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3-(2-Pyridyl)-*N*-*p*-tolylindolizin-1-amine

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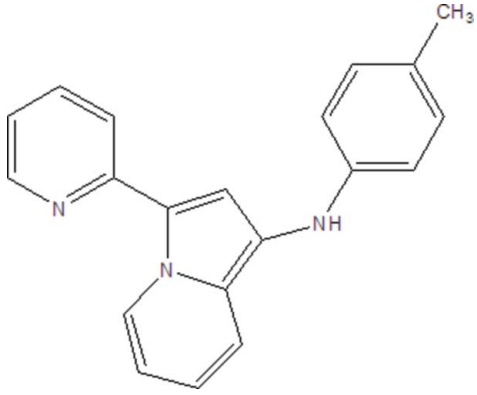
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; R factor = 0.052; wR factor = 0.137; data-to-parameter ratio = 6.7.

In the title compound, $C_{20}H_{17}N_3$, there are four molecules in the asymmetric unit. The dihedral angles between the indolizine ring system and the pyridyl ring are 6.6 (2), 7.4 (1), 4.0 (1) and 10.1 (4) in the four molecules. There are no further important differences between the independent molecules. In each molecule, there is an intramolecular C—H···N hydrogen bond. The whole structure is stabilized by N—H···π and C—H···π interactions.

Related literature

For related literature, see: Hema *et al.* (2003, 2004).



Experimental

Crystal data

$C_{20}H_{17}N_3$
M_r = 299.37
Monoclinic, *Cc*
a = 11.090 (4) Å
b = 11.140 (2) Å
c = 51.061 (3) Å
β = 95.41 (3)°
V = 6280 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.40 × 0.30 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
16297 measured reflections
5538 independent reflections
3417 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.136
S = 1.01
5538 reflections
831 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 is the centroid of the benzene ring C2–C7 and *Cg*2 is the centroid of the five-membered ring N2/C9/C8/C15/C14.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13*A*···N3	0.93	2.30	2.878 (8)	120 (1)
C33—H33*A*···N6	0.93	2.32	2.902 (8)	121 (1)
C53—H53*A*···N9	0.93	2.29	2.867 (7)	120 (1)
C73—H73*A*···N12	0.93	2.35	2.917 (8)	119 (1)
N7—H7*B*···*Cg*1^{i}	0.86	2.83 (1)	3.673 (2)	169 (1)
C57—H57*A*···*Cg*2^{ii}	0.93	2.98 (1)	3.852 (3)	157 (1)

Symmetry codes: (i) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL/PC* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2055).

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supplementary materials

Acta Cryst. (2008). E**64**, o386 [**doi:10.1107/S1600536807068481**]

3-(2-Pyridyl)-*N*-*p*-tolylindolizin-1-amine

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Comment

Chemists are attracted by indolizines and their derivatives because of their importance as pharmaceutical drugs, such as potential central nervous system depressants, cardiovascular agents, calcium entry blockers, spectral sensitizers and novel dyes (Hema *et al.*, 2003). Due to the diverse properties of indolizine derivatives, the structure determination of the title compound, (I), was performed.

Scheme I

The asymmetric unit of (I) contains four crystallographic independent molecules (A, B, C and D) as shown in Fig. 1. The corresponding bond lengths and angles in the independent molecules agree with each other and are comparable to those in related structures (Hema *et al.*, 2003, 2004). For A, the indolizine ring makes dihedral angels of 6.6 (2)° and 66.6 (1)°, respectively, with the pyridine ring and phenyl ring. (7.4 (1)° and 66.2 (1)° for B, 4.0 (1)° and 67.6 (1)° for C and 10.1 (4)° and 66.0 (1)° for D). The crystal packing is stabilized by N—H···Π and C—H···Π interactions (Table 1). The shortest N—H···Π interaction is H7B···*Cg*1^{i} = 2.827 (2) Å, N7—H7B···*Cg*1^{i} = 168.5 (2)°; and the shortest C—H···Π interaction is H57A···*Cg*2^{ii} = 2.977 (2) Å, C57—H57A···*Cg*2^{ii} = 157.4 (1)°. *Cg*1 is the centroid of the benzene ring C2–C7; *Cg*2 is the centroid of the 5-membered ring N2/C9/C8/C15/C14. [symmetry code: (i) −1/2+*X*,-1/2+Y,*Z*; (ii) *X*,-1+Y,*Z*]

Experimental

The mixture of ethyl 1,3-di(pyridin-2-yl)prop-2-en-1-one (5 mmol/1.044 g) and *p*-toluidine (6 mmol/0.643 g) in toluene (20 ml) was stirred and refluxed, then the phosphotungstic acid (0.01 g) in water (10 ml) was added dropwise. After two hours, the insoluble materials were removed by filtration, and the filtrate was separated. Finally the organic layer was kept at room temperature about two days. Yellow-colored and block shaped single crystals suitable for *x*-ray measurements were obtained.

Refinement

All the H atoms were discernable in a difference Fourier map. The N—H distance was 0.86 Å and C—H distances were constrained to 0.93 to 0.98 Å, respectively, while U_{iso}(H) = 1.2U_{eq}(C). 3423 Friedel pairs were averaged before the final refinement as the absolute could not be determined unambiguously.

Figures

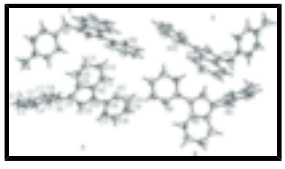


Fig. 1. The four independent molecules in the asymetric unit of (I) and atom-labeling scheme with the displacement ellipsoids drawn at the 30% probability level.

3-(2-Pyridyl)-*N*-*p*-tolylindolizin-1-amine

Crystal data

$C_{20}H_{17}N_3$	F_{000} = 2528
M_r = 299.37	D_x = 1.267 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 25 reflections
a = 11.090 (4) Å	θ = 1.6–28.4º
b = 11.140 (2) Å	μ = 0.08 mm^{-1}
c = 51.061 (3) Å	*T* = 295 (2) K
β = 95.41 (3)º	Block, yellow
V = 6280 (3) Å^3	0.40 × 0.30 × 0.12 mm
Z = 16	

Data collection

Bruker SMART CCD area-detector diffractometer	3417 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.050
Monochromator: graphite	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 1.6º
φ and ω scans	*h* = −12→13
Absorption correction: none	*k* = −13→12
16297 measured reflections	*l* = −58→60
5538 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.1752P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.136	$(\Delta/\sigma)_{max}$ = 0.011
S = 1.01	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
5538 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
831 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
2 restraints	Extinction coefficient: 0.00080 (13)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 3423 Friedel pairs
Secondary atom site location: difference Fourier map	

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}
N1	0.8702 (4)	0.3215 (4)	0.31351 (9)	0.0787 (14)
H1A	0.8720	0.3933	0.3197	0.094*
N2	0.7012 (4)	0.3065 (4)	0.24985 (9)	0.0608 (12)
N3	0.7434 (5)	0.2041 (5)	0.19954 (11)	0.0841 (15)
C1	1.0319 (7)	−0.0574 (6)	0.38255 (12)	0.110 (2)
H1B	1.0706	−0.0245	0.3986	0.164*
H1C	1.0886	−0.1064	0.3743	0.164*
H1D	0.9640	−0.1055	0.3864	0.164*
C2	0.9890 (6)	0.0429 (6)	0.36437 (11)	0.0741 (17)
C3	1.0091 (6)	0.1596 (6)	0.37080 (11)	0.0738 (16)
H3B	1.0495	0.1776	0.3871	0.089*
C4	0.9724 (5)	0.2527 (6)	0.35424 (10)	0.0696 (16)
H4A	0.9887	0.3316	0.3594	0.083*
C5	0.9113 (5)	0.2286 (5)	0.33001 (10)	0.0602 (14)
C6	0.8902 (5)	0.1097 (5)	0.32329 (11)	0.0662 (15)
H6A	0.8498	0.0906	0.3070	0.079*
C7	0.9284 (6)	0.0197 (5)	0.34038 (11)	0.0748 (16)
H7A	0.9125	−0.0596	0.3355	0.090*
C8	0.8258 (5)	0.3041 (5)	0.28723 (11)	0.0663 (15)
C9	0.7111 (5)	0.3368 (5)	0.27655 (11)	0.0621 (15)
C10	0.6124 (6)	0.3899 (5)	0.28682 (13)	0.0725 (17)
H10A	0.6170	0.4096	0.3046	0.087*
C11	0.5097 (6)	0.4132 (5)	0.27125 (15)	0.0812 (18)
H11A	0.4442	0.4497	0.2782	0.097*
C12	0.5030 (5)	0.3819 (5)	0.24475 (14)	0.0784 (17)
H12A	0.4319	0.3972	0.2341	0.094*
C13	0.5964 (5)	0.3301 (5)	0.23408 (12)	0.0697 (15)
H13A	0.5901	0.3105	0.2163	0.084*
C14	0.8086 (4)	0.2530 (4)	0.24408 (11)	0.0579 (13)
C15	0.8842 (5)	0.2535 (5)	0.26710 (11)	0.0651 (15)
H15A	0.9631	0.2242	0.2689	0.078*
C16	0.8322 (5)	0.2028 (5)	0.21916 (11)	0.0599 (14)
C17	0.9428 (5)	0.1527 (5)	0.21541 (12)	0.0744 (16)

H17A	1.0049	0.1543	0.2290	0.089*
C18	0.9618 (7)	0.1007 (6)	0.19205 (13)	0.0900 (19)
H18A	1.0365	0.0670	0.1895	0.108*
C19	0.8697 (8)	0.0989 (6)	0.17249 (13)	0.092 (2)
H19A	0.8792	0.0620	0.1565	0.111*
C20	0.7651 (8)	0.1517 (7)	0.17686 (15)	0.100 (2)
H20A	0.7033	0.1519	0.1632	0.120*
N4	0.5455 (4)	0.5425 (4)	−0.00222 (8)	0.0746 (14)
H4B	0.5423	0.6132	−0.0090	0.090*
N5	0.7094 (4)	0.5371 (3)	0.06191 (8)	0.0518 (11)
N6	0.6644 (5)	0.4385 (4)	0.11294 (10)	0.0770 (14)
C21	0.3945 (8)	0.1527 (7)	−0.06943 (13)	0.121 (3)
H21A	0.3530	0.1839	−0.0853	0.181*
H21B	0.3409	0.1014	−0.0608	0.181*
H21C	0.4640	0.1076	−0.0736	0.181*
C22	0.4350 (6)	0.2556 (6)	−0.05135 (11)	0.0741 (16)
C23	0.4128 (6)	0.3724 (6)	−0.05887 (12)	0.0801 (18)
H23A	0.3730	0.3882	−0.0754	0.096*
C24	0.4486 (5)	0.4670 (5)	−0.04242 (10)	0.0715 (16)
H24A	0.4318	0.5454	−0.0479	0.086*
C25	0.5086 (5)	0.4468 (5)	−0.01808 (10)	0.0543 (13)
C26	0.5321 (5)	0.3307 (5)	−0.01034 (10)	0.0625 (14)
H26A	0.5726	0.3151	0.0061	0.075*
C27	0.4957 (6)	0.2366 (5)	−0.02691 (10)	0.0748 (17)
H27A	0.5127	0.1584	−0.0214	0.090*
C28	0.5886 (5)	0.5302 (4)	0.02476 (10)	0.0579 (13)
C29	0.7024 (5)	0.5647 (5)	0.03511 (11)	0.0577 (14)
C30	0.8009 (6)	0.6197 (5)	0.02489 (12)	0.0718 (16)
H30A	0.7972	0.6387	0.0071	0.086*
C31	0.9021 (6)	0.6454 (5)	0.04093 (14)	0.0813 (17)
H31A	0.9685	0.6808	0.0342	0.098*
C32	0.9057 (5)	0.6185 (5)	0.06769 (13)	0.0740 (16)
H32A	0.9745	0.6380	0.0787	0.089*
C33	0.8120 (5)	0.5650 (5)	0.07788 (11)	0.0639 (14)
H33A	0.8167	0.5470	0.0957	0.077*
C34	0.6026 (5)	0.4835 (4)	0.06768 (10)	0.0529 (13)
C35	0.5289 (5)	0.4805 (4)	0.04439 (10)	0.0608 (13)
H35A	0.4508	0.4495	0.0423	0.073*
C36	0.5768 (5)	0.4394 (4)	0.09291 (11)	0.0576 (14)
C37	0.4624 (5)	0.3957 (5)	0.09660 (11)	0.0669 (15)
H37A	0.4012	0.3991	0.0829	0.080*
C38	0.4389 (6)	0.3478 (6)	0.12013 (12)	0.0831 (18)
H38A	0.3628	0.3165	0.1224	0.100*
C39	0.5289 (7)	0.3466 (6)	0.14023 (12)	0.087 (2)
H39A	0.5158	0.3150	0.1566	0.105*
C40	0.6374 (7)	0.3924 (6)	0.13573 (12)	0.087 (2)
H40A	0.6982	0.3917	0.1496	0.105*
N7	0.2351 (4)	0.1835 (4)	0.31743 (8)	0.0784 (14)
H7B	0.1674	0.1841	0.3244	0.094*

N8	0.2036 (4)	0.3160 (4)	0.25301 (8)	0.0551 (11)
N9	0.2663 (4)	0.2453 (4)	0.20166 (9)	0.0754 (13)
C41	0.6583 (7)	0.0627 (8)	0.38309 (13)	0.127 (3)
H41A	0.6362	0.0299	0.3994	0.191*
H41B	0.7068	0.1332	0.3866	0.191*
H41C	0.7037	0.0042	0.3743	0.191*
C42	0.5462 (6)	0.0949 (5)	0.36591 (11)	0.0718 (17)
C43	0.4346 (6)	0.0748 (5)	0.37313 (11)	0.0762 (18)
H43A	0.4266	0.0400	0.3894	0.091*
C44	0.3328 (6)	0.1037 (5)	0.35743 (10)	0.0695 (15)
H44A	0.2574	0.0895	0.3634	0.083*
C45	0.3385 (5)	0.1526 (5)	0.33324 (10)	0.0555 (13)
C46	0.4528 (5)	0.1748 (5)	0.32533 (10)	0.0633 (15)
H46A	0.4610	0.2099	0.3091	0.076*
C47	0.5528 (5)	0.1449 (5)	0.34158 (11)	0.0713 (15)
H47A	0.6288	0.1589	0.3359	0.086*
C48	0.2342 (5)	0.2138 (5)	0.29083 (11)	0.0616 (14)
C49	0.1925 (5)	0.3227 (5)	0.28004 (11)	0.0618 (15)
C50	0.1451 (5)	0.4263 (6)	0.29006 (13)	0.0742 (16)
H50A	0.1377	0.4321	0.3080	0.089*
C51	0.1101 (6)	0.5176 (5)	0.27438 (16)	0.0846 (18)
H51A	0.0780	0.5866	0.2813	0.102*
C52	0.1219 (5)	0.5090 (5)	0.24722 (14)	0.0779 (17)
H52A	0.0977	0.5732	0.2363	0.093*
C53	0.1670 (5)	0.4110 (5)	0.23683 (12)	0.0684 (15)
H53A	0.1738	0.4066	0.2188	0.082*
C54	0.2545 (5)	0.2072 (5)	0.24732 (10)	0.0553 (13)
C55	0.2706 (4)	0.1438 (5)	0.27082 (10)	0.0599 (13)
H55A	0.3012	0.0663	0.2727	0.072*
C56	0.2838 (5)	0.1672 (5)	0.22142 (10)	0.0598 (15)
C57	0.3280 (6)	0.0552 (5)	0.21804 (12)	0.0764 (16)
H57A	0.3378	0.0023	0.2322	0.092*
C58	0.3581 (7)	0.0202 (7)	0.19380 (15)	0.099 (2)
H58A	0.3901	−0.0556	0.1913	0.119*
C59	0.3398 (7)	0.0992 (9)	0.17338 (15)	0.103 (2)
H59A	0.3589	0.0785	0.1566	0.124*
C60	0.2935 (6)	0.2077 (8)	0.17817 (14)	0.096 (2)
H60A	0.2795	0.2603	0.1641	0.116*
N10	0.1844 (4)	0.4090 (5)	−0.00098 (10)	0.0818 (14)
H10B	0.2529	0.4104	−0.0076	0.098*
N11	0.2016 (4)	0.5450 (4)	0.06290 (9)	0.0580 (12)
N12	0.1146 (5)	0.4780 (4)	0.11300 (11)	0.0838 (15)
C61	−0.2288 (7)	0.2740 (8)	−0.06922 (14)	0.119 (3)
H61A	−0.2997	0.2754	−0.0598	0.178*
H61B	−0.2177	0.1947	−0.0759	0.178*
H61C	−0.2387	0.3299	−0.0836	0.178*
C62	−0.1199 (6)	0.3084 (6)	−0.05100 (12)	0.0759 (17)
C63	−0.0037 (6)	0.2915 (6)	−0.05796 (11)	0.0797 (18)
H63A	0.0072	0.2581	−0.0743	0.096*

C64	0.0966 (6)	0.3231 (5)	−0.04131 (11)	0.0741 (16)
H64A	0.1738	0.3092	−0.0463	0.089*
C65	0.0825 (5)	0.3754 (4)	−0.01716 (10)	0.0595 (14)
C66	−0.0325 (5)	0.3933 (5)	−0.01056 (11)	0.0657 (16)
H66A	−0.0444	0.4277	0.0056	0.079*
C67	−0.1307 (6)	0.3614 (5)	−0.02736 (11)	0.0771 (17)
H67A	−0.2078	0.3766	−0.0224	0.093*
C68	0.1821 (5)	0.4409 (5)	0.02563 (11)	0.0645 (14)
C69	0.2190 (5)	0.5481 (5)	0.03640 (11)	0.0613 (14)
C70	0.2701 (5)	0.6524 (6)	0.02631 (14)	0.0796 (18)
H70A	0.2822	0.6571	0.0086	0.096*
C71	0.3014 (5)	0.7460 (6)	0.04260 (15)	0.0811 (18)
H71A	0.3341	0.8155	0.0360	0.097*
C72	0.2844 (5)	0.7370 (5)	0.06911 (14)	0.0791 (17)
H72A	0.3074	0.8008	0.0802	0.095*
C73	0.2363 (5)	0.6400 (5)	0.07914 (12)	0.0663 (15)
H73A	0.2261	0.6364	0.0970	0.080*
C74	0.1514 (5)	0.4339 (4)	0.06860 (10)	0.0569 (13)
C75	0.1399 (5)	0.3708 (5)	0.04535 (11)	0.0631 (14)
H75A	0.1088	0.2935	0.0432	0.076*
C76	0.1158 (5)	0.3981 (5)	0.09363 (11)	0.0645 (14)
C77	0.0773 (6)	0.2824 (5)	0.09707 (12)	0.0790 (17)
H77A	0.0777	0.2279	0.0833	0.095*
C78	0.0385 (7)	0.2461 (6)	0.12032 (13)	0.0912 (19)
H78A	0.0126	0.1676	0.1225	0.109*
C79	0.0382 (7)	0.3279 (6)	0.14059 (12)	0.087 (2)
H79A	0.0128	0.3072	0.1568	0.105*
C80	0.0775 (7)	0.4408 (7)	0.13548 (13)	0.101 (2)
H80A	0.0781	0.4966	0.1490	0.121*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.107 (4)	0.058 (3)	0.068 (3)	0.001 (3)	−0.011 (3)	−0.009 (2)
N2	0.046 (3)	0.049 (3)	0.086 (3)	−0.002 (2)	0.000 (2)	0.008 (2)
N3	0.085 (4)	0.086 (4)	0.078 (4)	0.008 (3)	−0.008 (3)	−0.008 (3)
C1	0.148 (7)	0.097 (5)	0.084 (4)	0.030 (5)	0.012 (4)	0.023 (4)
C2	0.082 (5)	0.076 (4)	0.066 (4)	0.020 (3)	0.019 (3)	0.000 (3)
C3	0.074 (4)	0.083 (5)	0.063 (3)	0.003 (3)	−0.004 (3)	−0.010 (3)
C4	0.066 (4)	0.075 (4)	0.066 (4)	−0.006 (3)	−0.002 (3)	−0.022 (3)
C5	0.054 (3)	0.057 (3)	0.070 (3)	−0.003 (3)	0.008 (3)	−0.006 (3)
C6	0.066 (4)	0.063 (4)	0.070 (4)	−0.002 (3)	0.004 (3)	−0.015 (3)
C7	0.094 (5)	0.059 (4)	0.072 (4)	−0.005 (3)	0.012 (3)	−0.004 (3)
C8	0.065 (4)	0.051 (3)	0.083 (4)	−0.006 (3)	0.008 (3)	−0.001 (3)
C9	0.065 (4)	0.044 (3)	0.078 (4)	−0.009 (3)	0.011 (3)	0.004 (3)
C10	0.067 (4)	0.051 (4)	0.102 (5)	−0.004 (3)	0.023 (4)	−0.002 (3)
C11	0.057 (4)	0.072 (4)	0.118 (5)	−0.005 (3)	0.025 (4)	−0.001 (4)
C12	0.053 (4)	0.066 (4)	0.117 (5)	0.002 (3)	0.008 (4)	0.021 (4)

C13	0.055 (4)	0.055 (3)	0.098 (4)	0.002 (3)	0.004 (3)	0.015 (3)
C14	0.046 (3)	0.052 (3)	0.075 (4)	−0.002 (2)	−0.002 (3)	0.011 (3)
C15	0.051 (3)	0.058 (3)	0.084 (4)	0.003 (3)	−0.004 (3)	0.005 (3)
C16	0.061 (4)	0.051 (3)	0.065 (3)	−0.011 (3)	−0.008 (3)	0.011 (3)
C17	0.056 (4)	0.081 (4)	0.086 (4)	0.003 (3)	0.005 (3)	0.008 (3)
C18	0.092 (5)	0.099 (5)	0.082 (4)	0.002 (4)	0.024 (4)	−0.001 (4)
C19	0.118 (6)	0.092 (5)	0.068 (4)	−0.013 (5)	0.010 (5)	−0.010 (4)
C20	0.099 (6)	0.097 (5)	0.099 (6)	0.008 (5)	−0.014 (5)	−0.013 (4)
N4	0.108 (4)	0.052 (3)	0.061 (3)	0.002 (2)	−0.009 (3)	0.009 (2)
N5	0.048 (3)	0.042 (2)	0.065 (3)	0.004 (2)	0.001 (2)	−0.009 (2)
N6	0.071 (3)	0.085 (3)	0.071 (3)	−0.012 (3)	−0.016 (3)	0.001 (3)
C21	0.162 (8)	0.107 (6)	0.091 (5)	−0.024 (5)	0.006 (5)	−0.023 (4)
C22	0.076 (4)	0.072 (4)	0.075 (4)	−0.008 (3)	0.011 (3)	0.000 (3)
C23	0.077 (4)	0.099 (5)	0.062 (4)	−0.010 (4)	−0.004 (3)	0.006 (4)
C24	0.078 (4)	0.071 (4)	0.064 (4)	0.006 (3)	−0.001 (3)	0.013 (3)
C25	0.053 (3)	0.055 (3)	0.054 (3)	0.003 (3)	0.004 (3)	0.013 (3)
C26	0.070 (4)	0.061 (4)	0.056 (3)	0.003 (3)	0.003 (3)	0.004 (3)
C27	0.106 (5)	0.060 (4)	0.058 (3)	−0.001 (3)	0.006 (3)	0.008 (3)
C28	0.061 (4)	0.052 (3)	0.060 (3)	0.004 (3)	0.001 (3)	0.002 (2)
C29	0.062 (4)	0.046 (3)	0.065 (4)	0.006 (3)	0.007 (3)	0.002 (2)
C30	0.077 (4)	0.053 (4)	0.089 (4)	0.003 (3)	0.026 (4)	−0.002 (3)
C31	0.075 (4)	0.064 (4)	0.108 (5)	−0.003 (3)	0.025 (4)	−0.005 (4)
C32	0.054 (4)	0.060 (4)	0.107 (5)	0.000 (3)	0.004 (3)	−0.009 (3)
C33	0.049 (3)	0.058 (3)	0.083 (4)	0.003 (3)	0.003 (3)	−0.010 (3)
C34	0.049 (3)	0.054 (3)	0.055 (3)	0.001 (3)	−0.003 (3)	−0.005 (2)
C35	0.056 (3)	0.052 (3)	0.074 (4)	0.003 (3)	−0.002 (3)	−0.003 (3)
C36	0.049 (4)	0.051 (3)	0.071 (4)	0.004 (2)	0.000 (3)	−0.011 (3)
C37	0.060 (4)	0.074 (4)	0.066 (4)	0.010 (3)	0.004 (3)	0.002 (3)
C38	0.065 (4)	0.104 (5)	0.082 (4)	−0.005 (4)	0.014 (4)	0.005 (4)
C39	0.087 (5)	0.111 (5)	0.062 (4)	−0.007 (4)	0.000 (4)	0.005 (3)
C40	0.084 (5)	0.108 (5)	0.066 (4)	−0.012 (4)	−0.016 (4)	0.004 (4)
N7	0.059 (3)	0.119 (4)	0.058 (3)	0.001 (3)	0.013 (2)	0.013 (3)
N8	0.044 (3)	0.052 (3)	0.068 (3)	−0.007 (2)	−0.001 (2)	0.004 (2)
N9	0.079 (3)	0.085 (3)	0.063 (3)	0.007 (3)	0.013 (3)	0.014 (3)
C41	0.099 (6)	0.195 (8)	0.082 (5)	0.036 (6)	−0.022 (4)	0.005 (5)
C42	0.080 (5)	0.079 (4)	0.055 (4)	0.008 (3)	0.000 (3)	−0.004 (3)
C43	0.090 (5)	0.080 (4)	0.059 (4)	0.015 (4)	0.010 (4)	0.018 (3)
C44	0.068 (4)	0.080 (4)	0.063 (3)	−0.002 (3)	0.021 (3)	0.008 (3)
C45	0.053 (4)	0.062 (3)	0.051 (3)	−0.003 (3)	0.004 (3)	−0.001 (2)
C46	0.065 (4)	0.076 (4)	0.051 (3)	0.001 (3)	0.014 (3)	0.005 (3)
C47	0.057 (4)	0.091 (4)	0.067 (4)	0.001 (3)	0.010 (3)	−0.003 (3)
C48	0.050 (3)	0.073 (4)	0.063 (3)	−0.001 (3)	0.007 (3)	0.005 (3)
C49	0.047 (3)	0.065 (4)	0.074 (4)	−0.011 (3)	0.005 (3)	0.000 (3)
C50	0.060 (4)	0.068 (4)	0.095 (4)	−0.011 (3)	0.008 (3)	−0.021 (4)
C51	0.067 (4)	0.056 (4)	0.132 (6)	−0.004 (3)	0.011 (4)	−0.012 (4)
C52	0.060 (4)	0.060 (4)	0.112 (5)	−0.004 (3)	0.001 (4)	0.006 (3)
C53	0.056 (3)	0.054 (4)	0.094 (4)	−0.001 (3)	0.000 (3)	0.014 (3)
C54	0.054 (3)	0.048 (3)	0.065 (3)	−0.002 (2)	0.008 (3)	0.008 (3)
C55	0.054 (3)	0.059 (3)	0.066 (3)	−0.005 (3)	−0.001 (3)	0.011 (3)

C56	0.054 (3)	0.062 (4)	0.061 (3)	−0.013 (3)	−0.007 (3)	0.013 (3)
C57	0.089 (4)	0.064 (4)	0.078 (4)	−0.002 (3)	0.012 (3)	−0.001 (3)
C58	0.115 (6)	0.088 (5)	0.096 (5)	−0.001 (4)	0.019 (5)	−0.019 (4)
C59	0.104 (6)	0.129 (7)	0.078 (5)	−0.013 (5)	0.014 (4)	−0.013 (5)
C60	0.086 (5)	0.125 (7)	0.077 (5)	−0.005 (5)	0.003 (4)	0.012 (4)
N10	0.053 (3)	0.111 (4)	0.083 (3)	−0.006 (3)	0.014 (3)	−0.014 (3)
N11	0.042 (3)	0.052 (3)	0.078 (3)	0.001 (2)	−0.004 (2)	−0.001 (2)
N12	0.105 (4)	0.063 (3)	0.083 (4)	−0.017 (3)	0.008 (3)	−0.014 (3)
C61	0.088 (5)	0.168 (8)	0.098 (5)	−0.024 (5)	−0.003 (4)	−0.004 (5)
C62	0.070 (4)	0.081 (4)	0.075 (4)	−0.019 (3)	0.004 (3)	0.002 (3)
C63	0.082 (5)	0.090 (5)	0.068 (4)	−0.006 (4)	0.017 (4)	−0.004 (3)
C64	0.062 (4)	0.083 (4)	0.079 (4)	0.002 (3)	0.018 (3)	−0.006 (3)
C65	0.058 (4)	0.056 (3)	0.066 (3)	−0.004 (3)	0.012 (3)	0.002 (3)
C66	0.059 (4)	0.077 (4)	0.062 (3)	0.003 (3)	0.010 (3)	−0.006 (3)
C67	0.064 (4)	0.093 (5)	0.074 (4)	−0.002 (3)	0.009 (3)	0.012 (3)
C68	0.047 (3)	0.072 (4)	0.074 (4)	0.001 (3)	0.000 (3)	−0.005 (3)
C69	0.047 (3)	0.061 (4)	0.076 (4)	0.005 (3)	0.001 (3)	0.005 (3)
C70	0.052 (4)	0.080 (5)	0.108 (5)	0.015 (3)	0.015 (4)	0.016 (4)
C71	0.069 (4)	0.057 (4)	0.118 (5)	−0.003 (3)	0.009 (4)	0.009 (4)
C72	0.066 (4)	0.053 (4)	0.116 (5)	−0.003 (3)	−0.004 (4)	−0.007 (3)
C73	0.053 (3)	0.053 (3)	0.090 (4)	−0.003 (3)	−0.009 (3)	−0.010 (3)
C74	0.052 (3)	0.044 (3)	0.072 (4)	0.006 (2)	−0.005 (3)	−0.003 (3)
C75	0.053 (3)	0.054 (3)	0.083 (4)	0.000 (3)	0.011 (3)	−0.016 (3)
C76	0.058 (3)	0.053 (4)	0.080 (4)	0.002 (3)	−0.006 (3)	0.000 (3)
C77	0.102 (5)	0.056 (4)	0.080 (4)	−0.002 (3)	0.013 (4)	−0.005 (3)
C78	0.115 (6)	0.068 (4)	0.092 (5)	−0.003 (4)	0.014 (4)	0.010 (4)
C79	0.108 (6)	0.085 (5)	0.069 (4)	−0.013 (4)	0.010 (4)	0.007 (4)
C80	0.134 (7)	0.100 (6)	0.071 (4)	−0.022 (5)	0.016 (4)	−0.023 (4)

Geometric parameters (Å, °)

N1—C5	1.384 (6)	N7—C45	1.382 (6)
N1—C8	1.398 (7)	N7—C48	1.399 (7)
N1—H1A	0.8600	N7—H7B	0.8600
N2—C13	1.376 (6)	N8—C54	1.379 (6)
N2—C14	1.388 (6)	N8—C53	1.380 (6)
N2—C9	1.399 (7)	N8—C49	1.399 (6)
N3—C16	1.337 (7)	N9—C60	1.332 (8)
N3—C20	1.339 (8)	N9—C56	1.332 (6)
C1—C2	1.501 (8)	C41—C42	1.496 (9)
C1—H1B	0.9600	C41—H41A	0.9600
C1—H1C	0.9600	C41—H41B	0.9600
C1—H1D	0.9600	C41—H41C	0.9600
C2—C3	1.355 (8)	C42—C43	1.343 (8)
C2—C7	1.365 (8)	C42—C47	1.369 (7)
C3—C4	1.375 (8)	C43—C44	1.360 (8)
C3—H3B	0.9300	C43—H43A	0.9300
C4—C5	1.380 (7)	C44—C45	1.357 (7)
C4—H4A	0.9300	C44—H44A	0.9300

C5—C6	1.384 (7)	C45—C46	1.388 (7)
C6—C7	1.369 (7)	C46—C47	1.363 (7)
C6—H6A	0.9300	C46—H46A	0.9300
C7—H7A	0.9300	C47—H47A	0.9300
C8—C15	1.385 (7)	C48—C55	1.376 (7)
C8—C9	1.386 (7)	C48—C49	1.393 (8)
C9—C10	1.390 (8)	C49—C50	1.386 (8)
C10—C11	1.351 (8)	C50—C51	1.329 (8)
C10—H10A	0.9300	C50—H50A	0.9300
C11—C12	1.393 (8)	C51—C52	1.409 (8)
C11—H11A	0.9300	C51—H51A	0.9300
C12—C13	1.344 (8)	C52—C53	1.332 (7)
C12—H12A	0.9300	C52—H52A	0.9300
C13—H13A	0.9300	C53—H53A	0.9300
C14—C15	1.378 (7)	C54—C55	1.389 (7)
C14—C16	1.437 (7)	C54—C56	1.461 (7)
C15—H15A	0.9300	C55—H55A	0.9300
C16—C17	1.377 (8)	C56—C57	1.358 (7)
C17—C18	1.360 (8)	C57—C58	1.369 (8)
C17—H17A	0.9300	C57—H57A	0.9300
C18—C19	1.359 (9)	C58—C59	1.365 (10)
C18—H18A	0.9300	C58—H58A	0.9300
C19—C20	1.338 (10)	C59—C60	1.345 (10)
C19—H19A	0.9300	C59—H59A	0.9300
C20—H20A	0.9300	C60—H60A	0.9300
N4—C25	1.378 (6)	N10—C65	1.387 (7)
N4—C28	1.422 (6)	N10—C68	1.407 (7)
N4—H4B	0.8600	N10—H10B	0.8600
N5—C33	1.371 (6)	N11—C73	1.377 (6)
N5—C34	1.383 (6)	N11—C69	1.385 (6)
N5—C29	1.397 (6)	N11—C74	1.399 (6)
N6—C40	1.332 (7)	N12—C80	1.322 (8)
N6—C36	1.343 (6)	N12—C76	1.332 (7)
C21—C22	1.513 (8)	C61—C62	1.504 (8)
C21—H21A	0.9600	C61—H61A	0.9600
C21—H21B	0.9600	C61—H61B	0.9600
C21—H21C	0.9600	C61—H61C	0.9600
C22—C23	1.372 (8)	C62—C67	1.359 (8)
C22—C27	1.377 (8)	C62—C63	1.381 (8)
C23—C24	1.383 (8)	C63—C64	1.380 (8)
C23—H23A	0.9300	C63—H63A	0.9300
C24—C25	1.372 (7)	C64—C65	1.386 (7)
C24—H24A	0.9300	C64—H64A	0.9300
C25—C26	1.369 (7)	C65—C66	1.365 (7)
C26—C27	1.383 (7)	C66—C67	1.368 (8)
C26—H26A	0.9300	C66—H66A	0.9300
C27—H27A	0.9300	C67—H67A	0.9300
C28—C35	1.369 (7)	C68—C69	1.361 (7)
C28—C29	1.376 (7)	C68—C75	1.390 (7)

C29—C30	1.397 (8)	C69—C70	1.411 (8)
C30—C31	1.356 (8)	C70—C71	1.358 (9)
C30—H30A	0.9300	C70—H70A	0.9300
C31—C32	1.396 (8)	C71—C72	1.388 (9)
C31—H31A	0.9300	C71—H71A	0.9300
C32—C33	1.345 (7)	C72—C73	1.329 (8)
C32—H32A	0.9300	C72—H72A	0.9300
C33—H33A	0.9300	C73—H73A	0.9300
C34—C35	1.378 (7)	C74—C75	1.375 (7)
C34—C36	1.432 (7)	C74—C76	1.430 (7)
C35—H35A	0.9300	C75—H75A	0.9300
C36—C37	1.388 (7)	C76—C77	1.374 (7)
C37—C38	1.362 (8)	C77—C78	1.362 (8)
C37—H37A	0.9300	C77—H77A	0.9300
C38—C39	1.363 (8)	C78—C79	1.379 (8)
C38—H38A	0.9300	C78—H78A	0.9300
C39—C40	1.347 (9)	C79—C80	1.364 (9)
C39—H39A	0.9300	C79—H79A	0.9300
C40—H40A	0.9300	C80—H80A	0.9300
C5—N1—C8	123.1 (4)	C45—N7—C48	123.9 (5)
C5—N1—H1A	118.4	C45—N7—H7B	118.1
C8—N1—H1A	118.4	C48—N7—H7B	118.1
C13—N2—C14	130.8 (5)	C54—N8—C53	130.6 (5)
C13—N2—C9	120.5 (5)	C54—N8—C49	109.3 (4)
C14—N2—C9	108.7 (5)	C53—N8—C49	120.1 (5)
C16—N3—C20	117.6 (6)	C60—N9—C56	116.6 (6)
C2—C1—H1B	109.5	C42—C41—H41A	109.5
C2—C1—H1C	109.5	C42—C41—H41B	109.5
H1B—C1—H1C	109.5	H41A—C41—H41B	109.5
C2—C1—H1D	109.5	C42—C41—H41C	109.5
H1B—C1—H1D	109.5	H41A—C41—H41C	109.5
H1C—C1—H1D	109.5	H41B—C41—H41C	109.5
C3—C2—C7	117.0 (5)	C43—C42—C47	116.5 (6)
C3—C2—C1	122.0 (6)	C43—C42—C41	122.4 (6)
C7—C2—C1	121.0 (6)	C47—C42—C41	121.1 (7)
C2—C3—C4	122.8 (5)	C42—C43—C44	122.3 (5)
C2—C3—H3B	118.6	C42—C43—H43A	118.9
C4—C3—H3B	118.6	C44—C43—H43A	118.9
C3—C4—C5	119.8 (5)	C45—C44—C43	121.6 (6)
C3—C4—H4A	120.1	C45—C44—H44A	119.2
C5—C4—H4A	120.1	C43—C44—H44A	119.2
C4—C5—C6	117.7 (5)	C44—C45—N7	121.6 (5)
C4—C5—N1	120.4 (5)	C44—C45—C46	117.3 (5)
C6—C5—N1	121.8 (5)	N7—C45—C46	121.0 (5)
C7—C6—C5	120.5 (5)	C47—C46—C45	119.5 (5)
C7—C6—H6A	119.7	C47—C46—H46A	120.3
C5—C6—H6A	119.7	C45—C46—H46A	120.3
C2—C7—C6	122.0 (5)	C46—C47—C42	122.8 (6)
C2—C7—H7A	119.0	C46—C47—H47A	118.6

C6—C7—H7A	119.0	C42—C47—H47A	118.6
C15—C8—C9	106.9 (5)	C55—C48—C49	108.0 (5)
C15—C8—N1	128.5 (5)	C55—C48—N7	127.5 (5)
C9—C8—N1	124.6 (6)	C49—C48—N7	124.5 (5)
C8—C9—C10	133.7 (6)	C50—C49—C48	134.6 (6)
C8—C9—N2	107.7 (5)	C50—C49—N8	118.7 (5)
C10—C9—N2	118.6 (6)	C48—C49—N8	106.7 (5)
C11—C10—C9	120.7 (6)	C51—C50—C49	120.9 (6)
C11—C10—H10A	119.7	C51—C50—H50A	119.5
C9—C10—H10A	119.7	C49—C50—H50A	119.5
C10—C11—C12	119.2 (6)	C50—C51—C52	119.5 (6)
C10—C11—H11A	120.4	C50—C51—H51A	120.3
C12—C11—H11A	120.4	C52—C51—H51A	120.3
C13—C12—C11	121.9 (6)	C53—C52—C51	121.4 (6)
C13—C12—H12A	119.0	C53—C52—H52A	119.3
C11—C12—H12A	119.0	C51—C52—H52A	119.3
C12—C13—N2	119.0 (6)	C52—C53—N8	119.4 (6)
C12—C13—H13A	120.5	C52—C53—H53A	120.3
N2—C13—H13A	120.5	N8—C53—H53A	120.3
C15—C14—N2	106.4 (5)	N8—C54—C55	106.7 (5)
C15—C14—C16	127.6 (5)	N8—C54—C56	126.1 (5)
N2—C14—C16	125.9 (5)	C55—C54—C56	127.2 (5)
C14—C15—C8	110.2 (5)	C48—C55—C54	109.3 (5)
C14—C15—H15A	124.9	C48—C55—H55A	125.4
C8—C15—H15A	124.9	C54—C55—H55A	125.4
N3—C16—C17	120.2 (6)	N9—C56—C57	122.2 (6)
N3—C16—C14	118.5 (5)	N9—C56—C54	117.2 (5)
C17—C16—C14	121.3 (5)	C57—C56—C54	120.6 (5)
C18—C17—C16	120.5 (6)	C56—C57—C58	119.9 (6)
C18—C17—H17A	119.7	C56—C57—H57A	120.1
C16—C17—H17A	119.7	C58—C57—H57A	120.1
C19—C18—C17	118.9 (7)	C59—C58—C57	118.4 (7)
C19—C18—H18A	120.6	C59—C58—H58A	120.8
C17—C18—H18A	120.6	C57—C58—H58A	120.8
C20—C19—C18	118.3 (7)	C60—C59—C58	118.2 (7)
C20—C19—H19A	120.8	C60—C59—H59A	120.9
C18—C19—H19A	120.8	C58—C59—H59A	120.9
C19—C20—N3	124.4 (7)	N9—C60—C59	124.7 (7)
C19—C20—H20A	117.8	N9—C60—H60A	117.7
N3—C20—H20A	117.8	C59—C60—H60A	117.7
C25—N4—C28	123.3 (4)	C65—N10—C68	123.8 (5)
C25—N4—H4B	118.3	C65—N10—H10B	118.1
C28—N4—H4B	118.3	C68—N10—H10B	118.1
C33—N5—C34	130.6 (5)	C73—N11—C69	120.8 (5)
C33—N5—C29	119.9 (5)	C73—N11—C74	130.5 (5)
C34—N5—C29	109.5 (4)	C69—N11—C74	108.7 (4)
C40—N6—C36	117.5 (5)	C80—N12—C76	117.4 (6)
C22—C21—H21A	109.5	C62—C61—H61A	109.5
C22—C21—H21B	109.5	C62—C61—H61B	109.5

H21A—C21—H21B	109.5	H61A—C61—H61B	109.5
C22—C21—H21C	109.5	C62—C61—H61C	109.5
H21A—C21—H21C	109.5	H61A—C61—H61C	109.5
H21B—C21—H21C	109.5	H61B—C61—H61C	109.5
C23—C22—C27	117.3 (5)	C67—C62—C63	116.8 (6)
C23—C22—C21	120.8 (6)	C67—C62—C61	121.8 (6)
C27—C22—C21	121.9 (6)	C63—C62—C61	121.4 (6)
C22—C23—C24	121.3 (6)	C64—C63—C62	121.6 (6)
C22—C23—H23A	119.3	C64—C63—H63A	119.2
C24—C23—H23A	119.3	C62—C63—H63A	119.2
C25—C24—C23	120.8 (5)	C63—C64—C65	120.2 (6)
C25—C24—H24A	119.6	C63—C64—H64A	119.9
C23—C24—H24A	119.6	C65—C64—H64A	119.9
C26—C25—C24	118.7 (5)	C66—C65—C64	117.9 (5)
C26—C25—N4	121.5 (5)	C66—C65—N10	122.8 (5)
C24—C25—N4	119.8 (5)	C64—C65—N10	119.3 (5)
C25—C26—C27	120.1 (5)	C65—C66—C67	120.9 (5)
C25—C26—H26A	119.9	C65—C66—H66A	119.5
C27—C26—H26A	119.9	C67—C66—H66A	119.5
C22—C27—C26	121.9 (5)	C62—C67—C66	122.6 (6)
C22—C27—H27A	119.1	C62—C67—H67A	118.7
C26—C27—H27A	119.1	C66—C67—H67A	118.7
C35—C28—C29	108.7 (5)	C69—C68—C75	108.0 (5)
C35—C28—N4	127.4 (5)	C69—C68—N10	125.4 (6)
C29—C28—N4	123.9 (5)	C75—C68—N10	126.5 (5)
C28—C29—C30	134.5 (6)	C68—C69—N11	107.9 (5)
C28—C29—N5	106.2 (5)	C68—C69—C70	133.7 (6)
C30—C29—N5	119.3 (5)	N11—C69—C70	118.4 (5)
C31—C30—C29	119.9 (6)	C71—C70—C69	119.8 (7)
C31—C30—H30A	120.0	C71—C70—H70A	120.1
C29—C30—H30A	120.0	C69—C70—H70A	120.1
C30—C31—C32	119.5 (6)	C70—C71—C72	119.4 (6)
C30—C31—H31A	120.3	C70—C71—H71A	120.3
C32—C31—H31A	120.3	C72—C71—H71A	120.3
C33—C32—C31	121.4 (6)	C73—C72—C71	122.1 (6)
C33—C32—H32A	119.3	C73—C72—H72A	119.0
C31—C32—H32A	119.3	C71—C72—H72A	119.0
C32—C33—N5	119.9 (5)	C72—C73—N11	119.5 (6)
C32—C33—H33A	120.0	C72—C73—H73A	120.2
N5—C33—H33A	120.0	N11—C73—H73A	120.2
C35—C34—N5	106.0 (4)	C75—C74—N11	106.2 (5)
C35—C34—C36	128.0 (5)	C75—C74—C76	128.2 (5)
N5—C34—C36	126.0 (4)	N11—C74—C76	125.6 (5)
C28—C35—C34	109.5 (5)	C74—C75—C68	109.1 (5)
C28—C35—H35A	125.2	C74—C75—H75A	125.4
C34—C35—H35A	125.2	C68—C75—H75A	125.4
N6—C36—C37	119.9 (5)	N12—C76—C77	120.5 (6)
N6—C36—C34	119.7 (5)	N12—C76—C74	120.0 (5)
C37—C36—C34	120.3 (5)	C77—C76—C74	119.4 (5)

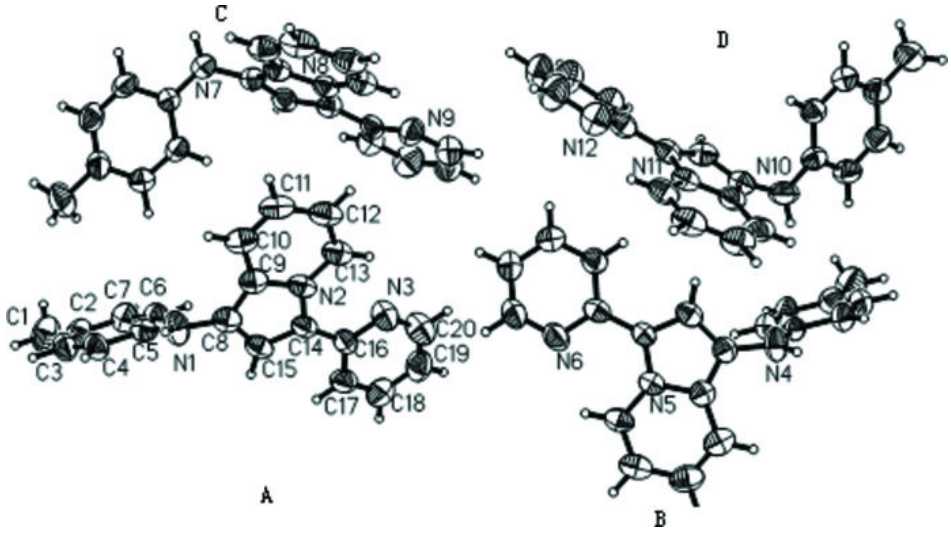
C38—C37—C36	120.7 (5)	C78—C77—C76	121.2 (6)
C38—C37—H37A	119.6	C78—C77—H77A	119.4
C36—C37—H37A	119.6	C76—C77—H77A	119.4
C37—C38—C39	118.7 (6)	C77—C78—C79	118.8 (6)
C37—C38—H38A	120.6	C77—C78—H78A	120.6
C39—C38—H38A	120.6	C79—C78—H78A	120.6
C40—C39—C38	118.1 (6)	C80—C79—C78	116.2 (6)
C40—C39—H39A	121.0	C80—C79—H79A	121.9
C38—C39—H39A	121.0	C78—C79—H79A	121.9
N6—C40—C39	125.0 (6)	N12—C80—C79	125.9 (6)
N6—C40—H40A	117.5	N12—C80—H80A	117.0
C39—C40—H40A	117.5	C79—C80—H80A	117.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···N3	0.93	2.30	2.878 (8)	120 (1)
C33—H33A···N6	0.93	2.32	2.902 (8)	121 (1)
C53—H53A···N9	0.93	2.29	2.867 (7)	120 (1)
C73—H73A···N12	0.93	2.35	2.917 (8)	119 (1)
N7—H7B···Cg1^{i}	0.86	2.83 (1)	3.673 (2)	169 (1)
C57—H57A···Cg2^{ii}	0.93	2.98 (1)	3.852 (3)	157 (1)

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

Fig. 1


C
D
N8
N7
N9
N12
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C11
C12
C10
C9
C13
N2
N3
C1
C2
C7
C6
C20
C19
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C4
C5
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C8
C15
C14
C16
C17
C18
N6
N5
N4
A
B