

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2,3-Dimethoxy-5,12-tetracenequinone

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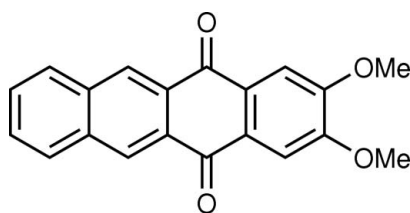
Received 17 December 2008; accepted 10 January 2009

Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.050; wR factor = 0.147; data-to-parameter ratio = 15.4.

The molecule of the title compound, $\text{C}_{20}\text{H}_{14}\text{O}_4$, is approximately planar [maximum deviation 0.168 (2) Å]. The two methoxy groups are slightly twisted relative to the plane of the 5,12-tetracenequinone system, with twist angles of 3.3 (3) and 5.6 (2)°. All O atoms are involved in intermolecular C—H···O interactions and the molecules are arranged into slipped face-to-face stacks along the b axis via π – π interactions with an interplanar distance of 3.407 (2) Å.

Related literature

For general background, see: Kitamura *et al.* (2008). For the synthetic procedures, see: McOmie & Perry (1973); Vets *et al.* (2004). For another synthetic method leading to the title compound, see: Reichwagen *et al.* (2005).



Experimental

Crystal data

$\text{C}_{20}\text{H}_{14}\text{O}_4$ $V = 1477.2$ (8) Å³
 $M_r = 318.31$ $Z = 4$
 Monoclinic, $P2_1/c$ Mo $K\alpha$ radiation
 $a = 8.290$ (3) Å $\mu = 0.1$ mm⁻¹
 $b = 6.9781$ (19) Å $T = 223$ K
 $c = 25.779$ (8) Å $0.5 \times 0.1 \times 0.05$ mm
 $\beta = 97.883$ (1)°

Data collection

Rigaku Mercury CCD area-detector 11405 measured reflections
 diffractometer 3370 independent reflections
 Absorption correction: numerical 2773 reflections with $I > 2\sigma(I)$
 (NUMABS; Higashi, 1999) $R_{\text{int}} = 0.033$
 $T_{\text{min}} = 0.988$, $T_{\text{max}} = 0.997$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$ 219 parameters
 $wR(F^2) = 0.147$ H-atom parameters constrained
 $S = 1.12$ $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 3370 reflections $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8}\cdots\text{O3}^{\text{i}}$	0.94	2.30	3.210 (2)	162
$\text{C15}-\text{H15}\cdots\text{O4}^{\text{ii}}$	0.94	2.60	3.383 (2)	141
$\text{C20}-\text{H20B}\cdots\text{O1}^{\text{iii}}$	0.97	2.55	3.486 (2)	162
$\text{C20}-\text{H20B}\cdots\text{O2}^{\text{iii}}$	0.97	2.48	3.206 (2)	131

Symmetry codes: (i) $-x + 1, -y, -z$; (ii) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 2, -y + 2, -z$.

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the Instrument Center of the Institute for Molecular Science for the X-ray structural analysis. This work was supported by a Grant-in-Aid (No. 20550128) for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2182).

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supplementary materials

Acta Cryst. (2009). E65, o324 [doi:10.1107/S1600536809001147]

2,3-Dimethoxy-5,12-tetracenequinone

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Comment

Although the title compound (I) was already synthesized (Reichwagen *et al.*, 2005), the X-ray structure was not reported. We prepared 2,3-dimethoxytetracene from 8,9-dimethoxy-5,12-tetracenequinone (McOmie & Perry, 1973), and attempted to perform the X-ray analysis of crystals made by recrystallization from a hot DMF solution under air and light. The analysis revealed that the molecule was not as expected 2,3-dimethoxytetracene but the title compound. Quinones have a weak dipole moment along the molecular long axis and are expected to take an antiparallel arrangement with respect to one another. The latter propensity may lead to the formation of face-to-face π -overlap along the stacking direction (Kitamura *et al.*, 2008).

The molecular structure is shown in Fig. 1. The molecule is approximately planar. The displacements of atoms O1, O2, O3, O4, C19, and C20 relative to the plane of the tetracene framework are -0.025 (1), -0.022 (1), -0.092 (1), 0.029 (1), -0.168 (2), and -0.113 (2) Å, respectively. The torsion angles of the two methoxy groups are -5.6 (2)° for C1—C2—O1—C19 and 3.3 (3)° for C4—C3—O2—C20, displaying that the C_{methyl}—O bonds are directed along the molecular short axis.

In the crystal structure, the molecules are linked through intermolecular C—H...O hydrogen bonds between the methoxy groups as well as between the tetracene groups (Table 1, Fig. 2). Interestingly, along the stacking direction, not antiparallel but just slipped π - π stacking can be found. The interplanar distance is 3.407 (2) Å. The dipole moment of (I) was calculated by MO calculations (B3LYP/6-31G*), which afforded an estimation of 0.01 debye. Thus, (I) is a non-polar molecule. Therefore, it seems reasonable to conclude that the electrostatic property can determine either an antiparallel or a non-antiparallel arrangement.

Experimental

8,9-Dimethoxy-5,12-tetracenequinone was prepared according to the method described by McOmie & Perry (1973). Transformation of tetracenequinone into tetracene was performed using two successive LiAlH₄ reductions by Vets *et al.* (2004). To a suspension of LiAlH₄ (224 mg, 5.9 mmol) in dry THF (15 ml), 8,9-dimethoxy-5,12-tetracenequinone (479 mg, 1.5 mmol) was added under nitrogen. The mixture was refluxed for 30 min, cooled to room temperature, and 6M HCl (7 ml) was added under cooling with ice. The residue was filtered, and washed with water, MeOH, and Et₂O. After drying, a yellow solid was isolated. The solid was added into a suspension of LiAlH₄ (235 mg, 6.2 mmol) in dry THF (15 ml). The mixture was again refluxed for 30 min, cooled to room temperature, and 6M HCl (7 ml) was added under cooling with ice. The product was filtered, and washed with water, MeOH, and Et₂O. After drying, 2,3-dimethoxytetracene was obtained (287 mg, 66%) as a yellow solid. Heating the tetracene in DMF under air and light, and then cooling the solution to room temperature resulted in deposition of brown crystals suitable for X-ray analysis.

Refinement

All H atoms were positioned geometrically and refined using a riding model approximation with C—H = 0.94 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C—H, and C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃.

Figures

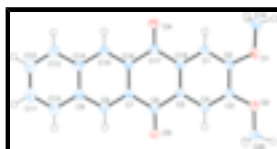


Fig. 1. The molecular structure of the title compound showing 50% probability displacement ellipsoids for non-H atoms.

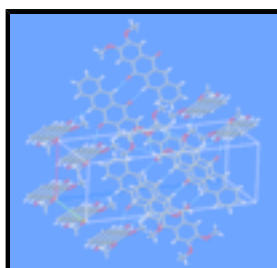


Fig. 2. The packing diagram of the title compound. C-H...O interactions are shown with dashed lines.

2,3-Dimethoxy-5,12-tetracenequinone

Crystal data

C₂₀H₁₄O₄

$M_r = 318.31$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.290$ (3) Å

$b = 6.9781$ (19) Å

$c = 25.779$ (8) Å

$\beta = 97.8830$ (10)°

$V = 1477.2$ (8) Å³

$Z = 4$

$F_{000} = 664$

$D_x = 1.431$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4021 reflections

$\theta = 3.0$ – 27.5°

$\mu = 0.1$ mm⁻¹

$T = 223$ K

Prism, brown

$0.5 \times 0.1 \times 0.05$ mm

Data collection

Rigaku Mercury CCD area-detector diffractometer

Radiation source: rotating-anode X-ray tube

Monochromator: graphite

Detector resolution: 14.7059 pixels mm⁻¹

$T = 223$ K

ϕ and ω scans

Absorption correction: numerical

3370 independent reflections

2773 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\text{max}} = 27.5^\circ$

$\theta_{\text{min}} = 3.0^\circ$

$h = -10 \rightarrow 10$

$k = -9 \rightarrow 5$

(NUMABS; Higashi, 1999)

$T_{\min} = 0.988$, $T_{\max} = 0.997$

$l = -33 \rightarrow 25$

11405 measured reflections

Refinement

Refinement on F^2

H-atom parameters constrained

Least-squares matrix: full

$$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.2183P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$R[F^2 > 2\sigma(F^2)] = 0.050$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$wR(F^2) = 0.147$$

$$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$$

$$S = 1.12$$

$$\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$$

3370 reflections

Extinction correction: none

219 parameters

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.00036 (17)	0.53181 (18)	0.14389 (6)	0.0275 (3)
H1	1.062	0.5387	0.1773	0.033*
C2	1.01106 (17)	0.67689 (19)	0.10804 (6)	0.0274 (3)
C3	0.91825 (18)	0.66693 (19)	0.05767 (6)	0.0287 (3)
C4	0.81764 (18)	0.51175 (19)	0.04488 (5)	0.0289 (3)
H4	0.7562	0.5042	0.0115	0.035*
C5	0.80647 (17)	0.36535 (18)	0.08134 (5)	0.0259 (3)
C6	0.69108 (19)	0.20757 (19)	0.06595 (5)	0.0291 (3)
C7	0.67888 (17)	0.05220 (18)	0.10459 (5)	0.0255 (3)
C8	0.57670 (18)	-0.09998 (19)	0.09083 (5)	0.0282 (3)
H8	0.5149	-0.103	0.0574	0.034*
C9	0.56328 (18)	-0.25179 (18)	0.12612 (6)	0.0268 (3)
C10	0.46090 (19)	-0.4123 (2)	0.11233 (6)	0.0341 (3)
H10	0.4002	-0.4192	0.0788	0.041*
C11	0.4501 (2)	-0.5567 (2)	0.14754 (7)	0.0384 (4)
H11	0.3814	-0.6619	0.1381	0.046*
C12	0.5408 (2)	-0.5489 (2)	0.19769 (6)	0.0386 (4)
H12	0.5326	-0.6492	0.2215	0.046*

supplementary materials

C13	0.6411 (2)	-0.3969 (2)	0.21228 (6)	0.0344 (4)
H13	0.7013	-0.3936	0.2459	0.041*
C14	0.65452 (17)	-0.24356 (18)	0.17669 (6)	0.0273 (3)
C15	0.75879 (18)	-0.08529 (19)	0.19038 (5)	0.0280 (3)
H15	0.8193	-0.0794	0.224	0.034*
C16	0.77246 (16)	0.05988 (18)	0.15515 (5)	0.0241 (3)
C17	0.88638 (17)	0.22181 (18)	0.16997 (5)	0.0260 (3)
C18	0.89773 (17)	0.37413 (18)	0.13063 (5)	0.0247 (3)
C19	1.1882 (2)	0.8638 (2)	0.16855 (6)	0.0360 (4)
H19A	1.1096	0.8696	0.1932	0.054*
H19B	1.2491	0.9828	0.1699	0.054*
H19C	1.2624	0.7579	0.1777	0.054*
C20	0.8334 (2)	0.8166 (2)	-0.02447 (6)	0.0398 (4)
H20A	0.8583	0.7051	-0.0444	0.06*
H20B	0.8538	0.932	-0.0435	0.06*
H20C	0.7199	0.8127	-0.0192	0.06*
O1	1.10487 (14)	0.83614 (14)	0.11692 (4)	0.0362 (3)
O2	0.93439 (14)	0.81632 (14)	0.02532 (4)	0.0378 (3)
O3	0.60656 (17)	0.20730 (16)	0.02332 (4)	0.0491 (4)
O4	0.96858 (15)	0.22784 (14)	0.21323 (4)	0.0401 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0273 (7)	0.0287 (7)	0.0248 (7)	-0.0028 (5)	-0.0018 (5)	-0.0021 (5)
C2	0.0268 (7)	0.0268 (6)	0.0283 (7)	-0.0069 (5)	0.0027 (6)	-0.0035 (5)
C3	0.0311 (8)	0.0287 (7)	0.0263 (7)	-0.0044 (5)	0.0042 (6)	0.0040 (5)
C4	0.0322 (8)	0.0306 (7)	0.0223 (7)	-0.0061 (6)	-0.0021 (6)	0.0023 (5)
C5	0.0276 (7)	0.0244 (6)	0.0247 (7)	-0.0025 (5)	0.0004 (6)	0.0008 (5)
C6	0.0352 (8)	0.0265 (6)	0.0234 (7)	-0.0061 (6)	-0.0035 (6)	0.0017 (5)
C7	0.0291 (7)	0.0238 (6)	0.0229 (7)	-0.0019 (5)	0.0007 (6)	0.0005 (5)
C8	0.0317 (8)	0.0269 (6)	0.0244 (7)	-0.0037 (5)	-0.0022 (6)	0.0007 (5)
C9	0.0275 (7)	0.0237 (6)	0.0295 (8)	0.0003 (5)	0.0047 (6)	-0.0002 (5)
C10	0.0355 (8)	0.0301 (7)	0.0364 (8)	-0.0049 (6)	0.0033 (7)	-0.0009 (6)
C11	0.0388 (9)	0.0271 (7)	0.0505 (10)	-0.0064 (6)	0.0107 (7)	0.0001 (6)
C12	0.0453 (9)	0.0287 (7)	0.0442 (10)	0.0007 (6)	0.0143 (8)	0.0117 (6)
C13	0.0396 (9)	0.0323 (7)	0.0315 (8)	0.0033 (6)	0.0057 (7)	0.0074 (6)
C14	0.0293 (8)	0.0244 (6)	0.0286 (8)	0.0033 (5)	0.0059 (6)	0.0034 (5)
C15	0.0317 (8)	0.0279 (6)	0.0231 (7)	0.0023 (5)	-0.0004 (6)	0.0021 (5)
C16	0.0267 (7)	0.0217 (6)	0.0232 (7)	0.0017 (5)	0.0008 (5)	-0.0005 (5)
C17	0.0289 (7)	0.0253 (6)	0.0222 (7)	0.0010 (5)	-0.0026 (6)	-0.0009 (5)
C18	0.0261 (7)	0.0239 (6)	0.0234 (7)	-0.0006 (5)	0.0009 (5)	-0.0009 (5)
C19	0.0372 (9)	0.0353 (7)	0.0345 (8)	-0.0117 (6)	0.0013 (7)	-0.0091 (6)
C20	0.0465 (10)	0.0386 (8)	0.0318 (8)	-0.0136 (7)	-0.0034 (7)	0.0106 (6)
O1	0.0425 (7)	0.0324 (5)	0.0320 (6)	-0.0160 (4)	-0.0008 (5)	-0.0007 (4)
O2	0.0448 (7)	0.0347 (5)	0.0314 (6)	-0.0160 (5)	-0.0034 (5)	0.0090 (4)
O3	0.0679 (9)	0.0436 (6)	0.0288 (6)	-0.0257 (6)	-0.0190 (6)	0.0104 (5)
O4	0.0514 (7)	0.0337 (5)	0.0294 (6)	-0.0079 (5)	-0.0149 (5)	0.0029 (4)

Geometric parameters (Å, °)

C1—C2	1.3818 (19)	C11—C12	1.405 (2)
C1—C18	1.4041 (18)	C11—H11	0.94
C1—H1	0.94	C12—C13	1.368 (2)
C2—O1	1.3577 (16)	C12—H12	0.94
C2—C3	1.417 (2)	C13—C14	1.4237 (19)
C3—O2	1.3530 (16)	C13—H13	0.94
C3—C4	1.3790 (19)	C14—C15	1.4170 (19)
C4—C5	1.3998 (19)	C15—C16	1.3757 (19)
C4—H4	0.94	C15—H15	0.94
C5—C18	1.3881 (19)	C16—C17	1.4885 (18)
C5—C6	1.4766 (18)	C17—O4	1.2254 (16)
C6—O3	1.2198 (17)	C17—C18	1.4810 (18)
C6—C7	1.4851 (18)	C19—O1	1.4262 (18)
C7—C8	1.3743 (18)	C19—H19A	0.97
C7—C16	1.4233 (18)	C19—H19B	0.97
C8—C9	1.4107 (19)	C19—H19C	0.97
C8—H8	0.94	C20—O2	1.4331 (18)
C9—C14	1.416 (2)	C20—H20A	0.97
C9—C10	1.4206 (19)	C20—H20B	0.97
C10—C11	1.368 (2)	C20—H20C	0.97
C10—H10	0.94		
C2—C1—C18	120.24 (12)	C13—C12—H12	119.6
C2—C1—H1	119.9	C11—C12—H12	119.6
C18—C1—H1	119.9	C12—C13—C14	120.25 (14)
O1—C2—C1	125.09 (13)	C12—C13—H13	119.9
O1—C2—C3	114.90 (12)	C14—C13—H13	119.9
C1—C2—C3	120.01 (12)	C9—C14—C15	119.45 (12)
O2—C3—C4	124.42 (13)	C9—C14—C13	118.93 (13)
O2—C3—C2	116.09 (12)	C15—C14—C13	121.61 (13)
C4—C3—C2	119.48 (12)	C16—C15—C14	120.81 (13)
C3—C4—C5	120.40 (13)	C16—C15—H15	119.6
C3—C4—H4	119.8	C14—C15—H15	119.6
C5—C4—H4	119.8	C15—C16—C7	119.53 (12)
C18—C5—C4	120.29 (12)	C15—C16—C17	119.76 (12)
C18—C5—C6	122.03 (12)	C7—C16—C17	120.70 (12)
C4—C5—C6	117.64 (12)	O4—C17—C18	121.27 (12)
O3—C6—C5	120.94 (12)	O4—C17—C16	120.91 (12)
O3—C6—C7	121.31 (12)	C18—C17—C16	117.82 (12)
C5—C6—C7	117.73 (12)	C5—C18—C1	119.56 (12)
C8—C7—C16	120.32 (12)	C5—C18—C17	121.15 (12)
C8—C7—C6	119.16 (12)	C1—C18—C17	119.27 (12)
C16—C7—C6	120.53 (12)	O1—C19—H19A	109.5
C7—C8—C9	120.93 (13)	O1—C19—H19B	109.5
C7—C8—H8	119.5	H19A—C19—H19B	109.5
C9—C8—H8	119.5	O1—C19—H19C	109.5
C8—C9—C14	118.95 (12)	H19A—C19—H19C	109.5

supplementary materials

C8—C9—C10	121.86 (13)	H19B—C19—H19C	109.5
C14—C9—C10	119.19 (13)	O2—C20—H20A	109.5
C11—C10—C9	120.42 (14)	O2—C20—H20B	109.5
C11—C10—H10	119.8	H20A—C20—H20B	109.5
C9—C10—H10	119.8	O2—C20—H20C	109.5
C10—C11—C12	120.41 (14)	H20A—C20—H20C	109.5
C10—C11—H11	119.8	H20B—C20—H20C	109.5
C12—C11—H11	119.8	C2—O1—C19	117.45 (11)
C13—C12—C11	120.79 (13)	C3—O2—C20	117.27 (11)
C18—C1—C2—O1	179.31 (13)	C10—C9—C14—C13	0.1 (2)
C18—C1—C2—C3	0.0 (2)	C12—C13—C14—C9	-0.3 (2)
O1—C2—C3—O2	-0.27 (19)	C12—C13—C14—C15	-179.20 (14)
C1—C2—C3—O2	179.11 (13)	C9—C14—C15—C16	-0.1 (2)
O1—C2—C3—C4	-179.36 (13)	C13—C14—C15—C16	178.82 (13)
C1—C2—C3—C4	0.0 (2)	C14—C15—C16—C7	0.9 (2)
O2—C3—C4—C5	-178.75 (14)	C14—C15—C16—C17	-178.27 (12)
C2—C3—C4—C5	0.3 (2)	C8—C7—C16—C15	-0.6 (2)
C3—C4—C5—C18	-0.6 (2)	C6—C7—C16—C15	179.76 (13)
C3—C4—C5—C6	177.37 (13)	C8—C7—C16—C17	178.55 (13)
C18—C5—C6—O3	176.55 (15)	C6—C7—C16—C17	-1.1 (2)
C4—C5—C6—O3	-1.3 (2)	C15—C16—C17—O4	0.0 (2)
C18—C5—C6—C7	-2.0 (2)	C7—C16—C17—O4	-179.14 (13)
C4—C5—C6—C7	-179.93 (13)	C15—C16—C17—C18	179.63 (12)
O3—C6—C7—C8	3.6 (2)	C7—C16—C17—C18	0.5 (2)
C5—C6—C7—C8	-177.82 (13)	C4—C5—C18—C1	0.6 (2)
O3—C6—C7—C16	-176.79 (14)	C6—C5—C18—C1	-177.27 (13)
C5—C6—C7—C16	1.8 (2)	C4—C5—C18—C17	179.34 (13)
C16—C7—C8—C9	-0.5 (2)	C6—C5—C18—C17	1.5 (2)
C6—C7—C8—C9	179.12 (13)	C2—C1—C18—C5	-0.3 (2)
C7—C8—C9—C14	1.3 (2)	C2—C1—C18—C17	-179.09 (13)
C7—C8—C9—C10	-178.72 (13)	O4—C17—C18—C5	178.92 (13)
C8—C9—C10—C11	-179.71 (14)	C16—C17—C18—C5	-0.7 (2)
C14—C9—C10—C11	0.3 (2)	O4—C17—C18—C1	-2.3 (2)
C9—C10—C11—C12	-0.4 (2)	C16—C17—C18—C1	178.11 (12)
C10—C11—C12—C13	0.2 (2)	C1—C2—O1—C19	-5.6 (2)
C11—C12—C13—C14	0.1 (2)	C3—C2—O1—C19	173.78 (13)
C8—C9—C14—C15	-1.0 (2)	C4—C3—O2—C20	3.3 (2)
C10—C9—C14—C15	179.02 (13)	C2—C3—O2—C20	-175.73 (13)
C8—C9—C14—C13	-179.95 (13)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C8—H8...O3 ⁱ	0.94	2.30	3.210 (2)	162
C15—H15...O4 ⁱⁱ	0.94	2.60	3.383 (2)	141
C20—H20B...O1 ⁱⁱⁱ	0.97	2.55	3.486 (2)	162
C20—H20B...O2 ⁱⁱⁱ	0.97	2.48	3.206 (2)	131

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x+2, y-1/2, -z+1/2$; (iii) $-x+2, -y+2, -z$.

Fig. 1

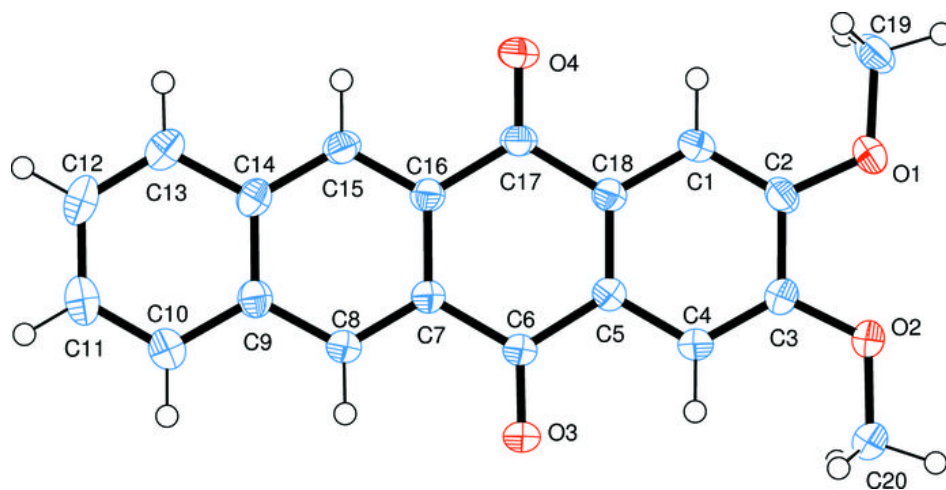


Fig. 2

