Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-[2-(2-Phenylindolizin-3-yl)-1-(1,2,4-triazol-1-yl)vinyl]benzonitrile

Li-Juan Tang,[a] Wei-Wei Liu,[a]* Bao-Hua Qian,[a] Ling Wang[a] and Da-Qi Wang[b]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, and [b]Department of Chemistry, Liaocheng University, Liaocheng 252059, People's Republic of China
Correspondence e-mail: Liuww323@yahoo.com.cn

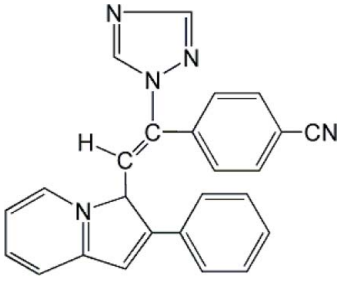
Received 10 July 2007; accepted 21 July 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 12.8.

In the title compound, $C_{25}H_{17}N_5$, the two bulky substituents, *viz*. 4-cyanophenyl and 2-phenylindolizin-3-yl, are situated on the same side of the C=C double bond, resulting in an *E* configuration. The crystal packing is stabilized by weak non-classical intermolecular C—H···N hydrogen bonds and slipped π–π stacking interactions.

Related literature

For related literature, see: Clive *et al.* (1999); Ebeid *et al.* (1997); Gundersen *et al.* (2007); Itoh *et al.* (2007); Malonne *et al.* (1998); Mehta & Parrick (1995).



Experimental

Crystal data

$C_{25}H_{17}N_5$
M_r = 387.44
Triclinic, $P\overline{1}$
a = 9.947 (5) Å
b = 9.996 (5) Å
c = 10.833 (5) Å
α = 83.381 (5)°
β = 74.695 (6)°
γ = 76.924 (6)°
V = 1010.2 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.58 × 0.50 × 0.37 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.956, T_{max} = 0.972
5230 measured reflections
3492 independent reflections
2413 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.02
3492 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···N5^{i}	0.93	2.54	3.448 (3)	165
C19—H19···N3^{ii}	0.93	2.62	3.462 (3)	152
C24—H24···N4^{iii}	0.93	2.67	3.492 (3)	148

Symmetry codes: (i) $x, y, z-1$; (ii) $-x, -y+1, -z+2$; (iii) $-x, -y+2, -z+1$.

Table 2
Intra- and intermolecular π–π interactions (Å).

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1/C1–C4, N1/C4–C8, C9–C14 and C17–C22 rings, respectively.

Interaction	Centroid-to-centroid	Plane-to-plane	Slippage
*Cg*1···*Cg*2^{i}	3.724 (2)	3.622	0.867
*Cg*3···*Cg*4	3.724 (2)	3.536	1.168

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*.

This work was supported by the Education Department of the Natural Science Foundation of Jiangsu Province (grant No. 06KJD150015), the Key Laboratory of the Marine Biotechnology Foundation of Jiangsu Province (grant No. 2006HS014) and the Huaihai Institute of Technology Disciplinary Construction Foundation (grant No. XK200309).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2219).

References

Bruker (2000). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Clive, D., Coltart, D. & Zhou, Y. (1999). *J. Org. Chem.* **64**, 1447–1454.
Ebeid, M. Y., Moghazyaly, S. M., Hanna, M. M., Romeih, F. A. & Barsoum, F. F. (1997). *Bull. Fac. Pharm. Cairo Univ.* **35**, 171–183.
Gundersen, L.-L., Charnock, C., Negussie, A. H., Rise, F. & Teklu, S. (2007). *Eur. J. Pharm. Sci.* **30**, 26–35.
Itoh, M., Ohta, M. & Muramatsu, H. (2007). Int. Patent WO 2007 007 688.
Malonne, H., Hanuise, J. & Fontaine, J. (1998). *Pharm. Pharmacol. Commun.* **4**, 241–243.
Mehta, L. & Parrick, J. (1995). *J. Heterocycl. Chem.* **32**, 27–30.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807035672

supplementary materials

Acta Cryst. (2007). E**63**, o3608 [**doi:10.1107/S1600536807035672**]

(*E*)-4-[2-(2-Phenylindolizin-3-yl)-1-(1,2,4-triazol-1-yl)vinyl]benzonitrile

L.-J. Tang, W.-W. Liu, B.-H. Qian, L. Wang and D.-Q. Wang

Comment

Indolizines and triazoles are important heterocyclic nitrogen compounds which display a wide range of biological activity. The synthetic indolozine (Gundersen *et al.*, 2007) and triazole (Itoh *et al.*, 2007) derivatives, have been used as antitumor (Mehta *et al.*, 1995), anti–inflammatory (Malonne *et al.*, 1998), antiviral agent (Ebeid *et al.*, 1997) and also as antihypertensive (Clive *et al.*, 1999). We report here the structure and stereochemistry of the title compound (I), which resulted from the condensation of 3-thioformylindolizine with 4-[(1*H*-1,2,4-triazol-1- yl)methyl] benzonitrile containing indolizine and triazole ring.

Compound (I) (Fig.1) assumes an E-conformation. There is a twist in the molecule as seen in the C1—C15—C16—C17 and the C15—C1—C2—C9 torsion angles of −9.8 (3)° and −3.0 (3)°, respectively. This is also reflected in the dihedral angles of 68.347 (76)° and 43.322 (53)° formed between C23—C24/N2—N3 and C17—C22 and C9—C14 and C1—C8/N1 respectively.

The two bulky substituted indolizinyl and 4-cyanophenyl rings are on the same side. Such conformation results from the occurrence of weak intramolecular π···π interactions (Table 2, Fig.1). There are also intermolecular slippest π···π stacking and weak C—H···N hydrogen-bonding resulting in the formation of pseudo-dimers across inversion centers (Fig.2, Tables 1 and 2) which are further interconnected to form a three dimensional network.

Experimental

A solution of 4-[(1*H*-1,2,4-triazol-1-yl)methyl]benzonitrile(0.24 g, 1.30 mmol), sodium hydroxide (0.05 g, 1.25 mmol) and 2-phenyl-3-thioformylindolizine(0.237 g, 1.00 mmol) in anhydrous dimethylformamide(15 ml) was stirred at ~343- 358 K, until all the thial had disappeared (monitored by thin-layer chromatography). The resulting mixture was chromatographed on a column of silica gel with petroleum ether and ethyl acetate as eluents for stepwise elution. Evaporation of the eluents gave the title compound as yellow solid. Single crystals of (I) suitable for *x*-ray crystallographic analysis were obtained by recrystallization from a mixture of petroleum ether and ethyl acetate.

Refinement

All H atoms were fixed geometrically and treated as riding on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

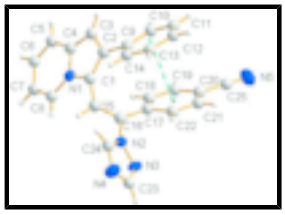


Fig. 1. A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level and H atoms are represented by spheres of arbitrary radii. Dashed line represent the intramolecular π-π stacking.

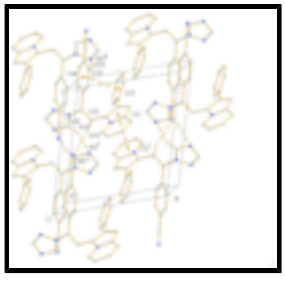


Fig. 2. Part of the crystal structure of (I), showing the formation of intermolecular π···π (dashed lines) interaction. H atoms have been omitted for clarity. [Symmetry codes: (i) 1 − *x*, 1 − *y*, 1 − *z*; (ii) −*x*, 1 − *y*, 1 − *z*; (iii) −*x*, 1 − *y*, 2 − *z*; (iv) *x*, *y*, *z* − 1].

(*E*)-4-[2-(2-Phenylindolizin-3-yl)-1-(1,2,4-triazol-1-yl)vinyl]benzonitrile

Crystal data

$C_{25}H_{17}N_5$	$Z = 2$
$M_r = 387.44$	$F_{000} = 404$
Triclinic, $P\bar{1}$	$D_x = 1.274$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 9.947$ (5) Å	Cell parameters from 1975 reflections
$b = 9.996$ (5) Å	θ = 2.5–27.1º
$c = 10.833$ (5) Å	μ = 0.08 mm^{-1}
α = 83.381 (5)º	$T = 298$ (2) K
β = 74.695 (6)º	Prism, yellow
γ = 76.924 (6)º	0.58 × 0.50 × 0.37 mm
$V = 1010.2$ (9) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3492 independent reflections
Radiation source: fine-focus sealed tube	2413 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 298(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -6 \rightarrow 11$
$T_{min} = 0.956$, $T_{max} = 0.972$	$k = -10 \rightarrow 11$
5230 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.1782P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.122$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
3492 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
272 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.036 (4)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.38641 (16)	0.43743 (16)	0.64233 (14)	0.0410 (4)
N2	−0.03197 (16)	0.79181 (15)	0.73271 (14)	0.0399 (4)
N3	−0.16952 (17)	0.78722 (18)	0.79478 (16)	0.0508 (5)
N4	−0.1620 (2)	0.9431 (2)	0.62648 (18)	0.0661 (6)
N5	0.0589 (3)	0.6483 (3)	1.4102 (2)	0.0964 (8)
C1	0.3291 (2)	0.56631 (19)	0.68966 (17)	0.0400 (5)
C2	0.4254 (2)	0.5964 (2)	0.75032 (17)	0.0423 (5)
C3	0.5397 (2)	0.4840 (2)	0.74142 (19)	0.0499 (5)
H3	0.6183	0.4772	0.7746	0.060*
C4	0.5164 (2)	0.3841 (2)	0.67480 (18)	0.0463 (5)
C5	0.5885 (2)	0.2513 (2)	0.63865 (19)	0.0549 (6)
H5	0.6766	0.2148	0.6561	0.066*
C6	0.5305 (3)	0.1764 (2)	0.5786 (2)	0.0612 (6)
H6	0.5774	0.0875	0.5571	0.073*
C7	0.3985 (3)	0.2329 (2)	0.5484 (2)	0.0604 (6)
H7	0.3598	0.1814	0.5059	0.072*

C8	0.3282 (2)	0.3609 (2)	0.58079 (18)	0.0504 (5)
H8	0.2408	0.3971	0.5616	0.060*
C9	0.4068 (2)	0.7238 (2)	0.81463 (18)	0.0438 (5)
C10	0.4369 (2)	0.7183 (2)	0.9333 (2)	0.0583 (6)
H10	0.4740	0.6339	0.9700	0.070*
C11	0.4124 (3)	0.8362 (3)	0.9976 (2)	0.0713 (7)
H11	0.4323	0.8304	1.0774	0.086*
C12	0.3592 (3)	0.9612 (3)	0.9449 (2)	0.0681 (7)
H12	0.3408	1.0401	0.9895	0.082*
C13	0.3329 (2)	0.9699 (2)	0.8258 (2)	0.0580 (6)
H13	0.3001	1.0553	0.7883	0.070*
C14	0.3552 (2)	0.8519 (2)	0.76121 (19)	0.0486 (5)
H14	0.3353	0.8586	0.6812	0.058*
C15	0.1904 (2)	0.64008 (19)	0.67592 (18)	0.0424 (5)
H15	0.1724	0.6450	0.5954	0.051*
C16	0.08603 (19)	0.70170 (18)	0.76966 (17)	0.0370 (4)
C17	0.08146 (18)	0.69058 (19)	0.90751 (17)	0.0369 (4)
C18	0.13747 (19)	0.5670 (2)	0.96614 (18)	0.0417 (5)
H18	0.1789	0.4909	0.9172	0.050*
C19	0.1329 (2)	0.5549 (2)	1.09464 (19)	0.0468 (5)
H19	0.1705	0.4713	1.1322	0.056*
C20	0.0721 (2)	0.6680 (2)	1.16816 (18)	0.0486 (5)
C21	0.0155 (2)	0.7910 (2)	1.11187 (19)	0.0546 (6)
H21	−0.0254	0.8669	1.1611	0.066*
C22	0.0191 (2)	0.8026 (2)	0.98321 (19)	0.0482 (5)
H22	−0.0206	0.8859	0.9465	0.058*
C23	−0.2408 (2)	0.8792 (2)	0.7270 (2)	0.0556 (6)
H23	−0.3398	0.8993	0.7468	0.067*
C24	−0.0326 (2)	0.8845 (2)	0.6342 (2)	0.0561 (6)
H24	0.0492	0.9052	0.5776	0.067*
C25	0.0644 (2)	0.6565 (3)	1.3034 (2)	0.0658 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0360 (9)	0.0447 (10)	0.0383 (9)	−0.0013 (7)	−0.0068 (7)	−0.0048 (7)
N2	0.0330 (9)	0.0432 (9)	0.0408 (9)	−0.0017 (7)	−0.0115 (7)	0.0018 (7)
N3	0.0307 (9)	0.0608 (11)	0.0566 (10)	−0.0058 (8)	−0.0096 (8)	0.0046 (8)
N4	0.0479 (12)	0.0727 (13)	0.0618 (12)	0.0113 (10)	−0.0141 (9)	0.0143 (10)
N5	0.0971 (19)	0.151 (2)	0.0522 (13)	−0.0378 (17)	−0.0296 (13)	0.0002 (14)
C1	0.0368 (11)	0.0423 (11)	0.0380 (10)	−0.0016 (9)	−0.0093 (8)	−0.0038 (8)
C2	0.0350 (11)	0.0489 (12)	0.0428 (11)	−0.0081 (9)	−0.0110 (9)	0.0000 (9)
C3	0.0347 (11)	0.0577 (13)	0.0570 (13)	−0.0046 (10)	−0.0177 (10)	0.0032 (10)
C4	0.0359 (11)	0.0483 (12)	0.0469 (11)	0.0012 (9)	−0.0072 (9)	0.0027 (9)
C5	0.0447 (13)	0.0532 (13)	0.0533 (13)	0.0061 (11)	−0.0049 (10)	0.0028 (10)
C6	0.0712 (17)	0.0484 (13)	0.0506 (13)	0.0065 (12)	−0.0067 (12)	−0.0057 (10)
C7	0.0732 (17)	0.0543 (14)	0.0503 (13)	−0.0062 (12)	−0.0112 (11)	−0.0128 (10)
C8	0.0496 (13)	0.0571 (13)	0.0438 (11)	−0.0064 (11)	−0.0126 (10)	−0.0069 (10)

C9	0.0319 (11)	0.0544 (13)	0.0459 (11)	−0.0135 (9)	−0.0075 (9)	−0.0013 (9)
C10	0.0631 (15)	0.0640 (15)	0.0586 (14)	−0.0280 (12)	−0.0241 (11)	0.0048 (11)
C11	0.0860 (19)	0.087 (2)	0.0572 (14)	−0.0423 (16)	−0.0224 (13)	−0.0077 (14)
C12	0.0664 (16)	0.0744 (18)	0.0677 (16)	−0.0329 (14)	0.0001 (13)	−0.0241 (13)
C13	0.0459 (13)	0.0517 (13)	0.0718 (16)	−0.0155 (11)	−0.0001 (11)	−0.0074 (11)
C14	0.0384 (12)	0.0563 (14)	0.0497 (12)	−0.0110 (10)	−0.0071 (9)	−0.0036 (10)
C15	0.0399 (11)	0.0480 (12)	0.0408 (11)	−0.0029 (9)	−0.0168 (9)	−0.0050 (9)
C16	0.0321 (10)	0.0386 (10)	0.0419 (10)	−0.0060 (8)	−0.0135 (8)	−0.0004 (8)
C17	0.0278 (10)	0.0433 (11)	0.0406 (10)	−0.0096 (8)	−0.0097 (8)	0.0010 (8)
C18	0.0357 (11)	0.0440 (11)	0.0478 (11)	−0.0118 (9)	−0.0135 (9)	0.0021 (9)
C19	0.0415 (12)	0.0531 (13)	0.0519 (12)	−0.0187 (10)	−0.0212 (10)	0.0134 (10)
C20	0.0408 (12)	0.0694 (15)	0.0412 (11)	−0.0210 (11)	−0.0140 (9)	0.0029 (10)
C21	0.0535 (14)	0.0615 (14)	0.0487 (12)	−0.0068 (11)	−0.0120 (10)	−0.0134 (10)
C22	0.0476 (13)	0.0459 (12)	0.0496 (12)	−0.0021 (10)	−0.0162 (10)	−0.0021 (9)
C23	0.0345 (12)	0.0652 (14)	0.0609 (14)	0.0055 (11)	−0.0160 (10)	0.0010 (11)
C24	0.0452 (13)	0.0592 (13)	0.0532 (13)	0.0027 (11)	−0.0114 (10)	0.0120 (11)
C25	0.0553 (15)	0.098 (2)	0.0529 (14)	−0.0252 (13)	−0.0229 (12)	0.0029 (13)

Geometric parameters (Å, °)

N1—C8	1.374 (3)	C10—C11	1.380 (3)
N1—C1	1.383 (2)	C10—H10	0.9300
N1—C4	1.402 (2)	C11—C12	1.365 (3)
N2—C24	1.330 (2)	C11—H11	0.9300
N2—N3	1.364 (2)	C12—C13	1.371 (3)
N2—C16	1.427 (2)	C12—H12	0.9300
N3—C23	1.308 (2)	C13—C14	1.386 (3)
N4—C24	1.308 (3)	C13—H13	0.9300
N4—C23	1.351 (3)	C14—H14	0.9300
N5—C25	1.138 (3)	C15—C16	1.337 (3)
C1—C2	1.395 (3)	C15—H15	0.9300
C1—C15	1.446 (3)	C16—C17	1.474 (3)
C2—C3	1.397 (3)	C17—C18	1.391 (2)
C2—C9	1.474 (3)	C17—C22	1.393 (3)
C3—C4	1.390 (3)	C18—C19	1.373 (3)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.403 (3)	C19—C20	1.386 (3)
C5—C6	1.350 (3)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.377 (3)
C6—C7	1.413 (3)	C20—C25	1.439 (3)
C6—H6	0.9300	C21—C22	1.377 (3)
C7—C8	1.348 (3)	C21—H21	0.9300
C7—H7	0.9300	C22—H22	0.9300
C8—H8	0.9300	C23—H23	0.9300
C9—C10	1.387 (3)	C24—H24	0.9300
C9—C14	1.388 (3)		
C8—N1—C1	128.76 (17)	C11—C12—C13	119.6 (2)
C8—N1—C4	121.32 (17)	C11—C12—H12	120.2
C1—N1—C4	109.75 (16)	C13—C12—H12	120.2

C24—N2—N3	108.51 (16)	C12—C13—C14	120.3 (2)
C24—N2—C16	129.20 (17)	C12—C13—H13	119.9
N3—N2—C16	122.18 (15)	C14—C13—H13	119.9
C23—N3—N2	102.02 (16)	C13—C14—C9	120.7 (2)
C24—N4—C23	101.48 (18)	C13—C14—H14	119.7
N1—C1—C2	107.01 (16)	C9—C14—H14	119.7
N1—C1—C15	120.65 (17)	C16—C15—C1	125.28 (17)
C2—C1—C15	132.28 (18)	C16—C15—H15	117.4
C1—C2—C3	108.12 (18)	C1—C15—H15	117.4
C1—C2—C9	125.41 (17)	C15—C16—N2	116.93 (16)
C3—C2—C9	126.46 (18)	C15—C16—C17	127.03 (17)
C4—C3—C2	108.75 (17)	N2—C16—C17	116.00 (15)
C4—C3—H3	125.6	C18—C17—C22	118.07 (17)
C2—C3—H3	125.6	C18—C17—C16	120.82 (17)
C3—C4—N1	106.36 (17)	C22—C17—C16	121.10 (16)
C3—C4—C5	135.6 (2)	C19—C18—C17	121.42 (19)
N1—C4—C5	118.1 (2)	C19—C18—H18	119.3
C6—C5—C4	120.3 (2)	C17—C18—H18	119.3
C6—C5—H5	119.8	C18—C19—C20	119.70 (18)
C4—C5—H5	119.8	C18—C19—H19	120.2
C5—C6—C7	120.1 (2)	C20—C19—H19	120.2
C5—C6—H6	120.0	C21—C20—C19	119.68 (18)
C7—C6—H6	120.0	C21—C20—C25	119.9 (2)
C8—C7—C6	120.6 (2)	C19—C20—C25	120.4 (2)
C8—C7—H7	119.7	C20—C21—C22	120.5 (2)
C6—C7—H7	119.7	C20—C21—H21	119.7
C7—C8—N1	119.5 (2)	C22—C21—H21	119.7
C7—C8—H8	120.2	C21—C22—C17	120.59 (19)
N1—C8—H8	120.2	C21—C22—H22	119.7
C10—C9—C14	118.0 (2)	C17—C22—H22	119.7
C10—C9—C2	120.40 (18)	N3—C23—N4	115.99 (19)
C14—C9—C2	121.62 (18)	N3—C23—H23	122.0
C11—C10—C9	120.9 (2)	N4—C23—H23	122.0
C11—C10—H10	119.6	N4—C24—N2	112.00 (19)
C9—C10—H10	119.6	N4—C24—H24	124.0
C12—C11—C10	120.5 (2)	N2—C24—H24	124.0
C12—C11—H11	119.7	N5—C25—C20	179.4 (3)
C10—C11—H11	119.7		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N5^{i}	0.93	2.54	3.448 (3)	165
C19—H19···N3^{ii}	0.93	2.62	3.462 (3)	152
C24—H24···N4^{iii}	0.93	2.67	3.492 (3)	148

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*, −*y*+1, −*z*+2; (iii) −*x*, −*y*+2, −*z*+1.

Intra- and intermolecular π–π interactions (Å)

Centroids	Centroid-to-centroid	Plane-to-plane	Slippage
*Cg*1···*Cg*2^{i}	3.724 (2)	3.622	0.867
*Cg*3···*Cg*4	3.724 (2)	3.536	1.168

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1/C1–C4, N1/C4–C8, C9–C14 and C17–C22 rings, respectively. [Symmetry code: (i) $1-x, 1-y, 1-z$]

Fig. 1

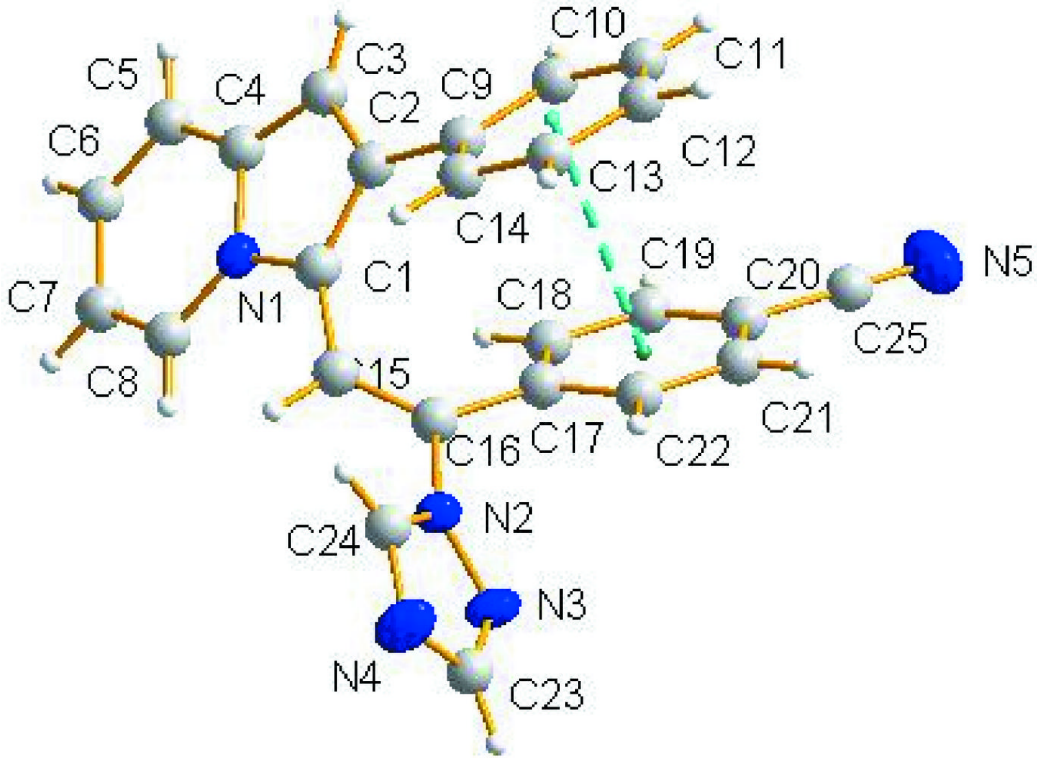

C10
C11
C5
C4
C3
C9
C2
C6
C12
C13
C14
C19
C20
N5
C7
N1
C1
C18
C25
C8
C15
C21
C16
C17
C22
N2
C24
N3
N4
C23

Fig. 2