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# 4,4′-[Propane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile–4,4′-[ethane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile [0.796 (2)/0.204 (2)]

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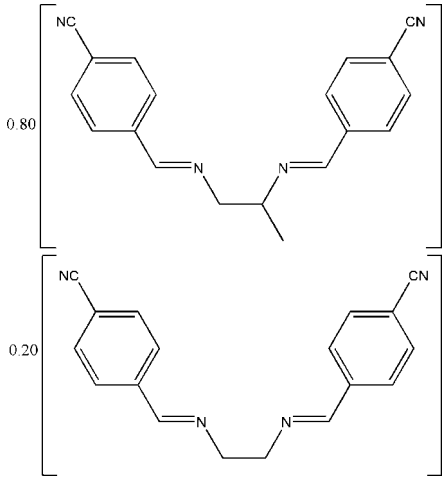
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.059; $wR$ factor = 0.182; data-to-parameter ratio = 20.1.

The title cocrystal, $0.796C_{19}H_{16}N_4{\cdot}0.204C_{18}H_{14}N_4$, is a disordered mixture of two potentially bidentate Schiff base ligands. The difference in the two components of the cocrystal is the replacement of the methyl group in the linkage between the imine N atoms in the major component of the Schiff base ligand by an H atom. The imino (C=N) functional groups are coplanar with the benzene rings (only the major component) and extend in opposite directions (both components). Intermolecular $\pi$–$\pi$ interactions with a centroid-to-centroid distance of 3.7371 (8) Å are observed in the crystal packing.

## Related literature

For values of bond lengths, see: Allen *et al.* (1987). For related structures, see, for example: Li *et al.* (2005); Bomfim *et al.* (2005); Glidewell *et al.* (2005, 2006); Sun *et al.* (2004); Fun, Kia & Kargar (2008); Fun, Kargar & Kia (2008).




## Experimental

### Crystal data

$0.796C_{19}H_{16}N_4{\cdot}0.204C_{18}H_{14}N_4$
$M_r$ = 297.68
Triclinic, $P\overline{1}$
$a$ = 9.2370 (2) Å
$b$ = 9.7769 (2) Å
$c$ = 9.8169 (2) Å
$\alpha$ = 81.846 (1)°
$\beta$ = 75.098 (1)°
$\gamma$ = 67.421 (1)°
$V$ = 790.15 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 100.0 (1) K
0.39 × 0.38 × 0.27 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.890, $T_{max}$ = 0.979
17295 measured reflections
4628 independent reflections
3746 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.182
$S$ = 1.04
4628 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: EZ2140).

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# supplementary materials

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# 4,4'-[Propane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile-4,4'-[ethane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile [0.796 (2)/0.204 (2)]

**H.-K. Fun, R. Kia and H. Kargar**

## Comment

Schiff bases are among the most prevalent mixed-donor ligands in the field of coordination chemistry. They play an important role in the development of catalysts and enzymatic reactions, magnetic materials and supramolecular architectures. Structures of Schiff bases derived from substituted benzaldehydes and closely related to the title compound have been reported recently (Li *et al.*, 2005; Bomfim *et al.*, 2005; Glidewell *et al.*, 2005, 2006; Sun *et al.*, 2004; Fun, Kargar & Kia, 2008; Fun, Kia & Kargar, 2008).

The title cocrystal consists of two bidentate Schiff base ligands. The bond lengths and angles in the two molecules (I, Fig. 1) are within normal ranges (Allen *et al.*, 1987). In the major component, the imino (C=N) functional groups are coplanar with the benzene rings. The difference in the two components of the co-crystal, which are disordered over two sites, is the replacement of the methyl group in the major component by a hydrogen atom in the linkage between the imino N atoms. The ratio of the refined site occupancy factors of the major and minor components is 0.796 (2)/0.204 (2). The short distance between the centroids of the six-membered rings indicates the existence of π-π interactions (Fig. 2), with a *Cg*1···*Cg*1 distance of 3.7371 (8) Å (symmetry code: -*x*, -*y*, 2 - *z*; *Cg*1 is the centroid of the C11–C16 benzene ring).

## Experimental

The synthetic method has been described previously (Fun, Kargar & Kia, 2008). Single crystals suitable for *X*-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

## Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å. The $U_{iso}$ values were constrained to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating-group model was used for the methyl groups. Incorrect bond lengths of the methylene bridge, plus the presence of large peaks in the difference Fourier map near to the methylene bridge, led us to suspect positional disorder of this segment of the title compound. The refined ratio of the site-occupany factors for the disorder parts is 0.796 (2)/0.204 (2).

## Figures

Fig. 1. The molecular structure of the title cocrystal, with atom labels and 50% probability ellipsoids for non-H atoms. Open bonds indicate the minor component.

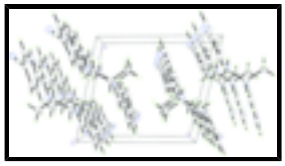

Fig. 2. The crystal packing of the major component of (I), viewed down the *b*-axis.

### 4,4'-[propane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile– 4,4'-[ethane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile [0.796 (2)/0.204 (2)]

*Crystal data*

| | |
|---|---|
| $0.796C_{19}H_{16}N_4{\cdot}0.204C_{18}H_{14}N_4$ | $Z = 2$ |
| $M_r = 297.68$ | $F_{000} = 313$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.251$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 9.2370$ (2) Å | Cell parameters from 6569 reflections |
| $b = 9.7769$ (2) Å | $\theta = 3.2$–$30.8°$ |
| $c = 9.8169$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $\alpha = 81.846$ (1)° | $T = 100.0$ (1) K |
| $\beta = 75.098$ (1)° | Block, colourless |
| $\gamma = 67.421$ (1)° | 0.39 × 0.38 × 0.27 mm |
| $V = 790.15$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 4628 independent reflections |
| Radiation source: fine-focus sealed tube | 3746 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 100.0(1)$ K | $\theta_{max} = 30.1°$ |
| φ and ω scans | $\theta_{min} = 2.2°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $h = -13\rightarrow13$ |
| $T_{min} = 0.890$, $T_{max} = 0.979$ | $k = -13\rightarrow13$ |
| 17295 measured reflections | $l = -13\rightarrow13$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.059$ | H-atom parameters constrained |
| $wR(F^2) = 0.182$ | $w = 1/[\sigma^2(F_o^2) + (0.0996P)^2 + 0.2311P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 4628 reflections | $\Delta\rho_{max} = 0.57$ e Å$^{-3}$ |

| | |
|---|---|
| 230 parameters | $\Delta\rho_{min} = -0.48$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

**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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| N1A | 0.44472 (19) | 0.58449 (16) | 0.76563 (18) | 0.0277 (3) | 0.796 (2) |
| N2A | 0.31537 (17) | 0.28586 (16) | 0.96983 (15) | 0.0294 (3) | 0.796 (2) |
| C8A | 0.41965 (19) | 0.44248 (17) | 0.78683 (17) | 0.0276 (3) | 0.796 (2) |
| H8AA | 0.5235 | 0.3602 | 0.7675 | 0.033* | 0.796 (2) |
| C9A | 0.3328 (2) | 0.42957 (19) | 0.93985 (17) | 0.0311 (4) | 0.796 (2) |
| H9AA | 0.3933 | 0.4409 | 1.0021 | 0.037* | 0.796 (2) |
| H9AB | 0.2275 | 0.5079 | 0.9569 | 0.037* | 0.796 (2) |
| C19A | 0.3162 (2) | 0.44326 (18) | 0.68371 (15) | 0.0302 (4) | 0.796 (2) |
| H19A | 0.3770 | 0.4426 | 0.5883 | 0.045* | 0.796 (2) |
| H19B | 0.2204 | 0.5308 | 0.6954 | 0.045* | 0.796 (2) |
| H19C | 0.2873 | 0.3569 | 0.7039 | 0.045* | 0.796 (2) |
| N1B | 0.4751 (7) | 0.5817 (7) | 0.8069 (6) | 0.0236 (13)* | 0.204 (2) |
| N2B | 0.2894 (7) | 0.2948 (6) | 0.8959 (6) | 0.0294 (3) | 0.204 (2) |
| C8B | 0.4619 (7) | 0.4375 (6) | 0.8536 (6) | 0.0225 (11)* | 0.204 (2) |
| H8BA | 0.4726 | 0.4144 | 0.9508 | 0.027* | 0.204 (2) |
| H8BB | 0.5478 | 0.3612 | 0.7959 | 0.027* | 0.204 (2) |
| C9B | 0.2974 (6) | 0.4397 (6) | 0.8414 (6) | 0.0203 (10) | 0.204 (2) |
| H9BA | 0.2106 | 0.5179 | 0.8962 | 0.024* | 0.204 (2) |
| H9BB | 0.2881 | 0.4571 | 0.7437 | 0.024* | 0.204 (2) |
| N3 | 0.77232 (14) | 1.20704 (14) | 0.53274 (13) | 0.0356 (3) | |
| N4 | 0.04293 (17) | −0.36229 (15) | 1.22228 (16) | 0.0481 (4) | |
| C1 | 0.77783 (15) | 0.70764 (15) | 0.59144 (14) | 0.0310 (3) | |
| H1A | 0.8552 | 0.6156 | 0.5652 | 0.037* | |
| C2 | 0.81727 (15) | 0.83368 (15) | 0.55783 (13) | 0.0301 (3) | |
| H2A | 0.9207 | 0.8263 | 0.5101 | 0.036* | |
| C3 | 0.70001 (14) | 0.97147 (14) | 0.59648 (12) | 0.0250 (2) | |
| C4 | 0.54475 (14) | 0.98285 (14) | 0.66949 (13) | 0.0281 (3) | |
| H4A | 0.4671 | 1.0749 | 0.6957 | 0.034* | |

| | | | | | |
|---|---|---|---|---|---|
| C5 | 0.50763 (14) | 0.85626 (14) | 0.70243 (13) | 0.0274 (3) | |
| H5A | 0.4043 | 0.8635 | 0.7507 | 0.033* | |
| C6 | 0.62345 (14) | 0.71778 (14) | 0.66410 (12) | 0.0248 (2) | |
| C7 | 0.58542 (16) | 0.58172 (14) | 0.69901 (14) | 0.0302 (3) | |
| H7A | 0.6682 | 0.4882 | 0.6713 | 0.036* | 0.796 (2) |
| H7B | 0.6427 | 0.4971 | 0.6419 | 0.036* | 0.204 (2) |
| C10 | 0.18277 (17) | 0.28390 (16) | 1.04041 (17) | 0.0379 (3) | |
| H10A | 0.0979 | 0.3754 | 1.0711 | 0.045* | 0.796 (2) |
| H10B | 0.1389 | 0.3631 | 1.1042 | 0.045* | 0.204 (2) |
| C11 | 0.15451 (14) | 0.14439 (14) | 1.07915 (13) | 0.0269 (3) | |
| C12 | 0.00891 (15) | 0.14545 (14) | 1.16669 (14) | 0.0309 (3) | |
| H12A | −0.0691 | 0.2345 | 1.2005 | 0.037* | |
| C13 | −0.02034 (15) | 0.01501 (14) | 1.20368 (13) | 0.0285 (3) | |
| H13A | −0.1174 | 0.0161 | 1.2625 | 0.034* | |
| C14 | 0.09638 (15) | −0.11766 (14) | 1.15229 (13) | 0.0269 (3) | |
| C15 | 0.24291 (15) | −0.12015 (15) | 1.06462 (14) | 0.0316 (3) | |
| H15A | 0.3205 | −0.2092 | 1.0303 | 0.038* | |
| C16 | 0.27163 (14) | 0.01010 (14) | 1.02930 (13) | 0.0283 (3) | |
| H16A | 0.3695 | 0.0086 | 0.9720 | 0.034* | |
| C17 | 0.73983 (15) | 1.10277 (15) | 0.56153 (13) | 0.0281 (3) | |
| C18 | 0.06622 (17) | −0.25355 (16) | 1.19090 (15) | 0.0348 (3) | |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1A | 0.0290 (7) | 0.0270 (7) | 0.0282 (7) | −0.0139 (5) | −0.0013 (6) | −0.0031 (5) |
| N2A | 0.0304 (6) | 0.0287 (6) | 0.0298 (7) | −0.0149 (5) | −0.0010 (5) | −0.0024 (5) |
| C8A | 0.0276 (7) | 0.0234 (7) | 0.0311 (8) | −0.0119 (6) | −0.0002 (6) | −0.0034 (6) |
| C9A | 0.0340 (8) | 0.0303 (8) | 0.0313 (8) | −0.0176 (6) | 0.0008 (6) | −0.0062 (6) |
| C19A | 0.0537 (10) | 0.0276 (7) | 0.0222 (7) | −0.0273 (7) | −0.0126 (6) | 0.0023 (5) |
| N2B | 0.0304 (6) | 0.0287 (6) | 0.0298 (7) | −0.0149 (5) | −0.0010 (5) | −0.0024 (5) |
| C9B | 0.024 (2) | 0.016 (2) | 0.021 (2) | −0.0076 (19) | −0.0053 (18) | 0.0005 (18) |
| N3 | 0.0337 (6) | 0.0363 (6) | 0.0387 (6) | −0.0187 (5) | 0.0002 (5) | −0.0055 (5) |
| N4 | 0.0457 (7) | 0.0340 (7) | 0.0585 (8) | −0.0165 (6) | 0.0000 (6) | 0.0008 (6) |
| C1 | 0.0258 (6) | 0.0283 (6) | 0.0341 (6) | −0.0090 (5) | 0.0027 (5) | −0.0060 (5) |
| C2 | 0.0239 (5) | 0.0335 (7) | 0.0312 (6) | −0.0127 (5) | 0.0020 (4) | −0.0046 (5) |
| C3 | 0.0253 (5) | 0.0294 (6) | 0.0229 (5) | −0.0134 (5) | −0.0033 (4) | −0.0031 (4) |
| C4 | 0.0235 (5) | 0.0265 (6) | 0.0325 (6) | −0.0096 (4) | −0.0006 (4) | −0.0051 (5) |
| C5 | 0.0225 (5) | 0.0294 (6) | 0.0298 (6) | −0.0116 (5) | −0.0006 (4) | −0.0036 (5) |
| C6 | 0.0252 (5) | 0.0268 (6) | 0.0219 (5) | −0.0112 (4) | −0.0011 (4) | −0.0029 (4) |
| C7 | 0.0304 (6) | 0.0258 (6) | 0.0308 (6) | −0.0108 (5) | 0.0010 (5) | −0.0025 (5) |
| C10 | 0.0293 (6) | 0.0273 (6) | 0.0558 (9) | −0.0129 (5) | 0.0018 (6) | −0.0112 (6) |
| C11 | 0.0248 (5) | 0.0261 (6) | 0.0312 (6) | −0.0105 (4) | −0.0043 (4) | −0.0055 (4) |
| C12 | 0.0260 (6) | 0.0257 (6) | 0.0360 (6) | −0.0066 (5) | 0.0000 (5) | −0.0066 (5) |
| C13 | 0.0236 (5) | 0.0305 (6) | 0.0283 (6) | −0.0094 (5) | −0.0015 (4) | −0.0008 (5) |
| C14 | 0.0269 (6) | 0.0263 (6) | 0.0263 (5) | −0.0094 (5) | −0.0046 (4) | −0.0005 (4) |
| C15 | 0.0271 (6) | 0.0265 (6) | 0.0358 (6) | −0.0072 (5) | 0.0004 (5) | −0.0057 (5) |
| C16 | 0.0232 (5) | 0.0299 (6) | 0.0303 (6) | −0.0100 (5) | −0.0006 (4) | −0.0054 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.0256 (5) | 0.0330 (6) | 0.0269 (6) | −0.0134 (5) | −0.0013 (4) | −0.0054 (5) |
| C18 | 0.0326 (6) | 0.0304 (7) | 0.0372 (7) | −0.0113 (5) | −0.0012 (5) | −0.0005 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1A—C7 | 1.2878 (18) | C2—C3 | 1.3947 (18) |
| N1A—C8A | 1.4714 (19) | C2—H2A | 0.9300 |
| N2A—C10 | 1.2484 (18) | C3—C4 | 1.3979 (16) |
| N2A—C9A | 1.455 (2) | C3—C17 | 1.4400 (16) |
| C8A—C9A | 1.523 (2) | C4—C5 | 1.3818 (16) |
| C8A—C19A | 1.558 (2) | C4—H4A | 0.9300 |
| C8A—H8AA | 0.9800 | C5—C6 | 1.3944 (17) |
| C9A—H9AA | 0.9700 | C5—H5A | 0.9300 |
| C9A—H9AB | 0.9700 | C6—C7 | 1.4758 (16) |
| C19A—H19A | 0.9600 | C7—H7A | 0.9600 |
| C19A—H19B | 0.9600 | C7—H7B | 0.9600 |
| C19A—H19C | 0.9600 | C10—C11 | 1.4658 (17) |
| N1B—C7 | 1.267 (6) | C10—H10A | 0.9600 |
| N1B—C8B | 1.460 (8) | C10—H10B | 0.9600 |
| N2B—C9B | 1.464 (7) | C11—C12 | 1.3945 (17) |
| N2B—C10 | 1.521 (6) | C11—C16 | 1.3975 (17) |
| C8B—C9B | 1.546 (8) | C12—C13 | 1.3834 (17) |
| C8B—H8BA | 0.9700 | C12—H12A | 0.9300 |
| C8B—H8BB | 0.9700 | C13—C14 | 1.3897 (17) |
| C9B—H9BA | 0.9700 | C13—H13A | 0.9300 |
| C9B—H9BB | 0.9700 | C14—C15 | 1.3982 (17) |
| N3—C17 | 1.1484 (17) | C14—C18 | 1.4400 (18) |
| N4—C18 | 1.1489 (19) | C15—C16 | 1.3781 (17) |
| C1—C2 | 1.3883 (17) | C15—H15A | 0.9300 |
| C1—C6 | 1.3930 (16) | C16—H16A | 0.9300 |
| C1—H1A | 0.9300 | | |
| C7—N1A—C8A | 116.77 (13) | C1—C6—C5 | 119.43 (11) |
| C10—N2A—C9A | 117.17 (13) | C1—C6—C7 | 119.38 (11) |
| N1A—C8A—C9A | 107.68 (13) | C5—C6—C7 | 121.19 (10) |
| N1A—C8A—C19A | 108.24 (13) | N1B—C7—N1A | 24.5 (2) |
| C9A—C8A—C19A | 111.02 (13) | N1B—C7—C6 | 117.3 (3) |
| N1A—C8A—H8AA | 110.0 | N1A—C7—C6 | 122.07 (12) |
| C9A—C8A—H8AA | 110.0 | N1B—C7—H7A | 117.8 |
| C19A—C8A—H8AA | 110.0 | N1A—C7—H7A | 119.0 |
| N2A—C9A—C8A | 110.09 (13) | C6—C7—H7A | 119.0 |
| N2A—C9A—H9AA | 109.6 | N1B—C7—H7B | 121.9 |
| C8A—C9A—H9AA | 109.6 | N1A—C7—H7B | 111.9 |
| N2A—C9A—H9AB | 109.6 | C6—C7—H7B | 120.8 |
| C8A—C9A—H9AB | 109.6 | H7A—C7—H7B | 23.9 |
| H9AA—C9A—H9AB | 108.2 | N2A—C10—C11 | 121.33 (13) |
| C7—N1B—C8B | 115.5 (5) | N2A—C10—N2B | 31.9 (2) |
| C9B—N2B—C10 | 118.6 (4) | C11—C10—N2B | 116.6 (2) |
| N1B—C8B—C9B | 110.0 (5) | N2A—C10—H10A | 119.5 |
| N1B—C8B—H8BA | 109.7 | C11—C10—H10A | 119.2 |

| | | | |
|---|---|---|---|
| C9B—C8B—H8BA | 109.7 | N2B—C10—H10A | 114.8 |
| N1B—C8B—H8BB | 109.7 | N2A—C10—H10B | 107.4 |
| C9B—C8B—H8BB | 109.7 | C11—C10—H10B | 121.7 |
| H8BA—C8B—H8BB | 108.2 | N2B—C10—H10B | 121.8 |
| N2B—C9B—C8B | 107.0 (4) | H10A—C10—H10B | 32.0 |
| N2B—C9B—H9BA | 110.3 | C12—C11—C16 | 119.49 (11) |
| C8B—C9B—H9BA | 110.3 | C12—C11—C10 | 119.68 (11) |
| N2B—C9B—H9BB | 110.3 | C16—C11—C10 | 120.83 (11) |
| C8B—C9B—H9BB | 110.3 | C13—C12—C11 | 120.51 (11) |
| H9BA—C9B—H9BB | 108.6 | C13—C12—H12A | 119.7 |
| C2—C1—C6 | 120.64 (11) | C11—C12—H12A | 119.7 |
| C2—C1—H1A | 119.7 | C12—C13—C14 | 119.49 (11) |
| C6—C1—H1A | 119.7 | C12—C13—H13A | 120.3 |
| C1—C2—C3 | 119.28 (11) | C14—C13—H13A | 120.3 |
| C1—C2—H2A | 120.4 | C13—C14—C15 | 120.52 (12) |
| C3—C2—H2A | 120.4 | C13—C14—C18 | 119.56 (11) |
| C2—C3—C4 | 120.53 (11) | C15—C14—C18 | 119.92 (11) |
| C2—C3—C17 | 119.61 (10) | C16—C15—C14 | 119.61 (11) |
| C4—C3—C17 | 119.86 (11) | C16—C15—H15A | 120.2 |
| C5—C4—C3 | 119.44 (11) | C14—C15—H15A | 120.2 |
| C5—C4—H4A | 120.3 | C15—C16—C11 | 120.37 (11) |
| C3—C4—H4A | 120.3 | C15—C16—H16A | 119.8 |
| C4—C5—C6 | 120.68 (11) | C11—C16—H16A | 119.8 |
| C4—C5—H5A | 119.7 | N3—C17—C3 | 179.50 (14) |
| C6—C5—H5A | 119.7 | N4—C18—C14 | 179.53 (16) |
| C7—N1A—C8A—C9A | 134.28 (16) | C1—C6—C7—N1B | 152.5 (3) |
| C7—N1A—C8A—C19A | −105.62 (18) | C5—C6—C7—N1B | −27.5 (4) |
| C10—N2A—C9A—C8A | −136.91 (16) | C1—C6—C7—N1A | −179.80 (14) |
| N1A—C8A—C9A—N2A | −175.76 (13) | C5—C6—C7—N1A | 0.2 (2) |
| C19A—C8A—C9A—N2A | 65.92 (17) | C9A—N2A—C10—C11 | −178.46 (13) |
| C7—N1B—C8B—C9B | −116.7 (5) | C9A—N2A—C10—N2B | 90.8 (4) |
| C10—N2B—C9B—C8B | 105.6 (5) | C9B—N2B—C10—N2A | −83.9 (6) |
| N1B—C8B—C9B—N2B | −177.4 (5) | C9B—N2B—C10—C11 | 168.8 (4) |
| C6—C1—C2—C3 | −0.6 (2) | N2A—C10—C11—C12 | 175.33 (15) |
| C1—C2—C3—C4 | 0.61 (19) | N2B—C10—C11—C12 | −148.5 (3) |
| C1—C2—C3—C17 | −179.77 (11) | N2A—C10—C11—C16 | −4.8 (2) |
| C2—C3—C4—C5 | −0.45 (19) | N2B—C10—C11—C16 | 31.4 (3) |
| C17—C3—C4—C5 | 179.94 (11) | C16—C11—C12—C13 | −0.31 (19) |
| C3—C4—C5—C6 | 0.25 (19) | C10—C11—C12—C13 | 179.60 (12) |
| C2—C1—C6—C5 | 0.38 (19) | C11—C12—C13—C14 | −0.35 (19) |
| C2—C1—C6—C7 | −179.66 (11) | C12—C13—C14—C15 | 0.44 (19) |
| C4—C5—C6—C1 | −0.22 (19) | C12—C13—C14—C18 | 179.89 (12) |
| C4—C5—C6—C7 | 179.83 (11) | C13—C14—C15—C16 | 0.1 (2) |
| C8B—N1B—C7—N1A | 83.2 (8) | C18—C14—C15—C16 | −179.31 (12) |
| C8B—N1B—C7—C6 | −168.7 (4) | C14—C15—C16—C11 | −0.8 (2) |
| C8A—N1A—C7—N1B | −97.6 (8) | C12—C11—C16—C15 | 0.90 (19) |
| C8A—N1A—C7—C6 | 176.59 (13) | C10—C11—C16—C15 | −179.01 (12) |

**Fig. 1**

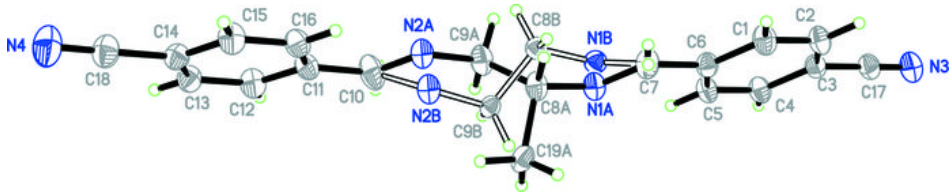
N4
C18
C14
C15
C16
C13
C12
C11
C10
N2A
C9A
N2B
C9B
C8B
C8A
N1B
N1A
C7
C6
C1
C2
C5
C4
C3
C17
N3
C19A

**Fig. 2**