organic compounds

4-Chloro-*N*-(pyrazin-2-yl)aniline

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

In the title compound, $C_{10}H_8ClN_3$, the dihedral angle between the aromatic rings is 43.0 (1)° and the bridging C—N—C angle is 128.19 (16)°. The amino N atom of one molecule forms a hydrogen bond to the 1-N atom of an adjacent pyrazinyl ring, generating an inversion dimer.

Related literature

For the two polymorphs of *N*-(pyrazin-2-yl)aniline, see: Wan Saffiee *et al.* (2008*a*); Abdullah & Ng (2008). For *N*-(pyrazin-2-yl)-4-toluidine; see: Wan Saffiee *et al.* (2008*b*).
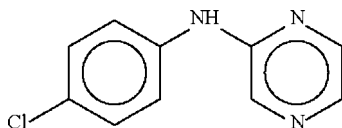
Experimental

Crystal data

$C_{10}H_8ClN_3$
M_r = 205.64
Monoclinic, $P2_1/c$
a = 12.1257 (3) Å
b = 3.7944 (1) Å
c = 19.7242 (5) Å
β = 91.370 (2)°

V = 907.25 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 100 (2) K
$0.25 \times 0.05 \times 0.01$ mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.912, T_{max} = 0.996

7922 measured reflections
2073 independent reflections
1633 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.128
S = 1.14
2073 reflections
131 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$N2^i	0.88 (1)	2.15 (1)	3.023 (2)	171 (2)

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

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, 2009).

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.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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*a*). *Acta Cryst.* E**64**, o2105.
Wan Saffiee, W. A. M., Idris, A., Aiyub, Z., Abdullah, Z. & Ng, S. W. (2008*b*). *Acta Cryst.* E**64**, o2440.
Westrip, S. P. (2009). *publCIF*. In preparation.

4-Chloro-*N*-(pyrazin-2-yl)aniline

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

S1. Experimental

2-Chloropyrazine (1.15 g, 10 mmol) and 4-chloroaniline (1.28 g, 10 mmol) were mixed with ethanol (2 ml) and the mixture heated at 423–433 K for 3 h. The product was dissolved in water and the solution extracted with ether. The ether phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped crystals along with some unidentified brown material.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) set to $1.2U_{eq}$(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; its temperature factor was freely refined.
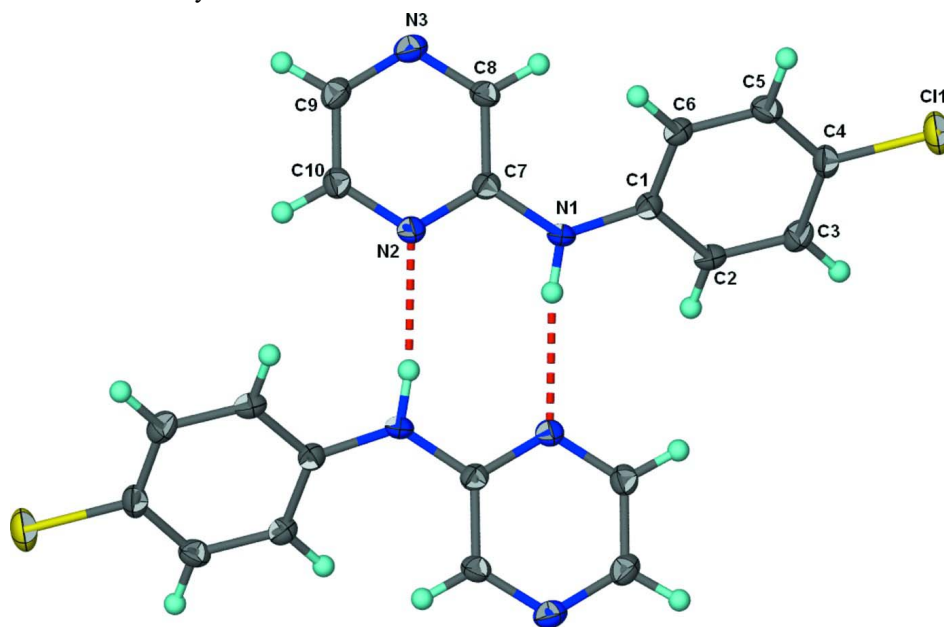
Figure 1

Thermal ellipsoid plot (Barbour, 2001) of hydrogen-bonded dimeric structure of $C_{10}H_8ClN_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are shown as red dashed lines.

4-Chloro-*N*-(pyrazin-2-yl)aniline

Crystal data

$C_{10}H_8ClN_3$	$F(000) = 424$
$M_r = 205.64$	$D_x = 1.506$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2160 reflections
$a = 12.1257$ (3) Å	$\theta = 2.6–28.1°$
$b = 3.7944$ (1) Å	$\mu = 0.38$ mm^{-1}
$c = 19.7242$ (5) Å	$T = 100$ K
$\beta = 91.370$ (2)°	Plate, yellow
$V = 907.25$ (4) Å^3	$0.25 \times 0.05 \times 0.01$ mm
$Z = 4$	

Data collection

Bruker SMART APEX diffractometer	7922 measured reflections
Radiation source: fine-focus sealed tube	2073 independent reflections
Graphite monochromator	1633 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.033$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$T_{min} = 0.912$, $T_{max} = 0.996$	$h = -15 \rightarrow 15$
	$k = -4 \rightarrow 4$
	$l = -25 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.0551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	
2073 reflections	$(\Delta/\sigma)_{max} = 0.001$
131 parameters	$\Delta\rho_{max} = 0.39$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.28$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.04801 (4)	−0.07942 (15)	0.36089 (3)	0.0269 (2)
N1	0.59098 (13)	0.2944 (5)	0.43167 (8)	0.0173 (4)
H1	0.5832 (19)	0.359 (6)	0.4742 (6)	0.019 (6)*
N2	0.40848 (13)	0.4535 (5)	0.42294 (8)	0.0152 (4)
N3	0.39085 (14)	0.1755 (5)	0.29204 (8)	0.0182 (4)
C1	0.69716 (16)	0.1986 (5)	0.41131 (10)	0.0147 (4)
C2	0.76584 (16)	0.0278 (5)	0.45861 (10)	0.0165 (4)
H2	0.7381	−0.0315	0.5018	0.020*
C3	0.87334 (16)	−0.0565 (5)	0.44384 (10)	0.0181 (4)
H3	0.9196	−0.1710	0.4766	0.022*
C4	0.91273 (16)	0.0283 (5)	0.38059 (11)	0.0173 (4)
C5	0.84635 (16)	0.1980 (5)	0.33265 (10)	0.0176 (4)

H5	0.8745	0.2545	0.2894	0.021*
C6	0.73893 (16)	0.2849 (5)	0.34796 (10)	0.0155 (4)
H6	0.6935	0.4033	0.3154	0.019*
C7	0.49564 (16)	0.3053 (5)	0.39334 (9)	0.0141 (4)
C8	0.48498 (16)	0.1632 (5)	0.32725 (10)	0.0159 (4)
H8	0.5473	0.0556	0.3075	0.019*
C9	0.30456 (17)	0.3280 (6)	0.32195 (10)	0.0185 (4)
H9	0.2360	0.3451	0.2979	0.022*
C10	0.31373 (16)	0.4595 (5)	0.38676 (10)	0.0168 (4)
H10	0.2503	0.5588	0.4067	0.020*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0139 (3)	0.0324 (3)	0.0346 (3)	0.0038 (2)	0.0035 (2)	−0.0016 (2)
N1	0.0157 (8)	0.0266 (9)	0.0096 (8)	0.0025 (7)	0.0006 (6)	−0.0028 (7)
N2	0.0154 (8)	0.0179 (8)	0.0124 (8)	0.0017 (6)	0.0004 (6)	0.0011 (6)
N3	0.0190 (9)	0.0222 (9)	0.0134 (8)	−0.0051 (7)	−0.0009 (6)	0.0010 (7)
C1	0.0134 (9)	0.0158 (9)	0.0148 (9)	−0.0009 (7)	−0.0007 (7)	−0.0024 (7)
C2	0.0194 (10)	0.0181 (10)	0.0121 (9)	−0.0008 (8)	−0.0014 (7)	0.0000 (7)
C3	0.0180 (10)	0.0168 (10)	0.0192 (10)	0.0019 (8)	−0.0039 (8)	0.0009 (8)
C4	0.0121 (9)	0.0178 (10)	0.0219 (10)	−0.0001 (7)	0.0004 (7)	−0.0040 (8)
C5	0.0177 (10)	0.0203 (10)	0.0148 (9)	−0.0034 (8)	0.0028 (7)	−0.0018 (8)
C6	0.0155 (9)	0.0166 (9)	0.0142 (9)	−0.0008 (7)	−0.0017 (7)	0.0005 (7)
C7	0.0143 (9)	0.0154 (9)	0.0125 (9)	−0.0014 (7)	0.0003 (7)	0.0020 (7)
C8	0.0164 (10)	0.0186 (10)	0.0129 (9)	−0.0012 (8)	0.0024 (7)	−0.0008 (8)
C9	0.0154 (10)	0.0236 (10)	0.0163 (10)	−0.0025 (8)	−0.0018 (7)	0.0045 (8)
C10	0.0145 (9)	0.0192 (10)	0.0167 (10)	0.0008 (8)	0.0013 (7)	0.0026 (8)

Geometric parameters (Å, º)

Cl1—C4	1.743 (2)	C3—C4	1.385 (3)
N1—C7	1.367 (2)	C3—H3	0.9500
N1—C1	1.406 (2)	C4—C5	1.386 (3)
N1—H1	0.881 (10)	C5—C6	1.384 (3)
N2—C10	1.338 (2)	C5—H5	0.9500
N2—C7	1.343 (2)	C6—H6	0.9500
N3—C8	1.323 (3)	C7—C8	1.414 (3)
N3—C9	1.344 (3)	C8—H8	0.9500
C1—C2	1.395 (3)	C9—C10	1.374 (3)
C1—C6	1.398 (3)	C9—H9	0.9500
C2—C3	1.380 (3)	C10—H10	0.9500
C2—H2	0.9500		
C7—N1—C1	128.19 (16)	C6—C5—H5	120.1
C7—N1—H1	114.2 (15)	C4—C5—H5	120.1
C1—N1—H1	117.6 (15)	C5—C6—C1	120.14 (18)
C10—N2—C7	116.74 (16)	C5—C6—H6	119.9

C8—N3—C9	117.11 (17)	C1—C6—H6	119.9
C2—C1—C6	118.89 (18)	N2—C7—N1	115.87 (17)
C2—C1—N1	117.73 (17)	N2—C7—C8	120.33 (17)
C6—C1—N1	123.26 (17)	N1—C7—C8	123.78 (18)
C3—C2—C1	121.21 (18)	N3—C8—C7	121.97 (18)
C3—C2—H2	119.4	N3—C8—H8	119.0
C1—C2—H2	119.4	C7—C8—H8	119.0
C2—C3—C4	118.96 (18)	N3—C9—C10	121.19 (19)
C2—C3—H3	120.5	N3—C9—H9	119.4
C4—C3—H3	120.5	C10—C9—H9	119.4
C3—C4—C5	121.05 (18)	N2—C10—C9	122.63 (18)
C3—C4—Cl1	119.53 (16)	N2—C10—H10	118.7
C5—C4—Cl1	119.42 (16)	C9—C10—H10	118.7
C6—C5—C4	119.75 (19)		
C7—N1—C1—C2	−146.4 (2)	N1—C1—C6—C5	176.58 (18)
C7—N1—C1—C6	37.6 (3)	C10—N2—C7—N1	−178.56 (17)
C6—C1—C2—C3	−0.1 (3)	C10—N2—C7—C8	−0.4 (3)
N1—C1—C2—C3	−176.21 (19)	C1—N1—C7—N2	−171.00 (19)
C1—C2—C3—C4	−0.5 (3)	C1—N1—C7—C8	10.9 (3)
C2—C3—C4—C5	0.6 (3)	C9—N3—C8—C7	−0.4 (3)
C2—C3—C4—Cl1	−179.50 (16)	N2—C7—C8—N3	1.2 (3)
C3—C4—C5—C6	0.0 (3)	N1—C7—C8—N3	179.22 (19)
Cl1—C4—C5—C6	−179.91 (15)	C8—N3—C9—C10	−1.1 (3)
C4—C5—C6—C1	−0.6 (3)	C7—N2—C10—C9	−1.1 (3)
C2—C1—C6—C5	0.7 (3)	N3—C9—C10—N2	1.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2[i]	0.88 (1)	2.15 (1)	3.023 (2)	171 (2)

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