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1-Hydroxy-3-methyl-9*H*-carbazole-2-carbaldehyde

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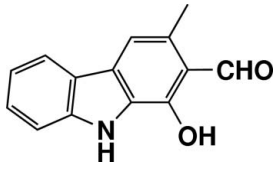
Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.148; data-to-parameter ratio = 14.4.

The carbazole unit of the title molecule, $C_{14}H_{11}NO_2$, is planar. The hydroxy group at position 1, carbaldehyde group at position 2, and methyl group at position 3 (with the exception of two H atoms) are coplanar with the attached benzene ring. The dihedral angle between the two benzene rings is 3.57 (8)°. The pyrrole ring makes dihedral angles of 1.53 (9) and 2.06 (9)° with the unsubstituted and substituted benzene rings, respectively. The structure is stabilized by inter- and intramolecular N—H···O and O—H···O hydrogen bonds.

Related literature

For related literature, see: Borek-Dohalska *et al.* (2004); Chakraborty (1977); Chakraborty & Roy (1991); Chmielewski *et al.* (2004); Hagg *et al.* (2004); Hedin *et al.* (2000); Hirata *et al.* (1999); Knolker & Reddy (2002); Saturnino *et al.* (2003); Thomas *et al.* (2001); Van Dijken *et al.* (2004); Wang *et al.* (2005).



Experimental

Crystal data

$C_{14}H_{11}NO_2$
M_r = 225.24
Monoclinic, $P2_1/n$
a = 12.1859 (6) Å
b = 6.6703 (3) Å
c = 14.1899 (7) Å
β = 113.469 (2)°
V = 1057.99 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 160 (1) K
0.25 × 0.25 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
25678 measured reflections
2424 independent reflections
1803 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.148
S = 1.04
2424 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O21	1.00 (4)	1.66 (3)	2.544 (2)	145 (2)
N9—H9···O1^{i}	0.91 (2)	2.06 (2)	2.9160 (19)	157.0 (19)

Symmetry code: (i) $-x, -y+1, -z$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zürich. His help is gratefully acknowledged by AT. AT thanks the UGC, India, for the award of a Minor Research Project [File No. MRP-2355/06(UGC-SERO), Link No. 2355, 10/01/2007].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2137).

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supplementary materials

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1-Hydroxy-3-methyl-9*H*-carbazole-2-carbaldehyde

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Comment

Carbazoles are ubiquitous structural subunits of numerous naturally occurring compounds as well as synthetic materials. Over the past four decades, a wide range of biologically active carbazole alkaloids have been isolated from plant sources. Among the ten naturally occurring simple carbazole alkaloids, five have oxygen function at C1 (or its equivalent C8) and most of them are having substituents in the third position (Chakraborty, 1977; Chakraborty & Roy, 1991). Many of these natural products display biological properties such as antitumor (Saturnino *et al.*, 2003; Borek-Dohalska *et al.*, 2004; Hagg *et al.*, 2004; Hedin *et al.*, 2000), anti-HIV properties (Hirata *et al.*, 1999; Wang *et al.*, 2005), psychotropic, anti-inflammatory, antihistaminic, antibiotic and antioxidative activities (Knolker *et al.*, 2002). As synthetic materials many carbazoles exhibit photo-reactive, photoconductive and light-emitting properties (Van Dijken *et al.*, 2004; Thomas *et al.*, 2001). Carbazoles have also been recognized as a useful scaffold in anion binding studies (Chmielewski *et al.*, 2004). Here we report the crystal structure of 1-hydroxy-3-methyl-9*H*- carbazole-2-carbaldehyde, (I).

The carbazole unit of the title molecule, (I), (Fig. 1), is planar. The attached hydroxy group at position 1, carbaldehyde group at position 2, and methyl group at position 3 have coplanar orientations with the benzene ring. The dihedral angle between the two benzene rings is 3.57 (8)°. The pyrrole ring makes a dihedral angles of 1.53 (9)° and 2.06 (9)° with the unsubstituted and substituted benzene respectively. The structure is stabilized by inter- and intramolecular N9–H9···O1(-*x*,1 - *y*,-*z*) and O1–H1···O21 hydrogen bonds respectively as shown in Fig. 2 and Fig. 3.

Experimental

30% Sodium hydride in mineral oil (2.4 g) was washed with dry benzene and taken in a round bottomed flask containing dry benzene (100 ml). The flask was kept in an ice bath with stirring. Ethyl formate (8 ml) was added drop wise over the period of 10 minutes to the solution. Then 3-methyl-2,3,4,9-tetrahydro-1*H*- carbazol-1-one (1.6 g, 0.008 mol) in dry benzene (25 ml) was added slowly and the reaction mixture was allowed to stir for another 36 h. The reaction was monitored by TLC. After the completion of the reaction the benzene was removed and the contents in the flask were transferred to a beaker containing water. It was neutralized with dilute HCl, filtered, washed with water and dried to get the crude 1-hydroxy-3-methyl-9*H*-carbazole-2- carbaldehyde (I). It was purified by column chromatography over silica using petroleum ether:ethyl acetate (98:2) as eluant. The yellow pure product obtained was recrystallized using glacial acetic acid (52%, 0.940 g).

Refinement

H1, H9, and H21 atoms were located in a difference map and refined isotropically [O1–H1 = 1.00 (4), N9–H9 = 0.91 (2) and C21–H21 = 1.02 (2) Å]. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.95-0.98 Å and with U_{iso}(H) = 1.2-1.5 times U_{eq}(C).

Figures

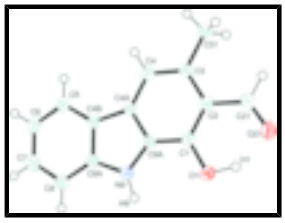


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. H atoms involved in hydrogen bonding have been labelled.

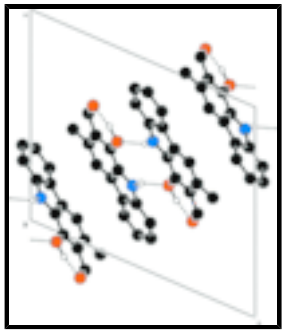


Fig. 2. The packing of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

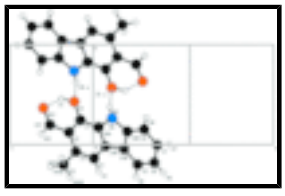


Fig. 3. The packing of (I), viewed down the *c* axis. Dashed lines indicate hydrogen bonds. The O1–H1···O21 intramolecular hydrogen bond forms a 6-membered ring and the N9–H9···O1(-*x*,1 - *y*,-*z*) intermolecular hydrogen bond forms a 10-membered ring; these favour the planarity of the title molecule (I).

1-Hydroxy-3-methyl-9*H*-carbazole-2-carbaldehyde

Crystal data

$C_{14}H_{11}NO_2$	F_{000} = 472
M_r = 225.24	D_x = 1.414 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 442(1) K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.1859 (6) Å	Cell parameters from 2612 reflections
b = 6.6703 (3) Å	θ = 2.0–27.5º
c = 14.1899 (7) Å	μ = 0.10 mm^{-1}
β = 113.469 (2)º	*T* = 160 (1) K
V = 1057.99 (9) Å^3	Needle, dark_brown
Z = 4	0.25 × 0.25 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer	2424 independent reflections
Radiation source: Nonius FR590 sealed tube generator	1803 reflections with $I > 2\sigma(I)$

Monochromator: horizontally mounted graphite crystal	R_{int} = 0.083
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 27.5º
T = 160(1) K	θ_{min} = 2.8º
φ and ω scans with κ offsets	h = −15→15
Absorption correction: none	k = −8→8
25678 measured reflections	l = −18→16

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0768P)^2 + 0.3576P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.148	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
2424 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
168 parameters	Extinction coefficient: 0.030 (6)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	−0.05055 (11)	0.43004 (18)	0.11451 (10)	0.0297 (4)
O21	−0.17265 (12)	0.3665 (2)	0.22106 (10)	0.0357 (5)
N9	0.12632 (13)	0.2634 (2)	0.04520 (11)	0.0253 (5)
C1	−0.00308 (15)	0.2454 (3)	0.14466 (13)	0.0229 (5)
C2	−0.03616 (14)	0.1239 (3)	0.20958 (12)	0.0227 (5)
C3	0.01660 (15)	−0.0705 (3)	0.24040 (12)	0.0240 (5)
C4	0.10098 (15)	−0.1368 (3)	0.20630 (13)	0.0244 (5)
C4A	0.13332 (14)	−0.0161 (2)	0.13988 (12)	0.0212 (5)

C4B	0.21270 (14)	−0.0436 (3)	0.08768 (12)	0.0238 (5)
C5	0.28668 (15)	−0.1995 (3)	0.08392 (13)	0.0296 (6)
C6	0.34962 (16)	−0.1795 (3)	0.02211 (14)	0.0333 (6)
C7	0.33931 (15)	−0.0049 (3)	−0.03579 (14)	0.0319 (6)
C8	0.26765 (15)	0.1521 (3)	−0.03319 (13)	0.0284 (6)
C8A	0.20392 (14)	0.1315 (3)	0.02920 (12)	0.0239 (5)
C9A	0.08162 (14)	0.1734 (3)	0.11020 (12)	0.0224 (5)
C21	−0.12595 (16)	0.1981 (3)	0.24268 (14)	0.0297 (6)
C31	−0.01876 (17)	−0.2000 (3)	0.31074 (14)	0.0315 (6)
H1	−0.106 (3)	0.460 (4)	0.149 (2)	0.081 (9)*
H4	0.13758	−0.26405	0.22743	0.0292*
H5	0.29383	−0.31779	0.12321	0.0355*
H6	0.40031	−0.28510	0.01884	0.0400*
H7	0.38310	0.00514	−0.07800	0.0382*
H8	0.26164	0.27031	−0.07232	0.0340*
H9	0.0972 (18)	0.377 (3)	0.0086 (16)	0.037 (6)*
H21	−0.1541 (18)	0.109 (3)	0.2875 (15)	0.036 (5)*
H31A	0.02338	−0.32857	0.32138	0.0473*
H31B	−0.10528	−0.22344	0.27962	0.0473*
H31C	0.00264	−0.13214	0.37695	0.0473*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0363 (7)	0.0229 (7)	0.0353 (7)	0.0073 (5)	0.0199 (6)	0.0055 (5)
O21	0.0362 (8)	0.0332 (8)	0.0439 (8)	0.0032 (6)	0.0224 (6)	−0.0032 (6)
N9	0.0270 (8)	0.0259 (8)	0.0256 (8)	0.0022 (6)	0.0132 (6)	0.0057 (6)
C1	0.0225 (8)	0.0207 (8)	0.0232 (8)	−0.0003 (7)	0.0066 (7)	−0.0021 (7)
C2	0.0205 (8)	0.0250 (9)	0.0218 (8)	−0.0030 (7)	0.0077 (7)	−0.0028 (7)
C3	0.0217 (8)	0.0266 (9)	0.0218 (8)	−0.0049 (7)	0.0066 (7)	0.0002 (7)
C4	0.0239 (9)	0.0231 (9)	0.0241 (9)	−0.0006 (7)	0.0074 (7)	0.0014 (7)
C4A	0.0179 (8)	0.0237 (8)	0.0205 (8)	−0.0017 (7)	0.0061 (6)	−0.0008 (7)
C4B	0.0189 (8)	0.0291 (9)	0.0216 (8)	−0.0003 (7)	0.0062 (7)	−0.0008 (7)
C5	0.0251 (9)	0.0321 (10)	0.0295 (10)	0.0036 (8)	0.0086 (7)	−0.0006 (8)
C6	0.0245 (9)	0.0421 (11)	0.0332 (10)	0.0066 (8)	0.0113 (8)	−0.0037 (9)
C7	0.0237 (9)	0.0472 (12)	0.0255 (9)	−0.0003 (8)	0.0107 (7)	−0.0038 (8)
C8	0.0238 (9)	0.0374 (11)	0.0238 (9)	−0.0014 (7)	0.0093 (7)	0.0013 (7)
C8A	0.0194 (8)	0.0302 (10)	0.0207 (8)	−0.0010 (7)	0.0065 (7)	0.0000 (7)
C9A	0.0207 (8)	0.0238 (9)	0.0221 (8)	−0.0017 (7)	0.0080 (7)	0.0011 (7)
C21	0.0287 (10)	0.0326 (10)	0.0299 (10)	−0.0035 (8)	0.0138 (8)	−0.0038 (8)
C31	0.0324 (10)	0.0331 (10)	0.0319 (10)	−0.0027 (8)	0.0159 (8)	0.0072 (8)

Geometric parameters (Å, °)

O1—C1	1.356 (2)	C4B—C8A	1.412 (3)
O21—C21	1.241 (2)	C4B—C5	1.391 (3)
O1—H1	1.00 (4)	C5—C6	1.382 (3)
N9—C8A	1.375 (2)	C6—C7	1.402 (3)
N9—C9A	1.381 (2)	C7—C8	1.373 (3)

N9—H9	0.91 (2)	C8—C8A	1.398 (3)
C1—C9A	1.392 (3)	C4—H4	0.9500
C1—C2	1.401 (3)	C5—H5	0.9500
C2—C21	1.440 (3)	C6—H6	0.9500
C2—C3	1.436 (3)	C7—H7	0.9500
C3—C4	1.372 (3)	C8—H8	0.9500
C3—C31	1.507 (3)	C21—H21	1.02 (2)
C4—C4A	1.410 (2)	C31—H31A	0.9800
C4A—C4B	1.445 (3)	C31—H31B	0.9800
C4A—C9A	1.400 (2)	C31—H31C	0.9800
O1···O21	2.544 (2)	C21···H31C	2.9300
O1···N9	2.922 (2)	C21···H31B	2.8500
O1···C4^{i}	3.397 (2)	C21···H1	2.27 (3)
O1···N9^{ii}	2.9160 (19)	C31···H1^{vii}	3.10 (3)
O21···O1	2.544 (2)	C31···H21	2.58 (2)
O21···C31^{i}	3.405 (2)	C31···H7^{ix}	3.0900
O1···H9^{ii}	2.06 (2)	H1···O21	1.66 (3)
O1···H9	2.79 (2)	H1···C21	2.27 (3)
O21···H1	1.66 (3)	H1···C31^{i}	3.10 (3)
O21···H31B^{i}	2.8800	H1···H8^{ii}	2.5200
O21···H21^{iii}	2.62 (2)	H1···H9^{ii}	2.53 (4)
O21···H31B^{iii}	2.7700	H4···H31A	2.3200
O21···H7^{iv}	2.7900	H5···C2^{viii}	2.9900
N9···O1	2.922 (2)	H5···C3^{viii}	2.8900
N9···O1^{ii}	2.9160 (19)	H5···C4^{viii}	3.0900
C1···C4B^{v}	3.535 (2)	H7···O21^{x}	2.7900
C2···C5^{vi}	3.482 (2)	H7···C31^{xi}	3.0900
C2···C8^{v}	3.462 (3)	H8···H1^{ii}	2.5200
C3···C8^{v}	3.582 (3)	H9···O1	2.79 (2)
C4···O1^{vii}	3.397 (2)	H9···O1^{ii}	2.06 (2)
C4B···C1^{v}	3.535 (2)	H9···H1^{ii}	2.53 (4)
C5···C2^{viii}	3.482 (2)	H21···C31	2.58 (2)
C7···C21^{v}	3.311 (3)	H21···H31B	2.3100
C8···C2^{v}	3.462 (3)	H21···H31C	2.4300
C8···C31^{vi}	3.551 (3)	H21···O21^{xii}	2.62 (2)
C8···C3^{v}	3.582 (3)	H31A···H4	2.3200
C21···C7^{v}	3.311 (3)	H31A···C7^{viii}	3.0600
C31···O21^{vii}	3.405 (2)	H31A···C8^{viii}	3.0700
C31···C8^{viii}	3.551 (3)	H31B···O21^{vii}	2.8800
C2···H5^{vi}	2.9900	H31B···C21	2.8500
C3···H5^{vi}	2.8900	H31B···H21	2.3100
C4···H5^{vi}	3.0900	H31B···O21^{xii}	2.7700
C7···H31A^{vi}	3.0600	H31C···C21	2.9300

C8···H31A^{vi}	3.0700	H31C···H21	2.4300
C1—O1—H1	108.3 (15)	N9—C8A—C4B	109.17 (15)
C8A—N9—C9A	108.19 (14)	N9—C8A—C8	129.33 (17)
C9A—N9—H9	125.2 (15)	N9—C9A—C1	129.01 (18)
C8A—N9—H9	125.3 (15)	N9—C9A—C4A	110.08 (16)
O1—C1—C9A	119.05 (17)	C1—C9A—C4A	120.91 (17)
O1—C1—C2	122.32 (17)	O21—C21—C2	124.32 (18)
C2—C1—C9A	118.63 (18)	C3—C4—H4	120.00
C1—C2—C3	120.75 (17)	C4A—C4—H4	120.00
C1—C2—C21	118.08 (18)	C4B—C5—H5	121.00
C3—C2—C21	121.16 (17)	C6—C5—H5	121.00
C4—C3—C31	120.06 (18)	C5—C6—H6	120.00
C2—C3—C4	119.41 (17)	C7—C6—H6	120.00
C2—C3—C31	120.53 (17)	C6—C7—H7	119.00
C3—C4—C4A	119.99 (17)	C8—C7—H7	119.00
C4—C4A—C4B	133.83 (15)	C7—C8—H8	121.00
C4—C4A—C9A	120.30 (16)	C8A—C8—H8	121.00
C4B—C4A—C9A	105.86 (14)	O21—C21—H21	116.4 (12)
C5—C4B—C8A	119.63 (16)	C2—C21—H21	119.3 (12)
C4A—C4B—C8A	106.66 (16)	C3—C31—H31A	109.00
C4A—C4B—C5	133.69 (17)	C3—C31—H31B	109.00
C4B—C5—C6	118.94 (18)	C3—C31—H31C	109.00
C5—C6—C7	120.61 (19)	H31A—C31—H31B	109.00
C6—C7—C8	121.82 (18)	H31A—C31—H31C	109.00
C7—C8—C8A	117.50 (18)	H31B—C31—H31C	109.00
C4B—C8A—C8	121.50 (18)		
C9A—N9—C8A—C8	177.63 (18)	C3—C4—C4A—C9A	1.4 (3)
C8A—N9—C9A—C1	−177.12 (18)	C4—C4A—C4B—C8A	178.29 (18)
C8A—N9—C9A—C4A	2.04 (19)	C9A—C4A—C4B—C5	−178.54 (19)
C9A—N9—C8A—C4B	−2.10 (19)	C9A—C4A—C4B—C8A	−0.13 (18)
O1—C1—C9A—N9	−1.2 (3)	C4—C4A—C4B—C5	−0.1 (3)
O1—C1—C9A—C4A	179.69 (16)	C4B—C4A—C9A—C1	178.08 (16)
C9A—C1—C2—C21	−178.53 (16)	C4—C4A—C9A—N9	−179.83 (15)
O1—C1—C2—C3	−179.63 (16)	C4—C4A—C9A—C1	−0.6 (3)
O1—C1—C2—C21	1.5 (3)	C4B—C4A—C9A—N9	−1.16 (19)
C9A—C1—C2—C3	0.3 (3)	C8A—C4B—C5—C6	−0.4 (3)
C2—C1—C9A—C4A	−0.2 (3)	C4A—C4B—C8A—N9	1.37 (19)
C2—C1—C9A—N9	178.83 (17)	C4A—C4B—C8A—C8	−178.39 (16)
C21—C2—C3—C31	−1.6 (3)	C4A—C4B—C5—C6	177.86 (18)
C21—C2—C3—C4	179.28 (17)	C5—C4B—C8A—N9	−179.95 (17)
C1—C2—C3—C4	0.5 (3)	C5—C4B—C8A—C8	0.3 (3)
C1—C2—C21—O21	−3.2 (3)	C4B—C5—C6—C7	0.1 (3)
C3—C2—C21—O21	177.99 (17)	C5—C6—C7—C8	0.3 (3)
C1—C2—C3—C31	179.63 (16)	C6—C7—C8—C8A	−0.4 (3)
C2—C3—C4—C4A	−1.3 (3)	C7—C8—C8A—N9	−179.57 (18)
C31—C3—C4—C4A	179.53 (16)	C7—C8—C8A—C4B	0.1 (3)
C3—C4—C4A—C4B	−176.84 (18)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*−1/2, *y*+1/2, −*z*+1/2; (iv) *x*−1/2, −*y*+1/2, *z*+1/2; (v) −*x*, −*y*, −*z*; (vi) −*x*+1/2, *y*+1/2, −*z*+1/2; (vii) *x*, *y*−1, *z*; (viii) −*x*+1/2, *y*−1/2, −*z*+1/2; (ix) *x*−1/2, −*y*−1/2, *z*+1/2; (x) *x*+1/2, −*y*+1/2, *z*−1/2; (xi) *x*+1/2, −*y*−1/2, *z*−1/2; (xii) −*x*−1/2, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O21	1.00 (4)	1.66 (3)	2.544 (2)	145 (2)
N9—H9···O1^{ii}	0.91 (2)	2.06 (2)	2.9160 (19)	157.0 (19)

Symmetry codes: (ii) −*x*, −*y*+1, −*z*.

Fig. 1

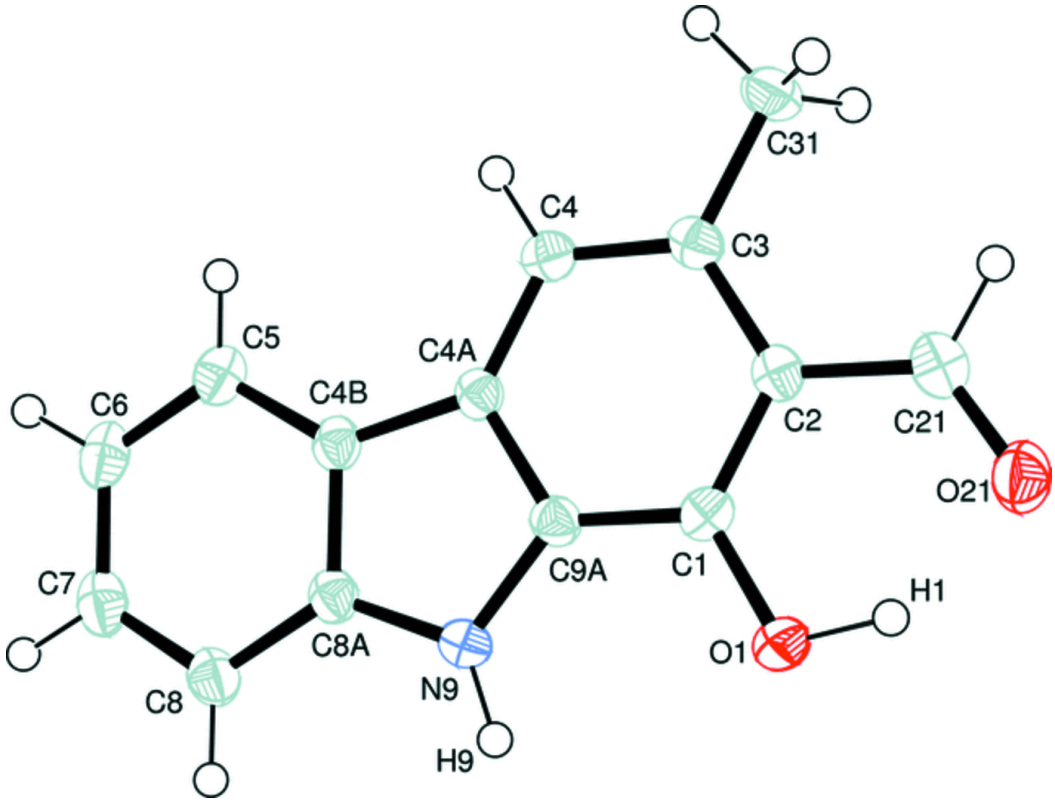


Fig. 2

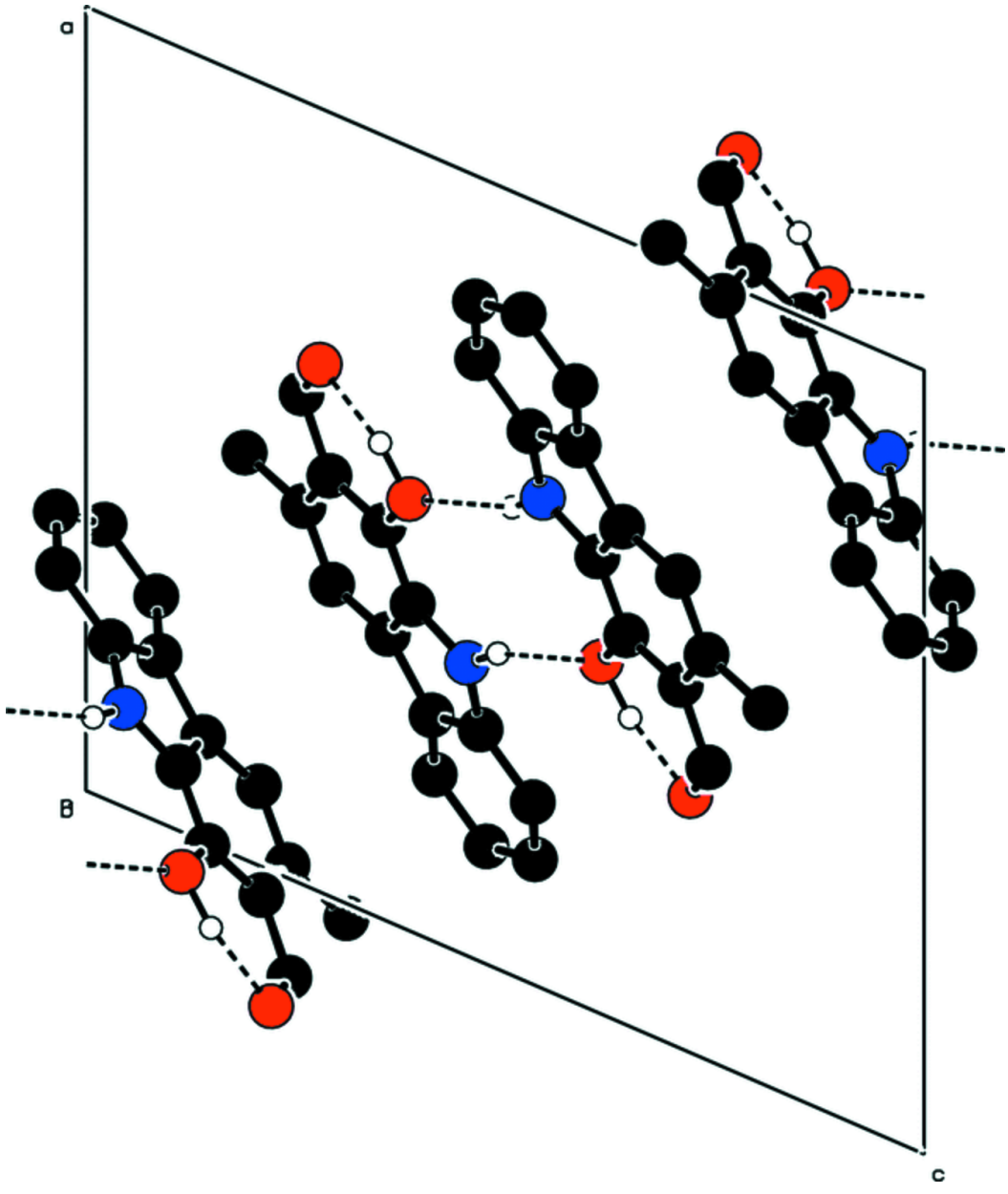
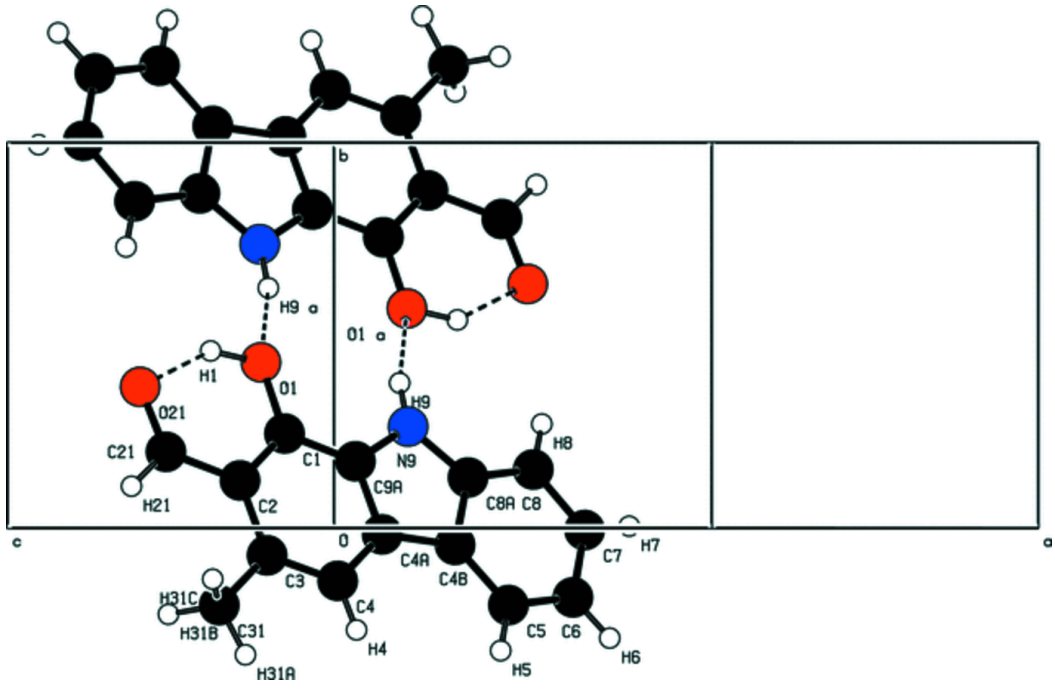


Fig. 3


b
H9 a
O1 a
H1
O1
O21
C21
C1
H9
N9
H8
C9A
C8A C8
H21
C2
c
0
a
C7
H7
C4A
C4B
C3
H31C
C4
H31B
C31
H4
C5
C6
H6
H5
H31A