

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

 4-Chloro-*N*-(pyrazin-2-yl)aniline

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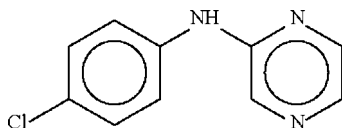
Received 4 December 2008; accepted 5 December 2008

 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.128; data-to-parameter ratio = 15.8.

In the title compound,  $\text{C}_{10}\text{H}_8\text{ClN}_3$ , the dihedral angle between the aromatic rings is  $43.0(1)^\circ$  and the bridging  $\text{C}-\text{N}-\text{C}$  angle is  $128.19(16)^\circ$ . The amino N atom of one molecule forms a hydrogen bond to the 1-N atom of an adjacent pyrazinyl ring, generating an inversion dimer.

## Related literature

For the two polymorphs of *N*-(pyrazin-2-yl)aniline, see: Wan Saffiee *et al.* (2008a); Abdullah & Ng (2008). For *N*-(pyrazin-2-yl)-4-toluidine; see: Wan Saffiee *et al.* (2008b).



## Experimental

## Crystal data

 $\text{C}_{10}\text{H}_8\text{ClN}_3$   
 $M_r = 205.64$   
 Monoclinic,  $P2_1/c$   
 $a = 12.1257(3)$  Å  
 $b = 3.7944(1)$  Å  
 $c = 19.7242(5)$  Å  
 $\beta = 91.370(2)^\circ$ 
 $V = 907.25(4)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.38$  mm<sup>-1</sup>  
 $T = 100(2)$  K  
 $0.25 \times 0.05 \times 0.01$  mm

## Data collection

 Bruker SMART APEX  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.912$ ,  $T_{\max} = 0.996$ 

 7922 measured reflections  
 2073 independent reflections  
 1633 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.128$   
 $S = 1.14$   
 2073 reflections  
 131 parameters  
 1 restraint

 H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $\Delta\rho_{\max} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.28$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                          | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------------|----------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{N2}^i$ | 0.88 (1) | 2.15 (1)    | 3.023 (2)   | 171 (2)       |

 Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

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, 2009).

We thank the University of Malaya for supporting this study (FS205/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2340).

## References

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**supplementary materials**

*Acta Cryst.* (2009). E65, o113 [ doi:10.1107/S1600536808041172 ]

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

W. A. M. Wan Saffiee, A. Idris, Z. Aiyub, Z. Abdullah and S. W. Ng

### Comment

(type here to add)

### Experimental

2-Chloropyrazine (1.15 g, 10 mmol) and 4-chloroaniline (1.28 g, 10 mmol) were mixed with ethanol (2 ml) and the mixture heated at 423–433 K for 3 h. The product was dissolved in water and the solution extracted with ether. The ether phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped crystals along with some unidentified brown material.

### 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  $U(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C})$ .

The amino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N—H 0.88±0.01 Å; its temperature factor was freely refined.

### Figures

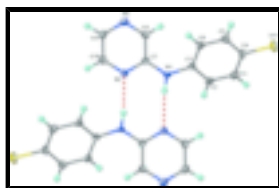


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of hydrogen-bonded dimeric structure of  $\text{C}_{10}\text{H}_8\text{ClN}_3$  at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Hydrogen bonds are shown as red dashed lines.

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

### Crystal data

$\text{C}_{10}\text{H}_8\text{ClN}_3$

$M_r = 205.64$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.1257 (3) \text{ \AA}$

$b = 3.7944 (1) \text{ \AA}$

$c = 19.7242 (5) \text{ \AA}$

$F_{000} = 424$

$D_x = 1.506 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2160 reflections

$\theta = 2.6\text{--}28.1^\circ$

$\mu = 0.38 \text{ mm}^{-1}$

$T = 100 (2) \text{ K}$

# supplementary materials

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$\beta = 91.370 (2)^\circ$  Plate, yellow  
 $V = 907.25 (4) \text{ \AA}^3$   $0.25 \times 0.05 \times 0.01 \text{ mm}$   
 $Z = 4$

## Data collection

|                                                             |                                        |
|-------------------------------------------------------------|----------------------------------------|
| Bruker SMART APEX diffractometer                            | 2073 independent reflections           |
| Radiation source: fine-focus sealed tube                    | 1633 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite                                     | $R_{\text{int}} = 0.033$               |
| $T = 100(2) \text{ K}$                                      | $\theta_{\text{max}} = 27.5^\circ$     |
| $\omega$ scans                                              | $\theta_{\text{min}} = 1.7^\circ$      |
| Absorption correction: Multi-scan (SADABS; Sheldrick, 1996) | $h = -15 \rightarrow 15$               |
| $T_{\text{min}} = 0.912$ , $T_{\text{max}} = 0.996$         | $k = -4 \rightarrow 4$                 |
| 7922 measured reflections                                   | $l = -25 \rightarrow 24$               |

## Refinement

|                                                                |                                                                        |
|----------------------------------------------------------------|------------------------------------------------------------------------|
| Refinement on $F^2$                                            | Secondary atom site location: difference Fourier map                   |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites               |
| $R[F^2 > 2\sigma(F^2)] = 0.037$                                | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.128$                                              | $w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.0551P]$                      |
| $S = 1.14$                                                     | where $P = (F_o^2 + 2F_c^2)/3$                                         |
| 2073 reflections                                               | $(\Delta/\sigma)_{\text{max}} = 0.001$                                 |
| 131 parameters                                                 | $\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$                    |
| 1 restraint                                                    | $\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$                   |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none                                            |

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

|     | <i>x</i>     | <i>y</i>      | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| C11 | 1.04801 (4)  | -0.07942 (15) | 0.36089 (3)  | 0.0269 (2)                       |
| N1  | 0.59098 (13) | 0.2944 (5)    | 0.43167 (8)  | 0.0173 (4)                       |
| H1  | 0.5832 (19)  | 0.359 (6)     | 0.4742 (6)   | 0.019 (6)*                       |
| N2  | 0.40848 (13) | 0.4535 (5)    | 0.42294 (8)  | 0.0152 (4)                       |
| N3  | 0.39085 (14) | 0.1755 (5)    | 0.29204 (8)  | 0.0182 (4)                       |
| C1  | 0.69716 (16) | 0.1986 (5)    | 0.41131 (10) | 0.0147 (4)                       |
| C2  | 0.76584 (16) | 0.0278 (5)    | 0.45861 (10) | 0.0165 (4)                       |
| H2  | 0.7381       | -0.0315       | 0.5018       | 0.020*                           |
| C3  | 0.87334 (16) | -0.0565 (5)   | 0.44384 (10) | 0.0181 (4)                       |
| H3  | 0.9196       | -0.1710       | 0.4766       | 0.022*                           |
| C4  | 0.91273 (16) | 0.0283 (5)    | 0.38059 (11) | 0.0173 (4)                       |
| C5  | 0.84635 (16) | 0.1980 (5)    | 0.33265 (10) | 0.0176 (4)                       |

|     |              |            |              |            |
|-----|--------------|------------|--------------|------------|
| H5  | 0.8745       | 0.2545     | 0.2894       | 0.021*     |
| C6  | 0.73893 (16) | 0.2849 (5) | 0.34796 (10) | 0.0155 (4) |
| H6  | 0.6935       | 0.4033     | 0.3154       | 0.019*     |
| C7  | 0.49564 (16) | 0.3053 (5) | 0.39334 (9)  | 0.0141 (4) |
| C8  | 0.48498 (16) | 0.1632 (5) | 0.32725 (10) | 0.0159 (4) |
| H8  | 0.5473       | 0.0556     | 0.3075       | 0.019*     |
| C9  | 0.30456 (17) | 0.3280 (6) | 0.32195 (10) | 0.0185 (4) |
| H9  | 0.2360       | 0.3451     | 0.2979       | 0.022*     |
| C10 | 0.31373 (16) | 0.4595 (5) | 0.38676 (10) | 0.0168 (4) |
| H10 | 0.2503       | 0.5588     | 0.4067       | 0.020*     |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C11 | 0.0139 (3)  | 0.0324 (3)  | 0.0346 (3)  | 0.0038 (2)  | 0.0035 (2)  | -0.0016 (2) |
| N1  | 0.0157 (8)  | 0.0266 (9)  | 0.0096 (8)  | 0.0025 (7)  | 0.0006 (6)  | -0.0028 (7) |
| N2  | 0.0154 (8)  | 0.0179 (8)  | 0.0124 (8)  | 0.0017 (6)  | 0.0004 (6)  | 0.0011 (6)  |
| N3  | 0.0190 (9)  | 0.0222 (9)  | 0.0134 (8)  | -0.0051 (7) | -0.0009 (6) | 0.0010 (7)  |
| C1  | 0.0134 (9)  | 0.0158 (9)  | 0.0148 (9)  | -0.0009 (7) | -0.0007 (7) | -0.0024 (7) |
| C2  | 0.0194 (10) | 0.0181 (10) | 0.0121 (9)  | -0.0008 (8) | -0.0014 (7) | 0.0000 (7)  |
| C3  | 0.0180 (10) | 0.0168 (10) | 0.0192 (10) | 0.0019 (8)  | -0.0039 (8) | 0.0009 (8)  |
| C4  | 0.0121 (9)  | 0.0178 (10) | 0.0219 (10) | -0.0001 (7) | 0.0004 (7)  | -0.0040 (8) |
| C5  | 0.0177 (10) | 0.0203 (10) | 0.0148 (9)  | -0.0034 (8) | 0.0028 (7)  | -0.0018 (8) |
| C6  | 0.0155 (9)  | 0.0166 (9)  | 0.0142 (9)  | -0.0008 (7) | -0.0017 (7) | 0.0005 (7)  |
| C7  | 0.0143 (9)  | 0.0154 (9)  | 0.0125 (9)  | -0.0014 (7) | 0.0003 (7)  | 0.0020 (7)  |
| C8  | 0.0164 (10) | 0.0186 (10) | 0.0129 (9)  | -0.0012 (8) | 0.0024 (7)  | -0.0008 (8) |
| C9  | 0.0154 (10) | 0.0236 (10) | 0.0163 (10) | -0.0025 (8) | -0.0018 (7) | 0.0045 (8)  |
| C10 | 0.0145 (9)  | 0.0192 (10) | 0.0167 (10) | 0.0008 (8)  | 0.0013 (7)  | 0.0026 (8)  |

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

|           |             |          |             |
|-----------|-------------|----------|-------------|
| C11—C4    | 1.743 (2)   | C3—C4    | 1.385 (3)   |
| N1—C7     | 1.367 (2)   | C3—H3    | 0.9500      |
| N1—C1     | 1.406 (2)   | C4—C5    | 1.386 (3)   |
| N1—H1     | 0.881 (10)  | C5—C6    | 1.384 (3)   |
| N2—C10    | 1.338 (2)   | C5—H5    | 0.9500      |
| N2—C7     | 1.343 (2)   | C6—H6    | 0.9500      |
| N3—C8     | 1.323 (3)   | C7—C8    | 1.414 (3)   |
| N3—C9     | 1.344 (3)   | C8—H8    | 0.9500      |
| C1—C2     | 1.395 (3)   | C9—C10   | 1.374 (3)   |
| C1—C6     | 1.398 (3)   | C9—H9    | 0.9500      |
| C2—C3     | 1.380 (3)   | C10—H10  | 0.9500      |
| C2—H2     | 0.9500      |          |             |
| C7—N1—C1  | 128.19 (16) | C6—C5—H5 | 120.1       |
| C7—N1—H1  | 114.2 (15)  | C4—C5—H5 | 120.1       |
| C1—N1—H1  | 117.6 (15)  | C5—C6—C1 | 120.14 (18) |
| C10—N2—C7 | 116.74 (16) | C5—C6—H6 | 119.9       |
| C8—N3—C9  | 117.11 (17) | C1—C6—H6 | 119.9       |

## supplementary materials

|              |              |              |              |
|--------------|--------------|--------------|--------------|
| C2—C1—C6     | 118.89 (18)  | N2—C7—N1     | 115.87 (17)  |
| C2—C1—N1     | 117.73 (17)  | N2—C7—C8     | 120.33 (17)  |
| C6—C1—N1     | 123.26 (17)  | N1—C7—C8     | 123.78 (18)  |
| C3—C2—C1     | 121.21 (18)  | N3—C8—C7     | 121.97 (18)  |
| C3—C2—H2     | 119.4        | N3—C8—H8     | 119.0        |
| C1—C2—H2     | 119.4        | C7—C8—H8     | 119.0        |
| C2—C3—C4     | 118.96 (18)  | N3—C9—C10    | 121.19 (19)  |
| C2—C3—H3     | 120.5        | N3—C9—H9     | 119.4        |
| C4—C3—H3     | 120.5        | C10—C9—H9    | 119.4        |
| C3—C4—C5     | 121.05 (18)  | N2—C10—C9    | 122.63 (18)  |
| C3—C4—C11    | 119.53 (16)  | N2—C10—H10   | 118.7        |
| C5—C4—C11    | 119.42 (16)  | C9—C10—H10   | 118.7        |
| C6—C5—C4     | 119.75 (19)  |              |              |
| C7—N1—C1—C2  | -146.4 (2)   | N1—C1—C6—C5  | 176.58 (18)  |
| C7—N1—C1—C6  | 37.6 (3)     | C10—N2—C7—N1 | -178.56 (17) |
| C6—C1—C2—C3  | -0.1 (3)     | C10—N2—C7—C8 | -0.4 (3)     |
| N1—C1—C2—C3  | -176.21 (19) | C1—N1—C7—N2  | -171.00 (19) |
| C1—C2—C3—C4  | -0.5 (3)     | C1—N1—C7—C8  | 10.9 (3)     |
| C2—C3—C4—C5  | 0.6 (3)      | C9—N3—C8—C7  | -0.4 (3)     |
| C2—C3—C4—C11 | -179.50 (16) | N2—C7—C8—N3  | 1.2 (3)      |
| C3—C4—C5—C6  | 0.0 (3)      | N1—C7—C8—N3  | 179.22 (19)  |
| C11—C4—C5—C6 | -179.91 (15) | C8—N3—C9—C10 | -1.1 (3)     |
| C4—C5—C6—C1  | -0.6 (3)     | C7—N2—C10—C9 | -1.1 (3)     |
| C2—C1—C6—C5  | 0.7 (3)      | N3—C9—C10—N2 | 1.9 (3)      |

### Hydrogen-bond geometry (Å, °)

| $D-H\cdots A$      | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|----------|-------------|-------------|---------------|
| $N1-H1\cdots N2^i$ | 0.88 (1) | 2.15 (1)    | 3.023 (2)   | 171 (2)       |

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

Fig. 1

