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## A second monoclinic polymorph of *N*-(pyrazin-2-yl)aniline

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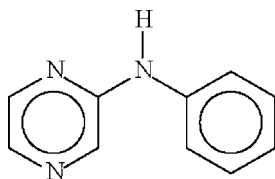
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  
 $R$  factor = 0.042;  $wR$  factor = 0.113; data-to-parameter ratio = 15.8.

The two aromatic rings in the title compound,  $\text{C}_{10}\text{H}_9\text{N}_3$ , are aligned at  $23.4(1)^\circ$  and the bridging  $\text{C}-\text{N}-\text{C}$  angle is  $128.9(1)^\circ$ . In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds result in a chain motif, the repeat distance of which is half the  $b$  axial length of 8.8851 (3) Å.

### Related literature

In the  $P2_1/c$  modification, the aromatic rings are aligned at  $15.2(1)^\circ$ , and the repeat distance of the helical chain is half the  $b$ -axial length of 7.8423 (3) Å; see: Wan Saffiee *et al.* (2008).



### Experimental

#### Crystal data

$\text{C}_{10}\text{H}_9\text{N}_3$   
 $M_r = 171.20$   
Monoclinic,  $P2_1/n$

$a = 8.2194(3)$  Å  
 $b = 8.8851(3)$  Å  
 $c = 11.8395(4)$  Å

$\beta = 104.643(2)^\circ$   
 $V = 836.56(5)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation

$\mu = 0.09$  mm<sup>-1</sup>  
 $T = 100(2)$  K  
 $0.25 \times 0.05 \times 0.03$  mm

#### Data collection

Bruker SMART APEX  
diffractometer  
Absorption correction: none  
7621 measured reflections

1922 independent reflections  
1389 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.113$   
 $S = 1.03$   
1922 reflections  
122 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{N3}^i$	0.90 (2)	2.17 (2)	3.062 (2)	175 (2)

Symmetry code: (i)  $-x + \frac{5}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ .

Data collection: *APEX2* (Bruker, 2007); cell refinement: *S SAINT* (Bruker, 2007); data reduction: *S 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: PK2124).

### References

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**supplementary materials**

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## A second monoclinic polymorph of *N*-(pyrazin-2-yl)aniline

Z. Abdullah and S. W. Ng

### Comment

The cell dimensions of the reported monoclinic  $P2_1/c$  modification are:  $a = 10.0644$  (3),  $b = 7.8423$  (3),  $c = 10.8907$  (3) Å;  $\beta = 116.439$  (2)° (Wan Saffie *et al.*, 2008). The cell dimensions of the present modification (Scheme I, Fig. 1), after transformation to the standard  $P2_1/c$  setting, are:  $a = 8.2194$  (3),  $b = 8.8851$  (3),  $c = 12.5909$  (4) Å,  $\beta = 114.525$  (2)°.

### Experimental

The  $P2_1/c$  modification of 2-pyrazinyl-*N*-aniline (0.10 g, 0.4 mmol), zinc acetate (0.09 g, 0.4 mmol) and water (18 ml) were heated in a 23-ml Teflon-lined Parr bomb at 403 K for 2 days. The bomb was cooled to room temperature at 5 K min<sup>-1</sup>. Several faint yellow prisms were picked out manually from the cool solution.

### 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 freely refined.

### Figures

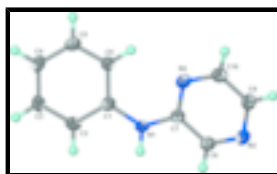


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of  $\text{C}_{10}\text{H}_9\text{N}_3$  at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

### *N*-(pyrazin-2-yl)aniline

#### Crystal data

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

$M_r = 171.20$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 8.2194$  (3) Å

$b = 8.8851$  (3) Å

$c = 11.8395$  (4) Å

$\beta = 104.643$  (2)°

$F_{000} = 360$

$D_x = 1.359$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 1282 reflections

$\theta = 2.7\text{--}26.1^\circ$

$\mu = 0.09$  mm<sup>-1</sup>

$T = 100$  (2) K

Prism, pale yellow

# supplementary materials

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$V = 836.56 (5) \text{ \AA}^3$   
 $Z = 4$

$0.25 \times 0.05 \times 0.03 \text{ mm}$

## Data collection

Bruker SMART APEX diffractometer	1389 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.045$
Monochromator: graphite	$\theta_{\text{max}} = 27.5^\circ$
$T = 100(2) \text{ K}$	$\theta_{\text{min}} = 2.7^\circ$
$\omega$ scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -11 \rightarrow 11$
7621 measured reflections	$l = -15 \rightarrow 14$
1922 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
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.1331P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
1922 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
122 parameters	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
	Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	1.00115 (16)	0.42084 (14)	0.63143 (11)	0.0216 (3)
H1	1.103 (2)	0.377 (2)	0.6527 (15)	0.035 (5)*
N2	0.84988 (15)	0.63197 (14)	0.66840 (11)	0.0230 (3)
N3	1.15770 (16)	0.76478 (14)	0.78284 (11)	0.0228 (3)
C1	0.86787 (18)	0.33136 (16)	0.56827 (12)	0.0193 (3)
C2	0.89595 (19)	0.17682 (17)	0.56499 (13)	0.0254 (4)
H2	1.0021	0.1367	0.6049	0.030*
C3	0.7717 (2)	0.08147 (17)	0.50462 (14)	0.0264 (4)
H3	0.7933	-0.0235	0.5030	0.032*
C4	0.61582 (19)	0.13750 (17)	0.44633 (13)	0.0232 (3)
H4	0.5296	0.0717	0.4058	0.028*
C5	0.58777 (19)	0.29106 (17)	0.44814 (13)	0.0222 (3)
H5	0.4815	0.3305	0.4079	0.027*
C6	0.71238 (18)	0.38836 (16)	0.50783 (13)	0.0211 (3)
H6	0.6916	0.4936	0.5074	0.025*

C7	0.99583 (18)	0.56191 (16)	0.67668 (13)	0.0192 (3)
C8	1.14967 (18)	0.63040 (16)	0.73478 (13)	0.0213 (3)
H8	1.2514	0.5772	0.7393	0.026*
C9	1.00948 (18)	0.83515 (18)	0.77382 (13)	0.0248 (4)
H9	1.0085	0.9325	0.8069	0.030*
C10	0.8604 (2)	0.76892 (17)	0.71788 (14)	0.0254 (4)
H10	0.7592	0.8226	0.7139	0.030*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0144 (7)	0.0200 (7)	0.0276 (7)	0.0019 (5)	0.0003 (5)	-0.0014 (5)
N2	0.0173 (6)	0.0230 (7)	0.0272 (7)	0.0004 (5)	0.0027 (5)	-0.0036 (5)
N3	0.0195 (7)	0.0228 (7)	0.0251 (7)	-0.0033 (5)	0.0037 (5)	-0.0011 (5)
C1	0.0180 (7)	0.0205 (7)	0.0193 (7)	-0.0010 (6)	0.0048 (6)	-0.0009 (6)
C2	0.0217 (8)	0.0227 (8)	0.0289 (8)	0.0040 (6)	0.0012 (6)	0.0000 (6)
C3	0.0293 (9)	0.0176 (8)	0.0307 (9)	0.0005 (6)	0.0043 (7)	-0.0019 (6)
C4	0.0217 (8)	0.0233 (8)	0.0244 (8)	-0.0059 (6)	0.0053 (6)	-0.0035 (6)
C5	0.0173 (7)	0.0251 (8)	0.0229 (8)	0.0005 (6)	0.0026 (6)	-0.0006 (6)
C6	0.0195 (8)	0.0190 (7)	0.0237 (8)	0.0005 (6)	0.0031 (6)	-0.0011 (6)
C7	0.0175 (7)	0.0198 (7)	0.0194 (7)	0.0004 (6)	0.0030 (6)	0.0020 (6)
C8	0.0177 (7)	0.0224 (8)	0.0233 (8)	-0.0001 (6)	0.0041 (6)	0.0015 (6)
C9	0.0228 (8)	0.0220 (8)	0.0284 (8)	-0.0016 (6)	0.0047 (6)	-0.0049 (6)
C10	0.0202 (8)	0.0241 (8)	0.0307 (9)	0.0032 (6)	0.0043 (6)	-0.0041 (7)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

N1—C7	1.3681 (19)	C3—H3	0.9500
N1—C1	1.4061 (19)	C4—C5	1.385 (2)
N1—H1	0.897 (18)	C4—H4	0.9500
N2—C7	1.3330 (18)	C5—C6	1.389 (2)
N2—C10	1.3438 (19)	C5—H5	0.9500
N3—C8	1.3171 (19)	C6—H6	0.9500
N3—C9	1.3494 (19)	C7—C8	1.415 (2)
C1—C6	1.393 (2)	C8—H8	0.9500
C1—C2	1.395 (2)	C9—C10	1.370 (2)
C2—C3	1.379 (2)	C9—H9	0.9500
C2—H2	0.9500	C10—H10	0.9500
C3—C4	1.385 (2)		
C7—N1—C1	128.94 (13)	C4—C5—H5	119.4
C7—N1—H1	114.0 (12)	C6—C5—H5	119.4
C1—N1—H1	116.7 (11)	C5—C6—C1	119.86 (14)
C7—N2—C10	115.67 (13)	C5—C6—H6	120.1
C8—N3—C9	116.12 (13)	C1—C6—H6	120.1
C6—C1—C2	118.72 (13)	N2—C7—N1	121.09 (13)
C6—C1—N1	123.92 (13)	N2—C7—C8	120.79 (13)
C2—C1—N1	117.35 (13)	N1—C7—C8	118.11 (13)
C3—C2—C1	120.88 (14)	N3—C8—C7	122.74 (13)

## supplementary materials

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C3—C2—H2	119.6	N3—C8—H8	118.6
C1—C2—H2	119.6	C7—C8—H8	118.6
C2—C3—C4	120.52 (14)	N3—C9—C10	121.23 (14)
C2—C3—H3	119.7	N3—C9—H9	119.4
C4—C3—H3	119.7	C10—C9—H9	119.4
C5—C4—C3	118.88 (14)	N2—C10—C9	123.44 (14)
C5—C4—H4	120.6	N2—C10—H10	118.3
C3—C4—H4	120.6	C9—C10—H10	118.3
C4—C5—C6	121.11 (14)		
C7—N1—C1—C6	21.9 (2)	C10—N2—C7—N1	178.88 (14)
C7—N1—C1—C2	-159.27 (15)	C10—N2—C7—C8	0.2 (2)
C6—C1—C2—C3	-1.0 (2)	C1—N1—C7—N2	2.9 (2)
N1—C1—C2—C3	-179.81 (14)	C1—N1—C7—C8	-178.36 (14)
C1—C2—C3—C4	-0.3 (2)	C9—N3—C8—C7	0.0 (2)
C2—C3—C4—C5	1.0 (2)	N2—C7—C8—N3	-0.2 (2)
C3—C4—C5—C6	-0.5 (2)	N1—C7—C8—N3	-178.92 (13)
C4—C5—C6—C1	-0.8 (2)	C8—N3—C9—C10	0.1 (2)
C2—C1—C6—C5	1.5 (2)	C7—N2—C10—C9	0.0 (2)
N1—C1—C6—C5	-179.75 (13)	N3—C9—C10—N2	-0.1 (2)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ N3 <sup>i</sup>	0.90 (2)	2.17 (2)	3.062 (2)	175 (2)

Symmetry codes: (i)  $-x+5/2, y-1/2, -z+3/2$ .

Fig. 1

