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# 2,5-Bis[(dimethylamino)methyl]-1*H*-pyrrole

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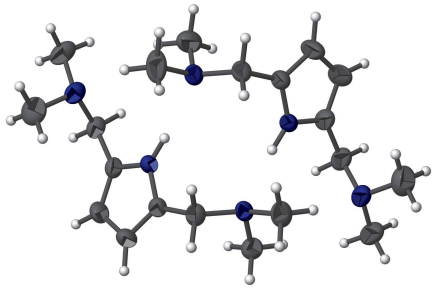
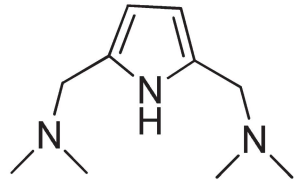
**Structural data**: full structural data are available from iucrdata.iucr.org

The asymmetric unit contains two independent molecules, $C_{10}H_{19}N_3$, which are linked into dimers by two $N_{pyrrole}—H\cdots N_{amine}$ hydrogen bonds.

**3D view**



**Chemical scheme**




## Structure description

Over the past few years, pincer ligands with three nitrogen donor functions {NNN} have played an increasingly important role in coordination chemistry. Due to their high thermal stability, unusual reactivity and high degree of flexibility concerning steric and electronic properties, they have been synthesized for making metal complexes to study catalysis of organic transformation reactions and used in inorganic coordination chemistry (Guo *et al.*, 2015). Among them, the monoanionic tridentate pyrrolyl ligand containing saturated methylene moieties, 2,5-bis[(dimethylamino)methylene]-1*H*-pyrrole, is a representative example. It is in a liquid state at room temperature. Many organometallic compounds formed by this auxiliary ligand with aluminium (Liu *et al.*, 2013) and zinc (Hsiao *et al.*, 2012) or transition metals including Ti (Li *et al.*, 2005), Zr (Hsu *et al.*, 2012), Hf (Lee *et al.*, 2011), Ga (Wang *et al.*, 2013), In (Kuo *et al.*, 2003), Y (Kuo *et al.*, 2005) and Mo (Huang *et al.*, 2001) have been reported and there are several reports of the crystal structures of organometallic compounds containing 2,5-bis[(dimethylamino)methylene]-1*H*-pyrrole as a ligand (Xia *et al.*, 2002; Lee *et al.*, 2011; Chang *et al.*, 2011; Wang *et al.*, 2012). However, although 2,5-bis[(dimethylamino)methylene]-1*H*-pyrrole has been prepared and studied for a long time, its crystal structure has not been reported so far. As a part of our studies on organometallic complexes incorporating substituted symmetrical tridentate pyrrolyl ligands and their application, we have determined its structure.

The asymmetric unit of the title compound is shown in Fig. 1. The two independent molecules are linked into dimers by $N_{pyrrole}—H\cdots N_{amine}$ hydrogen bonds (Table 1, Fig. 2).

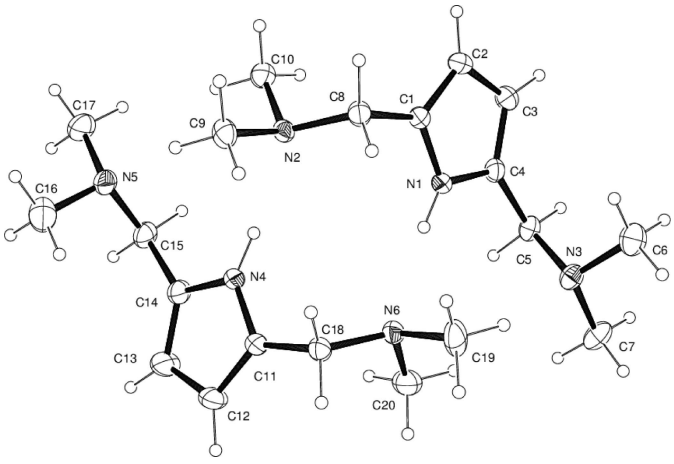



**Figure 1**
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

## Synthesis and crystallization

The title compound was prepared following a modified literature procedure (Herz *et al.*, 1947). A 250 ml flask was charged with formaldehyde (37%, 14.0 ml, 0.2 mol) and dimethylamine hydrochloride (16.3 g, 0.2 mol) and cooled to 273 K in an ice bath for 30 minutes with stirring. To the stirred solution, pyrrole (6.7 g, 0.1 mol) was added dropwise and the combined solution was warmed to room temperature and stirred for 24 h. The brown solution was neutralized with 30 ml aqueous sodium hydroxide (8 g, 0.2 mol) solution. The organic layer was separated, and the aqueous layer was extracted with 50 ml diethyl ether in three portions. The combined organic portion was dried over anhydrous $MgSO_4$ and filtered, and the solvent was removed under reduced pressure. The resultant residue was distilled under vacuum, yielding a colorless liquid (14.71 g, 78%). Crystals suitable for X-ray diffraction analysis were obtained from diethyl ether at 278 K. $^1$H NMR (300 MHz, $CDCl_3$): 2.22 (*s*, 12H, $NMe_2$), 3.39 (*s*, 4H, $CH_2NMe_2$), 5.92 (*s*, 2H, pyrrolyl C*H*), 8.7 (*br*, 1H, pyrrolyl N*H*).

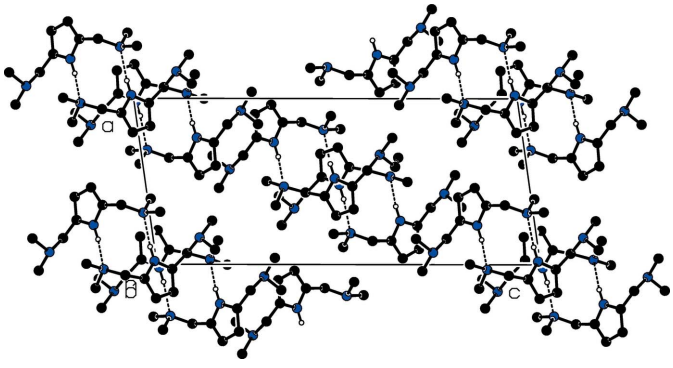


**Figure 2**
The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines. Only H atoms involved in hydrogen bonding are shown.

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H21···N6 | 0.886 (17) | 2.094 (17) | 2.9699 (16) | 169.8 (14) |
| N4—H20···N2 | 0.926 (16) | 2.095 (17) | 2.9939 (16) | 163.5 (14) |

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{10}H_{19}N_3$ |
| $M_r$ | 181.28 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 200 |
| $a$, $b$, $c$ (Å) | 9.8203 (4), 10.6193 (4), 22.5202 (9) |
| $\beta$ (°) | 98.098 (1) |
| $V$ (Å$^3$) | 2325.09 (16) |
| $Z$ | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.06 |
| Crystal size (mm) | 0.25 × 0.20 × 0.20 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2013) |
| $T_{min}$, $T_{max}$ | 0.984, 0.987 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 16645, 4102, 3463 |
| $R_{int}$ | 0.031 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.596 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.048, 0.120, 1.00 |
| No. of reflections | 4102 |
| No. of parameters | 251 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.14, −0.29 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2016). **1**, x161617 [https://doi.org/10.1107/S2414314616016175]

## 2,5-Bis[(dimethylamino)methyl]-1*H*-pyrrole

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### 2,5-Bis[(dimethylamino)methyl]-1*H*-pyrrole

*Crystal data*

$C_{10}H_{19}N_3$
$M_r$ = 181.28
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 9.8203 (4) Å
$b$ = 10.6193 (4) Å
$c$ = 22.5202 (9) Å
$\beta$ = 98.098 (1)°
$V$ = 2325.09 (16) Å$^3$
$Z$ = 8
$F(000)$ = 800
$D_x$ = 1.036 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9945 reflections
$\theta$ = 2.9–28.3°
$\mu$ = 0.06 mm$^{-1}$
$T$ = 200 K
Block, colorless
0.25 × 0.20 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min}$ = 0.984, $T_{max}$ = 0.987
16645 measured reflections
4102 independent reflections
3463 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.9°
$h$ = −11→9
$k$ = −12→12
$l$ = −26→26

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.120
$S$ = 1.00
4102 reflections
251 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.51916 (12) | 0.27259 (11) | 0.49505 (5) | 0.0330 (3) |
| N2 | 0.46921 (11) | 0.18139 (10) | 0.35956 (5) | 0.0329 (3) |
| N3 | 0.66223 (13) | 0.33577 (11) | 0.62140 (5) | 0.0406 (3) |
| N4 | 0.73647 (12) | 0.30961 (11) | 0.34942 (5) | 0.0349 (3) |
| N5 | 0.57265 (13) | 0.37168 (13) | 0.22458 (5) | 0.0462 (3) |
| N6 | 0.81107 (12) | 0.21866 (12) | 0.48359 (5) | 0.0380 (3) |
| C1 | 0.41230 (14) | 0.20883 (14) | 0.46275 (6) | 0.0373 (3) |
| C2 | 0.29505 (15) | 0.24217 (17) | 0.48545 (7) | 0.0490 (4) |
| H2 | 0.2046 | 0.2133 | 0.4716 | 0.059* |
| C3 | 0.33301 (15) | 0.32738 (17) | 0.53326 (7) | 0.0485 (4) |
| H3 | 0.2727 | 0.3657 | 0.5574 | 0.058* |
| C4 | 0.47210 (14) | 0.34452 (14) | 0.53839 (6) | 0.0372 (3) |
| C5 | 0.56728 (15) | 0.41779 (14) | 0.58293 (6) | 0.0396 (3) |
| H5A | 0.6209 | 0.4771 | 0.5614 | 0.047* |
| H5B | 0.5128 | 0.4679 | 0.6082 | 0.047* |
| C6 | 0.5889 (2) | 0.25212 (16) | 0.65700 (8) | 0.0590 (5) |
| H6A | 0.6549 | 0.1973 | 0.6814 | 0.088* |
| H6B | 0.5240 | 0.2005 | 0.6303 | 0.088* |
| H6C | 0.5385 | 0.3022 | 0.6833 | 0.088* |
| C7 | 0.76343 (19) | 0.40912 (16) | 0.66004 (7) | 0.0552 (4) |
| H7A | 0.7171 | 0.4591 | 0.6879 | 0.083* |
| H7B | 0.8115 | 0.4655 | 0.6355 | 0.083* |
| H7C | 0.8300 | 0.3523 | 0.6829 | 0.083* |
| C8 | 0.43384 (16) | 0.11967 (14) | 0.41380 (6) | 0.0393 (3) |
| H8A | 0.5085 | 0.0605 | 0.4291 | 0.047* |
| H8B | 0.3489 | 0.0697 | 0.4029 | 0.047* |
| C9 | 0.50189 (17) | 0.08705 (14) | 0.31653 (7) | 0.0451 (4) |
| H9A | 0.4207 | 0.0348 | 0.3040 | 0.068* |
| H9B | 0.5774 | 0.0338 | 0.3353 | 0.068* |
| H9C | 0.5295 | 0.1293 | 0.2814 | 0.068* |
| C10 | 0.35561 (16) | 0.25880 (15) | 0.33159 (7) | 0.0439 (4) |
| H10A | 0.3820 | 0.3005 | 0.2961 | 0.066* |
| H10B | 0.3334 | 0.3225 | 0.3602 | 0.066* |
| H10C | 0.2750 | 0.2055 | 0.3196 | 0.066* |
| C11 | 0.85627 (14) | 0.26252 (15) | 0.37998 (6) | 0.0404 (4) |
| C12 | 0.96231 (16) | 0.3169 (2) | 0.35660 (8) | 0.0666 (6) |
| H12 | 1.0575 | 0.3025 | 0.3692 | 0.080* |
| C13 | 0.90529 (18) | 0.3985 (2) | 0.31040 (8) | 0.0707 (6) |
| H13 | 0.9554 | 0.4485 | 0.2860 | 0.085* |
| C14 | 0.76571 (16) | 0.39331 (15) | 0.30672 (7) | 0.0458 (4) |

| | | | | |
|---|---|---|---|---|
| C15 | 0.65633 (17) | 0.45768 (16) | 0.26511 (7) | 0.0476 (4) |
| H15A | 0.5956 | 0.5042 | 0.2890 | 0.057* |
| H15B | 0.6998 | 0.5200 | 0.2410 | 0.057* |
| C16 | 0.6545 (2) | 0.3079 (2) | 0.18498 (9) | 0.0700 (5) |
| H16A | 0.6931 | 0.3700 | 0.1599 | 0.105* |
| H16B | 0.5962 | 0.2488 | 0.1594 | 0.105* |
| H16C | 0.7293 | 0.2617 | 0.2089 | 0.105* |
| C17 | 0.46052 (19) | 0.4411 (2) | 0.18979 (8) | 0.0663 (5) |
| H17A | 0.4985 | 0.5057 | 0.1657 | 0.099* |
| H17B | 0.4043 | 0.4814 | 0.2171 | 0.099* |
| H17C | 0.4034 | 0.3829 | 0.1632 | 0.099* |
| C18 | 0.85787 (15) | 0.16923 (14) | 0.42902 (6) | 0.0393 (3) |
| H18A | 0.7985 | 0.0973 | 0.4142 | 0.047* |
| H18B | 0.9528 | 0.1369 | 0.4395 | 0.047* |
| C19 | 0.8157 (2) | 0.11775 (19) | 0.52785 (8) | 0.0661 (6) |
| H19A | 0.9108 | 0.0889 | 0.5385 | 0.099* |
| H19B | 0.7583 | 0.0474 | 0.5109 | 0.099* |
| H19C | 0.7811 | 0.1492 | 0.5638 | 0.099* |
| C20 | 0.89513 (18) | 0.3249 (2) | 0.50799 (8) | 0.0625 (5) |
| H20A | 0.8625 | 0.3548 | 0.5447 | 0.094* |
| H20B | 0.8881 | 0.3931 | 0.4784 | 0.094* |
| H20C | 0.9913 | 0.2981 | 0.5173 | 0.094* |
| H20 | 0.6493 (17) | 0.2851 (14) | 0.3558 (7) | 0.043 (4)* |
| H21 | 0.6060 (17) | 0.2653 (14) | 0.4890 (7) | 0.041 (4)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0285 (6) | 0.0417 (7) | 0.0296 (6) | −0.0026 (5) | 0.0065 (5) | −0.0023 (5) |
| N2 | 0.0341 (6) | 0.0344 (6) | 0.0313 (6) | −0.0056 (5) | 0.0089 (5) | −0.0064 (5) |
| N3 | 0.0475 (7) | 0.0375 (6) | 0.0351 (6) | 0.0031 (5) | −0.0001 (5) | −0.0050 (5) |
| N4 | 0.0295 (6) | 0.0445 (7) | 0.0308 (6) | −0.0035 (5) | 0.0047 (5) | 0.0056 (5) |
| N5 | 0.0467 (7) | 0.0568 (8) | 0.0343 (7) | −0.0057 (6) | 0.0025 (5) | 0.0107 (6) |
| N6 | 0.0340 (6) | 0.0474 (7) | 0.0332 (6) | 0.0068 (5) | 0.0077 (5) | 0.0083 (5) |
| C1 | 0.0342 (7) | 0.0474 (8) | 0.0307 (7) | −0.0086 (6) | 0.0063 (6) | −0.0022 (6) |
| C2 | 0.0313 (7) | 0.0744 (11) | 0.0421 (8) | −0.0096 (7) | 0.0081 (6) | −0.0073 (8) |
| C3 | 0.0383 (8) | 0.0698 (11) | 0.0399 (8) | 0.0049 (8) | 0.0137 (6) | −0.0077 (8) |
| C4 | 0.0403 (8) | 0.0431 (8) | 0.0288 (7) | 0.0023 (6) | 0.0072 (6) | −0.0020 (6) |
| C5 | 0.0484 (8) | 0.0382 (8) | 0.0316 (7) | 0.0022 (6) | 0.0038 (6) | −0.0024 (6) |
| C6 | 0.0730 (12) | 0.0494 (10) | 0.0539 (10) | 0.0039 (9) | 0.0066 (9) | 0.0128 (8) |
| C7 | 0.0630 (11) | 0.0518 (10) | 0.0453 (9) | 0.0061 (8) | −0.0117 (8) | −0.0119 (8) |
| C8 | 0.0445 (8) | 0.0400 (8) | 0.0342 (7) | −0.0105 (6) | 0.0080 (6) | −0.0033 (6) |
| C9 | 0.0548 (9) | 0.0420 (8) | 0.0406 (8) | −0.0034 (7) | 0.0141 (7) | −0.0112 (7) |
| C10 | 0.0435 (8) | 0.0469 (8) | 0.0410 (8) | 0.0006 (7) | 0.0053 (7) | −0.0030 (7) |
| C11 | 0.0307 (7) | 0.0562 (9) | 0.0345 (7) | −0.0002 (6) | 0.0057 (6) | 0.0080 (7) |
| C12 | 0.0313 (8) | 0.1101 (16) | 0.0584 (11) | −0.0065 (9) | 0.0062 (7) | 0.0342 (11) |
| C13 | 0.0435 (9) | 0.1081 (16) | 0.0603 (11) | −0.0204 (10) | 0.0060 (8) | 0.0423 (11) |
| C14 | 0.0438 (8) | 0.0559 (9) | 0.0367 (8) | −0.0095 (7) | 0.0025 (6) | 0.0136 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.0535 (9) | 0.0504 (9) | 0.0375 (8) | −0.0030 (7) | 0.0015 (7) | 0.0110 (7) |
| C16 | 0.0836 (14) | 0.0752 (13) | 0.0530 (11) | −0.0044 (11) | 0.0158 (10) | −0.0043 (10) |
| C17 | 0.0569 (10) | 0.0914 (14) | 0.0467 (10) | −0.0045 (10) | −0.0065 (8) | 0.0234 (10) |
| C18 | 0.0353 (7) | 0.0477 (8) | 0.0357 (7) | 0.0070 (6) | 0.0077 (6) | 0.0066 (6) |
| C19 | 0.0795 (13) | 0.0785 (13) | 0.0444 (9) | 0.0340 (11) | 0.0229 (9) | 0.0284 (9) |
| C20 | 0.0444 (9) | 0.0851 (13) | 0.0582 (11) | −0.0051 (9) | 0.0077 (8) | −0.0207 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.3689 (17) | C7—H7C | 0.9800 |
| N1—C4 | 1.3700 (17) | C8—H8A | 0.9900 |
| N1—H21 | 0.886 (17) | C8—H8B | 0.9900 |
| N2—C10 | 1.4557 (18) | C9—H9A | 0.9800 |
| N2—C9 | 1.4605 (17) | C9—H9B | 0.9800 |
| N2—C8 | 1.4704 (17) | C9—H9C | 0.9800 |
| N3—C7 | 1.4519 (19) | C10—H10A | 0.9800 |
| N3—C6 | 1.453 (2) | C10—H10B | 0.9800 |
| N3—C5 | 1.4666 (18) | C10—H10C | 0.9800 |
| N4—C11 | 1.3710 (18) | C11—C12 | 1.360 (2) |
| N4—C14 | 1.3693 (18) | C11—C18 | 1.4820 (19) |
| N4—H20 | 0.926 (16) | C12—C13 | 1.408 (2) |
| N5—C16 | 1.450 (2) | C12—H12 | 0.9500 |
| N5—C15 | 1.460 (2) | C13—C14 | 1.363 (2) |
| N5—C17 | 1.458 (2) | C13—H13 | 0.9500 |
| N6—C19 | 1.4599 (19) | C14—C15 | 1.489 (2) |
| N6—C20 | 1.459 (2) | C15—H15A | 0.9900 |
| N6—C18 | 1.4683 (17) | C15—H15B | 0.9900 |
| C1—C2 | 1.370 (2) | C16—H16A | 0.9800 |
| C1—C8 | 1.4906 (19) | C16—H16B | 0.9800 |
| C2—C3 | 1.416 (2) | C16—H16C | 0.9800 |
| C2—H2 | 0.9500 | C17—H17A | 0.9800 |
| C3—C4 | 1.367 (2) | C17—H17B | 0.9800 |
| C3—H3 | 0.9500 | C17—H17C | 0.9800 |
| C4—C5 | 1.4903 (19) | C18—H18A | 0.9900 |
| C5—H5A | 0.9900 | C18—H18B | 0.9900 |
| C5—H5B | 0.9900 | C19—H19A | 0.9800 |
| C6—H6A | 0.9800 | C19—H19B | 0.9800 |
| C6—H6B | 0.9800 | C19—H19C | 0.9800 |
| C6—H6C | 0.9800 | C20—H20A | 0.9800 |
| C7—H7A | 0.9800 | C20—H20B | 0.9800 |
| C7—H7B | 0.9800 | C20—H20C | 0.9800 |
| | | | |
| C1—N1—C4 | 110.12 (12) | N2—C9—H9C | 109.5 |
| C1—N1—H21 | 123.9 (10) | H9A—C9—H9C | 109.5 |
| C4—N1—H21 | 126.0 (10) | H9B—C9—H9C | 109.5 |
| C10—N2—C9 | 109.09 (11) | N2—C10—H10A | 109.5 |
| C10—N2—C8 | 110.78 (11) | N2—C10—H10B | 109.5 |
| C9—N2—C8 | 110.19 (11) | H10A—C10—H10B | 109.5 |

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|---|---|---|---|
| C7—N3—C6 | 110.34 (13) | N2—C10—H10C | 109.5 |
| C7—N3—C5 | 111.10 (12) | H10A—C10—H10C | 109.5 |
| C6—N3—C5 | 111.45 (13) | H10B—C10—H10C | 109.5 |
| C11—N4—C14 | 109.83 (12) | C12—C11—N4 | 107.49 (13) |
| C11—N4—H20 | 124.5 (10) | C12—C11—C18 | 130.10 (14) |
| C14—N4—H20 | 125.6 (10) | N4—C11—C18 | 122.42 (12) |
| C16—N5—C15 | 111.41 (14) | C11—C12—C13 | 107.51 (14) |
| C16—N5—C17 | 110.36 (14) | C11—C12—H12 | 126.2 |
| C15—N5—C17 | 109.61 (14) | C13—C12—H12 | 126.2 |
| C19—N6—C20 | 110.40 (14) | C14—C13—C12 | 108.17 (14) |
| C19—N6—C18 | 109.01 (12) | C14—C13—H13 | 125.9 |
| C20—N6—C18 | 111.38 (12) | C12—C13—H13 | 125.9 |
| C2—C1—N1 | 107.18 (13) | C13—C14—N4 | 106.99 (13) |
| C2—C1—C8 | 130.86 (13) | C13—C14—C15 | 130.55 (14) |
| N1—C1—C8 | 121.94 (12) | N4—C14—C15 | 122.42 (13) |
| C1—C2—C3 | 107.69 (13) | N5—C15—C14 | 113.52 (13) |
| C1—C2—H2 | 126.2 | N5—C15—H15A | 108.9 |
| C3—C2—H2 | 126.2 | C14—C15—H15A | 108.9 |
| C4—C3—C2 | 107.60 (13) | N5—C15—H15B | 108.9 |
| C4—C3—H3 | 126.2 | C14—C15—H15B | 108.9 |
| C2—C3—H3 | 126.2 | H15A—C15—H15B | 107.7 |
| C3—C4—N1 | 107.40 (13) | N5—C16—H16A | 109.5 |
| C3—C4—C5 | 130.62 (13) | N5—C16—H16B | 109.5 |
| N1—C4—C5 | 121.87 (12) | H16A—C16—H16B | 109.5 |
| N3—C5—C4 | 111.95 (12) | N5—C16—H16C | 109.5 |
| N3—C5—H5A | 109.2 | H16A—C16—H16C | 109.5 |
| C4—C5—H5A | 109.2 | H16B—C16—H16C | 109.5 |
| N3—C5—H5B | 109.2 | N5—C17—H17A | 109.5 |
| C4—C5—H5B | 109.2 | N5—C17—H17B | 109.5 |
| H5A—C5—H5B | 107.9 | H17A—C17—H17B | 109.5 |
| N3—C6—H6A | 109.5 | N5—C17—H17C | 109.5 |
| N3—C6—H6B | 109.5 | H17A—C17—H17C | 109.5 |
| H6A—C6—H6B | 109.5 | H17B—C17—H17C | 109.5 |
| N3—C6—H6C | 109.5 | N6—C18—C11 | 114.39 (12) |
| H6A—C6—H6C | 109.5 | N6—C18—H18A | 108.7 |
| H6B—C6—H6C | 109.5 | C11—C18—H18A | 108.7 |
| N3—C7—H7A | 109.5 | N6—C18—H18B | 108.7 |
| N3—C7—H7B | 109.5 | C11—C18—H18B | 108.7 |
| H7A—C7—H7B | 109.5 | H18A—C18—H18B | 107.6 |
| N3—C7—H7C | 109.5 | N6—C19—H19A | 109.5 |
| H7A—C7—H7C | 109.5 | N6—C19—H19B | 109.5 |
| H7B—C7—H7C | 109.5 | H19A—C19—H19B | 109.5 |
| N2—C8—C1 | 113.95 (11) | N6—C19—H19C | 109.5 |
| N2—C8—H8A | 108.8 | H19A—C19—H19C | 109.5 |
| C1—C8—H8A | 108.8 | H19B—C19—H19C | 109.5 |
| N2—C8—H8B | 108.8 | N6—C20—H20A | 109.5 |
| C1—C8—H8B | 108.8 | N6—C20—H20B | 109.5 |
| H8A—C8—H8B | 107.7 | H20A—C20—H20B | 109.5 |

| | | | |
|---|---|---|---|
| N2—C9—H9A | 109.5 | N6—C20—H20C | 109.5 |
| N2—C9—H9B | 109.5 | H20A—C20—H20C | 109.5 |
| H9A—C9—H9B | 109.5 | H20B—C20—H20C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H21···N6 | 0.886 (17) | 2.094 (17) | 2.9699 (16) | 169.8 (14) |
| N4—H20···N2 | 0.926 (16) | 2.095 (17) | 2.9939 (16) | 163.5 (14) |