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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

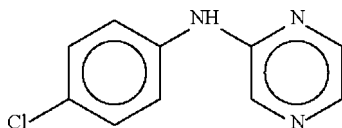
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.037; wR factor = 0.128; data-to-parameter ratio = 15.8.

In the title compound, $\text{C}_{10}\text{H}_8\text{ClN}_3$, the dihedral angle between the aromatic rings is $43.0(1)^\circ$ and the bridging $\text{C}-\text{N}-\text{C}$ angle is $128.19(16)^\circ$. 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.* (2008a); Abdullah & Ng (2008). For *N*-(pyrazin-2-yl)-4-toluidine; see: Wan Saffiee *et al.* (2008b).



Experimental

Crystal data

$\text{C}_{10}\text{H}_8\text{ClN}_3$
 $M_r = 205.64$
Monoclinic, $P2_1/c$
 $a = 12.1257(3)$ Å
 $b = 3.7944(1)$ Å
 $c = 19.7242(5)$ Å
 $\beta = 91.370(2)^\circ$

$V = 907.25(4)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.38$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

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, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{N2}^i$	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: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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).

We thank the University of Malaya for supporting this study (FS205/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2340).

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supplementary materials

Acta Cryst. (2009). E65, o113 [doi:10.1107/S1600536808041172]

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

W. A. M. Wan Saffie, A. Idris, Z. Aiyub, Z. Abdullah and S. W. Ng

Comment

(type here to add)

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.

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 $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

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.

Figures

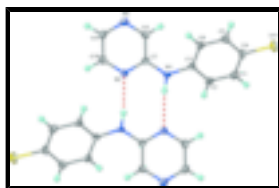


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of hydrogen-bonded dimeric structure of $\text{C}_{10}\text{H}_8\text{ClN}_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are shown as red dashed lines.

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

Crystal data

$\text{C}_{10}\text{H}_8\text{ClN}_3$
 $M_r = 205.64$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc
 $a = 12.1257 (3) \text{ \AA}$
 $b = 3.7944 (1) \text{ \AA}$
 $c = 19.7242 (5) \text{ \AA}$

$F_{000} = 424$

$D_x = 1.506 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2160 reflections

$\theta = 2.6\text{--}28.1^\circ$

$\mu = 0.38 \text{ mm}^{-1}$

$T = 100 (2) \text{ K}$

supplementary materials

$\beta = 91.370 (2)^\circ$ Plate, yellow
 $V = 907.25 (4) \text{ \AA}^3$ $0.25 \times 0.05 \times 0.01 \text{ mm}$
 $Z = 4$

Data collection

Bruker SMART APEX diffractometer	2073 independent reflections
Radiation source: fine-focus sealed tube	1633 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.033$
$T = 100(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 15$
$T_{\text{min}} = 0.912$, $T_{\text{max}} = 0.996$	$k = -4 \rightarrow 4$
7922 measured reflections	$l = -25 \rightarrow 24$

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
$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.0551P]$
$S = 1.14$	where $P = (F_o^2 + 2F_c^2)/3$
2073 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
131 parameters	$\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	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 (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	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 (\AA , $^\circ$)

C11—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

supplementary materials

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—C11	119.53 (16)	N2—C10—H10	118.7
C5—C4—C11	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—C11	-179.50 (16)	N2—C7—C8—N3	1.2 (3)
C3—C4—C5—C6	0.0 (3)	N1—C7—C8—N3	179.22 (19)
C11—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 (\AA , $^\circ$)

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

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

Fig. 1

