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

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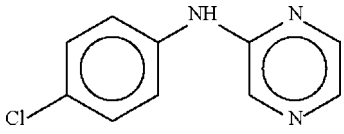
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.128; data-to-parameter ratio = 15.8.

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 × 0.05 × 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···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) $-x+1, -y+1, -z+1$.

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).

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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). E**65**, o113 [**doi:10.1107/S1600536808041172**]

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

W. A. M. Wan Saffiee, 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(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.

Figures

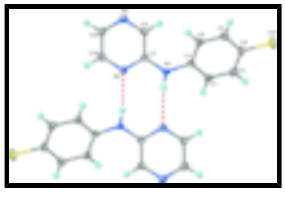

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of hydrogen-bonded dimeric structure of $C_{10}H_8ClN_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are shown as red dashed lines.

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 λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2160 reflections
a = 12.1257 (3) Å	θ = 2.6–28.1°
b = 3.7944 (1) Å	μ = 0.38 mm^{-1}
c = 19.7242 (5) Å	T = 100 (2) K

β = 91.370 (2)°	Plate, yellow
V = 907.25 (4) Å^3	0.25 × 0.05 × 0.01 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_{int} = 0.033
T = 100(2) K	θ_{max} = 27.5°
ω scans	θ_{min} = 1.7°
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.912, T_{max} = 0.996	k = −4→4
7922 measured reflections	l = −25→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	$(\Delta/\sigma)_{max}$ = 0.001
2073 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
131 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
1 restraint	Extinction correction: none
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 (Å^2)

	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, °)

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, °)

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 codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1