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N-(Pyrazin-2-yl)aniline

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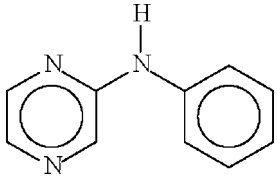
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 15.9.

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 $K\alpha$ 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).

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

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supporting information

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

N-(Pyrazin-2-yl)aniline

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S1. 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.

S2. 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.

S3. 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.

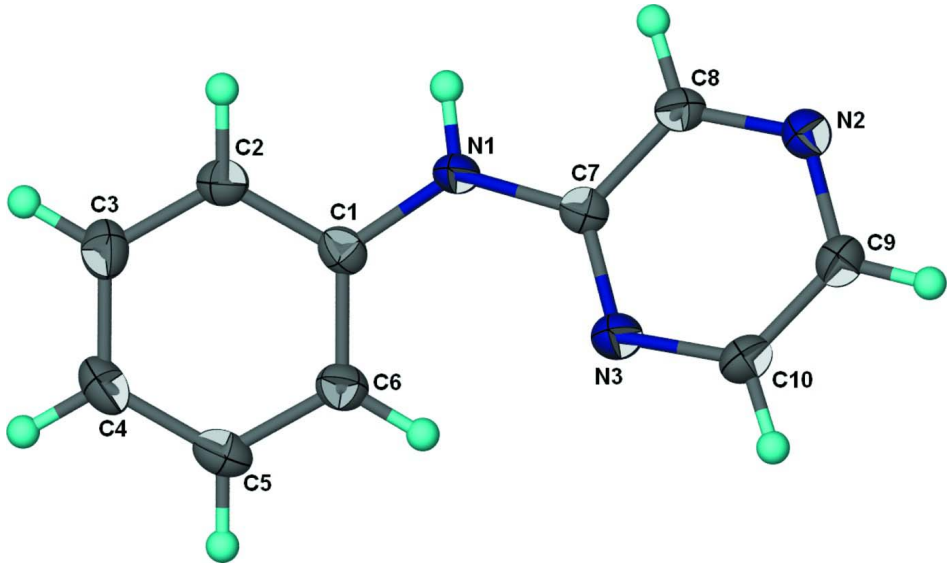

Figure 1

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

$C_{10}H_9N_3$
$M_r = 171.20$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.0644\ (3)$ Å
$b = 7.8423\ (3)$ Å
$c = 10.8907\ (3)$ Å
$\beta = 116.439\ (2)°$
$V = 846.15\ (5)$ Å^3
$Z = 4$

$F(000) = 360$
$D_x = 1.344$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3723 reflections
$\theta = 3.3–26.4°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Prism, colourless
0.20 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
5664 measured reflections
1934 independent reflections

1463 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -14\rightarrow14$
$k = -10\rightarrow10$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.101$
$S = 1.03$
1934 reflections
122 parameters
1 restraint

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.247P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	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 (Å²)

	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, º)

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, º)

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*−1/2, −*z*+3/2.