Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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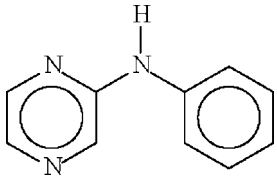
Received 23 September 2008; accepted 4 October 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.113; data-to-parameter ratio = 15.8.

The two aromatic rings in the title compound, $C_{10}H_9N_3$, are aligned at 23.4 (1)° and the bridging C—N—C angle is 128.9 (1)°. In the crystal structure, intermolecular N—H···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)°, 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

$C_{10}H_9N_3$
M_r = 171.20
Monoclinic, $P2_1/n$
a = 8.2194 (3) Å
b = 8.8851 (3) Å
c = 11.8395 (4) Å
β = 104.643 (2)°
V = 836.56 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.25 × 0.05 × 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_{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
$\Delta\rho_{max}$ = 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···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: *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: PK2124).

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Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o2106 [doi:10.1107/S1600536808031954]

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

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S1. 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; β = 116.439 (2)° (Wan Saffiee *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, β = 114.525 (2)°.

S2. 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^{-1}. Several faint yellow prisms were picked out manually from the cool solution.

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 freely refined.

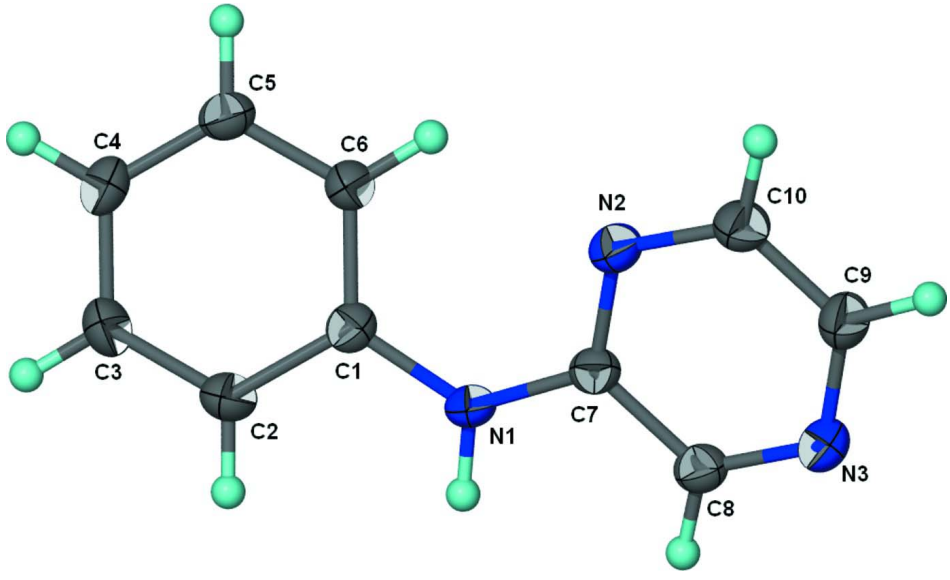

Figure 1

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, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.2194$ (3) Å
$b = 8.8851$ (3) Å
$c = 11.8395$ (4) Å
$\beta = 104.643$ (2)°
$V = 836.56$ (5) Å^3
$Z = 4$
$F(000) = 360$
$D_x = 1.359$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1282 reflections
$\theta = 2.7$–$26.1°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Prism, pale yellow
0.25 × 0.05 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
7621 measured reflections
1922 independent reflections
1389 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.113$
$S = 1.03$
1922 reflections
122 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.1331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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)
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.90 (2)	2.17 (2)	3.062 (2)	175 (2)

Symmetry code: (i) −*x*+5/2, *y*−1/2, −*z*+3/2.