

1,4,11,12-Tetrahydro-9,10-anthraquinone

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Key indicators

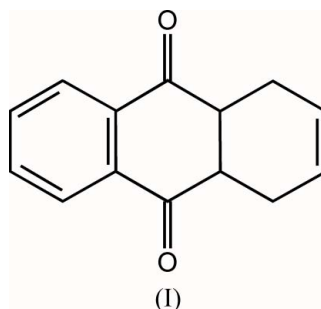
Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.048
 wR factor = 0.138
Data-to-parameter ratio = 15.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the title compound, $\text{C}_{14}\text{H}_{12}\text{O}_2$, the cyclohexene ring adopts
an envelope conformation, while the remaining fragment of
the anthraquinone skeleton is planar.

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Comment

The title compound, (I), is an important precursor for the
generation of the 1,4-dihydro-9,10-anthrasemiquinone radical,
(II), as observed by electron paramagnetic resonance spec-
troscopy (Mattar & Stephens, 1999). The proposed planar
structure of (II) is in stark contrast to the conformation
observed in (I).

The molecular structure of (I) is illustrated in Fig. 1. To our knowledge it is the only example of a crystallographically characterized, partially hydrogenated, unsubstituted anthraquinone. The cyclohexene ring in (I) adopts an envelope conformation, resulting in a planar C5–C9 fragment [maximum deviation = 0.0802 (2) Å], with atom C10, as the flap of the envelope, displaced by 0.633 (2) Å from this plane. The remaining carbon skeleton is planar to within 0.0145 (7) Å. The C5–C10 bond is twisted with respect to this plane, such that atom C5 is 0.353 (2) Å above and atom C10 is 0.339 (2) Å below this plane.

Experimental

Compound (I) was purchased from Aldrich and was recrystallized from methanol.

Crystal data

 $\text{C}_{14}\text{H}_{12}\text{O}_2$
 $M_r = 212.24$
 Triclinic, $P\bar{1}$
 $a = 5.0708$ (3) Å
 $b = 9.6094$ (6) Å
 $c = 11.9258$ (8) Å
 $\alpha = 66.348$ (1)°
 $\beta = 86.081$ (1)°
 $\gamma = 80.935$ (2)°
 $V = 525.64$ (6) Å³
 $Z = 2$
 $D_x = 1.341$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2887
 reflections
 $\theta = 2.3$ – 32.5 °
 $\mu = 0.09$ mm⁻¹
 $T = 296$ (1) K
 Block, colourless
 0.25 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2143 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.013$
Absorption correction: none	$\theta_{\text{max}} = 30.0^\circ$
5145 measured reflections	$h = -6 \rightarrow 7$
3052 independent reflections	$k = -13 \rightarrow 13$
	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0864P)^2]$
$wR(F^2) = 0.138$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} = 0.002$
3052 reflections	$\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$
193 parameters	$\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{\AA}^{-3}$

H atoms were located in difference Fourier maps and refined with isotropic displacement parameters; C–H distances are in the range 0.945 (18)–1.029 (18) Å.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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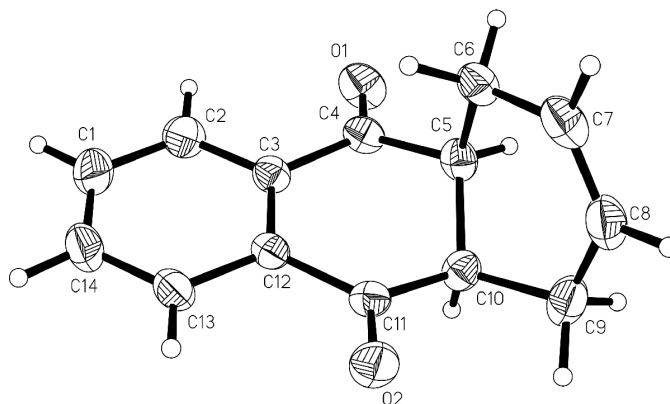


Figure 1
A view of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

References

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