Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 7,9-Dimethyl-3-phenylnaphtho[1,2-*b*]-furan-4,5-dione

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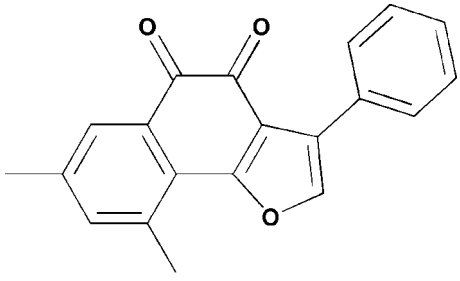
Received 4 September 2007; accepted 14 September 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.040; $wR$ factor = 0.119; data-to-parameter ratio = 15.1.

In the title compound, $C_{20}H_{14}O_3$, $\pi$–$\pi$ stacking interactions [3.474 (2)–3.789 (2) Å] dominate the crystal structure. The dihedral angle between the phenyl ring and fused-ring system is 32.3 (3)°.

## Related literature

For related literature, see: Chang *et al.* (1991); Janiak (2000); Ng *et al.* (2000); Kongkathip *et al.* (2003); Park *et al.* (1999); Shen *et al.* (2005).



## Experimental

### Crystal data

$C_{20}H_{14}O_3$
$M_r$ = 302.31
Monoclinic, $P2_1/c$
$a$ = 7.792 (2) Å
$b$ = 7.602 (2) Å
$c$ = 24.746 (7) Å
$\beta$ = 93.610 (5)°
$V$ = 1463.0 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 (2) K
0.50 × 0.38 × 0.27 mm

### Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.956, $T_{max}$ = 0.976
9844 measured reflections
3174 independent reflections
2534 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
$S$ = 1.03
3174 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by Guangdong Provincical Science Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2097).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4125 [ **doi:10.1107/S1600536807045059** ]

# 7,9-Dimethyl-3-phenylnaphtho[1,2-*b*]furan-4,5-dione

**Y. Shen, Y.-X. Tian and X.-Z. Bu**

## Comment

Polycyclic *ortho*-quinonoid structures constitute a large category of significant compounds which possess a broad spectrum of biological activities such as antioxidant activity (Ng *et al.*, 2000), cytotoxicity (Park *et al.*, 1999), antifungal activity (Chang *et al.*, 1991), antineoplastic activity (Kongkathip *et al.*, 2003). Recently, we are engaged in a program directed at searching for new bioactive *ortho*-quinoid compounds. As part of our investigation (Shen *et al.*, 2005), we reported the synthesis and single-crystal structure of 7, 9-dimethyl-3-phenylnaphtho [1, 2 − b] furan-4, 5-dione (I).

The X-ray study of (I) confirms the previously proposed molecular structure based on spectroscopic data (Figure. 1).

The C—C, C=C, C—O and C=O distances show no remarkable features, except that the bond C10—C11(1.548 (2) Å) is significantly longer than normal distance of C—C bond.

A structural feature of (I) is the presence of intermolecular strong π-π stacking interactions between adjacent molecules. The geometric parameters are within the acceptable range (Janiak, 2000). The *Cg*1···*Cg*2$^{i}$, *Cg*1···*Cg*3$^{ii}$ and *Cg*2···*Cg*3$^{ii}$ distances are 3.474 (2), 3.789 (2) and 3.690 (2)Å respectively [symmetry code: (i) −*x*, 1 − *y*, 2 − *z*, (ii)-*x*, −*y*, 2 − *z*, *Cg*1, *Cg*2 and *Cg*3 are centroids of the C10-containing ring, C13-containing ring and the O1-containing ring] (Figure. 2).

The naphtho[1,2-*b*]furan-4,5-dione part of the title molecule is approximately coplanar, the interplanar distances between neighbouring 13-membered ring planes are 3.458 (2) and 3.527 (2) Å.

Obviously, aromatic π-π stacking interactions play a key role in assembling the supramolecular structure.

## Experimental

The title compound was prepared from 3-phenylbenzofuran-4,5-dione and *N*-(2-methylpenta-1,3-dienyl)acetamide by the strategy of Diels-Alder. *N*-(2-methylpenta-1,3-dienyl)acetamide (0.139 g, 1 mmol) and 3-phenylbenzofuran-4,5-dione (0.240 g, 1 mmol) were added to benzene (30 ml), and refluxed for 5 h. Then, silica gel (10 g, 80–120 mesh) was added to the solution and the solvent was removed in vacuum at 45°C.

The resulted dry reaction-mixture-coated silica gel was then stirred at 45°C for 24 h. Purification by chromatography on silica gel ($CHCl_3$/$CH_3OH$) gave target compound (I) in 65% yield.

Crystals of (I) suitable for X-ray analysis were grown from $CDCl_3$ solution.

$^1$H-NMR (300 MHz, $CDCl_3$, TMS): δ 2.35(s, 3H), 2.67(s, 3H), 7.23(s, 1H), 7.35–7.42(m, 3H), 7.59(s, 1H), 7.64 (d, 1H), 7.75(s, 1H).

$^{13}$C NMR (75 MHz, $CDCl_3$): δ 21.16, 21.68, 118.71, 124.14, 127.19, 128.29, 128.30, 128.33, 128.34, 128.35, 129.09, 129.46, 129.63, 135.47, 139.33, 140.19, 140.81, 163.30, 174.84, 181.10.

ESI-MS(m/*z*): 303 ($[M+H]^+$).

### Refinement

All H atoms were positioned geometrically and refined with a riding model, with distances 0.96 ($CH_3$) and 0.93Å (CH) with $U_{iso}$(H) = 1.2 (1.5 for methyl groups) times $U_{eq}$(C).

### Figures

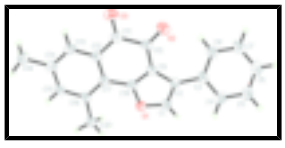

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

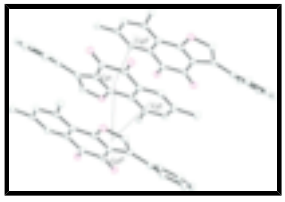

Fig. 2. Part of the crystal structure of (I) formed by π-π stacking interactions. Labels *Cg* represent the centroids of rings. H atoms have been omitted for clarity. Symmetry code:(i) −*x*, 1 − *y*, 2 − *z*, (ii) −*x*, −*y*, 2 − *z*.

### 7,9-Dimethyl-3-phenylnaphtho[1,2-*b*]furan-4,5-dione

*Crystal data*

| | |
|---|---|
| $C_{20}H_{14}O_3$ | $F_{000}$ = 632 |
| $M_r$ = 302.31 | $D_x$ = 1.373 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1012 reflections |
| *a* = 7.792 (2) Å | θ = 2.8–26.9º |
| *b* = 7.602 (2) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 24.746 (7) Å | *T* = 293 (2) K |
| β = 93.610 (5)º | Block, red |
| *V* = 1463.0 (7) Å$^3$ | 0.50 × 0.38 × 0.27 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART 1K CCD area-detector diffractometer | 3174 independent reflections |
| Radiation source: fine-focus sealed tube | 2534 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.015 |
| *T* = 293(2) K | $\theta_{max}$ = 27.1º |

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min}$ = 0.956, $T_{max}$ = 0.976

9844 measured reflections

$\theta_{min}$ = 2.6°

$h$ = −9→9

$k$ = −9→9

$l$ = −31→30

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.040

$wR(F^2)$ = 0.119

$S$ = 1.03

3174 reflections

210 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.3061P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$

$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

Extinction correction: none

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.33460 (19) | 0.0790 (2) | 0.94412 (6) | 0.0528 (4) |
| H1 | 0.4424 | 0.0311 | 0.9392 | 0.063* |
| C2 | 0.21428 (17) | 0.10566 (18) | 0.90371 (5) | 0.0454 (3) |
| C3 | 0.24088 (19) | 0.06386 (18) | 0.84666 (5) | 0.0482 (3) |
| C4 | 0.4054 (2) | 0.0779 (2) | 0.82849 (6) | 0.0577 (4) |
| H4 | 0.4939 | 0.1223 | 0.8515 | 0.069* |
| C5 | 0.4389 (2) | 0.0267 (3) | 0.77658 (7) | 0.0717 (5) |
| H5 | 0.5498 | 0.0361 | 0.7650 | 0.086* |
| C6 | 0.3096 (3) | −0.0379 (3) | 0.74210 (7) | 0.0749 (5) |
| H6 | 0.3328 | −0.0736 | 0.7074 | 0.090* |
| C7 | 0.1453 (3) | −0.0498 (2) | 0.75908 (7) | 0.0695 (5) |
| H7 | 0.0574 | −0.0931 | 0.7356 | 0.083* |
| C8 | 0.1096 (2) | 0.0023 (2) | 0.81090 (6) | 0.0579 (4) |

| | | | | |
|---|---|---|---|---|
| H8 | −0.0023 | −0.0040 | 0.8218 | 0.069* |
| C9 | 0.06983 (16) | 0.17866 (17) | 0.93019 (5) | 0.0422 (3) |
| C10 | −0.09938 (18) | 0.23874 (19) | 0.91119 (6) | 0.0486 (3) |
| C11 | −0.21411 (17) | 0.30834 (18) | 0.95534 (6) | 0.0493 (3) |
| C12 | −0.14654 (17) | 0.31760 (17) | 1.01237 (5) | 0.0440 (3) |
| C13 | −0.25251 (18) | 0.38256 (18) | 1.05073 (6) | 0.0500 (3) |
| H13 | −0.3638 | 0.4180 | 1.0401 | 0.060* |
| C14 | −0.19467 (19) | 0.39517 (18) | 1.10448 (6) | 0.0505 (3) |
| C15 | −0.02604 (19) | 0.34631 (18) | 1.11827 (6) | 0.0496 (3) |
| H15 | 0.0150 | 0.3590 | 1.1542 | 0.059* |
| C16 | 0.08540 (17) | 0.27926 (17) | 1.08151 (5) | 0.0450 (3) |
| C17 | 0.02245 (16) | 0.26205 (16) | 1.02753 (5) | 0.0405 (3) |
| C18 | 0.11923 (16) | 0.19215 (17) | 0.98400 (5) | 0.0412 (3) |
| C19 | −0.3093 (2) | 0.4566 (2) | 1.14715 (7) | 0.0664 (4) |
| H19A | −0.4067 | 0.5171 | 1.1303 | 0.100* |
| H19B | −0.2465 | 0.5349 | 1.1715 | 0.100* |
| H19C | −0.3480 | 0.3570 | 1.1669 | 0.100* |
| C20 | 0.2641 (2) | 0.2282 (2) | 1.10205 (6) | 0.0600 (4) |
| H20A | 0.2802 | 0.2562 | 1.1399 | 0.090* |
| H20B | 0.3465 | 0.2916 | 1.0824 | 0.090* |
| H20C | 0.2799 | 0.1041 | 1.0971 | 0.090* |
| O1 | 0.28067 (12) | 0.13026 (14) | 0.99344 (4) | 0.0518 (3) |
| O2 | −0.15827 (15) | 0.23743 (19) | 0.86475 (4) | 0.0759 (4) |
| O3 | −0.35925 (14) | 0.35313 (18) | 0.94093 (5) | 0.0736 (4) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0484 (7) | 0.0687 (9) | 0.0413 (7) | 0.0050 (7) | 0.0042 (6) | −0.0011 (7) |
| C2 | 0.0484 (7) | 0.0455 (7) | 0.0423 (7) | −0.0051 (6) | 0.0027 (5) | 0.0041 (6) |
| C3 | 0.0602 (8) | 0.0444 (7) | 0.0398 (7) | −0.0017 (6) | 0.0017 (6) | 0.0050 (6) |
| C4 | 0.0627 (9) | 0.0629 (9) | 0.0479 (8) | −0.0017 (7) | 0.0065 (7) | −0.0002 (7) |
| C5 | 0.0794 (12) | 0.0828 (12) | 0.0548 (10) | 0.0027 (9) | 0.0181 (8) | 0.0006 (9) |
| C6 | 0.1036 (14) | 0.0796 (12) | 0.0421 (9) | 0.0043 (10) | 0.0096 (9) | −0.0019 (8) |
| C7 | 0.0918 (13) | 0.0705 (11) | 0.0444 (8) | −0.0075 (9) | −0.0095 (8) | 0.0001 (8) |
| C8 | 0.0670 (9) | 0.0598 (9) | 0.0460 (8) | −0.0077 (7) | −0.0029 (7) | 0.0057 (7) |
| C9 | 0.0450 (7) | 0.0410 (7) | 0.0401 (7) | −0.0064 (5) | −0.0009 (5) | 0.0063 (5) |
| C10 | 0.0491 (7) | 0.0497 (7) | 0.0459 (8) | −0.0045 (6) | −0.0056 (6) | 0.0082 (6) |
| C11 | 0.0431 (7) | 0.0486 (8) | 0.0555 (8) | −0.0039 (6) | −0.0036 (6) | 0.0087 (6) |
| C12 | 0.0439 (7) | 0.0393 (7) | 0.0486 (8) | −0.0061 (5) | 0.0022 (5) | 0.0063 (5) |
| C13 | 0.0443 (7) | 0.0456 (7) | 0.0603 (9) | −0.0009 (6) | 0.0055 (6) | 0.0046 (6) |
| C14 | 0.0554 (8) | 0.0393 (7) | 0.0577 (9) | −0.0035 (6) | 0.0113 (6) | 0.0000 (6) |
| C15 | 0.0579 (8) | 0.0457 (7) | 0.0452 (7) | −0.0057 (6) | 0.0039 (6) | −0.0020 (6) |
| C16 | 0.0487 (7) | 0.0418 (7) | 0.0441 (7) | −0.0058 (5) | 0.0003 (6) | 0.0016 (5) |
| C17 | 0.0424 (7) | 0.0366 (6) | 0.0425 (7) | −0.0063 (5) | 0.0023 (5) | 0.0050 (5) |
| C18 | 0.0403 (6) | 0.0414 (7) | 0.0415 (7) | −0.0044 (5) | −0.0001 (5) | 0.0056 (5) |
| C19 | 0.0674 (10) | 0.0653 (10) | 0.0681 (11) | 0.0055 (8) | 0.0161 (8) | −0.0080 (8) |
| C20 | 0.0544 (8) | 0.0803 (11) | 0.0442 (8) | 0.0030 (8) | −0.0051 (6) | −0.0052 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0449 (5) | 0.0695 (6) | 0.0404 (5) | 0.0060 (4) | −0.0017 (4) | −0.0002 (4) |
| O2 | 0.0706 (7) | 0.1068 (10) | 0.0479 (6) | 0.0163 (7) | −0.0150 (5) | 0.0029 (6) |
| O3 | 0.0486 (6) | 0.1003 (10) | 0.0703 (8) | 0.0121 (6) | −0.0092 (5) | 0.0031 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.342 (2) | C11—O3 | 1.2130 (17) |
| C1—O1 | 1.3721 (17) | C11—C12 | 1.476 (2) |
| C1—H1 | 0.9300 | C12—C13 | 1.388 (2) |
| C2—C9 | 1.4480 (19) | C12—C17 | 1.4110 (19) |
| C2—C3 | 1.474 (2) | C13—C14 | 1.381 (2) |
| C3—C4 | 1.389 (2) | C13—H13 | 0.9300 |
| C3—C8 | 1.391 (2) | C14—C15 | 1.387 (2) |
| C4—C5 | 1.383 (2) | C14—C19 | 1.500 (2) |
| C4—H4 | 0.9300 | C15—C16 | 1.393 (2) |
| C5—C6 | 1.370 (3) | C15—H15 | 0.9300 |
| C5—H5 | 0.9300 | C16—C17 | 1.3999 (19) |
| C6—C7 | 1.375 (3) | C16—C20 | 1.503 (2) |
| C6—H6 | 0.9300 | C17—C18 | 1.4538 (18) |
| C7—C8 | 1.387 (2) | C18—O1 | 1.3496 (16) |
| C7—H7 | 0.9300 | C19—H19A | 0.9600 |
| C8—H8 | 0.9300 | C19—H19B | 0.9600 |
| C9—C18 | 1.3666 (18) | C19—H19C | 0.9600 |
| C9—C10 | 1.4457 (19) | C20—H20A | 0.9600 |
| C10—O2 | 1.2105 (17) | C20—H20B | 0.9600 |
| C10—C11 | 1.548 (2) | C20—H20C | 0.9600 |
| C2—C1—O1 | 112.39 (13) | C13—C12—C11 | 118.62 (13) |
| C2—C1—H1 | 123.8 | C17—C12—C11 | 120.70 (12) |
| O1—C1—H1 | 123.8 | C14—C13—C12 | 120.77 (13) |
| C1—C2—C9 | 104.32 (12) | C14—C13—H13 | 119.6 |
| C1—C2—C3 | 123.16 (13) | C12—C13—H13 | 119.6 |
| C9—C2—C3 | 132.53 (12) | C13—C14—C15 | 117.72 (13) |
| C4—C3—C8 | 118.45 (14) | C13—C14—C19 | 121.81 (14) |
| C4—C3—C2 | 118.80 (13) | C15—C14—C19 | 120.46 (14) |
| C8—C3—C2 | 122.66 (14) | C14—C15—C16 | 123.84 (14) |
| C5—C4—C3 | 120.75 (16) | C14—C15—H15 | 118.1 |
| C5—C4—H4 | 119.6 | C16—C15—H15 | 118.1 |
| C3—C4—H4 | 119.6 | C15—C16—C17 | 117.52 (13) |
| C6—C5—C4 | 120.33 (17) | C15—C16—C20 | 118.41 (13) |
| C6—C5—H5 | 119.8 | C17—C16—C20 | 124.07 (12) |
| C4—C5—H5 | 119.8 | C16—C17—C12 | 119.40 (12) |
| C5—C6—C7 | 119.72 (17) | C16—C17—C18 | 125.04 (12) |
| C5—C6—H6 | 120.1 | C12—C17—C18 | 115.55 (12) |
| C7—C6—H6 | 120.1 | O1—C18—C9 | 110.17 (11) |
| C6—C7—C8 | 120.56 (17) | O1—C18—C17 | 121.37 (11) |
| C6—C7—H7 | 119.7 | C9—C18—C17 | 128.46 (12) |
| C8—C7—H7 | 119.7 | C14—C19—H19A | 109.5 |
| C7—C8—C3 | 120.15 (16) | C14—C19—H19B | 109.5 |
| C7—C8—H8 | 119.9 | H19A—C19—H19B | 109.5 |

| | | | |
|---|---|---|---|
| C3—C8—H8 | 119.9 | C14—C19—H19C | 109.5 |
| C18—C9—C10 | 119.23 (12) | H19A—C19—H19C | 109.5 |
| C18—C9—C2 | 106.88 (11) | H19B—C19—H19C | 109.5 |
| C10—C9—C2 | 133.87 (12) | C16—C20—H20A | 109.5 |
| O2—C10—C9 | 126.13 (14) | C16—C20—H20B | 109.5 |
| O2—C10—C11 | 118.14 (13) | H20A—C20—H20B | 109.5 |
| C9—C10—C11 | 115.72 (12) | C16—C20—H20C | 109.5 |
| O3—C11—C12 | 122.51 (14) | H20A—C20—H20C | 109.5 |
| O3—C11—C10 | 117.24 (13) | H20B—C20—H20C | 109.5 |
| C12—C11—C10 | 120.25 (12) | C18—O1—C1 | 106.23 (10) |
| C13—C12—C17 | 120.68 (13) | | |
| O1—C1—C2—C9 | −0.80 (17) | C10—C11—C12—C17 | −0.52 (19) |
| O1—C1—C2—C3 | 179.16 (12) | C17—C12—C13—C14 | 0.4 (2) |
| C1—C2—C3—C4 | −31.4 (2) | C11—C12—C13—C14 | −179.45 (12) |
| C9—C2—C3—C4 | 148.53 (15) | C12—C13—C14—C15 | 2.1 (2) |
| C1—C2—C3—C8 | 145.23 (16) | C12—C13—C14—C19 | −176.95 (13) |
| C9—C2—C3—C8 | −34.8 (2) | C13—C14—C15—C16 | −2.6 (2) |
| C8—C3—C4—C5 | −2.0 (2) | C19—C14—C15—C16 | 176.49 (14) |
| C2—C3—C4—C5 | 174.80 (15) | C14—C15—C16—C17 | 0.5 (2) |
| C3—C4—C5—C6 | 0.4 (3) | C14—C15—C16—C20 | −178.85 (13) |
| C4—C5—C6—C7 | 0.8 (3) | C15—C16—C17—C12 | 2.02 (18) |
| C5—C6—C7—C8 | −0.3 (3) | C20—C16—C17—C12 | −178.68 (13) |
| C6—C7—C8—C3 | −1.3 (3) | C15—C16—C17—C18 | −178.94 (12) |
| C4—C3—C8—C7 | 2.4 (2) | C20—C16—C17—C18 | 0.4 (2) |
| C2—C3—C8—C7 | −174.24 (14) | C13—C12—C17—C16 | −2.48 (19) |
| C1—C2—C9—C18 | 1.27 (15) | C11—C12—C17—C16 | 177.34 (12) |
| C3—C2—C9—C18 | −178.68 (14) | C13—C12—C17—C18 | 178.39 (11) |
| C1—C2—C9—C10 | 179.28 (15) | C11—C12—C17—C18 | −1.80 (17) |
| C3—C2—C9—C10 | −0.7 (3) | C10—C9—C18—O1 | −179.68 (11) |
| C18—C9—C10—O2 | 178.62 (15) | C2—C9—C18—O1 | −1.32 (14) |
| C2—C9—C10—O2 | 0.8 (3) | C10—C9—C18—C17 | −0.2 (2) |
| C18—C9—C10—C11 | −2.22 (18) | C2—C9—C18—C17 | 178.16 (12) |
| C2—C9—C10—C11 | 179.96 (13) | C16—C17—C18—O1 | 2.71 (19) |
| O2—C10—C11—O3 | 2.1 (2) | C12—C17—C18—O1 | −178.22 (11) |
| C9—C10—C11—O3 | −177.14 (13) | C16—C17—C18—C9 | −176.72 (13) |
| O2—C10—C11—C12 | −178.18 (14) | C12—C17—C18—C9 | 2.35 (19) |
| C9—C10—C11—C12 | 2.59 (19) | C9—C18—O1—C1 | 0.84 (15) |
| O3—C11—C12—C13 | −1.0 (2) | C17—C18—O1—C1 | −178.69 (12) |
| C10—C11—C12—C13 | 179.29 (12) | C2—C1—O1—C18 | 0.02 (17) |
| O3—C11—C12—C17 | 179.19 (14) | | |

**Fig. 1**

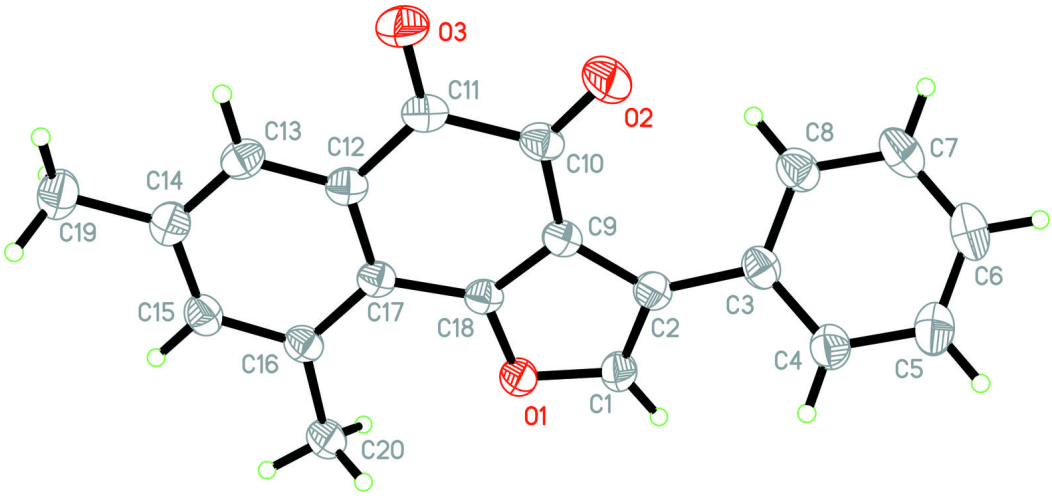
O3
C11
O2
C13
C12
C10
C8
C7
C14
C19
C9
C6
C15
C17
C18
C2
C3
C16
C4
C5
O1
C1
C20

**Fig. 2**