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N-[1-(1H-Pyrrol-2-yl)ethylidene]aniline

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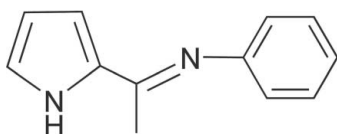
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.048; wR factor = 0.142; data-to-parameter ratio = 14.3.

There are two independent molecules in the asymmetric unit of the title compound, $\text{C}_{12}\text{H}_{12}\text{N}_2$, in which the pyrrole and benzene rings form dihedral angles of 72.37 (7) and 82.34 (8)°. The imino N—C bond lengths in the two molecules are equal [1.286 (2) Å] and indicate C=N character. In the crystal, each molecule forms a dimer with an inversion-related molecule through a pair of classical N—H...N hydrogen bonds.

Related literature

For general background to the iminopyrrole unit, see: Small *et al.* (1998); Su *et al.* (2009*a,b*); Britovsek *et al.* (2003); Dawson *et al.* (2000). For the pyrrole diimine unit, see: Matsuo *et al.* (2001) and for the pyrrole monoimine unit, see: He *et al.* (2009).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_{12}\text{N}_2$ $M_r = 184.24$ Triclinic, $P\bar{1}$ $a = 8.2236$ (14) Å $b = 11.3306$ (19) Å $c = 11.913$ (2) Å $\alpha = 95.984$ (3)° $\beta = 93.202$ (3)° $\gamma = 109.274$ (3)° $V = 1037.3$ (3) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.07$ mm⁻¹ $T = 296$ K $0.37 \times 0.25 \times 0.19$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.974$, $T_{\max} = 0.987$

5277 measured reflections
3655 independent reflections
2567 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.142$
 $S = 1.10$
3655 reflections

256 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N2}^i$	0.86	2.38	3.150 (2)	150
$\text{N3}-\text{H3A}\cdots\text{N4}^{ii}$	0.86	2.27	3.065 (2)	153

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2378).

References

- Britovsek, G. J. P., Gibson, V. C., Hoarau, O. D., Spitzmesser, S. K., White, A. J. P. & Williams, D. J. (2003). *Inorg. Chem.* **42**, 3454–3465.
- Bruker (2008). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dawson, D. M., Walker, D. A., Thornton-Pett, M. & Bochmann, M. (2000). *J. Chem. Soc. Dalton Trans.* pp. 459–466.
- He, L.-P., Liu, J.-Y., Pan, L., Wu, J.-Q., Xu, B.-C. & Li, Y.-S. (2009). *J. Polym. Sci. Part A Polym. Chem.* **47**, 713–721.
- Matsuo, Y., Mashima, K. & Tani, K. (2001). *Organometallics*, **20**, 3510–3518.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Small, B. L., Bennett, A. M. A. & Brookhart, M. (1998). *J. Am. Chem. Soc.* **120**, 4049–4050.
- Su, B.-Y., Zhao, J.-S., Zhang, Q.-Z. & Qin, W.-L. (2009*a*). *Synth. Commun.* **39**, 4429–4440.
- Su, B.-Y., Zhao, J.-S., Zhang, Q.-Z. & Qin, W.-L. (2009*b*). *Polym. Int.* **58**, 1051–1057.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

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N*-[1-(1*H*-Pyrrol-2-yl)ethylidene]aniline*Bi-Yun Su, Lei Li, Jia-Xiang Wang and Xuan-Yan Li****S1. Comment**

In recent years, the bis(imino)pyridine incorporated late transition metal catalysts have received considerable attention because of their antioxidant property and outstanding activity for olefin polymerization (Small *et al.*, 1998; Su *et al.*, 2009*a,b*). As the five-membered ring substitute of pyridine six-membered ring (Matsuo *et al.*, 2001; He *et al.*, 2009), pyrrole was frequently introduced into the skeleton of bis(imino)pyridine ligand to design new ligand and corresponding metal complexes (Britovsek *et al.*, 2003; Dawson *et al.*, 2000). Bis(imino)pyrrole was usually prepared from Schiff base condensation of 2,5-diacetylpyrrole and the aromatic amine (Matsuo *et al.*, 2001). As a contribution to this research field, we report herein the synthesis of mono(imino)pyrrole from 2-acetyl pyrrole and aromatic amine, as well as the crystal structure of the title compound 2-(1-phenyliminoethyl)pyrrole.

The asymmetric unit of the title compound (Fig. 1) comprises of two crystallographically independent molecules *A* and *B*. In each molecule the pyrrole ring and benzene ring are essentially perpendicular, with dihedral angles of 72.37 (7)° and 82.34 (8)° respectively. The benzene ring of molecules *A* are nearly parallel with the benzene ring of molecules *B* with dihedral angle of 14.33 (14)°, but pyrrole ring of molecules *A* forms a comparative large 39.42 (9)° dihedral angle with the pyrrole ring of molecules *B*. On the whole, bond lengths and angles in both molecules are equal in the s.u. range. The crystal packing is stabilized by N–H⋯N classical intermolecular hydrogen bonds (Table 1, Fig. 2).

S2. Experimental

The 2-acetyl pyrrole (0.1313 g, 1.20 mmol), aniline (0.1118 g, 1.20 mmol) were placed in a 50 ml flask, after a few drops of acetic acid were added in, the mixture was subjected to radiation in a 800 W microwave oven for 2 min and 3 min on a medium-heat setting. The reaction was monitored by *TLC*, and the crude product was purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate, 5:1 *v/v*), the colourless or light yellow crystals of the title compound were at last obtained by recrystallization from ethanol (yield 0.063 g, 28.4%). M.p. 405.25–406.85 K. The purity and the composition of the compound were checked and characterized by IR spectrum, ¹H NMR spectrum, mass spectrum, as well as elemental analysis. IR (KBr): $\nu_{\text{C}=\text{N}}$ 1653 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ 7.33 (t, H, benzene ring aromatic H), 7.15 (t, 2H, benzene ring aromatic H), 7.02 (d, 2H, benzene ring aromatic H), 6.97 (t, 1H, pyrrole ring aromatic H), 6.33 (d, 1H, pyrrole ring aromatic H), 6.10 (d, 1H, pyrrole ring aromatic H), 2.03 (s, 3H, -N=C(CH₃)-). MS (EI): *m/z* 184 (*M*). Anal. Calcd for C₁₂H₁₂N₂: C, 78.23; H, 6.57; N, 15.21. Found: C, 78.50; H, 7.01; N, 14.96.

Plate like colourless single crystals used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation of the solvent at room temperature.

S3. Refinement

All H atoms were placed at calculated positions and refined as riding, with C–H = 0.93–0.96 Å, N–H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

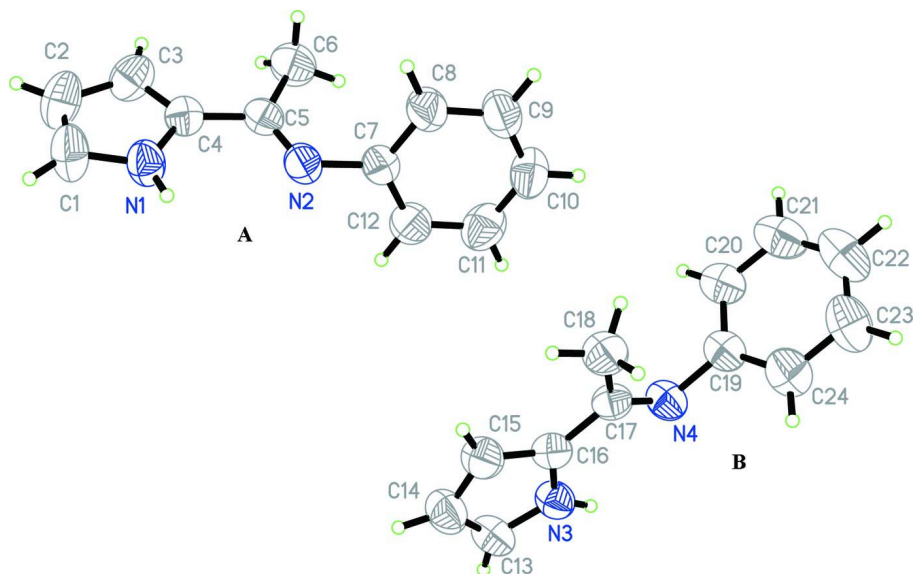


Figure 1

Two independent molecules in the asymmetric unit of the title compound showing the atomic numbering scheme.

Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

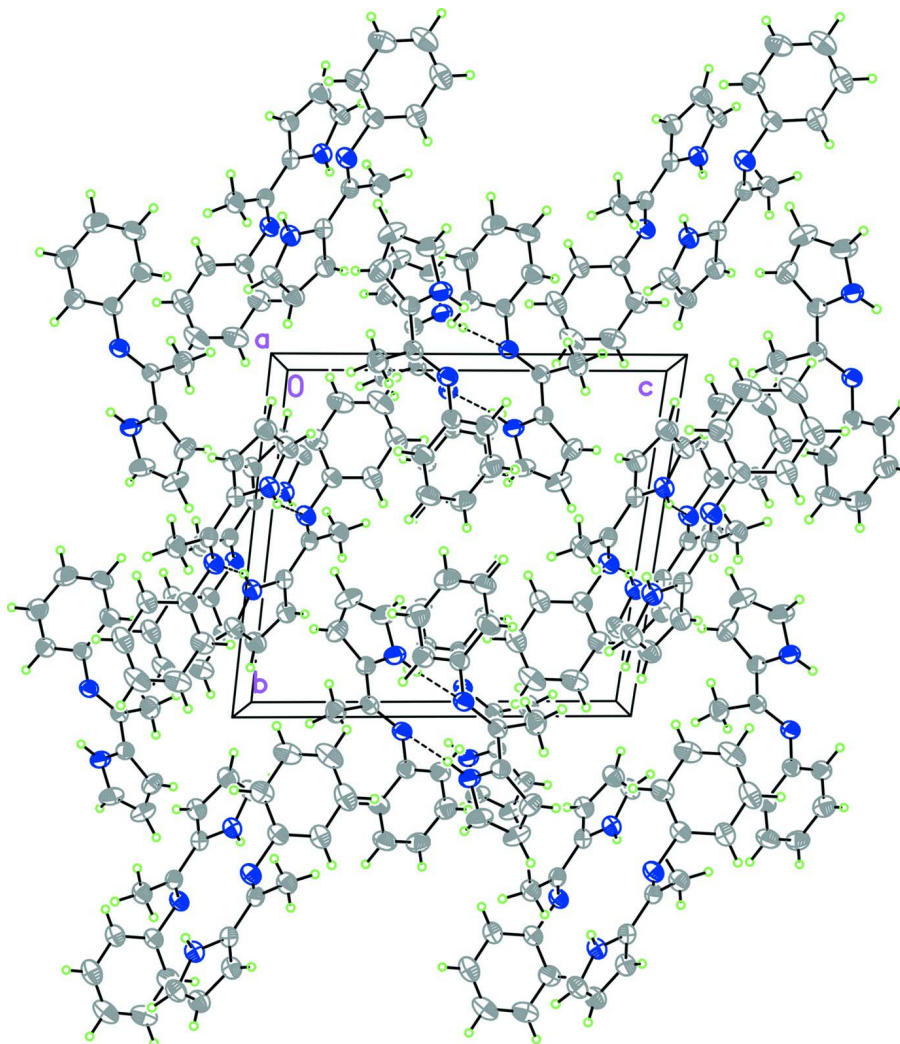


Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-[1-(1*H*-Pyrrol-2-yl)ethylidene]aniline

Crystal data

$C_{12}H_{12}N_2$

$M_r = 184.24$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.2236$ (14) Å

$b = 11.3306$ (19) Å

$c = 11.913$ (2) Å

$\alpha = 95.984$ (3)°

$\beta = 93.202$ (3)°

$\gamma = 109.274$ (3)°

$V = 1037.3$ (3) Å³

$Z = 4$

$F(000) = 392$

$D_x = 1.180$ Mg m⁻³

Melting point = 405.25–406.85 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1351 reflections

$\theta = 2.4$ – 25.1 °

$\mu = 0.07$ mm⁻¹

$T = 296$ K

Block, colourless

$0.37 \times 0.25 \times 0.19$ mm

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2008)
 $T_{\min} = 0.974$, $T_{\max} = 0.987$

5277 measured reflections
3655 independent reflections
2567 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 25.1^\circ$, $\theta_{\text{min}} = 2.4^\circ$
 $h = -9 \rightarrow 9$
 $k = -9 \rightarrow 13$
 $l = -14 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.142$
 $S = 1.10$
3655 reflections
256 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
 $w = 1/[\sigma^2(F_o^2) + (0.0689P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.20 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.13 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.043 (5)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.1204 (2)	1.17200 (13)	0.61426 (13)	0.0613 (4)
H1A	0.0627	1.1263	0.5534	0.074*
N2	0.19520 (19)	0.94813 (13)	0.57233 (12)	0.0557 (4)
N3	0.38995 (19)	0.64751 (14)	-0.01282 (12)	0.0557 (4)
H3A	0.4486	0.6007	-0.0354	0.067*
N4	0.31361 (19)	0.43111 (14)	0.10218 (13)	0.0569 (4)
C1	0.1184 (3)	1.28776 (18)	0.6531 (2)	0.0780 (6)
H1	0.0539	1.3305	0.6192	0.094*
C2	0.2261 (3)	1.3311 (2)	0.7498 (2)	0.0812 (7)
H2	0.2502	1.4089	0.7935	0.097*
C3	0.2940 (3)	1.23792 (19)	0.77152 (17)	0.0699 (6)
H3	0.3710	1.2419	0.8332	0.084*
C4	0.2279 (2)	1.13853 (16)	0.68614 (15)	0.0524 (5)
C5	0.2640 (2)	1.02211 (16)	0.66444 (14)	0.0519 (5)
C6	0.3844 (3)	0.9990 (2)	0.75197 (17)	0.0783 (6)

H6A	0.3216	0.9665	0.8140	0.117*
H6B	0.4757	1.0767	0.7793	0.117*
H6C	0.4331	0.9389	0.7187	0.117*
C7	0.2301 (2)	0.83354 (16)	0.54888 (15)	0.0525 (5)
C8	0.1630 (3)	0.73360 (18)	0.60871 (18)	0.0726 (6)
H8	0.0976	0.7418	0.6684	0.087*
C9	0.1917 (3)	0.62193 (19)	0.5811 (2)	0.0814 (7)
H9	0.1457	0.5553	0.6224	0.098*
C10	0.2873 (3)	0.6075 (2)	0.4936 (2)	0.0781 (6)
H10	0.3072	0.5319	0.4756	0.094*
C11	0.3536 (3)	0.7066 (2)	0.43257 (19)	0.0772 (6)
H11	0.4184	0.6980	0.3727	0.093*
C12	0.3241 (3)	0.81884 (18)	0.46002 (17)	0.0664 (5)
H12	0.3683	0.8850	0.4179	0.080*
C13	0.4041 (3)	0.76033 (19)	-0.04693 (17)	0.0651 (5)
H13	0.4783	0.8000	-0.0982	0.078*
C14	0.2908 (3)	0.8061 (2)	0.00674 (18)	0.0698 (6)
H14	0.2736	0.8820	-0.0013	0.084*
C15	0.2060 (3)	0.71803 (18)	0.07579 (17)	0.0627 (5)
H15	0.1218	0.7249	0.1225	0.075*
C16	0.2679 (2)	0.61897 (16)	0.06320 (14)	0.0507 (4)
C17	0.2239 (2)	0.50444 (16)	0.11674 (14)	0.0503 (4)
C18	0.0726 (3)	0.47986 (18)	0.18618 (16)	0.0656 (5)
H18A	-0.0259	0.4157	0.1446	0.098*
H18B	0.0462	0.5560	0.2025	0.098*
H18C	0.1006	0.4522	0.2559	0.098*
C19	0.2680 (2)	0.31984 (17)	0.15675 (16)	0.0561 (5)
C20	0.3454 (3)	0.3213 (2)	0.26340 (17)	0.0708 (6)
H20	0.4238	0.3961	0.3014	0.085*
C21	0.3063 (3)	0.2120 (3)	0.3132 (2)	0.0850 (7)
H21	0.3581	0.2136	0.3851	0.102*
C22	0.1926 (3)	0.1014 (2)	0.2583 (2)	0.0873 (7)
H22	0.1663	0.0283	0.2927	0.105*
C23	0.1175 (3)	0.0987 (2)	0.1524 (2)	0.0869 (7)
H23	0.0404	0.0233	0.1147	0.104*
C24	0.1551 (3)	0.2071 (2)	0.10094 (19)	0.0730 (6)
H24	0.1042	0.2042	0.0285	0.088*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0669 (10)	0.0474 (9)	0.0668 (10)	0.0195 (8)	-0.0074 (8)	0.0011 (7)
N2	0.0601 (9)	0.0484 (8)	0.0593 (9)	0.0191 (7)	0.0030 (8)	0.0102 (7)
N3	0.0549 (9)	0.0621 (10)	0.0579 (9)	0.0271 (7)	0.0110 (7)	0.0155 (7)
N4	0.0530 (9)	0.0618 (9)	0.0627 (9)	0.0236 (8)	0.0156 (7)	0.0197 (7)
C1	0.0800 (15)	0.0517 (12)	0.1002 (17)	0.0274 (11)	-0.0127 (13)	-0.0059 (11)
C2	0.0714 (14)	0.0616 (13)	0.1009 (17)	0.0213 (11)	-0.0030 (13)	-0.0218 (12)
C3	0.0603 (12)	0.0749 (14)	0.0679 (13)	0.0209 (11)	-0.0028 (10)	-0.0087 (11)

C4	0.0485 (10)	0.0518 (10)	0.0555 (11)	0.0150 (8)	0.0054 (8)	0.0070 (8)
C5	0.0497 (10)	0.0543 (11)	0.0520 (10)	0.0155 (8)	0.0071 (8)	0.0141 (9)
C6	0.0889 (16)	0.0862 (15)	0.0665 (13)	0.0400 (13)	-0.0089 (12)	0.0134 (11)
C7	0.0519 (10)	0.0509 (10)	0.0556 (10)	0.0183 (8)	0.0031 (8)	0.0092 (8)
C8	0.0878 (15)	0.0604 (12)	0.0798 (14)	0.0309 (11)	0.0335 (12)	0.0210 (10)
C9	0.1039 (18)	0.0574 (13)	0.0943 (16)	0.0343 (12)	0.0340 (14)	0.0233 (11)
C10	0.0847 (16)	0.0590 (13)	0.0935 (16)	0.0301 (12)	0.0134 (13)	0.0005 (12)
C11	0.0715 (14)	0.0779 (15)	0.0800 (15)	0.0235 (12)	0.0208 (12)	-0.0006 (12)
C12	0.0682 (13)	0.0598 (12)	0.0673 (13)	0.0145 (10)	0.0140 (10)	0.0109 (10)
C13	0.0620 (12)	0.0718 (13)	0.0703 (13)	0.0282 (10)	0.0107 (10)	0.0277 (10)
C14	0.0744 (14)	0.0705 (13)	0.0780 (14)	0.0382 (11)	0.0132 (11)	0.0213 (11)
C15	0.0641 (12)	0.0711 (13)	0.0634 (12)	0.0339 (10)	0.0145 (10)	0.0142 (10)
C16	0.0457 (10)	0.0615 (11)	0.0473 (10)	0.0208 (8)	0.0051 (8)	0.0084 (8)
C17	0.0472 (10)	0.0583 (11)	0.0457 (10)	0.0188 (8)	0.0033 (8)	0.0055 (8)
C18	0.0647 (12)	0.0725 (13)	0.0672 (12)	0.0293 (10)	0.0216 (10)	0.0146 (10)
C19	0.0474 (10)	0.0639 (12)	0.0649 (12)	0.0248 (9)	0.0165 (9)	0.0176 (9)
C20	0.0742 (14)	0.0770 (14)	0.0659 (13)	0.0280 (11)	0.0095 (11)	0.0200 (11)
C21	0.0857 (17)	0.1045 (19)	0.0803 (15)	0.0435 (15)	0.0171 (13)	0.0376 (14)
C22	0.0747 (16)	0.0889 (18)	0.118 (2)	0.0381 (14)	0.0315 (15)	0.0529 (16)
C23	0.0701 (15)	0.0685 (14)	0.121 (2)	0.0177 (11)	0.0122 (14)	0.0271 (14)
C24	0.0618 (13)	0.0717 (14)	0.0846 (15)	0.0196 (11)	0.0001 (11)	0.0195 (11)

Geometric parameters (Å, °)

N1—C1	1.350 (2)	C10—C11	1.378 (3)
N1—C4	1.365 (2)	C10—H10	0.9300
N1—H1A	0.8600	C11—C12	1.381 (3)
N2—C5	1.286 (2)	C11—H11	0.9300
N2—C7	1.423 (2)	C12—H12	0.9300
N3—C13	1.352 (2)	C13—C14	1.364 (3)
N3—C16	1.371 (2)	C13—H13	0.9300
N3—H3A	0.8600	C14—C15	1.391 (3)
N4—C17	1.286 (2)	C14—H14	0.9300
N4—C19	1.428 (2)	C15—C16	1.376 (2)
C1—C2	1.355 (3)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.453 (2)
C2—C3	1.387 (3)	C17—C18	1.498 (2)
C2—H2	0.9300	C18—H18A	0.9600
C3—C4	1.376 (2)	C18—H18B	0.9600
C3—H3	0.9300	C18—H18C	0.9600
C4—C5	1.446 (2)	C19—C24	1.381 (3)
C5—C6	1.500 (3)	C19—C20	1.385 (3)
C6—H6A	0.9600	C20—C21	1.379 (3)
C6—H6B	0.9600	C20—H20	0.9300
C6—H6C	0.9600	C21—C22	1.363 (3)
C7—C12	1.373 (3)	C21—H21	0.9300
C7—C8	1.376 (3)	C22—C23	1.366 (3)
C8—C9	1.373 (3)	C22—H22	0.9300

C8—H8	0.9300	C23—C24	1.381 (3)
C9—C10	1.368 (3)	C23—H23	0.9300
C9—H9	0.9300	C24—H24	0.9300
C1—N1—C4	109.71 (17)	C12—C11—H11	119.9
C1—N1—H1A	125.1	C7—C12—C11	120.60 (19)
C4—N1—H1A	125.1	C7—C12—H12	119.7
C5—N2—C7	119.64 (15)	C11—C12—H12	119.7
C13—N3—C16	109.70 (15)	N3—C13—C14	108.30 (18)
C13—N3—H3A	125.2	N3—C13—H13	125.9
C16—N3—H3A	125.2	C14—C13—H13	125.9
C17—N4—C19	118.11 (15)	C13—C14—C15	107.20 (18)
N1—C1—C2	108.44 (19)	C13—C14—H14	126.4
N1—C1—H1	125.8	C15—C14—H14	126.4
C2—C1—H1	125.8	C16—C15—C14	108.33 (17)
C1—C2—C3	107.24 (18)	C16—C15—H15	125.8
C1—C2—H2	126.4	C14—C15—H15	125.8
C3—C2—H2	126.4	N3—C16—C15	106.47 (15)
C4—C3—C2	108.29 (18)	N3—C16—C17	123.18 (15)
C4—C3—H3	125.9	C15—C16—C17	130.35 (16)
C2—C3—H3	125.9	N4—C17—C16	119.49 (16)
N1—C4—C3	106.31 (16)	N4—C17—C18	124.21 (16)
N1—C4—C5	122.82 (16)	C16—C17—C18	116.31 (15)
C3—C4—C5	130.76 (18)	C17—C18—H18A	109.5
N2—C5—C4	118.71 (16)	C17—C18—H18B	109.5
N2—C5—C6	124.98 (17)	H18A—C18—H18B	109.5
C4—C5—C6	116.29 (16)	C17—C18—H18C	109.5
C5—C6—H6A	109.5	H18A—C18—H18C	109.5
C5—C6—H6B	109.5	H18B—C18—H18C	109.5
H6A—C6—H6B	109.5	C24—C19—C20	118.90 (19)
C5—C6—H6C	109.5	C24—C19—N4	120.50 (18)
H6A—C6—H6C	109.5	C20—C19—N4	120.46 (17)
H6B—C6—H6C	109.5	C21—C20—C19	120.0 (2)
C12—C7—C8	118.78 (17)	C21—C20—H20	120.0
C12—C7—N2	119.48 (16)	C19—C20—H20	120.0
C8—C7—N2	121.62 (17)	C22—C21—C20	120.7 (2)
C9—C8—C7	120.61 (19)	C22—C21—H21	119.6
C9—C8—H8	119.7	C20—C21—H21	119.6
C7—C8—H8	119.7	C23—C22—C21	119.7 (2)
C10—C9—C8	120.8 (2)	C23—C22—H22	120.2
C10—C9—H9	119.6	C21—C22—H22	120.2
C8—C9—H9	119.6	C22—C23—C24	120.5 (2)
C9—C10—C11	119.0 (2)	C22—C23—H23	119.7
C9—C10—H10	120.5	C24—C23—H23	119.7
C11—C10—H10	120.5	C19—C24—C23	120.2 (2)
C10—C11—C12	120.2 (2)	C19—C24—H24	119.9
C10—C11—H11	119.9	C23—C24—H24	119.9

C4—N1—C1—C2	0.7 (2)	C16—N3—C13—C14	-0.1 (2)
N1—C1—C2—C3	-0.9 (3)	N3—C13—C14—C15	0.2 (2)
C1—C2—C3—C4	0.8 (2)	C13—C14—C15—C16	-0.2 (2)
C1—N1—C4—C3	-0.2 (2)	C13—N3—C16—C15	-0.1 (2)
C1—N1—C4—C5	-176.80 (17)	C13—N3—C16—C17	-179.24 (16)
C2—C3—C4—N1	-0.3 (2)	C14—C15—C16—N3	0.2 (2)
C2—C3—C4—C5	175.84 (19)	C14—C15—C16—C17	179.27 (18)
C7—N2—C5—C4	179.53 (15)	C19—N4—C17—C16	179.47 (15)
C7—N2—C5—C6	1.0 (3)	C19—N4—C17—C18	-0.9 (3)
N1—C4—C5—N2	1.6 (3)	N3—C16—C17—N4	7.2 (3)
C3—C4—C5—N2	-174.05 (19)	C15—C16—C17—N4	-171.75 (18)
N1—C4—C5—C6	-179.77 (17)	N3—C16—C17—C18	-172.52 (16)
C3—C4—C5—C6	4.6 (3)	C15—C16—C17—C18	8.6 (3)
C5—N2—C7—C12	-112.9 (2)	C17—N4—C19—C24	92.6 (2)
C5—N2—C7—C8	71.2 (2)	C17—N4—C19—C20	-91.9 (2)
C12—C7—C8—C9	1.0 (3)	C24—C19—C20—C21	-1.4 (3)
N2—C7—C8—C9	176.9 (2)	N4—C19—C20—C21	-177.05 (18)
C7—C8—C9—C10	-0.1 (4)	C19—C20—C21—C22	0.4 (3)
C8—C9—C10—C11	-0.5 (4)	C20—C21—C22—C23	0.5 (4)
C9—C10—C11—C12	0.2 (3)	C21—C22—C23—C24	-0.4 (4)
C8—C7—C12—C11	-1.2 (3)	C20—C19—C24—C23	1.5 (3)
N2—C7—C12—C11	-177.28 (17)	N4—C19—C24—C23	177.15 (18)
C10—C11—C12—C7	0.6 (3)	C22—C23—C24—C19	-0.7 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1 <i>A</i> ...N2 ⁱ	0.86	2.38	3.150 (2)	150
N3—H3 <i>A</i> ...N4 ⁱⁱ	0.86	2.27	3.065 (2)	153

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