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2-Methoxynaphthalene-1,4-dione

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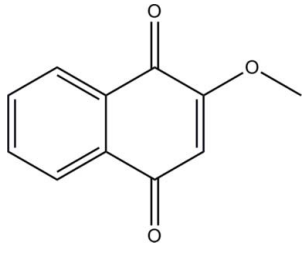
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.136; data-to-parameter ratio = 16.3.

The title compound, $C_{11}H_8O_3$, was isolated from *Impatiens balsamina* plants (balsam, LIB) grown in our laboratory. The two six-membered rings of the naphthalene-1,4-dione unit are coplanar [maximum deviation = 0.009 (1) Å]. The O and C atoms of the methoxy substituent also lie close to the naphthalene plane, with deviations of 0.0090 (2) and 0.047 (2) Å, respectively.

Related literature

For background to compounds extracted from *Impatiens balsamina*, see: Ding *et al.* (2008). For the antimicrobial activity of flavonol and naphthoquinone derivatives, see: Yang *et al.* (2001). For their anti-anaphylaxis properties, see: Yoshimi *et al.* (2003); Ishiguro *et al.* (1994) and for their use as anti-inflammatories, see: Hisae & Kyoko (2002). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_8O_3$
M_r = 188.17
Monoclinic, $P2_1/c$
a = 3.904 (3) Å
b = 7.662 (6) Å
c = 28.81 (2) Å
β = 93.562 (7)°
V = 860.1 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968.
T_{min} = 0.979, T_{max} = 0.989
7068 measured reflections
2082 independent reflections
1458 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.136
S = 1.08
2082 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: SJ5115).

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supporting information

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2-Methoxynaphthalene-1,4-dione

Bo Jin, Zhong-Cheng Song, Fu-Sheng Jiang, Wen-Hong Liu and Zhi-Shan Ding

S1. Comment

Modern chemical and pharmacological studies have identified flavonol and naphthoquinone derivatives, some of which have strong antimicrobial (Yang *et al.*, 2001) anti-anaphylaxis (Yoshimi *et al.*, 2003, Ishiguro *et al.*, 1994) and anti-inflammatory properties (Hisae & Kyoko, 2002). We have purified and identified an active component of the *Impatiens balsamina* plant (balsam, LIB) which was grown in our laboratory (Ding *et al.*, 2008) and authenticated by Professor Yao Zhensheng (Zhejiang Traditional Chinese Medicinal University). The molecular structure of the title compound is shown in Fig. 1. In the crystal, all bond lengths are within normal ranges (Allen *et al.*, 1987). The C1···C4,C9,C10 and C5···C10 rings of the naphthalene-1,4-dione unit are co-planar, maximum deviation 0.009 (1) Å. The O2 and C11 atoms of the methoxy substituent also lie close to the naphthalene plane with deviations of 0.0090 (2) Å and 0.047 (2) Å respectively.

S2. Experimental

Dried leaves (200 g) of *Impatiens balsamina* were crushed, soaked with 55% alcohol (1500 ml) for 24 h and then reflux extracted for 40 min (1500 ml\3). Extracts were filtered and vacuum evaporated. In addition, 200 g of dried leaves were directly reflux extracted using chloroform (3000 ml\2). Next these extracts were filtered, combined, vacuum evaporated and the residue dried for further use. A portion of residue was re-chromatographed on silica gel using a petroleum ether-acetone (8:2) system and the isolated product was recrystallized from chloroform to yield the active component as light yellow crystals.

S3. Refinement

H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.93–0.97 Å, O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(O).

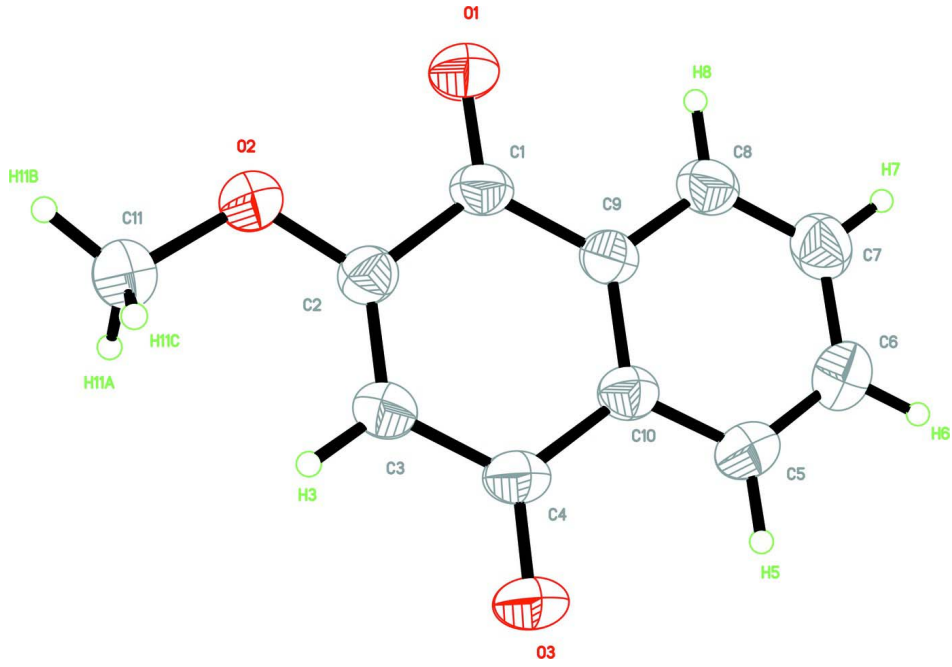

Figure 1

The molecular structure of the title compounds with atom labels and 50% probability displacement ellipsoids for non-hydrogen atoms.

2-Methoxynaphthalene-1,4-dione

Crystal data

$C_{11}H_8O_3$
M_r = 188.17
Monoclinic, $P2_1/c$
Hall symbol: -p 2ybc
a = 3.904 (3) Å
b = 7.662 (6) Å
c = 28.81 (2) Å
β = 93.562 (7)°
V = 860.1 (12) Å^3
Z = 4
$F(000)$ = 392
D_x = 1.453 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1421 reflections
θ = 3.0–26.7°
μ = 0.11 mm^{-1}
T = 296 K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Enrfa–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968.
T_{min} = 0.979, T_{max} = 0.989
7068 measured reflections
2082 independent reflections
1458 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 28.3°, θ_{min} = 2.8°
h = −5→5
k = −10→10
l = −38→36
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.136$
$S = 1.08$
2082 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 0.5448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.5248 (4)	1.29754 (19)	0.09145 (5)	0.0460 (4)
C10	0.8859 (5)	0.7924 (3)	0.12534 (7)	0.0351 (5)
C1	0.6106 (5)	1.0740 (3)	0.14687 (7)	0.0389 (5)
C9	0.7444 (5)	0.8979 (3)	0.15900 (7)	0.0347 (4)
C2	0.6487 (5)	1.1357 (3)	0.09790 (7)	0.0369 (5)
O3	1.0374 (5)	0.7687 (2)	0.04711 (5)	0.0549 (5)
C5	1.0035 (6)	0.6270 (3)	0.13751 (8)	0.0423 (5)
H5	1.0976	0.5566	0.1153	0.051*
O1	0.4735 (5)	1.1666 (2)	0.17443 (6)	0.0636 (5)
C3	0.7874 (5)	1.0345 (3)	0.06610 (7)	0.0393 (5)
H3	0.8047	1.0774	0.0361	0.047*
C6	0.9824 (6)	0.5657 (3)	0.18238 (8)	0.0483 (6)
H6	1.0607	0.4542	0.1902	0.058*
C4	0.9122 (5)	0.8589 (3)	0.07713 (7)	0.0384 (5)
C7	0.8444 (6)	0.6705 (3)	0.21567 (8)	0.0482 (6)
H7	0.8321	0.6295	0.2459	0.058*
C8	0.7251 (6)	0.8354 (3)	0.20418 (7)	0.0426 (5)
H8	0.6317	0.9049	0.2266	0.051*
C11	0.5484 (6)	1.3721 (3)	0.04595 (8)	0.0508 (6)
H11A	0.7849	1.3784	0.0388	0.076*
H11B	0.4516	1.4874	0.0454	0.076*
H11C	0.4243	1.3005	0.0233	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0583 (10)	0.0385 (8)	0.0422 (8)	0.0075 (7)	0.0122 (7)	−0.0003 (7)
C10	0.0342 (11)	0.0366 (11)	0.0347 (10)	−0.0011 (8)	0.0035 (8)	−0.0051 (8)
C1	0.0426 (12)	0.0375 (11)	0.0379 (11)	−0.0023 (9)	0.0124 (9)	−0.0080 (9)
C9	0.0341 (10)	0.0352 (10)	0.0354 (10)	−0.0059 (8)	0.0057 (8)	−0.0060 (8)
C2	0.0383 (11)	0.0331 (11)	0.0395 (11)	−0.0010 (8)	0.0053 (9)	−0.0030 (8)
O3	0.0747 (12)	0.0500 (10)	0.0418 (9)	0.0127 (9)	0.0185 (8)	−0.0096 (7)
C5	0.0440 (12)	0.0378 (11)	0.0453 (12)	0.0035 (9)	0.0037 (9)	−0.0076 (9)
O1	0.0953 (14)	0.0488 (10)	0.0502 (10)	0.0166 (9)	0.0325 (9)	−0.0034 (8)
C3	0.0444 (12)	0.0416 (11)	0.0324 (10)	0.0007 (9)	0.0070 (9)	−0.0023 (9)
C6	0.0534 (14)	0.0383 (12)	0.0528 (14)	0.0013 (10)	−0.0003 (11)	0.0024 (10)
C4	0.0372 (11)	0.0406 (12)	0.0379 (11)	−0.0007 (9)	0.0076 (9)	−0.0091 (9)
C7	0.0553 (14)	0.0495 (13)	0.0400 (12)	−0.0014 (11)	0.0037 (10)	0.0053 (10)
C8	0.0473 (13)	0.0440 (12)	0.0375 (11)	−0.0036 (10)	0.0102 (9)	−0.0049 (9)
C11	0.0607 (15)	0.0482 (13)	0.0442 (13)	0.0094 (11)	0.0090 (11)	0.0078 (10)

Geometric parameters (Å, º)

O2—C2	1.340 (3)	C5—H5	0.9300
O2—C11	1.438 (3)	C3—C4	1.459 (3)
C10—C5	1.386 (3)	C3—H3	0.9300
C10—C9	1.402 (3)	C6—C7	1.385 (3)
C10—C4	1.489 (3)	C6—H6	0.9300
C1—O1	1.213 (2)	C7—C8	1.380 (3)
C1—C9	1.481 (3)	C7—H7	0.9300
C1—C2	1.504 (3)	C8—H8	0.9300
C9—C8	1.394 (3)	C11—H11A	0.9600
C2—C3	1.340 (3)	C11—H11B	0.9600
O3—C4	1.232 (2)	C11—H11C	0.9600
C5—C6	1.383 (3)		
C2—O2—C11	116.82 (16)	C5—C6—C7	119.9 (2)
C5—C10—C9	119.40 (19)	C5—C6—H6	120.0
C5—C10—C4	120.52 (18)	C7—C6—H6	120.0
C9—C10—C4	120.07 (19)	O3—C4—C3	120.4 (2)
O1—C1—C9	122.80 (19)	O3—C4—C10	121.1 (2)
O1—C1—C2	120.2 (2)	C3—C4—C10	118.50 (17)
C9—C1—C2	116.96 (16)	C8—C7—C6	120.3 (2)
C8—C9—C10	119.6 (2)	C8—C7—H7	119.8
C8—C9—C1	119.66 (18)	C6—C7—H7	119.8
C10—C9—C1	120.70 (18)	C7—C8—C9	120.1 (2)
O2—C2—C3	126.77 (19)	C7—C8—H8	119.9
O2—C2—C1	111.40 (16)	C9—C8—H8	119.9
C3—C2—C1	121.83 (19)	O2—C11—H11A	109.5
C6—C5—C10	120.6 (2)	O2—C11—H11B	109.5
C6—C5—H5	119.7	H11A—C11—H11B	109.5

C10—C5—H5	119.7	O2—C11—H11C	109.5
C2—C3—C4	121.89 (19)	H11A—C11—H11C	109.5
C2—C3—H3	119.1	H11B—C11—H11C	109.5
C4—C3—H3	119.1		
C5—C10—C9—C8	0.2 (3)	C4—C10—C5—C6	179.4 (2)
C4—C10—C9—C8	−179.15 (19)	O2—C2—C3—C4	−179.6 (2)
C5—C10—C9—C1	−178.86 (19)	C1—C2—C3—C4	−0.5 (3)
C4—C10—C9—C1	1.8 (3)	C10—C5—C6—C7	−0.4 (3)
O1—C1—C9—C8	−2.2 (3)	C2—C3—C4—O3	179.7 (2)
C2—C1—C9—C8	178.25 (19)	C2—C3—C4—C10	−0.5 (3)
O1—C1—C9—C10	176.9 (2)	C5—C10—C4—O3	0.2 (3)
C2—C1—C9—C10	−2.7 (3)	C9—C10—C4—O3	179.6 (2)
C11—O2—C2—C3	−1.2 (3)	C5—C10—C4—C3	−179.5 (2)
C11—O2—C2—C1	179.59 (18)	C9—C10—C4—C3	−0.1 (3)
O1—C1—C2—O2	1.7 (3)	C5—C6—C7—C8	0.6 (4)
C9—C1—C2—O2	−178.74 (17)	C6—C7—C8—C9	−0.3 (3)
O1—C1—C2—C3	−177.6 (2)	C10—C9—C8—C7	−0.1 (3)
C9—C1—C2—C3	2.0 (3)	C1—C9—C8—C7	179.0 (2)
C9—C10—C5—C6	0.0 (3)		