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3,4,5-Trimethoxy-1-methylbenzene

Jian Li,[a] Zu-Pei Liang,[a]* Ai-Yu Wan[b] and Wu-Lan Zeng[a]

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and [b]Qingdao Huaren Pharmaceutical Co. Ltd., Qingdao 266101, People's Republic of China
Correspondence e-mail: zupeiliang@yahoo.com.cn

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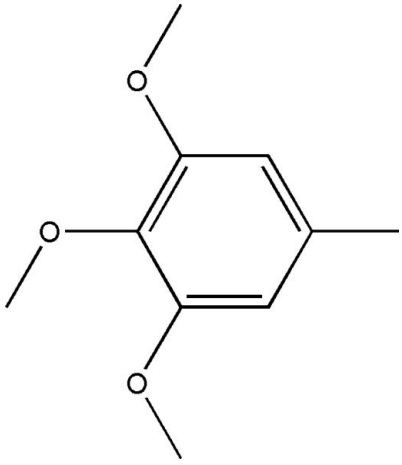
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.146; data-to-parameter ratio = 14.6.

The asymmetric unit of the title compound, $C_{10}H_{14}O_3$, comprises two independent molecules. All bond lengths and angles are within normal ranges.

Related literature

For related literature, see: Cheng *et al.* (2004); Zhang *et al.* (2005).



Experimental

Crystal data

$C_{10}H_{14}O_3$
M_r = 182.21
Monoclinic, $P2_1/n$
a = 13.902 (11) Å
b = 8.123 (7) Å
c = 18.021 (14) Å
β = 98.883 (14)°
V = 2011 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.978, T_{max} = 0.981
10097 measured reflections
3556 independent reflections
2019 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.146
S = 1.00
3556 reflections
243 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Selected torsion angles (°).

O1—C4—C5—O2	3.6 (3)	O4—C14—C15—O5	−2.2 (3)
O2—C5—C6—O3	−2.4 (3)	O5—C15—C16—O6	3.2 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BX2079).

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supplementary materials

Acta Cryst. (2007). E**63**, o2765 [**doi:10.1107/S1600536807020648**]

3,4,5-Trimethoxy-1-methylbenzene

J. Li, Z.-P. Liang, A.-Y. Wan and W.-L. Zeng

Comment

Coenzyme Q_0 is the simplest ubiquinone that has no isoprenyl side chain. Its importance lies in the use of synthesizing other coenzyme Q compounds, especially coenzyme Q_{10} which plays a central role in the two important biological electron-transfer reactions–respiration and photosynthesis. 3,4,5-trimethoxy-methylbenzene is the intermediate in the synthesis of Coenzyme Qo. We report here the structure of the title compound, (I), Fig 1. The bond lengths and angles of the title compound agree with those in the related compound 2,3,4-Trimethoxy-6-methylbenzaldehyde (Zhang *et al.*, 2005) as representative example. (Table 1).

Experimental

The compound was obtained as Colourless block crystals using the tecnique described by Cheng *et al.*, 2004.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(methyl C).

Figures

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids.

3,4,5-Trimethoxy-1-methylbenzene

Crystal data

$C_{10}H_{14}O_3$	F_{000} = 784
M_r = 182.21	D_x = 1.204 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2724 reflections
a = 13.902 (11) Å	θ = 2.8–22.5º
b = 8.123 (7) Å	μ = 0.09 mm^{-1}
c = 18.021 (14) Å	T = 294 (2) K
β = 98.883 (14)º	Block, colourless
V = 2011 (3) Å^3	0.26 × 0.24 × 0.22 mm

$Z = 8$

Data collection

Bruker SMART CCD area-detector diffractometer	3556 independent reflections
Radiation source: fine-focus sealed tube	2019 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
$T = 294(2)$ K	$\theta_{max} = 25.0^{o}$
φ and ω scans	$\theta_{min} = 1.7^{o}$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -10\rightarrow16$
$T_{min} = 0.978$, $T_{max} = 0.981$	$k = -9\rightarrow9$
10097 measured reflections	$l = -21\rightarrow20$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 0.3999P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.146$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.15$ e Å^{-3}
3556 reflections	Extinction correction: SHELXL97, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
243 parameters	Extinction coefficient: 0.0160 (19)
12 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.02646 (13)	0.7944 (2)	0.93359 (11)	0.0811 (6)
O2	0.17759 (12)	0.6040 (2)	0.98496 (9)	0.0737 (5)
O3	0.35210 (14)	0.6563 (2)	0.94730 (11)	0.0850 (6)
O4	0.31318 (13)	0.2503 (2)	0.08410 (9)	0.0780 (5)
O5	0.37108 (12)	0.37561 (18)	0.22006 (9)	0.0646 (5)
O6	0.47742 (12)	0.20326 (19)	0.32750 (9)	0.0687 (5)
C1	0.2257 (3)	1.1155 (4)	0.78266 (19)	0.1166 (12)
H1A	0.2632	1.0745	0.7462	0.175*
H1B	0.2590	1.2069	0.8089	0.175*
H1C	0.1630	1.1509	0.7578	0.175*
C2	0.2127 (2)	0.9804 (3)	0.83815 (13)	0.0715 (7)
C3	0.12352 (19)	0.9533 (3)	0.85913 (13)	0.0666 (7)
H3	0.0706	1.0181	0.8393	0.080*
C4	0.11210 (18)	0.8303 (3)	0.90965 (13)	0.0603 (6)
C5	0.19031 (18)	0.7328 (3)	0.93873 (12)	0.0565 (6)
C6	0.27995 (19)	0.7610 (3)	0.91703 (13)	0.0612 (6)
C7	0.2911 (2)	0.8853 (3)	0.86754 (13)	0.0687 (7)
H7	0.3519	0.9053	0.8539	0.082*
C8	−0.0564 (2)	0.8845 (4)	0.90251 (19)	0.1051 (11)
H8A	−0.0490	0.9972	0.9184	0.158*
H8B	−0.1130	0.8386	0.9192	0.158*
H8C	−0.0639	0.8793	0.8487	0.158*
C9	0.2051 (2)	0.6352 (4)	1.06233 (15)	0.0933 (9)
H9A	0.2725	0.6660	1.0720	0.140*
H9B	0.1953	0.5377	1.0904	0.140*
H9C	0.1660	0.7230	1.0773	0.140*
C10	0.4437 (2)	0.6752 (5)	0.9263 (2)	0.1088 (11)
H10A	0.4389	0.6599	0.8730	0.163*
H10B	0.4875	0.5950	0.9519	0.163*
H10C	0.4678	0.7838	0.9394	0.163*
C11	0.4870 (2)	−0.2676 (3)	0.15599 (17)	0.0894 (9)
H11A	0.5209	−0.3176	0.2008	0.134*
H11B	0.5295	−0.2618	0.1188	0.134*
H11C	0.4309	−0.3326	0.1371	0.134*
C12	0.45528 (17)	−0.0966 (3)	0.17368 (14)	0.0625 (6)
C13	0.39781 (17)	−0.0057 (3)	0.11903 (14)	0.0640 (7)
H13	0.3789	−0.0504	0.0715	0.077*
C14	0.36843 (16)	0.1505 (3)	0.13461 (13)	0.0564 (6)
C15	0.39629 (15)	0.2174 (3)	0.20540 (12)	0.0505 (6)
C16	0.45387 (15)	0.1268 (3)	0.25996 (12)	0.0517 (6)
C17	0.48328 (16)	−0.0301 (3)	0.24381 (14)	0.0601 (6)
H17	0.5222	−0.0910	0.2806	0.072*
C18	0.2924 (2)	0.1991 (4)	0.00807 (15)	0.0917 (9)
H18A	0.3522	0.1777	−0.0106	0.138*
H18B	0.2571	0.2844	−0.0214	0.138*
H18C	0.2538	0.1007	0.0047	0.138*
C19	0.2803 (2)	0.3894 (3)	0.24503 (16)	0.0835 (8)
H19A	0.2306	0.3419	0.2084	0.125*
H19B	0.2658	0.5035	0.2519	0.125*

H19C	0.2825	0.3322	0.2919	0.125*
C20	0.5391 (2)	0.1175 (4)	0.38557 (15)	0.0885 (9)
H20A	0.5069	0.0195	0.3985	0.133*
H20B	0.5531	0.1870	0.4290	0.133*
H20C	0.5987	0.0883	0.3682	0.133*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0687 (12)	0.0801 (12)	0.0936 (14)	−0.0031 (10)	0.0094 (10)	0.0109 (10)
O2	0.0848 (12)	0.0626 (11)	0.0695 (11)	−0.0120 (9)	−0.0015 (9)	0.0113 (9)
O3	0.0781 (13)	0.0901 (14)	0.0876 (13)	0.0125 (10)	0.0148 (10)	0.0178 (11)
O4	0.0978 (13)	0.0760 (12)	0.0544 (10)	0.0159 (10)	−0.0066 (9)	0.0013 (9)
O5	0.0778 (11)	0.0439 (9)	0.0709 (11)	0.0034 (8)	0.0079 (9)	0.0009 (8)
O6	0.0840 (12)	0.0566 (10)	0.0592 (10)	0.0067 (8)	−0.0086 (8)	−0.0028 (8)
C1	0.135 (3)	0.114 (3)	0.104 (2)	0.009 (2)	0.029 (2)	0.054 (2)
C2	0.096 (2)	0.0670 (17)	0.0517 (15)	−0.0009 (15)	0.0120 (14)	0.0062 (13)
C3	0.0778 (18)	0.0611 (16)	0.0579 (15)	0.0044 (13)	0.0011 (13)	0.0029 (13)
C4	0.0671 (16)	0.0553 (15)	0.0562 (15)	−0.0058 (12)	0.0022 (12)	−0.0048 (12)
C5	0.0702 (16)	0.0484 (14)	0.0486 (13)	−0.0057 (12)	0.0013 (12)	0.0026 (11)
C6	0.0721 (17)	0.0634 (16)	0.0466 (13)	0.0052 (13)	0.0041 (12)	−0.0010 (12)
C7	0.0826 (18)	0.0694 (17)	0.0569 (15)	−0.0006 (14)	0.0200 (13)	0.0000 (13)
C8	0.0640 (18)	0.116 (3)	0.132 (3)	0.0141 (17)	0.0053 (18)	0.012 (2)
C9	0.118 (2)	0.101 (2)	0.0594 (18)	−0.0078 (18)	0.0089 (16)	0.0130 (16)
C10	0.083 (2)	0.133 (3)	0.115 (3)	0.0250 (19)	0.0279 (19)	0.019 (2)
C11	0.102 (2)	0.0650 (18)	0.101 (2)	0.0152 (15)	0.0164 (17)	−0.0127 (16)
C12	0.0645 (15)	0.0518 (14)	0.0724 (17)	0.0016 (12)	0.0145 (13)	−0.0049 (13)
C13	0.0726 (16)	0.0616 (16)	0.0577 (15)	−0.0027 (13)	0.0095 (12)	−0.0094 (12)
C14	0.0584 (14)	0.0546 (15)	0.0553 (14)	0.0004 (11)	0.0056 (11)	0.0039 (12)
C15	0.0543 (13)	0.0408 (13)	0.0572 (14)	−0.0029 (10)	0.0106 (11)	0.0022 (11)
C16	0.0538 (13)	0.0475 (13)	0.0532 (14)	−0.0044 (10)	0.0067 (11)	−0.0002 (11)
C17	0.0586 (14)	0.0528 (15)	0.0682 (16)	0.0034 (11)	0.0082 (12)	0.0068 (12)
C18	0.102 (2)	0.111 (2)	0.0554 (16)	0.0090 (18)	−0.0089 (15)	−0.0018 (16)
C19	0.090 (2)	0.0728 (18)	0.090 (2)	0.0231 (15)	0.0200 (16)	−0.0050 (16)
C20	0.109 (2)	0.0823 (19)	0.0639 (17)	0.0138 (17)	−0.0203 (15)	0.0012 (15)

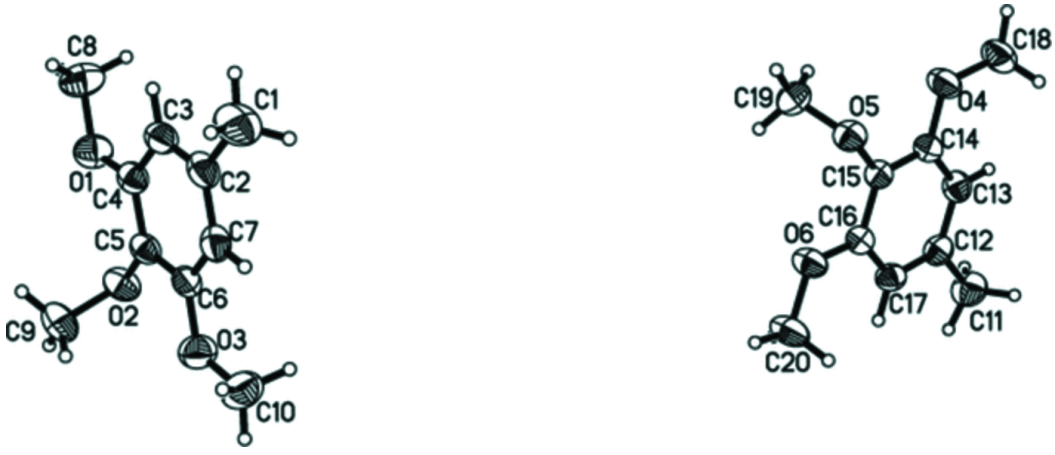
Geometric parameters (Å, °)

O1—C4	1.359 (3)	C9—H9A	0.9600
O1—C8	1.407 (3)	C9—H9B	0.9600
O2—C5	1.366 (3)	C9—H9C	0.9600
O2—C9	1.411 (3)	C10—H10A	0.9600
O3—C6	1.363 (3)	C10—H10B	0.9600
O3—C10	1.392 (4)	C10—H10C	0.9600
O4—C14	1.364 (3)	C11—C12	1.507 (4)
O4—C18	1.418 (3)	C11—H11A	0.9600
O5—C15	1.368 (3)	C11—H11B	0.9600
O5—C19	1.409 (3)	C11—H11C	0.9600
O6—C16	1.361 (3)	C12—C17	1.374 (3)

O6—C20	1.428 (3)	C12—C13	1.382 (3)
C1—C2	1.514 (4)	C13—C14	1.375 (3)
C1—H1A	0.9600	C13—H13	0.9300
C1—H1B	0.9600	C14—C15	1.386 (3)
C1—H1C	0.9600	C15—C16	1.381 (3)
C2—C3	1.368 (4)	C16—C17	1.383 (3)
C2—C7	1.374 (4)	C17—H17	0.9300
C3—C4	1.378 (3)	C18—H18A	0.9600
C3—H3	0.9300	C18—H18B	0.9600
C4—C5	1.381 (3)	C18—H18C	0.9600
C5—C6	1.382 (3)	C19—H19A	0.9600
C6—C7	1.372 (3)	C19—H19B	0.9600
C7—H7	0.9300	C19—H19C	0.9600
C8—H8A	0.9600	C20—H20A	0.9600
C8—H8B	0.9600	C20—H20B	0.9600
C8—H8C	0.9600	C20—H20C	0.9600
?···?	?		
C4—O1—C8	117.8 (2)	O3—C10—H10C	109.5
C5—O2—C9	115.1 (2)	H10A—C10—H10C	109.5
C6—O3—C10	118.0 (2)	H10B—C10—H10C	109.5
C14—O4—C18	118.7 (2)	C12—C11—H11A	109.5
C15—O5—C19	113.90 (18)	C12—C11—H11B	109.5
C16—O6—C20	117.85 (19)	H11A—C11—H11B	109.5
C2—C1—H1A	109.5	C12—C11—H11C	109.5
C2—C1—H1B	109.5	H11A—C11—H11C	109.5
H1A—C1—H1B	109.5	H11B—C11—H11C	109.5
C2—C1—H1C	109.5	C17—C12—C13	119.8 (2)
H1A—C1—H1C	109.5	C17—C12—C11	120.4 (2)
H1B—C1—H1C	109.5	C13—C12—C11	119.8 (2)
C3—C2—C7	120.1 (2)	C14—C13—C12	120.3 (2)
C3—C2—C1	120.3 (3)	C14—C13—H13	119.9
C7—C2—C1	119.6 (3)	C12—C13—H13	119.9
C2—C3—C4	120.1 (2)	O4—C14—C13	124.5 (2)
C2—C3—H3	120.0	O4—C14—C15	115.4 (2)
C4—C3—H3	120.0	C13—C14—C15	120.0 (2)
O1—C4—C3	124.2 (2)	O5—C15—C16	120.0 (2)
O1—C4—C5	115.7 (2)	O5—C15—C14	120.2 (2)
C3—C4—C5	120.2 (2)	C16—C15—C14	119.7 (2)
O2—C5—C4	120.1 (2)	O6—C16—C15	115.2 (2)
O2—C5—C6	120.5 (2)	O6—C16—C17	124.8 (2)
C4—C5—C6	119.3 (2)	C15—C16—C17	119.9 (2)
O3—C6—C7	124.7 (2)	C12—C17—C16	120.3 (2)
O3—C6—C5	115.1 (2)	C12—C17—H17	119.9
C7—C6—C5	120.2 (2)	C16—C17—H17	119.9
C6—C7—C2	120.1 (2)	O4—C18—H18A	109.5
C6—C7—H7	119.9	O4—C18—H18B	109.5
C2—C7—H7	119.9	H18A—C18—H18B	109.5
O1—C8—H8A	109.5	O4—C18—H18C	109.5

O1—C8—H8B	109.5	H18A—C18—H18C	109.5
H8A—C8—H8B	109.5	H18B—C18—H18C	109.5
O1—C8—H8C	109.5	O5—C19—H19A	109.5
H8A—C8—H8C	109.5	O5—C19—H19B	109.5
H8B—C8—H8C	109.5	H19A—C19—H19B	109.5
O2—C9—H9A	109.5	O5—C19—H19C	109.5
O2—C9—H9B	109.5	H19A—C19—H19C	109.5
H9A—C9—H9B	109.5	H19B—C19—H19C	109.5
O2—C9—H9C	109.5	O6—C20—H20A	109.5
H9A—C9—H9C	109.5	O6—C20—H20B	109.5
H9B—C9—H9C	109.5	H20A—C20—H20B	109.5
O3—C10—H10A	109.5	O6—C20—H20C	109.5
O3—C10—H10B	109.5	H20A—C20—H20C	109.5
H10A—C10—H10B	109.5	H20B—C20—H20C	109.5
C7—C2—C3—C4	−0.2 (4)	C17—C12—C13—C14	−0.1 (4)
C1—C2—C3—C4	−180.0 (2)	C11—C12—C13—C14	180.0 (2)
C8—O1—C4—C3	2.6 (4)	C18—O4—C14—C13	−7.0 (4)
C8—O1—C4—C5	−176.7 (2)	C18—O4—C14—C15	172.0 (2)
C2—C3—C4—O1	−179.9 (2)	C12—C13—C14—O4	178.8 (2)
C2—C3—C4—C5	−0.6 (4)	C12—C13—C14—C15	−0.1 (4)
C9—O2—C5—C4	−100.0 (3)	C19—O5—C15—C16	−94.5 (2)
C9—O2—C5—C6	83.9 (3)	C19—O5—C15—C14	88.9 (3)
O1—C4—C5—O2	3.6 (3)	O4—C14—C15—O5	−2.2 (3)
C3—C4—C5—O2	−175.7 (2)	C13—C14—C15—O5	176.9 (2)
O1—C4—C5—C6	179.8 (2)	O4—C14—C15—C16	−178.81 (19)
C3—C4—C5—C6	0.5 (3)	C13—C14—C15—C16	0.2 (3)
C10—O3—C6—C7	−0.6 (4)	C20—O6—C16—C15	−178.3 (2)
C10—O3—C6—C5	178.4 (2)	C20—O6—C16—C17	1.7 (3)
O2—C5—C6—O3	−2.4 (3)	O5—C15—C16—O6	3.2 (3)
C4—C5—C6—O3	−178.6 (2)	C14—C15—C16—O6	179.90 (19)
O2—C5—C6—C7	176.6 (2)	O5—C15—C16—C17	−176.78 (19)
C4—C5—C6—C7	0.5 (3)	C14—C15—C16—C17	−0.1 (3)
O3—C6—C7—C2	177.6 (2)	C13—C12—C17—C16	0.3 (3)
C5—C6—C7—C2	−1.3 (4)	C11—C12—C17—C16	−179.9 (2)
C3—C2—C7—C6	1.1 (4)	O6—C16—C17—C12	179.8 (2)
C1—C2—C7—C6	−179.1 (2)	C15—C16—C17—C12	−0.1 (3)

Fig. 1


C8
C3
C1
O1
C4
C2
C5
C7
O2
C6
C9
O3
C10
C18
C19
O5
O4
C14
C15
C13
C16
O6
C12
C17
C11
C20