Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-2,3-Bis(2-phenylindolizin-3-yl)-2-butenedinitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.065
wR factor = 0.137
Data-to-parameter ratio = 11.7

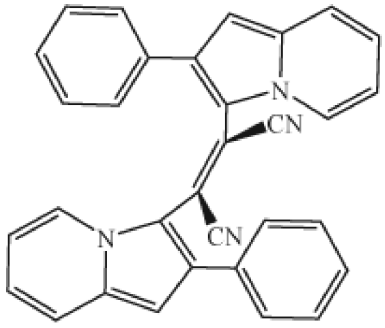
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 January 2005
Accepted 18 January 2005
Online 29 January 2005

The title compound, $C_{32}H_{20}N_4$, shows a *Z* configuration for the two 2-phenylindolizin-3-yl substituents. There are two intramolecular π–π interactions. The molecule self-assembles into a three-dimensional framework structure through one intermolecular π–π interaction and two weak intermolecular C—H···N interactions.

Comment

Organic electroluminescent devices are of both academic and industrial interest due to their potential applications in display technology (Ziemelis, 1999). The advantages of these organic materials over inorganic materials are high fluorescent efficiencies, wide ranges of emission wavelengths and the fact that they can be easily fabricated into large films (Kido, 1999). Recently, research on these compounds has focused on their fluorescent efficiency and solubility with different donor–acceptor substituents (Park *et al.*, 2000; Brabec *et al.*, 2001). We report here the X-ray crystal structure of (*Z*)-2,3-bis(2-phenylindolizin-3-yl)-2-butenedinitrile, (I), in which the donor–acceptor substituent is 2-phenyl-3-indolizinylcyano.



(I)

The title compound shows a *Z* configuration for the two 2-phenyl-3-indolizinyl substituents (Fig. 1 and Table 1). The eight atoms (N3/C10–C8/N4/C26–C24) around the C9═C25 double bond are nearly coplanar, with a maximum deviation of 0.022 (2) Å for atom N2.

There are two intramolecular π–π interactions between benzene rings and neighboring indolizinyl rings [*Cg*1···*Cg*2 = 3.490 (2) Å and *Cg*3···*Cg*4 = 3.496 (2) Å] (*Cg*2 and *Cg*3 are the mid-points of the C21—N2 and C5—N1 bonds, respectively, and *Cg*1 and *Cg*4 are the centroids of the benzene rings C11–C16 and C27–C32, respectively).

The crystal structure of (I) exhibits an intermolecular π–π interaction and two weak intermolecular C—H···N interactions, as shown in Fig. 2 and Table 2. Zigzag chains of molecules are formed along the *a* axis through one weak

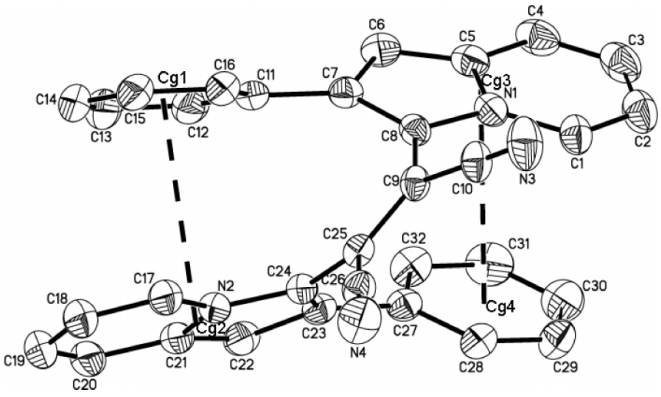


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate π–π interactions.

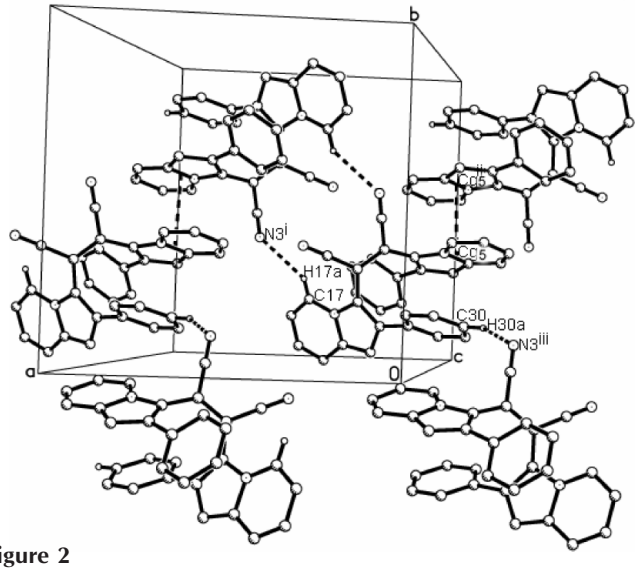


Figure 2
The intermolecular π–π interactions and weak intermolecular interactions (dashed lines) in the structure of the title compound [symmetry codes: (i) $1-x, 1-y, 2-z$; (ii) $-x, 1-y, 2-z$; (iii) $-x, -\frac{1}{2}+y, \frac{3}{2}-z$].

intermolecular interactions (C17—H17$A\cdots$N3^{i}) and one intermolecular π–π interaction [$Cg5\cdots Cg5^{ii}$ = 3.627 (2) Å] [$Cg5$ is the mid-point of the C5—N1 bond; symmetry codes: (i) $1-x, 1-y, 2-z$; (ii) $-x, 1-y, 2-z$]. Neighboring chains of molecules are connected through an additional weak intermolecular interaction [C30—H30$A\cdots$N3^{iii}; symmetry code: (iii) $-x, -\frac{1}{2}+y, \frac{3}{2}-z$], resulting in a three-dimensional framework structure (Fig. 3).

Experimental

A solution of 2-phenylindolizine-3-acetonitrile (0.12 g, 0.5 mmol) and sodium hydroxide (0.02 g, 0.5 mmol) in dimethylformamide (5 ml) was treated with oxygen at room temperature for 24 h. The resulting mixture was chromatographed on a column of alumina with petroleum ether/ethyl acetate as eluants. Evaporation of the eluants gave the title compound as a dark purple solid. Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization from acetone.

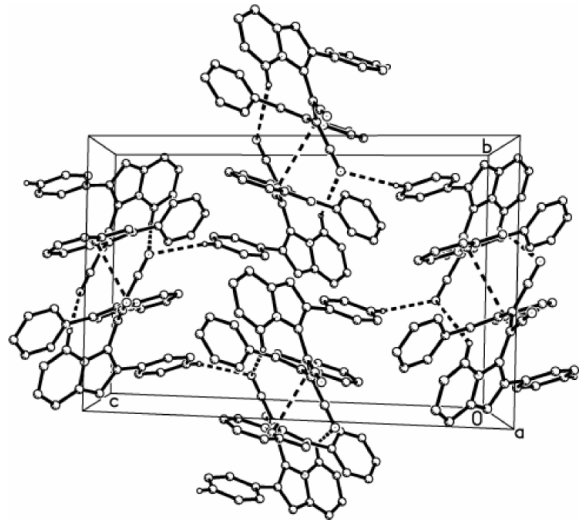


Figure 3
The three-dimensional framework of the title compound. Dashed lines indicate π–π interactions and weak intermolecular C—H$\cdots$N interactions.

Crystal data

$C_{32}H_{20}N_4$	D_x = 1.268 Mg m^{-3}
M_r = 460.52	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3716 reflections
a = 11.663 (2) Å	θ = 2.3–22.6°
b = 11.695 (2) Å	μ = 0.08 mm^{-1}
c = 18.348 (4) Å	T = 293 (2) K
β = 105.38 (3)°	Block, purple
V = 2413.0 (9) Å^3	0.32 × 0.26 × 0.24 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4719 independent reflections
	3207 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.043
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	θ_{max} = 26.0°
	$h = -13 \rightarrow 13$
T_{min} = 0.97, T_{max} = 0.98	$k = -14 \rightarrow 12$
15789 measured reflections	$l = -22 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.66P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.065	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.137	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
4719 reflections	
405 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

C8—C9	1.449 (3)	C24—C25	1.447 (3)
C9—C25	1.375 (3)	C25—C26	1.441 (3)
C9—C10	1.440 (3)		
C25—C9—C10	117.6 (2)	C9—C25—C26	117.5 (2)
C25—C9—C8	124.6 (2)	C9—C25—C24	124.3 (2)
C10—C9—C8	117.7 (2)	C26—C25—C24	118.2 (2)
C10—C9—C25—C26	6.5 (3)	C10—C9—C25—C24	−170.5 (2)
C8—C9—C25—C26	−170.8 (2)	C8—C9—C25—C24	12.1 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17A···N3^{i}	0.92 (3)	2.62 (3)	3.386 (4)	140 (2)
C30—H30A···N3^{ii}	0.90 (4)	2.73 (4)	3.498 (4)	144 (3)

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

All H atoms were located in difference Fourier maps and refined isotropically, the C—H distances being in the range 0.86 (3)–1.03 (4) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Education Department, Natural Science Foundation of Jiangsu Province of the People's Republic of China (grant No. 03KJB150009).

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