

N-[(E)-(9-Ethyl-9H-carbazol-3-yl)methylidene]aniline

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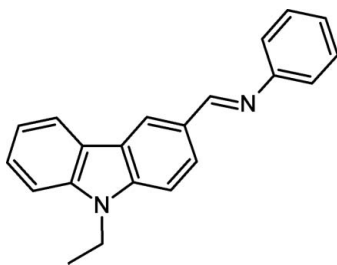
Received 3 May 2010; accepted 19 May 2010

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.062; wR factor = 0.148; data-to-parameter ratio = 13.6.

The title compound, $\text{C}_{21}\text{H}_{18}\text{N}_2$, was obtained as the product of the reaction between 9-ethyl-9H-carbazole-3-carbaldehyde and aniline in ethanol. The crystal packing is stabilized mainly by $\text{C}-\text{H}\cdots\pi$ interactions between the carbazole benzene rings and the methylene H atoms.

Related literature

For background to photoconductive properties see: Segura (1998); Grigoras & Antonoaia (2005). For geometrical parameters in related structures, see: Wang *et al.* (2008); Huang *et al.* (2008).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{18}\text{N}_2$
 $M_r = 298.37$
 Monoclinic, $P2_1/n$
 $a = 15.3350$ (3) Å

$b = 5.9692$ (10) Å
 $c = 17.5447$ (3) Å
 $\beta = 91.162$ (1)°
 $V = 1605.7$ (3) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹

$T = 295$ K
 $0.6 \times 0.4 \times 0.2$ mm

Data collection

Rigaku R-Axis RAPID S diffractometer
 28963 measured reflections

2838 independent reflections
 2821 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$
 $wR(F^2) = 0.148$
 $S = 1.41$
 2838 reflections

209 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ and $Cg2$ are the centroids of the $C1-C4/C4A/C9A$ and $C4B/C5-C8/C8A$ rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------|-------|-------------|-------------|---------------|
| $C5-H5\cdots Cg1^i$ | 0.93 | 2.87 | 3.587 (3) | 135 |
| $C12-H12\cdots Cg2^i$ | 0.93 | 2.98 | 3.660 (3) | 131 |
| $C10-H10A\cdots Cg2^{ii}$ | 0.97 | 3.25 | 4.050 (4) | 142 |

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

Data collection: *CrystalStructure* (Rigaku & Rigaku/MS, 2003); cell refinement: *CrystalStructure*; data reduction: *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Scientific Research Projects Department (BAP) at Balıkesir University for financial support (Project No. 08/06).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2337).

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supplementary materials

Acta Cryst. (2010). E66, o1456 [doi:10.1107/S1600536810018660]

N-[(*E*)-(9-Ethyl-9*H*-carbazol-3-yl)methylidene]aniline

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Comment

The structure of the title compound is depicted in (Fig. 1). The bond lengths and internal bond angles of the carbazole skeleton are comparable to those of related molecules (Wang *et al.*, 2008; Huang *et al.*, 2008). The carbazole and phenyl skeletons are essentially planar with r.m.s deviations of 0.021 Å (carbazole ring) and 0.008 Å (phenyl ring). The phenyl ring is twisted away from the carbazole ring by 67.45 (05)°. The ethyl group protrudes out of the plane of the carbazole skeleton as indicated by the C9A—N9—C10—C11 torsion angle of 86.0 (3)°. The only force that stack the molecules appears to be π -ring C—H...Cg intermolecular interactions among the benzene rings of carbazole and the hydrogen atoms H5, H10A and H12 (Fig. 2).

Experimental

The title compound was synthesized via the imine reaction between aniline and 9-ethyl-9*H*-carbazol-3-carbaldehyde in ethanol. In a round bottom flask fitted with a magnetic stirrer a solution was prepared from 9-ethyl-9*H*-carbazol-3-carbaldehyde (1.116 g, 5 mmol) and aniline (0.70 g, 7.5 mmol) in 50 ml ethanol at ambient temperature. After stirring for 2 h, the solution was left for crystallization overnight, after which time the product was precipitated as yellow crystals. The crude product was separated by filtration and washed with ethanol. Yellow, transparent crystals suitable for the X-ray diffraction analysis were grown from tetrahydrofuran by slow evaporation technique at ambient temperature, mp. 407 K. FT—IR (KBr) ν_{\max} (cm⁻¹): 3048 (Ar—H), 2973 (—CH₃), 2930 (—CH₂—), 1618 (C=N), 1587, 1567 (Ar—N), 1489, 1473, 1461 (Ar C=C); ¹HNMR (300 MHz, CDCl₃, ppm): 1.46 (t, J = 7.3 Hz, 3H, CH₃), 4.38 (q, J = 7.3 Hz, 2H, —CH₂—), 7.21-7.59 (m, 9H, ArH), 8.07 (dd, J = 8.5 and 1.8 Hz, 1H, H2), 8.18 (dt, J = 7.9 and 0.8 Hz, 1H, H5), 8.64 (s, 1H, H12), 8.65 (d, J = 1.8, 1H, H4). UV-Vis, [EtOH, λ_{\max} (nm), (ϵ)] = 238 (25800), 293 (22100), 338 (18500).

Refinement

All non-hydrogen atoms were refined anisotropically; the hydrogen atoms were positioned geometrically and allowed to ride on their corresponding parent atoms with C—H distances of 0.93 Å (aromatic), 0.96 Å (methyl), and 0.97 Å (methylene) with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ of the parent atom for the methyl group and $1.2U_{\text{eq}}(\text{C})$ for the rest.

Figures

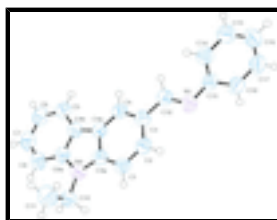


Fig. 1. The structure of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level and arbitrary spheres are shown for the H atoms.

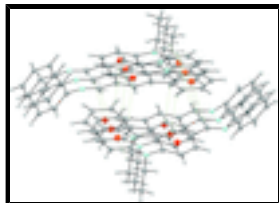


Fig. 2. Packing diagram of showing C—H...Cg intermolecular interactions; red spheres represent ring centroids.

N-[(*E*)-(9-Ethyl-9*H*-carbazol-3-yl)methylidene]aniline

Crystal data

| | |
|--------------------------------|---|
| $C_{21}H_{18}N_2$ | $F(000) = 632$ |
| $M_r = 298.37$ | $D_x = 1.234 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: $-P 2_1/n$ | Cell parameters from 8828 reflections |
| $a = 15.3350 (3) \text{ \AA}$ | $\theta = 2.3\text{--}25.3^\circ$ |
| $b = 5.9692 (10) \text{ \AA}$ | $\mu = 0.07 \text{ mm}^{-1}$ |
| $c = 17.5447 (3) \text{ \AA}$ | $T = 295 \text{ K}$ |
| $\beta = 91.162 (1)^\circ$ | Prism, yellow |
| $V = 1605.7 (3) \text{ \AA}^3$ | $0.6 \times 0.4 \times 0.2 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|--|--|
| Rigaku R-AXIS RAPID S diffractometer | $R_{\text{int}} = 0.030$ |
| graphite | $\theta_{\text{max}} = 25.2^\circ$, $\theta_{\text{min}} = 2.3^\circ$ |
| ω scans | $h = -18 \rightarrow 18$ |
| 28963 measured reflections | $k = -6 \rightarrow 7$ |
| 2838 independent reflections | $l = -20 \rightarrow 20$ |
| 2821 reflections with $I > 2\sigma(I)$ | |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.062$ | H-atom parameters constrained |
| $wR(F^2) = 0.148$ | $w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.4831P]$ |
| $S = 1.41$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2838 reflections | $(\Delta/\sigma)_{\text{max}} = 0.002$ |
| 209 parameters | $\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008) |
| | Extinction coefficient: 0.0123 (17) |

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|-------------|--------------|----------------------------------|
| N1 | 0.53644 (12) | -0.2326 (3) | 0.39241 (11) | 0.0627 (5) |
| N9 | 0.15252 (12) | 0.1918 (3) | 0.39179 (10) | 0.0567 (5) |
| C1 | 0.31091 (15) | 0.1662 (4) | 0.42835 (13) | 0.0583 (6) |
| H1 | 0.3127 | 0.2991 | 0.456 | 0.07* |
| C2 | 0.38396 (14) | 0.0359 (4) | 0.42111 (12) | 0.0580 (6) |
| H2 | 0.436 | 0.0829 | 0.444 | 0.07* |
| C3 | 0.38256 (14) | -0.1669 (4) | 0.38000 (12) | 0.0530 (5) |
| C4 | 0.30554 (14) | -0.2380 (4) | 0.34500 (12) | 0.0531 (5) |
| H4 | 0.304 | -0.3717 | 0.3178 | 0.064* |
| C4A | 0.23047 (13) | -0.1080 (4) | 0.35070 (11) | 0.0511 (5) |
| C4B | 0.14167 (13) | -0.1318 (4) | 0.32328 (11) | 0.0520 (5) |
| C5 | 0.09773 (15) | -0.2925 (4) | 0.27965 (12) | 0.0611 (6) |
| H5 | 0.1274 | -0.4154 | 0.2605 | 0.073* |
| C6 | 0.00979 (16) | -0.2669 (5) | 0.26525 (14) | 0.0678 (7) |
| H6 | -0.0202 | -0.3737 | 0.2364 | 0.081* |
| C7 | -0.03468 (16) | -0.0827 (5) | 0.29346 (14) | 0.0684 (7) |
| H7 | -0.0942 | -0.0697 | 0.2833 | 0.082* |
| C8 | 0.00672 (15) | 0.0809 (4) | 0.33593 (13) | 0.0636 (6) |
| H8 | -0.0235 | 0.2044 | 0.354 | 0.076* |
| C8A | 0.09549 (14) | 0.0541 (4) | 0.35072 (11) | 0.0542 (5) |
| C9A | 0.23398 (14) | 0.0931 (4) | 0.39289 (11) | 0.0522 (5) |
| C10 | 0.12624 (16) | 0.3717 (4) | 0.44220 (14) | 0.0651 (6) |
| H10A | 0.0808 | 0.4594 | 0.4171 | 0.078* |
| H10B | 0.1757 | 0.4697 | 0.452 | 0.078* |
| C11 | 0.0931 (2) | 0.2849 (5) | 0.51707 (15) | 0.0874 (9) |
| H11A | 0.0766 | 0.4088 | 0.5486 | 0.131* |
| H11B | 0.1382 | 0.2003 | 0.5425 | 0.131* |
| H11C | 0.0434 | 0.1904 | 0.5077 | 0.131* |
| C12 | 0.46110 (14) | -0.3017 (4) | 0.37283 (12) | 0.0553 (5) |
| H12 | 0.4557 | -0.4456 | 0.3529 | 0.066* |
| C13 | 0.60811 (14) | -0.3801 (4) | 0.38491 (12) | 0.0550 (5) |
| C14 | 0.61128 (15) | -0.5881 (4) | 0.41922 (13) | 0.0636 (6) |
| H14 | 0.5646 | -0.6363 | 0.448 | 0.076* |

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|-----|--------------|-------------|--------------|------------|
| C15 | 0.68271 (18) | -0.7249 (5) | 0.41133 (16) | 0.0767 (7) |
| H15 | 0.6844 | -0.8639 | 0.4352 | 0.092* |
| C16 | 0.75146 (18) | -0.6566 (5) | 0.36830 (18) | 0.0818 (8) |
| H16 | 0.7992 | -0.7505 | 0.362 | 0.098* |
| C17 | 0.74958 (16) | -0.4498 (5) | 0.33467 (16) | 0.0795 (8) |
| H17 | 0.7964 | -0.4032 | 0.3057 | 0.095* |
| C18 | 0.67877 (15) | -0.3096 (4) | 0.34333 (14) | 0.0674 (6) |
| H18 | 0.6786 | -0.1679 | 0.3212 | 0.081* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| N1 | 0.0557 (11) | 0.0652 (12) | 0.0671 (12) | 0.0002 (9) | -0.0018 (9) | -0.0068 (10) |
| N9 | 0.0579 (11) | 0.0550 (11) | 0.0573 (10) | 0.0052 (9) | 0.0051 (8) | -0.0043 (9) |
| C1 | 0.0646 (13) | 0.0538 (13) | 0.0566 (12) | -0.0033 (11) | 0.0010 (10) | -0.0071 (10) |
| C2 | 0.0570 (12) | 0.0616 (14) | 0.0553 (12) | -0.0056 (11) | -0.0028 (10) | -0.0016 (11) |
| C3 | 0.0549 (12) | 0.0564 (13) | 0.0477 (11) | 0.0000 (10) | 0.0020 (9) | 0.0005 (10) |
| C4 | 0.0592 (12) | 0.0516 (12) | 0.0485 (11) | -0.0004 (10) | 0.0014 (9) | -0.0044 (9) |
| C4A | 0.0549 (12) | 0.0514 (12) | 0.0470 (11) | -0.0026 (10) | 0.0012 (9) | 0.0000 (9) |
| C4B | 0.0558 (12) | 0.0567 (12) | 0.0435 (10) | -0.0015 (10) | 0.0022 (9) | 0.0047 (9) |
| C5 | 0.0686 (14) | 0.0626 (14) | 0.0519 (12) | -0.0042 (11) | -0.0041 (10) | -0.0013 (11) |
| C6 | 0.0647 (14) | 0.0795 (17) | 0.0589 (13) | -0.0129 (13) | -0.0095 (11) | 0.0054 (12) |
| C7 | 0.0551 (13) | 0.0889 (19) | 0.0611 (14) | -0.0045 (13) | -0.0032 (11) | 0.0162 (13) |
| C8 | 0.0590 (13) | 0.0738 (16) | 0.0582 (13) | 0.0065 (12) | 0.0053 (10) | 0.0093 (12) |
| C8A | 0.0573 (12) | 0.0593 (13) | 0.0461 (11) | -0.0012 (10) | 0.0037 (9) | 0.0062 (10) |
| C9A | 0.0569 (12) | 0.0518 (12) | 0.0480 (11) | 0.0003 (10) | 0.0051 (9) | 0.0009 (9) |
| C10 | 0.0702 (15) | 0.0567 (13) | 0.0688 (15) | 0.0077 (12) | 0.0092 (12) | -0.0066 (11) |
| C11 | 0.101 (2) | 0.102 (2) | 0.0603 (15) | 0.0029 (18) | 0.0132 (14) | -0.0073 (15) |
| C12 | 0.0577 (13) | 0.0579 (13) | 0.0505 (12) | -0.0021 (10) | 0.0031 (9) | -0.0029 (10) |
| C13 | 0.0519 (12) | 0.0608 (13) | 0.0524 (12) | -0.0049 (10) | -0.0024 (9) | -0.0068 (10) |
| C14 | 0.0626 (14) | 0.0665 (15) | 0.0619 (14) | -0.0044 (12) | 0.0076 (11) | -0.0003 (11) |
| C15 | 0.0802 (17) | 0.0668 (16) | 0.0833 (18) | 0.0074 (14) | 0.0044 (14) | 0.0030 (14) |
| C16 | 0.0649 (16) | 0.082 (2) | 0.099 (2) | 0.0120 (14) | 0.0043 (14) | -0.0125 (17) |
| C17 | 0.0560 (14) | 0.093 (2) | 0.0902 (19) | -0.0115 (14) | 0.0155 (13) | -0.0126 (16) |
| C18 | 0.0640 (14) | 0.0665 (15) | 0.0720 (15) | -0.0111 (12) | 0.0052 (12) | -0.0017 (12) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|----------|-----------|
| N1—C12 | 1.268 (3) | C7—C8 | 1.376 (3) |
| N1—C13 | 1.416 (3) | C7—H7 | 0.93 |
| N9—C9A | 1.381 (3) | C8—C8A | 1.390 (3) |
| N9—C8A | 1.391 (3) | C8—H8 | 0.93 |
| N9—C10 | 1.453 (3) | C10—C11 | 1.510 (3) |
| C1—C2 | 1.372 (3) | C10—H10A | 0.97 |
| C1—C9A | 1.393 (3) | C10—H10B | 0.97 |
| C1—H1 | 0.93 | C11—H11A | 0.96 |
| C2—C3 | 1.409 (3) | C11—H11B | 0.96 |
| C2—H2 | 0.93 | C11—H11C | 0.96 |
| C3—C4 | 1.386 (3) | C12—H12 | 0.93 |

| | | | |
|-------------|-------------|---------------|-------------|
| C3—C12 | 1.456 (3) | C13—C14 | 1.380 (3) |
| C4—C4A | 1.393 (3) | C13—C18 | 1.384 (3) |
| C4—H4 | 0.93 | C14—C15 | 1.375 (3) |
| C4A—C9A | 1.411 (3) | C14—H14 | 0.93 |
| C4A—C4B | 1.442 (3) | C15—C16 | 1.371 (4) |
| C4B—C5 | 1.393 (3) | C15—H15 | 0.93 |
| C4B—C8A | 1.407 (3) | C16—C17 | 1.368 (4) |
| C5—C6 | 1.376 (3) | C16—H16 | 0.93 |
| C5—H5 | 0.93 | C17—C18 | 1.382 (4) |
| C6—C7 | 1.390 (4) | C17—H17 | 0.93 |
| C6—H6 | 0.93 | C18—H18 | 0.93 |
| C12—N1—C13 | 118.5 (2) | N9—C9A—C1 | 129.1 (2) |
| C9A—N9—C8A | 108.32 (18) | N9—C9A—C4A | 109.32 (18) |
| C9A—N9—C10 | 124.65 (19) | C1—C9A—C4A | 121.6 (2) |
| C8A—N9—C10 | 124.95 (19) | N9—C10—C11 | 112.2 (2) |
| C2—C1—C9A | 117.8 (2) | N9—C10—H10A | 109.2 |
| C2—C1—H1 | 121.1 | C11—C10—H10A | 109.2 |
| C9A—C1—H1 | 121.1 | N9—C10—H10B | 109.2 |
| C1—C2—C3 | 122.0 (2) | C11—C10—H10B | 109.2 |
| C1—C2—H2 | 119 | H10A—C10—H10B | 107.9 |
| C3—C2—H2 | 119 | C10—C11—H11A | 109.5 |
| C4—C3—C2 | 119.6 (2) | C10—C11—H11B | 109.5 |
| C4—C3—C12 | 119.4 (2) | H11A—C11—H11B | 109.5 |
| C2—C3—C12 | 121.0 (2) | C10—C11—H11C | 109.5 |
| C3—C4—C4A | 119.7 (2) | H11A—C11—H11C | 109.5 |
| C3—C4—H4 | 120.1 | H11B—C11—H11C | 109.5 |
| C4A—C4—H4 | 120.1 | N1—C12—C3 | 123.2 (2) |
| C4—C4A—C9A | 119.24 (19) | N1—C12—H12 | 118.4 |
| C4—C4A—C4B | 134.2 (2) | C3—C12—H12 | 118.4 |
| C9A—C4A—C4B | 106.53 (18) | C14—C13—C18 | 118.8 (2) |
| C5—C4B—C8A | 119.4 (2) | C14—C13—N1 | 122.6 (2) |
| C5—C4B—C4A | 134.0 (2) | C18—C13—N1 | 118.5 (2) |
| C8A—C4B—C4A | 106.66 (19) | C15—C14—C13 | 120.7 (2) |
| C6—C5—C4B | 119.1 (2) | C15—C14—H14 | 119.6 |
| C6—C5—H5 | 120.5 | C13—C14—H14 | 119.6 |
| C4B—C5—H5 | 120.5 | C16—C15—C14 | 120.1 (3) |
| C5—C6—C7 | 120.6 (2) | C16—C15—H15 | 119.9 |
| C5—C6—H6 | 119.7 | C14—C15—H15 | 119.9 |
| C7—C6—H6 | 119.7 | C17—C16—C15 | 119.7 (3) |
| C8—C7—C6 | 122.0 (2) | C17—C16—H16 | 120.1 |
| C8—C7—H7 | 119 | C15—C16—H16 | 120.1 |
| C6—C7—H7 | 119 | C16—C17—C18 | 120.6 (2) |
| C7—C8—C8A | 117.3 (2) | C16—C17—H17 | 119.7 |
| C7—C8—H8 | 121.3 | C18—C17—H17 | 119.7 |
| C8A—C8—H8 | 121.3 | C17—C18—C13 | 119.9 (2) |
| N9—C8A—C8 | 129.2 (2) | C17—C18—H18 | 120 |
| N9—C8A—C4B | 109.14 (18) | C13—C18—H18 | 120 |
| C8—C8A—C4B | 121.7 (2) | | |

supplementary materials

| | | | |
|-----------------|--------------|-----------------|--------------|
| C9A—C1—C2—C3 | -0.6 (3) | C8A—N9—C9A—C1 | -178.4 (2) |
| C1—C2—C3—C4 | 0.5 (3) | C10—N9—C9A—C1 | -14.2 (4) |
| C1—C2—C3—C12 | 179.7 (2) | C8A—N9—C9A—C4A | 1.4 (2) |
| C2—C3—C4—C4A | 0.1 (3) | C10—N9—C9A—C4A | 165.58 (19) |
| C12—C3—C4—C4A | -179.05 (19) | C2—C1—C9A—N9 | 179.7 (2) |
| C3—C4—C4A—C9A | -0.7 (3) | C2—C1—C9A—C4A | 0.0 (3) |
| C3—C4—C4A—C4B | -178.9 (2) | C4—C4A—C9A—N9 | -179.11 (19) |
| C4—C4A—C4B—C5 | -1.2 (4) | C4B—C4A—C9A—N9 | -0.5 (2) |
| C9A—C4A—C4B—C5 | -179.6 (2) | C4—C4A—C9A—C1 | 0.7 (3) |
| C4—C4A—C4B—C8A | 177.8 (2) | C4B—C4A—C9A—C1 | 179.34 (19) |
| C9A—C4A—C4B—C8A | -0.6 (2) | C9A—N9—C10—C11 | -86.0 (3) |
| C8A—C4B—C5—C6 | -0.8 (3) | C8A—N9—C10—C11 | 75.7 (3) |
| C4A—C4B—C5—C6 | 178.0 (2) | C13—N1—C12—C3 | 178.29 (19) |
| C4B—C5—C6—C7 | 0.3 (3) | C4—C3—C12—N1 | 168.4 (2) |
| C5—C6—C7—C8 | 0.5 (4) | C2—C3—C12—N1 | -10.7 (3) |
| C6—C7—C8—C8A | -0.8 (3) | C12—N1—C13—C14 | -56.6 (3) |
| C9A—N9—C8A—C8 | 178.3 (2) | C12—N1—C13—C18 | 125.4 (2) |
| C10—N9—C8A—C8 | 14.1 (4) | C18—C13—C14—C15 | -1.0 (3) |
| C9A—N9—C8A—C4B | -1.7 (2) | N1—C13—C14—C15 | -179.1 (2) |
| C10—N9—C8A—C4B | -165.92 (19) | C13—C14—C15—C16 | -0.8 (4) |
| C7—C8—C8A—N9 | -179.8 (2) | C14—C15—C16—C17 | 1.5 (4) |
| C7—C8—C8A—C4B | 0.3 (3) | C15—C16—C17—C18 | -0.4 (4) |
| C5—C4B—C8A—N9 | -179.41 (18) | C16—C17—C18—C13 | -1.5 (4) |
| C4A—C4B—C8A—N9 | 1.4 (2) | C14—C13—C18—C17 | 2.1 (3) |
| C5—C4B—C8A—C8 | 0.5 (3) | N1—C13—C18—C17 | -179.7 (2) |
| C4A—C4B—C8A—C8 | -178.60 (19) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C1—C4/C4A/C9A and C4B/C5—C8/C8A rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|-------|-------------|-------------|---------------|
| C5—H5 \cdots Cg1 ⁱ | 0.93 | 2.87 | 3.587 (3) | 135. |
| C12—H12 \cdots Cg2 ⁱ | 0.93 | 2.98 | 3.660 (3) | 131. |
| C10—H10A \cdots Cg2 ⁱⁱ | 0.97 | 3.25 | 4.050 (4) | 142. |

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

Fig. 1

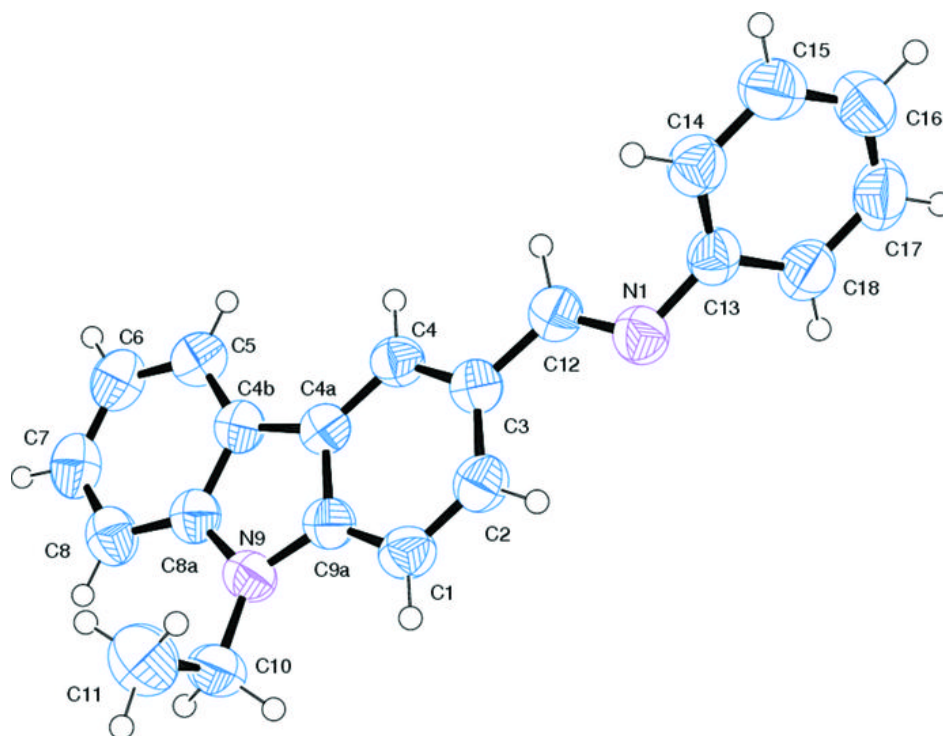


Fig. 2

