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3,9-Dimethyl-10*H*-isoxazolo[5,4-*a*]-carbazole

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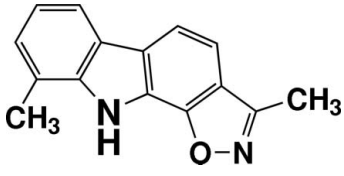
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.120; data-to-parameter ratio = 22.5.

The title molecule, $C_{15}H_{12}N_2O$, is essentially planar, except for the methyl H atoms. The mean plane of the isoxazole ring forms dihedral angles of 2.27 (9), 0.66 (8) and 3.97 (9)° with the pyrrole, fused benzene and methyl-substituted benzene rings, respectively. There is a short intermolecular contact between inversion-related isoxazole O atoms [O···O = 2.696 (1) Å]. In the crystal structure, molecules are stabilized by intermolecular N—H···O and N—H···N hydrogen bonds.

Related literature

For related literature, see: Gunaseelan *et al.* (2007); Haider *et al.* (1998); Hirata *et al.* (1999); Knolker & Reddy (2002); Kondo *et al.* (1986); Martin *et al.* (2007); Meragelman *et al.* (2000); Te Paske *et al.* (1989).



Experimental

Crystal data

$C_{15}H_{12}N_2O$
M_r = 236.27
Monoclinic, $I2/a$
a = 23.640 (2) Å
b = 5.0840 (5) Å
c = 19.2139 (19) Å
β = 93.974 (10)°
V = 2303.7 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 203 (2) K
0.43 × 0.35 × 0.17 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.649, T_{max} = 1.000 (expected range 0.962–0.985)
9488 measured reflections
3809 independent reflections
1239 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.120
S = 0.80
3809 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10···O1^{i}	0.852 (16)	2.496 (17)	3.1822 (19)	138.2 (14)
N10—H10···N2^{i}	0.852 (16)	2.223 (16)	3.062 (2)	168.0 (16)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2462).

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supplementary materials

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3,9-Dimethyl-10*H*-isoxazolo[5,4-*a*]carbazole

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Comment

The carbazole alkaloids and heterofused carbazoles like pyrido-, pyrimido-, indolo-, pyrazolo- and isoxazolo-carbazoles can exhibit high pharmacological properties such as anticancer, anti-HIV, antibiotic, cytotoxic and antiviral (Hirata *et al.*, 1999; Haider, 1998; Knolker & Reddy, 2002; Meragelman *et al.*, 2000; Kondo *et al.*, 1986; Te Paske *et al.*, 1989). The above properties have motivated us to study the X-ray crystal structures of these types of compounds (Gunaseelan *et al.*, 2007; Martin *et al.*, 2007).

The molecular structure of the title compound, with atomic numbering scheme, is shown in Fig. 1. The heterofused carbazole unit is essentially planar. The mean plane of the isoxazole ring forms dihedral angles of 2.27 (9)°, 0.66 (8)° and 3.97 (9)° with the pyrrole, fused benzene and methyl substituted benzene rings, respectively. There is a short intermolecular contact between inversion related isoxazole O atoms [O···O^{i} = 2.696 (1) Å]. In the crystal structure, molecules are stabilized by intermolecular N10—H10···O1^{i} and N10—H10···N2^{i} [symmetry code: (i)-*x*, −*y* + 1, −*z* + 1] hydrogen bonds (Fig. 2).

Experimental

A mixture of 2-acetyl-8-methyl-2,3,4,9-tetrahydrocarbazol-1-one (240 mg, 0.001 mol) and hydroxylamine hydrochloride (140 mg, 0.002 mol) in glacial acetic acid (15 ml) was refluxed on an oil bath for 4 h. The reaction was monitored by TLC. After the completion of the reaction the contents were poured into crushed ice. It was extracted using ethyl acetate washed with water and dried over anhydrous sodium sulfate. It was purified by column chromatography over silica gel using petroleum ether:ethyl acetate (98:2 *v*/*v*) as eluant (140 mg, 60%).

Refinement

H atom bonded to N10 was located in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.94–0.97 Å and U_{iso}(H) = 1.2–1.5 times U_{eq}(C).

Figures

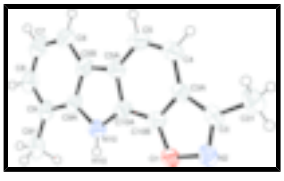

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

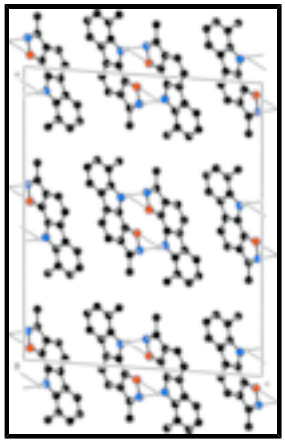

Fig. 2. The molecular packing of the title compound, viewed down the *b* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

3,9-Dimethyl-10*H*-isoxazolo[5,4-*a*]carbazole

Crystal data

$C_{15}H_{12}N_2O$	F_{000} = 992
M_r = 236.27	D_x = 1.362 Mg m^{-3}
Monoclinic, *I*2/*a*	Melting point: 472(1) K
Hall symbol: -I 2ya	Mo *K*α radiation λ = 0.71073 Å
a = 23.640 (2) Å	Cell parameters from 1857 reflections
b = 5.0840 (5) Å	θ = 4.6–32.5º
c = 19.2139 (19) Å	μ = 0.09 mm^{-1}
β = 93.974 (10)º	*T* = 203 (2) K
V = 2303.7 (4) Å^3	Needle, colourless
Z = 8	0.43 × 0.35 × 0.17 mm

Data collection

Oxford Diffraction Gemini diffractometer	1239 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.063
Monochromator: graphite	θ_{max} = 32.5º
T = 203(2) K	θ_{min} = 4.7º
φ and ω scans	*h* = −35→34
Absorption correction: multi-scan (Crysalis RED; Oxford Diffraction, 2007)	*k* = −7→7
T_{min} = 0.649, T_{max} = 1.000	*l* = −28→28
9488 measured reflections	Standard reflections: ?
3809 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.80$	$(\Delta/\sigma)_{max} < 0.001$
3809 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
169 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 e.s.d.'s 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 $F^2 > 2$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	−0.04155 (4)	0.3394 (2)	0.47379 (6)	0.0424 (4)
N2	−0.09963 (5)	0.2931 (3)	0.48477 (7)	0.0457 (5)
N10	0.07711 (6)	0.2663 (3)	0.40825 (8)	0.0398 (5)
C3	−0.11601 (7)	0.0942 (3)	0.44424 (9)	0.0411 (6)
C3A	−0.07096 (7)	0.0021 (3)	0.40550 (8)	0.0381 (5)
C4	−0.06581 (8)	−0.1975 (3)	0.35538 (9)	0.0474 (6)
C5	−0.01438 (8)	−0.2287 (3)	0.32738 (9)	0.0472 (6)
C5A	0.03141 (7)	−0.0642 (3)	0.34754 (8)	0.0389 (6)
C5B	0.08782 (7)	−0.0459 (3)	0.32571 (8)	0.0407 (6)
C6	0.11742 (8)	−0.1786 (3)	0.27566 (9)	0.0510 (7)
C7	0.17254 (9)	−0.1040 (4)	0.26672 (10)	0.0583 (8)
C8	0.19864 (8)	0.0958 (4)	0.30696 (10)	0.0527 (7)
C9	0.17104 (7)	0.2330 (3)	0.35633 (9)	0.0435 (6)
C9A	0.11525 (7)	0.1591 (3)	0.36421 (8)	0.0407 (6)
C10A	0.02666 (7)	0.1346 (3)	0.39816 (8)	0.0366 (5)
C10B	−0.02632 (7)	0.1618 (3)	0.42522 (8)	0.0375 (6)
C31	−0.17529 (7)	−0.0051 (4)	0.44370 (10)	0.0618 (8)
C91	0.19968 (7)	0.4476 (3)	0.39940 (10)	0.0555 (7)
H4	−0.09673	−0.30622	0.34154	0.0569*
H5	−0.00982	−0.36194	0.29430	0.0566*
H6	0.10015	−0.31494	0.24885	0.0612*
H7	0.19286	−0.18935	0.23293	0.0700*
H8	0.23654	0.13845	0.30015	0.0632*
H10	0.0847 (7)	0.403 (3)	0.4328 (9)	0.047 (6)*

H31A	−0.19423	0.07606	0.48141	0.0926*
H31B	−0.17484	−0.19453	0.44984	0.0926*
H31C	−0.19542	0.03834	0.39949	0.0926*
H91A	0.23628	0.48590	0.38185	0.0832*
H91B	0.20494	0.39078	0.44762	0.0832*
H91C	0.17631	0.60453	0.39656	0.0832*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0344 (7)	0.0473 (7)	0.0456 (7)	−0.0078 (5)	0.0044 (5)	−0.0079 (6)
N2	0.0345 (9)	0.0541 (9)	0.0486 (9)	−0.0051 (7)	0.0041 (7)	0.0006 (8)
N10	0.0386 (9)	0.0382 (8)	0.0427 (9)	−0.0007 (7)	0.0043 (7)	−0.0021 (7)
C3	0.0375 (10)	0.0438 (10)	0.0410 (10)	−0.0076 (8)	−0.0047 (8)	0.0082 (8)
C3A	0.0409 (10)	0.0369 (9)	0.0354 (9)	−0.0026 (8)	−0.0050 (8)	0.0057 (8)
C4	0.0525 (12)	0.0426 (10)	0.0460 (11)	−0.0077 (9)	−0.0049 (9)	−0.0018 (9)
C5	0.0668 (13)	0.0373 (9)	0.0364 (10)	0.0013 (9)	−0.0033 (9)	−0.0032 (8)
C5A	0.0467 (11)	0.0373 (9)	0.0320 (9)	0.0022 (8)	−0.0030 (8)	0.0035 (8)
C5B	0.0510 (11)	0.0393 (10)	0.0317 (9)	0.0096 (9)	0.0013 (8)	0.0059 (8)
C6	0.0639 (13)	0.0536 (11)	0.0351 (10)	0.0164 (10)	0.0005 (9)	−0.0004 (9)
C7	0.0636 (14)	0.0697 (14)	0.0435 (11)	0.0262 (11)	0.0166 (10)	0.0075 (11)
C8	0.0457 (11)	0.0638 (13)	0.0496 (12)	0.0135 (10)	0.0101 (10)	0.0171 (11)
C9	0.0415 (11)	0.0477 (10)	0.0411 (10)	0.0078 (9)	0.0022 (8)	0.0128 (9)
C9A	0.0452 (11)	0.0397 (9)	0.0377 (10)	0.0114 (9)	0.0074 (8)	0.0094 (8)
C10A	0.0393 (10)	0.0332 (9)	0.0374 (9)	0.0012 (8)	0.0026 (8)	0.0023 (8)
C10B	0.0472 (11)	0.0323 (9)	0.0324 (9)	−0.0007 (8)	−0.0014 (8)	−0.0013 (8)
C31	0.0473 (12)	0.0735 (14)	0.0638 (13)	−0.0156 (10)	−0.0013 (10)	0.0033 (11)
C91	0.0431 (11)	0.0622 (12)	0.0617 (13)	0.0042 (10)	0.0071 (9)	0.0192 (11)

Geometric parameters (Å, °)

O1—N2	1.4231 (15)	C7—C8	1.394 (3)
O1—C10B	1.3647 (19)	C8—C9	1.378 (3)
N2—C3	1.318 (2)	C9—C91	1.502 (2)
N10—C9A	1.390 (2)	C9—C9A	1.390 (2)
N10—C10A	1.370 (2)	C10A—C10B	1.396 (2)
N10—H10	0.852 (16)	C4—H4	0.9400
C3—C3A	1.420 (2)	C5—H5	0.9400
C3—C31	1.489 (2)	C6—H6	0.9400
C3A—C10B	1.364 (2)	C7—H7	0.9400
C3A—C4	1.410 (2)	C8—H8	0.9400
C4—C5	1.372 (3)	C31—H31A	0.9700
C5—C5A	1.401 (2)	C31—H31B	0.9700
C5A—C10A	1.413 (2)	C31—H31C	0.9700
C5A—C5B	1.428 (2)	C91—H91A	0.9700
C5B—C6	1.401 (2)	C91—H91B	0.9700
C5B—C9A	1.410 (2)	C91—H91C	0.9700
C6—C7	1.379 (3)		

O1···N10	3.1753 (18)	C8···H31C^{vii}	3.0500
O1···C4^{i}	3.297 (2)	C8···H91C^{iv}	3.1000
O1···O1^{ii}	2.6956 (14)	C31···H91B^{iii}	2.9800
O1···N10^{ii}	3.1822 (19)	C91···H10	2.845 (17)
O1···H10^{ii}	2.496 (17)	H4···C6^{viii}	2.9600
N2···N10^{ii}	3.062 (2)	H4···C7^{viii}	3.0500
N10···O1^{ii}	3.1822 (19)	H5···C5^{viii}	3.0700
N10···O1	3.1753 (18)	H5···C5A^{viii}	2.9200
N10···C3^{iii}	3.446 (2)	H5···C5B^{viii}	3.0000
N10···N2^{ii}	3.062 (2)	H6···C4^{viii}	2.8700
N2···H10^{ii}	2.223 (16)	H8···H91A	2.3600
N10···H91C	2.9300	H8···H31C^{vii}	2.5700
C3···N10^{iii}	3.446 (2)	H8···C8^{vi}	2.9700
C4···O1^{iv}	3.297 (2)	H8···H8^{vi}	2.3600
C6···C91^{iv}	3.522 (2)	H10···C91	2.845 (17)
C6···C9^{iv}	3.562 (2)	H10···H91C	2.5400
C7···C91^{iv}	3.447 (3)	H10···O1^{ii}	2.496 (17)
C9···C6^{i}	3.562 (2)	H10···N2^{ii}	2.223 (16)
C10B···C10B^{iii}	3.467 (2)	H31B···H91B^{iii}	2.3600
C91···C7^{i}	3.447 (3)	H31C···C8^{ix}	3.0500
C91···C6^{i}	3.522 (2)	H31C···H8^{ix}	2.5700
C4···H6^{v}	2.8700	H91A···H8	2.3600
C5···H5^{v}	3.0700	H91B···C31^{iii}	2.9800
C5A···H5^{v}	2.9200	H91B···H31B^{iii}	2.3600
C5B···H91C^{iv}	3.0000	H91C···N10	2.9300
C5B···H5^{v}	3.0000	H91C···C5B^{i}	3.0000
C6···H91C^{iv}	2.8500	H91C···C6^{i}	2.8500
C6···H4^{v}	2.9600	H91C···C7^{i}	2.9000
C7···H91C^{iv}	2.9000	H91C···C8^{i}	3.1000
C7···H4^{v}	3.0500	H91C···H10	2.5400
C8···H8^{vi}	2.9700		
N2—O1—C10B	107.15 (11)	N10—C10A—C10B	133.93 (15)
O1—N2—C3	106.64 (12)	C5A—C10A—C10B	116.33 (14)
C9A—N10—C10A	108.50 (14)	N10—C10A—C5A	109.71 (14)
C10A—N10—H10	128.7 (11)	C3A—C10B—C10A	122.30 (14)
C9A—N10—H10	122.4 (11)	O1—C10B—C3A	110.37 (14)
C3A—C3—C31	128.62 (15)	O1—C10B—C10A	127.33 (14)
N2—C3—C31	120.14 (15)	C3A—C4—H4	121.00
N2—C3—C3A	111.24 (14)	C5—C4—H4	121.00
C3—C3A—C4	134.31 (16)	C4—C5—H5	120.00
C3—C3A—C10B	104.59 (14)	C5A—C5—H5	120.00
C4—C3A—C10B	121.08 (16)	C5B—C6—H6	121.00

C3A—C4—C5	118.14 (16)	C7—C6—H6	121.00
C4—C5—C5A	120.74 (15)	C6—C7—H7	119.00
C5—C5A—C10A	121.38 (15)	C8—C7—H7	119.00
C5B—C5A—C10A	106.02 (14)	C7—C8—H8	119.00
C5—C5A—C5B	132.59 (15)	C9—C8—H8	119.00
C6—C5B—C9A	118.86 (15)	C3—C31—H31A	109.00
C5A—C5B—C6	133.71 (15)	C3—C31—H31B	109.00
C5A—C5B—C9A	107.39 (14)	C3—C31—H31C	109.00
C5B—C6—C7	118.31 (16)	H31A—C31—H31B	109.00
C6—C7—C8	121.12 (18)	H31A—C31—H31C	109.00
C7—C8—C9	122.56 (18)	H31B—C31—H31C	109.00
C8—C9—C91	122.02 (16)	C9—C91—H91A	109.00
C8—C9—C9A	115.88 (15)	C9—C91—H91B	109.00
C9A—C9—C91	122.10 (15)	C9—C91—H91C	109.00
N10—C9A—C9	128.38 (15)	H91A—C91—H91B	109.00
N10—C9A—C5B	108.37 (14)	H91A—C91—H91C	109.00
C5B—C9A—C9	123.24 (15)	H91B—C91—H91C	109.00
C10B—O1—N2—C3	0.70 (16)	C10A—C5A—C5B—C6	−177.00 (17)
N2—O1—C10B—C3A	−1.06 (16)	C10A—C5A—C5B—C9A	0.78 (17)
N2—O1—C10B—C10A	179.77 (15)	C5—C5A—C10A—N10	−179.98 (15)
O1—N2—C3—C3A	−0.11 (18)	C5—C5A—C10A—C10B	−1.7 (2)
O1—N2—C3—C31	179.71 (14)	C5B—C5A—C10A—N10	−0.91 (18)
C10A—N10—C9A—C5B	−0.18 (18)	C5B—C5A—C10A—C10B	177.39 (14)
C10A—N10—C9A—C9	179.22 (16)	C5A—C5B—C6—C7	178.20 (18)
C9A—N10—C10A—C5A	0.69 (18)	C9A—C5B—C6—C7	0.6 (2)
C9A—N10—C10A—C10B	−177.19 (17)	C5A—C5B—C9A—N10	−0.39 (18)
N2—C3—C3A—C4	−179.01 (17)	C5A—C5B—C9A—C9	−179.83 (15)
N2—C3—C3A—C10B	−0.53 (19)	C6—C5B—C9A—N10	177.79 (14)
C31—C3—C3A—C4	1.2 (3)	C6—C5B—C9A—C9	−1.7 (2)
C31—C3—C3A—C10B	179.68 (17)	C5B—C6—C7—C8	0.9 (3)
C3—C3A—C4—C5	178.94 (17)	C6—C7—C8—C9	−1.4 (3)
C10B—C3A—C4—C5	0.6 (2)	C7—C8—C9—C9A	0.4 (3)
C3—C3A—C10B—O1	0.97 (17)	C7—C8—C9—C91	179.92 (18)
C3—C3A—C10B—C10A	−179.81 (15)	C8—C9—C9A—N10	−178.21 (17)
C4—C3A—C10B—O1	179.71 (14)	C8—C9—C9A—C5B	1.1 (2)
C4—C3A—C10B—C10A	−1.1 (2)	C91—C9—C9A—N10	2.3 (3)
C3A—C4—C5—C5A	−0.8 (2)	C91—C9—C9A—C5B	−178.37 (15)
C4—C5—C5A—C5B	−177.42 (17)	N10—C10A—C10B—O1	−1.6 (3)
C4—C5—C5A—C10A	1.4 (2)	N10—C10A—C10B—C3A	179.33 (17)
C5—C5A—C5B—C6	1.9 (3)	C5A—C10A—C10B—O1	−179.37 (14)
C5—C5A—C5B—C9A	179.71 (17)	C5A—C10A—C10B—C3A	1.6 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···O1^{ii}	0.852 (16)	2.496 (17)	3.1822 (19)	138.2 (14)
N10—H10···N2^{ii}	0.852 (16)	2.223 (16)	3.062 (2)	168.0 (16)

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

Fig. 1

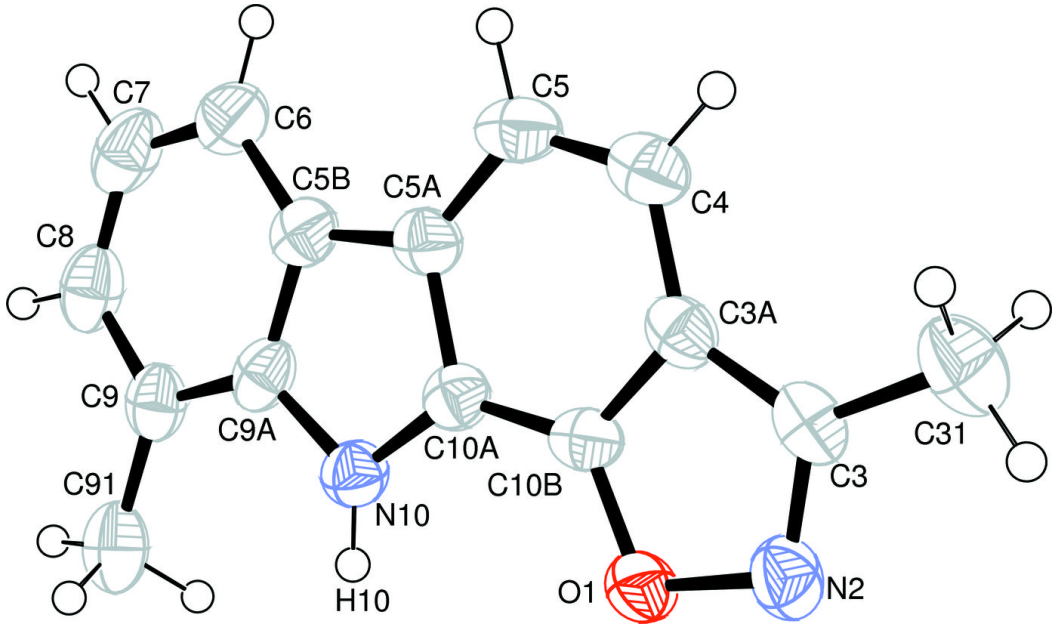

Fig. 2