Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Methyl-2-pyridyl)-*p*-toluidine

Zainal Abidin Fairuz, Zaharah Aiyub, Zanariah Abdullah and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

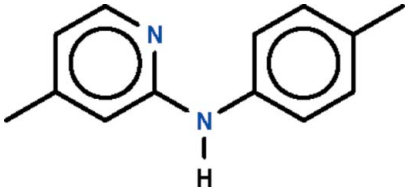
Received 12 December 2009; accepted 30 December 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.142; data-to-parameter ratio = 17.7.

In the title compound, $C_{13}H_{14}N_2$, the dihedral angle between the aromatic rings is 48.1 (1)° and the bridging C—N—C bond angle is 127.24 (12)°. In the crystal, intermolecular N—H···N hydrogen bonding about a center of inversion generates a hydrogen-bonded dimer.

Related literature

For the structure of *N*-(2-pyridyl)-4-toluidine, see: Fairuz *et al.* (2008).



Experimental

Crystal data

$C_{13}H_{14}N_2$
M_r = 198.26
Monoclinic, $P2_1/n$
a = 10.9385 (11) Å
b = 7.5708 (8) Å
c = 13.4372 (14) Å
β = 95.246 (2)°
V = 1108.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 K
0.45 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
6758 measured reflections
2528 independent reflections
1797 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.142
S = 1.05
2528 reflections
143 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.87 (1)	2.18 (1)	3.041 (2)	170 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank the University of Malaya (grant No. RG027/09AFR, PS374/09 A) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2710).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fairuz, Z. A., Aiyub, Z., Abdullah, Z. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o2441.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *publCIF*. In preparation.

supporting information

Acta Cryst. (2010). E**66**, o371 [https://doi.org/10.1107/S160053680905586X]

N-(4-Methyl-2-pyridyl)-*p*-toluidine

Zainal Abidin Fairuz, Zaharah Aiyub, Zanariah Abdullah and Seik Weng Ng

S1. Experimental

2-Chloro-4-methylpyridine (1 ml, 0.01 mol) and *p*-toluidine (1.2 g, 0.01 mol) were heated for 4 h. The product was dissolved in water and the solution extracted with ether. The ether extract was dried over sodium sulfate. Evaporation of the solvent gave large blocks of dark brown crystals. The crystals, when the outer parts were removed, were colorless.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C). The amino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N–H 0.86±0.01 Å; its temperature factor was refined.

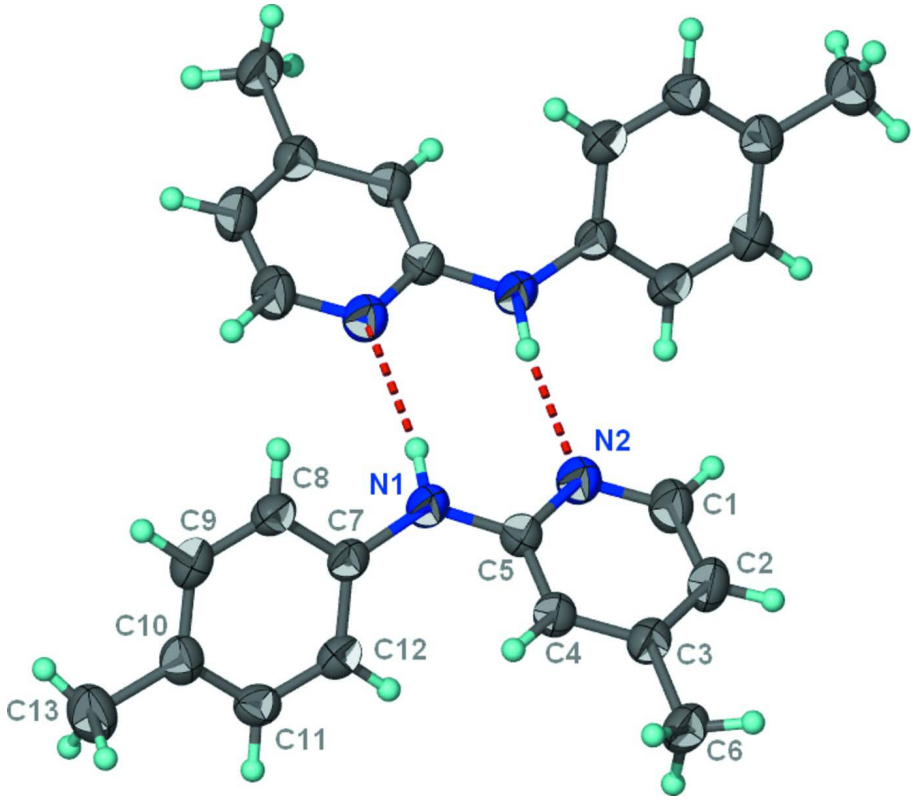


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the hydrogen-bonded $C_{13}H_{14}N_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Dashed lines denote hydrogen bonds.

N-(4-Methyl-2-pyridyl)-*p*-toluidine

Crystal data

$C_{13}H_{14}N_2$
$M_r = 198.26$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.9385$ (11) Å
$b = 7.5708$ (8) Å
$c = 13.4372$ (14) Å
$\beta = 95.246$ (2)°
$V = 1108.1$ (2) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.188$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2289 reflections
$\theta = 2.5$–$28.1°$
$\mu = 0.07$ mm^{-1}
$T = 295$ K
Irregular block, colorless
0.45 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6758 measured reflections
2528 independent reflections
1797 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -14 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.142$
$S = 1.05$
2528 reflections
143 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 0.1529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.044 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.51269 (11)	0.54344 (19)	0.64065 (9)	0.0571 (4)
H1	0.4682 (13)	0.546 (2)	0.5832 (8)	0.063 (5)*
N2	0.66732 (12)	0.46482 (18)	0.54571 (9)	0.0554 (4)
C1	0.78715 (15)	0.4383 (2)	0.53779 (12)	0.0642 (5)
H1A	0.8107	0.4072	0.4754	0.077*
C2	0.87740 (14)	0.4535 (2)	0.61487 (13)	0.0619 (4)
H2	0.9588	0.4288	0.6052	0.074*
C3	0.84502 (13)	0.50645 (19)	0.70755 (11)	0.0490 (4)
C4	0.72299 (13)	0.53940 (19)	0.71698 (11)	0.0471 (3)
H4	0.6985	0.5788	0.7776	0.056*
C5	0.63566 (13)	0.51384 (18)	0.63552 (10)	0.0458 (3)
C6	0.93890 (14)	0.5264 (2)	0.79563 (12)	0.0607 (4)

H6A	0.9168	0.6239	0.8360	0.091*
H6B	1.0180	0.5479	0.7725	0.091*
H6C	0.9418	0.4201	0.8347	0.091*
C7	0.45006 (12)	0.55349 (19)	0.72722 (10)	0.0447 (3)
C8	0.35038 (12)	0.6665 (2)	0.72803 (11)	0.0516 (4)
H8	0.3294	0.7385	0.6731	0.062*
C9	0.28208 (13)	0.6735 (2)	0.80914 (11)	0.0547 (4)
H9	0.2153	0.7498	0.8077	0.066*
C10	0.31070 (13)	0.5694 (2)	0.89293 (11)	0.0526 (4)
C11	0.41089 (13)	0.4573 (2)	0.89151 (11)	0.0502 (4)
H11	0.4322	0.3860	0.9467	0.060*
C12	0.47974 (13)	0.44843 (19)	0.81091 (10)	0.0477 (4)
H12	0.5464	0.3719	0.8124	0.057*
C13	0.23520 (17)	0.5750 (3)	0.98106 (13)	0.0757 (5)
H13A	0.1631	0.6452	0.9646	0.113*
H13B	0.2829	0.6262	1.0373	0.113*
H13C	0.2115	0.4572	0.9974	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0418 (7)	0.0866 (10)	0.0424 (7)	0.0084 (6)	0.0001 (5)	0.0006 (6)
N2	0.0492 (7)	0.0675 (8)	0.0496 (7)	0.0037 (6)	0.0048 (5)	−0.0037 (6)
C1	0.0536 (9)	0.0824 (12)	0.0583 (9)	0.0073 (8)	0.0136 (7)	−0.0093 (8)
C2	0.0426 (8)	0.0744 (11)	0.0698 (10)	0.0060 (7)	0.0104 (7)	−0.0040 (8)
C3	0.0433 (8)	0.0435 (8)	0.0599 (9)	−0.0004 (6)	0.0025 (6)	0.0045 (6)
C4	0.0439 (7)	0.0494 (8)	0.0479 (7)	0.0008 (6)	0.0049 (6)	−0.0010 (6)
C5	0.0427 (7)	0.0476 (8)	0.0471 (7)	0.0022 (6)	0.0049 (6)	0.0029 (6)
C6	0.0435 (8)	0.0664 (10)	0.0706 (10)	−0.0005 (7)	−0.0032 (7)	0.0044 (8)
C7	0.0363 (7)	0.0533 (8)	0.0434 (7)	−0.0015 (6)	−0.0023 (5)	−0.0024 (6)
C8	0.0424 (7)	0.0570 (9)	0.0542 (8)	0.0033 (6)	−0.0022 (6)	0.0070 (7)
C9	0.0411 (7)	0.0585 (9)	0.0643 (9)	0.0052 (6)	0.0031 (6)	−0.0040 (7)
C10	0.0452 (8)	0.0625 (9)	0.0500 (8)	−0.0080 (7)	0.0034 (6)	−0.0102 (7)
C11	0.0479 (8)	0.0559 (9)	0.0450 (7)	−0.0082 (6)	−0.0047 (6)	0.0031 (6)
C12	0.0408 (7)	0.0497 (8)	0.0512 (8)	0.0021 (6)	−0.0036 (6)	−0.0022 (6)
C13	0.0698 (11)	0.0969 (14)	0.0623 (10)	−0.0047 (10)	0.0172 (8)	−0.0109 (10)

Geometric parameters (Å, º)

N1—C5	1.3716 (18)	C6—H6C	0.9600
N1—C7	1.4051 (18)	C7—C8	1.3867 (19)
N1—H1	0.875 (9)	C7—C12	1.391 (2)
N2—C1	1.340 (2)	C8—C9	1.378 (2)
N2—C5	1.3380 (18)	C8—H8	0.9300
C1—C2	1.369 (2)	C9—C10	1.386 (2)
C1—H1A	0.9300	C9—H9	0.9300
C2—C3	1.385 (2)	C10—C11	1.388 (2)
C2—H2	0.9300	C10—C13	1.505 (2)

C3—C4	1.375 (2)	C11—C12	1.376 (2)
C3—C6	1.502 (2)	C11—H11	0.9300
C4—C5	1.399 (2)	C12—H12	0.9300
C4—H4	0.9300	C13—H13A	0.9600
C6—H6A	0.9600	C13—H13B	0.9600
C6—H6B	0.9600	C13—H13C	0.9600

C5—N1—C7	127.24 (12)	C8—C7—C12	118.16 (13)
C5—N1—H1	115.4 (11)	C8—C7—N1	118.89 (13)
C7—N1—H1	117.1 (11)	C12—C7—N1	122.87 (13)
C1—N2—C5	116.68 (13)	C9—C8—C7	120.90 (13)
N2—C1—C2	124.77 (15)	C9—C8—H8	119.5
N2—C1—H1A	117.6	C7—C8—H8	119.5
C2—C1—H1A	117.6	C8—C9—C10	121.47 (14)
C1—C2—C3	118.61 (14)	C8—C9—H9	119.3
C1—C2—H2	120.7	C10—C9—H9	119.3
C3—C2—H2	120.7	C9—C10—C11	117.16 (14)
C4—C3—C2	117.75 (14)	C9—C10—C13	121.57 (15)
C4—C3—C6	120.58 (14)	C11—C10—C13	121.26 (15)
C2—C3—C6	121.67 (14)	C12—C11—C10	122.03 (14)
C3—C4—C5	120.13 (13)	C12—C11—H11	119.0
C3—C4—H4	119.9	C10—C11—H11	119.0
C5—C4—H4	119.9	C11—C12—C7	120.27 (13)
N2—C5—N1	115.25 (12)	C11—C12—H12	119.9
N2—C5—C4	121.97 (13)	C7—C12—H12	119.9
N1—C5—C4	122.73 (13)	C10—C13—H13A	109.5
C3—C6—H6A	109.5	C10—C13—H13B	109.5
C3—C6—H6B	109.5	H13A—C13—H13B	109.5
H6A—C6—H6B	109.5	C10—C13—H13C	109.5
C3—C6—H6C	109.5	H13A—C13—H13C	109.5
H6A—C6—H6C	109.5	H13B—C13—H13C	109.5
H6B—C6—H6C	109.5		

C5—N2—C1—C2	1.7 (3)	C5—N1—C7—C8	146.94 (15)
N2—C1—C2—C3	−2.5 (3)	C5—N1—C7—C12	−36.3 (2)
C1—C2—C3—C4	0.6 (2)	C12—C7—C8—C9	−0.5 (2)
C1—C2—C3—C6	−179.91 (16)	N1—C7—C8—C9	176.39 (13)
C2—C3—C4—C5	2.0 (2)	C7—C8—C9—C10	0.5 (2)
C6—C3—C4—C5	−177.51 (13)	C8—C9—C10—C11	−0.2 (2)
C1—N2—C5—N1	178.72 (14)	C8—C9—C10—C13	−179.16 (15)
C1—N2—C5—C4	1.1 (2)	C9—C10—C11—C12	0.0 (2)
C7—N1—C5—N2	163.28 (14)	C13—C10—C11—C12	178.95 (14)
C7—N1—C5—C4	−19.1 (2)	C10—C11—C12—C7	0.0 (2)
C3—C4—C5—N2	−3.0 (2)	C8—C7—C12—C11	0.3 (2)
C3—C4—C5—N1	179.59 (14)	N1—C7—C12—C11	−176.47 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.87 (1)	2.18 (1)	3.041 (2)	170 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.