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12-(4-Methoxyphenyl)-9,10-dihydrobenzo[*b*][4,7]phenanthrolin-11(7*H*,8*H*,12*H*)-one

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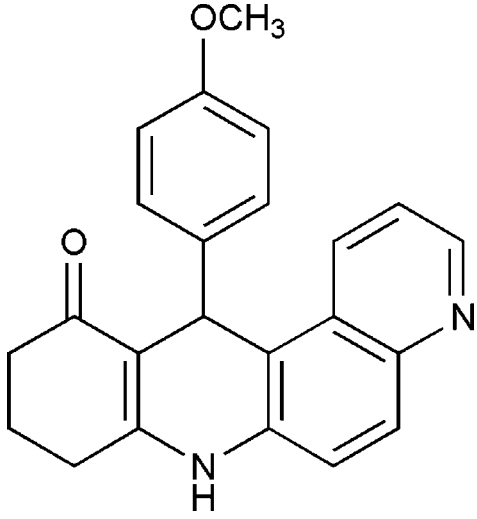
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.074; wR factor = 0.179; data-to-parameter ratio = 14.6.

In the molecule of the title compound, $C_{23}H_{20}N_2O_2$, the dihydropyridine ring has a boat conformation, while the cyclohexene ring adopts an envelope conformation. In the crystal structure there are intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Hall *et al.* (1977); Cassady & Floss (1977); Jastrzebska-Glapa *et al.* (1979). For bond-length data, see: Allen *et al.* (1987). For ring-conformation puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{23}H_{20}N_2O_2$
M_r = 356.41
Monoclinic, $C2/c$
a = 25.072 (3) Å
b = 7.3183 (16) Å
c = 23.335 (2) Å
β = 107.922 (2)°
V = 4073.9 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.25 × 0.22 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.987
9763 measured reflections
3561 independent reflections
1506 reflections with $I > 2\sigma(I)$
R_{int} = 0.091

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.179
S = 0.90
3561 reflections
244 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	1.99	2.842 (4)	170

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2333).

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supplementary materials

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12-(4-Methoxyphenyl)-9,10-dihydrobenzo[*b*][4,7]phenanthrolin-11(7*H*,8*H*,12*H*)-one

X. Zhang, D. Zhou, S. Tu, Q. Shao and C. Li

Comment

Compounds with the 4,7-phenanthroline motif, analogs of ergot alkaloids, possess high and versatile pharmacological effects, such as serotonin antagonism, vasoconstriction, oxytocic and psychotropic activities (Hall *et al.*, 1977). And they are also used as inhibitors of the pituitary hormone prolactin (Cassady & Floss, 1977) and fungicides (Jastrzebska-Glapa *et al.*, 1979). We report herein the crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

Rings A (C1—C6) and B (N1/C1/C6—C8/C13) are not planar, having total puckering amplitudes, Q_T, of 0.442 (2) and 0.218 (2) Å, respectively [φ = 121.08 (7)°, θ = 59.96 (5)° and φ = −7.63 (6)°, θ = 105.09 (5)°, respectively] (Cremer & Pople, 1975). Ring B has a boat conformation, while ring A adopts an envelope conformation with atom C3 displaced by 0.611 (3) Å from the plane of the other ring atoms. Rings C (C8—C13), D (N2/C9/C10/C14—C16) and E (C17—C22) are, of course, planar and the dihedral angles between them are C/D = 2.48 (3)°, C/E = 81.78 (2)° and D/E = 82.14 (2)°.

In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound, (I), was prepared by the reaction of 4-methoxybenzaldehyde (136 mg, 1 mmol), 6-aminoquinaldine (114 mg, 1 mmol) with 1,3-cyclohexanedione (112 mg, 1 mmol) in water (2 ml) at 393 K under microwave irradiation (maximum power 250 W, initial power 200 W) for 6 min (yield; 339 mg, 95%, m.p. > 573 K). Single crystals suitable for X-ray analysis were obtained from an ethanol solution (95%) by slow evaporation.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 (for NH) and C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

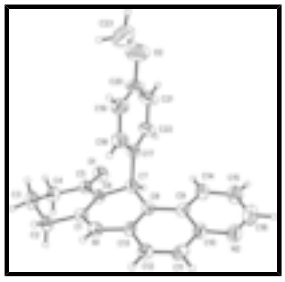

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

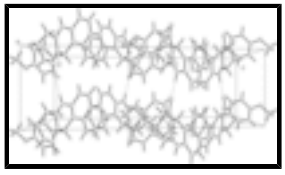

Fig. 2. A packing diagram of (I).

12-(4-Methoxyphenyl)-9,10-dihydrobenzo[*b*][4,7]phenanthrolin-11(7*H*,8H,12*H*)-one

Crystal data

$C_{23}H_{20}N_2O_2$	F_{000} = 1504
M_r = 356.41	D_x = 1.162 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: > 573 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 25.072 (3) Å	Cell parameters from 1054 reflections
b = 7.3183 (16) Å	θ = 3.1–25.0º
c = 23.335 (2) Å	μ = 0.08 mm^{-1}
β = 107.922 (2)º	*T* = 298 (2) K
V = 4073.9 (11) Å^3	Block, yellow
Z = 8	0.25 × 0.22 × 0.17 mm

Data collection

Bruker CCD area-detector diffractometer	3561 independent reflections
Radiation source: fine-focus sealed tube	1506 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.091
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −27→29
T_{min} = 0.982, T_{max} = 0.987	*k* = −6→8
9763 measured reflections	*l* = −27→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H-atom parameters constrained
$wR(F^2) = 0.179$	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.90$	$(\Delta/\sigma)_{max} < 0.001$
3561 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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}
N1	0.25058 (12)	0.2112 (4)	0.12759 (13)	0.0527 (8)
H1	0.2592	0.1025	0.1196	0.063*
N2	0.12094 (15)	0.2715 (6)	0.27923 (16)	0.0776 (11)
O1	0.26478 (10)	0.8398 (4)	0.09987 (12)	0.0660 (8)
O2	0.00632 (15)	0.7318 (7)	−0.06119 (19)	0.1331 (16)
C1	0.27071 (14)	0.3551 (5)	0.10386 (16)	0.0473 (9)
C2	0.31553 (15)	0.3166 (6)	0.07644 (17)	0.0587 (11)
H2A	0.3072	0.2023	0.0544	0.070*
H2B	0.3508	0.3016	0.1083	0.070*
C3	0.32208 (18)	0.4638 (6)	0.0345 (2)	0.0752 (13)
H3A	0.2910	0.4590	−0.0025	0.090*
H3B	0.3564	0.4443	0.0245	0.090*
C4	0.32379 (16)	0.6511 (5)	0.06386 (18)	0.0629 (11)
H4A	0.3596	0.6649	0.0949	0.076*
H4B	0.3216	0.7445	0.0337	0.076*
C5	0.27826 (15)	0.6826 (6)	0.09107 (16)	0.0519 (10)
C6	0.25135 (14)	0.5270 (5)	0.10778 (15)	0.0458 (9)

C7	0.20182 (14)	0.5607 (5)	0.13040 (15)	0.0489 (10)
H7	0.2102	0.6688	0.1564	0.059*
C8	0.19323 (14)	0.4004 (5)	0.16820 (15)	0.0456 (9)
C9	0.16183 (14)	0.4200 (5)	0.20860 (15)	0.0484 (10)
C10	0.15200 (16)	0.2680 (6)	0.24086 (17)	0.0579 (11)
C11	0.17668 (16)	0.0988 (6)	0.23468 (17)	0.0614 (11)
H11	0.1712	−0.0021	0.2564	0.074*
C12	0.20816 (15)	0.0827 (6)	0.19748 (17)	0.0558 (10)
H12	0.2243	−0.0294	0.1940	0.067*
C13	0.21689 (14)	0.2323 (5)	0.16396 (15)	0.0458 (9)
C14	0.13782 (15)	0.5875 (6)	0.21876 (17)	0.0631 (11)
H14	0.1423	0.6927	0.1983	0.076*
C15	0.10836 (18)	0.5925 (7)	0.2585 (2)	0.0820 (14)
H15	0.0934	0.7023	0.2666	0.098*
C16	0.1004 (2)	0.4308 (9)	0.2875 (2)	0.0910 (16)
H16	0.0793	0.4372	0.3141	0.109*
C17	0.14855 (15)	0.6003 (6)	0.07851 (17)	0.0549 (10)
C18	0.12516 (18)	0.4690 (7)	0.03605 (18)	0.0704 (13)
H18	0.1413	0.3534	0.0398	0.084*
C19	0.07762 (19)	0.5063 (9)	−0.0126 (2)	0.0852 (15)
H19	0.0624	0.4180	−0.0417	0.102*
C20	0.05397 (19)	0.6772 (10)	−0.0163 (2)	0.0864 (18)
C21	0.07634 (19)	0.8092 (8)	0.0256 (2)	0.0856 (16)
H21	0.0597	0.9239	0.0223	0.103*
C22	0.12300 (17)	0.7715 (6)	0.07178 (19)	0.0683 (12)
H22	0.1385	0.8624	0.0998	0.082*
C23	−0.0179 (3)	0.6087 (10)	−0.1060 (3)	0.142 (2)
H23A	0.0081	0.5787	−0.1274	0.213*
H23B	−0.0511	0.6614	−0.1335	0.213*
H23C	−0.0277	0.4998	−0.0887	0.213*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.070 (2)	0.030 (2)	0.062 (2)	0.0002 (15)	0.0266 (18)	0.0000 (16)
N2	0.093 (3)	0.077 (3)	0.073 (2)	0.007 (2)	0.040 (2)	0.000 (2)
O1	0.0811 (19)	0.0320 (18)	0.089 (2)	0.0003 (14)	0.0326 (16)	−0.0026 (16)
O2	0.078 (3)	0.183 (5)	0.118 (3)	−0.016 (2)	0.000 (2)	0.036 (3)
C1	0.048 (2)	0.040 (3)	0.053 (2)	−0.0018 (19)	0.0146 (19)	−0.003 (2)
C2	0.067 (3)	0.045 (3)	0.072 (3)	−0.0010 (19)	0.033 (2)	−0.009 (2)
C3	0.097 (3)	0.056 (3)	0.092 (3)	−0.005 (2)	0.057 (3)	−0.004 (3)
C4	0.080 (3)	0.045 (3)	0.072 (3)	−0.008 (2)	0.034 (2)	−0.001 (2)
C5	0.063 (3)	0.039 (3)	0.058 (2)	0.002 (2)	0.024 (2)	0.000 (2)
C6	0.056 (2)	0.034 (2)	0.053 (2)	−0.0009 (18)	0.0246 (19)	−0.0066 (19)
C7	0.055 (2)	0.038 (2)	0.053 (2)	−0.0003 (18)	0.0152 (19)	−0.0037 (19)
C8	0.044 (2)	0.045 (2)	0.047 (2)	−0.0066 (18)	0.0126 (18)	−0.006 (2)
C9	0.057 (2)	0.045 (3)	0.044 (2)	−0.0070 (19)	0.0175 (19)	−0.003 (2)
C10	0.061 (3)	0.069 (3)	0.046 (2)	−0.003 (2)	0.020 (2)	−0.003 (2)

C11	0.073 (3)	0.053 (3)	0.058 (2)	−0.011 (2)	0.019 (2)	0.009 (2)
C12	0.064 (3)	0.046 (3)	0.059 (2)	−0.0018 (19)	0.021 (2)	0.000 (2)
C13	0.050 (2)	0.044 (3)	0.048 (2)	−0.0054 (18)	0.0223 (19)	−0.002 (2)
C14	0.067 (3)	0.061 (3)	0.068 (3)	0.002 (2)	0.030 (2)	−0.007 (2)
C15	0.098 (4)	0.070 (4)	0.092 (3)	0.010 (3)	0.049 (3)	−0.008 (3)
C16	0.095 (4)	0.107 (5)	0.086 (4)	−0.010 (3)	0.050 (3)	−0.008 (4)
C17	0.051 (2)	0.057 (3)	0.060 (2)	0.001 (2)	0.023 (2)	0.003 (2)
C18	0.070 (3)	0.074 (3)	0.065 (3)	−0.003 (2)	0.017 (2)	−0.005 (3)
C19	0.059 (3)	0.120 (5)	0.069 (3)	−0.017 (3)	0.009 (3)	0.003 (3)
C20	0.037 (3)	0.138 (6)	0.073 (3)	0.000 (3)	0.000 (2)	0.037 (4)
C21	0.050 (3)	0.093 (4)	0.109 (4)	0.008 (3)	0.017 (3)	0.035 (4)
C22	0.049 (3)	0.071 (4)	0.082 (3)	0.009 (2)	0.016 (2)	0.011 (3)
C23	0.128 (5)	0.202 (7)	0.090 (4)	−0.034 (4)	0.026 (4)	0.005 (4)

Geometric parameters (Å, °)

N1—C1	1.357 (4)	C9—C10	1.407 (5)
N1—C13	1.378 (4)	C9—C14	1.418 (5)
N1—H1	0.8600	C10—C11	1.411 (5)
N2—C16	1.313 (6)	C11—C12	1.346 (5)
N2—C10	1.356 (5)	C11—H11	0.9300
O1—C5	1.234 (4)	C12—C13	1.402 (5)
O2—C23	1.373 (6)	C12—H12	0.9300
O2—C20	1.384 (5)	C14—C15	1.352 (5)
C1—C6	1.362 (5)	C14—H14	0.9300
C1—C2	1.481 (5)	C15—C16	1.409 (6)
C2—C3	1.497 (5)	C15—H15	0.9300
C2—H2A	0.9700	C16—H16	0.9300
C2—H2B	0.9700	C17—C18	1.375 (5)
C3—C4	1.527 (5)	C17—C22	1.394 (5)
C3—H3A	0.9700	C18—C19	1.397 (6)
C3—H3B	0.9700	C18—H18	0.9300
C4—C5	1.485 (5)	C19—C20	1.375 (7)
C4—H4A	0.9700	C19—H19	0.9300
C4—H4B	0.9700	C20—C21	1.365 (7)
C5—C6	1.437 (5)	C21—C22	1.353 (5)
C6—C7	1.512 (5)	C21—H21	0.9300
C7—C8	1.522 (5)	C22—H22	0.9300
C7—C17	1.529 (5)	C23—H23A	0.9600
C7—H7	0.9800	C23—H23B	0.9600
C8—C13	1.383 (5)	C23—H23C	0.9600
C8—C9	1.409 (5)		
C1—N1—C13	122.7 (3)	N2—C10—C9	124.7 (4)
C1—N1—H1	118.7	C11—C10—C9	119.0 (4)
C13—N1—H1	118.7	C12—C11—C10	120.4 (4)
C16—N2—C10	116.5 (4)	C12—C11—H11	119.8
C23—O2—C20	117.7 (6)	C10—C11—H11	119.8
N1—C1—C6	120.3 (3)	C11—C12—C13	121.0 (4)
N1—C1—C2	117.1 (3)	C11—C12—H12	119.5

C6—C1—C2	122.6 (4)	C13—C12—H12	119.5
C1—C2—C3	113.3 (3)	C8—C13—N1	120.1 (3)
C1—C2—H2A	108.9	C8—C13—C12	120.7 (4)
C3—C2—H2A	108.9	N1—C13—C12	119.1 (4)
C1—C2—H2B	108.9	C15—C14—C9	119.2 (4)
C3—C2—H2B	108.9	C15—C14—H14	120.4
H2A—C2—H2B	107.7	C9—C14—H14	120.4
C2—C3—C4	110.3 (3)	C14—C15—C16	119.7 (5)
C2—C3—H3A	109.6	C14—C15—H15	120.2
C4—C3—H3A	109.6	C16—C15—H15	120.2
C2—C3—H3B	109.6	N2—C16—C15	123.7 (5)
C4—C3—H3B	109.6	N2—C16—H16	118.1
H3A—C3—H3B	108.1	C15—C16—H16	118.1
C5—C4—C3	114.3 (3)	C18—C17—C22	117.9 (4)
C5—C4—H4A	108.7	C18—C17—C7	120.8 (4)
C3—C4—H4A	108.7	C22—C17—C7	121.3 (4)
C5—C4—H4B	108.7	C17—C18—C19	121.1 (5)
C3—C4—H4B	108.7	C17—C18—H18	119.4
H4A—C4—H4B	107.6	C19—C18—H18	119.4
O1—C5—C6	121.2 (3)	C20—C19—C18	118.2 (5)
O1—C5—C4	120.1 (4)	C20—C19—H19	120.9
C6—C5—C4	118.7 (4)	C18—C19—H19	120.9
C1—C6—C5	120.5 (3)	C19—C20—C21	121.6 (5)
C1—C6—C7	121.5 (3)	C19—C20—O2	124.4 (6)
C5—C6—C7	118.1 (3)	C21—C20—O2	114.0 (6)
C6—C7—C8	110.8 (3)	C22—C21—C20	119.3 (5)
C6—C7—C17	111.4 (3)	C22—C21—H21	120.3
C8—C7—C17	111.1 (3)	C20—C21—H21	120.3
C6—C7—H7	107.8	C21—C22—C17	121.8 (4)
C8—C7—H7	107.8	C21—C22—H22	119.1
C17—C7—H7	107.8	C17—C22—H22	119.1
C13—C8—C9	118.6 (4)	O2—C23—H23A	109.5
C13—C8—C7	120.2 (3)	O2—C23—H23B	109.5
C9—C8—C7	121.2 (3)	H23A—C23—H23B	109.5
C10—C9—C8	120.3 (4)	O2—C23—H23C	109.5
C10—C9—C14	116.2 (4)	H23A—C23—H23C	109.5
C8—C9—C14	123.6 (4)	H23B—C23—H23C	109.5
N2—C10—C11	116.3 (4)		
C13—N1—C1—C6	−10.0 (5)	C14—C9—C10—C11	−177.4 (3)
C13—N1—C1—C2	167.6 (3)	N2—C10—C11—C12	179.9 (3)
N1—C1—C2—C3	161.1 (3)	C9—C10—C11—C12	−1.4 (5)
C6—C1—C2—C3	−21.4 (5)	C10—C11—C12—C13	−0.3 (5)
C1—C2—C3—C4	47.6 (4)	C9—C8—C13—N1	−176.2 (3)
C2—C3—C4—C5	−48.7 (5)	C7—C8—C13—N1	3.1 (5)
C3—C4—C5—O1	−158.6 (4)	C9—C8—C13—C12	2.3 (5)
C3—C4—C5—C6	22.6 (5)	C7—C8—C13—C12	−178.5 (3)
N1—C1—C6—C5	170.5 (3)	C1—N1—C13—C8	12.8 (5)
C2—C1—C6—C5	−6.9 (5)	C1—N1—C13—C12	−165.7 (3)
N1—C1—C6—C7	−8.6 (5)	C11—C12—C13—C8	−0.2 (5)

C2—C1—C6—C7	174.0 (3)	C11—C12—C13—N1	178.3 (3)
O1—C5—C6—C1	−172.8 (3)	C10—C9—C14—C15	1.0 (5)
C4—C5—C6—C1	6.0 (5)	C8—C9—C14—C15	−180.0 (3)
O1—C5—C6—C7	6.4 (5)	C9—C14—C15—C16	−2.1 (6)
C4—C5—C6—C7	−174.8 (3)	C10—N2—C16—C15	0.9 (7)
C1—C6—C7—C8	21.6 (4)	C14—C15—C16—N2	1.2 (7)
C5—C6—C7—C8	−157.6 (3)	C6—C7—C17—C18	64.9 (4)
C1—C6—C7—C17	−102.7 (4)	C8—C7—C17—C18	−59.2 (4)
C5—C6—C7—C17	78.2 (4)	C6—C7—C17—C22	−113.4 (4)
C6—C7—C8—C13	−18.6 (4)	C8—C7—C17—C22	122.5 (4)
C17—C7—C8—C13	105.9 (4)	C22—C17—C18—C19	0.6 (6)
C6—C7—C8—C9	160.6 (3)	C7—C17—C18—C19	−177.8 (3)
C17—C7—C8—C9	−74.9 (4)	C17—C18—C19—C20	−1.4 (6)
C13—C8—C9—C10	−4.0 (5)	C18—C19—C20—C21	1.1 (7)
C7—C8—C9—C10	176.8 (3)	C18—C19—C20—O2	−178.7 (4)
C13—C8—C9—C14	177.0 (3)	C23—O2—C20—C19	−2.0 (7)
C7—C8—C9—C14	−2.2 (5)	C23—O2—C20—C21	178.2 (4)
C16—N2—C10—C11	176.5 (4)	C19—C20—C21—C22	0.1 (7)
C16—N2—C10—C9	−2.1 (6)	O2—C20—C21—C22	179.9 (4)
C8—C9—C10—N2	−177.8 (3)	C20—C21—C22—C17	−1.0 (6)
C14—C9—C10—N2	1.2 (5)	C18—C17—C22—C21	0.6 (6)
C8—C9—C10—C11	3.6 (5)	C7—C17—C22—C21	179.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	1.99	2.842 (4)	170

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

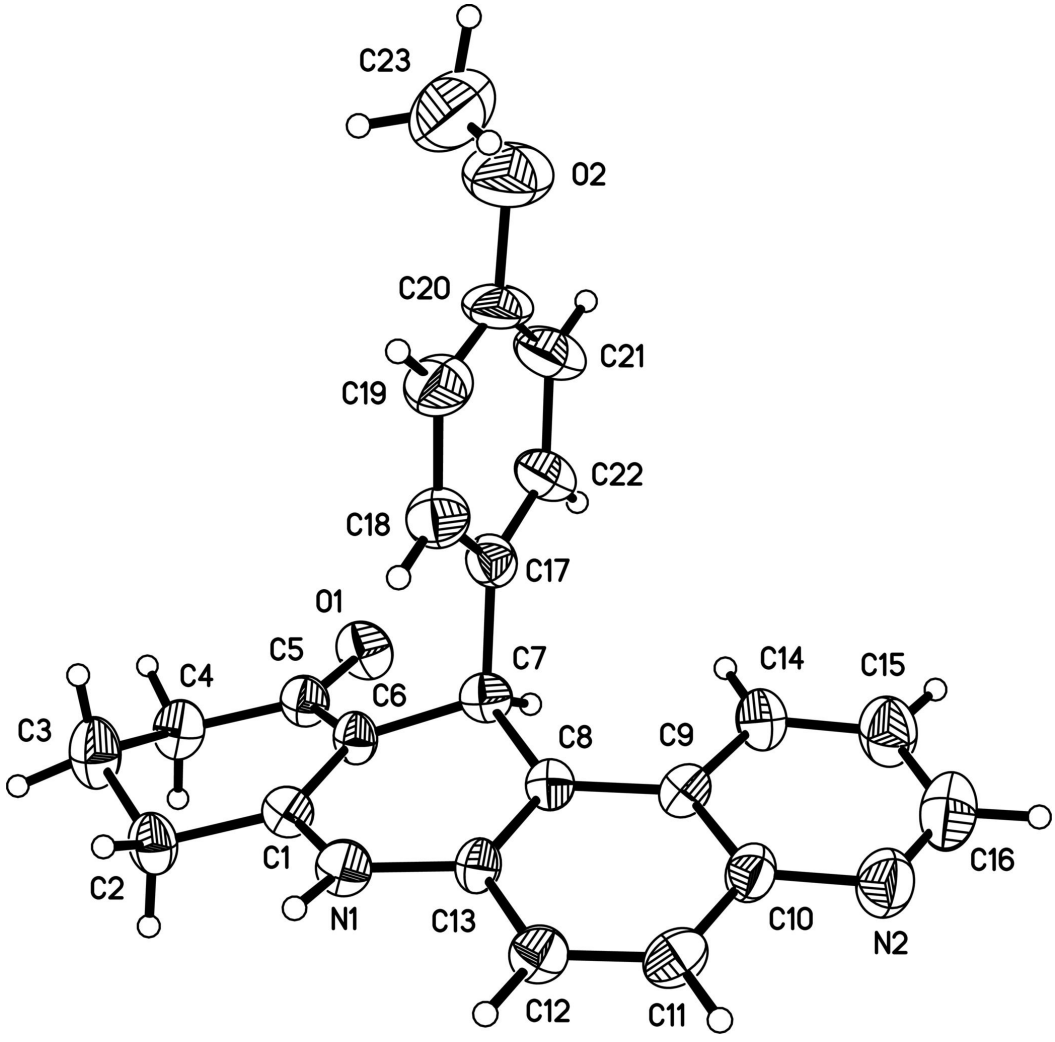
C23
O2
C20
C21
C19
C22
C18
C17
O1
C5
C7
C14
C15
C4
C6
C3
C8
C9
C1
C16
C2
N1
C13
C10
N2
C12
C11

Fig. 2