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3-[(*E*)-2-Phenylethenyl]-1*H*-indole-6-carbonitrile

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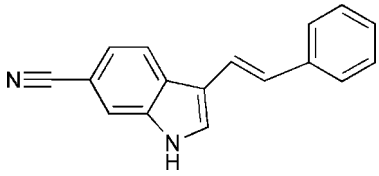
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.127; data-to-parameter ratio = 13.2.

In the title compound, $C_{17}H_{12}N_2$, the interplanar angle between the indole mean plane [max.deviation 0.030 (1) Å] and the phenyl ring is 24.32 (7)°. In the crystal, intermolecular N—H···N≡C hydrogen bonds form zigzag chains in the *a*-axis direction augmented by weak C—H···N≡C contacts.

Related literature

For indole derivatives as drug intermediates, see: Kunzer & Wendt (2011).



Experimental

Crystal data

$C_{17}H_{12}N_2$ M_r = 244.29
Orthorhombic, *Pbca*
a = 9.689 (8) Å
b = 7.440 (6) Å
c = 35.53 (3) Å
V = 2561 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.985, T_{max} = 0.985
16536 measured reflections
2263 independent reflections
1867 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.127
S = 1.16
2263 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.90	2.19	3.043 (3)	158
C5—H5A···N2^{ii}	0.93	2.66	3.416 (4)	138

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2065).

References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Kunzer, A. R. & Wendt, M. D. (2011). *Tetrahedron*, **52**, 1815–1818.
Rigaku. (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o207 [doi:10.1107/S1600536811054225]

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S1. Comment

Derivatives of indole are important chemical materials because they are excellent drug intermediates for many pharmaceutical products (Kunzer, *et al.*,2011). As part of our interest in these materials, we report here the crystal structure of the title compound $C_{17}H_{12}N_2$.

The molecular structure of the title compound is shown in Fig. 1. a dihedral angle of 24.32 (7)° between the planes of the indole and benzene rings is observed.

In the crystal, there are intermolecular N—H···O hydrogen bonds and no significant intermolecular π–π interactions [minimum ring centroid separation, 7.440 (5) Å]. (Fig. 2).

S2. Experimental

The title compound *E*-3-phenyl vinyl-6-cynaindole was obtained economically, Crystals of of it suitable for X-ray diffraction were obstained by slow evaporation of a ethanol solution.

S3. Refinement

All H atoms attached to C atoms and O atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH) and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(C and N).

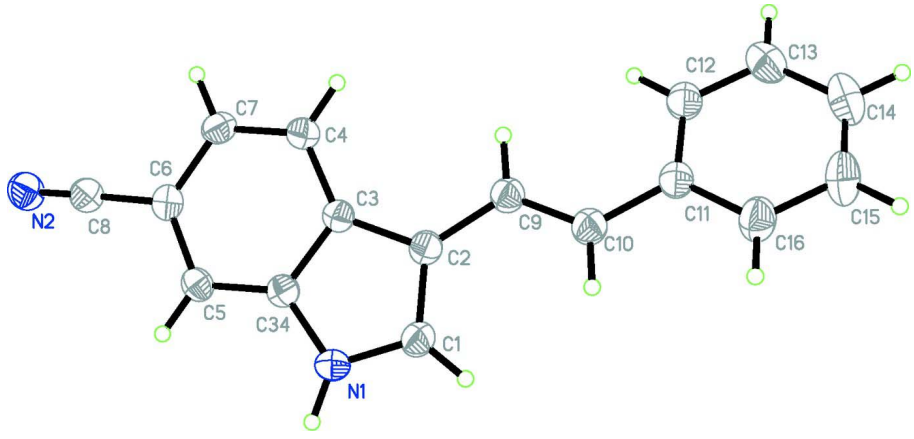

Figure 1

The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

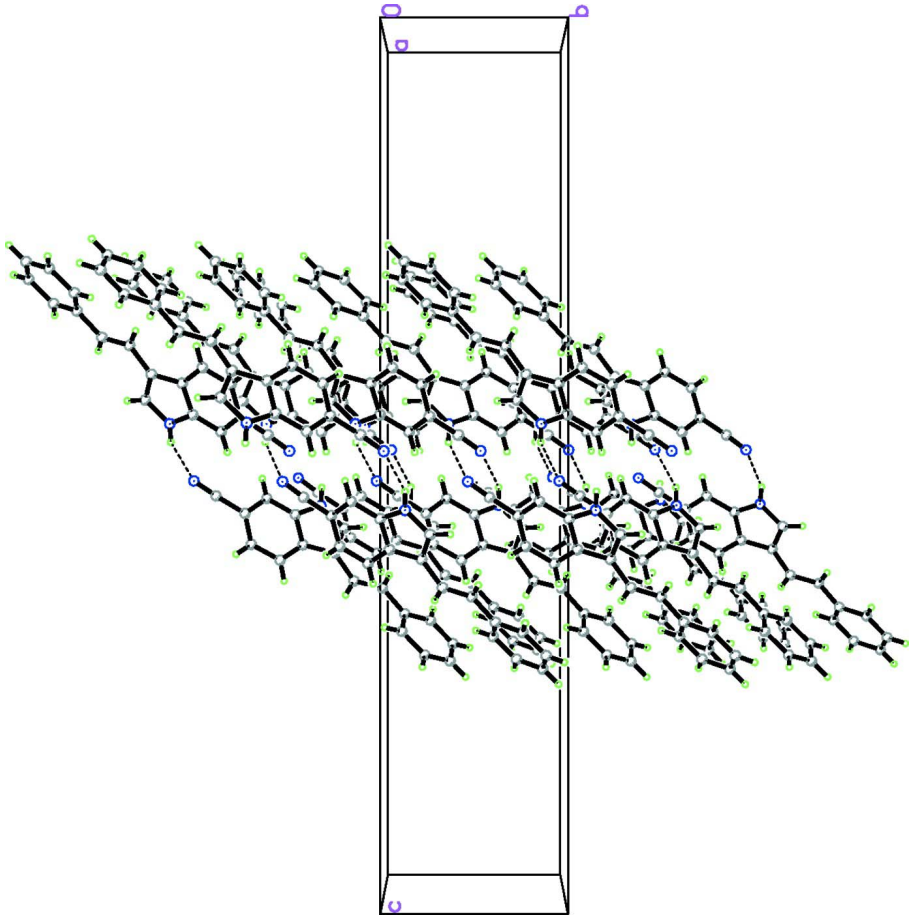

Figure 2

A packing view down the *a* axis showing the three dimensionnal network. Intermolecular hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{17}H_{12}N_2$
$M_r = 244.29$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.689\ (8)$ Å
$b = 7.440\ (6)$ Å
$c = 35.53\ (3)$ Å
$V = 2561\ (4)$ Å^3
$Z = 8$
$F(000) = 1024$
$D_x = 1.267$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2263 reflections
$\theta = 1.2–25.0°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, blue
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.985$, $T_{max} = 0.985$
16536 measured reflections
2263 independent reflections
1867 reflections with $I > 2\sigma(I)$

R_{int} = 0.027
θ_{max} = 25.0°, θ_{min} = 1.2°
h = −11→11
k = −7→8
l = −42→42

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.127
S = 1.16
2263 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.3176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	−0.14124 (13)	0.36176 (18)	0.04780 (4)	0.0497 (4)
H1A	−0.1933	0.3603	0.0268	0.060*
N2	0.17232 (16)	1.0338 (2)	0.01757 (4)	0.0620 (4)
C1	−0.13711 (17)	0.2312 (2)	0.07463 (5)	0.0515 (4)
H1B	−0.1876	0.1250	0.0738	0.062*
C2	−0.04867 (15)	0.2774 (2)	0.10301 (4)	0.0437 (4)
C3	0.00642 (14)	0.4503 (2)	0.09281 (4)	0.0388 (4)
C4	0.09969 (16)	0.5690 (2)	0.10937 (4)	0.0448 (4)
H4A	0.1368	0.5438	0.1329	0.054*
C5	−0.01787 (14)	0.6535 (2)	0.03886 (4)	0.0426 (4)
H5A	−0.0577	0.6824	0.0158	0.051*
C6	0.07849 (15)	0.7645 (2)	0.05558 (4)	0.0435 (4)
C7	0.13635 (17)	0.7231 (2)	0.09078 (4)	0.0477 (4)
H7A	0.2001	0.8010	0.1016	0.057*
C8	0.12868 (16)	0.9173 (2)	0.03509 (4)	0.0486 (4)
C9	−0.00992 (16)	0.1678 (2)	0.13506 (4)	0.0470 (4)
H9A	0.0605	0.2106	0.1504	0.056*
C10	−0.06676 (17)	0.0115 (2)	0.14427 (5)	0.0508 (4)
H10A	−0.1435	−0.0224	0.1302	0.061*
C11	−0.02405 (17)	−0.1135 (2)	0.17358 (4)	0.0469 (4)
C12	0.10257 (18)	−0.1029 (2)	0.19183 (5)	0.0534 (4)
H12A	0.1627	−0.0094	0.1861	0.064*

C13	0.1402 (2)	−0.2282 (3)	0.21825 (5)	0.0649 (5)
H13A	0.2253	−0.2186	0.2302	0.078*
C14	0.0534 (2)	−0.3680 (3)	0.22722 (6)	0.0756 (6)
H14A	0.0794	−0.4527	0.2451	0.091*
C15	−0.0719 (2)	−0.3811 (3)	0.20954 (6)	0.0795 (7)
H15A	−0.1315	−0.4749	0.2155	0.095*
C16	−0.1100 (2)	−0.2561 (3)	0.18295 (5)	0.0639 (5)
H16A	−0.1949	−0.2673	0.1710	0.077*
C34	−0.05265 (14)	0.4975 (2)	0.05786 (4)	0.0403 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0468 (7)	0.0499 (8)	0.0525 (8)	−0.0053 (6)	−0.0124 (6)	0.0016 (6)
N2	0.0596 (9)	0.0647 (10)	0.0618 (9)	−0.0127 (8)	−0.0015 (7)	0.0148 (8)
C1	0.0481 (9)	0.0448 (10)	0.0616 (10)	−0.0067 (7)	−0.0061 (8)	0.0041 (8)
C2	0.0403 (8)	0.0420 (9)	0.0487 (9)	0.0003 (7)	−0.0001 (7)	0.0007 (7)
C3	0.0354 (7)	0.0397 (8)	0.0412 (8)	0.0043 (6)	0.0014 (6)	−0.0011 (6)
C4	0.0484 (9)	0.0457 (9)	0.0402 (8)	0.0001 (7)	−0.0032 (7)	−0.0013 (7)
C5	0.0398 (8)	0.0457 (9)	0.0423 (8)	0.0066 (7)	0.0012 (6)	0.0023 (7)
C6	0.0417 (8)	0.0417 (9)	0.0472 (8)	0.0023 (7)	0.0076 (7)	0.0019 (7)
C7	0.0490 (9)	0.0466 (9)	0.0476 (9)	−0.0072 (7)	−0.0015 (7)	−0.0044 (7)
C8	0.0459 (9)	0.0509 (10)	0.0491 (9)	−0.0018 (8)	0.0015 (7)	0.0021 (8)
C9	0.0457 (8)	0.0454 (9)	0.0498 (9)	−0.0013 (7)	−0.0007 (7)	0.0016 (7)
C10	0.0488 (9)	0.0495 (10)	0.0540 (9)	−0.0028 (8)	−0.0021 (7)	0.0032 (8)
C11	0.0532 (9)	0.0432 (9)	0.0443 (9)	0.0014 (7)	0.0061 (7)	−0.0008 (7)
C12	0.0602 (10)	0.0498 (10)	0.0503 (9)	0.0006 (8)	0.0041 (8)	−0.0005 (8)
C13	0.0706 (12)	0.0697 (13)	0.0543 (10)	0.0150 (10)	−0.0015 (9)	0.0040 (9)
C14	0.0897 (15)	0.0720 (15)	0.0653 (12)	0.0171 (12)	0.0135 (11)	0.0233 (10)
C15	0.0866 (15)	0.0673 (14)	0.0845 (15)	−0.0052 (11)	0.0183 (12)	0.0279 (12)
C16	0.0609 (11)	0.0588 (12)	0.0722 (12)	−0.0072 (9)	0.0046 (9)	0.0116 (10)
C34	0.0347 (7)	0.0417 (8)	0.0446 (8)	0.0037 (6)	0.0009 (6)	−0.0016 (7)

Geometric parameters (Å, º)

N1—C1	1.361 (2)	C7—H7A	0.9300
N1—C34	1.372 (2)	C9—C10	1.328 (2)
N1—H1A	0.8999	C9—H9A	0.9300
N2—C8	1.148 (2)	C10—C11	1.457 (2)
C1—C2	1.367 (2)	C10—H10A	0.9300
C1—H1B	0.9300	C11—C12	1.390 (3)
C2—C3	1.439 (2)	C11—C16	1.389 (3)
C2—C9	1.450 (2)	C12—C13	1.373 (3)
C3—C34	1.412 (2)	C12—H12A	0.9300
C3—C4	1.394 (2)	C13—C14	1.375 (3)
C4—C7	1.370 (2)	C13—H13A	0.9300
C4—H4A	0.9300	C14—C15	1.370 (3)
C5—C34	1.385 (2)	C14—H14A	0.9300

C5—C6	1.380 (2)	C15—C16	1.376 (3)
C5—H5A	0.9300	C15—H15A	0.9300
C6—C7	1.405 (2)	C16—H16A	0.9300
C6—C8	1.435 (2)		

C1—N1—C34	108.91 (14)	C10—C9—H9A	117.3
C1—N1—H1A	126.0	C2—C9—H9A	117.3
C34—N1—H1A	125.1	C9—C10—C11	128.16 (16)
N1—C1—C2	110.82 (15)	C9—C10—H10A	115.9
N1—C1—H1B	124.6	C11—C10—H10A	115.9
C2—C1—H1B	124.6	C12—C11—C16	117.45 (16)
C1—C2—C3	105.76 (14)	C12—C11—C10	123.22 (15)
C1—C2—C9	126.88 (16)	C16—C11—C10	119.26 (16)
C3—C2—C9	127.18 (14)	C13—C12—C11	120.99 (18)
C34—C3—C4	118.45 (14)	C13—C12—H12A	119.5
C34—C3—C2	107.06 (13)	C11—C12—H12A	119.5
C4—C3—C2	134.49 (14)	C12—C13—C14	120.6 (2)
C7—C4—C3	119.67 (15)	C12—C13—H13A	119.7
C7—C4—H4A	120.2	C14—C13—H13A	119.7
C3—C4—H4A	120.2	C15—C14—C13	119.32 (19)
C34—C5—C6	117.15 (14)	C15—C14—H14A	120.3
C34—C5—H5A	121.4	C13—C14—H14A	120.3
C6—C5—H5A	121.4	C16—C15—C14	120.3 (2)
C5—C6—C7	121.46 (15)	C16—C15—H15A	119.9
C5—C6—C8	119.00 (15)	C14—C15—H15A	119.9
C7—C6—C8	119.34 (15)	C15—C16—C11	121.3 (2)
C4—C7—C6	120.61 (15)	C15—C16—H16A	119.3
C4—C7—H7A	119.7	C11—C16—H16A	119.3
C6—C7—H7A	119.7	N1—C34—C5	129.96 (14)
N2—C8—C6	176.59 (18)	N1—C34—C3	107.43 (14)
C10—C9—C2	125.35 (16)	C5—C34—C3	122.59 (14)

C34—N1—C1—C2	0.90 (19)	C9—C10—C11—C16	169.56 (17)
N1—C1—C2—C3	−0.13 (18)	C16—C11—C12—C13	−0.4 (2)
N1—C1—C2—C9	−175.44 (15)	C10—C11—C12—C13	−177.41 (16)
C1—C2—C3—C34	−0.66 (16)	C11—C12—C13—C14	0.2 (3)
C9—C2—C3—C34	174.63 (14)	C12—C13—C14—C15	−0.1 (3)
C1—C2—C3—C4	179.82 (17)	C13—C14—C15—C16	0.3 (3)
C9—C2—C3—C4	−4.9 (3)	C14—C15—C16—C11	−0.6 (3)
C34—C3—C4—C7	−3.0 (2)	C12—C11—C16—C15	0.6 (3)
C2—C3—C4—C7	176.51 (15)	C10—C11—C16—C15	177.75 (18)
C34—C5—C6—C7	−1.5 (2)	C1—N1—C34—C5	177.01 (15)
C34—C5—C6—C8	173.32 (13)	C1—N1—C34—C3	−1.29 (17)
C3—C4—C7—C6	1.4 (2)	C6—C5—C34—N1	−178.20 (15)
C5—C6—C7—C4	0.9 (2)	C6—C5—C34—C3	−0.1 (2)
C8—C6—C7—C4	−173.94 (15)	C4—C3—C34—N1	−179.20 (13)
C1—C2—C9—C10	−8.2 (3)	C2—C3—C34—N1	1.20 (16)
C3—C2—C9—C10	177.49 (15)	C4—C3—C34—C5	2.3 (2)

C2—C9—C10—C11	173.21 (15)	C2—C3—C34—C5	−177.26 (13)
C9—C10—C11—C12	−13.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{i}	0.90	2.19	3.043 (3)	158
C5—H5*A*···N2^{ii}	0.93	2.66	3.416 (4)	138

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