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N-(Pyrazin-2-yl)aniline

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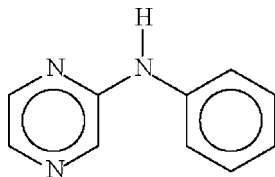
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 15.9.

 The two aromatic rings in the title compound, $\text{C}_{10}\text{H}_9\text{N}_3$, are inclined at $15.2(1)^\circ$ to each other; this opens up the angle at the amino N atom to $130.4(1)^\circ$. 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

 $\text{C}_{10}\text{H}_9\text{N}_3$
 $M_r = 171.20$
 Monoclinic, $P2_1/c$
 $a = 11.0644(3)$ Å

 $b = 7.8423(3)$ Å
 $c = 10.8907(3)$ Å
 $\beta = 116.439(2)^\circ$
 $V = 846.15(5)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 100(2)$ K
 $0.20 \times 0.10 \times 0.05$ mm

Data collection

 Bruker SMART APEX
 diffractometer
 Absorption correction: none
 5664 measured reflections

 1934 independent reflections
 1463 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

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

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{N2}^i$	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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supplementary materials

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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 $U(\text{H})$ fixed at $1.2U(\text{C})$. 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

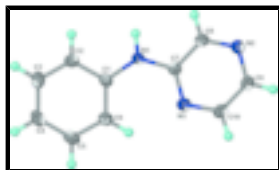


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $\text{C}_{10}\text{H}_9\text{N}_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(pyrazin-2-yl)aniline

Crystal data

$\text{C}_{10}\text{H}_9\text{N}_3$

$M_r = 171.20$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.0644$ (3) Å

$b = 7.8423$ (3) Å

$c = 10.8907$ (3) Å

$F_{000} = 360$

$D_x = 1.344$ 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

$T = 100$ (2) K

supplementary materials

$\beta = 116.439 (2)^\circ$
 $V = 846.15 (5) \text{ \AA}^3$
 $Z = 4$

Prism, colourless
 $0.20 \times 0.10 \times 0.05 \text{ mm}$

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 100(2) \text{ K}$
 ω scans
Absorption correction: none
5664 measured reflections
1934 independent reflections

1463 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\text{max}} = 27.5^\circ$
 $\theta_{\text{min}} = 3.3^\circ$
 $h = -14 \rightarrow 14$
 $k = -10 \rightarrow 10$
 $l = -14 \rightarrow 14$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^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 (\AA , $^\circ$)

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)

supplementary materials

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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots 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

