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6-[(*E*)-2-Phenylvinyl]-1*H*-indole

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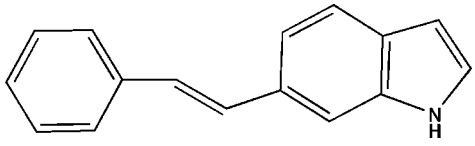
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.132; data-to-parameter ratio = 12.7.

The title compound, $C_{16}H_{13}N$, is essentially planar [maximum deviation from the least-squares plane = 0.081 (3) Å], with a dihedral angle of 1.65 (13)° between the planes of the indole and benzene rings. In the crystal, there are no significant intermolecular π–π interactions [minimum ring centroid–centroid separation = 4.217 (5) Å].

Related literature

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



Experimental

Crystal data

$C_{16}H_{13}N$
M_r = 219.29
Orthorhombic, $Pna2_1$
a = 8.254 (8) Å
b = 5.626 (6) Å
c = 25.74 (3) Å
V = 1195 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.10 mm

Data collection

Rigaku SCXmini CCD-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.982, T_{max} = 0.993
7653 measured reflections
1954 independent reflections
1627 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.08
1954 reflections
154 parameters
19 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2163).

References

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supporting information

Acta Cryst. (2012). E**68**, o73 [doi:10.1107/S1600536811051750]

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S1. Comment

The derivatives of indole are important chemical materials, because they are excellent drug intermediates for many pharmaceutical products (Kunzer & Wendt, 2011). As part of our interest in these materials, we report here the crystal structure of the title compound $C_{16}H_{13}N$ (Fig. 1).

This compound is essentially planar [maximum deviation from the least-squares plane 0.081 (3) Å (for C1)], with a dihedral angle of 1.65 (13)° between the planes of the indole and benzene ring systems. With the absence of no acceptor atoms in the molecule, no intermolecular hydrogen bonds are found in the crystal packing. Also, there are no significant intermolecular π–π interactions [minimum ring centroid separation, 4.217 (5) Å].

S2. Experimental

Crystals of 6-phenylvinylindole suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

S3. Refinement

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

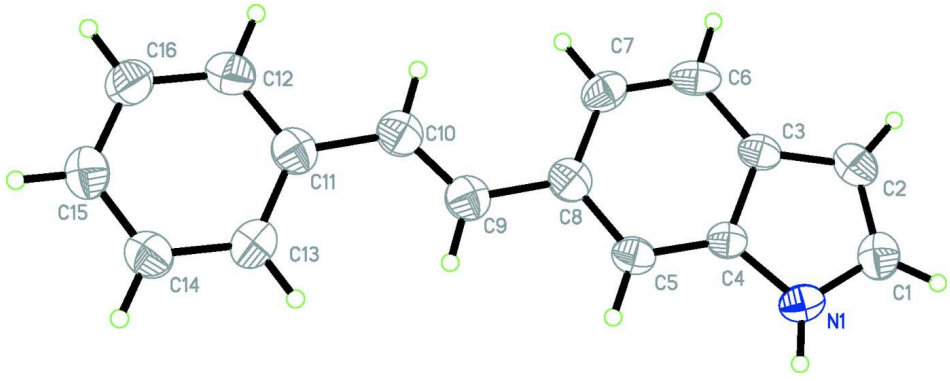

Figure 1

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.

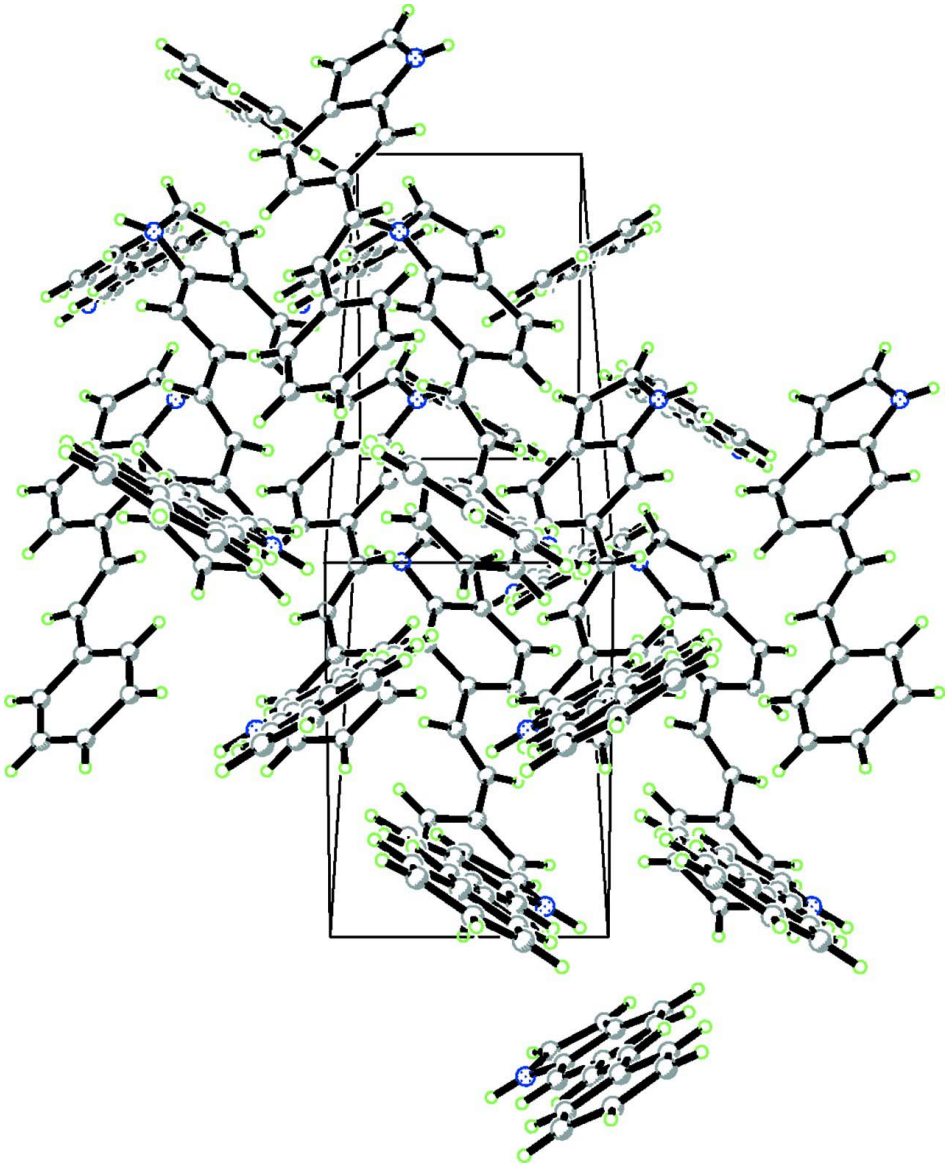

Figure 2

A packing in the unit cell viewed down the *a* axis.

6-[(*E*)-2-Phenylvinyl]-1*H*-indole

Crystal data

$C_{16}H_{13}N$
$M_r = 219.29$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 8.254$ (8) Å
$b = 5.626$ (6) Å
$c = 25.74$ (3) Å
$V = 1195$ (2) Å^3
$Z = 4$

$F(000) = 464$
$D_x = 1.218$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1954 reflections
$\theta = 3.2$–$25.0°$
$\mu = 0.07$ mm^{-1}
$T = 296$ K
Prism, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Rigaku SCXmini CCD-detector 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} = 0.982, T_{max} = 0.993
7653 measured reflections
1954 independent reflections
1627 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°, θ_{min} = 3.2°
h = −9→9
k = −6→6
l = −27→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.08
1954 reflections
154 parameters
19 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
$w = 1/[\sigma^2(F_o^2) + (0.0665P)^2 + 0.2586P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C2	−0.0689 (4)	0.5222 (6)	0.31498 (14)	0.0656 (8)
H2A	−0.0588	0.6242	0.2867	0.079*
C8	0.0968 (4)	0.4941 (5)	0.46948 (12)	0.0597 (6)
C7	0.1442 (3)	0.6940 (5)	0.43984 (13)	0.0623 (8)
H7A	0.2102	0.8076	0.4553	0.075*
C15	0.4035 (4)	0.4885 (6)	0.70717 (14)	0.0687 (9)
H15A	0.4359	0.4764	0.7417	0.082*
C5	−0.0018 (3)	0.3276 (5)	0.44626 (11)	0.0538 (7)
H5A	−0.0369	0.1955	0.4648	0.065*
C3	0.0004 (3)	0.5547 (5)	0.36510 (11)	0.0510 (6)
N1	−0.1423 (3)	0.2156 (4)	0.36424 (10)	0.0594 (6)
H1A	−0.1875	0.0850	0.3738	0.071*
C6	0.0972 (3)	0.7280 (5)	0.38924 (13)	0.0613 (8)
H6A	0.1289	0.8635	0.3712	0.074*
C10	0.2538 (4)	0.5725 (6)	0.55023 (12)	0.0658 (5)
H10A	0.3012	0.7004	0.5331	0.079*

C4	−0.0482 (3)	0.3585 (4)	0.39512 (11)	0.0471 (6)
C9	0.1498 (4)	0.4487 (6)	0.52418 (13)	0.0636 (5)
H9A	0.1036	0.3191	0.5410	0.076*
C12	0.4050 (4)	0.6954 (6)	0.62754 (15)	0.0720 (9)
H12A	0.4403	0.8245	0.6080	0.086*
C13	0.2544 (4)	0.3359 (6)	0.63444 (13)	0.0709 (9)
H13A	0.1880	0.2199	0.6200	0.085*
C11	0.3047 (4)	0.5306 (6)	0.60460 (13)	0.0640 (6)
C14	0.3045 (4)	0.3175 (6)	0.68583 (14)	0.0716 (9)
H14A	0.2710	0.1891	0.7059	0.086*
C16	0.4541 (4)	0.6758 (7)	0.67764 (14)	0.0745 (9)
H16A	0.5223	0.7901	0.6919	0.089*
C1	−0.1528 (4)	0.3136 (6)	0.31610 (14)	0.0672 (8)
H1B	−0.2087	0.2483	0.2882	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0589 (17)	0.074 (2)	0.0634 (19)	0.0063 (16)	0.0072 (14)	0.0118 (17)
C8	0.0534 (11)	0.0637 (12)	0.0620 (12)	0.0073 (10)	0.0089 (9)	−0.0038 (11)
C7	0.0517 (15)	0.0564 (17)	0.079 (2)	−0.0009 (13)	0.0019 (15)	−0.0132 (16)
C15	0.0648 (19)	0.078 (2)	0.063 (2)	0.0144 (17)	−0.0019 (16)	−0.0018 (18)
C5	0.0495 (14)	0.0506 (14)	0.0612 (19)	0.0012 (12)	0.0077 (13)	0.0047 (14)
C3	0.0395 (12)	0.0517 (14)	0.0618 (17)	0.0039 (11)	0.0095 (13)	0.0058 (13)
N1	0.0490 (12)	0.0554 (13)	0.0739 (18)	−0.0070 (10)	0.0006 (12)	−0.0002 (13)
C6	0.0507 (14)	0.0428 (13)	0.090 (2)	0.0006 (12)	0.0138 (16)	0.0090 (16)
C10	0.0604 (10)	0.0708 (11)	0.0661 (10)	0.0047 (9)	0.0093 (8)	−0.0033 (9)
C4	0.0389 (12)	0.0474 (13)	0.0550 (16)	0.0029 (10)	0.0045 (12)	0.0009 (12)
C9	0.0579 (9)	0.0675 (11)	0.0654 (10)	0.0049 (9)	0.0093 (8)	−0.0047 (9)
C12	0.0658 (19)	0.074 (2)	0.077 (2)	−0.0057 (16)	0.0101 (18)	0.0082 (19)
C13	0.0671 (19)	0.071 (2)	0.074 (2)	−0.0016 (16)	−0.0065 (18)	−0.0103 (18)
C11	0.0590 (11)	0.0707 (12)	0.0624 (12)	0.0082 (11)	0.0107 (10)	−0.0022 (11)
C14	0.073 (2)	0.070 (2)	0.072 (2)	0.0003 (16)	0.0026 (17)	0.0096 (17)
C16	0.067 (2)	0.078 (2)	0.078 (3)	−0.0089 (17)	−0.0027 (18)	−0.0035 (19)
C1	0.0569 (17)	0.082 (2)	0.0630 (19)	0.0074 (16)	−0.0034 (15)	−0.0041 (18)

Geometric parameters (Å, º)

C2—C1	1.363 (5)	N1—C4	1.372 (4)
C2—C3	1.423 (5)	N1—H1A	0.8600
C2—H2A	0.9300	C6—H6A	0.9300
C8—C5	1.377 (4)	C10—C9	1.293 (4)
C8—C7	1.415 (4)	C10—C11	1.480 (5)
C8—C9	1.497 (5)	C10—H10A	0.9300
C7—C6	1.372 (5)	C9—H9A	0.9300
C7—H7A	0.9300	C12—C16	1.356 (5)
C15—C16	1.365 (5)	C12—C11	1.376 (5)
C15—C14	1.377 (5)	C12—H12A	0.9300

C15—H15A	0.9300	C13—C14	1.390 (5)
C5—C4	1.382 (4)	C13—C11	1.401 (4)
C5—H5A	0.9300	C13—H13A	0.9300
C3—C4	1.406 (4)	C14—H14A	0.9300
C3—C6	1.405 (4)	C16—H16A	0.9300
N1—C1	1.359 (4)	C1—H1B	0.9300
C1—C2—C3	107.2 (3)	C11—C10—H10A	116.8
C1—C2—H2A	126.4	N1—C4—C5	129.5 (2)
C3—C2—H2A	126.4	N1—C4—C3	107.7 (3)
C5—C8—C7	118.0 (3)	C5—C4—C3	122.9 (3)
C5—C8—C9	117.7 (3)	C10—C9—C8	126.2 (3)
C7—C8—C9	124.2 (3)	C10—C9—H9A	116.9
C6—C7—C8	123.0 (3)	C8—C9—H9A	116.9
C6—C7—H7A	118.5	C16—C12—C11	122.2 (3)
C8—C7—H7A	118.5	C16—C12—H12A	118.9
C16—C15—C14	119.9 (3)	C11—C12—H12A	118.9
C16—C15—H15A	120.0	C14—C13—C11	119.5 (3)
C14—C15—H15A	120.0	C14—C13—H13A	120.3
C8—C5—C4	119.5 (3)	C11—C13—H13A	120.3
C8—C5—H5A	120.3	C12—C11—C13	118.0 (3)
C4—C5—H5A	120.3	C12—C11—C10	118.0 (3)
C4—C3—C6	117.7 (3)	C13—C11—C10	124.0 (3)
C4—C3—C2	106.4 (3)	C15—C14—C13	120.3 (3)
C6—C3—C2	135.9 (3)	C15—C14—H14A	119.9
C1—N1—C4	109.1 (2)	C13—C14—H14A	119.9
C1—N1—H1A	125.5	C12—C16—C15	120.1 (3)
C4—N1—H1A	125.5	C12—C16—H16A	120.0
C7—C6—C3	118.9 (3)	C15—C16—H16A	120.0
C7—C6—H6A	120.5	N1—C1—C2	109.7 (3)
C3—C6—H6A	120.5	N1—C1—H1B	125.2
C9—C10—C11	126.4 (3)	C2—C1—H1B	125.2
C9—C10—H10A	116.8		