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4′-(4-Methylphenyl)-2,2′:6′,2″-terpyridine

Han-Guo Liu, Yong-Cai Qiu and Jian-Zhong Wu*

Department of Chemistry, School of Chemistry and the Environment, South China Normal University, Guangzhou 510631, People's Republic of China
Correspondence e-mail: wujzh@scnu.edu.cn

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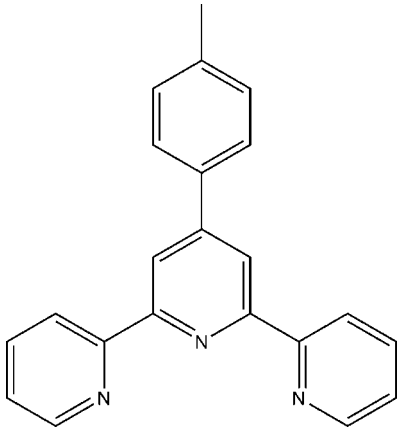
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.131; data-to-parameter ratio = 17.7.

There are two crystallographically independent molecules in the asymmetric unit of the title compound, $C_{22}H_{17}N_3$. In each molecule, the three pyridyl groups are nearly coplanar, whereas the tolyl groups are twisted out of the plane of the attached pyridyl rings by *ca* 28°. The molecular components are assembled through C—H$\cdots\pi$ and π–π interactions [centroid–centroid distances are 3.677 (4) and 3.707 (7) Å] into a one-dimensional chain running in the *a*-axis direction.

Related literature

For related literature, see Cargill Thompson (1997); Collin *et al.* (1991); Liu *et al.* (2007); Thummel (2004); Wang *et al.* (2007); Samnes & Yahioglu (1994).



Experimental

Crystal data

$C_{22}H_{17}N_3$
M_r = 323.39
Monoclinic, $P2_1/c$
a = 9.4575 (4) Å
b = 33.8005 (15) Å
c = 11.3730 (5) Å
β = 112.357 (3)°
V = 3362.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.26 × 0.23 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: none
54997 measured reflections
8020 independent reflections
4866 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.131
S = 1.03
8020 reflections
453 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
C—H$\cdots\pi$ interactions (Å, °).

*Cg*1 and *Cg*2 are the centroids of rings C38–C43 and C16–C21, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C18—H18$\cdots$*Cg*1	0.93	2.82	3.5303 (1)	134 (2)
C21—H21$\cdots$*Cg*1^{i}	0.93	2.87	3.5767 (1)	133 (2)
C39—H39$\cdots$*Cg*2^{ii}	0.93	2.93	3.5398 (1)	125 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: KJ2073).

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supplementary materials

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4'-(4-Methylphenyl)-2,2':6',2''-terpyridine

H.-G. Liu, Y.-C. Qiu and J.-Z. Wu

Comment

Organic molecules bearing the 2,2':6',2"-terpyridine (ttp) group have a geometry favourable for accepting various metal centres, therefore such molecules are used widely in coordination chemistry (Samnes & Yahioglu, 1994; Thummel, 2004; Cargill Thompson, 1997). However, the crystal structure of the title compound has not been reported until now.

As illustrated in Fig. 1, in an asymmetric unit there are two crystallographically independent molecules, which are slightly distinct. In each molecule the three pyridyl moieties are nearly coplanar. The tolyl groups are twisted out of their connected pyridyls by 28.7 (4)° and 27.8 (9)°, respectively, which is somewhat different from the values reported for $[Mn(ttp)_2](ClO_4)_2$ [35.62 (4)° and 20.23 (6), Liu *et al.* (2007)]. In the asymmetric unit, the two terpyridyl moieties are parellel and staggered, whereas the two benzene rings make a dihedral angle of 55.6 (5)°. The crystal packing involves three short C—H···π contacts. A list, with geometric details, is given in Table 1. THe crystal packing also involves π-π stacking for some pyridyl rings: the centroid-centroid distances are 3.677 (4) Å between ring(N2, C6—C10) and ring(N4, C23—C27), and 3.707 (7) Å between ring(N3, C11—C15) and ring(N5, C28—C32)[−1 + *x*, *y*, *z*]. The C—H···π and π-π stacking interactions join the molecules into a one-dimensional chain, running in the a-direction (Fig. 2).

Experimental

4'-(4-methylphenyl)-2,2':6',2"-terpyridine (ttp) was prepared by an improved Kröhnke condensation method (Wang *et al.*, 2007; Collin *et al.*, 1991). A mixture of ttp (2 mmol) and water/ethanol(10 ml, 1:1) was placed in a 25 ml of Teflon-lined stainless steel vessel and heated under autogenous pressure at 413 K for 3 days, followed by cooling to room temperature at a rate of 5 K/h. Colorless block crystals were obtained.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

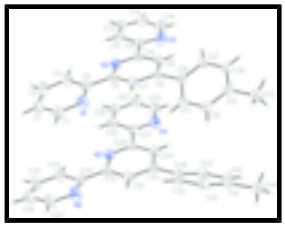

Fig. 1. The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

Fig. 2. The packing view of (I). C—H···π and π···π interactions are shown as dashed lines. H atoms not involved in close contacts are omitted for clarity.

4'-(4-Methylphenyl)-2,2':6',2''-terpyridine

Crystal data

$C_{22}H_{17}N_3$	F_{000} = 1360
M_r = 323.39	D_x = 1.278 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5600 reflections
a = 9.4575 (4) Å	θ = 1.4–28.0º
b = 33.8005 (15) Å	μ = 0.08 mm^{-1}
c = 11.3730 (5) Å	T = 293 (2) K
β = 112.357 (3)º	Block, colourless
V = 3362.3 (3) Å^3	0.26 × 0.23 × 0.19 mm
Z = 8	

Data collection

Bruker APEXII area-detector diffractometer	4866 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.045
Monochromator: graphite	θ_{max} = 27.9º
T = 293(2) K	θ_{min} = 2.0º
φ and ω scan	h = −12→12
Absorption correction: none	k = −44→43
54997 measured reflections	l = −14→14
8020 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained

$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.4806P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
8020 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
453 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.7759 (2)	0.11297 (6)	0.48780 (16)	0.0696 (5)
H1	0.7122	0.0961	0.5098	0.083*
C2	0.8596 (2)	0.13996 (6)	0.57595 (16)	0.0701 (5)
H2	0.8524	0.1416	0.6551	0.084*
C3	0.9539 (3)	0.16431 (6)	0.54450 (17)	0.0816 (6)
H3	1.0143	0.1827	0.6028	0.098*
C4	0.9591 (2)	0.16147 (6)	0.42549 (16)	0.0728 (5)
H4	1.0226	0.1781	0.4023	0.087*
C5	0.86928 (18)	0.13385 (4)	0.34122 (14)	0.0497 (4)
C6	0.86531 (17)	0.13101 (4)	0.20943 (14)	0.0466 (4)
C7	0.77995 (17)	0.10220 (4)	0.12563 (14)	0.0475 (4)
H7	0.7269	0.0834	0.1525	0.057*
C8	0.77361 (16)	0.10132 (4)	0.00176 (13)	0.0449 (3)
C9	0.85548 (17)	0.13028 (4)	−0.03174 (14)	0.0495 (4)
H9	0.8538	0.1311	−0.1140	0.059*
C10	0.93975 (17)	0.15801 (4)	0.05723 (14)	0.0474 (4)
C11	1.02934 (17)	0.18938 (4)	0.02493 (14)	0.0498 (4)
C12	1.12666 (19)	0.21366 (5)	0.11818 (16)	0.0580 (4)
H12	1.1365	0.2107	0.2022	0.070*
C13	1.2091 (2)	0.24222 (5)	0.08585 (18)	0.0659 (5)
H13	1.2750	0.2589	0.1476	0.079*
C14	1.1930 (2)	0.24576 (5)	−0.03759 (18)	0.0681 (5)
H14	1.2477	0.2647	−0.0623	0.082*
C15	1.0942 (2)	0.22076 (6)	−0.12404 (18)	0.0806 (6)
H15	1.0830	0.2234	−0.2085	0.097*

C16	0.68526 (16)	0.07058 (4)	−0.08986 (13)	0.0444 (3)
C17	0.55910 (17)	0.05249 (5)	−0.07901 (14)	0.0506 (4)
H17	0.5280	0.0601	−0.0139	0.061*
C18	0.47891 (17)	0.02341 (5)	−0.16333 (14)	0.0533 (4)
H18	0.3945	0.0119	−0.1540	0.064*
C19	0.52101 (17)	0.01106 (5)	−0.26110 (14)	0.0511 (4)
C20	0.64724 (18)	0.02899 (5)	−0.27141 (14)	0.0556 (4)
H20	0.6784	0.0212	−0.3362	0.067*
C21	0.72812 (17)	0.05812 (5)	−0.18789 (14)	0.0518 (4)
H21	0.8126	0.0696	−0.1974	0.062*
C22	0.4345 (2)	−0.02102 (6)	−0.35164 (17)	0.0729 (5)
H22A	0.3543	−0.0094	−0.4231	0.109*
H22B	0.3910	−0.0389	−0.3090	0.109*
H22C	0.5030	−0.0352	−0.3806	0.109*
C23	0.5999 (2)	0.21967 (6)	−0.08254 (19)	0.0766 (6)
H23	0.5938	0.2216	−0.1659	0.092*
C24	0.6915 (2)	0.24603 (5)	0.00338 (19)	0.0700 (5)
H24	0.7459	0.2652	−0.0206	0.084*
C25	0.7009 (2)	0.24337 (5)	0.12568 (19)	0.0686 (5)
H25	0.7615	0.2609	0.1871	0.082*
C26	0.61903 (19)	0.21428 (5)	0.15698 (16)	0.0589 (4)
H26	0.6251	0.2117	0.2402	0.071*
C27	0.52811 (17)	0.18903 (4)	0.06361 (14)	0.0484 (4)
C28	0.43590 (16)	0.15754 (4)	0.09245 (14)	0.0459 (3)
C29	0.35440 (16)	0.13027 (4)	0.00119 (14)	0.0471 (4)
H29	0.3562	0.1316	−0.0799	0.057*
C30	0.26990 (16)	0.10085 (4)	0.02985 (13)	0.0439 (3)
C31	0.27262 (17)	0.10065 (4)	0.15311 (14)	0.0476 (4)
H31	0.2176	0.0817	0.1771	0.057*
C32	0.35749 (17)	0.12881 (4)	0.24004 (14)	0.0465 (4)
C33	0.36472 (18)	0.12913 (5)	0.37347 (14)	0.0510 (4)
C34	0.4341 (2)	0.15961 (5)	0.45523 (16)	0.0684 (5)
H34	0.4736	0.1812	0.4271	0.082*
C35	0.4444 (2)	0.15775 (7)	0.57910 (18)	0.0813 (6)
H35	0.4906	0.1781	0.6356	0.098*
C36	0.3861 (2)	0.12569 (7)	0.61817 (18)	0.0804 (6)
H36	0.3936	0.1234	0.7018	0.096*
C37	0.3164 (3)	0.09704 (6)	0.53035 (17)	0.0815 (6)
H37	0.2745	0.0755	0.5565	0.098*
C38	0.18624 (16)	0.07058 (4)	−0.06589 (13)	0.0430 (3)
C39	0.16367 (16)	0.03240 (4)	−0.03040 (13)	0.0478 (4)
H39	0.1968	0.0260	0.0555	0.057*
C40	0.09327 (16)	0.00391 (4)	−0.11997 (14)	0.0492 (4)
H40	0.0788	−0.0212	−0.0931	0.059*
C41	0.04346 (16)	0.01154 (4)	−0.24868 (14)	0.0481 (4)
C42	0.06321 (17)	0.04971 (5)	−0.28435 (14)	0.0520 (4)
H42	0.0287	0.0560	−0.3703	0.062*
C43	0.13286 (17)	0.07865 (5)	−0.19547 (14)	0.0508 (4)
H43	0.1443	0.1040	−0.2227	0.061*

C44	−0.0281 (2)	−0.02038 (5)	−0.34506 (16)	0.0656 (5)
H44A	−0.0878	−0.0085	−0.4254	0.098*
H44B	−0.0929	−0.0365	−0.3171	0.098*
H44C	0.0507	−0.0365	−0.3542	0.098*
N1	0.77916 (16)	0.10912 (4)	0.37216 (12)	0.0611 (4)
N2	0.94561 (14)	0.15852 (4)	0.17656 (11)	0.0497 (3)
N3	1.01214 (18)	0.19271 (4)	−0.09654 (13)	0.0711 (4)
N4	0.51837 (17)	0.19136 (4)	−0.05618 (13)	0.0663 (4)
N5	0.43839 (14)	0.15705 (4)	0.21117 (11)	0.0493 (3)
N6	0.30441 (18)	0.09797 (4)	0.40976 (13)	0.0687 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0820 (13)	0.0769 (13)	0.0565 (11)	0.0047 (10)	0.0340 (9)	0.0042 (9)
C2	0.0920 (14)	0.0748 (13)	0.0457 (9)	0.0182 (11)	0.0287 (10)	0.0024 (9)
C3	0.1102 (16)	0.0774 (14)	0.0517 (11)	−0.0114 (12)	0.0247 (11)	−0.0163 (10)
C4	0.0951 (14)	0.0686 (12)	0.0562 (11)	−0.0184 (10)	0.0304 (10)	−0.0118 (9)
C5	0.0567 (9)	0.0460 (9)	0.0464 (8)	0.0075 (7)	0.0195 (7)	0.0003 (7)
C6	0.0511 (8)	0.0433 (9)	0.0465 (8)	0.0056 (7)	0.0197 (7)	−0.0002 (7)
C7	0.0516 (9)	0.0451 (9)	0.0480 (8)	0.0020 (7)	0.0214 (7)	0.0023 (7)
C8	0.0456 (8)	0.0436 (8)	0.0460 (8)	0.0047 (7)	0.0180 (6)	0.0005 (7)
C9	0.0559 (9)	0.0502 (9)	0.0448 (8)	0.0029 (7)	0.0219 (7)	0.0006 (7)
C10	0.0494 (8)	0.0423 (8)	0.0512 (9)	0.0039 (7)	0.0199 (7)	0.0008 (7)
C11	0.0526 (9)	0.0436 (9)	0.0544 (9)	0.0054 (7)	0.0216 (7)	0.0016 (7)
C12	0.0625 (10)	0.0522 (10)	0.0599 (10)	−0.0030 (8)	0.0240 (8)	−0.0035 (8)
C13	0.0617 (11)	0.0547 (11)	0.0780 (13)	−0.0069 (8)	0.0228 (9)	−0.0062 (9)
C14	0.0708 (12)	0.0547 (11)	0.0811 (13)	−0.0083 (9)	0.0316 (10)	0.0087 (9)
C15	0.1039 (16)	0.0778 (13)	0.0638 (12)	−0.0254 (12)	0.0358 (11)	0.0056 (10)
C16	0.0449 (8)	0.0472 (9)	0.0409 (8)	0.0046 (6)	0.0161 (6)	0.0005 (6)
C17	0.0482 (9)	0.0587 (10)	0.0498 (9)	0.0031 (7)	0.0241 (7)	−0.0033 (7)
C18	0.0432 (8)	0.0615 (10)	0.0563 (9)	−0.0028 (7)	0.0201 (7)	−0.0021 (8)
C19	0.0475 (9)	0.0551 (10)	0.0451 (8)	0.0005 (7)	0.0113 (7)	−0.0018 (7)
C20	0.0586 (10)	0.0670 (11)	0.0457 (8)	−0.0008 (8)	0.0248 (7)	−0.0073 (8)
C21	0.0502 (9)	0.0605 (10)	0.0486 (9)	−0.0054 (7)	0.0230 (7)	−0.0038 (7)
C22	0.0701 (12)	0.0765 (13)	0.0655 (11)	−0.0142 (10)	0.0185 (9)	−0.0156 (10)
C23	0.1024 (15)	0.0667 (12)	0.0709 (12)	−0.0243 (11)	0.0446 (11)	−0.0012 (10)
C24	0.0744 (12)	0.0543 (11)	0.0869 (14)	−0.0122 (9)	0.0372 (11)	0.0025 (10)
C25	0.0680 (11)	0.0541 (11)	0.0800 (13)	−0.0127 (9)	0.0241 (10)	−0.0101 (9)
C26	0.0625 (10)	0.0535 (10)	0.0614 (10)	−0.0034 (8)	0.0243 (8)	−0.0040 (8)
C27	0.0513 (9)	0.0410 (8)	0.0553 (9)	0.0044 (7)	0.0229 (7)	0.0002 (7)
C28	0.0486 (8)	0.0414 (8)	0.0503 (9)	0.0058 (7)	0.0219 (7)	0.0017 (7)
C29	0.0530 (9)	0.0468 (9)	0.0450 (8)	0.0027 (7)	0.0224 (7)	0.0017 (7)
C30	0.0435 (8)	0.0435 (8)	0.0461 (8)	0.0048 (6)	0.0186 (6)	0.0025 (6)
C31	0.0502 (8)	0.0460 (9)	0.0485 (8)	0.0000 (7)	0.0210 (7)	0.0029 (7)
C32	0.0502 (8)	0.0442 (9)	0.0468 (8)	0.0066 (7)	0.0203 (7)	0.0025 (7)
C33	0.0553 (9)	0.0515 (9)	0.0479 (9)	0.0054 (7)	0.0215 (7)	0.0007 (7)
C34	0.0871 (13)	0.0642 (11)	0.0596 (11)	−0.0078 (10)	0.0344 (10)	−0.0104 (9)

C35	0.0947 (15)	0.0931 (16)	0.0575 (12)	−0.0080 (12)	0.0306 (11)	−0.0209 (11)
C36	0.0967 (15)	0.1012 (16)	0.0484 (10)	0.0077 (13)	0.0333 (10)	0.0013 (11)
C37	0.1110 (16)	0.0863 (14)	0.0567 (11)	−0.0095 (12)	0.0426 (11)	0.0037 (10)
C38	0.0425 (8)	0.0447 (8)	0.0437 (8)	0.0025 (6)	0.0185 (6)	0.0026 (6)
C39	0.0498 (8)	0.0505 (9)	0.0428 (8)	0.0032 (7)	0.0175 (7)	0.0064 (7)
C40	0.0501 (9)	0.0441 (8)	0.0538 (9)	−0.0015 (7)	0.0203 (7)	0.0030 (7)
C41	0.0435 (8)	0.0521 (9)	0.0492 (9)	0.0016 (7)	0.0180 (7)	−0.0018 (7)
C42	0.0540 (9)	0.0598 (10)	0.0410 (8)	−0.0002 (7)	0.0167 (7)	0.0033 (7)
C43	0.0544 (9)	0.0498 (9)	0.0488 (9)	−0.0014 (7)	0.0202 (7)	0.0077 (7)
C44	0.0693 (11)	0.0649 (11)	0.0597 (10)	−0.0053 (9)	0.0214 (9)	−0.0093 (8)
N1	0.0718 (9)	0.0650 (9)	0.0507 (8)	−0.0017 (7)	0.0281 (7)	−0.0004 (7)
N2	0.0554 (8)	0.0458 (7)	0.0493 (7)	0.0023 (6)	0.0212 (6)	−0.0017 (6)
N3	0.0888 (11)	0.0702 (10)	0.0556 (9)	−0.0222 (8)	0.0291 (8)	0.0002 (7)
N4	0.0849 (10)	0.0605 (9)	0.0617 (9)	−0.0195 (8)	0.0370 (8)	−0.0042 (7)
N5	0.0535 (7)	0.0459 (7)	0.0499 (7)	0.0034 (6)	0.0212 (6)	−0.0001 (6)
N6	0.0913 (11)	0.0678 (10)	0.0528 (8)	−0.0086 (8)	0.0340 (8)	0.0002 (7)

Geometric parameters (Å, °)

C1—N1	1.334 (2)	C23—N4	1.333 (2)
C1—C2	1.364 (3)	C23—C24	1.362 (2)
C1—H1	0.9300	C23—H23	0.9300
C2—C3	1.358 (3)	C24—C25	1.363 (2)
C2—H2	0.9300	C24—H24	0.9300
C3—C4	1.376 (2)	C25—C26	1.379 (2)
C3—H3	0.9300	C25—H25	0.9300
C4—C5	1.376 (2)	C26—C27	1.379 (2)
C4—H4	0.9300	C26—H26	0.9300
C5—N1	1.333 (2)	C27—N4	1.3324 (19)
C5—C6	1.488 (2)	C27—C28	1.489 (2)
C6—N2	1.3407 (18)	C28—N5	1.3415 (18)
C6—C7	1.387 (2)	C28—C29	1.383 (2)
C7—C8	1.3875 (19)	C29—C30	1.3898 (19)
C7—H7	0.9300	C29—H29	0.9300
C8—C9	1.388 (2)	C30—C31	1.3923 (19)
C8—C16	1.4835 (19)	C30—C38	1.484 (2)
C9—C10	1.387 (2)	C31—C32	1.387 (2)
C9—H9	0.9300	C31—H31	0.9300
C10—N2	1.3371 (18)	C32—N5	1.3399 (18)
C10—C11	1.488 (2)	C32—C33	1.493 (2)
C11—N3	1.3329 (19)	C33—N6	1.336 (2)
C11—C12	1.379 (2)	C33—C34	1.376 (2)
C12—C13	1.376 (2)	C34—C35	1.376 (2)
C12—H12	0.9300	C34—H34	0.9300
C13—C14	1.358 (2)	C35—C36	1.364 (3)
C13—H13	0.9300	C35—H35	0.9300
C14—C15	1.362 (2)	C36—C37	1.367 (3)
C14—H14	0.9300	C36—H36	0.9300
C15—N3	1.335 (2)	C37—N6	1.333 (2)

C15—H15	0.9300	C37—H37	0.9300
C16—C17	1.387 (2)	C38—C43	1.3910 (19)
C16—C21	1.389 (2)	C38—C39	1.3925 (19)
C17—C18	1.381 (2)	C39—C40	1.376 (2)
C17—H17	0.9300	C39—H39	0.9300
C18—C19	1.381 (2)	C40—C41	1.381 (2)
C18—H18	0.9300	C40—H40	0.9300
C19—C20	1.383 (2)	C41—C42	1.386 (2)
C19—C22	1.505 (2)	C41—C44	1.503 (2)
C20—C21	1.380 (2)	C42—C43	1.381 (2)
C20—H20	0.9300	C42—H42	0.9300
C21—H21	0.9300	C43—H43	0.9300
C22—H22A	0.9600	C44—H44A	0.9600
C22—H22B	0.9600	C44—H44B	0.9600
C22—H22C	0.9600	C44—H44C	0.9600
N1—C1—C2	124.41 (18)	C23—C24—C25	117.76 (17)
N1—C1—H1	117.8	C23—C24—H24	121.1
C2—C1—H1	117.8	C25—C24—H24	121.1
C3—C2—C1	117.89 (17)	C24—C25—C26	119.05 (17)
C3—C2—H2	121.1	C24—C25—H25	120.5
C1—C2—H2	121.1	C26—C25—H25	120.5
C2—C3—C4	119.31 (18)	C27—C26—C25	119.30 (16)
C2—C3—H3	120.3	C27—C26—H26	120.4
C4—C3—H3	120.3	C25—C26—H26	120.4
C5—C4—C3	119.28 (18)	N4—C27—C26	122.10 (15)
C5—C4—H4	120.4	N4—C27—C28	116.66 (13)
C3—C4—H4	120.4	C26—C27—C28	121.24 (14)
N1—C5—C4	121.93 (15)	N5—C28—C29	122.58 (14)
N1—C5—C6	116.85 (14)	N5—C28—C27	116.29 (13)
C4—C5—C6	121.20 (15)	C29—C28—C27	121.13 (13)
N2—C6—C7	122.61 (14)	C28—C29—C30	120.46 (14)
N2—C6—C5	115.86 (13)	C28—C29—H29	119.8
C7—C6—C5	121.51 (14)	C30—C29—H29	119.8
C6—C7—C8	120.12 (14)	C29—C30—C31	116.59 (13)
C6—C7—H7	119.9	C29—C30—C38	120.98 (13)
C8—C7—H7	119.9	C31—C30—C38	122.40 (13)
C7—C8—C9	116.77 (13)	C32—C31—C30	119.89 (14)
C7—C8—C16	121.56 (13)	C32—C31—H31	120.1
C9—C8—C16	121.67 (13)	C30—C31—H31	120.1
C10—C9—C8	120.12 (14)	N5—C32—C31	122.94 (14)
C10—C9—H9	119.9	N5—C32—C33	115.74 (13)
C8—C9—H9	119.9	C31—C32—C33	121.32 (14)
N2—C10—C9	122.67 (14)	N6—C33—C34	122.12 (15)
N2—C10—C11	115.70 (13)	N6—C33—C32	116.66 (14)
C9—C10—C11	121.63 (14)	C34—C33—C32	121.20 (15)
N3—C11—C12	121.97 (15)	C33—C34—C35	119.17 (18)
N3—C11—C10	117.35 (14)	C33—C34—H34	120.4
C12—C11—C10	120.68 (14)	C35—C34—H34	120.4
C13—C12—C11	119.48 (16)	C36—C35—C34	119.33 (18)

C13—C12—H12	120.3	C36—C35—H35	120.3
C11—C12—H12	120.3	C34—C35—H35	120.3
C14—C13—C12	119.06 (17)	C35—C36—C37	117.83 (18)
C14—C13—H13	120.5	C35—C36—H36	121.1
C12—C13—H13	120.5	C37—C36—H36	121.1
C13—C14—C15	117.88 (17)	N6—C37—C36	124.31 (19)
C13—C14—H14	121.1	N6—C37—H37	117.8
C15—C14—H14	121.1	C36—C37—H37	117.8
N3—C15—C14	124.88 (18)	C43—C38—C39	117.06 (13)
N3—C15—H15	117.6	C43—C38—C30	121.29 (13)
C14—C15—H15	117.6	C39—C38—C30	121.59 (13)
C17—C16—C21	117.46 (14)	C40—C39—C38	121.22 (13)
C17—C16—C8	121.33 (13)	C40—C39—H39	119.4
C21—C16—C8	121.19 (13)	C38—C39—H39	119.4
C18—C17—C16	121.04 (14)	C39—C40—C41	121.90 (14)
C18—C17—H17	119.5	C39—C40—H40	119.1
C16—C17—H17	119.5	C41—C40—H40	119.1
C19—C18—C17	121.60 (14)	C40—C41—C42	117.02 (14)
C19—C18—H18	119.2	C40—C41—C44	121.10 (14)
C17—C18—H18	119.2	C42—C41—C44	121.88 (14)
C18—C19—C20	117.29 (14)	C43—C42—C41	121.67 (14)
C18—C19—C22	121.39 (15)	C43—C42—H42	119.2
C20—C19—C22	121.32 (15)	C41—C42—H42	119.2
C21—C20—C19	121.65 (14)	C42—C43—C38	121.10 (14)
C21—C20—H20	119.2	C42—C43—H43	119.4
C19—C20—H20	119.2	C38—C43—H43	119.4
C20—C21—C16	120.96 (14)	C41—C44—H44A	109.5
C20—C21—H21	119.5	C41—C44—H44B	109.5
C16—C21—H21	119.5	H44A—C44—H44B	109.5
C19—C22—H22A	109.5	C41—C44—H44C	109.5
C19—C22—H22B	109.5	H44A—C44—H44C	109.5
H22A—C22—H22B	109.5	H44B—C44—H44C	109.5
C19—C22—H22C	109.5	C5—N1—C1	117.14 (15)
H22A—C22—H22C	109.5	C10—N2—C6	117.70 (13)
H22B—C22—H22C	109.5	C11—N3—C15	116.73 (15)
N4—C23—C24	124.95 (18)	C27—N4—C23	116.84 (15)
N4—C23—H23	117.5	C32—N5—C28	117.55 (13)
C24—C23—H23	117.5	C37—N6—C33	117.22 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···Cg1	0.93	2.82	3.5303 (1)	134 (2)
C21—H21···Cg1^{i}	0.93	2.87	3.5767 (1)	133 (2)
C39—H39···Cg2^{ii}	0.93	2.93	3.5398 (1)	125 (2)

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

Fig. 1

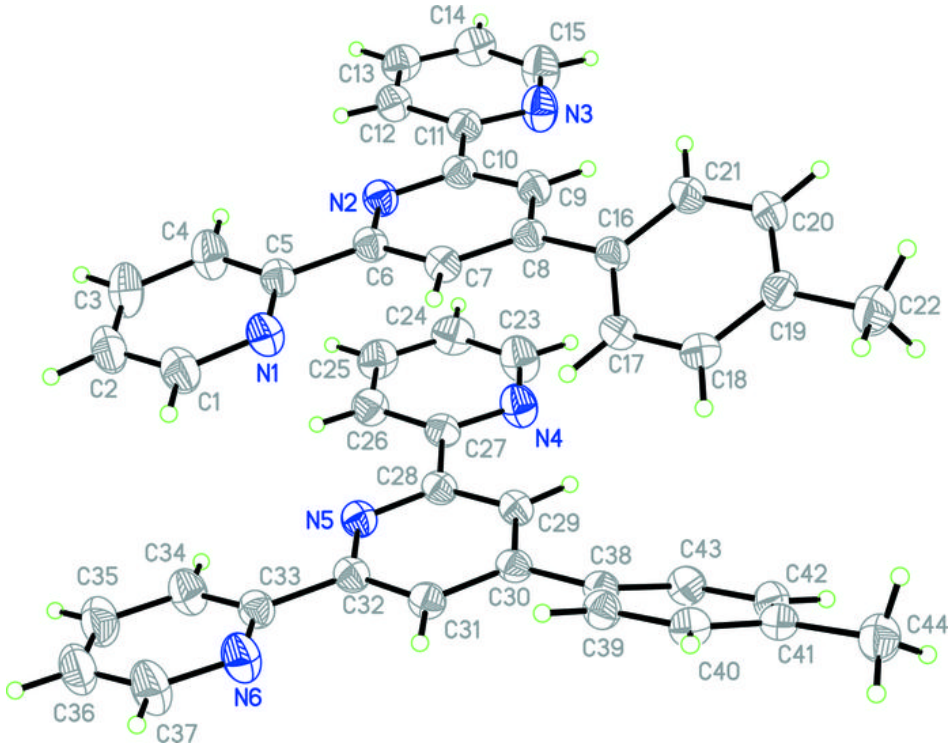
C14
C15
C13
N3
C12
C11
C10
C21
N2
C9
C16
C20
C4
C5
C6
C7
C8
C3
C22
C24
C23
C19
N1
C25
C17
C2
C1
C18
C26
C27
N4
C28
N5
C29
C34
C38
C43
C35
C33
C32
C30
C42
C31
C44
C39
C41
N6
C40
C36
C37

Fig. 2