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(1*S**,2*S**,5*R**,8*S**,11*S**,14*R**,17*S**,20*R**)-14-Methyl-6-methylene-10,16,18-trioxahexacyclo[12.5.1.1^{5,8}.0^{1,11}.0^{2,8}.0^{17,20}]henicosane-7,9-dione: natural diterpenoid macrocalyxoformin B

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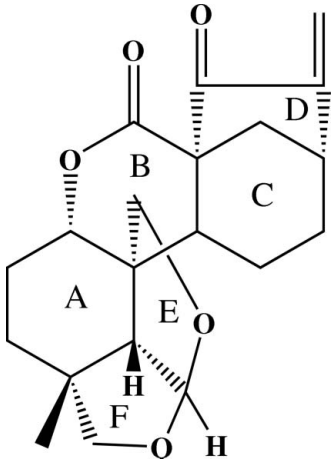
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.062; wR factor = 0.159; data-to-parameter ratio = 7.5.

The title compound, $C_{20}H_{24}O_5$, isolated from *Rabdosia* var. *lophanthoides* Hara, is built up from six fused rings. Cyclohexane ring *A* adopts a chair conformation, ring *B* exists in a screw-boat conformation and ring *C* adopts a boat conformation; the three five-membered rings *D*, *E* and *F* adopt envelope conformations.

Related literature

For related literature, see: Wang *et al.* (1986). For ring puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{20}H_{24}O_5$
M_r = 344.39
Orthorhombic, $P2_12_12_1$
a = 7.8450 (10) Å
b = 13.1365 (17) Å
c = 16.178 (2) Å
V = 1667.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.20 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.981, T_{max} = 0.987
7324 measured reflections
1707 independent reflections
1158 reflections with $I > 2\sigma(I)$
R_{int} = 0.151

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.159
S = 0.99
1707 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Puckering parameters (Å, °).

Ring	Q	θ	φ
A	0.478 (5)	24.8 (6)	126.4 (14)
B	0.664 (5)	106.1 (4)	89.3 (4)
C	0.821 (5)	100.1 (3)	54.3 (4)

	$Q2$	$\varphi2$
D	0.473 (5)	324.5 (6)
E	0.365 (5)	321.7 (7)
F	0.330 (5)	140.1 (9)

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: *PLATON* (Spek, 2003); 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: DN2278).

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supporting information

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(1*S**,2*S**,5*R**,8*S**,11*S**,14*R**,17*S**,20*R**)-14-Methyl-6-methylene-10,16,18-trioxahexacyclo[12.5.1.1^{5,8}.0^{1,11}.0^{2,8}.0^{17,20}]henicosane-7,9-dione: natural diterpenoid macrocalyxoformin B

Hao Shi

S1. Comment

The diterpenoid macrocalyxoformin B, (I), has been previously isolated from Rabdosia macrocalyx Hara (Wang *et al., 1986*) and its structure was established from the spectroscopic and chemical evidence. Recently, it was for the first time isolated from Rabdosia var lophanthoides Hara, and its structure was confirmed by an X-ray diffraction study.

The molecule is built up from six fused rings, three six membered and three five membered rings (Fig. 1). Some geometrical features of these rings were investigated using *PLATON* (Spek, 2003).

Cyclohexane ring A (C1/C11—C14/C20) adopts a chair conformation (Cremer & Pople, 1975), ring B (O10/C9/C8/C2/C1/C11) exists in a screw-boat conformation, ring C (C2—C5/C21/C8) adopts the boat conformation. All the three five-membered rings adopt envelope conformation.

S2. Experimental

The title compound (I) was isolated from Rabdosia var lophanthoides Hara and crystals suitable for X-ray structure analysis were obtained by slow evaporation from a solution of methanol at room temperature.

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (=CH_2); 0.96 Å (methy), 0.97 Å(methylene) or 0.98 Å (methine) with U_{iso}(H) = 1.2U_{eq}(=CH_2, methylene, methine) or U_{iso}(H) = 1.5U_{eq}(methyl).

In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined from the X-ray analyses and the Friedel pairs were merged, relative stereochemistry is shown in the Scheme and figures.

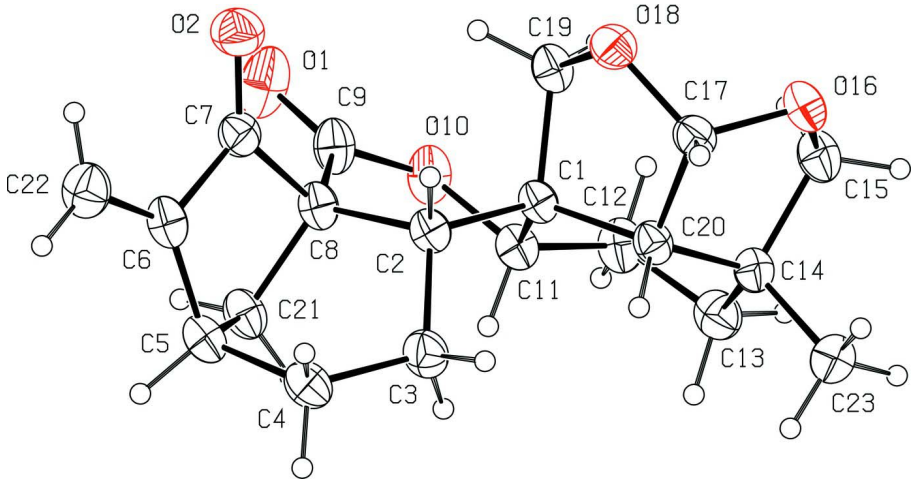

Figure 1

Molecular view of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

(1*S,2*S**,5*R**,8*S**,11*S**,14*R**, 17*S**,20*R**)-14-Methyl-6-methylene-10,16,18-trioxahexacyclo[12.5.1.1^{5,8}.0^{1,11}.0^{2,8}.0^{17,20}]henicosane-7,9-dione**

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Hall symbol: P 2ac 2ab
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c = 16.178 (2) Å
V = 1667.2 (4) Å^3
Z = 4
F(000) = 736
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1585 reflections
θ = 2.5–24.9°
μ = 0.10 mm^{-1}
T = 298 K
Plate, colorless
0.20 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.981, T_{max} = 0.987
7324 measured reflections
1707 independent reflections
1158 reflections with $I > 2\sigma(I)$
R_{int} = 0.151
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −8→9
k = −9→15
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.159
S = 0.99
1707 reflections
228 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

$w = 1/[\sigma^2(F_o^2) + (0.0846P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.2722 (6)	0.1295 (3)	0.8777 (3)	0.0774 (13)
O2	0.1286 (5)	0.3379 (3)	0.8514 (2)	0.0648 (11)
O10	0.5239 (5)	0.1278 (3)	0.8173 (2)	0.0528 (10)
O16	0.6881 (4)	0.3328 (3)	0.54354 (19)	0.0531 (10)
O18	0.4526 (4)	0.3456 (3)	0.6322 (2)	0.0485 (9)
C1	0.6034 (6)	0.2829 (4)	0.7468 (3)	0.0374 (11)
C2	0.5314 (6)	0.3540 (4)	0.8156 (3)	0.0403 (12)
H2	0.4508	0.4005	0.7890	0.048*
C3	0.6638 (7)	0.4202 (4)	0.8615 (3)	0.0517 (14)
H3A	0.7590	0.3776	0.8779	0.062*
H3B	0.7069	0.4715	0.8238	0.062*
C4	0.5914 (7)	0.4733 (4)	0.9387 (3)	0.0528 (14)
H4A	0.5317	0.5345	0.9217	0.063*
H4B	0.6853	0.4937	0.9740	0.063*
C5	0.4682 (7)	0.4057 (4)	0.9889 (3)	0.0490 (14)
H5	0.4809	0.4174	1.0485	0.059*
C6	0.2874 (7)	0.4183 (4)	0.9622 (3)	0.0475 (13)
C7	0.2569 (7)	0.3448 (4)	0.8912 (3)	0.0443 (12)
C8	0.4269 (6)	0.2882 (4)	0.8792 (3)	0.0421 (12)
C9	0.3966 (7)	0.1760 (4)	0.8572 (3)	0.0510 (14)
C11	0.6700 (7)	0.1866 (4)	0.7881 (3)	0.0427 (12)
H11	0.7402	0.2059	0.8357	0.051*
C12	0.7723 (7)	0.1176 (4)	0.7328 (3)	0.0523 (14)
H12A	0.7007	0.0926	0.6883	0.063*
H12B	0.8129	0.0596	0.7642	0.063*
C13	0.9228 (7)	0.1754 (5)	0.6971 (3)	0.0547 (15)
H13A	0.9869	0.1302	0.6613	0.066*
H13B	0.9972	0.1962	0.7418	0.066*
C14	0.8695 (6)	0.2705 (4)	0.6473 (3)	0.0439 (13)
C15	0.7866 (7)	0.2448 (4)	0.5647 (3)	0.0542 (15)
H15A	0.8725	0.2315	0.5230	0.065*
H15B	0.7140	0.1853	0.5699	0.065*

C17	0.6237 (7)	0.3750 (4)	0.6172 (3)	0.0442 (12)
H17	0.6306	0.4494	0.6142	0.053*
C19	0.4542 (7)	0.2586 (4)	0.6866 (3)	0.0437 (12)
H19A	0.4755	0.1963	0.6562	0.052*
H19B	0.3471	0.2523	0.7162	0.052*
C20	0.7337 (6)	0.3367 (4)	0.6893 (3)	0.0400 (11)
H20	0.7872	0.3941	0.7180	0.048*
C21	0.5012 (7)	0.2938 (4)	0.9666 (3)	0.0483 (13)
H21A	0.6221	0.2782	0.9668	0.058*
H21B	0.4425	0.2480	1.0041	0.058*
C22	0.1647 (7)	0.4771 (5)	0.9914 (4)	0.0605 (16)
H22A	0.1859	0.5197	1.0361	0.073*
H22B	0.0572	0.4758	0.9672	0.073*
C23	1.0269 (7)	0.3360 (5)	0.6295 (3)	0.0599 (15)
H23A	1.1118	0.2954	0.6023	0.090*
H23B	1.0722	0.3616	0.6806	0.090*
H23C	0.9955	0.3920	0.5945	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.091 (3)	0.042 (2)	0.099 (3)	−0.013 (2)	0.041 (3)	−0.008 (2)
O2	0.057 (2)	0.072 (3)	0.065 (2)	0.008 (2)	−0.006 (2)	−0.013 (2)
O10	0.071 (2)	0.0318 (19)	0.0556 (19)	0.0020 (19)	0.017 (2)	0.0054 (17)
O16	0.067 (2)	0.058 (2)	0.0344 (17)	0.002 (2)	0.0020 (17)	0.0028 (17)
O18	0.049 (2)	0.051 (2)	0.0454 (18)	0.0031 (19)	−0.0048 (17)	0.0100 (17)
C1	0.047 (3)	0.031 (3)	0.034 (2)	0.001 (2)	0.001 (2)	−0.001 (2)
C2	0.049 (3)	0.034 (3)	0.038 (2)	0.002 (2)	0.001 (2)	−0.001 (2)
C3	0.061 (3)	0.047 (3)	0.048 (3)	−0.009 (3)	0.004 (3)	−0.009 (3)
C4	0.064 (3)	0.047 (3)	0.047 (3)	0.000 (3)	−0.003 (3)	−0.011 (3)
C5	0.063 (3)	0.048 (3)	0.036 (2)	0.004 (3)	−0.001 (3)	−0.004 (2)
C6	0.064 (3)	0.039 (3)	0.039 (3)	0.002 (3)	0.008 (3)	0.001 (2)
C7	0.047 (3)	0.046 (3)	0.040 (2)	0.001 (3)	0.001 (2)	0.007 (2)
C8	0.054 (3)	0.033 (3)	0.039 (3)	0.003 (2)	0.006 (2)	−0.001 (2)
C9	0.067 (4)	0.039 (3)	0.047 (3)	0.002 (3)	0.014 (3)	0.006 (3)
C11	0.052 (3)	0.036 (3)	0.040 (2)	0.005 (3)	0.000 (2)	0.002 (2)
C12	0.063 (3)	0.039 (3)	0.055 (3)	0.014 (3)	0.008 (3)	0.001 (2)
C13	0.058 (3)	0.054 (4)	0.052 (3)	0.014 (3)	−0.001 (3)	−0.008 (3)
C14	0.045 (3)	0.047 (3)	0.040 (2)	0.001 (3)	0.004 (2)	−0.003 (2)
C15	0.065 (4)	0.054 (4)	0.044 (3)	0.008 (3)	0.006 (3)	−0.005 (3)
C17	0.050 (3)	0.044 (3)	0.039 (3)	−0.004 (3)	−0.002 (2)	−0.002 (2)
C19	0.059 (3)	0.033 (3)	0.039 (2)	−0.003 (3)	0.005 (3)	0.002 (2)
C20	0.049 (3)	0.036 (3)	0.035 (2)	−0.003 (2)	0.002 (2)	0.002 (2)
C21	0.063 (3)	0.045 (3)	0.037 (2)	0.007 (3)	0.000 (3)	0.007 (2)
C22	0.066 (4)	0.050 (4)	0.065 (4)	0.002 (3)	0.010 (3)	−0.009 (3)
C23	0.049 (3)	0.075 (4)	0.056 (3)	−0.001 (3)	0.006 (3)	−0.005 (3)

Geometric parameters (Å, º)

O1—C9	1.199 (7)	C8—C21	1.531 (7)
O2—C7	1.199 (6)	C8—C9	1.534 (7)
O10—C9	1.348 (6)	C11—C12	1.505 (7)
O10—C11	1.461 (6)	C11—H11	0.9800
O16—C17	1.408 (6)	C12—C13	1.518 (7)
O16—C15	1.432 (6)	C12—H12A	0.9700
O18—C17	1.418 (6)	C12—H12B	0.9700
O18—C19	1.443 (6)	C13—C14	1.544 (7)
C1—C11	1.523 (7)	C13—H13A	0.9700
C1—C20	1.552 (6)	C13—H13B	0.9700
C1—C19	1.555 (7)	C14—C15	1.523 (7)
C1—C2	1.558 (6)	C14—C23	1.533 (8)
C2—C3	1.545 (7)	C14—C20	1.534 (7)
C2—C8	1.575 (7)	C15—H15A	0.9700
C2—H2	0.9800	C15—H15B	0.9700
C3—C4	1.539 (7)	C17—C20	1.536 (7)
C3—H3A	0.9700	C17—H17	0.9800
C3—H3B	0.9700	C19—H19A	0.9700
C4—C5	1.544 (8)	C19—H19B	0.9700
C4—H4A	0.9700	C20—H20	0.9800
C4—H4B	0.9700	C21—H21A	0.9700
C5—C6	1.492 (8)	C21—H21B	0.9700
C5—C21	1.536 (7)	C22—H22A	0.9300
C5—H5	0.9800	C22—H22B	0.9300
C6—C22	1.321 (7)	C23—H23A	0.9600
C6—C7	1.520 (7)	C23—H23B	0.9600
C7—C8	1.539 (7)	C23—H23C	0.9600
C9—O10—C11	119.2 (4)	C13—C12—H12A	109.7
C17—O16—C15	108.0 (4)	C11—C12—H12B	109.7
C17—O18—C19	108.2 (4)	C13—C12—H12B	109.7
C11—C1—C20	114.5 (4)	H12A—C12—H12B	108.2
C11—C1—C19	111.3 (4)	C12—C13—C14	113.1 (4)
C20—C1—C19	102.4 (4)	C12—C13—H13A	109.0
C11—C1—C2	108.0 (4)	C14—C13—H13A	109.0
C20—C1—C2	113.2 (4)	C12—C13—H13B	109.0
C19—C1—C2	107.3 (4)	C14—C13—H13B	109.0
C3—C2—C1	115.9 (4)	H13A—C13—H13B	107.8
C3—C2—C8	110.2 (4)	C15—C14—C23	107.7 (4)
C1—C2—C8	109.1 (4)	C15—C14—C20	102.6 (4)
C3—C2—H2	107.1	C23—C14—C20	109.0 (4)
C1—C2—H2	107.1	C15—C14—C13	113.2 (5)
C8—C2—H2	107.1	C23—C14—C13	109.5 (4)
C4—C3—C2	113.4 (4)	C20—C14—C13	114.5 (4)
C4—C3—H3A	108.9	O16—C15—C14	105.1 (4)
C2—C3—H3A	108.9	O16—C15—H15A	110.7

C4—C3—H3B	108.9	C14—C15—H15A	110.7
C2—C3—H3B	108.9	O16—C15—H15B	110.7
H3A—C3—H3B	107.7	C14—C15—H15B	110.7
C3—C4—C5	113.5 (4)	H15A—C15—H15B	108.8
C3—C4—H4A	108.9	O16—C17—O18	112.2 (4)
C5—C4—H4A	108.9	O16—C17—C20	108.2 (4)
C3—C4—H4B	108.9	O18—C17—C20	108.2 (4)
C5—C4—H4B	108.9	O16—C17—H17	109.4
H4A—C4—H4B	107.7	O18—C17—H17	109.4
C6—C5—C21	101.4 (5)	C20—C17—H17	109.4
C6—C5—C4	112.3 (4)	O18—C19—C1	103.1 (4)
C21—C5—C4	108.7 (4)	O18—C19—H19A	111.2
C6—C5—H5	111.3	C1—C19—H19A	111.2
C21—C5—H5	111.3	O18—C19—H19B	111.2
C4—C5—H5	111.3	C1—C19—H19B	111.2
C22—C6—C5	130.8 (5)	H19A—C19—H19B	109.1
C22—C6—C7	121.8 (5)	C14—C20—C17	103.8 (4)
C5—C6—C7	107.3 (4)	C14—C20—C1	117.7 (4)
O2—C7—C6	125.9 (5)	C17—C20—C1	103.5 (4)
O2—C7—C8	128.5 (5)	C14—C20—H20	110.4
C6—C7—C8	105.4 (4)	C17—C20—H20	110.4
C21—C8—C9	108.7 (4)	C1—C20—H20	110.4
C21—C8—C7	101.0 (4)	C8—C21—C5	101.5 (4)
C9—C8—C7	111.1 (4)	C8—C21—H21A	111.5
C21—C8—C2	112.2 (4)	C5—C21—H21A	111.5
C9—C8—C2	117.1 (4)	C8—C21—H21B	111.5
C7—C8—C2	105.6 (4)	C5—C21—H21B	111.5
O1—C9—O10	119.7 (5)	H21A—C21—H21B	109.3
O1—C9—C8	123.5 (5)	C6—C22—H22A	120.0
O10—C9—C8	116.6 (5)	C6—C22—H22B	120.0
O10—C11—C12	107.0 (4)	H22A—C22—H22B	120.0
O10—C11—C1	108.2 (4)	C14—C23—H23A	109.5
C12—C11—C1	115.0 (4)	C14—C23—H23B	109.5
O10—C11—H11	108.9	H23A—C23—H23B	109.5
C12—C11—H11	108.9	C14—C23—H23C	109.5
C1—C11—H11	108.9	H23A—C23—H23C	109.5
C11—C12—C13	109.9 (4)	H23B—C23—H23C	109.5
C11—C12—H12A	109.7		

C11—C1—C2—C3	82.7 (5)	C2—C1—C11—O10	71.0 (5)
C20—C1—C2—C3	−45.1 (5)	C20—C1—C11—C12	−42.5 (6)
C19—C1—C2—C3	−157.3 (4)	C19—C1—C11—C12	73.0 (5)
C11—C1—C2—C8	−42.3 (5)	C2—C1—C11—C12	−169.5 (4)
C20—C1—C2—C8	−170.1 (4)	O10—C11—C12—C13	177.5 (4)
C19—C1—C2—C8	77.7 (4)	C1—C11—C12—C13	57.4 (6)
C1—C2—C3—C4	−169.3 (4)	C11—C12—C13—C14	−58.3 (6)
C8—C2—C3—C4	−44.8 (6)	C12—C13—C14—C15	−71.9 (6)
C2—C3—C4—C5	39.5 (6)	C12—C13—C14—C23	168.0 (5)

C3—C4—C5—C6	−91.0 (6)	C12—C13—C14—C20	45.3 (6)
C3—C4—C5—C21	20.4 (6)	C17—O16—C15—C14	−34.5 (5)
C21—C5—C6—C22	149.2 (6)	C23—C14—C15—O16	−81.1 (5)
C4—C5—C6—C22	−95.0 (6)	C20—C14—C15—O16	33.8 (5)
C21—C5—C6—C7	−28.9 (5)	C13—C14—C15—O16	157.7 (4)
C4—C5—C6—C7	86.9 (5)	C15—O16—C17—O18	−98.7 (5)
C22—C6—C7—O2	6.0 (8)	C15—O16—C17—C20	20.6 (5)
C5—C6—C7—O2	−175.7 (5)	C19—O18—C17—O16	95.5 (5)
C22—C6—C7—C8	−177.4 (5)	C19—O18—C17—C20	−23.9 (5)
C5—C6—C7—C8	0.9 (5)	C17—O18—C19—C1	37.8 (5)
O2—C7—C8—C21	−156.0 (6)	C11—C1—C19—O18	−158.8 (4)
C6—C7—C8—C21	27.5 (5)	C20—C1—C19—O18	−36.1 (5)
O2—C7—C8—C9	−40.9 (7)	C2—C1—C19—O18	83.3 (4)
C6—C7—C8—C9	142.6 (4)	C15—C14—C20—C17	−20.9 (5)
O2—C7—C8—C2	87.0 (6)	C23—C14—C20—C17	93.1 (5)
C6—C7—C8—C2	−89.5 (4)	C13—C14—C20—C17	−143.9 (5)
C3—C2—C8—C21	−9.1 (6)	C15—C14—C20—C1	92.7 (5)
C1—C2—C8—C21	119.2 (4)	C23—C14—C20—C1	−153.3 (4)
C3—C2—C8—C9	−135.8 (5)	C13—C14—C20—C1	−30.3 (6)
C1—C2—C8—C9	−7.5 (6)	O16—C17—C20—C14	1.4 (5)
C3—C2—C8—C7	100.0 (5)	O18—C17—C20—C14	123.2 (4)
C1—C2—C8—C7	−131.7 (4)	O16—C17—C20—C1	−122.1 (4)
C11—O10—C9—O1	176.3 (5)	O18—C17—C20—C1	−0.3 (5)
C11—O10—C9—C8	−8.0 (6)	C11—C1—C20—C14	28.6 (5)
C21—C8—C9—O1	82.9 (7)	C19—C1—C20—C14	−91.9 (4)
C7—C8—C9—O1	−27.3 (7)	C2—C1—C20—C14	152.9 (4)
C2—C8—C9—O1	−148.7 (5)	C11—C1—C20—C17	142.4 (4)
C21—C8—C9—O10	−92.6 (5)	C19—C1—C20—C17	21.8 (5)
C7—C8—C9—O10	157.1 (4)	C2—C1—C20—C17	−93.3 (4)
C2—C8—C9—O10	35.8 (6)	C9—C8—C21—C5	−162.2 (4)
C9—O10—C11—C12	−169.4 (4)	C7—C8—C21—C5	−45.3 (5)
C9—O10—C11—C1	−45.0 (5)	C2—C8—C21—C5	66.7 (5)
C20—C1—C11—O10	−162.0 (4)	C6—C5—C21—C8	46.3 (5)
C19—C1—C11—O10	−46.5 (5)	C4—C5—C21—C8	−72.2 (5)