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9(10*H*)-Acridone

Graham D. Potts

Department of Chemical Engineering, UMIST,
PO Box 88, Manchester M60 1QD, England

William Jones

Department of Chemistry, University of Cambridge,
Lensfield Road, Cambridge CB2 1EW, England

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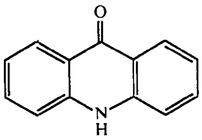
Abstract

The molecular packing arrangement in $C_{13}H_9NO$ is characterized by two major interaction types. The first comprises N—H···O hydrogen bonds between glide-related molecules, with an N···O distance of 2.782 (3) Å, such that each molecule is hydrogen bonded to two adjacent molecules. The second consists of π–π interactions between molecules stacked along the short crystal axis.

Comment

The structure determination of the title compound, (I), was undertaken as part of an investigation into the importance of specific intermolecular interactions in relation to the observed packing arrangement adopted by planar aromatic systems.



(I)

The molecule is planar with no atoms deviating by more than 0.02 Å from the molecular plane defined by the non-H ring atoms and the O atom; all torsion angles lie within ±1.5° of 0 or 180°. The molecules adopt a herringbone packing arrangement very similar to that found in anthraquinone (Lenstra & van Loock, 1984), indigo (Suesse, Steins & Kupcik, 1988) and quinacridone (Potts, Jones, Bullock, Andrews & Maginn, in preparation). Hydrogen bonding is maximized in such structures.

Overall hydrogen bonding and π–π interactions are the dominant factors controlling the crystal arrangement (Fig. 2).

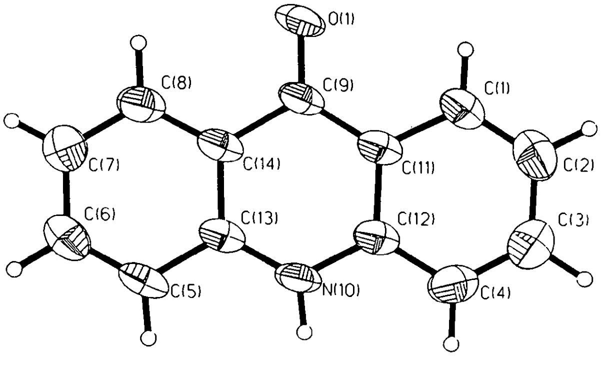


Fig. 1. *SHELXTL-Plus* (Sheldrick, 1990*b*) view of the molecule with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

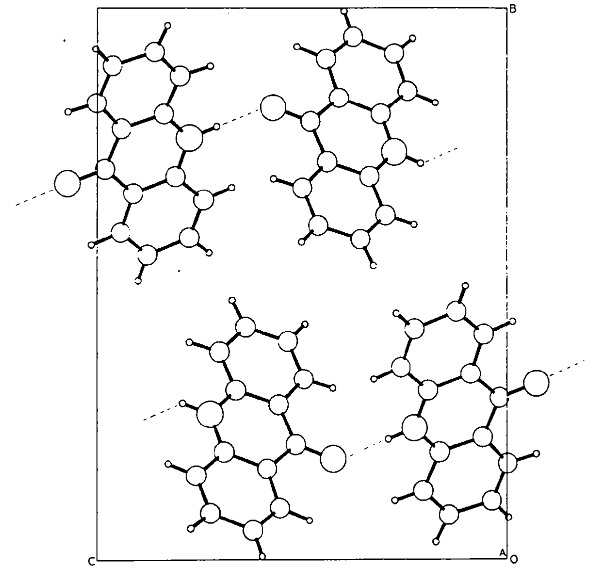


Fig. 2. Crystal structure viewed down the *a* axis with the hydrogen bonds shown.

Experimental

Crystal data

$C_{13}H_9NO$
M_r = 195.21
Monoclinic
$P2_1/n$
a = 4.5330 (10) Å
b = 16.537 (3) Å
c = 12.687 (3) Å
β = 97.22 (3)°

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 8–15°
μ = 0.088 mm^{-1}
T = 296 (2) K
Plate

$V = 943.5$ (3) Å^3
$Z = 4$
$D_x = 1.374$ Mg m^{-3}

0.40 × 0.40 × 0.06 mm
Yellow
Crystal source: Aldrich

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1738 measured reflections
1664 independent reflections
1029 observed reflections [$I > 2\sigma(I)$]

$R_{\rm int} = 0.0296$
$\theta_{\rm max} = 24.98°$
$h = -5 \rightarrow 5$
$k = 0 \rightarrow 19$
$l = 0 \rightarrow 15$
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0543$
$wR(F^2) = 0.1759$
$S = 0.786$
1664 reflections
172 parameters
$w = 1/[\sigma^2(F_o^2) + (0.2096P)^2 + 0.1467P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = -0.062$
$\Delta\rho_{\rm max} = 0.154$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.253$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{\rm eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	$U_{\rm eq}$
N10	−0.0070 (5)	0.23733 (15)	0.2255 (2)	0.0473 (7)
C14	−0.3202 (6)	0.2200 (2)	0.0597 (2)	0.0414 (7)
C11	0.0230 (6)	0.3362 (2)	0.0888 (2)	0.0419 (7)
C13	−0.2183 (6)	0.1939 (2)	0.1638 (2)	0.0426 (7)
C9	−0.2017 (6)	0.2928 (2)	0.0185 (2)	0.0441 (7)
C12	0.1149 (6)	0.30593 (15)	0.1917 (2)	0.0400 (7)
C5	−0.3350 (7)	0.1234 (2)	0.2031 (2)	0.0565 (8)
O1	−0.2819 (5)	0.31831 (12)	−0.07342 (13)	0.0641 (7)
C4	0.3352 (6)	0.3476 (2)	0.2584 (2)	0.0511 (8)
C8	−0.5374 (7)	0.1732 (2)	−0.0014 (2)	0.0515 (8)
C1	0.1504 (7)	0.4071 (2)	0.0573 (2)	0.0503 (7)
C2	0.3601 (7)	0.4480 (2)	0.1235 (2)	0.0603 (8)
C7	−0.6469 (7)	0.1050 (2)	0.0375 (3)	0.0644 (9)
C6	−0.5450 (8)	0.0796 (2)	0.1412 (3)	0.0660 (9)
C3	0.4538 (7)	0.4167 (2)	0.2247 (2)	0.0566 (8)

Table 2. *Selected geometric parameters* (Å, °)

Angles at C other than those given below are in the range 118–122°.

N10—C12	1.355 (4)	C13—C5	1.398 (4)
N10—C13	1.363 (3)	C9—O1	1.250 (3)
N10—H10	0.96 (4)	C12—C4	1.406 (4)
C14—C8	1.406 (4)	C5—C6	1.363 (5)
C14—C13	1.411 (3)	C4—C3	1.354 (5)
C14—C9	1.443 (4)	C8—C7	1.350 (4)
C11—C1	1.389 (4)	C1—C2	1.366 (4)
C11—C12	1.410 (3)	C2—C3	1.400 (4)
C11—C9	1.456 (4)	C7—C6	1.402 (5)
C12—N10—C13	123.0 (2)	C14—C9—C11	116.9 (2)
O1—C9—C14	122.8 (2)		

All nine H atoms were located from the Fourier difference map and their positions and isotropic displacement parameters were refined.

Data collection: CAD-4 diffractometer software. Cell refinement: CAD-4 diffractometer software. Data reduction: CAD-4 diffractometer software. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990*a*). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1122). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(1β,5α,6β)-10,10-(1,2-Ethylenedioxy)-1,5-dimethylbicyclo[4.4.0]decan-4-one

KWANGYONG PARK AND DALE C. SWENSON

Department of Chemistry, University of Iowa,
Iowa City, Iowa 52242, USA

WILLIAM J. SCOTT

Miles Inc., Pharmaceutical Division,
Institute for Chemistry, 400 Morgan Lane, West Haven,
CT 06516-4175, USA

DAVID F. WIEMER

Department of Chemistry, University of Iowa,
Iowa City, Iowa 52242, USA

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Abstract

The title compound (1) [alternative name: 5,8a-dimethyl(decahydronaphthalene)-1-spiro-2′-(1′,3′-dioxolan)-6-one, $C_{14}H_{22}O_3$] was obtained as the major prod-