

## 9,9'-Biacridine

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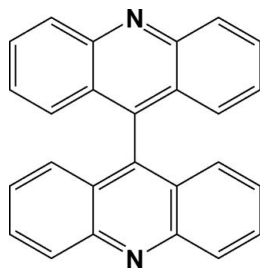
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.060;  $wR$  factor = 0.113; data-to-parameter ratio = 12.5.

The title molecule,  $\text{C}_{26}\text{H}_{16}\text{N}_2$ , is nonplanar, the dihedral angle between the two acridine ring systems being  $84.67$  ( $7$ )°. In the crystal structure, intermolecular  $\text{C}-\text{H}\cdots\text{N}$  and  $\text{C}-\text{H}\cdots\pi$  hydrogen-bonding interactions link the adjacent molecules into a two-dimensional network parallel to the  $ab$  plane.

### Related literature

For related literature, see: Boyer *et al.* (1999); Bu *et al.* (2004); Kitagawa *et al.* (2004); Liu *et al.* (2006); Steel (2005). For relevant papers on hydrogen bonds, see: Desiraju & Steiner (1999); Sony & Ponnuswamy (2006).



### Experimental

#### Crystal data

$\text{C}_{26}\text{H}_{16}\text{N}_2$   
 $M_r = 356.41$   
 Monoclinic,  $C2/c$   
 $a = 24.427$  (8) Å  
 $b = 9.463$  (3) Å  
 $c = 15.644$  (5) Å  
 $\beta = 98.253$  (6)°

$V = 3578.9$  (19) Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.30 \times 0.25 \times 0.25$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 1998)  
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.981$   
 8953 measured reflections  
 3166 independent reflections  
 1342 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.099$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.113$   
 $S = 0.96$   
 3166 reflections  
 253 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the N1/C9–C13 pyridine ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8–H8A $\cdots$ N2 <sup>i</sup>	0.93	2.49	3.374 (5)	159
C21–H21A $\cdots$ N1 <sup>ii</sup>	0.93	2.53	3.419 (4)	159
C19–H19A $\cdots$ Cg1 <sup>iii</sup>	0.93	2.88	3.764 (4)	159

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2445).

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**supplementary materials**

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## 9,9'-Biacridine

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### Comment

N-containing heterocyclic aromatic compounds are extensively used as bridging ligands in coordination and metallocsupramolecular chemistry (Steel, 2005). The most frequently used neutral bridging ligands are 4,4'-bipyridine and its derivatives (Kitagawa *et al.*, 2004). In comparison with other N-containing heterocyclic ligands, acridine-based ligands have some primary structural characteristics: (a) acridine ring has larger conjugated  $\pi$ -systems, therefore  $\pi$ - $\pi$  stacking interactions may play important roles in the formations of their metal complexes and (b) the larger conjugated  $\pi$ -systems and the steric hindrance of H atoms of the adjacent benzene rings may probably affect the coordination abilities of the acridine N donor atom (Bu *et al.*, 2004; Liu *et al.*, 2006). Recently, we synthesized a 4,4'-bipyridyl-like linear diamine bridging ligand, 9,9'-biacridine, (I). We report here the crystal structure of (I).

Bond distances and angles in (I) (Fig. 1) have normal values, and are comparable to those observed for similar acridine-based molecules (Boyer *et al.*, 1999; Liu *et al.*, 2006). Each of the acridine ring system is essentially planar. The two acridine ring systems are twisted away from one another by an angle of 84.67 (7)°.

In the crystal structure, the adjacent molecules are linked into a chain along the [1 1 0] direction by intermolecular C—H $\cdots$ N hydrogen-bonding interactions (Fig. 2 and Table 1) (Desiraju *et al.*, 1999). The adjacent chains are cross-linked *via* intermolecular C—H $\cdots$  $\pi$  interactions (Table 1) involving the N1/C9—C13 pyridine ring (centroid Cg1), forming a two-dimensional network parallel to the *ab* plane (Fig. 3). In the adjacent chains the acridine rings are arranged in an edge-to-face orientation (Sony *et al.*, 2006).

### Experimental

Compound (I) was synthesized according to the method reported in the literature (Boyer *et al.*, 1999). A solution of (I) (0.1 mmol) in methanol (15 ml) was filtered off and the resulting solution was kept at room temperature. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield: 30%). Analysis calculated for C<sub>26</sub>H<sub>16</sub>N<sub>2</sub>: C 87.62, H 4.52, N 7.86%; found: C 87.75, H 4.59, N 7.77%.

### Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Figures

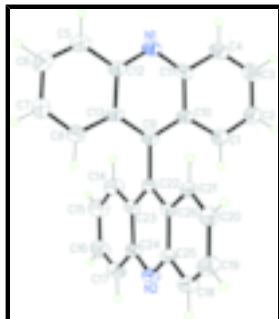


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

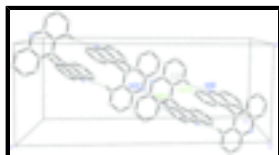


Fig. 2. Part of the crystal packing in the title compound, showing a C—H...N hydrogen-bonded (dashed lines) chain. The atoms labelled with the suffixes B and C are generated by the symmetry operations  $(1/2 - x, 3/2 - y, -z)$  and  $(-x, 2 - y, -z)$ , respectively. For clarity, only H atoms involved in the interactions are shown.

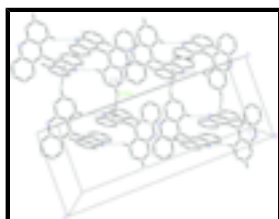


Fig. 3. View of the two-dimensional network formed by intermolecular C—H... $\pi$  interactions (dashed lines).

**9,9'-Biacridine**

*Crystal data*

$C_{26}H_{16}N_2$

$M_r = 356.41$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 24.427\ (8)\ \text{\AA}$

$b = 9.463\ (3)\ \text{\AA}$

$c = 15.644\ (5)\ \text{\AA}$

$\beta = 98.253\ (6)^\circ$

$V = 3578.9\ (19)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 1488$

$D_x = 1.323\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 881 reflections

$\theta = 2.3\text{--}21.3^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, yellow

$0.30 \times 0.25 \times 0.25\ \text{mm}$

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ (2)\ \text{K}$

$\phi$  and  $\omega$  scans

3166 independent reflections

1342 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.099$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 1.7^\circ$

Absorption correction: multi-scan  
(SADABS; Bruker, 1998)  $h = -28 \rightarrow 28$   
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.981$   $k = -8 \rightarrow 11$   
8953 measured reflections  $l = -14 \rightarrow 18$

### Refinement

Refinement on  $F^2$  Secondary atom site location: difference Fourier map  
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites  
 $R[F^2 > 2\sigma(F^2)] = 0.060$  H-atom parameters constrained  
 $wR(F^2) = 0.113$   $w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $S = 0.96$   $(\Delta/\sigma)_{\max} = 0.002$   
3166 reflections  $\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$   
253 parameters  $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$   
Primary atom site location: structure-invariant direct methods Extinction correction: none

### 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.19370 (14)	0.7778 (3)	0.2003 (2)	0.0500 (10)
H1A	0.1676	0.8395	0.2173	0.060*
C2	0.23874 (15)	0.7408 (4)	0.2580 (2)	0.0572 (10)
H2A	0.2432	0.7773	0.3137	0.069*
C3	0.27834 (15)	0.6474 (4)	0.2331 (2)	0.0612 (11)
H3A	0.3093	0.6241	0.2724	0.073*
C4	0.27214 (13)	0.5911 (3)	0.1531 (2)	0.0544 (10)
H4A	0.2984	0.5277	0.1385	0.065*
C5	0.17604 (14)	0.5463 (4)	-0.1308 (2)	0.0545 (10)
H5A	0.2026	0.4810	-0.1420	0.065*
C6	0.13522 (16)	0.5805 (4)	-0.1946 (2)	0.0636 (11)
H6A	0.1339	0.5399	-0.2490	0.076*
C7	0.09413 (14)	0.6788 (4)	-0.1784 (2)	0.0569 (10)
H7A	0.0661	0.7030	-0.2227	0.068*

## supplementary materials

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C8	0.09507 (14)	0.7383 (4)	-0.0992 (2)	0.0489 (9)
H8A	0.0675	0.8017	-0.0894	0.059*
C9	0.14161 (12)	0.7630 (3)	0.0516 (2)	0.0375 (8)
C10	0.18597 (13)	0.7233 (3)	0.1144 (2)	0.0391 (8)
C11	0.22609 (13)	0.6270 (3)	0.0906 (2)	0.0410 (9)
C12	0.17990 (13)	0.6065 (3)	-0.0472 (2)	0.0407 (9)
C13	0.13817 (12)	0.7038 (3)	-0.0310 (2)	0.0388 (8)
C14	0.03651 (14)	0.6738 (4)	0.1059 (2)	0.0566 (10)
H14A	0.0611	0.6050	0.0924	0.068*
C15	-0.01240 (15)	0.6344 (4)	0.1313 (2)	0.0662 (11)
H15A	-0.0209	0.5389	0.1345	0.079*
C16	-0.05029 (15)	0.7365 (5)	0.1529 (2)	0.0647 (11)
H16A	-0.0834	0.7081	0.1702	0.078*
C17	-0.03851 (13)	0.8749 (4)	0.1484 (2)	0.0550 (10)
H17A	-0.0637	0.9413	0.1630	0.066*
C18	0.07636 (15)	1.2536 (4)	0.08545 (19)	0.0542 (10)
H18A	0.0501	1.3163	0.1007	0.065*
C19	0.12268 (15)	1.3040 (4)	0.0582 (2)	0.0610 (10)
H19A	0.1277	1.4011	0.0545	0.073*
C20	0.16333 (14)	1.2119 (4)	0.0353 (2)	0.0532 (10)
H20A	0.1949	1.2487	0.0166	0.064*
C21	0.15701 (12)	1.0701 (3)	0.04014 (18)	0.0429 (9)
H21A	0.1843	1.0102	0.0252	0.052*
C22	0.09950 (12)	0.8657 (3)	0.07359 (18)	0.0377 (8)
C23	0.05018 (12)	0.8194 (4)	0.09971 (18)	0.0403 (8)
C24	0.01180 (13)	0.9217 (4)	0.12164 (19)	0.0415 (8)
C25	0.06751 (13)	1.1060 (3)	0.09096 (18)	0.0397 (8)
C26	0.10848 (12)	1.0121 (3)	0.06823 (17)	0.0365 (8)
N1	0.22283 (10)	0.5684 (3)	0.01215 (18)	0.0449 (8)
N2	0.02041 (10)	1.0618 (3)	0.11775 (15)	0.0447 (7)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.055 (2)	0.038 (2)	0.057 (3)	0.0051 (19)	0.008 (2)	-0.001 (2)
C2	0.067 (3)	0.046 (3)	0.056 (3)	0.004 (2)	0.000 (2)	0.003 (2)
C3	0.057 (3)	0.055 (3)	0.068 (3)	0.010 (2)	-0.005 (2)	0.009 (2)
C4	0.046 (2)	0.042 (2)	0.076 (3)	0.0075 (19)	0.011 (2)	0.011 (2)
C5	0.059 (3)	0.045 (2)	0.063 (3)	0.004 (2)	0.022 (2)	-0.004 (2)
C6	0.077 (3)	0.061 (3)	0.056 (3)	-0.004 (2)	0.018 (2)	-0.010 (2)
C7	0.056 (3)	0.061 (3)	0.052 (2)	-0.004 (2)	0.0015 (19)	-0.001 (2)
C8	0.044 (2)	0.047 (2)	0.056 (2)	0.0013 (18)	0.0086 (19)	0.000 (2)
C9	0.0324 (19)	0.032 (2)	0.050 (2)	-0.0002 (17)	0.0128 (17)	0.0045 (18)
C10	0.038 (2)	0.030 (2)	0.050 (2)	0.0020 (17)	0.0116 (18)	0.0023 (18)
C11	0.0330 (19)	0.030 (2)	0.060 (3)	0.0017 (17)	0.0083 (18)	0.0112 (19)
C12	0.041 (2)	0.035 (2)	0.048 (2)	-0.0007 (18)	0.0153 (18)	0.0001 (18)
C13	0.034 (2)	0.030 (2)	0.055 (2)	-0.0009 (17)	0.0164 (18)	0.0012 (18)
C14	0.055 (2)	0.043 (3)	0.077 (3)	-0.002 (2)	0.025 (2)	0.005 (2)

C15	0.062 (3)	0.052 (3)	0.089 (3)	-0.009 (2)	0.024 (2)	0.006 (2)
C16	0.045 (2)	0.072 (3)	0.081 (3)	-0.003 (2)	0.024 (2)	0.010 (2)
C17	0.040 (2)	0.068 (3)	0.060 (3)	0.008 (2)	0.0170 (18)	0.007 (2)
C18	0.059 (3)	0.042 (3)	0.063 (3)	0.010 (2)	0.017 (2)	0.001 (2)
C19	0.071 (3)	0.037 (2)	0.078 (3)	0.000 (2)	0.020 (2)	0.004 (2)
C20	0.048 (2)	0.047 (3)	0.066 (2)	-0.005 (2)	0.0140 (18)	0.000 (2)
C21	0.041 (2)	0.037 (2)	0.051 (2)	0.0045 (19)	0.0097 (16)	-0.0013 (18)
C22	0.0327 (19)	0.040 (2)	0.041 (2)	0.0063 (18)	0.0058 (16)	-0.0002 (17)
C23	0.036 (2)	0.040 (2)	0.045 (2)	0.0037 (19)	0.0062 (16)	0.0031 (17)
C24	0.034 (2)	0.044 (2)	0.048 (2)	0.0020 (19)	0.0086 (16)	0.0021 (18)
C25	0.040 (2)	0.038 (2)	0.041 (2)	0.0056 (19)	0.0074 (16)	0.0003 (17)
C26	0.0338 (19)	0.037 (2)	0.039 (2)	0.0054 (18)	0.0066 (15)	0.0013 (17)
N1	0.0439 (18)	0.0339 (18)	0.059 (2)	0.0049 (15)	0.0141 (16)	0.0017 (16)
N2	0.0401 (18)	0.043 (2)	0.0533 (19)	0.0086 (16)	0.0131 (14)	0.0037 (15)

*Geometric parameters (Å, °)*

C1—C2	1.365 (4)	C14—C15	1.364 (4)
C1—C10	1.427 (4)	C14—C23	1.425 (4)
C1—H1A	0.93	C14—H14A	0.93
C2—C3	1.406 (4)	C15—C16	1.412 (4)
C2—H2A	0.93	C15—H15A	0.93
C3—C4	1.349 (4)	C16—C17	1.345 (4)
C3—H3A	0.93	C16—H16A	0.93
C4—C11	1.421 (4)	C17—C24	1.424 (4)
C4—H4A	0.93	C17—H17A	0.93
C5—C6	1.345 (4)	C18—C19	1.352 (4)
C5—C12	1.418 (4)	C18—C25	1.419 (4)
C5—H5A	0.93	C18—H18A	0.93
C6—C7	1.418 (4)	C19—C20	1.406 (4)
C6—H6A	0.93	C19—H19A	0.93
C7—C8	1.358 (4)	C20—C21	1.354 (4)
C7—H7A	0.93	C20—H20A	0.93
C8—C13	1.425 (4)	C21—C26	1.432 (4)
C8—H8A	0.93	C21—H21A	0.93
C9—C13	1.399 (4)	C22—C23	1.397 (4)
C9—C10	1.405 (4)	C22—C26	1.407 (4)
C9—C22	1.491 (4)	C23—C24	1.423 (4)
C10—C11	1.426 (4)	C24—N2	1.345 (4)
C11—N1	1.339 (4)	C25—N2	1.346 (3)
C12—N1	1.346 (4)	C25—C26	1.421 (4)
C12—C13	1.423 (4)		
C2—C1—C10	121.0 (3)	C15—C14—H14A	119.8
C2—C1—H1A	119.5	C23—C14—H14A	119.8
C10—C1—H1A	119.5	C14—C15—C16	120.9 (4)
C1—C2—C3	120.0 (3)	C14—C15—H15A	119.5
C1—C2—H2A	120.0	C16—C15—H15A	119.5
C3—C2—H2A	120.0	C17—C16—C15	120.1 (4)
C4—C3—C2	121.0 (3)	C17—C16—H16A	119.9

## supplementary materials

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C4—C3—H3A	119.5	C15—C16—H16A	119.9
C2—C3—H3A	119.5	C16—C17—C24	121.2 (3)
C3—C4—C11	121.0 (3)	C16—C17—H17A	119.4
C3—C4—H4A	119.5	C24—C17—H17A	119.4
C11—C4—H4A	119.5	C19—C18—C25	120.5 (3)
C6—C5—C12	122.1 (4)	C19—C18—H18A	119.7
C6—C5—H5A	119.0	C25—C18—H18A	119.7
C12—C5—H5A	119.0	C18—C19—C20	121.0 (3)
C5—C6—C7	119.6 (4)	C18—C19—H19A	119.5
C5—C6—H6A	120.2	C20—C19—H19A	119.5
C7—C6—H6A	120.2	C21—C20—C19	120.6 (3)
C8—C7—C6	121.0 (3)	C21—C20—H20A	119.7
C8—C7—H7A	119.5	C19—C20—H20A	119.7
C6—C7—H7A	119.5	C20—C21—C26	120.2 (3)
C7—C8—C13	120.1 (3)	C20—C21—H21A	119.9
C7—C8—H8A	119.9	C26—C21—H21A	119.9
C13—C8—H8A	119.9	C23—C22—C26	118.3 (3)
C13—C9—C10	118.5 (3)	C23—C22—C9	121.0 (3)
C13—C9—C22	121.5 (3)	C26—C22—C9	120.7 (3)
C10—C9—C22	120.1 (3)	C22—C23—C24	118.8 (3)
C9—C10—C11	118.6 (3)	C22—C23—C14	122.9 (3)
C9—C10—C1	123.1 (3)	C24—C23—C14	118.2 (3)
C11—C10—C1	118.3 (3)	N2—C24—C23	123.2 (3)
N1—C11—C4	117.9 (3)	N2—C24—C17	117.8 (3)
N1—C11—C10	123.4 (3)	C23—C24—C17	119.0 (3)
C4—C11—C10	118.7 (3)	N2—C25—C18	118.0 (3)
N1—C12—C5	118.1 (3)	N2—C25—C26	123.2 (3)
N1—C12—C13	123.9 (3)	C18—C25—C26	118.8 (3)
C5—C12—C13	118.1 (3)	C22—C26—C25	118.6 (3)
C9—C13—C12	118.3 (3)	C22—C26—C21	122.6 (3)
C9—C13—C8	122.7 (3)	C25—C26—C21	118.8 (3)
C12—C13—C8	119.1 (3)	C11—N1—C12	117.3 (3)
C15—C14—C23	120.5 (3)	C24—N2—C25	117.8 (3)
C10—C1—C2—C3	-0.1 (5)	C13—C9—C22—C23	84.9 (4)
C1—C2—C3—C4	-1.3 (5)	C10—C9—C22—C23	-95.0 (4)
C2—C3—C4—C11	1.6 (5)	C13—C9—C22—C26	-94.8 (4)
C12—C5—C6—C7	-0.6 (5)	C10—C9—C22—C26	85.2 (4)
C5—C6—C7—C8	-0.5 (5)	C26—C22—C23—C24	-1.4 (4)
C6—C7—C8—C13	0.8 (5)	C9—C22—C23—C24	178.8 (3)
C13—C9—C10—C11	1.3 (4)	C26—C22—C23—C14	178.9 (3)
C22—C9—C10—C11	-178.8 (3)	C9—C22—C23—C14	-0.9 (4)
C13—C9—C10—C1	179.5 (3)	C15—C14—C23—C22	-179.7 (3)
C22—C9—C10—C1	-0.5 (4)	C15—C14—C23—C24	0.6 (5)
C2—C1—C10—C9	-177.1 (3)	C22—C23—C24—N2	0.6 (5)
C2—C1—C10—C11	1.1 (4)	C14—C23—C24—N2	-179.7 (3)
C3—C4—C11—N1	179.3 (3)	C22—C23—C24—C17	-180.0 (3)
C3—C4—C11—C10	-0.6 (5)	C14—C23—C24—C17	-0.2 (4)
C9—C10—C11—N1	-2.3 (4)	C16—C17—C24—N2	179.2 (3)
C1—C10—C11—N1	179.4 (3)	C16—C17—C24—C23	-0.2 (5)



C9—C10—C11—C4	177.6 (3)	C19—C18—C25—N2	-179.4 (3)
C1—C10—C11—C4	-0.8 (4)	C19—C18—C25—C26	0.7 (5)
C6—C5—C12—N1	-178.6 (3)	C23—C22—C26—C25	1.1 (4)
C6—C5—C12—C13	1.4 (5)	C9—C22—C26—C25	-179.2 (3)
C10—C9—C13—C12	-0.1 (4)	C23—C22—C26—C21	-178.4 (3)
C22—C9—C13—C12	180.0 (3)	C9—C22—C26—C21	1.3 (4)
C10—C9—C13—C8	-179.4 (3)	N2—C25—C26—C22	0.2 (4)
C22—C9—C13—C8	0.7 (4)	C18—C25—C26—C22	-179.9 (3)
N1—C12—C13—C9	-0.4 (5)	N2—C25—C26—C21	179.7 (3)
C5—C12—C13—C9	179.6 (3)	C18—C25—C26—C21	-0.3 (4)
N1—C12—C13—C8	178.9 (3)	C20—C21—C26—C22	179.3 (3)
C5—C12—C13—C8	-1.0 (4)	C20—C21—C26—C25	-0.2 (4)
C7—C8—C13—C9	179.3 (3)	C4—C11—N1—C12	-178.1 (3)
C7—C8—C13—C12	0.0 (4)	C10—C11—N1—C12	1.8 (4)
C23—C14—C15—C16	-0.6 (5)	C5—C12—N1—C11	179.5 (3)
C14—C15—C16—C17	0.1 (6)	C13—C12—N1—C11	-0.4 (4)
C15—C16—C17—C24	0.3 (5)	C23—C24—N2—C25	0.6 (4)
C25—C18—C19—C20	-0.5 (5)	C17—C24—N2—C25	-178.8 (3)
C18—C19—C20—C21	-0.1 (5)	C18—C25—N2—C24	179.0 (3)
C19—C20—C21—C26	0.4 (5)	C26—C25—N2—C24	-1.1 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A $\cdots$ N2 <sup>i</sup>	0.93	2.49	3.374 (5)	159
C21—H21A $\cdots$ N1 <sup>ii</sup>	0.93	2.53	3.419 (4)	159
C19—H19A $\cdots$ Cg1 <sup>iii</sup>	0.93	2.88	3.764 (4)	159

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



Fig. 2

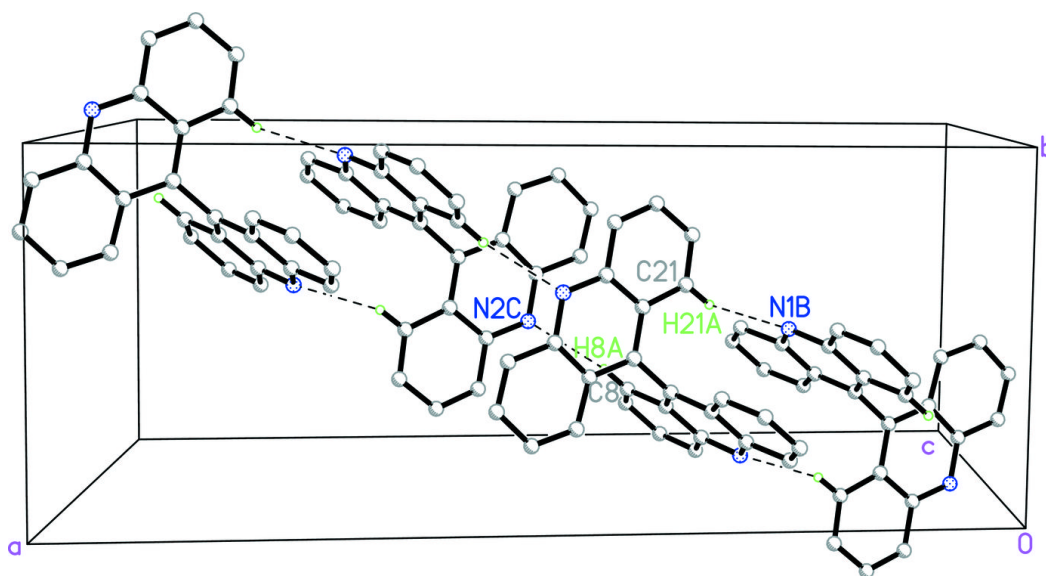


Fig. 3

