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(*E*)-2-Phenyl-3-(2-phenylindolizin-3-yl)acrylonitrile

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Key indicators

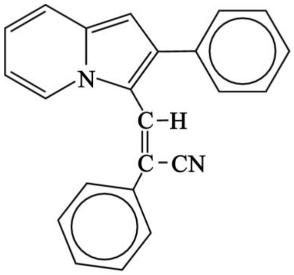
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.122
Data-to-parameter ratio = 15.6

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

In the title compound, $C_{23}H_{16}N_2$, the two bulky substituents, phenyl and 2-phenylindolizin-3-yl are situated on the same side of the C═C double bond, resulting in an *E* configuration. This configuration minimizes the interatomic contacts. There are weak C—H$\cdots\pi$ interactions between neighboring molecules related by an inversion center.

Comment

Organic electroluminescent devices are of both academic and industrial interest due to their potential application in display technology (Ziemelis, 1999). The advantages of these organic materials over inorganic materials are their high fluorescent efficiency, wide range of emission wavelengths and the fact that they can be easily fabricated into large films (Kido, 1999). Recent research in organic electroluminescent materials has focused on changing the color, the fluorescent efficiency (Park *et al.*, 2000) and solubility (Christoph *et al.*, 2001) with donor/acceptor substituents. We report here the X-ray crystal structure of the title compound, (I), in which the donor and acceptor substituents are 2-phenylindolizin-3-yl and cyano.



(I)

In (I), the phenyl and 2-phenylindolizin-3-yl substituents are situated on the same side of the C═C double bond (Fig. 1). Such a conformation minimizes the intraatomic contacts. The dihedral angles between the C18–C23 phenyl ring and acrylonitrile, the indolizinyl plane and acrylonitrile, and the C1–C6 phenyl ring and indolizinyl are 18.4, 44.0 and 45.6°, respectively.

There are weak C22—H22$\cdots\pi$ interactions, resulting in the formation of layers packed parallel to the *ab* and *ac* planes (Fig. 2). The phenyl and pyridine rings act as acceptors and atoms C11, C19, C20 and C22 as donors (Table 1).

Experimental

A solution of benzyl cyanide (0.12 g, 1.02 mmol), sodium hydroxide (0.02 g, 0.50 mmol) and 2-phenyl-3-thioformylindolizine (0.22 g, 0.94 mmol) in anhydrous dimethylformamide (15 ml) was stirred at

328–333 K, until all the thiol had disappeared (monitored by thin-layer chromatography). The resulting mixture was column chromatographed on alumina gel, using a petroleum ether/ethyl acetate gradient as eluant, followed by recrystallization from a mixture of petroleum ether and ethyl acetate to give the title compound as yellow crystals.

Crystal data

$C_{23}H_{16}N_2$
$M_r = 320.38$
Orthorhombic, *Pbca*
$a = 12.175$ (2) Å
$b = 16.548$ (3) Å
$c = 17.111$ (3) Å
$V = 3447.5$ (11) Å^3

$Z = 8$
$D_x = 1.235$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 294$ (2) K
Prism, yellow
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.976$, $T_{\max} = 0.987$

18419 measured reflections
3548 independent reflections
1379 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.075$
$\theta_{\max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.122$
$S = 0.97$
3548 reflections
227 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.6402P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 0.11$ e Å^{-3}
$\Delta\rho_{\min} = -0.10$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0012 (3)

Table 1
C—H···π interactions (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···$Cg3^{\rm i}$	0.93	3.15	3.557 (3)	109
C19—H19···$Cg1^{\rm ii}$	0.93	3.25	3.816 (3)	121
C20—H20···$Cg1^{\rm ii}$	0.93	3.17	3.771 (3)	124
C22—H22···$Cg2^{\rm iii}$	0.93	3.04	3.728 (3)	132

Symmetry codes: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, z$; (ii) $x - \frac{1}{2}, y, -z + \frac{3}{2}$; (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$. *Cg*1, *Cg*2 and *Cg*3 represent the centroids of the C1–C6, N1–C13 and C19–C22 rings respectively.

All H atoms were included in calculated positions and refined using a riding model, with C—H= 0.93 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

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

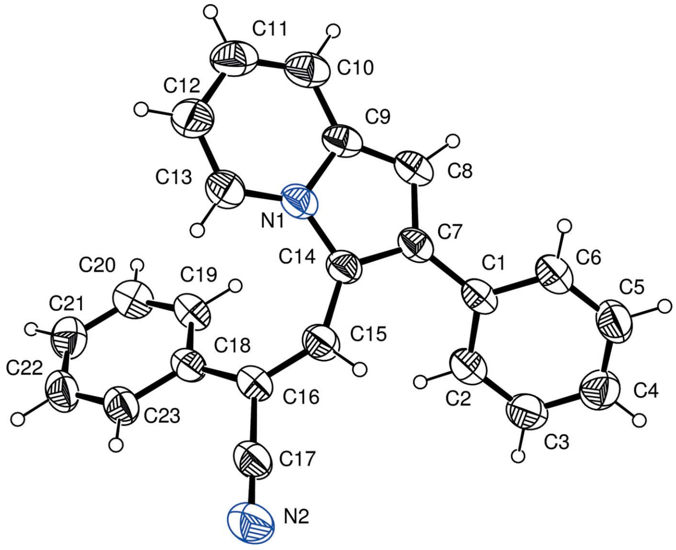


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

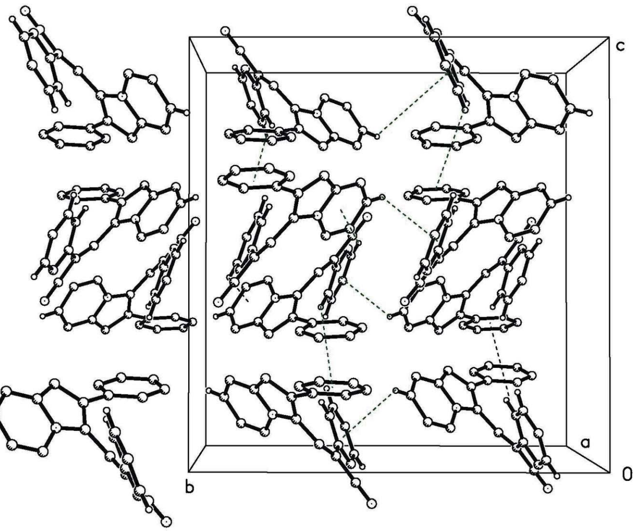


Figure 2
Packing diagram, viewed down the *a* axis, showing the weak C—H···π interactions as dashed lines. H atoms not involved in these interactions have been omitted.

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