Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-(±)-Phenyl[2,4,5-tri-2-pyridyl-4,5-dihydroimidazol-1-yl]methanone

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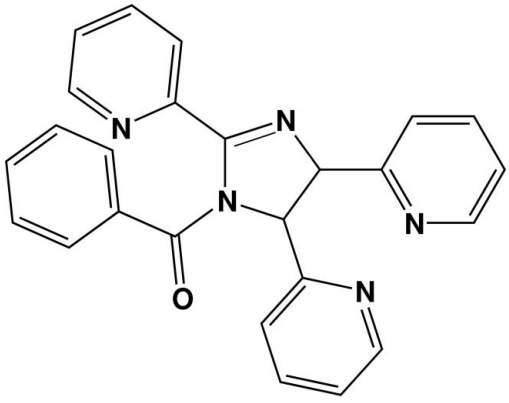
Received 11 May 2007; accepted 30 May 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.057; wR factor = 0.140; data-to-parameter ratio = 12.4.

In the title compound, $C_{25}H_{19}N_5O$, two types of intermolecular interactions are observed. Edge-to-face C—H$\cdots\pi$ interactions between neighbouring molecules form a one-dimensional network, while C—H$\cdots$N and C—H$\cdots$O interactions form a two-dimensional network.

Related literature

For related literature on supramolecular structures, see: Albrechet (2001); Leininger *et al.* (2000); on hydrogen bonding, see: Burchell & Puddephatt (2006); Gallego *et al.* (2004); Thallapally *et al.* (2003); on π–π interactions, see: Zou *et al.* (2006); Liu *et al.* (2005); on C—H$\cdots\pi$ interactions, see: Chen & Liu (2002); Janiak (2000); Planas *et al.* (2006); on properties of supramolecular architectures, see: Lehn (1995); Séneque *et al.* (2001); on related compounds, see: Campos-Gaxiola *et al.* (2007); Itoh *et al.* (2005); Jayaraman *et al.* (2006); Jennings *et al.* (2001); Kapildev *et al.* (2005); Larter *et al.* (1998); Majumder *et al.* (2006); Oxtoby *et al.* (2003); Parra-Hake *et al.* (2000); Reger *et al.* (2001); Roesky & Andruh (2003); Wang *et al.* (2006); Yang *et al.* (2006).



Experimental

Crystal data

$C_{25}H_{19}N_5O$
M_r = 405.45
Triclinic, $P\overline{1}$
a = 8.004 (3) Å
b = 10.085 (4) Å
c = 13.432 (4) Å
α = 108.65 (4)°
β = 93.56 (3)°
γ = 99.84 (4)°
V = 1004.2 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.5 × 0.42 × 0.14 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: none
3758 measured reflections
3483 independent reflections
1931 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
every 97 reflections
intensity decay: 13.7%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.140
S = 0.99
3483 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C13—H13$A\cdots$O1^{i}	0.93	2.57	3.469 (5)	163
C15—H15$A\cdots$N4^{i}	0.93	2.56	3.483 (5)	171
C5—H5$B\cdots$N4^{ii}	0.93	2.69	3.515 (5)	149
C21—H21$A\cdots$N3^{iii}	0.93	2.56	3.413 (5)	153
C5—H5$B\cdots Cg1^{iv}$	0.93	3.24	3.906 (3)	129
C22—H22$A\cdots Cg2^{v}$	0.93	2.91	3.775 (4)	153

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+1, -y, -z+2$; (v) $-x+1, -y+1, -z+2$. Notes: $Cg1$ and $Cg2$ are the centroids of rings C9–C13/N4 and C14–C18/N5, respectively.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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*.

This work was supported by the Consejo del Sistema Nacional de Educación Tecnológica (COSNET) (grant No. 418.03-P). Support from the Consejo Nacional de Ciencia y Tecnología (CONACYT) in the form of a fellowship for JJCG is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2022).

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supplementary materials

Acta Cryst. (2007). E**63**, o3126-o3127 [**doi:10.1107/S1600536807026414**]

cis-(±)-Phenyl[2,4,5-tri-2-pyridyl-4,5-dihydroimidazol-1-yl]methanone

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Comment

The coordination chemistry of transition metals with polypyridyl ligands has progressed considerably during the last decade, and has been widely used for the construction of coordination polymers and other supramolecular structures (Itoh *et al.*, 2005; Albrechy, 2001; Leininger *et al.*, 2000). Complex metal-organic coordination polymers, macrocycles, networks and other metallosupramolecular structures can be constructed by self-assembly from small, easily prepared building blocks, which are combined either through coordinative bonds, hydrogen bonding (Majumder *et al.*, 2006; Burchell *et al.* 2006; Gallego *et al.* 2004), π-π (Zou *et al.*, 2006; Liu *et al.*, 2005; Roesky *et al.*, 2003; Wang *et al*., 2006) or CH/π interactions (Chen *et al.*, 2002; Janiak *et al*., 2000). Such supramolecular architectures have attracted considerable attention due to the useful electronic, magnetic, optical and catalytic properties of these materials (Lehn, 1995; Séneque *et al.*, 2001). In this direction, previous work in our laboratory has been focused on the coordination chemistry of the ligand *cis*-(±)2-(2,5-di(pyridin-2-yl)-4,5-dihydro-1*H*-imidazol-4-yl)pyridine (Larter *et al.*, 1998) with transition metals such as Ni(II), Cu(II), Zn(II) (Parra-Hake *et al.*, 2000) and Cd(II) (Campos-Gaxiola *et al.*, 2007).

As part of our ongoing research on the chemistry of polypyridine ligands we have synthesized *Cis*-(±)-phenyl[2,4,5-tri(pyridin-2-yl)-4,5- dihydroimidazol-1-yl]methanone (**I**) in order to modify the coordination environment that could assist in the formation of coordination macromolecules. To gain insight on the new coordination capabilities, the X-ray crystal structure of the title compound has been carried out (Fig. 1).

In the crystal structure, adjacent units are linked together by strong and weak edge-to-face C—H···π interactions (Fig. 2) between pyridyl protons and the pyridyl ring [H···π 3.250 (4) Å and C—H···π 129.3 (2)°], phenyl protons and the pyridyl ring [H···π 2.917 (4) Å and C—H···π 154.0 (2)°](Yang *et al.*, 2006; Jennings *et al.*, 2001; Planas *et al.*, 2006; Jayaraman *et al.*, 2006; Reger *et al.*, 2001), to form one-dimensional chains along the [001] direction. In addition, adjacent units are arranged into a two-dimensional network propagated along the (011) plane *via* intermolecular C—H···N hydrogen bond interactions between the H-atoms of phenyl or pyridyl rings and pyridyl N atoms as well as C—H···O interactions between pyridyl protons and the O atom of carbonyl group (Fig. 3). The hydrogen bond distances are within the range found for other reported structures (Oxtoby *et al.*, 2003; Thallapally *et al.*, 2003; Kapildev *et al.*, 2005). These interactions may be attributed to the orientation of the aromatic rings, which help to stabilize the structure.

Experimental

To a stirring solution of *cis*-(±)2-(2,5-di(pyridin-2-yl)-4,5-dihydro-1*H*-imidazol-4-yl)pyridine (0.3 g, 0.9966 mmol) in dichloromethane (10 ml) was added Et_3N (0.5 g, 4.9807 mmol). After an additional 5 min, benzoyl chloride (0.28 g, 1.9931 mmol) and 4-dimethylaminopyridine (0.012 g, 0.0982 mmol) was added. The solution was stirred for 22 h at room temperature. The resulting mixture was washed with 0.1 N NaOH (3 × 10 ml). The organic layer was dried over $MgSO_4$, filtered, and the solvent removed under reduced pressure. The remaining solid was crystallized from CH_2Cl_2/pentane by gas phase diffusion providing colourless crystals that were dried under high vacuum. Yield (0.1930 g, 48%) Mp: 248–250 °K. IR

(KBr): 3039, 2929, 2852, 1651, 1613, 1589, 1473, 1438, 1354, 1147, 996, 784, 704 cm^{-1}. ^1H NMR ($CDCl_3$, 500 MHz): d8.34 (ta, *J* = 4.8, 2H), 8.24 (da, *J* = 4.6, 2.0, 0.8 Hz,1*H*), 7.85 (d, *J* = 7.5 Hz,1*H*), 7.62 (td, *J* = 7.7, 2.0 Hz, 1H), 7.42–7.38 (m, 3H),7.32 (td, *J* = 7.5, 1.6, Hz, 1H), 7.23–7.16 (m, 2H), 7.15 (ddd, *J* = 7.6,4.8, 1.1 Hz, 1H), 7.09 (t, *J* = 7.6 Hz, 3H), 6.95(ddd, *J* = 7.4, *J* = 4.9, *J* = 1.0 Hz,1*H*), 6.91(ddd, *J* = 7.5,4.8, 1.0 Hz, 1H), 6.08 (d, *J* = 9.1 Hz, 1H), 6.05 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR ($CDCl_3$ 125.7 MHz): 168.83, 161.43, 157.52, 156.53, 150.14, 149.04, 148.96, 148.89, 148.33, 136.11, 135.88, 153.47, 131.04, 128.43, 127.77, 124.41, 122.85, 122.34, 121.97, 121.90, 75.40, 70.36. EMIES *m/e* (int. *rel*.): $[M+H]^+$ 406 (100%).

Refinement

The sample partially decomposed in the X-ray beam (13% decay). Refinement of H atoms was carried out using a riding model, with distances constrained to 0.93 Å for aromatic CH, 0.98 Å for methine CH. Isotropic U parameters were fixed at $U_{iso}(H) = 1.2U_{eq}$(carrier atom) for aromatic CH and methine CH.

Figures

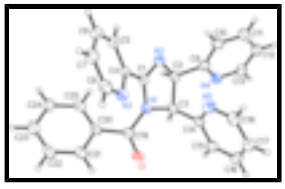

Fig. 1. Molecular structure of (I) with 30% thermal ellipsoid and labeling schemes.

Fig. 2. Edge-to-face C—H···π interactions between neighboring molecules form chains along the [001] direction. All interactions are indicated by dashed lines.

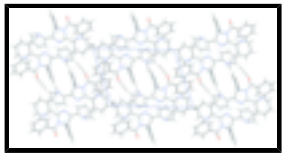

Fig. 3. C—H···N and C—H···O interactions form two-dimensional networks along the (011) plane. All interactions are indicated by dashed lines.

cis-(±)-Phenyl[2,4,5-tri-2-pyridyl-4,5-dihydroimidazol-1-yl]methanone

Crystal data

$C_{25}H_{19}N_5O$	$Z = 2$
$M_r = 405.45$	$F_{000} = 424$
Triclinic, $P\overline{1}$	$D_x = 1.341$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.004$ (3) Å	Cell parameters from 39 reflections
$b = 10.085$ (4) Å	$\theta = 4.6–11.6°$
$c = 13.432$ (4) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 108.65$ (4)°	$T = 298$ (2) K
$\beta = 93.56$ (3)°	Prismatic, colourless
$\gamma = 99.84$ (4)°	0.5 × 0.42 × 0.14 mm
$V = 1004.2$ (7) $Å^3$	

Data collection

Bruker P4 diffractometer	R_{int} = 0.030
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.2º
T = 298(2) K	h = 0→9
2θ/ω scans	k = −11→11
Absorption correction: none	l = −15→15
3758 measured reflections	3 standard reflections
3483 independent reflections	every 97 reflections
1931 reflections with $I > 2\sigma(I)$	intensity decay: 13.7%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.140	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.010
3483 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
280 parameters	$\Delta\rho_{min}$ = −0.21 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4369 (4)	0.1653 (3)	0.7048 (2)	0.0388 (7)
C2	0.4347 (4)	0.1829 (3)	0.5448 (2)	0.0433 (8)
H2B	0.5467	0.1729	0.5211	0.052*
C3	0.4522 (4)	0.3372 (3)	0.6233 (2)	0.0435 (8)
H3B	0.5464	0.4015	0.6087	0.052*

C4	0.4006 (4)	0.1088 (3)	0.7916 (2)	0.0388 (7)
C5	0.3979 (4)	−0.0332 (3)	0.7776 (3)	0.0479 (8)
H5B	0.4261	−0.0932	0.7152	0.057*
C6	0.3527 (5)	−0.0842 (4)	0.8574 (3)	0.0589 (10)
H6A	0.3497	−0.1795	0.8500	0.071*
C7	0.3124 (4)	0.0069 (4)	0.9475 (3)	0.0578 (10)
H7A	0.2817	−0.0248	1.0029	0.069*
C8	0.3181 (4)	0.1471 (4)	0.9550 (3)	0.0539 (9)
H8A	0.2899	0.2086	1.0167	0.065*
C9	0.3068 (4)	0.1464 (3)	0.4479 (2)	0.0415 (8)
C10	0.1672 (4)	0.0362 (3)	0.4222 (3)	0.0513 (9)
H10A	0.1478	−0.0208	0.4644	0.062*
C11	0.0569 (5)	0.0117 (4)	0.3332 (3)	0.0625 (10)
H11A	−0.0397	−0.0612	0.3146	0.075*
C12	0.0912 (5)	0.0962 (4)	0.2719 (3)	0.0583 (10)
H12A	0.0182	0.0819	0.2112	0.070*
C13	0.2343 (5)	0.2014 (4)	0.3016 (3)	0.0557 (9)
H13A	0.2579	0.2573	0.2589	0.067*
C14	0.2925 (4)	0.3986 (3)	0.6281 (2)	0.0407 (8)
C15	0.2940 (5)	0.5330 (3)	0.6216 (3)	0.0561 (9)
H15A	0.3945	0.5878	0.6131	0.067*
C16	0.1466 (6)	0.5843 (4)	0.6277 (3)	0.0683 (11)
H16A	0.1453	0.6745	0.6236	0.082*
C17	0.0008 (5)	0.5011 (4)	0.6399 (3)	0.0669 (11)
H17A	−0.1013	0.5337	0.6449	0.080*
C18	0.0088 (5)	0.3687 (4)	0.6447 (3)	0.0587 (9)
H18A	−0.0912	0.3117	0.6514	0.070*
C19	0.5967 (4)	0.4186 (3)	0.8071 (2)	0.0459 (8)
C20	0.6959 (4)	0.3814 (3)	0.8878 (2)	0.0401 (8)
C21	0.7149 (4)	0.4693 (3)	0.9926 (3)	0.0479 (8)
H21A	0.6591	0.5457	1.0118	0.057*
C22	0.8166 (5)	0.4436 (4)	1.0685 (3)	0.0590 (10)
H22A	0.8246	0.5001	1.1392	0.071*
C23	0.9049 (5)	0.3364 (4)	1.0408 (3)	0.0632 (10)
H23A	0.9764	0.3222	1.0921	0.076*
C24	0.8890 (4)	0.2488 (4)	0.9372 (3)	0.0565 (9)
H24A	0.9488	0.1749	0.9185	0.068*
C25	0.7838 (4)	0.2708 (3)	0.8608 (3)	0.0465 (8)
H25A	0.7721	0.2107	0.7908	0.056*
N1	0.5004 (3)	0.3120 (2)	0.72264 (18)	0.0417 (6)
N2	0.3949 (3)	0.0892 (3)	0.6083 (2)	0.0443 (7)
N3	0.3616 (3)	0.1996 (3)	0.8789 (2)	0.0448 (7)
N4	0.3427 (3)	0.2286 (3)	0.3890 (2)	0.0505 (7)
N5	0.1514 (4)	0.3169 (3)	0.6402 (2)	0.0522 (7)
O1	0.6116 (3)	0.5423 (2)	0.80961 (17)	0.0641 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (18)	0.0368 (17)	0.0389 (18)	0.0068 (14)	0.0009 (14)	0.0105 (15)
C2	0.0434 (19)	0.0461 (18)	0.0357 (18)	0.0063 (15)	0.0033 (15)	0.0092 (15)
C3	0.047 (2)	0.0443 (18)	0.0369 (18)	0.0011 (15)	0.0008 (15)	0.0160 (14)
C4	0.0349 (17)	0.0384 (17)	0.0388 (18)	0.0022 (14)	−0.0060 (14)	0.0119 (15)
C5	0.053 (2)	0.0417 (19)	0.047 (2)	0.0091 (16)	−0.0030 (16)	0.0156 (16)
C6	0.069 (3)	0.043 (2)	0.063 (2)	0.0028 (18)	−0.011 (2)	0.0245 (19)
C7	0.061 (2)	0.060 (2)	0.053 (2)	−0.0052 (19)	−0.0043 (18)	0.0316 (19)
C8	0.056 (2)	0.064 (2)	0.042 (2)	0.0058 (18)	0.0062 (17)	0.0199 (18)
C9	0.048 (2)	0.0400 (18)	0.0363 (18)	0.0123 (16)	0.0086 (15)	0.0102 (15)
C10	0.052 (2)	0.051 (2)	0.048 (2)	0.0009 (17)	0.0044 (17)	0.0180 (17)
C11	0.050 (2)	0.064 (2)	0.059 (2)	−0.0017 (18)	−0.0064 (19)	0.009 (2)
C12	0.054 (2)	0.063 (2)	0.050 (2)	0.0173 (19)	−0.0115 (18)	0.0091 (19)
C13	0.069 (3)	0.055 (2)	0.046 (2)	0.016 (2)	−0.0006 (19)	0.0208 (18)
C14	0.048 (2)	0.0377 (18)	0.0313 (17)	0.0019 (15)	−0.0016 (14)	0.0093 (14)
C15	0.065 (2)	0.041 (2)	0.057 (2)	−0.0011 (18)	−0.0061 (18)	0.0183 (17)
C16	0.084 (3)	0.044 (2)	0.077 (3)	0.017 (2)	−0.013 (2)	0.024 (2)
C17	0.067 (3)	0.061 (2)	0.066 (3)	0.023 (2)	−0.003 (2)	0.008 (2)
C18	0.054 (2)	0.058 (2)	0.064 (2)	0.0099 (19)	0.0120 (19)	0.0217 (19)
C19	0.049 (2)	0.0395 (19)	0.0426 (19)	−0.0007 (16)	0.0011 (16)	0.0103 (15)
C20	0.0380 (18)	0.0421 (18)	0.0351 (18)	−0.0026 (15)	−0.0020 (14)	0.0129 (15)
C21	0.046 (2)	0.0458 (19)	0.046 (2)	0.0005 (16)	0.0052 (16)	0.0133 (16)
C22	0.065 (2)	0.063 (2)	0.0367 (19)	−0.005 (2)	−0.0083 (18)	0.0106 (17)
C23	0.059 (2)	0.070 (3)	0.058 (3)	−0.002 (2)	−0.0115 (19)	0.030 (2)
C24	0.050 (2)	0.053 (2)	0.067 (3)	0.0056 (17)	−0.0057 (19)	0.0248 (19)
C25	0.0432 (19)	0.049 (2)	0.0407 (19)	−0.0006 (16)	0.0011 (15)	0.0117 (15)
N1	0.0479 (16)	0.0360 (14)	0.0337 (14)	−0.0023 (12)	−0.0069 (12)	0.0095 (11)
N2	0.0532 (17)	0.0366 (14)	0.0405 (16)	0.0062 (12)	0.0007 (13)	0.0117 (12)
N3	0.0463 (16)	0.0445 (15)	0.0422 (16)	0.0042 (13)	0.0040 (13)	0.0157 (13)
N4	0.0567 (18)	0.0476 (16)	0.0436 (16)	0.0035 (14)	0.0008 (14)	0.0152 (14)
N5	0.0569 (19)	0.0499 (17)	0.0538 (18)	0.0121 (15)	0.0124 (15)	0.0213 (14)
O1	0.0910 (19)	0.0381 (14)	0.0542 (15)	−0.0024 (13)	−0.0156 (13)	0.0157 (11)

Geometric parameters (Å, °)

C1—N2	1.267 (4)	C12—H12A	0.9300
C1—N1	1.416 (4)	C13—N4	1.340 (4)
C1—C4	1.476 (4)	C13—H13A	0.9300
C2—N2	1.473 (4)	C14—N5	1.331 (4)
C2—C9	1.509 (4)	C14—C15	1.384 (4)
C2—C3	1.552 (4)	C15—C16	1.363 (5)
C2—H2B	0.9800	C15—H15A	0.9300
C3—N1	1.477 (4)	C16—C17	1.368 (5)
C3—C14	1.509 (4)	C16—H16A	0.9300
C3—H3B	0.9800	C17—C18	1.369 (5)
C4—N3	1.330 (4)	C17—H17A	0.9300

C4—C5	1.380 (4)	C18—N5	1.331 (4)
C5—C6	1.371 (4)	C18—H18A	0.9300
C5—H5B	0.9300	C19—O1	1.222 (3)
C6—C7	1.361 (5)	C19—N1	1.366 (4)
C6—H6A	0.9300	C19—C20	1.483 (4)
C7—C8	1.377 (4)	C20—C25	1.383 (4)
C7—H7A	0.9300	C20—C21	1.385 (4)
C8—N3	1.332 (4)	C21—C22	1.381 (4)
C8—H8A	0.9300	C21—H21A	0.9300
C9—N4	1.327 (4)	C22—C23	1.358 (5)
C9—C10	1.373 (4)	C22—H22A	0.9300
C10—C11	1.369 (4)	C23—C24	1.373 (5)
C10—H10A	0.9300	C23—H23A	0.9300
C11—C12	1.369 (5)	C24—C25	1.384 (4)
C11—H11A	0.9300	C24—H24A	0.9300
C12—C13	1.362 (5)	C25—H25A	0.9300
N2—C1—N1	114.6 (3)	C12—C13—H13A	118.3
N2—C1—C4	122.2 (3)	N5—C14—C15	122.2 (3)
N1—C1—C4	122.7 (3)	N5—C14—C3	116.2 (3)
N2—C2—C9	113.5 (3)	C15—C14—C3	121.6 (3)
N2—C2—C3	105.2 (2)	C16—C15—C14	119.3 (3)
C9—C2—C3	114.1 (2)	C16—C15—H15A	120.3
N2—C2—H2B	107.9	C14—C15—H15A	120.3
C9—C2—H2B	107.9	C15—C16—C17	119.0 (3)
C3—C2—H2B	107.9	C15—C16—H16A	120.5
N1—C3—C14	111.5 (2)	C17—C16—H16A	120.5
N1—C3—C2	98.9 (2)	C18—C17—C16	118.4 (4)
C14—C3—C2	115.8 (3)	C18—C17—H17A	120.8
N1—C3—H3B	110.1	C16—C17—H17A	120.8
C14—C3—H3B	110.1	N5—C18—C17	123.8 (4)
C2—C3—H3B	110.1	N5—C18—H18A	118.1
N3—C4—C5	123.3 (3)	C17—C18—H18A	118.1
N3—C4—C1	116.2 (3)	O1—C19—N1	119.1 (3)
C5—C4—C1	120.3 (3)	O1—C19—C20	121.1 (3)
C6—C5—C4	118.7 (3)	N1—C19—C20	119.5 (3)
C6—C5—H5B	120.6	C25—C20—C21	118.8 (3)
C4—C5—H5B	120.6	C25—C20—C19	122.2 (3)
C7—C6—C5	118.9 (3)	C21—C20—C19	118.7 (3)
C7—C6—H6A	120.5	C22—C21—C20	120.1 (3)
C5—C6—H6A	120.5	C22—C21—H21A	119.9
C6—C7—C8	118.6 (3)	C20—C21—H21A	119.9
C6—C7—H7A	120.7	C23—C22—C21	120.6 (3)
C8—C7—H7A	120.7	C23—C22—H22A	119.7
N3—C8—C7	123.8 (3)	C21—C22—H22A	119.7
N3—C8—H8A	118.1	C22—C23—C24	120.2 (3)
C7—C8—H8A	118.1	C22—C23—H23A	119.9
N4—C9—C10	123.1 (3)	C24—C23—H23A	119.9
N4—C9—C2	114.1 (3)	C23—C24—C25	119.9 (3)
C10—C9—C2	122.8 (3)	C23—C24—H24A	120.1

C11—C10—C9	118.8 (3)	C25—C24—H24A	120.1
C11—C10—H10A	120.6	C24—C25—C20	120.4 (3)
C9—C10—H10A	120.6	C24—C25—H25A	119.8
C10—C11—C12	118.9 (3)	C20—C25—H25A	119.8
C10—C11—H11A	120.5	C19—N1—C1	132.2 (3)
C12—C11—H11A	120.5	C19—N1—C3	121.1 (2)
C13—C12—C11	118.8 (3)	C1—N1—C3	106.6 (2)
C13—C12—H12A	120.6	C1—N2—C2	107.4 (2)
C11—C12—H12A	120.6	C4—N3—C8	116.6 (3)
N4—C13—C12	123.3 (3)	C9—N4—C13	117.1 (3)
N4—C13—H13A	118.3	C14—N5—C18	117.3 (3)
N2—C2—C3—N1	25.5 (3)	N1—C19—C20—C21	−145.6 (3)
C9—C2—C3—N1	150.6 (3)	C25—C20—C21—C22	−1.7 (5)
N2—C2—C3—C14	−93.6 (3)	C19—C20—C21—C22	−175.4 (3)
C9—C2—C3—C14	31.4 (4)	C20—C21—C22—C23	3.0 (5)
N2—C1—C4—N3	−144.7 (3)	C21—C22—C23—C24	−2.4 (6)
N1—C1—C4—N3	26.8 (4)	C22—C23—C24—C25	0.6 (5)
N2—C1—C4—C5	31.4 (4)	C23—C24—C25—C20	0.7 (5)
N1—C1—C4—C5	−157.1 (3)	C21—C20—C25—C24	−0.2 (5)
N3—C4—C5—C6	0.0 (5)	C19—C20—C25—C24	173.3 (3)
C1—C4—C5—C6	−175.8 (3)	O1—C19—N1—C1	−168.1 (3)
C4—C5—C6—C7	−0.1 (5)	C20—C19—N1—C1	18.4 (5)
C5—C6—C7—C8	0.2 (5)	O1—C19—N1—C3	16.1 (5)
C6—C7—C8—N3	−0.3 (5)	C20—C19—N1—C3	−157.4 (3)
N2—C2—C9—N4	−178.9 (3)	N2—C1—N1—C19	−160.5 (3)
C3—C2—C9—N4	60.5 (4)	C4—C1—N1—C19	27.4 (5)
N2—C2—C9—C10	0.0 (4)	N2—C1—N1—C3	15.7 (3)
C3—C2—C9—C10	−120.6 (3)	C4—C1—N1—C3	−156.4 (3)
N4—C9—C10—C11	−1.8 (5)	C14—C3—N1—C19	−85.2 (3)
C2—C9—C10—C11	179.4 (3)	C2—C3—N1—C19	152.4 (3)
C9—C10—C11—C12	1.2 (5)	C14—C3—N1—C1	98.1 (3)
C10—C11—C12—C13	0.2 (5)	C2—C3—N1—C1	−24.3 (3)
C11—C12—C13—N4	−1.1 (5)	N1—C1—N2—C2	2.3 (3)
N1—C3—C14—N5	−62.1 (3)	C4—C1—N2—C2	174.4 (3)
C2—C3—C14—N5	49.9 (4)	C9—C2—N2—C1	−143.8 (3)
N1—C3—C14—C15	117.1 (3)	C3—C2—N2—C1	−18.3 (3)
C2—C3—C14—C15	−130.9 (3)	C5—C4—N3—C8	−0.1 (4)
N5—C14—C15—C16	0.0 (5)	C1—C4—N3—C8	175.9 (3)
C3—C14—C15—C16	−179.2 (3)	C7—C8—N3—C4	0.2 (5)
C14—C15—C16—C17	−0.1 (5)	C10—C9—N4—C13	0.9 (5)
C15—C16—C17—C18	−0.5 (6)	C2—C9—N4—C13	179.8 (3)
C16—C17—C18—N5	1.4 (6)	C12—C13—N4—C9	0.6 (5)
O1—C19—C20—C25	−132.3 (3)	C15—C14—N5—C18	0.7 (4)
N1—C19—C20—C25	41.0 (4)	C3—C14—N5—C18	180.0 (3)
O1—C19—C20—C21	41.1 (5)	C17—C18—N5—C14	−1.5 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C13—H13A···O1^{i}	0.93	2.57	3.469 (5)	163
C15—H15A···N4^{i}	0.93	2.56	3.483 (5)	171
C5—H5B···N4^{ii}	0.93	2.69	3.515 (5)	149
C21—H21A···N3^{iii}	0.93	2.56	3.413 (5)	153

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+2.

Fig. 1

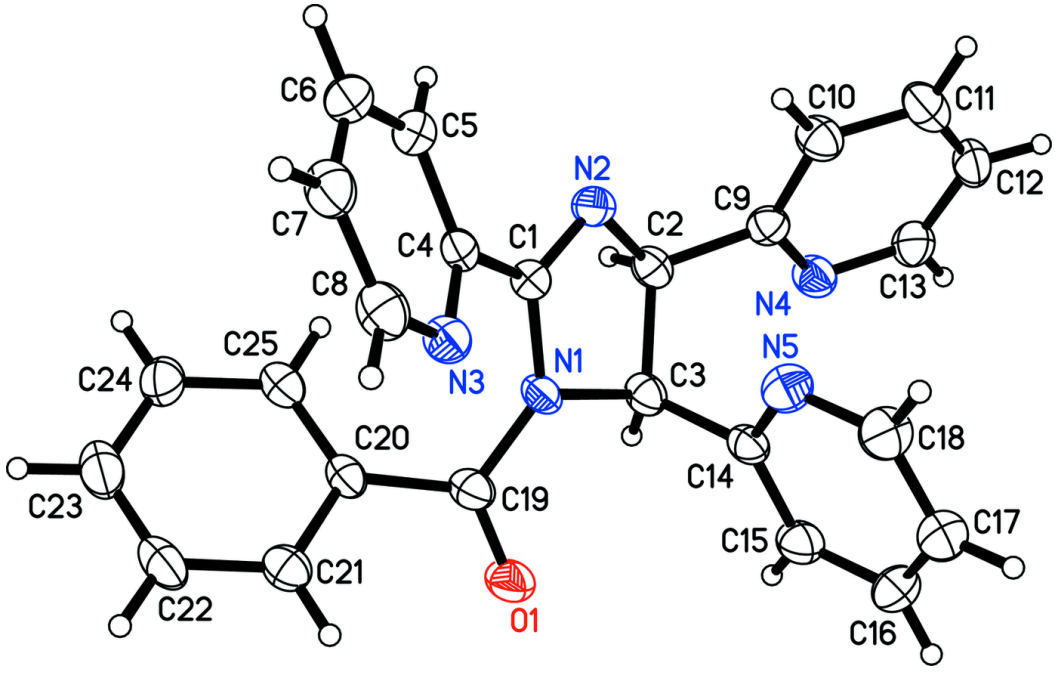
C6
C5
C10
C11
N2
C12
C9
C7
C4
C1
C2
C8
N4
C13
C25
N3
N1
C3
N5
C24
C20
C18
C14
C23
C19
C17
C15
C21
O1
C22
C16

Fig. 2

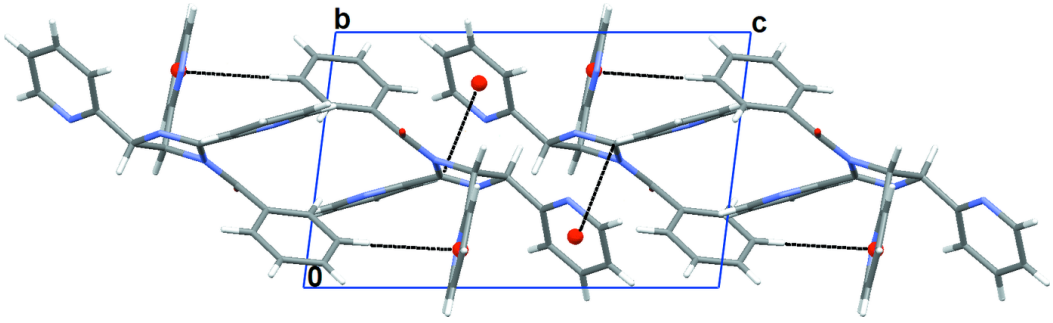

Fig. 3