.2066	0.039*
H25C	0.0528	0.1442	0.1525	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0172 (5)	0.0204 (5)	0.0174 (5)	−0.0028 (4)	0.0042 (4)	−0.0008 (4)
O2	0.0159 (5)	0.0221 (5)	0.0181 (5)	−0.0013 (4)	0.0044 (4)	−0.0033 (4)
C1	0.0206 (7)	0.0169 (7)	0.0162 (6)	−0.0041 (6)	0.0063 (6)	−0.0047 (5)
C2	0.0219 (7)	0.0204 (7)	0.0207 (7)	−0.0027 (6)	0.0068 (6)	−0.0014 (6)
C3	0.0340 (9)	0.0213 (8)	0.0204 (7)	−0.0075 (7)	0.0076 (6)	0.0004 (6)
C4	0.0339 (9)	0.0294 (9)	0.0226 (7)	−0.0150 (7)	0.0152 (7)	−0.0060 (6)
C5	0.0219 (8)	0.0283 (8)	0.0267 (8)	−0.0083 (6)	0.0113 (6)	−0.0099 (6)
C6	0.0224 (7)	0.0198 (7)	0.0218 (7)	−0.0034 (6)	0.0076 (6)	−0.0056 (6)
C7	0.0137 (7)	0.0143 (7)	0.0275 (7)	−0.0004 (5)	0.0031 (6)	−0.0001 (6)
C8	0.0158 (7)	0.0200 (7)	0.0330 (8)	−0.0008 (6)	0.0039 (6)	−0.0045 (6)
C9	0.0188 (8)	0.0197 (8)	0.0509 (11)	0.0021 (6)	0.0019 (7)	−0.0099 (7)
C10	0.0217 (8)	0.0151 (8)	0.0569 (11)	0.0009 (6)	−0.0045 (8)	0.0038 (8)
C11	0.0225 (8)	0.0232 (8)	0.0393 (9)	−0.0026 (7)	−0.0016 (7)	0.0110 (7)
C12	0.0196 (7)	0.0192 (7)	0.0287 (8)	−0.0020 (6)	0.0034 (6)	0.0038 (6)
C13	0.0191 (7)	0.0122 (7)	0.0176 (6)	−0.0023 (5)	0.0072 (5)	0.0021 (5)
C14	0.0175 (7)	0.0193 (7)	0.0218 (7)	0.0001 (6)	0.0074 (6)	0.0014 (6)
C15	0.0197 (7)	0.0250 (8)	0.0208 (7)	−0.0045 (6)	0.0042 (6)	0.0001 (6)
C16	0.0278 (8)	0.0189 (7)	0.0187 (7)	−0.0053 (6)	0.0096 (6)	−0.0028 (6)
C17	0.0252 (8)	0.0160 (7)	0.0213 (7)	0.0012 (6)	0.0106 (6)	0.0028 (6)
C18	0.0190 (7)	0.0168 (7)	0.0182 (7)	−0.0001 (6)	0.0053 (5)	0.0024 (5)
C19	0.0160 (7)	0.0139 (7)	0.0178 (7)	0.0002 (5)	0.0047 (5)	0.0006 (5)
C20	0.0158 (7)	0.0152 (7)	0.0166 (7)	0.0005 (5)	0.0042 (5)	−0.0003 (5)
C21	0.0165 (7)	0.0203 (7)	0.0200 (7)	−0.0014 (6)	0.0059 (6)	−0.0020 (6)
C22	0.0151 (7)	0.0217 (7)	0.0175 (7)	−0.0013 (6)	0.0039 (5)	0.0006 (6)
C23	0.0200 (7)	0.0150 (7)	0.0185 (7)	−0.0011 (6)	0.0067 (6)	−0.0012 (5)

C24	0.0198 (7)	0.0196 (7)	0.0204 (7)	−0.0001 (6)	0.0042 (6)	−0.0022 (6)
C25	0.0193 (7)	0.0286 (8)	0.0286 (8)	−0.0044 (6)	0.0064 (6)	−0.0006 (7)

Geometric parameters (Å, º)

O1—C23	1.4125 (16)	C13—C18	1.3899 (19)
O1—C21	1.4345 (15)	C13—C14	1.3994 (19)
O2—C23	1.4181 (15)	C13—C19	1.5509 (18)
O2—C22	1.4355 (15)	C14—C15	1.382 (2)
C1—C6	1.3959 (19)	C14—H14	0.9500
C1—C2	1.403 (2)	C15—C16	1.385 (2)
C1—C19	1.5465 (19)	C15—H15	0.9500
C2—C3	1.387 (2)	C16—C17	1.384 (2)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.387 (2)	C17—C18	1.3925 (19)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.381 (2)	C18—H18	0.9500
C4—H4	0.9500	C19—C20	1.5661 (18)
C5—C6	1.387 (2)	C20—C21	1.5264 (18)
C5—H5	0.9500	C20—C22	1.5287 (19)
C6—H6	0.9500	C20—H20	1.0000
C7—C8	1.395 (2)	C21—H21A	0.9900
C7—C12	1.395 (2)	C21—H21B	0.9900
C7—C19	1.5459 (19)	C22—H22A	0.9900
C8—C9	1.396 (2)	C22—H22B	0.9900
C8—H8	0.9500	C23—C24	1.5053 (18)
C9—C10	1.381 (3)	C23—H23A	1.0000
C9—H9	0.9500	C24—C25	1.523 (2)
C10—C11	1.376 (2)	C24—H24A	0.9900
C10—H10	0.9500	C24—H24B	0.9900
C11—C12	1.392 (2)	C25—H25A	0.9800
C11—H11	0.9500	C25—H25B	0.9800
C12—H12	0.9500	C25—H25C	0.9800
C23—O1—C21	111.18 (10)	C15—C16—H16	120.6
C23—O2—C22	109.94 (10)	C16—C17—C18	120.80 (13)
C6—C1—C2	117.39 (13)	C16—C17—H17	119.6
C6—C1—C19	121.83 (12)	C18—C17—H17	119.6
C2—C1—C19	120.33 (12)	C13—C18—C17	120.90 (13)
C3—C2—C1	121.06 (14)	C13—C18—H18	119.6
C3—C2—H2	119.5	C17—C18—H18	119.6
C1—C2—H2	119.5	C7—C19—C1	113.28 (11)
C4—C3—C2	120.50 (14)	C7—C19—C13	110.66 (11)
C4—C3—H3	119.7	C1—C19—C13	103.22 (10)
C2—C3—H3	119.7	C7—C19—C20	107.31 (11)
C5—C4—C3	119.17 (14)	C1—C19—C20	111.01 (10)
C5—C4—H4	120.4	C13—C19—C20	111.43 (11)
C3—C4—H4	120.4	C21—C20—C22	106.57 (11)

C4—C5—C6	120.53 (14)	C21—C20—C19	114.62 (11)
C4—C5—H5	119.7	C22—C20—C19	113.35 (10)
C6—C5—H5	119.7	C21—C20—H20	107.3
C5—C6—C1	121.34 (14)	C22—C20—H20	107.3
C5—C6—H6	119.3	C19—C20—H20	107.3
C1—C6—H6	119.3	O1—C21—C20	110.30 (11)
C8—C7—C12	117.57 (14)	O1—C21—H21A	109.6
C8—C7—C19	121.37 (13)	C20—C21—H21A	109.6
C12—C7—C19	120.78 (13)	O1—C21—H21B	109.6
C7—C8—C9	120.98 (15)	C20—C21—H21B	109.6
C7—C8—H8	119.5	H21A—C21—H21B	108.1
C9—C8—H8	119.5	O2—C22—C20	109.71 (10)
C10—C9—C8	120.36 (16)	O2—C22—H22A	109.7
C10—C9—H9	119.8	C20—C22—H22A	109.7
C8—C9—H9	119.8	O2—C22—H22B	109.7
C11—C10—C9	119.42 (15)	C20—C22—H22B	109.7
C11—C10—H10	120.3	H22A—C22—H22B	108.2
C9—C10—H10	120.3	O1—C23—O2	110.18 (10)
C10—C11—C12	120.42 (16)	O1—C23—C24	109.22 (11)
C10—C11—H11	119.8	O2—C23—C24	108.81 (11)
C12—C11—H11	119.8	O1—C23—H23A	109.5
C11—C12—C7	121.26 (15)	O2—C23—H23A	109.5
C11—C12—H12	119.4	C24—C23—H23A	109.5
C7—C12—H12	119.4	C23—C24—C25	111.50 (11)
C18—C13—C14	117.58 (12)	C23—C24—H24A	109.3
C18—C13—C19	123.54 (12)	C25—C24—H24A	109.3
C14—C13—C19	118.71 (12)	C23—C24—H24B	109.3
C15—C14—C13	121.43 (13)	C25—C24—H24B	109.3
C15—C14—H14	119.3	H24A—C24—H24B	108.0
C13—C14—H14	119.3	C24—C25—H25A	109.5
C14—C15—C16	120.50 (13)	C24—C25—H25B	109.5
C14—C15—H15	119.8	H25A—C25—H25B	109.5
C16—C15—H15	119.8	C24—C25—H25C	109.5
C17—C16—C15	118.78 (13)	H25A—C25—H25C	109.5
C17—C16—H16	120.6	H25B—C25—H25C	109.5

C6—C1—C2—C3	1.3 (2)	C6—C1—C19—C7	−28.71 (17)
C19—C1—C2—C3	173.68 (12)	C2—C1—C19—C7	159.22 (12)
C1—C2—C3—C4	−0.3 (2)	C6—C1—C19—C13	91.00 (14)
C2—C3—C4—C5	−0.6 (2)	C2—C1—C19—C13	−81.08 (14)
C3—C4—C5—C6	0.6 (2)	C6—C1—C19—C20	−149.52 (12)
C4—C5—C6—C1	0.4 (2)	C2—C1—C19—C20	38.41 (16)
C2—C1—C6—C5	−1.3 (2)	C18—C13—C19—C7	−136.57 (13)
C19—C1—C6—C5	−173.61 (12)	C14—C13—C19—C7	48.34 (16)
C12—C7—C8—C9	−0.2 (2)	C18—C13—C19—C1	101.94 (14)
C19—C7—C8—C9	−174.13 (13)	C14—C13—C19—C1	−73.15 (14)
C7—C8—C9—C10	−0.1 (2)	C18—C13—C19—C20	−17.26 (17)
C8—C9—C10—C11	0.3 (2)	C14—C13—C19—C20	167.65 (12)

C9—C10—C11—C12	−0.2 (2)	C7—C19—C20—C21	−68.12 (14)
C10—C11—C12—C7	−0.2 (2)	C1—C19—C20—C21	56.15 (15)
C8—C7—C12—C11	0.4 (2)	C13—C19—C20—C21	170.60 (11)
C19—C7—C12—C11	174.28 (13)	C7—C19—C20—C22	54.53 (14)
C18—C13—C14—C15	0.9 (2)	C1—C19—C20—C22	178.81 (11)
C19—C13—C14—C15	176.25 (12)	C13—C19—C20—C22	−66.75 (14)
C13—C14—C15—C16	−0.5 (2)	C23—O1—C21—C20	−58.77 (14)
C14—C15—C16—C17	0.3 (2)	C22—C20—C21—O1	54.60 (14)
C15—C16—C17—C18	−0.5 (2)	C19—C20—C21—O1	−179.15 (10)
C14—C13—C18—C17	−1.1 (2)	C23—O2—C22—C20	61.61 (14)
C19—C13—C18—C17	−176.24 (12)	C21—C20—C22—O2	−56.23 (14)
C16—C17—C18—C13	0.9 (2)	C19—C20—C22—O2	176.77 (10)
C8—C7—C19—C1	−39.96 (17)	C21—O1—C23—O2	62.29 (13)
C12—C7—C19—C1	146.35 (12)	C21—O1—C23—C24	−178.24 (11)
C8—C7—C19—C13	−155.31 (12)	C22—O2—C23—O1	−63.62 (13)
C12—C7—C19—C13	31.00 (17)	C22—O2—C23—C24	176.67 (11)
C8—C7—C19—C20	82.92 (15)	O1—C23—C24—C25	176.55 (12)
C12—C7—C19—C20	−90.77 (15)	O2—C23—C24—C25	−63.14 (15)