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

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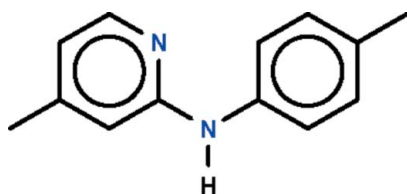
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.043; wR factor = 0.142; data-to-parameter ratio = 17.7.

In the title compound, $\text{C}_{13}\text{H}_{14}\text{N}_2$, the dihedral angle between the aromatic rings is $48.1(1)^\circ$ and the bridging $\text{C}-\text{N}-\text{C}$ bond angle is $127.24(12)^\circ$. In the crystal, intermolecular $\text{N}-\text{H}\cdots\text{N}$ 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

$\text{C}_{13}\text{H}_{14}\text{N}_2$
 $M_r = 198.26$
Monoclinic, $P2_1/n$
 $a = 10.9385(11)$ Å

$b = 7.5708(8)$ Å
 $c = 13.4372(14)$ Å
 $\beta = 95.246(2)^\circ$
 $V = 1108.1(2)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹

$T = 295$ K
 $0.45 \times 0.40 \times 0.30$ mm

Data collection

Bruker SMART APEX
diffractometer
6758 measured reflections

2528 independent reflections
1797 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

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
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{N2}^i$	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: *pubCIF* (Westrip, 2010).

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

References

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supplementary materials

Acta Cryst. (2010). E66, o371 [doi:10.1107/S160053680905586X]

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

Z. A. Fairuz, Z. Aiyub, Z. Abdullah and S. W. Ng

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.

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 $U(\text{H})$ set to 1.2–1.5 $U(\text{C})$. 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.

Figures

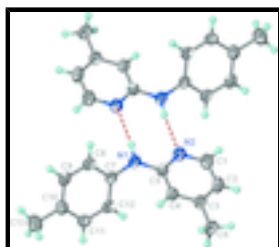


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the hydrogen-bonded $\text{C}_{13}\text{H}_{14}\text{N}_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Dashed lines denote hydrogen bonds.

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

Crystal data

$\text{C}_{13}\text{H}_{14}\text{N}_2$

$M_r = 198.26$

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) Å³

$Z = 4$

$F(000) = 424$

$D_x = 1.188$ 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

$0.45 \times 0.40 \times 0.30$ mm

supplementary materials

Data collection

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

Refinement

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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 (\AA , $^\circ$)

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

supplementary materials

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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots N2 ⁱ	0.87 (1)	2.18 (1)	3.041 (2)	170 (2)

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

Fig. 1

