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N,*N*′-Bis(2-pyridylethyl)pyromellitic diimide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.124
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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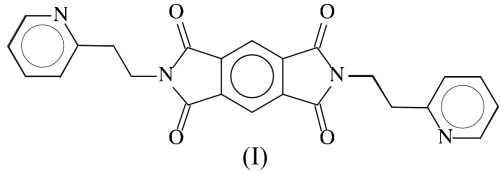
N,*N*′-Bis(2-pyridylethyl)pyromellitic diimide, $C_{24}H_{18}N_4O_4$, exists as a centrosymmetric monomeric molecule. Adjacent molecules are linked by weak C—H···O and C—H···N interactions into a linear ribbon-like structure. The $C_{pyridyl}—C_{methylene}—C_{methylene}—N_{imido}$ fragment is in an *anti* conformation [torsion angle = 168.3 (2)°].

Comment

A previous report has documented the structure of *N*,*N*′-bis(2-pyridylmethyl)pyromellitic diimide (Lü *et al.*, 2003), a compound whose heterocyclic portion is separated from the rigid aromatic system by a methylene linkage; the linkage permits free rotation of the heterocyclic rings. The centrosymmetric bidentate title compound, (I) (Fig. 1), possesses two ethylene linkages and is expected to be much more flexible. The coordination behaviour of the compound is being investigated. As the $C_{pyridyl}—C_{methylene}—C_{methylene}—N_{imido}$ fragment is in an *anti* conformation [torsion angle = 168.3 (2)°], the molecule is best described as being in an extended form. Selected bond distances and angles are given in Table 1.



(I)

In the crystal structure, adjacent molecules interact *via* weak C—H···O and C—H···N interactions, giving rise to a linear ribbon-like structure (Fig. 2).

Experimental

The title compound was prepared from the condensation of pyromelletic dianhydride and aminoethyl-2-pyridine in dimethylformamide (DMF), as described for the synthesis of *N*,*N*′-bis(2-pyridylmethyl)pyromellitic diimide by Lü *et al.* (2003). The resulting

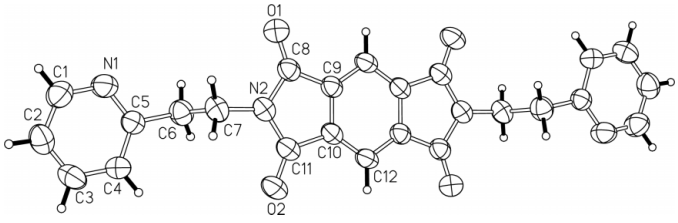


Figure 1
A view of (I), showing the labelling scheme and displacement ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

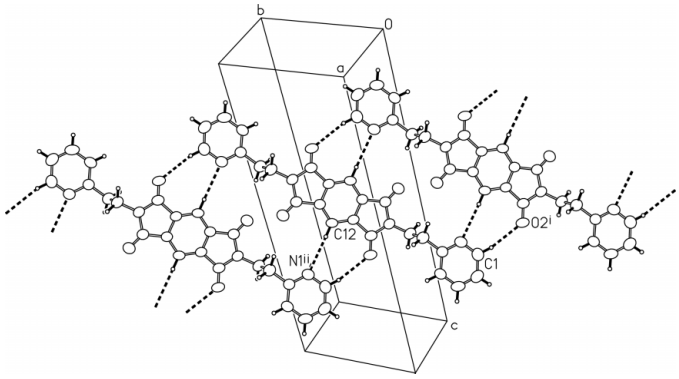


Figure 2
A packing diagram, showing the C—H···O interactions that link the molecules into a chain [C1···O2^{i} = 3.419 (2) Å and C12···N1^{ii} = 3.519 (2) Å]. [Symmetry codes: (i) $x-1, y-1, z$; (ii) $1+x, 1+y, z$.]

brown compound was purified by recrystallization from DMF and a second time from chloroform, giving pure colourless (I) in 70% yield.

Crystal data

$C_{24}H_{18}N_4O_4$	D_x = 1.422 Mg m^{-3}
M_r = 426.42	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 748 reflections
a = 5.2484 (7) Å	θ = 2.7–26.5°
b = 8.125 (1) Å	μ = 0.10 mm^{-1}
c = 23.398 (3) Å	T = 298 (2) K
β = 93.422 (2)°	Block, colorless
V = 996.0 (2) Å^3	0.50 × 0.17 × 0.15 mm
Z = 2	

Data collection

Bruker SMART area-detector diffractometer	1469 reflections with $I > 2\sigma(I)$
	R_{int} = 0.023
φ and ω scans	θ_{max} = 27.0°
Absorption correction: none	$h = -6 \rightarrow 6$
6073 measured reflections	$k = -8 \rightarrow 10$
2171 independent reflections	$l = -29 \rightarrow 29$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.0976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.124	
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2171 reflections	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.201 (2)	C3—C4	1.373 (3)
O2—C11	1.206 (2)	C4—C5	1.377 (2)
N1—C1	1.335 (2)	C5—C6	1.505 (2)
N1—C5	1.331 (2)	C6—C7	1.517 (2)
N2—C11	1.383 (2)	C8—C9	1.485 (2)
N2—C7	1.456 (2)	C9—C10	1.386 (2)
N2—C8	1.398 (2)	C9—C12^{iii}	1.385 (2)
C1—C2	1.365 (2)	C10—C11	1.492 (2)
C2—C3	1.362 (3)	C10—C12	1.379 (2)
C1—N1—C5	117.7 (2)	O1—C8—N2	125.0 (2)
C7—N2—C8	124.6 (1)	O1—C8—C9	129.4 (2)
C7—N2—C11	123.2 (1)	N2—C8—C9	105.6 (1)
C8—N2—C11	112.2 (1)	C8—C9—C10	108.4 (1)
N1—C1—C2	124.0 (2)	C8—C9—C12^{iii}	128.9 (2)
C1—C2—C3	118.1 (2)	C10—C9—C12^{iii}	122.7 (2)
C2—C3—C4	118.9 (2)	C9—C10—C11	107.7 (1)
C3—C4—C5	119.8 (2)	C9—C10—C12	122.6 (1)
N1—C5—C4	121.5 (2)	C11—C10—C12	129.8 (1)
N1—C5—C6	117.6 (2)	O2—C11—N2	124.8 (2)
C4—C5—C6	120.9 (2)	O2—C11—C10	129.1 (2)
C5—C6—C7	111.1 (1)	N2—C11—C10	106.1 (1)
N2—C7—C6	112.1 (1)		

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

H atoms were placed in calculated positions in the riding-model approximation (C—H = 0.93 Å for aromatic H atoms and C—H = 0.97 Å for aliphatic H atoms), and their U_{iso} values were set to $1.2U_{eq}$(parent C atom).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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