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Crystal structure of 2-isopropyl-8-methyl-phenanthrene-3,4-dione, C₁₈H₁₆O₂

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.25 × 0.15 × 0.12 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	27.4°, >98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5354, 1633, 0.044
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1148
$N(\text{param})_{\text{refined}}$:	120
Programs:	Bruker programs [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.39634(12)	0.2500	0.16579(14)	0.0641(7)
O2	0.35548(10)	0.2500	0.35240(13)	0.0450(5)
C1	0.63162(16)	0.4334(3)	0.05250(15)	0.0622(7)
H1A	0.5959	0.5504	0.0700	0.093*
H1B	0.6422	0.4320	-0.0179	0.093*
H1C	0.6911	0.4357	0.0865	0.093*
C2	0.57806(16)	0.2500	0.08192(19)	0.0412(7)
H2	0.5179	0.2500	0.0461	0.049*
C3	0.55741(15)	0.2500	0.19054(17)	0.0314(6)
C4	0.46070(14)	0.2500	0.22194(19)	0.0343(6)
C5	0.43752(14)	0.2500	0.33278(17)	0.0284(6)
C6	0.51392(13)	0.2500	0.40390(17)	0.0243(5)
C7	0.50008(14)	0.2500	0.50772(18)	0.0255(5)
C8	0.41131(14)	0.2500	0.55209(19)	0.0320(6)
H8	0.3573	0.2500	0.5128	0.038*
C9	0.40365(16)	0.2500	0.6513(2)	0.0392(7)
H9	0.3439	0.2500	0.6799	0.047*
C10	0.48182(17)	0.2500	0.7119(2)	0.0399(6)
H10	0.4739	0.2500	0.7806	0.048*
C11	0.56924(16)	0.2500	0.67383(18)	0.0330(6)
C12	0.57954(14)	0.2500	0.57007(17)	0.0274(5)
C13	0.66844(14)	0.2500	0.52706(19)	0.0321(6)
H13	0.7214	0.2500	0.5680	0.039*
C14	0.68025(14)	0.2500	0.42872(17)	0.0313(6)
H14	0.7409	0.2500	0.4023	0.038*
C15	0.60340(13)	0.2500	0.36562(17)	0.0261(5)
C16	0.62199(14)	0.2500	0.26074(17)	0.0317(6)
H16	0.6848	0.2500	0.2408	0.038*
C17	0.65239(19)	0.2500	0.74001(19)	0.0468(7)
H17A ^a	0.6319	0.2466	0.8080	0.070*
H17B ^a	0.6888	0.3691	0.7287	0.070*
H17C ^a	0.6905	0.1343	0.7264	0.070*

^aOccupancy: 0.5.

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Abstract

C₁₈H₁₆O₂, orthorhombic, *Pnma* (no. 62), $a = 14.474(6)$ Å, $b = 6.815(3)$ Å, $c = 13.738(6)$ Å, $V = 1355.1(10)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0583$, $wR_{\text{ref}}(F^2) = 0.1759$, $T = 173$ K.

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The crystal structure is shown in the figure ($i = x, 0.5 - y, z$). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The roots of *Salvia miltiorrhiza* Bunge (5.0 kg) were extracted with MeOH (×3) and filtered. The filtrate was concentrated and partitioned with EtOAc, then subjected to silica gel column (petroleum ether/EtOAc, 20:1) to provide five fractions (Fr. A–E). Fr. B was further purified on silica gel column and recrystallized with dichloromethane to obtain the title compound (120 mg).

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Experimental details

Hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms.

Discussion

Diterpenoid quinones are the main lipid-soluble components in the traditional medicinal plant *Salvia miltiorrhiza* Bunge that has been applied to treat coronary heart diseases and cerebrovascular diseases. The structure of diterpenoid quinones are classified into two series, the phenanthro[1, 2 – b] furan-10,11-dione series and the phenanthro[3, 2 – b] furan-7,11-dione series [4]. The title compound belongs to the former series and contains three six-membered rings, which geometric parameters are in the normal ranges (*cf.* the figure). The asymmetric unit contains one half of a molecule which is located on a mirror plane. The bond distances of C4–O1 and C5–O2 are 1.209(3) Å and 1.218(3) Å, which are typical for C=O groups.

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