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4-Chloro-*N*-(2-pyridyl)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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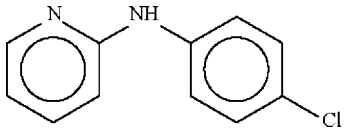
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.137; data-to-parameter ratio = 17.5.

There are two molecules in the asymmetric unit of the title compound, $C_{11}H_9ClN_2$, with dihedral angles of 41.84 (12) and 49.24 (12)° between the aromatic ring planes. The two molecules form a dimer *via* a pair of N—H···N hydrogen bonds.

Related literature

For the structures of the two modifications of *N*-(pyrazin-2-yl)aniline, see: Abdullah & Ng (2008); Wan Saffiee *et al.* (2008).



Experimental

Crystal data

$C_{11}H_9ClN_2$
M_r = 204.65
Monoclinic, $P2_1/n$
a = 15.5096 (4) Å
b = 7.5519 (2) Å
c = 17.6846 (4) Å
β = 106.284 (2)°
V = 1988.25 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 296 (2) K
0.42 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.870, T_{max} = 0.990
18472 measured reflections
4565 independent reflections
2369 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.137
S = 1.00
4565 reflections
261 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4	0.87 (1)	2.16 (1)	3.018 (3)	170 (2)
N3—H3···N2	0.86 (1)	2.22 (1)	3.071 (3)	171 (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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2855).

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 Göttigen, 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). *Acta Cryst.* E**64**, o2105.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2008). E**64**, o2437 [**doi:10.1107/S1600536808038658**]

4-Chloro-*N*-(2-pyridyl)aniline

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

Comment

For related structures, see: Abdullah & Ng (2008); Wan Saffiee *et al.* (2008). For the molecular structure of the title compound, (I), see Fig. 1. For hydrogen bond data, see Table 1.

Experimental

2-Chloropyrazine (0.11 g, 0.1 mmol) and 4-chloroaniline (0.13 g, 0.1 mmol) were heated at 423–433 K for 5 h. The mixture was cooled and dissolved in water. The solution was extracted with ether. The ether extract was dried over sodium sulfate and the solvent evaporated to yield a dark brown compound. Colourless rods of (I) were separated manually.

Refinement

The carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with U(H) = 1.2U(C). The amino H-atoms were located in a difference map, and were refined with a distance restraint of N–H = 0.88±0.01 Å.

Figures

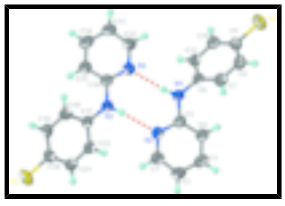


Fig. 1. The molecular structure of (I) drawn at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Chloro-*N*-(2-pyridyl)aniline

Crystal data

$C_{11}H_9ClN_2$	F_{000} = 848
M_r = 204.65	D_x = 1.367 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2114 reflections
a = 15.5096 (4) Å	θ = 2.4–21.4°
b = 7.5519 (2) Å	μ = 0.34 mm^{-1}
c = 17.6846 (4) Å	T = 296 (2) K
β = 106.284 (2)°	Rod, colourless
V = 1988.25 (9) Å^3	0.42 × 0.06 × 0.03 mm
Z = 8	

Data collection

Bruker SMART APEX CCD diffractometer	4565 independent reflections
Radiation source: fine-focus sealed tube	2369 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 100(2)$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 1.6^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -20\rightarrow20$
$T_{min} = 0.870$, $T_{max} = 0.990$	$k = -9\rightarrow9$
18472 measured reflections	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.3184P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4565 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
261 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
2 restraints	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	0.67109 (6)	0.86166 (11)	0.13818 (4)	0.0915 (3)
Cl2	0.52605 (6)	0.65436 (13)	0.94056 (4)	0.1027 (3)
N1	0.67429 (13)	0.7765 (3)	0.47124 (11)	0.0625 (5)
H1	0.6219 (9)	0.782 (3)	0.4794 (14)	0.074 (8)*
N2	0.72018 (12)	0.7057 (3)	0.60159 (11)	0.0625 (5)
N3	0.52408 (13)	0.6934 (3)	0.60693 (11)	0.0651 (6)
H3	0.5772 (9)	0.691 (3)	0.6004 (13)	0.064 (7)*
N4	0.48220 (12)	0.7816 (3)	0.47849 (11)	0.0634 (5)
C1	0.78370 (17)	0.6465 (4)	0.66437 (14)	0.0710 (7)
H1A	0.7688	0.6375	0.7116	0.085*
C2	0.86856 (17)	0.5984 (4)	0.66472 (15)	0.0743 (8)
H2	0.9099	0.5571	0.7102	0.089*
C3	0.89013 (16)	0.6137 (3)	0.59455 (15)	0.0693 (7)
H3A	0.9473	0.5828	0.5921	0.083*
C4	0.82822 (15)	0.6738 (3)	0.52878 (14)	0.0614 (6)

H4	0.8425	0.6842	0.4813	0.074*
C5	0.74264 (14)	0.7197 (3)	0.53411 (13)	0.0528 (6)
C6	0.67699 (14)	0.7960 (3)	0.39292 (12)	0.0517 (5)
C7	0.74402 (15)	0.8895 (3)	0.37290 (14)	0.0626 (6)
H7	0.7902	0.9407	0.4122	0.075*
C8	0.74268 (16)	0.9074 (3)	0.29468 (15)	0.0648 (7)
H8	0.7889	0.9670	0.2815	0.078*
C9	0.67292 (17)	0.8368 (3)	0.23664 (14)	0.0590 (6)
C10	0.60499 (15)	0.7467 (3)	0.25551 (13)	0.0571 (6)
H10	0.5576	0.7003	0.2160	0.069*
C11	0.60754 (14)	0.7255 (3)	0.33346 (13)	0.0532 (6)
H11	0.5619	0.6630	0.3463	0.064*
C12	0.41850 (17)	0.8195 (4)	0.41237 (14)	0.0756 (8)
H12	0.4368	0.8569	0.3692	0.091*
C13	0.32900 (18)	0.8074 (4)	0.40351 (15)	0.0787 (8)
H13	0.2873	0.8389	0.3565	0.094*
C14	0.30224 (16)	0.7468 (4)	0.46686 (15)	0.0747 (8)
H14	0.2415	0.7335	0.4628	0.090*
C15	0.36502 (15)	0.7066 (3)	0.53537 (14)	0.0654 (7)
H15	0.3478	0.6647	0.5784	0.078*
C16	0.45526 (14)	0.7290 (3)	0.54015 (13)	0.0546 (6)
C17	0.52001 (13)	0.6854 (3)	0.68456 (12)	0.0504 (5)
C18	0.45807 (15)	0.7767 (3)	0.71257 (13)	0.0573 (6)
H18	0.4151	0.8470	0.6784	0.069*
C19	0.45919 (16)	0.7647 (3)	0.79053 (14)	0.0614 (6)
H19	0.4161	0.8238	0.8084	0.074*
C20	0.52424 (16)	0.6652 (3)	0.84200 (13)	0.0601 (6)
C21	0.58698 (15)	0.5743 (3)	0.81581 (13)	0.0592 (6)
H21	0.6308	0.5071	0.8507	0.071*
C22	0.58459 (14)	0.5833 (3)	0.73756 (13)	0.0559 (6)
H22	0.6266	0.5205	0.7197	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1128 (6)	0.1099 (6)	0.0642 (4)	0.0274 (5)	0.0455 (4)	0.0168 (4)
Cl2	0.1127 (6)	0.1427 (8)	0.0617 (4)	0.0110 (5)	0.0395 (4)	0.0276 (4)
N1	0.0442 (11)	0.0929 (16)	0.0500 (11)	0.0058 (11)	0.0123 (10)	0.0067 (10)
N2	0.0496 (11)	0.0902 (15)	0.0470 (11)	−0.0002 (10)	0.0125 (9)	−0.0015 (10)
N3	0.0437 (11)	0.1038 (17)	0.0470 (11)	0.0070 (11)	0.0112 (9)	0.0061 (10)
N4	0.0528 (11)	0.0867 (15)	0.0499 (12)	0.0078 (10)	0.0132 (10)	0.0019 (10)
C1	0.0581 (15)	0.104 (2)	0.0467 (14)	−0.0025 (15)	0.0082 (12)	0.0000 (13)
C2	0.0530 (15)	0.101 (2)	0.0594 (16)	0.0018 (14)	0.0003 (12)	0.0038 (14)
C3	0.0453 (13)	0.0847 (19)	0.0717 (17)	0.0065 (13)	0.0062 (13)	−0.0064 (14)
C4	0.0501 (13)	0.0802 (18)	0.0535 (14)	0.0011 (12)	0.0136 (11)	−0.0050 (12)
C5	0.0437 (12)	0.0622 (14)	0.0499 (13)	−0.0034 (11)	0.0086 (11)	−0.0051 (11)
C6	0.0444 (12)	0.0614 (14)	0.0502 (13)	0.0000 (11)	0.0146 (10)	0.0030 (11)
C7	0.0509 (14)	0.0699 (16)	0.0649 (15)	−0.0099 (12)	0.0126 (12)	0.0014 (12)

C8	0.0565 (14)	0.0664 (16)	0.0782 (17)	−0.0024 (12)	0.0301 (13)	0.0124 (13)
C9	0.0627 (15)	0.0628 (16)	0.0556 (14)	0.0137 (12)	0.0231 (12)	0.0072 (11)
C10	0.0489 (13)	0.0655 (16)	0.0547 (14)	0.0020 (11)	0.0107 (11)	−0.0056 (11)
C11	0.0438 (12)	0.0596 (14)	0.0575 (14)	−0.0017 (11)	0.0162 (11)	0.0015 (11)
C12	0.0645 (17)	0.111 (2)	0.0505 (15)	0.0178 (15)	0.0148 (13)	0.0093 (14)
C13	0.0578 (16)	0.119 (2)	0.0516 (15)	0.0208 (16)	0.0031 (13)	0.0020 (15)
C14	0.0464 (14)	0.102 (2)	0.0685 (17)	0.0002 (14)	0.0049 (13)	−0.0065 (15)
C15	0.0488 (13)	0.0883 (18)	0.0560 (14)	−0.0067 (13)	0.0097 (11)	0.0019 (13)
C16	0.0478 (13)	0.0647 (15)	0.0496 (13)	0.0051 (11)	0.0106 (11)	−0.0018 (11)
C17	0.0384 (11)	0.0631 (14)	0.0489 (13)	−0.0045 (10)	0.0108 (10)	0.0009 (10)
C18	0.0499 (13)	0.0631 (15)	0.0555 (14)	0.0051 (11)	0.0094 (11)	0.0066 (11)
C19	0.0562 (14)	0.0704 (17)	0.0622 (15)	0.0023 (12)	0.0244 (12)	0.0011 (12)
C20	0.0603 (15)	0.0692 (16)	0.0526 (14)	−0.0064 (13)	0.0186 (12)	0.0107 (12)
C21	0.0486 (13)	0.0677 (16)	0.0586 (14)	−0.0023 (12)	0.0104 (11)	0.0153 (12)
C22	0.0420 (12)	0.0654 (15)	0.0585 (14)	0.0008 (11)	0.0114 (11)	0.0029 (11)

Geometric parameters (Å, °)

Cl1—C9	1.744 (2)	C8—C9	1.373 (3)
Cl2—C20	1.737 (2)	C8—H8	0.9300
N1—C5	1.372 (3)	C9—C10	1.371 (3)
N1—C6	1.405 (3)	C10—C11	1.377 (3)
N1—H1	0.865 (10)	C10—H10	0.9300
N2—C1	1.338 (3)	C11—H11	0.9300
N2—C5	1.338 (3)	C12—C13	1.356 (3)
N3—C16	1.378 (3)	C12—H12	0.9300
N3—C17	1.393 (3)	C13—C14	1.378 (3)
N3—H3	0.863 (9)	C13—H13	0.9300
N4—C12	1.333 (3)	C14—C15	1.359 (3)
N4—C16	1.333 (3)	C14—H14	0.9300
C1—C2	1.364 (3)	C15—C16	1.389 (3)
C1—H1A	0.9300	C15—H15	0.9300
C2—C3	1.378 (3)	C17—C18	1.382 (3)
C2—H2	0.9300	C17—C22	1.396 (3)
C3—C4	1.362 (3)	C18—C19	1.377 (3)
C3—H3A	0.9300	C18—H18	0.9300
C4—C5	1.400 (3)	C19—C20	1.377 (3)
C4—H4	0.9300	C19—H19	0.9300
C6—C7	1.382 (3)	C20—C21	1.373 (3)
C6—C11	1.383 (3)	C21—C22	1.376 (3)
C7—C8	1.384 (3)	C21—H21	0.9300
C7—H7	0.9300	C22—H22	0.9300
C5—N1—C6	127.0 (2)	C11—C10—H10	120.2
C5—N1—H1	115.4 (16)	C10—C11—C6	120.9 (2)
C6—N1—H1	116.6 (16)	C10—C11—H11	119.5
C1—N2—C5	116.8 (2)	C6—C11—H11	119.5
C16—N3—C17	127.9 (2)	N4—C12—C13	124.7 (2)
C16—N3—H3	115.4 (15)	N4—C12—H12	117.6
C17—N3—H3	116.0 (15)	C13—C12—H12	117.6

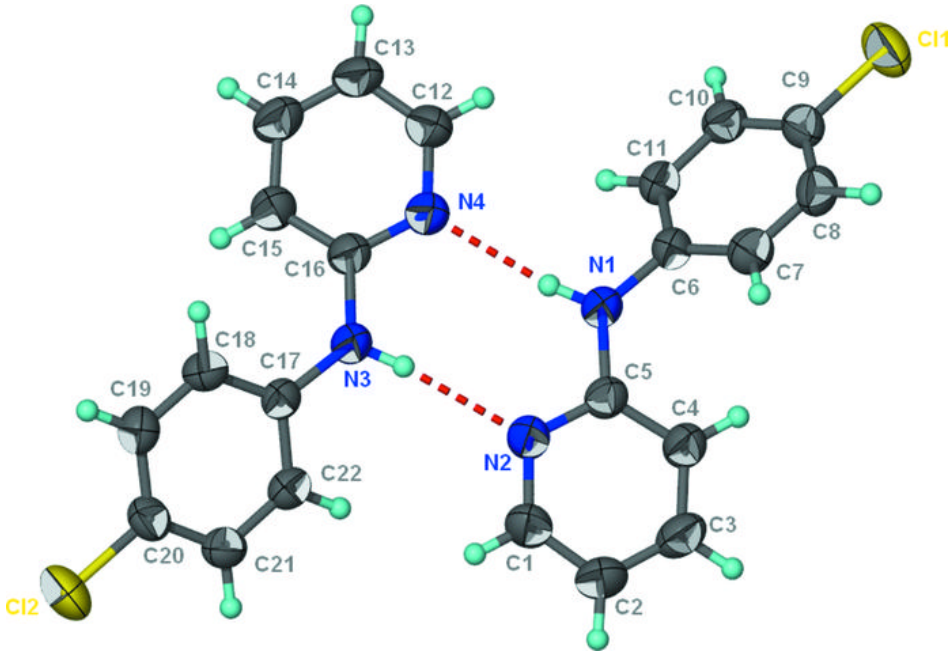
C12—N4—C16	117.2 (2)	C12—C13—C14	117.4 (2)
N2—C1—C2	125.3 (2)	C12—C13—H13	121.3
N2—C1—H1A	117.3	C14—C13—H13	121.3
C2—C1—H1A	117.3	C15—C14—C13	119.7 (2)
C1—C2—C3	116.8 (2)	C15—C14—H14	120.2
C1—C2—H2	121.6	C13—C14—H14	120.2
C3—C2—H2	121.6	C14—C15—C16	119.0 (2)
C4—C3—C2	120.4 (2)	C14—C15—H15	120.5
C4—C3—H3A	119.8	C16—C15—H15	120.5
C2—C3—H3A	119.8	N4—C16—N3	114.45 (19)
C3—C4—C5	118.7 (2)	N4—C16—C15	121.9 (2)
C3—C4—H4	120.7	N3—C16—C15	123.6 (2)
C5—C4—H4	120.7	C18—C17—N3	124.0 (2)
N2—C5—N1	114.34 (19)	C18—C17—C22	118.3 (2)
N2—C5—C4	122.0 (2)	N3—C17—C22	117.6 (2)
N1—C5—C4	123.7 (2)	C19—C18—C17	120.7 (2)
C7—C6—C11	118.9 (2)	C19—C18—H18	119.6
C7—C6—N1	122.6 (2)	C17—C18—H18	119.6
C11—C6—N1	118.5 (2)	C18—C19—C20	119.9 (2)
C6—C7—C8	120.3 (2)	C18—C19—H19	120.0
C6—C7—H7	119.9	C20—C19—H19	120.0
C8—C7—H7	119.9	C21—C20—C19	120.5 (2)
C9—C8—C7	119.8 (2)	C21—C20—Cl2	120.07 (18)
C9—C8—H8	120.1	C19—C20—Cl2	119.5 (2)
C7—C8—H8	120.1	C20—C21—C22	119.5 (2)
C10—C9—C8	120.6 (2)	C20—C21—H21	120.2
C10—C9—Cl1	119.87 (19)	C22—C21—H21	120.2
C8—C9—Cl1	119.55 (19)	C21—C22—C17	121.0 (2)
C9—C10—C11	119.5 (2)	C21—C22—H22	119.5
C9—C10—H10	120.2	C17—C22—H22	119.5
C5—N2—C1—C2	−0.6 (4)	C16—N4—C12—C13	−0.4 (4)
N2—C1—C2—C3	0.5 (4)	N4—C12—C13—C14	−1.9 (5)
C1—C2—C3—C4	−0.3 (4)	C12—C13—C14—C15	1.8 (4)
C2—C3—C4—C5	0.1 (4)	C13—C14—C15—C16	0.5 (4)
C1—N2—C5—N1	178.4 (2)	C12—N4—C16—N3	−179.4 (2)
C1—N2—C5—C4	0.3 (3)	C12—N4—C16—C15	2.8 (4)
C6—N1—C5—N2	−177.0 (2)	C17—N3—C16—N4	160.2 (2)
C6—N1—C5—C4	0.9 (4)	C17—N3—C16—C15	−22.0 (4)
C3—C4—C5—N2	−0.1 (4)	C14—C15—C16—N4	−2.9 (4)
C3—C4—C5—N1	−177.9 (2)	C14—C15—C16—N3	179.5 (2)
C5—N1—C6—C7	−51.1 (4)	C16—N3—C17—C18	−26.8 (4)
C5—N1—C6—C11	131.9 (3)	C16—N3—C17—C22	155.4 (2)
C11—C6—C7—C8	−1.9 (3)	N3—C17—C18—C19	−178.8 (2)
N1—C6—C7—C8	−178.9 (2)	C22—C17—C18—C19	−1.1 (3)
C6—C7—C8—C9	2.1 (4)	C17—C18—C19—C20	2.0 (4)
C7—C8—C9—C10	−0.8 (4)	C18—C19—C20—C21	−1.5 (4)
C7—C8—C9—Cl1	179.35 (19)	C18—C19—C20—Cl2	178.90 (18)
C8—C9—C10—C11	−0.7 (3)	C19—C20—C21—C22	0.1 (3)
Cl1—C9—C10—C11	179.13 (17)	Cl2—C20—C21—C22	179.70 (18)

C9—C10—C11—C6	0.9 (3)	C20—C21—C22—C17	0.8 (3)
C7—C6—C11—C10	0.4 (3)	C18—C17—C22—C21	−0.4 (3)
N1—C6—C11—C10	177.5 (2)	N3—C17—C22—C21	177.5 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4	0.87 (1)	2.16 (1)	3.018 (3)	170 (2)
N3—H3···N2	0.86 (1)	2.22 (1)	3.071 (3)	171 (2)

Fig. 1


C13
C14
C12
C15
C16
N4
N1
C10
C9
Cl1
C11
C8
C6
C7
C18
C17
N3
C5
C19
C4
N2
C22
C3
C20
C21
C1
C2
Cl2