Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(Pyrazin-2-yl)-4-toluidine

Wan Ainna Mardhiah Wan Saffiee, Azila Idris, 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

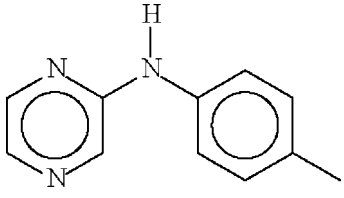
Received 19 October 2008; accepted 11 November 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 16.4.

The two aromatic systems in the title compound, $C_{11}H_{11}N_3$, are inclined by 19.1 (1)°, whilst the angle at the central amino N atom is 130.3 (2)°. The amino group forms a hydrogen bond to the pyrazine N-4 atom of an adjacent molecule, forming a chain motif.

Related literature

For the structure of aminopyrazine, see: Chao *et al.* (1976) and for that of *N*-(pyrazin-2-yl)-2-nitroaniline; see: Parsons *et al.* (2006). For two monoclinic modifications of *N*-(pyrazin-2-yl)-aniline, see: Abdullah & Ng (2008); Wan Saffiee *et al.* (2008).



Experimental

Crystal data

$C_{11}H_{11}N_3$
M_r = 185.23
Monoclinic, $C2/c$
a = 21.7179 (7) Å
b = 7.5323 (3) Å
c = 12.0073 (5) Å
β = 105.790 (3)°
V = 1890.1 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
6057 measured reflections
2165 independent reflections
1437 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.03
2165 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.89 (2)	2.10 (2)	2.963 (2)	163 (2)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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, 2008).

We thank the University of Malaya for supporting this study (grant No. FS 358/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2277).

References

Abdullah, Z. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o2106.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chao, M., Schempp, E. & Rosenstein, R. D. (1976). *Acta Cryst.* B**32**, 288–290.
Parsons, S., Wharton, S., McNab, H., Parkin, A. & Johnstone, R. (2006). Private communcation (refcode SEMSAF 610410). CCDC, Cambridge, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wan Saffiee, W. A. M., Idris, A., Abdullah, Z., Aiyub, Z. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o2105.
Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o2440 [doi:10.1107/S160053680803729X]

N-(Pyrazin-2-yl)-4-toluidine

Wan Ainna Mardhiah Wan Saffiee, Azila Idris, Zaharah Aiyub, Zanariah Abdullah and Seik Weng Ng

S1. Experimental

Chloropyrazine (1 ml, 1.1 mmol) and 4-toluidine (1.2 g, 1.1 mmol) were heated at 423–433 K for 3 h. The solid was dissolved in water. The compound was extracted with ether. The ether extract was dried over sodium sulfate; evaporation of the solvent gave colorless crystals among some unidentified dark brown materials.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) fixed at 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 0.88±0.01 Å.

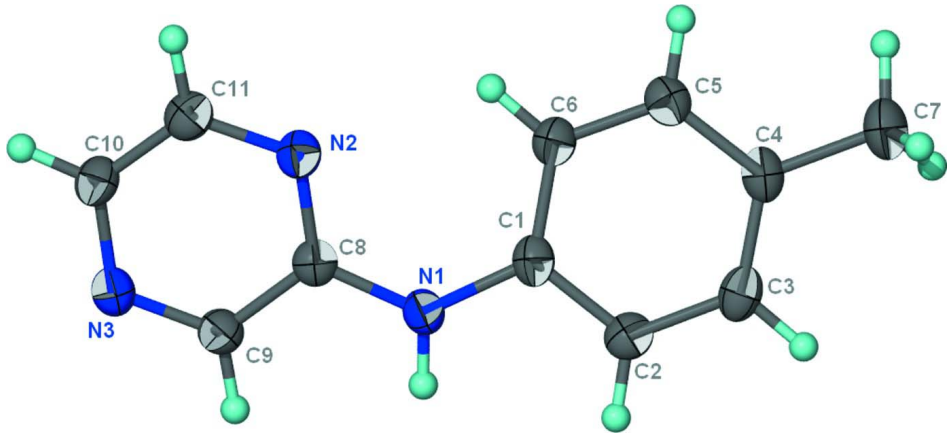


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{11}H_{11}N_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(Pyrazin-2-yl)-4-toluidine

Crystal data

$C_{11}H_{11}N_3$
M_r = 185.23
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 21.7179 (7) Å
b = 7.5323 (3) Å
c = 12.0073 (5) Å
β = 105.790 (3)°
V = 1890.1 (1) Å^3
Z = 8
F(000) = 784
D_x = 1.302 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1368 reflections
θ = 2.9–27.2°
μ = 0.08 mm^{-1}

T = 100 K
Prism, colorless

0.30 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6057 measured reflections
2165 independent reflections

1437 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 2.0°
h = −28→28
k = −9→9
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.03
2165 reflections
132 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.9346P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
N1	0.31486 (7)	0.7286 (2)	0.14663 (14)	0.0223 (4)
H1	0.2746 (10)	0.754 (3)	0.1433 (17)	0.025 (5)*
N2	0.39338 (7)	0.5068 (2)	0.20972 (13)	0.0215 (4)
N3	0.30867 (7)	0.3328 (2)	0.31234 (14)	0.0240 (4)
C1	0.34916 (8)	0.8610 (2)	0.10751 (15)	0.0209 (4)
C2	0.31332 (8)	0.9994 (2)	0.04370 (15)	0.0225 (4)
H2	0.2680	0.9977	0.0274	0.027*
C3	0.34299 (9)	1.1385 (2)	0.00420 (15)	0.0243 (4)
H3	0.3176	1.2305	−0.0396	0.029*
C4	0.40936 (9)	1.1472 (2)	0.02707 (15)	0.0231 (4)
C5	0.44431 (8)	1.0095 (2)	0.09091 (15)	0.0226 (4)
H5	0.4897	1.0127	0.1081	0.027*
C6	0.41565 (8)	0.8672 (2)	0.13069 (15)	0.0222 (4)
H6	0.4412	0.7745	0.1734	0.027*
C7	0.44137 (10)	1.3010 (3)	−0.01539 (18)	0.0302 (5)
H7A	0.4876	1.2958	0.0203	0.045*
H7B	0.4244	1.4129	0.0056	0.045*
H7C	0.4328	1.2941	−0.0997	0.045*
C8	0.33543 (8)	0.5719 (2)	0.20318 (15)	0.0201 (4)
C9	0.29286 (8)	0.4818 (2)	0.25360 (16)	0.0231 (4)
H9	0.2514	0.5298	0.2450	0.028*
C10	0.36764 (8)	0.2678 (2)	0.32060 (16)	0.0231 (4)
H10	0.3813	0.1616	0.3628	0.028*

C11	0.40806 (9)	0.3538 (2)	0.26845 (16)	0.0235 (4)
H11	0.4487	0.3022	0.2742	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0217 (8)	0.0194 (8)	0.0284 (9)	0.0007 (6)	0.0110 (7)	0.0031 (7)
N2	0.0249 (8)	0.0191 (8)	0.0223 (8)	0.0013 (6)	0.0095 (6)	−0.0011 (6)
N3	0.0254 (8)	0.0213 (8)	0.0262 (9)	−0.0016 (6)	0.0087 (7)	0.0019 (7)
C1	0.0275 (9)	0.0177 (9)	0.0191 (9)	−0.0009 (7)	0.0089 (7)	−0.0013 (7)
C2	0.0240 (9)	0.0224 (10)	0.0214 (10)	0.0019 (8)	0.0067 (7)	−0.0018 (8)
C3	0.0344 (10)	0.0191 (9)	0.0194 (10)	0.0024 (8)	0.0072 (8)	0.0004 (7)
C4	0.0316 (10)	0.0193 (9)	0.0200 (9)	−0.0032 (8)	0.0096 (8)	−0.0008 (7)
C5	0.0252 (9)	0.0222 (10)	0.0221 (10)	−0.0018 (8)	0.0093 (8)	−0.0018 (8)
C6	0.0261 (9)	0.0207 (9)	0.0204 (9)	0.0004 (7)	0.0071 (7)	0.0004 (7)
C7	0.0390 (11)	0.0250 (11)	0.0287 (11)	−0.0033 (9)	0.0128 (9)	0.0045 (8)
C8	0.0237 (9)	0.0196 (9)	0.0177 (9)	−0.0013 (7)	0.0065 (7)	−0.0023 (7)
C9	0.0222 (9)	0.0211 (9)	0.0267 (10)	0.0003 (7)	0.0079 (8)	0.0002 (8)
C10	0.0275 (9)	0.0187 (9)	0.0237 (10)	0.0022 (7)	0.0077 (8)	0.0003 (8)
C11	0.0264 (9)	0.0211 (10)	0.0238 (10)	0.0020 (8)	0.0080 (8)	−0.0020 (8)

Geometric parameters (Å, º)

N1—C8	1.374 (2)	C4—C5	1.386 (3)
N1—C1	1.401 (2)	C4—C7	1.509 (3)
N1—H1	0.89 (2)	C5—C6	1.388 (2)
N2—C8	1.333 (2)	C5—H5	0.9500
N2—C11	1.344 (2)	C6—H6	0.9500
N3—C9	1.320 (2)	C7—H7A	0.9800
N3—C10	1.349 (2)	C7—H7B	0.9800
C1—C6	1.395 (2)	C7—H7C	0.9800
C1—C2	1.398 (2)	C8—C9	1.410 (2)
C2—C3	1.380 (3)	C9—H9	0.9500
C2—H2	0.9500	C10—C11	1.372 (3)
C3—C4	1.393 (3)	C10—H10	0.9500
C3—H3	0.9500	C11—H11	0.9500
C8—N1—C1	130.28 (15)	C5—C6—H6	120.2
C8—N1—H1	113.3 (13)	C1—C6—H6	120.2
C1—N1—H1	115.9 (14)	C4—C7—H7A	109.5
C8—N2—C11	115.60 (15)	C4—C7—H7B	109.5
C9—N3—C10	116.84 (15)	H7A—C7—H7B	109.5
C6—C1—C2	118.44 (16)	C4—C7—H7C	109.5
C6—C1—N1	124.95 (16)	H7A—C7—H7C	109.5
C2—C1—N1	116.58 (15)	H7B—C7—H7C	109.5
C3—C2—C1	120.81 (16)	N2—C8—N1	121.33 (16)
C3—C2—H2	119.6	N2—C8—C9	121.10 (16)
C1—C2—H2	119.6	N1—C8—C9	117.57 (15)

C2—C3—C4	121.50 (17)	N3—C9—C8	122.23 (16)
C2—C3—H3	119.3	N3—C9—H9	118.9
C4—C3—H3	119.3	C8—C9—H9	118.9
C5—C4—C3	117.08 (16)	N3—C10—C11	120.51 (17)
C5—C4—C7	121.84 (16)	N3—C10—H10	119.7
C3—C4—C7	121.08 (17)	C11—C10—H10	119.7
C4—C5—C6	122.59 (16)	N2—C11—C10	123.68 (17)
C4—C5—H5	118.7	N2—C11—H11	118.2
C6—C5—H5	118.7	C10—C11—H11	118.2
C5—C6—C1	119.58 (17)		
C8—N1—C1—C6	−7.4 (3)	N1—C1—C6—C5	−177.39 (17)
C8—N1—C1—C2	174.81 (17)	C11—N2—C8—N1	179.29 (16)
C6—C1—C2—C3	0.2 (3)	C11—N2—C8—C9	−1.1 (2)
N1—C1—C2—C3	178.22 (16)	C1—N1—C8—N2	−13.4 (3)
C1—C2—C3—C4	−0.6 (3)	C1—N1—C8—C9	166.96 (17)
C2—C3—C4—C5	0.2 (3)	C10—N3—C9—C8	−1.1 (3)
C2—C3—C4—C7	−179.30 (17)	N2—C8—C9—N3	2.1 (3)
C3—C4—C5—C6	0.4 (3)	N1—C8—C9—N3	−178.20 (16)
C7—C4—C5—C6	179.96 (17)	C9—N3—C10—C11	−0.8 (3)
C4—C5—C6—C1	−0.7 (3)	C8—N2—C11—C10	−0.8 (3)
C2—C1—C6—C5	0.4 (3)	N3—C10—C11—N2	1.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.89 (2)	2.10 (2)	2.963 (2)	163 (2)

Symmetry code: (i) −*x*+1/2, *y*+1/2, −*z*+1/2.