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1,1′-(*N*-Methyliminodimethylene)di-2-naphthol

Xiu-Ling Chen,[a]‡ Xu-Hong Yang[b] and Ming-Hu Wu[b]*

[a]College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]Department of Chemistry and Life Sciences, Xianning College, Xianning 437100, People's Republic of China
Correspondence e-mail: minghuwu@hotmail.com

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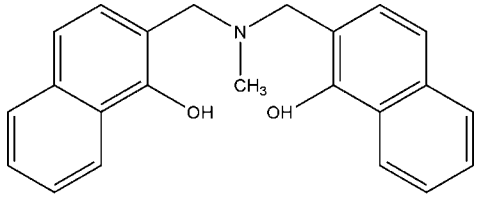
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.147; data-to-parameter ratio = 16.5.

In the title molecule, $C_{23}H_{21}NO_2$, the dihedral angle between the naphthalene ring systems is 70.71 (6)°. In the crystal structure, molecules are linked by intermolecular O—H···O hydrogen bonds to form one-dimensional chains along the c axis direction. In addition, weak C—H···π(arene) interactions help to stabilize the structure.

Related literature

We have recently determined the crystal structure of the closely related compound 4,4′-dimethyl-2,2′-(*N*-methyliminodimethylene)diphenol (Wu *et al.*, 2006). For related literature, see: Phongtamrug *et al.* (2004).



Experimental

Crystal data

$C_{23}H_{21}NO_2$
M_r = 343.41
Monoclinic, $P2_1/c$
a = 9.9947 (10) Å
b = 24.319 (3) Å
c = 8.0077 (8) Å
β = 111.745 (2)°
V = 1807.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 297 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.984, T_{max} = 0.984
10992 measured reflections
3931 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.148
S = 1.01
3931 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*1 is the centroid of the C1/C2/C7–C10 ring and *Cg*2 is the centroid of the C14–C18/C23 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.84	2.633 (2)	164
O2—H2···N1	0.82	1.83	2.557 (2)	148
C6—H6···*Cg*2^{ii}	0.93	2.82	3.698 (3)	158
C19—H19···*Cg*1^{iii}	0.93	2.78	3.564 (2)	143

Symmetry codes: (i) $x, y, z+1$; (ii) $x-1, y, z$; (iii) $-x+2, -y, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2426).

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‡ Current address: Xianning College, Xianning 437100, People's Republic of China.

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supplementary materials

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1,1'-(*N*-Methyliminodimethylene)di-2-naphthol

X.-L. Chen, X.-H. Yang and M.-H. Wu

Comment

Benzoxazine dimers, *e.g.*, *N*,*N*-bis(2-hydroxy-5-ethylbenzyl)cyclohexylamine, *N*,*N*-bis(2-hydroxy-5-methylbenzyl)propylamine, and *N*,*N*-bis(hydroxy-5-ethylbenzyl)cyclohexylamine have been prepared by Phongtamrug *et al.* (2004). The synthesis and X-ray crystal structure of 4,4'-Dimethyl-2,2'-(*N*-methyliminodimethylene)-diphenol from 4-methylphenol by Mannich reaction has been reported by Wu *et al.* (2006). We have recently synthesized the title compound by reaction of 2-naphthol, formaldehyde and methylamine, and its crystal structure is crystal structure is reported herein.

In the molecule the dihedral angle between the naphthyl rings is 70.71 (6)°. The torsional angles C2—C1—C11—N1 and N1—C13—C14—C15 are −81.52 (17)° and −37.61 (19)°, respectively, showing that the aminomethyl groups are *syn*-clinal to the corresponding attached phenyl ring plane.

In the crystal structure, molecules are linked by intermolecular O—H···O hydrogen bonds to form onr-dimensional chains along the *c* axis direction (Fig. 2). In addition, the structure is stabilized by two intermolecular C—H···π(arene) interactions *via* H6 to the centroid of C14—C18/C23 (*Cg*2) (−1 + *x*, *y*, *z*), and *via* H19 to the centroid of C1/C2/C7—C10 (*Cg*1) (2 − *x*,-*y*,-*z*).

Experimental

Formaldehyde (8 ml, 40%, 0.1 mol) was added slowly with stirring to a mixture of methanol (35 ml), methylamine (6.5 ml, 25–30%, 0.05 mol) and 2-naphthol (14.4 g, 0.1 mol) over 40 min. The mixture was stirred for additional 12 h at room temperature. The resulting bright yellow solid was filtered and washed with methanol. The solid residue was recrystallized from 1,4-dioxane-methanol (2:1/v:v) to give colorless crystals of the title compound in a yield 98% (m.p. 408 K), which were suitable for X-ray analysis. ^{1}H NMR ($CDCl_3$, 400 MHz), 8.00 (s, 2H, O—H), 7.07–7.98 (m, 12H, aromatic-H), 4.34 (s, 4H, N—CH_2), 2.45 (s, 3H, N—CH_3).

Refinement

All H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and included in the riding model approximation, with U_{iso} (H) = 1.2U_{iso} (C) or 1.5U_{eq}(methyl C).

Figures

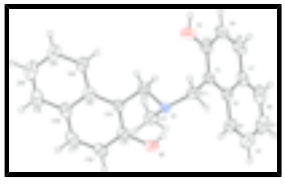

Fig. 1. The molecular structure with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

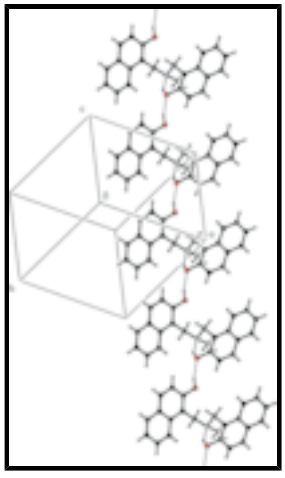

Fig. 2. Part of the crystal structure of (I). Hydrogen bonds are shown as dashed lines.

1,1'-(*N*-Methyliminodimethylene)di-2-naphthol

Crystal data

$C_{23}H_{21}NO_2$	F_{000} = 728
M_r = 343.41	D_x = 1.262 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2957 reflections
a = 9.9947 (10) Å	θ = 1.7–27.0º
b = 24.319 (3) Å	μ = 0.08 mm^{-1}
c = 8.0077 (8) Å	T = 297 (2) K
β = 111.745 (2)º	Block, colourless
V = 1807.9 (3) Å^3	0.20 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3931 independent reflections
Radiation source: fine-focus sealed tube	2738 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
T = 297(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −12→12
T_{min} = 0.984, T_{max} = 0.984	k = −31→30
10992 measured reflections	l = −8→10

Refinement

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

$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3931 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
238 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
C1	0.73724 (17)	0.18095 (6)	0.1033 (2)	0.0440 (4)
C2	0.60649 (18)	0.17833 (6)	−0.0501 (2)	0.0465 (4)
C3	0.5930 (2)	0.19982 (7)	−0.2203 (2)	0.0585 (5)
H3	0.6719	0.2166	−0.2340	0.070*
C4	0.4662 (2)	0.19623 (9)	−0.3641 (3)	0.0782 (6)
H4	0.4595	0.2108	−0.4743	0.094*
C5	0.3458 (2)	0.17075 (10)	−0.3475 (4)	0.0856 (7)
H5	0.2600	0.1681	−0.4467	0.103*
C6	0.3547 (2)	0.14998 (9)	−0.1864 (4)	0.0781 (6)
H6	0.2743	0.1334	−0.1762	0.094*
C7	0.4837 (2)	0.15312 (7)	−0.0340 (3)	0.0580 (5)
C8	0.4956 (2)	0.13167 (8)	0.1361 (3)	0.0692 (6)
H8	0.4158	0.1154	0.1487	0.083*
C9	0.6205 (3)	0.13447 (7)	0.2796 (3)	0.0642 (5)
H9	0.6258	0.1203	0.3897	0.077*
C10	0.7420 (2)	0.15858 (6)	0.2630 (2)	0.0499 (4)
C11	0.86922 (18)	0.20939 (6)	0.0976 (2)	0.0463 (4)
H11A	0.8392	0.2429	0.0279	0.056*
H11B	0.9295	0.2199	0.2191	0.056*
C12	1.08916 (19)	0.20732 (8)	0.0432 (2)	0.0589 (5)
H12A	1.1515	0.2071	0.1676	0.088*
H12B	1.0650	0.2446	0.0038	0.088*
H12C	1.1374	0.1903	−0.0272	0.088*
C13	0.99320 (18)	0.12140 (6)	0.1021 (2)	0.0458 (4)

H13A	0.9073	0.1047	0.1089	0.055*
H13B	1.0636	0.1249	0.2236	0.055*
C14	1.05305 (16)	0.08475 (6)	−0.0055 (2)	0.0427 (4)
C15	0.99667 (18)	0.08809 (7)	−0.1903 (2)	0.0488 (4)
C16	1.0473 (2)	0.05410 (8)	−0.2965 (2)	0.0618 (5)
H16	1.0078	0.0570	−0.4211	0.074*
C17	1.1534 (2)	0.01729 (8)	−0.2174 (3)	0.0666 (5)
H17	1.1870	−0.0045	−0.2889	0.080*
C18	1.21416 (19)	0.01128 (7)	−0.0292 (3)	0.0560 (5)
C19	1.3239 (2)	−0.02738 (8)	0.0550 (4)	0.0761 (6)
H19	1.3605	−0.0485	−0.0151	0.091*
C20	1.3767 (2)	−0.03431 (9)	0.2344 (4)	0.0855 (7)
H20	1.4486	−0.0602	0.2872	0.103*
C21	1.3235 (2)	−0.00268 (8)	0.3408 (3)	0.0724 (6)
H21	1.3590	−0.0082	0.4645	0.087*
C22	1.22052 (19)	0.03615 (7)	0.2667 (2)	0.0553 (4)
H22	1.1883	0.0573	0.3411	0.066*
C23	1.16151 (17)	0.04493 (6)	0.0789 (2)	0.0472 (4)
N1	0.95721 (13)	0.17670 (5)	0.02054 (16)	0.0413 (3)
O1	0.87029 (15)	0.16064 (5)	0.40481 (16)	0.0670 (4)
H1	0.8592	0.1499	0.4959	0.101*
O2	0.88986 (14)	0.12468 (5)	−0.27686 (14)	0.0606 (4)
H2	0.8808	0.1466	−0.2039	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0560 (10)	0.0320 (7)	0.0523 (10)	0.0033 (7)	0.0299 (8)	−0.0017 (6)
C2	0.0514 (10)	0.0336 (8)	0.0602 (11)	0.0048 (7)	0.0272 (8)	−0.0018 (7)
C3	0.0605 (12)	0.0494 (10)	0.0623 (12)	0.0041 (8)	0.0189 (10)	0.0065 (8)
C4	0.0783 (16)	0.0698 (13)	0.0725 (14)	0.0142 (11)	0.0118 (12)	0.0084 (10)
C5	0.0587 (14)	0.0797 (15)	0.0960 (19)	0.0101 (12)	0.0024 (13)	−0.0092 (13)
C6	0.0481 (12)	0.0705 (13)	0.1153 (19)	0.0005 (10)	0.0297 (12)	−0.0147 (13)
C7	0.0536 (11)	0.0428 (9)	0.0862 (14)	0.0029 (8)	0.0359 (10)	−0.0060 (9)
C8	0.0747 (14)	0.0551 (11)	0.1037 (17)	−0.0051 (10)	0.0631 (14)	−0.0021 (11)
C9	0.0902 (15)	0.0525 (10)	0.0726 (13)	0.0032 (10)	0.0566 (13)	0.0033 (9)
C10	0.0695 (12)	0.0392 (8)	0.0503 (10)	0.0052 (8)	0.0329 (9)	−0.0030 (7)
C11	0.0572 (10)	0.0370 (8)	0.0465 (9)	−0.0023 (7)	0.0214 (8)	−0.0020 (7)
C12	0.0535 (11)	0.0573 (10)	0.0665 (12)	−0.0080 (8)	0.0227 (9)	0.0066 (8)
C13	0.0555 (10)	0.0423 (8)	0.0422 (9)	0.0026 (7)	0.0211 (7)	0.0049 (6)
C14	0.0426 (9)	0.0415 (8)	0.0468 (9)	−0.0032 (7)	0.0197 (7)	−0.0025 (7)
C15	0.0497 (10)	0.0507 (9)	0.0476 (10)	−0.0046 (8)	0.0198 (8)	−0.0061 (7)
C16	0.0653 (13)	0.0703 (12)	0.0549 (11)	−0.0073 (10)	0.0285 (10)	−0.0163 (9)
C17	0.0682 (13)	0.0636 (12)	0.0785 (14)	−0.0082 (10)	0.0394 (11)	−0.0288 (10)
C18	0.0497 (10)	0.0443 (9)	0.0770 (13)	−0.0046 (8)	0.0269 (9)	−0.0139 (8)
C19	0.0614 (13)	0.0560 (11)	0.1095 (19)	0.0067 (10)	0.0301 (13)	−0.0209 (11)
C20	0.0643 (14)	0.0579 (12)	0.119 (2)	0.0163 (11)	0.0164 (14)	−0.0014 (13)
C21	0.0629 (13)	0.0599 (12)	0.0839 (14)	0.0095 (10)	0.0151 (11)	0.0084 (10)

C22	0.0519 (10)	0.0468 (9)	0.0643 (12)	0.0017 (8)	0.0183 (9)	0.0019 (8)
C23	0.0437 (9)	0.0384 (8)	0.0605 (11)	−0.0068 (7)	0.0205 (8)	−0.0051 (7)
N1	0.0455 (8)	0.0386 (7)	0.0418 (7)	−0.0007 (5)	0.0185 (6)	0.0047 (5)
O1	0.0897 (10)	0.0674 (8)	0.0474 (7)	−0.0020 (7)	0.0294 (7)	0.0016 (6)
O2	0.0686 (8)	0.0718 (8)	0.0389 (6)	0.0099 (7)	0.0171 (6)	−0.0005 (5)

Geometric parameters (Å, °)

C1—C10	1.374 (2)	C12—H12C	0.9600
C1—C2	1.425 (2)	C13—N1	1.4800 (19)
C1—C11	1.505 (2)	C13—C14	1.509 (2)
C2—C3	1.419 (2)	C13—H13A	0.9700
C2—C7	1.420 (2)	C13—H13B	0.9700
C3—C4	1.363 (3)	C14—C15	1.377 (2)
C3—H3	0.9300	C14—C23	1.424 (2)
C4—C5	1.403 (3)	C15—O2	1.365 (2)
C4—H4	0.9300	C15—C16	1.408 (2)
C5—C6	1.358 (3)	C16—C17	1.352 (3)
C5—H5	0.9300	C16—H16	0.9300
C6—C7	1.411 (3)	C17—C18	1.408 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.421 (3)	C18—C19	1.412 (3)
C8—C9	1.349 (3)	C18—C23	1.426 (2)
C8—H8	0.9300	C19—C20	1.345 (3)
C9—C10	1.398 (3)	C19—H19	0.9300
C9—H9	0.9300	C20—C21	1.391 (3)
C10—O1	1.363 (2)	C20—H20	0.9300
C11—N1	1.4793 (19)	C21—C22	1.361 (2)
C11—H11A	0.9700	C21—H21	0.9300
C11—H11B	0.9700	C22—C23	1.414 (2)
C12—N1	1.466 (2)	C22—H22	0.9300
C12—H12A	0.9600	O1—H1	0.8200
C12—H12B	0.9600	O2—H2	0.8200
C10—C1—C2	119.27 (15)	N1—C13—C14	111.57 (12)
C10—C1—C11	118.81 (15)	N1—C13—H13A	109.3
C2—C1—C11	121.88 (14)	C14—C13—H13A	109.3
C3—C2—C7	117.94 (17)	N1—C13—H13B	109.3
C3—C2—C1	122.84 (15)	C14—C13—H13B	109.3
C7—C2—C1	119.22 (15)	H13A—C13—H13B	108.0
C4—C3—C2	121.07 (19)	C15—C14—C23	119.13 (14)
C4—C3—H3	119.5	C15—C14—C13	119.20 (14)
C2—C3—H3	119.5	C23—C14—C13	121.60 (14)
C3—C4—C5	120.6 (2)	O2—C15—C14	121.05 (14)
C3—C4—H4	119.7	O2—C15—C16	117.68 (15)
C5—C4—H4	119.7	C14—C15—C16	121.27 (16)
C6—C5—C4	119.8 (2)	C17—C16—C15	120.03 (18)
C6—C5—H5	120.1	C17—C16—H16	120.0
C4—C5—H5	120.1	C15—C16—H16	120.0
C5—C6—C7	121.3 (2)	C16—C17—C18	121.51 (16)

C5—C6—H6	119.4	C16—C17—H17	119.2
C7—C6—H6	119.4	C18—C17—H17	119.2
C6—C7—C2	119.21 (18)	C17—C18—C19	122.06 (17)
C6—C7—C8	122.31 (19)	C17—C18—C23	118.70 (16)
C2—C7—C8	118.48 (18)	C19—C18—C23	119.24 (18)
C9—C8—C7	121.36 (17)	C20—C19—C18	121.42 (19)
C9—C8—H8	119.3	C20—C19—H19	119.3
C7—C8—H8	119.3	C18—C19—H19	119.3
C8—C9—C10	120.17 (17)	C19—C20—C21	119.81 (19)
C8—C9—H9	119.9	C19—C20—H20	120.1
C10—C9—H9	119.9	C21—C20—H20	120.1
O1—C10—C1	117.24 (15)	C22—C21—C20	121.1 (2)
O1—C10—C9	121.27 (16)	C22—C21—H21	119.5
C1—C10—C9	121.49 (18)	C20—C21—H21	119.5
N1—C11—C1	115.40 (12)	C21—C22—C23	121.22 (17)
N1—C11—H11A	108.4	C21—C22—H22	119.4
C1—C11—H11A	108.4	C23—C22—H22	119.4
N1—C11—H11B	108.4	C22—C23—C14	123.50 (14)
C1—C11—H11B	108.4	C22—C23—C18	117.19 (16)
H11A—C11—H11B	107.5	C14—C23—C18	119.30 (15)
N1—C12—H12A	109.5	C12—N1—C11	108.78 (12)
N1—C12—H12B	109.5	C12—N1—C13	110.28 (13)
H12A—C12—H12B	109.5	C11—N1—C13	112.90 (11)
N1—C12—H12C	109.5	C10—O1—H1	109.5
H12A—C12—H12C	109.5	C15—O2—H2	109.5
H12B—C12—H12C	109.5		
C10—C1—C2—C3	−179.24 (14)	C23—C14—C15—O2	178.26 (14)
C11—C1—C2—C3	3.0 (2)	C13—C14—C15—O2	1.3 (2)
C10—C1—C2—C7	0.6 (2)	C23—C14—C15—C16	−2.0 (2)
C11—C1—C2—C7	−177.12 (13)	C13—C14—C15—C16	−178.93 (14)
C7—C2—C3—C4	−0.2 (2)	O2—C15—C16—C17	179.75 (16)
C1—C2—C3—C4	179.62 (16)	C14—C15—C16—C17	0.0 (3)
C2—C3—C4—C5	−0.4 (3)	C15—C16—C17—C18	1.0 (3)
C3—C4—C5—C6	0.8 (3)	C16—C17—C18—C19	179.34 (18)
C4—C5—C6—C7	−0.4 (3)	C16—C17—C18—C23	0.1 (3)
C5—C6—C7—C2	−0.3 (3)	C17—C18—C19—C20	−177.14 (19)
C5—C6—C7—C8	−179.99 (18)	C23—C18—C19—C20	2.1 (3)
C3—C2—C7—C6	0.6 (2)	C18—C19—C20—C21	−0.4 (3)
C1—C2—C7—C6	−179.28 (15)	C19—C20—C21—C22	−1.3 (3)
C3—C2—C7—C8	−179.70 (14)	C20—C21—C22—C23	1.4 (3)
C1—C2—C7—C8	0.5 (2)	C21—C22—C23—C14	179.63 (16)
C6—C7—C8—C9	179.13 (18)	C21—C22—C23—C18	0.2 (2)
C2—C7—C8—C9	−0.6 (2)	C15—C14—C23—C22	−176.40 (15)
C7—C8—C9—C10	−0.3 (3)	C13—C14—C23—C22	0.5 (2)
C2—C1—C10—O1	178.20 (13)	C15—C14—C23—C18	3.0 (2)
C11—C1—C10—O1	−4.02 (19)	C13—C14—C23—C18	179.90 (13)
C2—C1—C10—C9	−1.5 (2)	C17—C18—C23—C22	177.33 (16)
C11—C1—C10—C9	176.24 (14)	C19—C18—C23—C22	−1.9 (2)
C8—C9—C10—O1	−178.31 (15)	C17—C18—C23—C14	−2.1 (2)

C8—C9—C10—C1	1.4 (3)	C19—C18—C23—C14	178.65 (16)
C10—C1—C11—N1	100.76 (16)	C1—C11—N1—C12	−173.60 (13)
C2—C1—C11—N1	−81.52 (17)	C1—C11—N1—C13	−50.84 (18)
N1—C13—C14—C15	−37.61 (19)	C14—C13—N1—C12	−70.89 (16)
N1—C13—C14—C23	145.50 (14)	C14—C13—N1—C11	167.19 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.84	2.633 (2)	164
O2—H2···N1	0.82	1.83	2.557 (2)	148
C6—H6···Cg2^{ii}	0.93	2.82	3.698 (3)	158
C19—H19···Cg1^{iii}	0.93	2.78	3.564 (2)	143

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*, −*z*.

Fig. 1

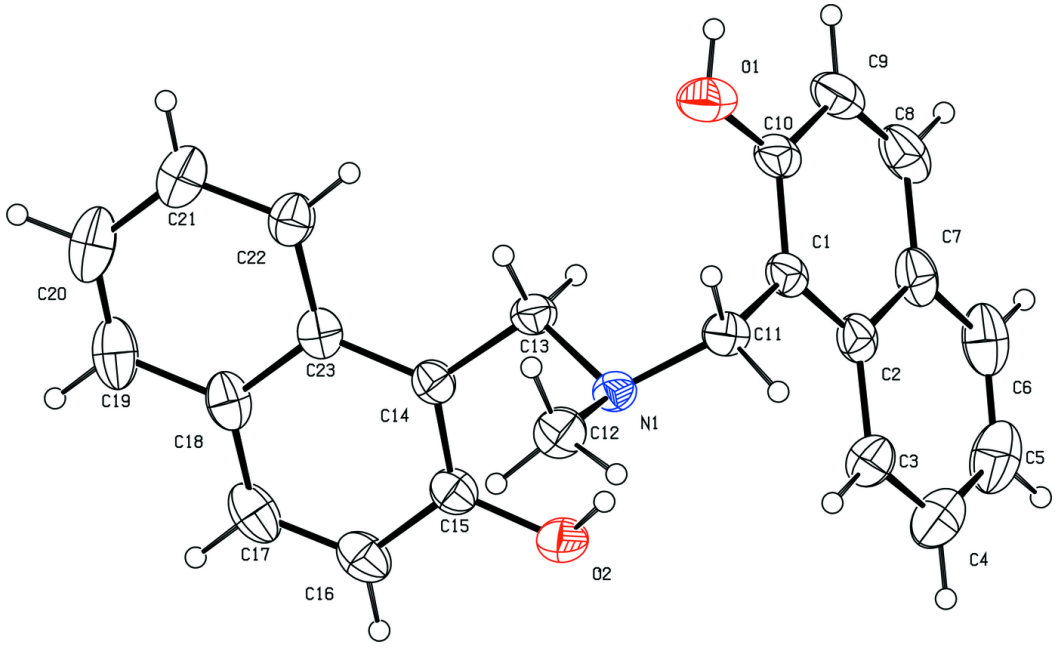
O1
C9
C10
C8
C1
C7
C11
C2
C6
C3
C5
C4
N1
C12
C13
C14
C15
O2
C16
C17
C18
C19
C20
C21
C22
C23

Fig. 2