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## Structure Reports

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2-Methyl-3-*p*-tolyl-3*H*-benzo[*e*]indole-1-carbonitrileJiang-Sheng Li,<sup>a\*</sup> Qi-Xi He<sup>b</sup> and Peng-Yu Li<sup>a</sup><sup>a</sup>School of Chemistry and Biological Engineering, Changsha University of Science & Technology, Changsha 410004, People's Republic of China, and <sup>b</sup>College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, People's Republic of China

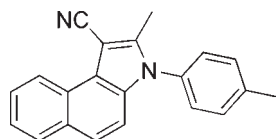
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.056;  $wR$  factor = 0.168; data-to-parameter ratio = 13.6.

In the title compound,  $\text{C}_{21}\text{H}_{16}\text{N}_2$ , the dihedral angle between the benzindole and tosyl ring systems is  $71.99(7)^\circ$ . In the crystal, molecules are linked into centrosymmetric dimers by pairs of  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds, generating  $R_2^2(16)$  loops.

## Related literature

For the synthesis, see: Du *et al.* (2006).

## Experimental

## Crystal data

 $\text{C}_{21}\text{H}_{16}\text{N}_2$   
 $M_r = 296.36$ Monoclinic,  $P2_1/n$   
 $a = 10.321(2)$  Å $b = 12.422(3)$  Å  
 $c = 13.258(3)$  Å  
 $\beta = 107.14(3)^\circ$   
 $V = 1624.4(6)$  Å<sup>3</sup>  
 $Z = 4$ Mo  $K\alpha$  radiation  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.28 \times 0.20 \times 0.18$  mm

## Data collection

Rigaku Saturn CCD diffractometer  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku/MS, 2005)  
 $T_{\min} = 0.980$ ,  $T_{\max} = 0.987$ 10714 measured reflections  
2858 independent reflections  
2092 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.168$   
 $S = 1.04$   
2858 reflections210 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.16$  e Å<sup>-3</sup>**Table 1**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C16}-\text{H16}\cdots\text{N2}^i$	0.93	2.60	3.480 (3)	158

Symmetry code: (i)  $-x, -y + 2, -z$ .

Data collection: *CrystalClear* (Rigaku/MS, 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5275).

## References

- Du, Y. F., Liu, R. H., Linn, G. & Zhao, K. (2006). *Org. Lett.* **8**, 5919–5922.  
Rigaku/MS (2005). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

*Acta Cryst.* (2010). E66, o111 [ doi:10.1107/S1600536809052441 ]

## 2-Methyl-3-*p*-tolyl-3*H*-benzo[*e*]indole-1-carbonitrile

J.-S. Li, Q.-X. He and P.-Y. Li

### Comment

The title compound, (I), comprises of a benzoindole ring and tosyl ring (Fig. 1). The dihedral angle of both rings is 71.99 (7)°.

In the crystal packing, molecules are linked into centrosymmetric dimers by C—H···N hydrogen bonds (Table 1). Weak C—H··· $\pi$  interactions help dimers pack. No significant  $\pi$ - $\pi$  stacking interaction was observed.

### Experimental

The compound was obtained according to the method of Du and his coworkers (2006). Colourless block of (I) was grown by slow evaporation of its ethanolic solution.

### Refinement

All H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{CH})$  or  $1.5U_{\text{eq}}(\text{CH}_3)$ .

### Figures

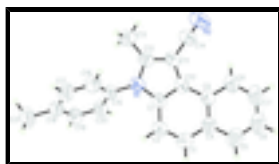


Fig. 1. The molecule of (I) showing displacement ellipsoids drawn at the 50% probability level.

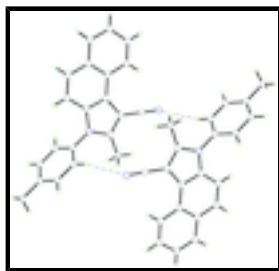


Fig. 2. Centrosymmetric dimers of (I) formed by C—H···N hydrogen bonds drawn as dashed lines.

## 2-Methyl-3-*p*-tolyl-3*H*-benzo[*e*]indole-1-carbonitrile

### Crystal data

C<sub>21</sub>H<sub>16</sub>N<sub>2</sub>

$M_r = 296.36$

Monoclinic,  $P2_1/n$

$F(000) = 624$

$D_x = 1.212 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

# supplementary materials

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Hall symbol: -P 2yn  
 $a = 10.321$  (2) Å  
 $b = 12.422$  (3) Å  
 $c = 13.258$  (3) Å  
 $\beta = 107.14$  (3)°  
 $V = 1624.4$  (6) Å<sup>3</sup>  
 $Z = 4$

Cell parameters from 3474 reflections  
 $\theta = 2.2$ – $27.5$ °  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 293$  K  
Block, colourless  
 $0.28 \times 0.20 \times 0.18$  mm

## Data collection

Rigaku Saturn CCD  
diffractometer

Radiation source: rotating anode  
confocal

Detector resolution: 7.31 pixels mm<sup>-1</sup>  
 $\omega$  and  $\varphi$  scans

Absorption correction: multi-scan  
(*CrystalClear*; Rigaku/MSO, 2005)

$T_{\min} = 0.980$ ,  $T_{\max} = 0.987$

10714 measured reflections

2858 independent reflections

2092 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 25.0$ °,  $\theta_{\min} = 2.2$ °

$h = -12 \rightarrow 11$

$k = -13 \rightarrow 14$

$l = -15 \rightarrow 14$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.056$

$wR(F^2) = 0.168$

$S = 1.04$

2858 reflections

210 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

$w = 1/[\sigma^2(F_o^2) + (0.1027P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.16$  e Å<sup>-3</sup>

Extinction correction: *SHELXL97* (Sheldrick, 2008),

$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.070 (10)

## 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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.10089 (15)	0.87702 (12)	0.23973 (11)	0.0575 (5)
N2	-0.2675 (2)	1.06928 (18)	0.01735 (16)	0.1025 (8)
C1	0.00439 (18)	0.79674 (14)	0.23281 (13)	0.0547 (5)
C2	0.0217 (2)	0.69469 (15)	0.27979 (14)	0.0629 (5)
H2	0.1053	0.6728	0.3241	0.075*
C3	-0.0883 (2)	0.62878 (16)	0.25826 (15)	0.0679 (6)
H3	-0.0790	0.5606	0.2885	0.081*
C4	-0.2171 (2)	0.66084 (17)	0.19091 (15)	0.0631 (6)
C5	-0.3298 (2)	0.5901 (2)	0.16630 (16)	0.0806 (7)
H5	-0.3197	0.5211	0.1947	0.097*
C6	-0.4540 (2)	0.6220 (2)	0.10095 (19)	0.0900 (8)
H6	-0.5266	0.5742	0.0854	0.108*
C7	-0.4715 (2)	0.7253 (2)	0.05799 (18)	0.0860 (7)
H7	-0.5561	0.7467	0.0150	0.103*
C8	-0.3656 (2)	0.79452 (19)	0.07884 (15)	0.0692 (6)
H8	-0.3783	0.8630	0.0491	0.083*
C9	-0.23647 (19)	0.76498 (16)	0.14464 (13)	0.0580 (5)
C10	-0.12000 (19)	0.83318 (14)	0.16682 (12)	0.0542 (5)
C11	-0.0941 (2)	0.93897 (14)	0.13370 (13)	0.0589 (5)
C12	0.0402 (2)	0.96343 (15)	0.17945 (14)	0.0608 (5)
C13	0.1146 (3)	1.06418 (17)	0.17368 (17)	0.0812 (7)
H13A	0.1546	1.0918	0.2436	0.122*
H13B	0.0529	1.1164	0.1323	0.122*
H13C	0.1847	1.0496	0.1414	0.122*
C14	-0.1898 (2)	1.01126 (18)	0.06895 (15)	0.0722 (6)
C15	0.24140 (19)	0.86902 (14)	0.29878 (14)	0.0556 (5)
C16	0.3392 (2)	0.85881 (17)	0.24716 (15)	0.0670 (6)
H16	0.3146	0.8569	0.1738	0.080*
C17	0.4734 (2)	0.85143 (16)	0.30554 (17)	0.0722 (6)
H17	0.5388	0.8442	0.2704	0.087*
C18	0.5142 (2)	0.85442 (15)	0.41425 (17)	0.0670 (6)
C19	0.4147 (2)	0.86356 (17)	0.46373 (16)	0.0717 (6)
H19	0.4395	0.8647	0.5371	0.086*
C20	0.2793 (2)	0.87108 (16)	0.40767 (14)	0.0661 (6)
H20	0.2140	0.8775	0.4430	0.079*
C21	0.6620 (2)	0.8465 (2)	0.4766 (2)	0.1000 (9)
H21A	0.6952	0.7759	0.4682	0.150*
H21B	0.6720	0.8594	0.5499	0.150*
H21C	0.7128	0.8993	0.4513	0.150*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0540 (10)	0.0542 (9)	0.0598 (9)	0.0010 (7)	0.0098 (7)	0.0032 (7)

## supplementary materials

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N2	0.1048 (18)	0.1026 (16)	0.0931 (13)	0.0401 (13)	0.0185 (12)	0.0307 (12)
C1	0.0532 (11)	0.0564 (11)	0.0521 (9)	0.0020 (9)	0.0115 (8)	0.0003 (8)
C2	0.0582 (12)	0.0630 (12)	0.0618 (11)	0.0065 (10)	0.0091 (9)	0.0085 (9)
C3	0.0706 (15)	0.0630 (12)	0.0686 (12)	-0.0020 (10)	0.0181 (10)	0.0123 (9)
C4	0.0561 (13)	0.0752 (14)	0.0595 (11)	-0.0083 (10)	0.0193 (9)	-0.0022 (9)
C5	0.0756 (17)	0.0909 (16)	0.0801 (13)	-0.0151 (13)	0.0306 (12)	-0.0002 (11)
C6	0.0581 (16)	0.124 (2)	0.0903 (16)	-0.0246 (14)	0.0249 (13)	-0.0114 (15)
C7	0.0544 (14)	0.123 (2)	0.0797 (14)	-0.0008 (13)	0.0185 (11)	-0.0047 (14)
C8	0.0516 (12)	0.0883 (15)	0.0654 (12)	0.0054 (11)	0.0137 (9)	-0.0024 (10)
C9	0.0517 (12)	0.0728 (13)	0.0502 (10)	0.0031 (9)	0.0162 (8)	-0.0029 (8)
C10	0.0531 (11)	0.0601 (11)	0.0475 (9)	0.0074 (9)	0.0120 (8)	-0.0010 (7)
C11	0.0616 (13)	0.0571 (11)	0.0550 (10)	0.0116 (9)	0.0128 (9)	0.0036 (8)
C12	0.0653 (13)	0.0532 (11)	0.0628 (10)	0.0061 (9)	0.0171 (9)	0.0013 (8)
C13	0.0884 (17)	0.0583 (13)	0.0960 (14)	-0.0013 (11)	0.0257 (13)	0.0075 (11)
C14	0.0755 (15)	0.0725 (14)	0.0667 (12)	0.0194 (11)	0.0181 (10)	0.0103 (10)
C15	0.0481 (11)	0.0550 (11)	0.0584 (10)	-0.0029 (8)	0.0078 (8)	-0.0001 (8)
C16	0.0665 (14)	0.0746 (13)	0.0614 (11)	0.0013 (10)	0.0213 (10)	-0.0024 (9)
C17	0.0578 (14)	0.0732 (14)	0.0902 (15)	0.0001 (10)	0.0288 (11)	-0.0033 (10)
C18	0.0535 (13)	0.0555 (12)	0.0852 (14)	-0.0010 (9)	0.0102 (11)	0.0016 (10)
C19	0.0628 (14)	0.0818 (14)	0.0627 (11)	-0.0043 (11)	0.0062 (10)	0.0005 (10)
C20	0.0564 (13)	0.0825 (14)	0.0593 (11)	-0.0021 (10)	0.0169 (9)	0.0014 (9)
C21	0.0563 (15)	0.0937 (18)	0.133 (2)	0.0003 (12)	0.0011 (14)	0.0023 (15)

### *Geometric parameters (Å, °)*

N1—C12	1.374 (2)	C10—C11	1.435 (3)
N1—C1	1.393 (2)	C11—C12	1.373 (3)
N1—C15	1.434 (2)	C11—C14	1.421 (3)
N2—C14	1.143 (2)	C12—C13	1.483 (3)
C1—C10	1.399 (2)	C13—H13A	0.9600
C1—C2	1.400 (2)	C13—H13B	0.9600
C2—C3	1.360 (3)	C13—H13C	0.9600
C2—H2	0.9300	C15—C20	1.380 (3)
C3—C4	1.422 (3)	C15—C16	1.382 (3)
C3—H3	0.9300	C16—C17	1.376 (3)
C4—C5	1.417 (3)	C16—H16	0.9300
C4—C9	1.420 (3)	C17—C18	1.378 (3)
C5—C6	1.377 (3)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.376 (3)
C6—C7	1.394 (4)	C18—C21	1.509 (3)
C6—H6	0.9300	C19—C20	1.379 (3)
C7—C8	1.354 (3)	C19—H19	0.9300
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.409 (3)	C21—H21A	0.9600
C8—H8	0.9300	C21—H21B	0.9600
C9—C10	1.429 (3)	C21—H21C	0.9600
C12—N1—C1	109.04 (15)	C14—C11—C10	127.20 (19)
C12—N1—C15	125.88 (15)	C11—C12—N1	108.18 (17)
C1—N1—C15	125.07 (14)	C11—C12—C13	129.44 (18)

N1—C1—C10	108.42 (15)	N1—C12—C13	122.34 (18)
N1—C1—C2	128.59 (17)	C12—C13—H13A	109.5
C10—C1—C2	122.97 (17)	C12—C13—H13B	109.5
C3—C2—C1	117.55 (18)	H13A—C13—H13B	109.5
C3—C2—H2	121.2	C12—C13—H13C	109.5
C1—C2—H2	121.2	H13A—C13—H13C	109.5
C2—C3—C4	122.07 (18)	H13B—C13—H13C	109.5
C2—C3—H3	119.0	N2—C14—C11	179.4 (3)
C4—C3—H3	119.0	C20—C15—C16	119.78 (18)
C5—C4—C9	117.6 (2)	C20—C15—N1	119.91 (18)
C5—C4—C3	121.5 (2)	C16—C15—N1	120.31 (16)
C9—C4—C3	120.85 (18)	C17—C16—C15	119.24 (17)
C6—C5—C4	121.0 (2)	C17—C16—H16	120.4
C6—C5—H5	119.5	C15—C16—H16	120.4
C4—C5—H5	119.5	C16—C17—C18	122.2 (2)
C5—C6—C7	120.4 (2)	C16—C17—H17	118.9
C5—C6—H6	119.8	C18—C17—H17	118.9
C7—C6—H6	119.8	C19—C18—C17	117.41 (19)
C8—C7—C6	120.1 (2)	C19—C18—C21	121.3 (2)
C8—C7—H7	120.0	C17—C18—C21	121.2 (2)
C6—C7—H7	120.0	C18—C19—C20	121.91 (19)
C7—C8—C9	121.4 (2)	C18—C19—H19	119.0
C7—C8—H8	119.3	C20—C19—H19	119.0
C9—C8—H8	119.3	C19—C20—C15	119.5 (2)
C8—C9—C4	119.45 (19)	C19—C20—H20	120.3
C8—C9—C10	123.90 (19)	C15—C20—H20	120.3
C4—C9—C10	116.63 (17)	C18—C21—H21A	109.5
C1—C10—C9	119.89 (17)	C18—C21—H21B	109.4
C1—C10—C11	105.56 (17)	H21A—C21—H21B	109.5
C9—C10—C11	134.53 (16)	C18—C21—H21C	109.4
C12—C11—C14	123.93 (19)	H21A—C21—H21C	109.5
C12—C11—C10	108.80 (15)	H21B—C21—H21C	109.5
C12—N1—C1—C10	-0.03 (19)	C1—C10—C11—C12	-0.5 (2)
C15—N1—C1—C10	-178.86 (14)	C9—C10—C11—C12	-178.67 (19)
C12—N1—C1—C2	178.88 (18)	C1—C10—C11—C14	-177.42 (17)
C15—N1—C1—C2	0.0 (3)	C9—C10—C11—C14	4.4 (3)
N1—C1—C2—C3	-177.95 (18)	C14—C11—C12—N1	177.53 (16)
C10—C1—C2—C3	0.8 (3)	C10—C11—C12—N1	0.5 (2)
C1—C2—C3—C4	-0.1 (3)	C14—C11—C12—C13	0.0 (3)
C2—C3—C4—C5	177.9 (2)	C10—C11—C12—C13	-177.0 (2)
C2—C3—C4—C9	-1.2 (3)	C1—N1—C12—C11	-0.3 (2)
C9—C4—C5—C6	-0.8 (3)	C15—N1—C12—C11	178.55 (16)
C3—C4—C5—C6	-179.95 (19)	C1—N1—C12—C13	177.43 (18)
C4—C5—C6—C7	-0.4 (4)	C15—N1—C12—C13	-3.8 (3)
C5—C6—C7—C8	1.2 (4)	C12—C11—C14—N2	-129 (29)
C6—C7—C8—C9	-0.7 (3)	C10—C11—C14—N2	47 (29)
C7—C8—C9—C4	-0.6 (3)	C12—N1—C15—C20	110.1 (2)
C7—C8—C9—C10	177.95 (18)	C1—N1—C15—C20	-71.3 (2)
C5—C4—C9—C8	1.3 (3)	C12—N1—C15—C16	-70.1 (2)

## supplementary materials

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C3—C4—C9—C8	-179.57 (17)	C1—N1—C15—C16	108.5 (2)
C5—C4—C9—C10	-177.31 (17)	C20—C15—C16—C17	-0.4 (3)
C3—C4—C9—C10	1.8 (3)	N1—C15—C16—C17	179.90 (17)
N1—C1—C10—C9	178.82 (15)	C15—C16—C17—C18	-0.3 (3)
C2—C1—C10—C9	-0.2 (3)	C16—C17—C18—C19	1.0 (3)
N1—C1—C10—C11	0.30 (19)	C16—C17—C18—C21	-179.8 (2)
C2—C1—C10—C11	-178.68 (16)	C17—C18—C19—C20	-0.9 (3)
C8—C9—C10—C1	-179.70 (15)	C21—C18—C19—C20	179.9 (2)
C4—C9—C10—C1	-1.1 (2)	C18—C19—C20—C15	0.3 (3)
C8—C9—C10—C11	-1.7 (3)	C16—C15—C20—C19	0.4 (3)
C4—C9—C10—C11	176.86 (18)	N1—C15—C20—C19	-179.86 (17)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16 $\cdots$ N2 <sup>i</sup>	0.93	2.60	3.480 (3)	158

Symmetry codes: (i)  $-x, -y+2, -z$ .



Fig. 1

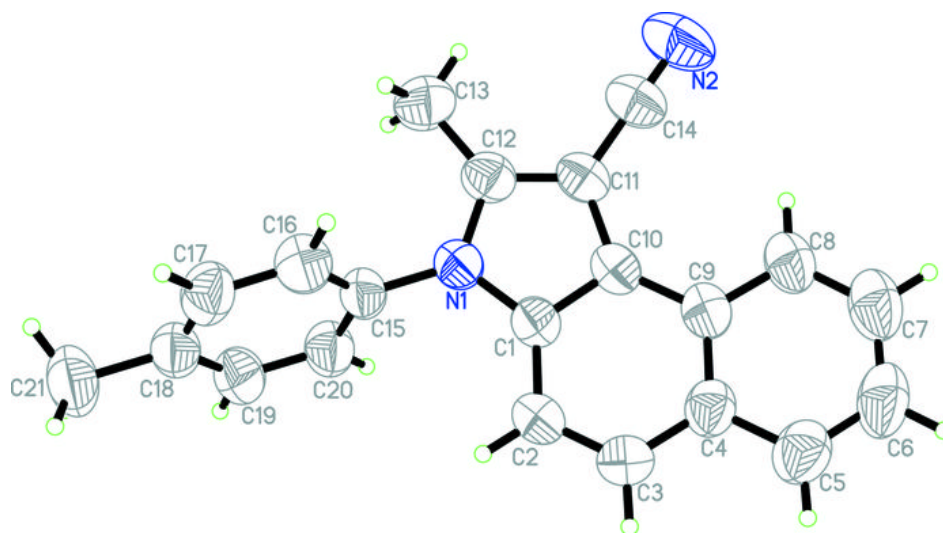


Fig. 2

