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Key indicators

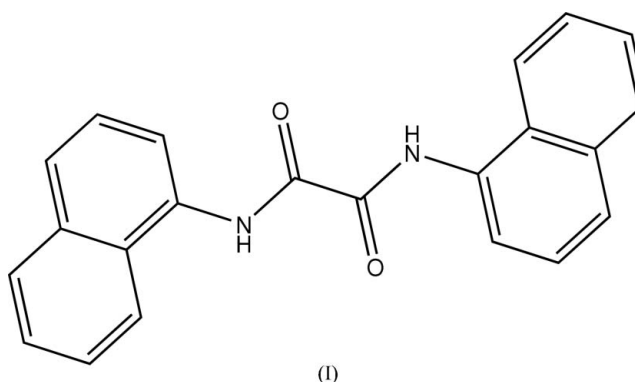
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.057
 wR factor = 0.157
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N,N'*-Di-1-naphthyloxamide

The molecule of the title compound, $\text{C}_{22}\text{H}_{16}\text{N}_2\text{O}_2$, lies on a crystallographically imposed center of symmetry at the midpoint of the C—C bond of the oxamide unit. In the crystal structure, intermolecular C—H···O and N—H···O hydrogen bonds link the molecules into ribbons along the c axis. The packing is further stabilized by C—H··· π interactions.

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Comment

In our ongoing studies of oxamide derivatives, the title compound, (I), was obtained. We report here its synthesis and crystal structure.



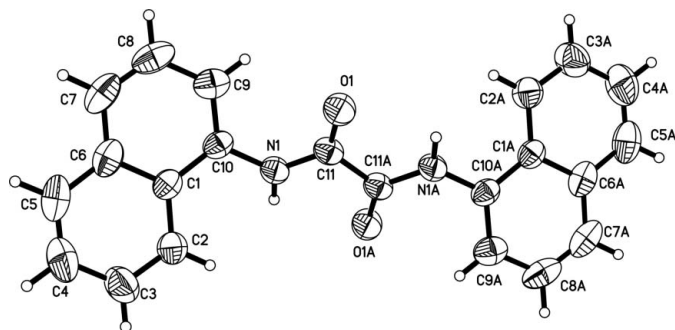
In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It has a crystallographically imposed center of symmetry at the mid-point of the C11—C11ⁱ bond [symmetry code: (i) $-x, 2 - y, 1 - z$] and an intramolecular C9—H9A···O1 hydrogen bond (Table 1) forms a six-membered ring.

The dihedral angle between the two benzene rings is $2.17(4)^\circ$. The naphthalene ring system and the O1/N1/C10/C11/O1ⁱ/N1ⁱ/C10ⁱ/C11ⁱ unit [symmetry code: (i) $-x, 2 - y, 1 - z$] are each nearly planar, having total puckering amplitudes, Q_T , of 0.0614 (3) and 0.0589 (4) Å, respectively (Cremer & Pople, 1975); the dihedral angle between them is $40.9(1)^\circ$.

As can be seen from the packing diagram (Fig. 2), intermolecular C—H···O and N—H···O hydrogen bonds (Table 1) link the molecules into ribbons along the c axis. The packing is further stabilized by C—H··· π interactions.

Experimental

To a solution of 1-naphthylamine (28.6 g, 0.2 mol) in benzene (70 ml) was added dropwise a solution of oxalyl chloride (6.4 g, 0.05 mol) in benzene (30 ml), and the mixture was stirred at 343 K for 6 h. After


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code $(-x, 2 - y, 1 - z)$.

cooling to room temperature, 50 ml of water was added to the reaction mixture and the organic phase was washed three times with water to give a solid. The title compound was obtained after drying the solid at room temperature for 3 d. Colorless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dimethylformamide solution over a period of 5 d.

Crystal data

$C_{22}H_{16}N_2O_2$
 $M_r = 340.37$
 Monoclinic, $P2_1/c$
 $a = 14.351$ (5) Å
 $b = 6.105$ (2) Å
 $c = 9.639$ (4) Å
 $\beta = 91.798$ (6)°
 $V = 844.1$ (5) Å³

$Z = 2$
 $D_x = 1.339$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 294$ (2) K
 Block, colorless
 $0.41 \times 0.25 \times 0.07$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.965$, $T_{\max} = 0.994$

4238 measured reflections
 1643 independent reflections
 993 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.157$
 $S = 1.04$
 1643 reflections
 118 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.0595P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

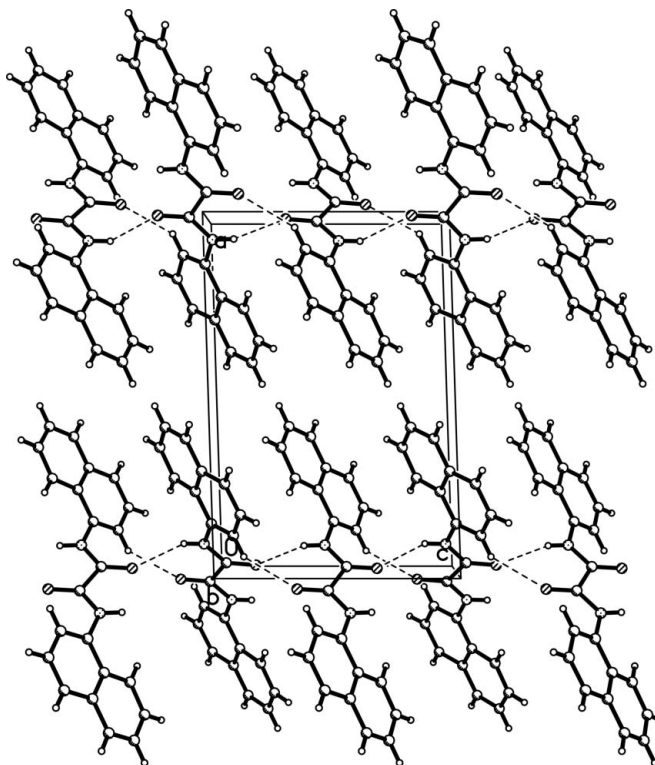
Table 1

Hydrogen-bond geometry (Å, °).

Cg_1 and Cg_2 are the centroids of atoms C1–C6 and C1/C6–C10, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2A\cdots Cg_2^{ii}$	0.93	2.97	3.548	122
$C7-H7A\cdots Cg_1^{iii}$	0.93	3.18	3.836	129
$N1-H1A\cdots O1^i$	0.86	2.30	2.700 (3)	108
$N1-H1A\cdots O1^{iv}$	0.86	2.54	3.116 (3)	125
$C9-H9A\cdots O1$	0.93	2.52	2.954 (3)	109
$C9-H9A\cdots O1^v$	0.93	2.49	3.272 (4)	141

Symmetry codes: (i) $-x, -y + 2, -z + 1$; (ii) $x, -y + \frac{1}{2}, z - \frac{3}{2}$; (iii) $x, -y - \frac{1}{2}, z - \frac{1}{2}$; (iv) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (v) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.


Figure 2

Packing diagram of (I). Hydrogen bonds are shown as dashed lines.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with $N-H = 0.86$ Å (for NH) and $C-H = 0.93$ Å for aromatic H atoms, and with $U_{\text{iso}}(H) = 1.2 U_{\text{eq}}(C, N)$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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