Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(Pyrazin-2-yl)aniline

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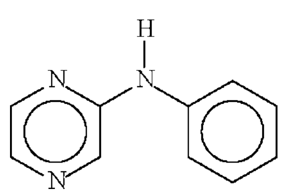
Received 10 September 2008; accepted 4 October 2008

Key indicators: single-crystal X-ray study; *T* = 100 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.041; *wR* factor = 0.101; data-to-parameter ratio = 15.9.

The two aromatic rings in the title compound, $C_{10}H_9N_3$, are inclined at 15.2 (1)° to each other; this opens up the angle at the amino N atom to 130.4 (1)°. The amino N atom forms a hydrogen bond to the 4-N atom of an adjacent molecule to create a chain motif.

Related literature

For the structure of aminopyrazine, see: Chao *et al.* (1976). For the structure of 2-pyrazinyl-*N*-2-nitrophenylaniline; see: Parsons *et al.* (2006).



Experimental

Crystal data

$C_{10}H_9N_3$
M_r = 171.20
Monoclinic, $P2_1/c$
a = 11.0644 (3) Å
b = 7.8423 (3) Å
c = 10.8907 (3) Å
β = 116.439 (2)°
V = 846.15 (5) Å^3
Z = 4
Mo *K*α radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.20 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
5664 measured reflections
1934 independent reflections
1463 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.101
S = 1.03
1934 reflections
122 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 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···N2^i	0.89 (1)	2.12 (1)	2.977 (2)	162 (1)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

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).

The authors thank the University of Malaya for supporting this study (grant Nos. FS 358/2008A and FA 067/2006A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2121).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chao, M., Schempp, E. & Rosenstein, R. D. (1976). *Acta Cryst.* B**32**, 288–290.
Parsons, S., Wharton, S., McNab, H., Parkin, A. & Johnstone, R. (2006). Private communication (Deposition No. 610410). CCDC, Union Road, Cambridge, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2008). E**64**, o2105 [**doi:10.1107/S1600536808031942**]

N-(Pyrazin-2-yl)aniline

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Comment

There are few structural examples of pyrazine compounds having an amino substituent; these are limited to, for example, aminopyrazine (Chao *et al.*, 1976) and pyrazinyl-*N*-2-nitrophenylaniline (Parsons *et al.*, 2006). In the title compound (Scheme I, Fig. 1), the two aromatic rings are aligned at 15.2 (1)°; these open up the angle at the amino nitrogen to 130.4 (1) °. The amino nitrogen forms a hydrogen bond to the 4-nitrogen atom of an adjacent molecule to furnish a chain motif.

Experimental

Chloropyrazine (1 ml, 1.1 mmol) and aniline (1 ml, 1.1 mmol) were heated at 423–433 K for 3 h. The solid was dissolved in water. The compound was extracted with ether. The ether extract was dried over sodium sulfate; evaporation of the solvent gave a colorless crystals among some unidentified dark brown materials.

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) fixed at 1.2*U*(C). The amino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N—H 0.88 (1) Å.

Figures

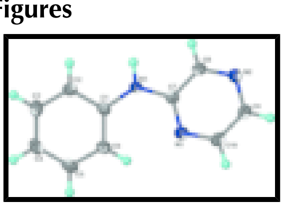

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{10}H_9N_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(pyrazin-2-yl)aniline

Crystal data

$C_{10}H_9N_3$	F_{000} = 360
M_r = 171.20	D_x = 1.344 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3723 reflections
a = 11.0644 (3) Å	θ = 3.3–26.4°
b = 7.8423 (3) Å	μ = 0.09 mm^{-1}
c = 10.8907 (3) Å	*T* = 100 (2) K

β = 116.439 (2)°	Prism, colourless
V = 846.15 (5) Å^3	0.20 × 0.10 × 0.05 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	1463 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.033
Monochromator: graphite	θ_{max} = 27.5°
T = 100(2) K	θ_{min} = 3.3°
ω scans	$h = -14 \rightarrow 14$
Absorption correction: none	$k = -10 \rightarrow 10$
5664 measured reflections	$l = -14 \rightarrow 14$
1934 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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.101	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.247P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
1934 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
122 parameters	$\Delta\rho_{min}$ = −0.23 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}
N1	0.36080 (11)	0.49391 (15)	0.56127 (12)	0.0188 (3)
H1	0.4485 (9)	0.479 (2)	0.6153 (13)	0.024 (4)*
N2	0.36741 (11)	0.89784 (15)	0.72193 (11)	0.0205 (3)
N3	0.18404 (11)	0.69151 (16)	0.51024 (12)	0.0221 (3)
C1	0.29407 (14)	0.36077 (18)	0.46992 (13)	0.0181 (3)
C2	0.37632 (14)	0.23785 (18)	0.45198 (14)	0.0201 (3)
H2	0.4717	0.2479	0.5007	0.024*
C3	0.32046 (15)	0.1019 (2)	0.36410 (15)	0.0246 (3)
H3	0.3775	0.0188	0.3534	0.029*
C4	0.18124 (15)	0.0862 (2)	0.29138 (15)	0.0255 (3)
H4	0.1427	−0.0058	0.2293	0.031*
C5	0.09930 (14)	0.20604 (19)	0.31037 (14)	0.0235 (3)
H5	0.0040	0.1948	0.2617	0.028*

C6	0.15425 (14)	0.34292 (18)	0.39962 (14)	0.0204 (3)
H6	0.0969	0.4236	0.4125	0.025*
C7	0.31216 (13)	0.64466 (17)	0.58462 (13)	0.0174 (3)
C8	0.40342 (13)	0.74982 (17)	0.69058 (14)	0.0184 (3)
H8	0.4941	0.7127	0.7412	0.022*
C9	0.23812 (14)	0.94629 (19)	0.64641 (14)	0.0232 (3)
H9	0.2078	1.0522	0.6649	0.028*
C10	0.14961 (14)	0.84350 (19)	0.54274 (15)	0.0245 (3)
H10	0.0594	0.8820	0.4914	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0140 (6)	0.0182 (6)	0.0186 (6)	0.0013 (5)	0.0023 (5)	−0.0019 (5)
N2	0.0201 (6)	0.0197 (6)	0.0210 (6)	−0.0006 (5)	0.0085 (5)	−0.0008 (5)
N3	0.0182 (6)	0.0214 (7)	0.0220 (6)	0.0020 (5)	0.0048 (5)	−0.0008 (5)
C1	0.0201 (7)	0.0171 (7)	0.0147 (6)	−0.0012 (5)	0.0057 (5)	0.0009 (5)
C2	0.0176 (7)	0.0223 (8)	0.0194 (7)	−0.0005 (6)	0.0074 (6)	0.0000 (6)
C3	0.0285 (8)	0.0227 (8)	0.0257 (8)	−0.0008 (6)	0.0150 (6)	−0.0045 (6)
C4	0.0286 (8)	0.0236 (8)	0.0233 (7)	−0.0072 (6)	0.0108 (6)	−0.0075 (6)
C5	0.0197 (7)	0.0251 (8)	0.0214 (7)	−0.0047 (6)	0.0051 (6)	−0.0003 (6)
C6	0.0189 (7)	0.0197 (7)	0.0194 (7)	−0.0005 (6)	0.0056 (6)	0.0008 (6)
C7	0.0180 (7)	0.0175 (7)	0.0164 (7)	−0.0003 (5)	0.0073 (5)	0.0019 (5)
C8	0.0155 (6)	0.0193 (7)	0.0187 (7)	0.0006 (5)	0.0060 (5)	0.0019 (5)
C9	0.0215 (7)	0.0211 (7)	0.0250 (7)	0.0039 (6)	0.0087 (6)	−0.0015 (6)
C10	0.0191 (7)	0.0237 (8)	0.0266 (8)	0.0058 (6)	0.0065 (6)	−0.0001 (6)

Geometric parameters (Å, °)

N1—C7	1.3689 (17)	C3—H3	0.9500
N1—C1	1.4039 (17)	C4—C5	1.384 (2)
N1—H1	0.891 (9)	C4—H4	0.9500
N2—C8	1.3207 (18)	C5—C6	1.393 (2)
N2—C9	1.3488 (17)	C5—H5	0.9500
N3—C7	1.3335 (17)	C6—H6	0.9500
N3—C10	1.3458 (19)	C7—C8	1.4120 (19)
C1—C6	1.3944 (18)	C8—H8	0.9500
C1—C2	1.3978 (19)	C9—C10	1.378 (2)
C2—C3	1.381 (2)	C9—H9	0.9500
C2—H2	0.9500	C10—H10	0.9500
C3—C4	1.389 (2)		
C7—N1—C1	130.38 (12)	C4—C5—H5	119.5
C7—N1—H1	113.3 (10)	C6—C5—H5	119.5
C1—N1—H1	116.3 (10)	C5—C6—C1	119.56 (13)
C8—N2—C9	116.75 (12)	C5—C6—H6	120.2
C7—N3—C10	115.67 (12)	C1—C6—H6	120.2
C6—C1—C2	119.09 (13)	N3—C7—N1	121.64 (12)
C6—C1—N1	124.65 (13)	N3—C7—C8	121.03 (12)

C2—C1—N1	116.25 (12)	N1—C7—C8	117.32 (12)
C3—C2—C1	120.72 (13)	N2—C8—C7	122.44 (12)
C3—C2—H2	119.6	N2—C8—H8	118.8
C1—C2—H2	119.6	C7—C8—H8	118.8
C2—C3—C4	120.26 (14)	N2—C9—C10	120.58 (13)
C2—C3—H3	119.9	N2—C9—H9	119.7
C4—C3—H3	119.9	C10—C9—H9	119.7
C5—C4—C3	119.26 (14)	N3—C10—C9	123.53 (13)
C5—C4—H4	120.4	N3—C10—H10	118.2
C3—C4—H4	120.4	C9—C10—H10	118.2
C4—C5—C6	121.08 (13)		

C7—N1—C1—C6	−12.7 (2)	C10—N3—C7—N1	−179.30 (12)
C7—N1—C1—C2	168.41 (13)	C10—N3—C7—C8	0.36 (19)
C6—C1—C2—C3	1.1 (2)	C1—N1—C7—N3	−4.2 (2)
N1—C1—C2—C3	−179.89 (12)	C1—N1—C7—C8	176.09 (13)
C1—C2—C3—C4	0.5 (2)	C9—N2—C8—C7	−0.73 (19)
C2—C3—C4—C5	−1.5 (2)	N3—C7—C8—N2	0.3 (2)
C3—C4—C5—C6	0.9 (2)	N1—C7—C8—N2	−179.99 (12)
C4—C5—C6—C1	0.7 (2)	C8—N2—C9—C10	0.4 (2)
C2—C1—C6—C5	−1.7 (2)	C7—N3—C10—C9	−0.7 (2)
N1—C1—C6—C5	179.40 (13)	N2—C9—C10—N3	0.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.89 (1)	2.12 (1)	2.977 (2)	162 (1)

Symmetry codes: (i) $-x+1, y-1/2, -z+3/2$.

Fig. 1