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Key indicators

Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.048
 wR factor = 0.126
Data-to-parameter ratio = 18.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*N*-Butyl-4-butylamino-1,8-naphthalimide

The crystal structure of the title compound, $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2$, establishes the intramolecular charge transfer state as the lowest electronic state in the molecule. The molecules are held together by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, giving rise to a polymeric chain.

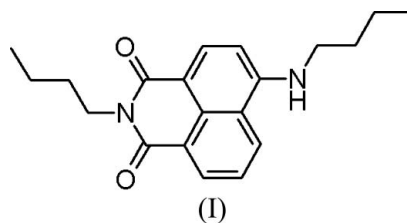
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Comment

4-Amino-1,8-naphthalimide and its derivatives possess conjugating electron donor and acceptor groups and therefore they are expected to have an intramolecular charge transfer (ICT) state as the lowest electronic state. This CT nature for the molecules has been elucidated by various photophysical studies. Crystal structures of such compounds are also equally important to understand their ground-state properties (Banthia & Samanta, 2005). The crystal structure of the title compound, (I) (Fig. 1), reported here, supports very well the existence of a CT character in the molecule. The short C4–N1 bond length, 1.3521 (15) Å, and bond angles around the amine N atom close to 120° (Table 1), suggest considerable double-bond character for the C–N bond, manifesting CT character in the ground state.



In the packing structure of (I), shown in Fig. 2, an intermolecular $\text{N1}-\text{H1}\cdots\text{O1}$ hydrogen bond (Table 2) connects the translated molecules, leading to an infinite polymeric chain.

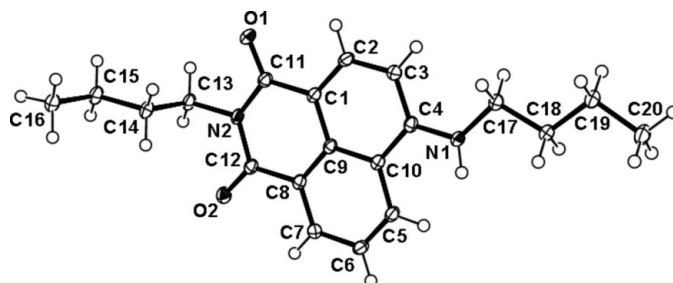


Figure 1

An ORTEP-3 (Farrugia, 1997) view of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

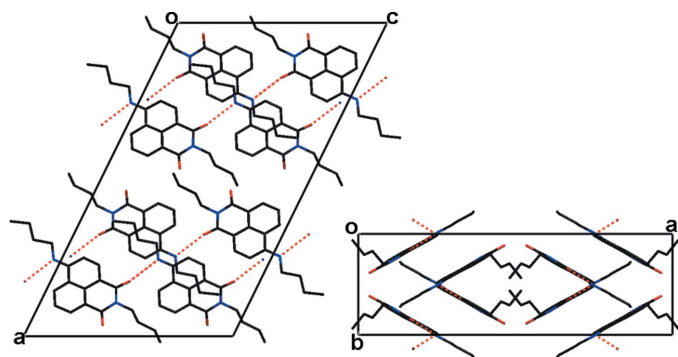


Figure 2
Packing diagrams of (I), illustrating the intermolecular hydrogen bonding, shown as dashed lines, between the amine and the carbonyl groups. H atoms have been omitted for clarity.

Experimental

The title compound was prepared according to standard procedures (Banthia *et al.*, 2005). Single crystals suitable for the X-ray diffraction study were grown by slow evaporation of a solution of (I) in chloroform.

Crystal data

$C_{20}H_{24}N_2O_2$	$D_x = 1.283 \text{ Mg m}^{-3}$
$M_r = 324.41$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6924 reflections
$a = 27.886 (3) \text{ \AA}$	$\theta = 2.5\text{--}28.2^\circ$
$b = 8.0475 (9) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 16.671 (2) \text{ \AA}$	$T = 100 (2) \text{ K}$
$\beta = 116.149 (2)^\circ$	Plate, yellow
$V = 3358.3 (7) \text{ \AA}^3$	$0.60 \times 0.18 \times 0.06 \text{ mm}$
$Z = 8$	

Data collection

Bruker SMART CCD area-detector diffractometer	4026 independent reflections
φ and ω scans	3477 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{\text{int}} = 0.031$
$T_{\text{min}} = 0.856$, $T_{\text{max}} = 0.995$	$\theta_{\text{max}} = 28.3^\circ$
18639 measured reflections	$h = -36 \rightarrow 36$
	$k = -10 \rightarrow 10$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 2.4226P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
4026 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
223 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (\AA , $^\circ$).

O1—C11	1.2309 (14)	N1—H1	0.877 (18)
O2—C12	1.2183 (15)	N2—C12	1.4001 (15)
N1—C4	1.3521 (15)	N2—C11	1.4003 (15)
N1—C17	1.4564 (15)	N2—C13	1.4767 (14)
C4—N1—C17	123.82 (10)	C2—C1—C11	120.50 (10)
C4—N1—H1	115.9 (11)	C9—C1—C11	120.59 (11)
C17—N1—H1	118.1 (11)	N1—C4—C3	121.40 (11)
C2—C1—C9	118.90 (10)	N1—C4—C10	119.87 (10)

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N1—H1 \cdots O1 ⁱ	0.88 (2)	2.26 (2)	3.0744 (14)	155 (2)

Symmetry code: (i) $x, -y + 2, z + \frac{1}{2}$.

The H atom attached to the amine N atom was located in a difference map and refined without any restraint, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$. Other H atoms were included in the refinement at calculated positions and refined as riding on their carrier atoms, with C—H set to 0.93 (aromatic), 0.97 (CH_2) or 0.96 \AA (CH_3), and with displacement parameters set to be isotropic with a value equal to 1.2 (aromatic CH, CH_2) or 1.5 (CH_3) times U_{eq} of the parent C atom.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and MERCURY (Bruno *et al.*, 2002); software used to prepare material for publication: SHELXTL (Bruker 2003).

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References

- Banthia, S. & Samanta, A. (2005). *Chem. Lett.* **34**, 722–723.
 Banthia, S., Sarkar, M. & Samanta, A. (2005). *Res. Chem. Intermed.* **31**, 25–38.
 Bruker (2003). SMART (Version 5.63), SAINT (Version 6.45) and SHELXTL (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* **B58**, 389–397.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (2002). SADABS. University of Göttingen, Germany.