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N-(Pyrimidin-2-yl)aniline

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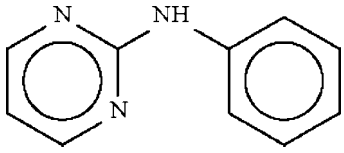
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 16.3.

There are two molecules in the asymmetric unit of the title compound, $C_{10}H_9N_3$, with inter-ring dihedral angles of 31.1 (1) and 35.3 (1)°. The bridging C—N—C bond angles are 128.2 (1) and 129.1 (1)°. In the crystal, the two independent molecules are linked into a dimer by two N—H···N hydrogen bonds.

Related literature

For the structure of 4-chloro-*N*-(pyrimidin-2-yl)aniline, see: Maizathul Akmam *et al.* (2009).



Experimental

Crystal data

$C_{10}H_9N_3$
M_r = 171.20
Triclinic, $P\overline{1}$
a = 8.8792 (2) Å
b = 9.9382 (2) Å
c = 10.2038 (2) Å
α = 93.186 (1)°
β = 103.665 (1)°
γ = 97.780 (1)°
V = 863.28 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 123 K
0.35 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
8238 measured reflections
3950 independent reflections
3144 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.03
3950 reflections
243 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N5	0.89 (1)	2.10 (1)	2.972 (1)	164 (1)
N4—H4···N2	0.89 (1)	2.15 (1)	3.020 (1)	165 (1)

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

The authors thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2492).

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supplementary materials

Acta Cryst. (2009). E**65**, o703 [**doi:10.1107/S1600536809007685**]

N-(Pyrimidin-2-yl)aniline

E. Badaruddin, N. Shah Bakhtiar, Z. Aiyub, Z. Abdullah and S. W. Ng

Experimental

2-Chloropyrimidine (0.05 mol), aniline (0.05 mol) and ethanol (5 ml) were 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 colorless 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_{iso}(H) set to 1.2U_{eq}(C). The amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H 0.88±0.01 Å; their isotropic temperature factors were refined.

Figures

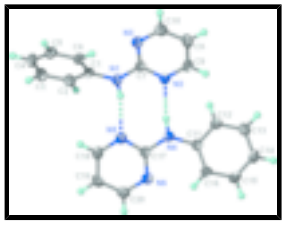


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_{10}H_9N_3$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Dashed lines denote hydrogen bonds.

N-(Pyrimidin-2-yl)aniline

Crystal data

$C_{10}H_9N_3$	$Z = 4$
$M_r = 171.20$	$F_{000} = 360$
Triclinic, $P\overline{1}$	$D_x = 1.317$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.8792$ (2) Å	Cell parameters from 3015 reflections
$b = 9.9382$ (2) Å	$\theta = 2.7$–28.3°
$c = 10.2038$ (2) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 93.186$ (1)°	$T = 123$ K
$\beta = 103.665$ (1)°	Prism, colorless
$\gamma = 97.780$ (1)°	0.35 × 0.20 × 0.10 mm
$V = 863.28$ (3) Å^3	

Data collection

Bruker SMART APEX diffractometer	3144 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.020$
Monochromator: graphite	$\theta_{max} = 27.5^o$
$T = 123$ K	$\theta_{min} = 2.1^o$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: None	$k = -12 \rightarrow 12$
8238 measured reflections	$l = -13 \rightarrow 12$
3950 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.1316P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3950 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
243 parameters	$\Delta\rho_{min} = -0.22$ 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}
N1	0.63241 (11)	0.69760 (10)	0.39973 (10)	0.0229 (2)
H1	0.5458 (13)	0.7328 (15)	0.4021 (15)	0.042 (4)*
N2	0.60532 (11)	0.62876 (10)	0.60461 (10)	0.0235 (2)
N3	0.82465 (11)	0.58169 (10)	0.51919 (10)	0.0257 (2)
N4	0.33475 (12)	0.78540 (10)	0.59499 (10)	0.0256 (2)
H4	0.4034 (15)	0.7306 (13)	0.5833 (14)	0.038 (4)*
N5	0.37902 (11)	0.86480 (10)	0.39948 (10)	0.0256 (2)
N6	0.18856 (11)	0.94997 (10)	0.50126 (10)	0.0245 (2)
C1	0.69680 (13)	0.72230 (11)	0.28811 (11)	0.0212 (2)
C2	0.59235 (14)	0.72964 (12)	0.16374 (12)	0.0259 (3)
H2	0.4827	0.7163	0.1571	0.031*
C3	0.64691 (15)	0.75616 (13)	0.04969 (12)	0.0305 (3)
H3	0.5748	0.7621	−0.0342	0.037*
C4	0.80703 (15)	0.77406 (13)	0.05803 (13)	0.0304 (3)
H4A	0.8449	0.7896	−0.0203	0.036*
C5	0.91044 (14)	0.76895 (12)	0.18192 (12)	0.0273 (3)

H5	1.0200	0.7824	0.1882	0.033*
C6	0.85757 (13)	0.74464 (11)	0.29708 (12)	0.0234 (2)
H6	0.9304	0.7432	0.3816	0.028*
C7	0.69174 (13)	0.63447 (11)	0.51132 (11)	0.0208 (2)
C8	0.66215 (14)	0.56772 (12)	0.71431 (12)	0.0269 (3)
H8	0.6055	0.5618	0.7825	0.032*
C9	0.79969 (15)	0.51238 (14)	0.73406 (13)	0.0321 (3)
H9	0.8393	0.4706	0.8140	0.039*
C10	0.87631 (14)	0.52129 (13)	0.63096 (13)	0.0309 (3)
H10	0.9700	0.4826	0.6402	0.037*
C11	0.27870 (12)	0.77031 (12)	0.71236 (11)	0.0219 (2)
C12	0.28250 (13)	0.64404 (12)	0.76560 (12)	0.0245 (3)
H12	0.3171	0.5728	0.7199	0.029*
C13	0.23654 (14)	0.62121 (13)	0.88390 (12)	0.0281 (3)
H13	0.2399	0.5349	0.9191	0.034*
C14	0.18554 (15)	0.72450 (14)	0.95093 (13)	0.0322 (3)
H14	0.1532	0.7093	1.0319	0.039*
C15	0.18214 (16)	0.84974 (14)	0.89877 (13)	0.0336 (3)
H15	0.1470	0.9204	0.9447	0.040*
C16	0.22895 (14)	0.87466 (12)	0.78070 (12)	0.0274 (3)
H16	0.2271	0.9617	0.7469	0.033*
C17	0.29837 (13)	0.87077 (11)	0.49672 (11)	0.0220 (2)
C18	0.34955 (14)	0.95120 (12)	0.30445 (12)	0.0277 (3)
H18	0.4052	0.9520	0.2356	0.033*
C19	0.24158 (14)	1.03965 (12)	0.30177 (12)	0.0281 (3)
H19	0.2233	1.1016	0.2342	0.034*
C20	0.16165 (14)	1.03296 (12)	0.40278 (12)	0.0271 (3)
H20	0.0840	1.0901	0.4020	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0200 (5)	0.0288 (5)	0.0229 (5)	0.0082 (4)	0.0084 (4)	0.0053 (4)
N2	0.0250 (5)	0.0245 (5)	0.0232 (5)	0.0057 (4)	0.0090 (4)	0.0032 (4)
N3	0.0237 (5)	0.0303 (5)	0.0251 (5)	0.0093 (4)	0.0068 (4)	0.0043 (4)
N4	0.0280 (5)	0.0276 (5)	0.0273 (5)	0.0120 (4)	0.0134 (4)	0.0068 (4)
N5	0.0250 (5)	0.0288 (5)	0.0260 (5)	0.0065 (4)	0.0102 (4)	0.0052 (4)
N6	0.0223 (5)	0.0262 (5)	0.0260 (5)	0.0066 (4)	0.0062 (4)	0.0031 (4)
C1	0.0246 (5)	0.0192 (5)	0.0215 (5)	0.0043 (4)	0.0086 (4)	0.0019 (4)
C2	0.0239 (6)	0.0279 (6)	0.0260 (6)	0.0052 (5)	0.0055 (5)	0.0043 (5)
C3	0.0364 (7)	0.0325 (7)	0.0221 (6)	0.0062 (5)	0.0054 (5)	0.0046 (5)
C4	0.0393 (7)	0.0294 (6)	0.0262 (6)	0.0035 (5)	0.0159 (5)	0.0041 (5)
C5	0.0273 (6)	0.0255 (6)	0.0319 (7)	0.0025 (5)	0.0140 (5)	0.0014 (5)
C6	0.0230 (5)	0.0241 (6)	0.0232 (6)	0.0032 (4)	0.0063 (4)	0.0007 (4)
C7	0.0208 (5)	0.0207 (5)	0.0206 (5)	0.0022 (4)	0.0055 (4)	−0.0003 (4)
C8	0.0319 (6)	0.0291 (6)	0.0220 (6)	0.0050 (5)	0.0107 (5)	0.0036 (5)
C9	0.0345 (7)	0.0394 (7)	0.0246 (6)	0.0114 (6)	0.0061 (5)	0.0114 (5)
C10	0.0263 (6)	0.0364 (7)	0.0317 (7)	0.0122 (5)	0.0055 (5)	0.0073 (5)

C11	0.0182 (5)	0.0257 (6)	0.0228 (6)	0.0043 (4)	0.0060 (4)	0.0035 (4)
C12	0.0245 (6)	0.0243 (6)	0.0259 (6)	0.0054 (4)	0.0080 (5)	0.0010 (5)
C13	0.0299 (6)	0.0269 (6)	0.0294 (6)	0.0042 (5)	0.0096 (5)	0.0075 (5)
C14	0.0363 (7)	0.0406 (7)	0.0259 (6)	0.0105 (6)	0.0160 (5)	0.0087 (5)
C15	0.0417 (7)	0.0368 (7)	0.0295 (7)	0.0172 (6)	0.0166 (6)	0.0036 (5)
C16	0.0328 (6)	0.0253 (6)	0.0275 (6)	0.0097 (5)	0.0104 (5)	0.0048 (5)
C17	0.0199 (5)	0.0228 (6)	0.0232 (6)	0.0025 (4)	0.0060 (4)	0.0017 (4)
C18	0.0291 (6)	0.0300 (6)	0.0254 (6)	0.0028 (5)	0.0102 (5)	0.0049 (5)
C19	0.0329 (6)	0.0254 (6)	0.0257 (6)	0.0047 (5)	0.0054 (5)	0.0074 (5)
C20	0.0268 (6)	0.0257 (6)	0.0287 (6)	0.0082 (5)	0.0042 (5)	0.0019 (5)

Geometric parameters (Å, °)

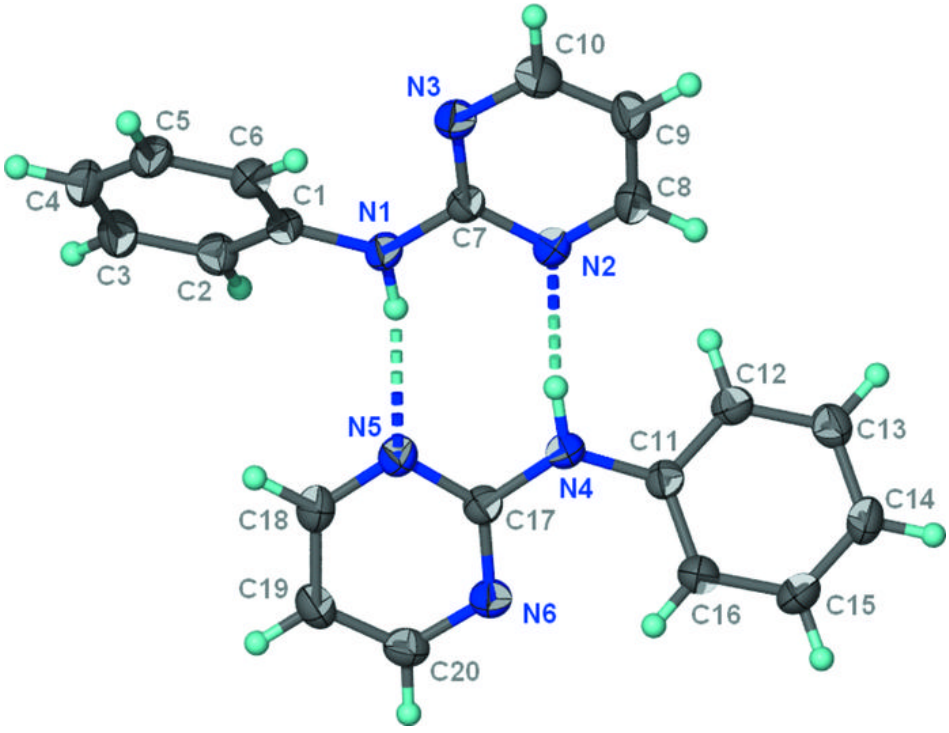
N1—C7	1.3613 (14)	C5—H5	0.9500
N1—C1	1.4090 (14)	C6—H6	0.9500
N1—H1	0.892 (9)	C8—C9	1.3829 (17)
N2—C8	1.3294 (15)	C8—H8	0.9500
N2—C7	1.3555 (14)	C9—C10	1.3819 (17)
N3—C10	1.3322 (15)	C9—H9	0.9500
N3—C7	1.3423 (14)	C10—H10	0.9500
N4—C17	1.3584 (15)	C11—C16	1.3950 (16)
N4—C11	1.4093 (14)	C11—C12	1.3963 (16)
N4—H4	0.894 (8)	C12—C13	1.3831 (16)
N5—C18	1.3339 (15)	C12—H12	0.9500
N5—C17	1.3570 (14)	C13—C14	1.3859 (17)
N6—C20	1.3338 (15)	C13—H13	0.9500
N6—C17	1.3407 (14)	C14—C15	1.3818 (18)
C1—C6	1.3949 (15)	C14—H14	0.9500
C1—C2	1.3958 (16)	C15—C16	1.3883 (17)
C2—C3	1.3873 (16)	C15—H15	0.9500
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.3903 (18)	C18—C19	1.3824 (17)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.3839 (18)	C19—C20	1.3824 (17)
C4—H4A	0.9500	C19—H19	0.9500
C5—C6	1.3860 (16)	C20—H20	0.9500
C7—N1—C1	128.19 (9)	C10—C9—H9	121.9
C7—N1—H1	114.6 (10)	C8—C9—H9	121.9
C1—N1—H1	117.0 (10)	N3—C10—C9	122.94 (11)
C8—N2—C7	115.61 (10)	N3—C10—H10	118.5
C10—N3—C7	116.06 (10)	C9—C10—H10	118.5
C17—N4—C11	129.13 (10)	C16—C11—C12	119.15 (10)
C17—N4—H4	115.5 (9)	C16—C11—N4	124.17 (10)
C11—N4—H4	115.4 (9)	C12—C11—N4	116.58 (10)
C18—N5—C17	115.71 (10)	C13—C12—C11	120.91 (11)
C20—N6—C17	115.97 (10)	C13—C12—H12	119.5
C6—C1—C2	119.10 (10)	C11—C12—H12	119.5
C6—C1—N1	123.56 (10)	C12—C13—C14	119.88 (11)
C2—C1—N1	117.30 (10)	C12—C13—H13	120.1

C3—C2—C1	120.70 (11)	C14—C13—H13	120.1
C3—C2—H2	119.7	C15—C14—C13	119.35 (11)
C1—C2—H2	119.7	C15—C14—H14	120.3
C2—C3—C4	120.04 (11)	C13—C14—H14	120.3
C2—C3—H3	120.0	C14—C15—C16	121.49 (11)
C4—C3—H3	120.0	C14—C15—H15	119.3
C5—C4—C3	119.13 (11)	C16—C15—H15	119.3
C5—C4—H4A	120.4	C15—C16—C11	119.20 (11)
C3—C4—H4A	120.4	C15—C16—H16	120.4
C4—C5—C6	121.39 (11)	C11—C16—H16	120.4
C4—C5—H5	119.3	N6—C17—N5	125.94 (11)
C6—C5—H5	119.3	N6—C17—N4	119.51 (10)
C5—C6—C1	119.59 (11)	N5—C17—N4	114.55 (10)
C5—C6—H6	120.2	N5—C18—C19	122.92 (11)
C1—C6—H6	120.2	N5—C18—H18	118.5
N3—C7—N2	125.92 (10)	C19—C18—H18	118.5
N3—C7—N1	119.10 (10)	C18—C19—C20	116.34 (11)
N2—C7—N1	114.96 (10)	C18—C19—H19	121.8
N2—C8—C9	123.22 (11)	C20—C19—H19	121.8
N2—C8—H8	118.4	N6—C20—C19	123.03 (11)
C9—C8—H8	118.4	N6—C20—H20	118.5
C10—C9—C8	116.22 (11)	C19—C20—H20	118.5
C7—N1—C1—C6	−31.08 (18)	C17—N4—C11—C16	−28.92 (18)
C7—N1—C1—C2	151.47 (11)	C17—N4—C11—C12	154.69 (11)
C6—C1—C2—C3	1.23 (17)	C16—C11—C12—C13	0.54 (17)
N1—C1—C2—C3	178.80 (10)	N4—C11—C12—C13	177.12 (10)
C1—C2—C3—C4	0.81 (18)	C11—C12—C13—C14	0.15 (18)
C2—C3—C4—C5	−1.85 (18)	C12—C13—C14—C15	−0.37 (19)
C3—C4—C5—C6	0.85 (18)	C13—C14—C15—C16	−0.1 (2)
C4—C5—C6—C1	1.19 (17)	C14—C15—C16—C11	0.8 (2)
C2—C1—C6—C5	−2.21 (17)	C12—C11—C16—C15	−1.00 (18)
N1—C1—C6—C5	−179.62 (10)	N4—C11—C16—C15	−177.30 (11)
C10—N3—C7—N2	−1.59 (17)	C20—N6—C17—N5	−2.37 (17)
C10—N3—C7—N1	−179.97 (10)	C20—N6—C17—N4	178.70 (10)
C8—N2—C7—N3	1.75 (16)	C18—N5—C17—N6	3.36 (17)
C8—N2—C7—N1	−179.81 (10)	C18—N5—C17—N4	−177.67 (10)
C1—N1—C7—N3	−3.22 (17)	C11—N4—C17—N6	−3.96 (18)
C1—N1—C7—N2	178.23 (10)	C11—N4—C17—N5	176.99 (11)
C7—N2—C8—C9	−0.28 (17)	C17—N5—C18—C19	−1.45 (17)
N2—C8—C9—C10	−1.14 (19)	N5—C18—C19—C20	−1.09 (18)
C7—N3—C10—C9	−0.06 (18)	C17—N6—C20—C19	−0.57 (17)
C8—C9—C10—N3	1.3 (2)	C18—C19—C20—N6	2.18 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N5	0.89 (1)	2.10 (1)	2.972 (1)	164 (1)
N4—H4···N2	0.89 (1)	2.15 (1)	3.020 (1)	165 (1)

Fig. 1


C10
N3
C5
C6
C9
C4
C1
C8
N1
C7
C3
C2
N2
C12
N5
C13
C11
N4
C14
C18
C17
C19
N6
C16
C15
C20