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3-(1,2-Diphenylethenyl)-2-phenyl-1*H*-indole

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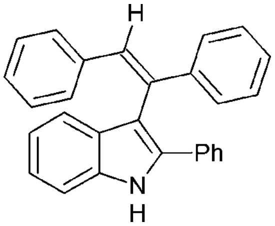
Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.070; *wR* factor = 0.221; data-to-parameter ratio = 17.6.

In the title compound, $C_{28}H_{21}N$, the planar pyrrole ring makes dihedral angles of 1.5 (2), 42.4 (2), 65.4 (2) and 79.7 (1)°, with the least squares planes of the four phenyl rings. The molecular structure and crystal packing are stabilized by weak inter- and intramolecular C—H⋯π interactions.

Related literature

For applications of heteroarenes, see: Ritleng *et al.* (2002). For their pharmaceutical properties and related reactions, see: Sundberg (1996); Ferrer *et al.* (2007); Nair *et al.* (2004; Sakai *et al.* (2006, 2008); Cheng *et al.* (2007); For standard bond lengths, see: Allen *et al.* (1987). For bond distances and angles in related structures, see: NizamMohideen *et al.* (2010*a*,*b*).



Experimental

Crystal data

$C_{28}H_{21}N$
M_r = 371.46
Monoclinic, $P2_1/c$
a = 11.4227 (6) Å
b = 8.6998 (5) Å
c = 20.6203 (13) Å
β = 94.413 (4)°
V = 2043.1 (2) Å^3
Z = 4
Mo *K*α radiation
μ = 0.07 mm^{-1}
T = 298 K
0.32 × 0.28 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer'
Absorption correction: multi-scan (*SADABS*; Bruker, 2004) T_{min} = 0.978, T_{max} = 0.985
14625 measured reflections
4674 independent reflections
1701 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.221
S = 1.01
4674 reflections
266 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N1/C1/C2/C3/C8 and C3–C8 rings, respectively.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C18—H18⋯*Cg*1	0.93	2.92	3.562 (2)	127
C20—H20⋯*Cg*2^{i}	0.93	2.92	3.825 (2)	164

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2059).

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supplementary materials

Acta Cryst. (2010). E**66**, o2745 [**doi:10.1107/S1600536810039309**]

3-(1,2-Diphenylethenyl)-2-phenyl-1*H*-indole

P. A. A. Mahaboob, M. NizamMohideen, G. Bhaskar and **P. T. Perumal**

Comment

The indole ring system exists ubiquitously in natural products, and exhibits biological and pharmaceutical properties (Sundberg, 1996). Ferrer and co-workers reported a systematic investigation on the gold-catalyzed intra- and intermolecular addition of indoles to alkynes (Ferrer *et al.*, 2007). Cheng and co-workers investigated the reaction of indoles with alkynyl alcohols employing platinum as a catalyst (Cheng *et al.*, 2007). Development of heteroarene functionalization has attracted much attention of their wide range of applications such as fluorescent dyes, synthetic analogues of natural products, and pharmaceuticals (Ritleng *et al.*, 2002). There has been considerable interest in the catalytic use of indium(III) halides in organic synthesis (Nair *et al.*, 2004), due to their unique properties such as non-toxicity, stability in air, and water tolerance (Sakai *et al.*, 2006). Indium(III) bromide is known to catalyze intramolecular cyclization of 2-alkynylanilines (Sakai *et al.*, 2008). In continuation of our work in this area, the title compound, $C_{28}H_{21}N$, (I) has been prepared and its crystal structure is reported.

In the title compound the pyrrole ring is planar, the maximum deviation from the least squares plane being -0.009 (1)Å for atom N1. The dihedral angle formed by the least squares planes of the pyrrole ring and the four benzene rings is 1.5 (2)° (C3—C8), 42.4 (2)° (C9—C14), 65.4 (2)° (C17—C22) and 79.7 (1)° (C23—C28), respectively. The dihedral angle between the phenyl rings C9—C14 and C23—C28 is 88.5 (2)°. The dihedral angle between benzene rings C3—C8 and C17—C22 is 66.7 (7)° and between rings C17—C22 and C23—C28 is 87.0 (2)°. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable with those in a previously reported structure (NizamMohideen *et al.*, 2010a,b). The molecular packing is stabilized by an intra and intermolecular C—H···π interactions (Table 1).

Experimental

A mixture of diphenylacetylene (2.4 mmol), 2-Phenyl indole (2 mmol), indium tribromide (0.2 mmol) in toluene (4 ml) was stirred at 383° K temperature for 2.5 h. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with water and extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4, concentrated *in vacuo* and purified by column chromatography on silica gel (Merck, 100 - 200 mesh) to afford the desired product after crystallization.

Refinement

H1N was located by a difference fourier map and refined isotropically. All other H atoms were positioned geometrically, with C—H = 0.93 and N—H = 0.89Å constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C, N)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all H atoms.

Figures

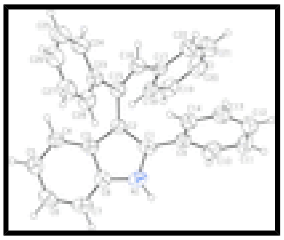

Fig. 1. The molecular structure of the title compound with the atom numbering scheme and 50% probability displacement ellipsoids. H atoms are presented as a small spheres of arbitrary radius.

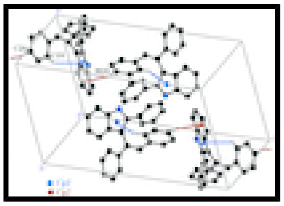

Fig. 2. C—H···π interactions (dashed lines) in the title compound. *Cg* denotes the ring centroid. [Symmetry codes: (i) *x*,y,*z*; (ii) *x*,1/2-y,-1/2+*z*]

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Crystal data

$C_{28}H_{21}N$
M_r = 371.46
Monoclinic, $P2_1/c$
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a = 11.4227 (6) Å
b = 8.6998 (5) Å
c = 20.6203 (13) Å
β = 94.413 (4)°
V = 2043.1 (2) Å^3
Z = 4

$F(000)$ = 784
D_x = 1.208 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1461 reflections
θ = 2.5–18.8°
μ = 0.07 mm^{-1}
T = 298 K
Block, colourless
0.32 × 0.28 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer'
Radiation source: fine-focus sealed tube
graphite
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.978, T_{max} = 0.985
14625 measured reflections

4674 independent reflections
1701 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 28.4°, θ_{min} = 2.5°
$h = -15 \rightarrow 13$
$k = -11 \rightarrow 10$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.070$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.221$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4674 reflections	$(\Delta/\sigma)_{max} < 0.001$
266 parameters	$\Delta\rho_{max} = 0.30$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.14$ 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*	$U_{iso}*/U_{eq}$
C1	0.6739 (3)	0.0471 (4)	0.09769 (15)	0.0597 (9)
C2	0.7394 (3)	0.1773 (4)	0.11004 (14)	0.0567 (8)
C3	0.6655 (3)	0.2848 (4)	0.14155 (14)	0.0553 (8)
C4	0.6798 (3)	0.4337 (4)	0.16344 (16)	0.0663 (9)
H4	0.7507	0.4842	0.1595	0.080*
C5	0.5896 (3)	0.5078 (4)	0.19108 (15)	0.0716 (10)
H5	0.6000	0.6082	0.2059	0.086*
C6	0.4831 (3)	0.4337 (5)	0.19703 (17)	0.0770 (11)
H6	0.4230	0.4842	0.2163	0.092*
C7	0.4662 (3)	0.2860 (5)	0.17452 (17)	0.0755 (11)
H7	0.3951	0.2356	0.1777	0.091*
C8	0.5580 (3)	0.2157 (4)	0.14725 (16)	0.0606 (9)
C9	0.7056 (3)	−0.1003 (4)	0.06783 (15)	0.0594 (9)
C10	0.6325 (3)	−0.1789 (5)	0.02351 (19)	0.0823 (11)
H10	0.5589	−0.1383	0.0111	0.099*
C11	0.6650 (4)	−0.3161 (5)	−0.0031 (2)	0.0910 (12)
H11	0.6136	−0.3684	−0.0325	0.109*
C12	0.7729 (5)	−0.3737 (5)	0.0142 (2)	0.0926 (13)
H12	0.7963	−0.4649	−0.0045	0.111*
C13	0.8484 (3)	−0.3000 (5)	0.0588 (2)	0.0807 (11)
H13	0.9214	−0.3426	0.0712	0.097*
C14	0.8157 (3)	−0.1631 (4)	0.08506 (17)	0.0687 (10)
H14	0.8675	−0.1119	0.1146	0.082*

C15	0.8582 (3)	0.2075 (4)	0.09030 (17)	0.0633 (9)
C16	0.8850 (3)	0.1954 (4)	0.02908 (16)	0.0647 (9)
H16	0.9649	0.1998	0.0233	0.078*
C17	0.8091 (3)	0.1761 (4)	−0.03113 (15)	0.0558 (8)
C18	0.6996 (3)	0.2448 (4)	−0.04003 (16)	0.0598 (9)
H18	0.6674	0.2921	−0.0051	0.072*
C19	0.6376 (3)	0.2438 (4)	−0.1002 (2)	0.0757 (10)
H19	0.5648	0.2918	−0.1059	0.091*
C20	0.6835 (4)	0.1720 (5)	−0.15140 (19)	0.0947 (13)
H20	0.6419	0.1727	−0.1920	0.114*
C21	0.7894 (4)	0.0995 (5)	−0.1438 (2)	0.0995 (13)
H21	0.8189	0.0484	−0.1787	0.119*
C22	0.8522 (3)	0.1024 (4)	−0.08424 (19)	0.0801 (11)
H22	0.9249	0.0541	−0.0793	0.096*
C23	0.9520 (3)	0.2436 (4)	0.14166 (17)	0.0627 (9)
C24	1.0480 (3)	0.3370 (5)	0.1295 (2)	0.0875 (12)
H24	1.0514	0.3805	0.0885	0.105*
C25	1.1354 (3)	0.3657 (5)	0.1754 (2)	0.1007 (14)
H25	1.1977	0.4287	0.1662	0.121*
C26	1.1321 (4)	0.3016 (6)	0.2357 (2)	0.1003 (14)
H26	1.1942	0.3174	0.2669	0.120*
C27	1.0389 (4)	0.2150 (5)	0.2505 (2)	0.0953 (13)
H27	1.0362	0.1739	0.2920	0.114*
C28	0.9482 (3)	0.1884 (4)	0.20368 (19)	0.0793 (11)
H28	0.8834	0.1320	0.2144	0.095*
N1	0.5641 (3)	0.0706 (4)	0.11907 (15)	0.0738 (9)
H1N	0.506 (3)	0.001 (5)	0.1187 (18)	0.107 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.051 (2)	0.076 (3)	0.053 (2)	0.0087 (17)	0.0059 (15)	0.0111 (17)
C2	0.061 (2)	0.065 (2)	0.0440 (19)	0.0007 (18)	0.0009 (15)	−0.0004 (16)
C3	0.0518 (19)	0.070 (2)	0.0433 (19)	−0.0028 (17)	−0.0002 (14)	0.0064 (17)
C4	0.067 (2)	0.072 (3)	0.060 (2)	−0.0061 (19)	0.0086 (17)	0.0030 (19)
C5	0.081 (3)	0.073 (2)	0.061 (2)	0.008 (2)	0.0041 (19)	−0.0043 (19)
C6	0.064 (2)	0.106 (3)	0.062 (2)	0.025 (2)	0.0081 (18)	0.001 (2)
C7	0.053 (2)	0.104 (3)	0.070 (3)	−0.004 (2)	0.0087 (17)	0.016 (2)
C8	0.059 (2)	0.063 (2)	0.059 (2)	0.0065 (18)	−0.0016 (16)	0.0055 (18)
C9	0.065 (2)	0.061 (2)	0.053 (2)	−0.0056 (18)	0.0043 (17)	0.0070 (17)
C10	0.076 (3)	0.085 (3)	0.083 (3)	−0.013 (2)	−0.010 (2)	0.004 (2)
C11	0.112 (4)	0.076 (3)	0.083 (3)	−0.020 (3)	−0.008 (3)	−0.017 (2)
C12	0.124 (4)	0.072 (3)	0.086 (3)	−0.013 (3)	0.036 (3)	−0.011 (2)
C13	0.084 (3)	0.071 (3)	0.089 (3)	0.000 (2)	0.020 (2)	0.009 (2)
C14	0.076 (3)	0.064 (2)	0.067 (2)	−0.0036 (19)	0.0091 (19)	0.0002 (19)
C15	0.058 (2)	0.074 (2)	0.058 (2)	0.0023 (16)	0.0013 (17)	−0.0049 (18)
C16	0.060 (2)	0.073 (2)	0.061 (2)	−0.0035 (17)	0.0036 (18)	−0.0031 (18)
C17	0.0472 (19)	0.068 (2)	0.051 (2)	−0.0121 (16)	−0.0044 (15)	−0.0015 (17)

C18	0.066 (2)	0.060 (2)	0.052 (2)	−0.0105 (17)	−0.0013 (17)	−0.0002 (16)
C19	0.079 (2)	0.072 (3)	0.073 (3)	−0.0073 (19)	−0.012 (2)	0.010 (2)
C20	0.115 (4)	0.113 (3)	0.052 (3)	−0.021 (3)	−0.011 (2)	−0.007 (2)
C21	0.100 (3)	0.136 (4)	0.063 (3)	−0.016 (3)	0.008 (2)	−0.032 (3)
C22	0.065 (2)	0.100 (3)	0.076 (3)	0.000 (2)	0.009 (2)	−0.022 (2)
C23	0.053 (2)	0.071 (2)	0.062 (2)	0.0034 (17)	−0.0091 (17)	−0.0047 (18)
C24	0.063 (2)	0.128 (4)	0.071 (3)	−0.006 (2)	0.002 (2)	−0.018 (2)
C25	0.058 (3)	0.152 (4)	0.091 (3)	−0.008 (2)	−0.002 (2)	−0.023 (3)
C26	0.062 (3)	0.146 (4)	0.089 (4)	0.014 (3)	−0.016 (2)	−0.030 (3)
C27	0.091 (3)	0.129 (4)	0.063 (3)	0.005 (3)	−0.011 (2)	−0.012 (2)
C28	0.076 (3)	0.092 (3)	0.067 (3)	−0.004 (2)	−0.013 (2)	0.000 (2)
N1	0.060 (2)	0.083 (2)	0.078 (2)	−0.0147 (18)	0.0016 (16)	0.0084 (18)

Geometric parameters (Å, °)

C1—C2	1.370 (4)	C15—C16	1.326 (4)
C1—N1	1.376 (4)	C15—C23	1.481 (5)
C1—C9	1.479 (4)	C16—C17	1.468 (4)
C2—C3	1.446 (4)	C16—H16	0.9300
C2—C15	1.470 (4)	C17—C18	1.386 (4)
C3—C4	1.377 (4)	C17—C22	1.391 (4)
C3—C8	1.380 (4)	C18—C19	1.381 (5)
C4—C5	1.376 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.365 (5)
C5—C6	1.392 (5)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.362 (5)
C6—C7	1.374 (5)	C20—H20	0.9300
C6—H6	0.9300	C21—C22	1.375 (5)
C7—C8	1.372 (4)	C21—H21	0.9300
C7—H7	0.9300	C22—H22	0.9300
C8—N1	1.393 (4)	C23—C28	1.370 (5)
C9—C10	1.372 (5)	C23—C24	1.404 (5)
C9—C14	1.392 (4)	C24—C25	1.345 (5)
C10—C11	1.377 (5)	C24—H24	0.9300
C10—H10	0.9300	C25—C26	1.365 (6)
C11—C12	1.352 (5)	C25—H25	0.9300
C11—H11	0.9300	C26—C27	1.358 (5)
C12—C13	1.371 (5)	C26—H26	0.9300
C12—H12	0.9300	C27—C28	1.380 (5)
C13—C14	1.372 (5)	C27—H27	0.9300
C13—H13	0.9300	C28—H28	0.9300
C14—H14	0.9300	N1—H1N	0.89 (4)
C2—C1—N1	108.4 (3)	C2—C15—C23	118.2 (3)
C2—C1—C9	130.3 (3)	C15—C16—C17	130.5 (3)
N1—C1—C9	121.4 (3)	C15—C16—H16	114.8
C1—C2—C3	106.8 (3)	C17—C16—H16	114.8
C1—C2—C15	126.7 (3)	C18—C17—C22	117.7 (3)
C3—C2—C15	126.3 (3)	C18—C17—C16	122.1 (3)
C4—C3—C8	117.8 (3)	C22—C17—C16	119.8 (3)

C4—C3—C2	134.2 (3)	C19—C18—C17	120.8 (3)
C8—C3—C2	108.0 (3)	C19—C18—H18	119.6
C5—C4—C3	120.2 (3)	C17—C18—H18	119.6
C5—C4—H4	119.9	C20—C19—C18	119.8 (4)
C3—C4—H4	119.9	C20—C19—H19	120.1
C4—C5—C6	120.5 (3)	C18—C19—H19	120.1
C4—C5—H5	119.8	C21—C20—C19	120.9 (4)
C6—C5—H5	119.8	C21—C20—H20	119.5
C7—C6—C5	120.3 (3)	C19—C20—H20	119.5
C7—C6—H6	119.9	C20—C21—C22	119.4 (4)
C5—C6—H6	119.9	C20—C21—H21	120.3
C8—C7—C6	117.6 (3)	C22—C21—H21	120.3
C8—C7—H7	121.2	C21—C22—C17	121.3 (4)
C6—C7—H7	121.2	C21—C22—H22	119.3
C7—C8—C3	123.6 (3)	C17—C22—H22	119.3
C7—C8—N1	129.8 (3)	C28—C23—C24	116.8 (3)
C3—C8—N1	106.6 (3)	C28—C23—C15	121.4 (3)
C10—C9—C14	117.7 (3)	C24—C23—C15	121.8 (3)
C10—C9—C1	123.6 (3)	C25—C24—C23	122.0 (4)
C14—C9—C1	118.6 (3)	C25—C24—H24	119.0
C9—C10—C11	121.9 (4)	C23—C24—H24	119.0
C9—C10—H10	119.0	C24—C25—C26	119.6 (4)
C11—C10—H10	119.0	C24—C25—H25	120.2
C12—C11—C10	119.0 (4)	C26—C25—H25	120.2
C12—C11—H11	120.5	C27—C26—C25	120.5 (4)
C10—C11—H11	120.5	C27—C26—H26	119.7
C11—C12—C13	121.1 (4)	C25—C26—H26	119.7
C11—C12—H12	119.4	C26—C27—C28	119.7 (4)
C13—C12—H12	119.4	C26—C27—H27	120.2
C12—C13—C14	119.6 (4)	C28—C27—H27	120.2
C12—C13—H13	120.2	C23—C28—C27	121.3 (4)
C14—C13—H13	120.2	C23—C28—H28	119.4
C13—C14—C9	120.5 (4)	C27—C28—H28	119.4
C13—C14—H14	119.7	C1—N1—C8	110.1 (3)
C9—C14—H14	119.7	C1—N1—H1N	126 (2)
C16—C15—C2	122.4 (3)	C8—N1—H1N	124 (2)
C16—C15—C23	119.4 (3)		

N1—C1—C2—C3	0.9 (3)	C3—C2—C15—C16	−120.7 (4)
C9—C1—C2—C3	−178.4 (3)	C1—C2—C15—C23	−122.5 (3)
N1—C1—C2—C15	−174.5 (3)	C3—C2—C15—C23	63.0 (4)
C9—C1—C2—C15	6.2 (5)	C2—C15—C16—C17	10.5 (6)
C1—C2—C3—C4	−177.6 (3)	C23—C15—C16—C17	−173.2 (3)
C15—C2—C3—C4	−2.2 (6)	C15—C16—C17—C18	35.3 (5)
C1—C2—C3—C8	0.1 (3)	C15—C16—C17—C22	−152.4 (4)
C15—C2—C3—C8	175.5 (3)	C22—C17—C18—C19	−2.0 (4)
C8—C3—C4—C5	1.2 (4)	C16—C17—C18—C19	170.4 (3)
C2—C3—C4—C5	178.8 (3)	C17—C18—C19—C20	1.2 (5)
C3—C4—C5—C6	−0.2 (5)	C18—C19—C20—C21	0.8 (6)
C4—C5—C6—C7	−0.9 (5)	C19—C20—C21—C22	−1.8 (6)

C5—C6—C7—C8	0.9 (5)	C20—C21—C22—C17	0.9 (6)
C6—C7—C8—C3	0.2 (5)	C18—C17—C22—C21	1.0 (5)
C6—C7—C8—N1	−177.8 (3)	C16—C17—C22—C21	−171.6 (3)
C4—C3—C8—C7	−1.3 (5)	C16—C15—C23—C28	−148.1 (3)
C2—C3—C8—C7	−179.4 (3)	C2—C15—C23—C28	28.3 (5)
C4—C3—C8—N1	177.1 (3)	C16—C15—C23—C24	32.6 (5)
C2—C3—C8—N1	−1.0 (3)	C2—C15—C23—C24	−150.9 (3)
C2—C1—C9—C10	−138.1 (4)	C28—C23—C24—C25	3.1 (5)
N1—C1—C9—C10	42.6 (5)	C15—C23—C24—C25	−177.6 (3)
C2—C1—C9—C14	41.5 (5)	C23—C24—C25—C26	0.5 (6)
N1—C1—C9—C14	−137.8 (3)	C24—C25—C26—C27	−3.0 (7)
C14—C9—C10—C11	0.6 (5)	C25—C26—C27—C28	1.7 (6)
C1—C9—C10—C11	−179.8 (3)	C24—C23—C28—C27	−4.4 (5)
C9—C10—C11—C12	−1.1 (6)	C15—C23—C28—C27	176.3 (3)
C10—C11—C12—C13	1.8 (6)	C26—C27—C28—C23	2.1 (6)
C11—C12—C13—C14	−2.0 (6)	C2—C1—N1—C8	−1.6 (4)
C12—C13—C14—C9	1.4 (5)	C9—C1—N1—C8	177.8 (3)
C10—C9—C14—C13	−0.7 (5)	C7—C8—N1—C1	179.9 (3)
C1—C9—C14—C13	179.6 (3)	C3—C8—N1—C1	1.6 (4)
C1—C2—C15—C16	53.8 (5)		

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the N1/C1/C2/C3/C8 and C3–C8 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···Cg1	0.93	2.92	3.562 (2)	127
C20—H20···Cg2^{i}	0.93	2.92	3.825 (2)	164

Symmetry codes: (i) $x, -y-1/2, z-3/2$.

Fig. 1

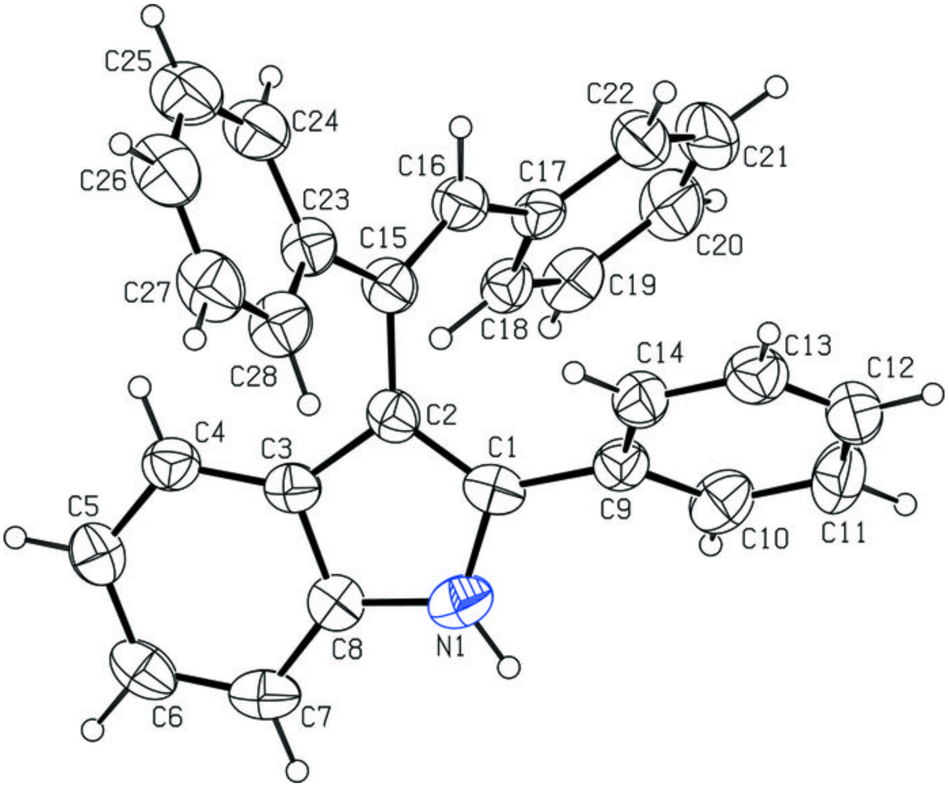
C25
C24
C26
C23
C16
C17
C22
C21
C20
C15
C27
C28
C18
C19
C14
C13
C12
C4
C3
C2
C1
C9
C5
C10
C11
C8
N1
C6
C7

Fig. 2