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N,*N*′-Dimethyl-*N*,*N*′-diphenylnaphthalene-1,4-dicarboxamide

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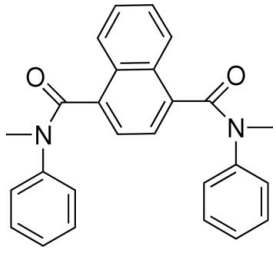
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.136; data-to-parameter ratio = 16.8.

In the title compound, $C_{26}H_{22}N_2O_2$, the two amide groups are twisted away from the attached naphthalene ring system by 63.94 (3) and 66.07 (3)°. The crystal packing is stabilized by C—H$\cdots\pi$ interactions.

Related literature

For applications of 1,4-naphthalenedicarboxylic acid derivatives, see: Fukuzumi *et al.* (1994); Tsukada *et al.* (1994). For related structures, see: Jing, Qin, Gu, Zhang & Lei (2006); Jing, Qin, Gu, Zhang & Mao (2006).



Experimental

Crystal data

$C_{26}H_{22}N_2O_2$
M_r = 394.46
Triclinic, $P\overline{1}$
a = 8.9970 (6) Å
b = 9.3627 (5) Å
c = 13.5538 (7) Å
α = 105.329 (1)°
β = 92.391 (2)°
γ = 111.656 (2)°
V = 1010.95 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 (2) K
0.55 × 0.33 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
9974 measured reflections
4593 independent reflections
3695 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.136
S = 1.00
4593 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 is the centroid of the C21–C26 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots$*Cg*1^{i}	0.95	2.82	3.614 (1)	142

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2482).

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supplementary materials

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N,*N*'-Dimethyl-*N*,*N*'-diphenylnaphthalene-1,4-dicarboxamide

L.-H. Jing and D.-B. Qin

Comment

1,4-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). Previously, we have reported the crystal structures of *N*,*N*'-bis(4-nitrophenyl)naphthalene-1,4-dicarboxamide dimethylsulfoxide disolvate (Jing, Qin, Gu, Zhang & Mao, 2006) and *N*,*N*'-bis(2-methoxyphenyl)naphthalene-1,4-dicarboxamide (Jing, Qin, Gu, Zhang & Lei, 2006). We now report the crystal structure of the title compound, (I).

The bond lengths and angles in (I) are normal. The naphthalene ring system is planar, with a maximum deviation of 0.017 (1) Å for atom C2. As a result of steric effects, two amide groups (O1/N1/C1/C11 and O2/N2/C4/C19) are twisted away from the naphthalene mean plane by 63.94 (3) and 66.07 (3)°, respectively (Fig. 1). The dihedral angle between the O1/N1/C1/C11 and C13—C18 planes is 65.80 (5)°, and that between the O2/N2/C4/C19 and C21—C26 planes is 56.36 (6)°. The crystal packing is stabilized by intermolecular C—H···π interactions involving the C21—C26 phenyl ring (centroid *Cg*1; Table 1).

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride (6 mmol) in dioxane (20 ml) were boiled under reflux for 6 h. The solution was distilled under reduced pressure and a yellow solid was formed. *N*-Methyl phenylamine (4 mmol) in tetrahydrofuran (20 ml) was added to the yellow solid and boiled under reflux for 1 d. The solution was then cooled to ambient temperature and filtered to remove the tetrahydrofuran. The precipitate was dissolved in dimethylsulfoxide and allowed to stand for one month at ambient temperature, after which time white single crystals of (I) suitable for X-ray diffraction were obtained.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.95 or 0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The methyl groups were allowed to rotate but not to tip.

Figures

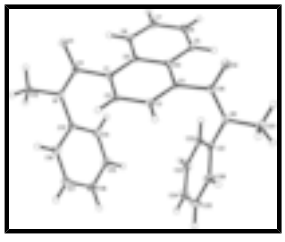


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

N,*N*'-Dimethyl-*N*,*N*'-diphenylnaphthalene-1,4- dicarboxamide

Crystal data

$C_{26}H_{22}N_2O_2$	$Z = 2$
$M_r = 394.46$	$F_{000} = 416$
Triclinic, $P\overline{1}$	$D_x = 1.296$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9970$ (6) Å	Cell parameters from 7714 reflections
$b = 9.3627$ (5) Å	$\theta = 3.1$–27.5º
$c = 13.5538$ (7) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 105.329$ (1)º	$T = 153$ (2) K
$\beta = 92.391$ (2)º	Block, colourless
$\gamma = 111.656$ (2)º	0.55 × 0.33 × 0.21 mm
$V = 1010.95$ (10) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	3695 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	$R_{int} = 0.017$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 153$(2) K	$\theta_{min} = 3.1$º
ω scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -12 \rightarrow 12$
9974 measured reflections	$l = -15 \rightarrow 17$
4593 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0828P)^2 + 0.279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.136$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.35$ e Å^{-3}
4593 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
274 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.017 (4)
Secondary atom site location: difference Fourier map	

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	0.78271 (13)	0.56379 (13)	−0.00270 (8)	0.0238 (2)
N2	0.77994 (13)	0.57326 (13)	0.52950 (8)	0.0258 (3)
O1	0.80460 (13)	0.32300 (11)	−0.03540 (7)	0.0323 (2)
O2	0.81029 (13)	0.33566 (11)	0.47733 (7)	0.0320 (2)
C1	0.78108 (15)	0.44480 (14)	0.13806 (9)	0.0211 (3)
C2	0.90138 (15)	0.56211 (14)	0.21448 (10)	0.0232 (3)
H2	0.9872	0.6429	0.1971	0.028*
C3	0.89866 (15)	0.56371 (14)	0.31845 (10)	0.0234 (3)
H3	0.9834	0.6451	0.3706	0.028*
C4	0.77506 (15)	0.44910 (14)	0.34541 (9)	0.0208 (3)
C5	0.51417 (15)	0.20772 (15)	0.29354 (10)	0.0239 (3)
H5	0.5098	0.2092	0.3637	0.029*
C6	0.39271 (16)	0.09150 (15)	0.21772 (11)	0.0281 (3)
H6	0.3048	0.0133	0.2356	0.034*
C7	0.39727 (16)	0.08714 (16)	0.11339 (11)	0.0281 (3)
H7	0.3130	0.0054	0.0612	0.034*
C8	0.52240 (15)	0.19998 (15)	0.08664 (10)	0.0239 (3)
H8	0.5236	0.1956	0.0159	0.029*
C9	0.65017 (14)	0.32318 (14)	0.16274 (9)	0.0201 (3)
C10	0.64688 (14)	0.32649 (13)	0.26882 (9)	0.0196 (3)
C11	0.79059 (15)	0.43809 (15)	0.02613 (10)	0.0228 (3)
C12	0.79649 (18)	0.56323 (18)	−0.11009 (10)	0.0314 (3)
H12A	0.9103	0.6186	−0.1159	0.038*
H12B	0.7331	0.6190	−0.1308	0.038*
H12C	0.7552	0.4518	−0.1554	0.038*
C13	0.78233 (16)	0.70820 (15)	0.06758 (10)	0.0233 (3)
C14	0.64906 (17)	0.70588 (17)	0.11556 (10)	0.0292 (3)
H14	0.5575	0.6077	0.1038	0.035*
C15	0.6503 (2)	0.84799 (19)	0.18088 (12)	0.0372 (4)
H15	0.5594	0.8469	0.2143	0.045*
C16	0.7831 (2)	0.99164 (19)	0.19777 (12)	0.0420 (4)
H16	0.7832	1.0887	0.2426	0.050*
C17	0.9154 (2)	0.99328 (18)	0.14922 (13)	0.0421 (4)

H17	1.0064	1.0918	0.1606	0.050*
C18	0.91587 (18)	0.85181 (16)	0.08391 (11)	0.0324 (3)
H18	1.0070	0.8531	0.0506	0.039*
C19	0.78729 (15)	0.44667 (15)	0.45572 (9)	0.0230 (3)
C20	0.81888 (19)	0.5865 (2)	0.63851 (10)	0.0377 (4)
H20A	0.7882	0.4784	0.6460	0.045*
H20B	0.7591	0.6420	0.6806	0.045*
H20C	0.9354	0.6478	0.6618	0.045*
C21	0.74327 (16)	0.69856 (15)	0.50824 (10)	0.0265 (3)
C22	0.60438 (17)	0.66366 (17)	0.44191 (11)	0.0298 (3)
H22	0.5337	0.5546	0.4088	0.036*
C23	0.5681 (2)	0.7869 (2)	0.42367 (14)	0.0452 (4)
H23	0.4733	0.7616	0.3776	0.054*
C24	0.6678 (3)	0.9448 (2)	0.47155 (18)	0.0592 (6)
H24	0.6428	1.0288	0.4584	0.071*
C25	0.8031 (3)	0.98039 (19)	0.53825 (18)	0.0631 (7)
H25	0.8711	1.0900	0.5720	0.076*
C26	0.8442 (2)	0.85844 (18)	0.55828 (14)	0.0451 (4)
H26	0.9387	0.8848	0.6049	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0268 (5)	0.0250 (5)	0.0212 (5)	0.0105 (4)	0.0082 (4)	0.0084 (4)
N2	0.0271 (6)	0.0300 (6)	0.0192 (5)	0.0122 (4)	0.0031 (4)	0.0043 (4)
O1	0.0445 (6)	0.0268 (5)	0.0272 (5)	0.0163 (4)	0.0127 (4)	0.0067 (4)
O2	0.0407 (6)	0.0317 (5)	0.0287 (5)	0.0183 (4)	0.0022 (4)	0.0120 (4)
C1	0.0233 (6)	0.0218 (6)	0.0223 (6)	0.0123 (5)	0.0060 (5)	0.0080 (5)
C2	0.0218 (6)	0.0202 (6)	0.0272 (6)	0.0072 (5)	0.0056 (5)	0.0080 (5)
C3	0.0223 (6)	0.0195 (6)	0.0259 (6)	0.0079 (5)	0.0019 (5)	0.0039 (5)
C4	0.0237 (6)	0.0199 (6)	0.0214 (6)	0.0119 (5)	0.0041 (5)	0.0055 (5)
C5	0.0258 (6)	0.0238 (6)	0.0238 (6)	0.0108 (5)	0.0081 (5)	0.0077 (5)
C6	0.0239 (6)	0.0236 (6)	0.0331 (7)	0.0059 (5)	0.0086 (5)	0.0072 (5)
C7	0.0230 (6)	0.0245 (6)	0.0297 (7)	0.0062 (5)	0.0010 (5)	0.0017 (5)
C8	0.0255 (6)	0.0247 (6)	0.0209 (6)	0.0112 (5)	0.0024 (5)	0.0040 (5)
C9	0.0208 (6)	0.0195 (6)	0.0219 (6)	0.0107 (5)	0.0044 (5)	0.0053 (5)
C10	0.0211 (6)	0.0184 (5)	0.0213 (6)	0.0107 (4)	0.0043 (4)	0.0047 (4)
C11	0.0210 (6)	0.0240 (6)	0.0220 (6)	0.0073 (5)	0.0049 (5)	0.0066 (5)
C12	0.0402 (8)	0.0383 (7)	0.0225 (6)	0.0190 (6)	0.0121 (6)	0.0139 (6)
C13	0.0280 (6)	0.0251 (6)	0.0216 (6)	0.0136 (5)	0.0045 (5)	0.0103 (5)
C14	0.0290 (7)	0.0358 (7)	0.0278 (7)	0.0162 (6)	0.0065 (5)	0.0123 (6)
C15	0.0438 (8)	0.0498 (9)	0.0317 (7)	0.0327 (7)	0.0111 (6)	0.0128 (7)
C16	0.0638 (11)	0.0347 (8)	0.0360 (8)	0.0318 (8)	0.0044 (7)	0.0065 (6)
C17	0.0513 (10)	0.0259 (7)	0.0440 (9)	0.0114 (6)	0.0032 (7)	0.0086 (6)
C18	0.0334 (7)	0.0295 (7)	0.0339 (7)	0.0103 (6)	0.0088 (6)	0.0116 (6)
C19	0.0212 (6)	0.0252 (6)	0.0215 (6)	0.0085 (5)	0.0017 (5)	0.0065 (5)
C20	0.0412 (8)	0.0539 (9)	0.0185 (6)	0.0246 (7)	0.0008 (6)	0.0037 (6)
C21	0.0293 (7)	0.0229 (6)	0.0264 (6)	0.0097 (5)	0.0135 (5)	0.0054 (5)

C22	0.0354 (7)	0.0320 (7)	0.0303 (7)	0.0181 (6)	0.0141 (6)	0.0139 (6)
C23	0.0608 (11)	0.0530 (10)	0.0519 (10)	0.0407 (9)	0.0329 (8)	0.0335 (8)
C24	0.0801 (15)	0.0446 (10)	0.0856 (15)	0.0423 (10)	0.0564 (13)	0.0394 (10)
C25	0.0787 (15)	0.0202 (7)	0.0832 (15)	0.0115 (8)	0.0504 (13)	0.0100 (8)
C26	0.0413 (9)	0.0280 (7)	0.0492 (9)	0.0028 (6)	0.0187 (7)	−0.0013 (7)

Geometric parameters (Å, °)

N1—C11	1.3583 (16)	C12—H12B	0.98
N1—C13	1.4347 (16)	C12—H12C	0.98
N1—C12	1.4647 (16)	C13—C14	1.3836 (19)
N2—C19	1.3587 (16)	C13—C18	1.3887 (18)
N2—C21	1.4229 (17)	C14—C15	1.385 (2)
N2—C20	1.4660 (17)	C14—H14	0.95
O1—C11	1.2273 (16)	C15—C16	1.384 (2)
O2—C19	1.2343 (15)	C15—H15	0.95
C1—C2	1.3704 (17)	C16—C17	1.381 (3)
C1—C9	1.4283 (16)	C16—H16	0.95
C1—C11	1.5091 (17)	C17—C18	1.387 (2)
C2—C3	1.4067 (18)	C17—H17	0.95
C2—H2	0.95	C18—H18	0.95
C3—C4	1.3719 (17)	C20—H20A	0.98
C3—H3	0.95	C20—H20B	0.98
C4—C10	1.4207 (16)	C20—H20C	0.98
C4—C19	1.5014 (17)	C21—C22	1.388 (2)
C5—C6	1.3681 (18)	C21—C26	1.3906 (19)
C5—C10	1.4230 (17)	C22—C23	1.386 (2)
C5—H5	0.95	C22—H22	0.95
C6—C7	1.4066 (19)	C23—C24	1.370 (3)
C6—H6	0.95	C23—H23	0.95
C7—C8	1.3688 (18)	C24—C25	1.364 (3)
C7—H7	0.95	C24—H24	0.95
C8—C9	1.4174 (17)	C25—C26	1.408 (3)
C8—H8	0.95	C25—H25	0.95
C9—C10	1.4317 (17)	C26—H26	0.95
C12—H12A	0.98		
C11—N1—C13	124.44 (10)	C14—C13—C18	120.41 (12)
C11—N1—C12	118.52 (11)	C14—C13—N1	120.69 (11)
C13—N1—C12	116.55 (10)	C18—C13—N1	118.86 (12)
C19—N2—C21	124.32 (11)	C13—C14—C15	119.45 (13)
C19—N2—C20	118.31 (11)	C13—C14—H14	120.3
C21—N2—C20	117.32 (11)	C15—C14—H14	120.3
C2—C1—C9	120.60 (11)	C16—C15—C14	120.51 (14)
C2—C1—C11	120.02 (11)	C16—C15—H15	119.7
C9—C1—C11	119.30 (11)	C14—C15—H15	119.7
C1—C2—C3	120.47 (11)	C17—C16—C15	119.75 (14)
C1—C2—H2	119.8	C17—C16—H16	120.1
C3—C2—H2	119.8	C15—C16—H16	120.1
C4—C3—C2	120.75 (11)	C16—C17—C18	120.32 (15)

C4—C3—H3	119.6	C16—C17—H17	119.8
C2—C3—H3	119.6	C18—C17—H17	119.8
C3—C4—C10	120.63 (11)	C17—C18—C13	119.55 (14)
C3—C4—C19	118.30 (11)	C17—C18—H18	120.2
C10—C4—C19	120.79 (11)	C13—C18—H18	120.2
C6—C5—C10	120.94 (12)	O2—C19—N2	122.19 (12)
C6—C5—H5	119.5	O2—C19—C4	120.00 (11)
C10—C5—H5	119.5	N2—C19—C4	117.74 (11)
C5—C6—C7	120.34 (12)	N2—C20—H20A	109.5
C5—C6—H6	119.8	N2—C20—H20B	109.5
C7—C6—H6	119.8	H20A—C20—H20B	109.5
C8—C7—C6	120.41 (12)	N2—C20—H20C	109.5
C8—C7—H7	119.8	H20A—C20—H20C	109.5
C6—C7—H7	119.8	H20B—C20—H20C	109.5
C7—C8—C9	121.13 (12)	C22—C21—C26	119.48 (14)
C7—C8—H8	119.4	C22—C21—N2	120.95 (11)
C9—C8—H8	119.4	C26—C21—N2	119.50 (14)
C8—C9—C1	122.74 (11)	C23—C22—C21	120.40 (15)
C8—C9—C10	118.54 (11)	C23—C22—H22	119.8
C1—C9—C10	118.72 (11)	C21—C22—H22	119.8
C4—C10—C5	122.54 (11)	C24—C23—C22	120.59 (18)
C4—C10—C9	118.83 (11)	C24—C23—H23	119.7
C5—C10—C9	118.63 (11)	C22—C23—H23	119.7
O1—C11—N1	122.12 (11)	C25—C24—C23	119.46 (17)
O1—C11—C1	120.70 (11)	C25—C24—H24	120.3
N1—C11—C1	117.18 (10)	C23—C24—H24	120.3
N1—C12—H12A	109.5	C24—C25—C26	121.53 (16)
N1—C12—H12B	109.5	C24—C25—H25	119.2
H12A—C12—H12B	109.5	C26—C25—H25	119.2
N1—C12—H12C	109.5	C21—C26—C25	118.52 (19)
H12A—C12—H12C	109.5	C21—C26—H26	120.7
H12B—C12—H12C	109.5	C25—C26—H26	120.7
C9—C1—C2—C3	0.62 (18)	C11—N1—C13—C14	−70.76 (17)
C11—C1—C2—C3	−176.18 (11)	C12—N1—C13—C14	117.40 (13)
C1—C2—C3—C4	−0.63 (19)	C11—N1—C13—C18	111.51 (14)
C2—C3—C4—C10	−0.15 (18)	C12—N1—C13—C18	−60.33 (16)
C2—C3—C4—C19	173.82 (11)	C18—C13—C14—C15	−0.5 (2)
C10—C5—C6—C7	0.19 (19)	N1—C13—C14—C15	−178.25 (12)
C5—C6—C7—C8	−0.6 (2)	C13—C14—C15—C16	0.4 (2)
C6—C7—C8—C9	0.2 (2)	C14—C15—C16—C17	−0.1 (2)
C7—C8—C9—C1	−178.76 (12)	C15—C16—C17—C18	−0.1 (2)
C7—C8—C9—C10	0.67 (18)	C16—C17—C18—C13	0.0 (2)
C2—C1—C9—C8	179.58 (11)	C14—C13—C18—C17	0.3 (2)
C11—C1—C9—C8	−3.59 (18)	N1—C13—C18—C17	178.08 (13)
C2—C1—C9—C10	0.16 (17)	C21—N2—C19—O2	−175.71 (12)
C11—C1—C9—C10	176.98 (10)	C20—N2—C19—O2	7.03 (19)
C3—C4—C10—C5	−178.34 (11)	C21—N2—C19—C4	7.42 (18)
C19—C4—C10—C5	7.84 (17)	C20—N2—C19—C4	−169.84 (12)
C3—C4—C10—C9	0.91 (17)	C3—C4—C19—O2	−109.93 (14)

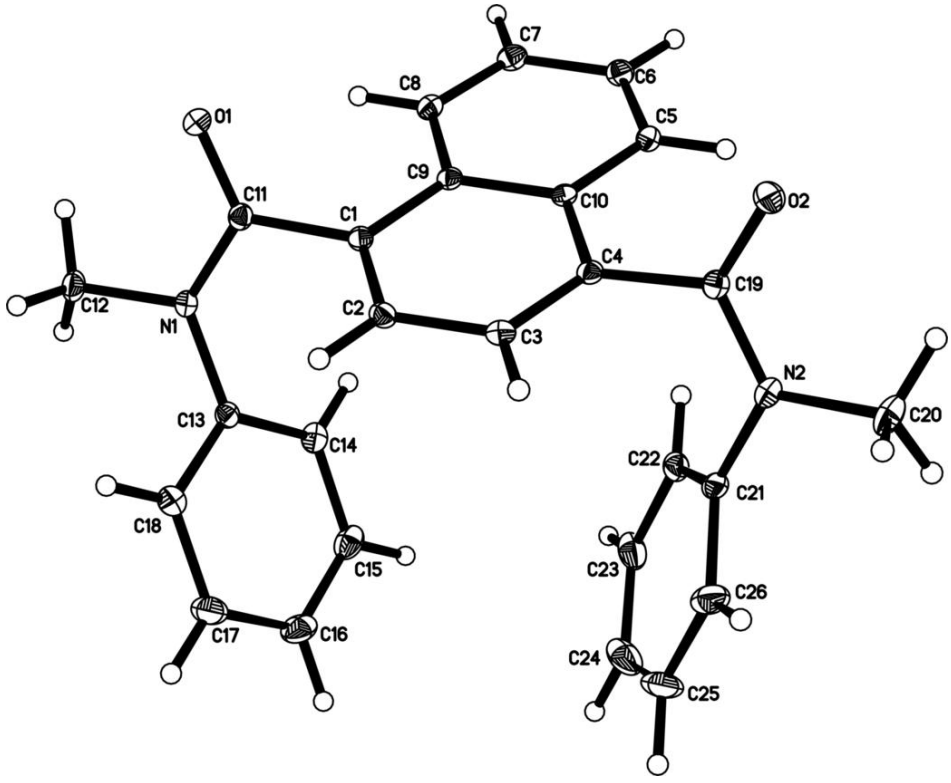
C19—C4—C10—C9	−172.90 (10)	C10—C4—C19—O2	64.03 (16)
C6—C5—C10—C4	179.92 (12)	C3—C4—C19—N2	67.01 (15)
C6—C5—C10—C9	0.66 (18)	C10—C4—C19—N2	−119.03 (13)
C8—C9—C10—C4	179.64 (10)	C19—N2—C21—C22	53.51 (18)
C1—C9—C10—C4	−0.91 (16)	C20—N2—C21—C22	−129.20 (14)
C8—C9—C10—C5	−1.07 (17)	C19—N2—C21—C26	−129.46 (14)
C1—C9—C10—C5	178.38 (10)	C20—N2—C21—C26	47.84 (17)
C13—N1—C11—O1	−173.60 (12)	C26—C21—C22—C23	1.5 (2)
C12—N1—C11—O1	−1.91 (18)	N2—C21—C22—C23	178.52 (12)
C13—N1—C11—C1	6.50 (17)	C21—C22—C23—C24	−0.7 (2)
C12—N1—C11—C1	178.19 (11)	C22—C23—C24—C25	−0.5 (3)
C2—C1—C11—O1	115.16 (14)	C23—C24—C25—C26	0.8 (3)
C9—C1—C11—O1	−61.68 (16)	C22—C21—C26—C25	−1.2 (2)
C2—C1—C11—N1	−64.93 (16)	N2—C21—C26—C25	−178.23 (13)
C9—C1—C11—N1	118.22 (12)	C24—C25—C26—C21	0.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Cg1^{i}	0.95	2.82	3.614 (1)	142

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

Fig. 1


C7
C6
C8
C5
O1
C9
C11
C10
O2
C1
C4
C12
C19
N1
C2
C3
N2
C20
C13
C14
C22
C21
C18
C15
C23
C26
C17
C16
C24
C25