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# 2,6-Bis[1-(2-methylphenylimino)ethyl]-pyridine

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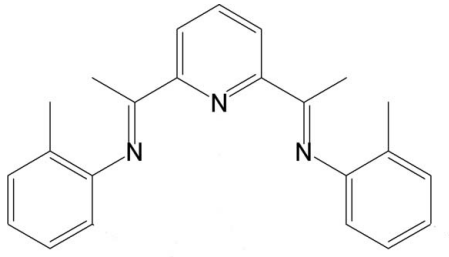
Key indicators: single-crystal X-ray study; $T$ = 193 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.051; $wR$ factor = 0.157; data-to-parameter ratio = 18.9.

The molecule of the title compound, $C_{23}H_{23}N_3$, which was synthesized by the condensation reaction between 2,6-diacetylpyridine and 2-dimethylaniline, adopts an $E$ configuration about both C=N imine bonds. The dihedral angles formed by the benzene rings with the pyridine ring are 89.68 (5) and 53.62 (6)°.

## Related literature

For the applications of pyridine-based ligands in sensor technologies and electro-luminescent devices, see: Tang & Vanslyke (1987); Wang (2001). For the crystal structures of related compounds, see: Mentes *et al.* (2001); Huang *et al.* (2006). For the synthesis, see: Fan *et al.* (2004).



## Experimental

### Crystal data

$C_{23}H_{23}N_3$
$M_r$ = 341.44
Monoclinic, $P2_1/n$
$a$ = 12.966 (3) Å
$b$ = 11.304 (2) Å
$c$ = 14.767 (3) Å
$\beta$ = 115.62 (3)°
$V$ = 1951.6 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 193 K
0.56 × 0.41 × 0.36 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.960, $T_{max}$ = 0.972
18526 measured reflections
4435 independent reflections
2804 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.157
$S$ = 1.06
4435 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2329).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o1480 [ **doi:10.1107/S1600536809020522** ]

# 2,6-Bis[1-(2-methylphenylimino)ethyl]pyridine

**R.-Q. Fan, X.-D. Ding, G.-P. Zhou and Y.-L. Yang**

## Comment

Luminescent coordination compounds based on pyridine-type ligands have attracted intensive attention due to their potential application in areas of sensor technologies and electro-luminescent devices (Tang & Vanslyke, 1987; Wang, 2001). In order to explore potential luminescent complexes of this type, we prepared a series of bis(iminoalkyl)pyridine ligands by the condensation reaction of 2,6-diacetylpyridine with the corresponding aniline in methanol (Fan *et al.*, 2004). It is still challenging to design and rationally synthesize ligands with unique structures and functions. In this regard, we report herein the synthesis and crystal structure of the title compound.

The molecule of the title compound (Fig. 1) possesses an approximate $C_s$ symmetry about a plane bisecting the pyridine ring. The pyridine ring is coplanar with the two imino groups, which show typical C═N double bond character (1.2606 (18) and 1.2674 (19) Å for N1═C1 and N3═C7, respectively). These values are in good agreement with those observed in 2,6-bis[1-(phenylimino)ethyl]pyridine (1.266 (4) Å; Mentes *et al.*, 2001) and in 2,6-bis[1-(2,6-dimethylphenylimino)ethyl]pyridine (1.265 (2) and 1.271 (2) Å; Huang *et al.*, 2006). The dihedral angles between the C10–C15 and C17–C22 benzene rings and the pyridine ring are 89.68 (5) and 53.62 (6)°, respectively. The crystal packing (Fig. 2) is stabilized only by van der Waals interactions.

## Experimental

The title compound was synthesized according to the literatute method (Fan *et al.*, 2004). To a solution of 2,6-diacetylpyridine (1.1 g, 6.7 mmol) in absolute methanol (25 ml) was added 2-dimethylaniline (2.2 ml, 20.5 mmol). After the addition of several drops of formic acid, the reaction mixture was refluxed for 24 h and then allowed to cool down to room temperature. The crude product precipitated as yellow powder. Yellow block crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a methanol solution in 85% yield (1.96 g).

## Refinement

All H atoms were positioned geometrically with C—H = 0.93–0.96 Å, and allowed to ride on their parent atoms with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(C) for methyl H atoms.

## Figures

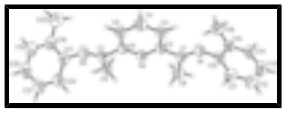


Fig. 1. The molecular structire of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

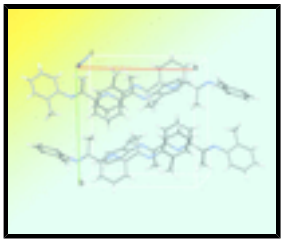


Fig. 2. Packing diagram of the title compound viewed along the *c* axis.

**2,6-bis[1-(2-methylphenylimino)ethyl]pyridine**

*Crystal data*

| | |
|---|---|
| $C_{23}H_{23}N_3$ | $F_{000}$ = 728 |
| $M_r$ = 341.44 | $D_x$ = 1.162 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 18526 reflections |
| $a$ = 12.966 (3) Å | θ = 3.1–27.5º |
| $b$ = 11.304 (2) Å | μ = 0.07 mm$^{-1}$ |
| $c$ = 14.767 (3) Å | $T$ = 193 K |
| β = 115.62 (3)º | Block, yellow |
| $V$ = 1951.6 (8) Å$^3$ | 0.56 × 0.41 × 0.36 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 4435 independent reflections |
| Radiation source: fine-focus sealed tube | 2804 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.037 |
| $T$ = 193 K | $\theta_{max}$ = 27.5º |
| phi and ω scans | $\theta_{min}$ = 3.1º |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h$ = −16→16 |
| $T_{min}$ = 0.960, $T_{max}$ = 0.972 | $k$ = −14→13 |
| 18526 measured reflections | $l$ = −19→19 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.051 | H-atom parameters constrained |
| $wR(F^2)$ = 0.157 | $w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 0.041P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.06 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4435 reflections | $\Delta\rho_{max}$ = 0.22 e Å$^{-3}$ |

| | |
|---|---|
| 235 parameters | $\Delta\rho_{min} = -0.16$ e Å$^{-3}$ |
| 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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N2 | 0.27847 (10) | 0.74889 (10) | 0.16139 (9) | 0.0458 (3) |
| N1 | −0.01920 (11) | 0.79913 (11) | 0.03667 (10) | 0.0527 (3) |
| C6 | 0.37804 (12) | 0.80381 (12) | 0.18433 (11) | 0.0448 (4) |
| N3 | 0.57761 (11) | 0.77842 (11) | 0.25205 (11) | 0.0565 (4) |
| C2 | 0.18145 (13) | 0.80916 (12) | 0.10943 (11) | 0.0457 (4) |
| C1 | 0.07290 (13) | 0.74430 (12) | 0.08606 (11) | 0.0476 (4) |
| C7 | 0.48407 (13) | 0.73369 (12) | 0.24317 (11) | 0.0466 (4) |
| C3 | 0.18154 (13) | 0.92576 (13) | 0.08007 (12) | 0.0524 (4) |
| H3B | 0.1130 | 0.9656 | 0.0444 | 0.063* |
| C5 | 0.38449 (14) | 0.92051 (13) | 0.15758 (13) | 0.0543 (4) |
| H5A | 0.4550 | 0.9567 | 0.1751 | 0.065* |
| C10 | −0.12858 (13) | 0.74706 (12) | 0.00704 (12) | 0.0489 (4) |
| C17 | 0.68397 (13) | 0.72253 (14) | 0.30780 (13) | 0.0523 (4) |
| C15 | −0.18677 (13) | 0.75912 (12) | 0.06699 (12) | 0.0522 (4) |
| C4 | 0.28403 (14) | 0.98142 (13) | 0.10444 (13) | 0.0586 (4) |
| H4A | 0.2858 | 1.0595 | 0.0853 | 0.070* |
| C14 | −0.29933 (15) | 0.72146 (15) | 0.02802 (15) | 0.0620 (5) |
| H14A | −0.3395 | 0.7298 | 0.0668 | 0.074* |
| C22 | 0.71360 (14) | 0.61751 (15) | 0.27656 (14) | 0.0633 (5) |
| H22A | 0.6602 | 0.5788 | 0.2202 | 0.076* |
| C9 | 0.47073 (15) | 0.62046 (14) | 0.28932 (15) | 0.0633 (5) |
| H9A | 0.5443 | 0.5840 | 0.3248 | 0.095* |
| H9B | 0.4213 | 0.5681 | 0.2375 | 0.095* |
| H9C | 0.4381 | 0.6366 | 0.3353 | 0.095* |
| C18 | 0.76376 (15) | 0.78082 (15) | 0.39198 (13) | 0.0579 (4) |
| C8 | 0.08130 (16) | 0.61968 (15) | 0.12366 (17) | 0.0764 (6) |
| H8A | 0.0058 | 0.5882 | 0.1037 | 0.115* |
| H8B | 0.1217 | 0.6191 | 0.1956 | 0.115* |
| H8C | 0.1217 | 0.5721 | 0.0958 | 0.115* |
| C13 | −0.35352 (16) | 0.67238 (16) | −0.06562 (16) | 0.0697 (5) |

| | | | | |
|---|---|---|---|---|
| H13A | −0.4295 | 0.6487 | −0.0902 | 0.084* |
| C11 | −0.18236 (16) | 0.69527 (15) | −0.08650 (14) | 0.0634 (5) |
| H11A | −0.1426 | 0.6850 | −0.1254 | 0.076* |
| C20 | 0.90039 (16) | 0.62620 (19) | 0.41061 (16) | 0.0742 (6) |
| H20A | 0.9733 | 0.5946 | 0.4454 | 0.089* |
| C12 | −0.29465 (17) | 0.65852 (17) | −0.12285 (15) | 0.0721 (5) |
| H12A | −0.3304 | 0.6243 | −0.1862 | 0.087* |
| C19 | 0.87169 (16) | 0.72988 (18) | 0.44214 (14) | 0.0708 (5) |
| H19A | 0.9259 | 0.7674 | 0.4988 | 0.085* |
| C16 | −0.12855 (18) | 0.81252 (18) | 0.17075 (15) | 0.0768 (6) |
| H16A | −0.1809 | 0.8138 | 0.2009 | 0.115* |
| H16B | −0.1049 | 0.8918 | 0.1659 | 0.115* |
| H16C | −0.0629 | 0.7659 | 0.2114 | 0.115* |
| C21 | 0.82176 (17) | 0.56955 (18) | 0.32815 (17) | 0.0744 (5) |
| H21A | 0.8407 | 0.4990 | 0.3066 | 0.089* |
| C23 | 0.7334 (2) | 0.89394 (18) | 0.42839 (17) | 0.0874 (6) |
| H23A | 0.6561 | 0.9154 | 0.3847 | 0.131* |
| H23B | 0.7842 | 0.9558 | 0.4283 | 0.131* |
| H23C | 0.7407 | 0.8829 | 0.4953 | 0.131* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N2 | 0.0389 (7) | 0.0437 (7) | 0.0531 (7) | 0.0021 (5) | 0.0183 (6) | 0.0030 (5) |
| N1 | 0.0407 (7) | 0.0476 (7) | 0.0659 (9) | 0.0017 (5) | 0.0193 (6) | 0.0079 (6) |
| C6 | 0.0412 (8) | 0.0442 (8) | 0.0508 (8) | 0.0034 (6) | 0.0217 (7) | 0.0030 (6) |
| N3 | 0.0409 (8) | 0.0550 (7) | 0.0719 (9) | 0.0030 (6) | 0.0227 (7) | 0.0109 (6) |
| C2 | 0.0413 (8) | 0.0460 (8) | 0.0493 (8) | 0.0043 (6) | 0.0191 (7) | 0.0026 (6) |
| C1 | 0.0423 (8) | 0.0458 (8) | 0.0533 (9) | 0.0019 (6) | 0.0193 (7) | 0.0031 (6) |
| C7 | 0.0421 (8) | 0.0441 (7) | 0.0537 (9) | 0.0027 (6) | 0.0208 (7) | −0.0005 (6) |
| C3 | 0.0439 (9) | 0.0460 (8) | 0.0631 (10) | 0.0072 (6) | 0.0191 (7) | 0.0075 (7) |
| C5 | 0.0434 (9) | 0.0472 (8) | 0.0721 (11) | −0.0002 (6) | 0.0247 (8) | 0.0068 (7) |
| C10 | 0.0394 (8) | 0.0399 (7) | 0.0619 (9) | 0.0040 (6) | 0.0166 (7) | 0.0108 (6) |
| C17 | 0.0384 (8) | 0.0541 (9) | 0.0654 (10) | 0.0012 (7) | 0.0234 (8) | 0.0113 (7) |
| C15 | 0.0446 (9) | 0.0435 (8) | 0.0658 (10) | 0.0024 (6) | 0.0212 (8) | 0.0074 (7) |
| C4 | 0.0521 (10) | 0.0421 (8) | 0.0790 (11) | 0.0036 (7) | 0.0260 (8) | 0.0122 (7) |
| C14 | 0.0454 (9) | 0.0622 (10) | 0.0774 (12) | 0.0018 (8) | 0.0256 (9) | 0.0112 (9) |
| C22 | 0.0455 (9) | 0.0639 (10) | 0.0785 (12) | 0.0029 (8) | 0.0248 (9) | 0.0004 (8) |
| C9 | 0.0487 (10) | 0.0548 (9) | 0.0876 (13) | 0.0091 (7) | 0.0305 (9) | 0.0182 (8) |
| C18 | 0.0542 (10) | 0.0614 (9) | 0.0583 (10) | −0.0042 (8) | 0.0245 (8) | 0.0091 (7) |
| C8 | 0.0511 (10) | 0.0542 (10) | 0.1118 (16) | 0.0021 (8) | 0.0239 (10) | 0.0249 (10) |
| C13 | 0.0429 (9) | 0.0704 (11) | 0.0806 (13) | −0.0085 (8) | 0.0125 (9) | 0.0122 (10) |
| C11 | 0.0589 (11) | 0.0667 (10) | 0.0621 (11) | −0.0051 (8) | 0.0238 (9) | 0.0013 (8) |
| C20 | 0.0415 (10) | 0.0890 (14) | 0.0863 (14) | 0.0123 (9) | 0.0222 (10) | 0.0223 (11) |
| C12 | 0.0647 (12) | 0.0717 (11) | 0.0630 (11) | −0.0148 (9) | 0.0116 (10) | −0.0010 (9) |
| C19 | 0.0518 (11) | 0.0886 (13) | 0.0613 (11) | −0.0094 (9) | 0.0143 (9) | 0.0121 (9) |
| C16 | 0.0730 (13) | 0.0819 (13) | 0.0805 (14) | −0.0175 (10) | 0.0380 (11) | −0.0189 (10) |
| C21 | 0.0567 (11) | 0.0729 (11) | 0.1024 (15) | 0.0155 (9) | 0.0428 (11) | 0.0108 (11) |

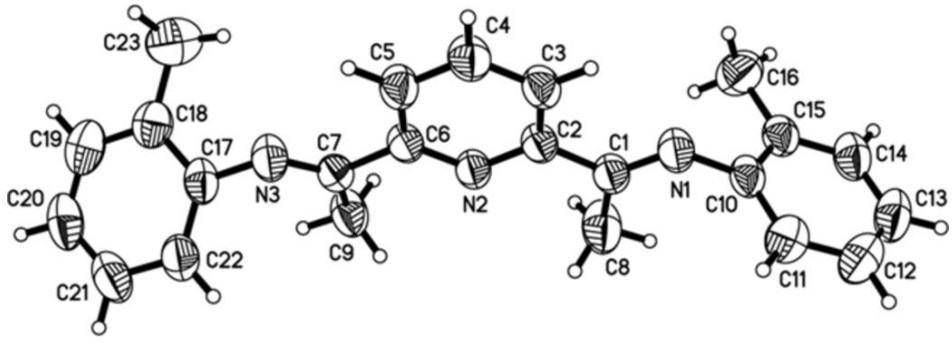
| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.1025 (18) | 0.0732 (12) | 0.0791 (14) | −0.0003 (12) | 0.0323 (13) | −0.0034 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N2—C6 | 1.3374 (18) | C22—H22A | 0.9300 |
| N2—C2 | 1.3420 (18) | C9—H9A | 0.9600 |
| N1—C1 | 1.2606 (18) | C9—H9B | 0.9600 |
| N1—C10 | 1.4187 (19) | C9—H9C | 0.9600 |
| C6—C5 | 1.390 (2) | C18—C19 | 1.394 (3) |
| C6—C7 | 1.497 (2) | C18—C23 | 1.504 (3) |
| N3—C7 | 1.2674 (19) | C8—H8A | 0.9600 |
| N3—C17 | 1.413 (2) | C8—H8B | 0.9600 |
| C2—C3 | 1.388 (2) | C8—H8C | 0.9600 |
| C2—C1 | 1.489 (2) | C13—C12 | 1.371 (3) |
| C1—C8 | 1.501 (2) | C13—H13A | 0.9300 |
| C7—C9 | 1.495 (2) | C11—C12 | 1.380 (3) |
| C3—C4 | 1.370 (2) | C11—H11A | 0.9300 |
| C3—H3B | 0.9300 | C20—C21 | 1.363 (3) |
| C5—C4 | 1.379 (2) | C20—C19 | 1.371 (3) |
| C5—H5A | 0.9300 | C20—H20A | 0.9300 |
| C10—C11 | 1.380 (2) | C12—H12A | 0.9300 |
| C10—C15 | 1.396 (2) | C19—H19A | 0.9300 |
| C17—C22 | 1.387 (2) | C16—H16A | 0.9600 |
| C17—C18 | 1.392 (2) | C16—H16B | 0.9600 |
| C15—C14 | 1.384 (2) | C16—H16C | 0.9600 |
| C15—C16 | 1.511 (3) | C21—H21A | 0.9300 |
| C4—H4A | 0.9300 | C23—H23A | 0.9600 |
| C14—C13 | 1.369 (3) | C23—H23B | 0.9600 |
| C14—H14A | 0.9300 | C23—H23C | 0.9600 |
| C22—C21 | 1.385 (2) | | |
| C6—N2—C2 | 118.22 (12) | C7—C9—H9C | 109.5 |
| C1—N1—C10 | 123.03 (12) | H9A—C9—H9C | 109.5 |
| N2—C6—C5 | 122.59 (13) | H9B—C9—H9C | 109.5 |
| N2—C6—C7 | 116.43 (12) | C17—C18—C19 | 117.84 (17) |
| C5—C6—C7 | 120.96 (13) | C17—C18—C23 | 120.89 (17) |
| C7—N3—C17 | 122.08 (13) | C19—C18—C23 | 121.26 (18) |
| N2—C2—C3 | 122.25 (14) | C1—C8—H8A | 109.5 |
| N2—C2—C1 | 116.17 (12) | C1—C8—H8B | 109.5 |
| C3—C2—C1 | 121.58 (13) | H8A—C8—H8B | 109.5 |
| N1—C1—C2 | 117.13 (13) | C1—C8—H8C | 109.5 |
| N1—C1—C8 | 125.07 (14) | H8A—C8—H8C | 109.5 |
| C2—C1—C8 | 117.79 (13) | H8B—C8—H8C | 109.5 |
| N3—C7—C9 | 126.06 (14) | C14—C13—C12 | 119.32 (17) |
| N3—C7—C6 | 116.53 (13) | C14—C13—H13A | 120.3 |
| C9—C7—C6 | 117.37 (13) | C12—C13—H13A | 120.3 |
| C4—C3—C2 | 119.07 (14) | C10—C11—C12 | 120.57 (19) |
| C4—C3—H3B | 120.5 | C10—C11—H11A | 119.7 |
| C2—C3—H3B | 120.5 | C12—C11—H11A | 119.7 |
| C4—C5—C6 | 118.51 (14) | C21—C20—C19 | 119.81 (17) |

| | | | |
|---|---|---|---|
| C4—C5—H5A | 120.7 | C21—C20—H20A | 120.1 |
| C6—C5—H5A | 120.7 | C19—C20—H20A | 120.1 |
| C11—C10—C15 | 119.90 (15) | C13—C12—C11 | 120.05 (18) |
| C11—C10—N1 | 119.33 (16) | C13—C12—H12A | 120.0 |
| C15—C10—N1 | 120.41 (15) | C11—C12—H12A | 120.0 |
| C22—C17—C18 | 119.76 (15) | C20—C19—C18 | 122.03 (18) |
| C22—C17—N3 | 121.99 (15) | C20—C19—H19A | 119.0 |
| C18—C17—N3 | 118.04 (15) | C18—C19—H19A | 119.0 |
| C14—C15—C10 | 117.91 (16) | C15—C16—H16A | 109.5 |
| C14—C15—C16 | 121.28 (17) | C15—C16—H16B | 109.5 |
| C10—C15—C16 | 120.81 (15) | H16A—C16—H16B | 109.5 |
| C3—C4—C5 | 119.35 (14) | C15—C16—H16C | 109.5 |
| C3—C4—H4A | 120.3 | H16A—C16—H16C | 109.5 |
| C5—C4—H4A | 120.3 | H16B—C16—H16C | 109.5 |
| C13—C14—C15 | 122.21 (18) | C20—C21—C22 | 119.73 (18) |
| C13—C14—H14A | 118.9 | C20—C21—H21A | 120.1 |
| C15—C14—H14A | 118.9 | C22—C21—H21A | 120.1 |
| C21—C22—C17 | 120.83 (17) | C18—C23—H23A | 109.5 |
| C21—C22—H22A | 119.6 | C18—C23—H23B | 109.5 |
| C17—C22—H22A | 119.6 | H23A—C23—H23B | 109.5 |
| C7—C9—H9A | 109.5 | C18—C23—H23C | 109.5 |
| C7—C9—H9B | 109.5 | H23A—C23—H23C | 109.5 |
| H9A—C9—H9B | 109.5 | H23B—C23—H23C | 109.5 |
| C2—N2—C6—C5 | 0.8 (2) | C11—C10—C15—C14 | −2.1 (2) |
| C2—N2—C6—C7 | 179.43 (13) | N1—C10—C15—C14 | 170.93 (13) |
| C6—N2—C2—C3 | −0.6 (2) | C11—C10—C15—C16 | 178.34 (15) |
| C6—N2—C2—C1 | −179.79 (13) | N1—C10—C15—C16 | −8.6 (2) |
| C10—N1—C1—C2 | 178.32 (14) | C2—C3—C4—C5 | −0.1 (3) |
| C10—N1—C1—C8 | −2.3 (3) | C6—C5—C4—C3 | 0.3 (3) |
| N2—C2—C1—N1 | −179.50 (14) | C10—C15—C14—C13 | 0.8 (2) |
| C3—C2—C1—N1 | 1.3 (2) | C16—C15—C14—C13 | −179.72 (16) |
| N2—C2—C1—C8 | 1.0 (2) | C18—C17—C22—C21 | 0.1 (3) |
| C3—C2—C1—C8 | −178.12 (16) | N3—C17—C22—C21 | 174.74 (16) |
| C17—N3—C7—C9 | 1.0 (3) | C22—C17—C18—C19 | −0.2 (2) |
| C17—N3—C7—C6 | 178.40 (14) | N3—C17—C18—C19 | −175.06 (15) |
| N2—C6—C7—N3 | 169.72 (14) | C22—C17—C18—C23 | −179.14 (17) |
| C5—C6—C7—N3 | −11.6 (2) | N3—C17—C18—C23 | 6.0 (2) |
| N2—C6—C7—C9 | −12.7 (2) | C15—C14—C13—C12 | 0.7 (3) |
| C5—C6—C7—C9 | 165.96 (16) | C15—C10—C11—C12 | 2.1 (2) |
| N2—C2—C3—C4 | 0.3 (2) | N1—C10—C11—C12 | −171.07 (15) |
| C1—C2—C3—C4 | 179.40 (15) | C14—C13—C12—C11 | −0.8 (3) |
| N2—C6—C5—C4 | −0.6 (2) | C10—C11—C12—C13 | −0.5 (3) |
| C7—C6—C5—C4 | −179.19 (15) | C21—C20—C19—C18 | −0.4 (3) |
| C1—N1—C10—C11 | −93.60 (19) | C17—C18—C19—C20 | 0.4 (3) |
| C1—N1—C10—C15 | 93.31 (19) | C23—C18—C19—C20 | 179.31 (19) |
| C7—N3—C17—C22 | 68.2 (2) | C19—C20—C21—C22 | 0.3 (3) |
| C7—N3—C17—C18 | −117.05 (18) | C17—C22—C21—C20 | −0.1 (3) |

**Fig. 1**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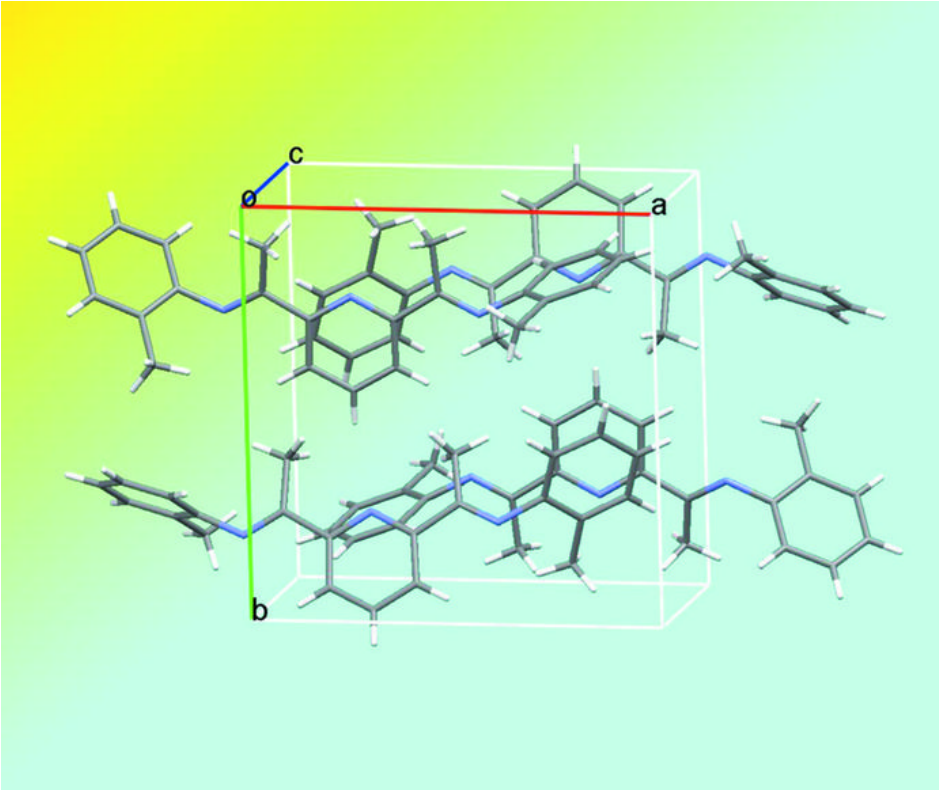
**Fig. 2**