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1,4-Dihydroxy-2-methoxy-7-methylanthracene-9,10-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.154
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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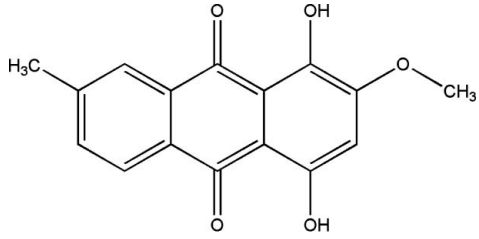
The title compound, $C_{16}H_{12}O_5$, was isolated from extracts of cultures of the estuarine fungus. The planar molecule shows normal bond distances and angles. Intramolecular hydrogen bonding occurs between the hydroxy and carbonyl groups.

Comment

The title compound, (I), was previously isolated from the genus *Cortinarius* (Archard *et al.*, 1985), and its structure was elucidated on the basis of spectroscopic analysis. We recently isolated (I) from extracts of cultures of the estuarine fungus (No. 1403) and obtained single crystals. Here we report the crystal structure of (I).



(I)

The molecular structure of (I) is shown in Fig. 1. It confirms the previously proposed molecular structure based on spectroscopic data. The non-H atoms of the molecule are coplanar; bond distances and angles are normal. The hydroxy groups form intramolecular hydrogen bonds with adjacent carbonyl groups (Table 1).

Experimental

The title compound, (I), was isolated from extracts of cultures of the estuarine fungus (No. 1403). The cultures (100 l) of the strain of fungus were filtered through cheesecloth. The filtrate was concentrated to 5 l below 323 K, then extracted three times by shaking with an equal volume of ethyl acetate. The extract was evaporated under reduced pressure. The combined organic extracts were subjected to silica-gel column chromatography, eluting with petroleum ether/ethyl acetate (1:4), to yield (I). Single crystals of (I) were obtained from a methanol solution.

Crystal data

$C_{16}H_{12}O_5$
M_r = 284.26
Monoclinic, $P2_1/c$
a = 8.637 (3) Å
b = 7.899 (3) Å
c = 18.622 (6) Å
β = 97.081 (6)°
V = 1260.8 (8) Å^3
Z = 4
D_x = 1.498 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
Plate, red
0.48 × 0.42 × 0.16 mm

Data collection

Bruker AXS SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.980
10150 measured reflections
2728 independent reflections
1551 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.154
S = 1.03
2728 reflections
194 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 0.221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3	0.82	1.81	2.536 (2)	147
O1—H1···O2	0.82	1.82	2.542 (2)	146

H atoms were placed in calculated positions, with C—H = 0.96 (methyl) or 0.93 Å (aromatic) and O—H = 0.82 Å. Torsion angles of methyl groups were refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

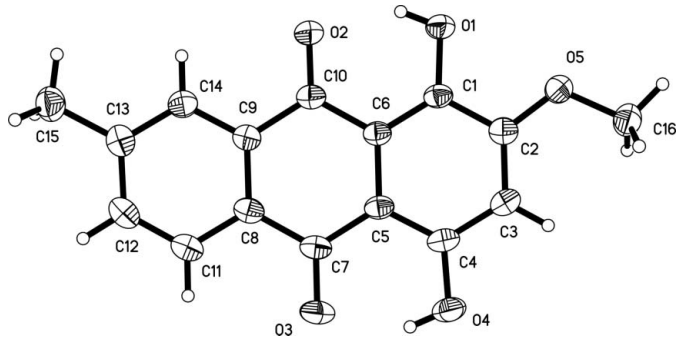


Figure 1
The molecular structure of (I) shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

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