

2-Benzyl-6-(benzylamino)-1*H*-benzo- [de]isoquinoline-1,3(2*H*)-dione

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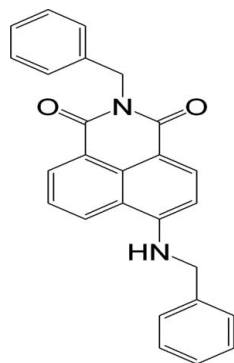
Received 11 September 2007; accepted 11 October 2007

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.051; wR factor = 0.136; data-to-parameter ratio = 13.3.

The title compound, $\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}_2$, is a 1,8-naphthalimide derivative. Molecules are arranged into stacks *via* π - π interactions between the naphthalimide systems, with interplanar distances of 3.379 (2) and 3.630 (2) Å. In addition, the crystal structure is stabilized by weak intermolecular C—H...O interactions.

Related literature

For related literature, see: Konstantinova *et al.* (2000); Mitchell *et al.* (1998); Sarma *et al.* (2007); Xu *et al.* (2004).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}_2$	$\gamma = 69.065$ (4)°
$M_r = 392.44$	$V = 984.1$ (5) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.354$ (2) Å	Mo $K\alpha$ radiation
$b = 10.314$ (3) Å	$\mu = 0.08$ mm ⁻¹
$c = 12.503$ (3) Å	$T = 298$ (2) K
$\alpha = 78.068$ (4)°	$0.27 \times 0.23 \times 0.14$ mm
$\beta = 87.225$ (4)°	

Data collection

Rigaku Mercury diffractometer	5185 measured reflections
Absorption correction: multi-scan (Jacobson, 1998)	3602 independent reflections
$T_{\min} = 0.978$, $T_{\max} = 0.988$	2545 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$	271 parameters
$wR(F^2) = 0.136$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.16$ e Å ⁻³
3602 reflections	$\Delta\rho_{\text{min}} = -0.15$ e Å ⁻³

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13B...O2	0.97	2.35	2.709 (2)	101
C17—H17...O2 ⁱ	0.93	2.49	3.287 (3)	144
C19—H19...O2	0.93	2.60	3.298 (3)	133
C22—H22...O1 ⁱⁱ	0.93	2.52	3.430 (3)	165
C24—H24...O2 ⁱⁱⁱ	0.93	2.51	3.407 (3)	162

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

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (grant Nos. 20362002, 20442005 and 20762001), the 100 Young and Middle-aged Disciplinary Leaders in Guangxi Higher Education Institutions and the Science Foundation of Guangxi Province (grant No. 0575046), as well as the Foundation of Guangxi Universities of the People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2103).

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supplementary materials

Acta Cryst. (2007). E63, o4336 [doi:10.1107/S1600536807049975]

2-Benzyl-6-(benzylamino)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione

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Comment

Since that the naphthalimide derivatives have been used as important dyes (Konstantinova *et al.*, 2000), fluorescent tags (Mitchell *et al.*, 1998) and photochemical DNA cleaving reagents (Xu *et al.*, 2004), the synthesis of naphthalimides has attracted a great deal of attention. Here we report the synthesis and crystal structure of a new naphthalimide derivative.

The molecular structure of the title compound is shown in Fig.1. The molecular geometry is comparable with that of 2-benzyl-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (Sarma *et al.*, 2007). The 1, 8-naphthalimide unit are almost planar.

Weak intermolecular C—H \cdots O hydrogen bonds and π - π stacking interactions stabilize the crystal packing (Fig. 2).

Experimental

The mixture of 4-bromo-1,8-naphthalic anhydride (0.28 g, 1 mmol), benzylamine (0.25 g, 2.3 mmol) and copper nitrate trihydrate (0.021 g, 0.1 mmol) was refluxed in ethylene glycol monomethyl ether (30 ml) for about 10 h, and cooled to afford the yellow powder of the title compound. Upon recrystallization from ethanol, yellow crystals were obtained (yield 46%, m.p. 428–430 K).

Refinement

H atoms bound to C atoms were positioned geometrically and included in the refinement in the riding-model approximation [$d(\text{C—H}) = 0.95$ and 0.99 Å for aromatic and CH_2 groups, respectively; $d(\text{N—H}) = 0.87$ Å], and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Figures

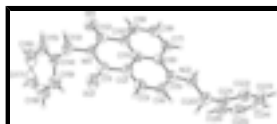


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom labelling scheme. H atoms are represented by small spheres of arbitrary radius.

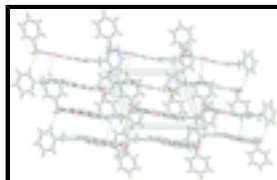


Fig. 2. Packing diagram with H bonds indicated by dashed lines.

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Crystal data

$C_{26}H_{20}N_2O_2$	$Z = 2$
$M_r = 392.44$	$F_{000} = 412$
Triclinic, $P\bar{1}$	$D_x = 1.324 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.354 (2) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 10.314 (3) \text{ \AA}$	Cell parameters from 1545 reflections
$c = 12.503 (3) \text{ \AA}$	$\theta = 2.5\text{--}26.6^\circ$
$\alpha = 78.068 (4)^\circ$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 87.225 (4)^\circ$	$T = 298 (2) \text{ K}$
$\gamma = 69.065 (4)^\circ$	Prism, yellow
$V = 984.1 (5) \text{ \AA}^3$	$0.27 \times 0.23 \times 0.14 \text{ mm}$

Data collection

Rigaku Mercury diffractometer	3602 independent reflections
Radiation source: fine-focus sealed tube	2545 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.017$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (Jacobson, 1998)	$h = -6 \rightarrow 10$
$T_{\text{min}} = 0.978, T_{\text{max}} = 0.988$	$k = -11 \rightarrow 12$
5185 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.0186P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
3602 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
271 parameters	$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
	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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2622 (2)	0.59547 (19)	0.71932 (14)	0.0512 (5)
C2	0.2342 (2)	0.49746 (18)	0.81289 (13)	0.0477 (4)
C3	0.1932 (2)	0.3848 (2)	0.79810 (14)	0.0578 (5)
H3	0.1755	0.3763	0.7274	0.069*
C4	0.1775 (3)	0.2837 (2)	0.88512 (14)	0.0594 (5)
H4	0.1497	0.2087	0.8718	0.071*
C5	0.2025 (2)	0.29171 (18)	0.99235 (13)	0.0491 (4)
C6	0.2351 (2)	0.41232 (17)	1.01200 (13)	0.0444 (4)
C7	0.2521 (2)	0.43494 (19)	1.11711 (13)	0.0517 (5)
H7	0.2387	0.3706	1.1778	0.062*
C8	0.2876 (3)	0.54894 (19)	1.13225 (14)	0.0591 (5)
H8	0.2980	0.5618	1.2027	0.071*
C9	0.3086 (2)	0.64652 (19)	1.04242 (15)	0.0568 (5)
H9	0.3353	0.7231	1.0533	0.068*
C10	0.2900 (2)	0.63026 (17)	0.93806 (13)	0.0470 (4)
C11	0.2517 (2)	0.51367 (17)	0.92052 (13)	0.0433 (4)
C12	0.3131 (2)	0.73448 (19)	0.84477 (15)	0.0525 (5)
C13	0.3202 (2)	0.81558 (18)	0.64637 (14)	0.0573 (5)
H13A	0.2690	0.9099	0.6620	0.069*
H13B	0.2606	0.8130	0.5826	0.069*
C14	0.5053 (2)	0.78830 (18)	0.62048 (13)	0.0507 (5)
C15	0.5796 (3)	0.8849 (2)	0.63119 (16)	0.0697 (6)
H15	0.5142	0.9672	0.6550	0.084*
C16	0.7474 (4)	0.8621 (3)	0.60742 (19)	0.0871 (8)
H16	0.7951	0.9286	0.6149	0.105*
C17	0.8459 (3)	0.7410 (3)	0.57247 (18)	0.0887 (8)
H17	0.9607	0.7247	0.5570	0.106*
C18	0.7732 (3)	0.6437 (3)	0.56048 (18)	0.0822 (7)
H18	0.8387	0.5617	0.5363	0.099*
C19	0.6045 (3)	0.6681 (2)	0.58416 (16)	0.0643 (5)
H19	0.5562	0.6023	0.5756	0.077*
C20	0.1766 (3)	0.0588 (2)	1.06164 (15)	0.0712 (6)
H20A	0.2599	0.0172	1.0101	0.085*

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H20B	0.0630	0.0818	1.0309	0.085*
C21	0.2003 (3)	-0.04668 (19)	1.16736 (14)	0.0555 (5)
C22	0.0616 (3)	-0.0690 (2)	1.22008 (15)	0.0632 (5)
H22	-0.0481	-0.0169	1.1904	0.076*
C23	0.0825 (3)	-0.1670 (2)	1.31597 (17)	0.0731 (6)
H23	-0.0128	-0.1805	1.3509	0.088*
C24	0.2425 (4)	-0.2446 (2)	1.36027 (17)	0.0772 (7)
H24	0.2564	-0.3111	1.4252	0.093*
C25	0.3827 (3)	-0.2244 (2)	1.30889 (18)	0.0779 (7)
H25	0.4920	-0.2773	1.3389	0.093*
C26	0.3621 (3)	-0.1256 (2)	1.21254 (16)	0.0684 (6)
H26	0.4577	-0.1122	1.1779	0.082*
N1	0.29555 (19)	0.71192 (14)	0.74032 (11)	0.0503 (4)
N2	0.1971 (2)	0.18745 (15)	1.07740 (11)	0.0610 (5)
H2	0.2061	0.1982	1.1430	0.073*
O1	0.34627 (19)	0.83731 (13)	0.85503 (10)	0.0699 (4)
O2	0.25983 (18)	0.58088 (14)	0.62488 (9)	0.0659 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0489 (11)	0.0597 (11)	0.0461 (10)	-0.0226 (9)	-0.0022 (8)	-0.0061 (8)
C2	0.0472 (11)	0.0534 (10)	0.0436 (9)	-0.0210 (9)	-0.0011 (8)	-0.0061 (8)
C3	0.0690 (14)	0.0725 (12)	0.0411 (10)	-0.0367 (11)	-0.0038 (9)	-0.0097 (9)
C4	0.0766 (14)	0.0662 (12)	0.0499 (11)	-0.0426 (11)	-0.0026 (9)	-0.0107 (9)
C5	0.0501 (11)	0.0532 (10)	0.0458 (10)	-0.0223 (9)	-0.0007 (8)	-0.0061 (8)
C6	0.0402 (10)	0.0487 (9)	0.0432 (9)	-0.0145 (8)	0.0012 (7)	-0.0095 (7)
C7	0.0569 (12)	0.0553 (10)	0.0413 (10)	-0.0190 (10)	0.0049 (8)	-0.0090 (8)
C8	0.0768 (14)	0.0615 (11)	0.0433 (10)	-0.0257 (11)	0.0048 (9)	-0.0188 (9)
C9	0.0698 (14)	0.0476 (10)	0.0556 (11)	-0.0185 (10)	0.0049 (9)	-0.0207 (9)
C10	0.0469 (11)	0.0445 (9)	0.0463 (10)	-0.0115 (8)	0.0029 (8)	-0.0111 (8)
C11	0.0368 (10)	0.0458 (9)	0.0452 (9)	-0.0122 (8)	0.0010 (7)	-0.0087 (7)
C12	0.0526 (12)	0.0448 (10)	0.0555 (11)	-0.0117 (9)	0.0039 (9)	-0.0107 (8)
C13	0.0657 (13)	0.0480 (10)	0.0511 (11)	-0.0179 (10)	0.0007 (9)	0.0015 (8)
C14	0.0622 (13)	0.0512 (10)	0.0387 (9)	-0.0243 (10)	-0.0013 (8)	-0.0010 (8)
C15	0.0874 (17)	0.0710 (13)	0.0614 (13)	-0.0424 (13)	0.0019 (11)	-0.0108 (10)
C16	0.095 (2)	0.120 (2)	0.0694 (15)	-0.0721 (19)	0.0012 (13)	-0.0072 (14)
C17	0.0613 (16)	0.143 (3)	0.0605 (14)	-0.0467 (18)	0.0057 (11)	0.0000 (15)
C18	0.0653 (16)	0.0978 (18)	0.0756 (15)	-0.0195 (15)	0.0112 (12)	-0.0200 (13)
C19	0.0647 (14)	0.0652 (12)	0.0647 (12)	-0.0246 (11)	0.0037 (10)	-0.0145 (10)
C20	0.1121 (19)	0.0646 (12)	0.0507 (11)	-0.0492 (13)	0.0010 (11)	-0.0089 (9)
C21	0.0787 (15)	0.0487 (10)	0.0465 (10)	-0.0296 (11)	0.0021 (10)	-0.0134 (8)
C22	0.0721 (15)	0.0583 (12)	0.0602 (12)	-0.0228 (11)	0.0038 (10)	-0.0151 (10)
C23	0.0967 (19)	0.0731 (14)	0.0591 (13)	-0.0431 (14)	0.0204 (12)	-0.0151 (11)
C24	0.128 (2)	0.0574 (13)	0.0464 (11)	-0.0338 (15)	0.0044 (14)	-0.0089 (9)
C25	0.0922 (18)	0.0687 (14)	0.0629 (13)	-0.0132 (13)	-0.0133 (13)	-0.0161 (11)
C26	0.0743 (15)	0.0782 (14)	0.0596 (12)	-0.0333 (13)	0.0089 (11)	-0.0194 (11)
N1	0.0542 (10)	0.0476 (8)	0.0455 (8)	-0.0172 (8)	0.0004 (7)	-0.0029 (6)

N2	0.0911 (13)	0.0584 (9)	0.0430 (8)	-0.0393 (9)	0.0003 (8)	-0.0078 (7)
O1	0.0988 (12)	0.0489 (7)	0.0684 (9)	-0.0333 (8)	0.0052 (8)	-0.0136 (6)
O2	0.0870 (11)	0.0811 (9)	0.0396 (7)	-0.0448 (9)	-0.0036 (6)	-0.0057 (6)

Geometric parameters (Å, °)

C1—O2	1.223 (2)	C14—C19	1.376 (3)
C1—N1	1.402 (2)	C14—C15	1.379 (2)
C1—C2	1.449 (2)	C15—C16	1.364 (3)
C2—C3	1.371 (2)	C15—H15	0.9300
C2—C11	1.411 (2)	C16—C17	1.372 (3)
C3—C4	1.380 (2)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.380 (3)
C4—C5	1.390 (2)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.369 (3)
C5—N2	1.359 (2)	C18—H18	0.9300
C5—C6	1.434 (2)	C19—H19	0.9300
C6—C7	1.404 (2)	C20—N2	1.450 (2)
C6—C11	1.419 (2)	C20—C21	1.499 (2)
C7—C8	1.361 (2)	C20—H20A	0.9700
C7—H7	0.9300	C20—H20B	0.9700
C8—C9	1.394 (2)	C21—C22	1.372 (3)
C8—H8	0.9300	C21—C26	1.381 (3)
C9—C10	1.372 (2)	C22—C23	1.372 (3)
C9—H9	0.9300	C22—H22	0.9300
C10—C11	1.410 (2)	C23—C24	1.363 (3)
C10—C12	1.470 (2)	C23—H23	0.9300
C12—O1	1.219 (2)	C24—C25	1.369 (3)
C12—N1	1.396 (2)	C24—H24	0.9300
C13—N1	1.4765 (19)	C25—C26	1.381 (3)
C13—C14	1.501 (3)	C25—H25	0.9300
C13—H13A	0.9700	C26—H26	0.9300
C13—H13B	0.9700	N2—H2	0.8600
O2—C1—N1	119.24 (15)	C16—C15—C14	121.2 (2)
O2—C1—C2	123.69 (17)	C16—C15—H15	119.4
N1—C1—C2	117.07 (15)	C14—C15—H15	119.4
C3—C2—C11	118.65 (15)	C15—C16—C17	120.2 (2)
C3—C2—C1	120.19 (16)	C15—C16—H16	119.9
C11—C2—C1	121.14 (16)	C17—C16—H16	119.9
C2—C3—C4	121.88 (16)	C16—C17—C18	119.4 (2)
C2—C3—H3	119.1	C16—C17—H17	120.3
C4—C3—H3	119.1	C18—C17—H17	120.3
C3—C4—C5	121.24 (17)	C19—C18—C17	119.9 (2)
C3—C4—H4	119.4	C19—C18—H18	120.0
C5—C4—H4	119.4	C17—C18—H18	120.0
N2—C5—C4	121.01 (16)	C18—C19—C14	121.1 (2)
N2—C5—C6	120.23 (15)	C18—C19—H19	119.5
C4—C5—C6	118.76 (15)	C14—C19—H19	119.5
C7—C6—C11	118.34 (16)	N2—C20—C21	111.32 (15)

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C7—C6—C5	123.34 (16)	N2—C20—H20A	109.4
C11—C6—C5	118.32 (15)	C21—C20—H20A	109.4
C8—C7—C6	121.49 (16)	N2—C20—H20B	109.4
C8—C7—H7	119.3	C21—C20—H20B	109.4
C6—C7—H7	119.3	H20A—C20—H20B	108.0
C7—C8—C9	120.20 (17)	C22—C21—C26	118.61 (18)
C7—C8—H8	119.9	C22—C21—C20	120.6 (2)
C9—C8—H8	119.9	C26—C21—C20	120.8 (2)
C10—C9—C8	120.39 (17)	C23—C22—C21	120.9 (2)
C10—C9—H9	119.8	C23—C22—H22	119.5
C8—C9—H9	119.8	C21—C22—H22	119.5
C9—C10—C11	120.33 (16)	C24—C23—C22	120.2 (2)
C9—C10—C12	119.31 (16)	C24—C23—H23	119.9
C11—C10—C12	120.35 (16)	C22—C23—H23	119.9
C10—C11—C2	119.83 (15)	C23—C24—C25	119.8 (2)
C10—C11—C6	119.21 (15)	C23—C24—H24	120.1
C2—C11—C6	120.94 (16)	C25—C24—H24	120.1
O1—C12—N1	119.74 (16)	C24—C25—C26	120.1 (2)
O1—C12—C10	123.19 (17)	C24—C25—H25	119.9
N1—C12—C10	117.07 (16)	C26—C25—H25	119.9
N1—C13—C14	113.22 (14)	C25—C26—C21	120.3 (2)
N1—C13—H13A	108.9	C25—C26—H26	119.8
C14—C13—H13A	108.9	C21—C26—H26	119.8
N1—C13—H13B	108.9	C12—N1—C1	124.40 (14)
C14—C13—H13B	108.9	C12—N1—C13	117.28 (14)
H13A—C13—H13B	107.7	C1—N1—C13	118.28 (14)
C19—C14—C15	118.26 (19)	C5—N2—C20	122.42 (15)
C19—C14—C13	121.24 (17)	C5—N2—H2	118.8
C15—C14—C13	120.49 (18)	C20—N2—H2	118.8
O2—C1—C2—C3	-3.7 (3)	C11—C10—C12—N1	-0.1 (3)
N1—C1—C2—C3	177.04 (15)	N1—C13—C14—C19	65.5 (2)
O2—C1—C2—C11	174.97 (17)	N1—C13—C14—C15	-115.45 (18)
N1—C1—C2—C11	-4.3 (3)	C19—C14—C15—C16	-0.5 (3)
C11—C2—C3—C4	-3.4 (3)	C13—C14—C15—C16	-179.64 (18)
C1—C2—C3—C4	175.33 (18)	C14—C15—C16—C17	-0.2 (3)
C2—C3—C4—C5	0.1 (3)	C15—C16—C17—C18	0.7 (3)
C3—C4—C5—N2	-176.01 (18)	C16—C17—C18—C19	-0.5 (3)
C3—C4—C5—C6	3.7 (3)	C17—C18—C19—C14	-0.3 (3)
N2—C5—C6—C7	-4.1 (3)	C15—C14—C19—C18	0.8 (3)
C4—C5—C6—C7	176.14 (17)	C13—C14—C19—C18	179.89 (18)
N2—C5—C6—C11	175.62 (16)	N2—C20—C21—C22	104.6 (2)
C4—C5—C6—C11	-4.1 (3)	N2—C20—C21—C26	-76.8 (2)
C11—C6—C7—C8	-1.6 (3)	C26—C21—C22—C23	0.3 (3)
C5—C6—C7—C8	178.19 (17)	C20—C21—C22—C23	178.92 (17)
C6—C7—C8—C9	-0.2 (3)	C21—C22—C23—C24	-0.3 (3)
C7—C8—C9—C10	1.4 (3)	C22—C23—C24—C25	0.1 (3)
C8—C9—C10—C11	-0.8 (3)	C23—C24—C25—C26	0.1 (3)
C8—C9—C10—C12	-179.88 (17)	C24—C25—C26—C21	0.0 (3)
C9—C10—C11—C2	-179.52 (16)	C22—C21—C26—C25	-0.2 (3)

C12—C10—C11—C2	-0.5 (3)	C20—C21—C26—C25	-178.77 (18)
C9—C10—C11—C6	-1.0 (3)	O1—C12—N1—C1	178.24 (17)
C12—C10—C11—C6	178.12 (16)	C10—C12—N1—C1	-1.8 (3)
C3—C2—C11—C10	-178.62 (16)	O1—C12—N1—C13	0.6 (2)
C1—C2—C11—C10	2.7 (3)	C10—C12—N1—C13	-179.45 (15)
C3—C2—C11—C6	2.8 (3)	O2—C1—N1—C12	-175.40 (16)
C1—C2—C11—C6	-175.87 (16)	C2—C1—N1—C12	3.9 (3)
C7—C6—C11—C10	2.1 (3)	O2—C1—N1—C13	2.3 (2)
C5—C6—C11—C10	-177.67 (15)	C2—C1—N1—C13	-178.47 (15)
C7—C6—C11—C2	-179.35 (15)	C14—C13—N1—C12	82.09 (19)
C5—C6—C11—C2	0.9 (3)	C14—C13—N1—C1	-95.74 (19)
C9—C10—C12—O1	-1.0 (3)	C4—C5—N2—C20	4.1 (3)
C11—C10—C12—O1	179.94 (16)	C6—C5—N2—C20	-175.57 (18)
C9—C10—C12—N1	179.02 (16)	C21—C20—N2—C5	171.73 (18)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C13—H13B \cdots O2	0.97	2.35	2.709 (2)	101
C17—H17 \cdots O2 ⁱ	0.93	2.49	3.287 (3)	144
C19—H19 \cdots O2	0.93	2.60	3.298 (3)	133
C22—H22 \cdots O1 ⁱⁱ	0.93	2.52	3.430 (3)	165
C24—H24 \cdots O2 ⁱⁱⁱ	0.93	2.51	3.407 (3)	162

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

Fig. 1

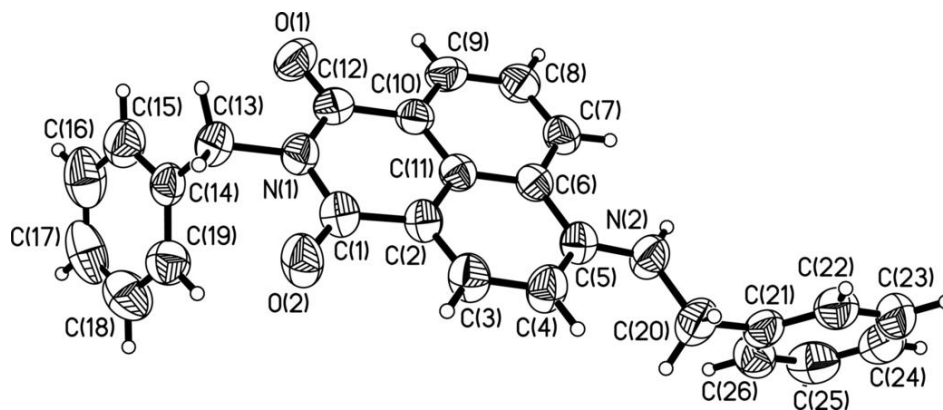


Fig. 2

