IUCrData

ISSN 2414-3146

# *N*′-[1-(Pyrazin-2-yl)ethylidene]pyrazine-2-carbohydrazide

**Zhaodong Wang***

Chongqing Key Laboratory of Environmental, Materials & Remediation Technologies, Chongqing University of Arts and Sciences, Yongchuan, Chongqing, 402160, People's Republic of China. *Correspondence e-mail: ouwzdong@qq.com

Received 10 August 2018
Accepted 12 August 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

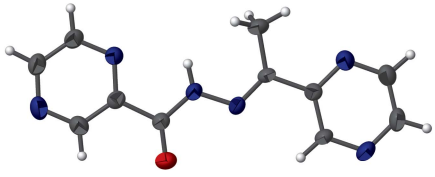
**Keywords:** crystal structure; pyrazine; acylhydrazone.

**CCDC reference**: 1852715

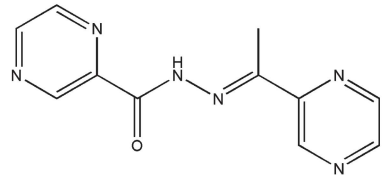
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compoud, $C_{11}H_{10}N_6O$, was synthesized by the condensation reaction of pyrazine-2-carbohydrazide with 2-acetylpyrazine in ethanol. The dihedral angle between the pyrazine rings is 4.7 (3)°. In the crystal, aromatic $\pi$–$\pi$ stacking [centroid–centroid separations = 3.606 (5) and 3.671 (5) Å] connect the molecules into stacks propagating in the [010] direction. A weak C—H···N interaction is also observed. The crystal studied was refined as a two-component twin.

**3D view**



**Chemical scheme**




## Structure description

The Schiff base acylhydrazone ligand has been well studied and used in supramolecular chemistry (Stadler & Harrowfield, 2009). Its applications have focused on molecular switches (Coskun *et al.*, 2012), sensors (Albelda *et al.*, 2012) and single molecular magnets (SMMs) (Anwar *et al.*, 2018). 2-Acetylpyrazine-based hydrazone ligands and their transition metal chemistry have also been reported (Hou *et al.*, 2018; Li *et al.*, 2015). As part of our studies in this area, we synthesized the title 2-acetylpyrazine-based hydrazone ligand with two pyrazine rings as a possible new ligand.

The dihedral angle between the pyrazine rings is 4.7 (3)° (Fig. 1). The C2—N2 bond length is 1.291 (7) Å, which is shorter than C1—N1 [1.362 (7) Å], showing that C2—N2 has strong double-bond character. The N—H grouping is sterically hindered from forming hydrogen bonds but a short intramolecular N—H···N contact occurs (Table 1). In the crystal, aromatic $\pi$–$\pi$ stacking [centroid–centroid separations = 3.606 (5) and 3.671 (5) Å] connect the molecules into stacks propagating in the [010] direction (Fig. 2). A weak C—H···N interaction is also observed (Table 1).

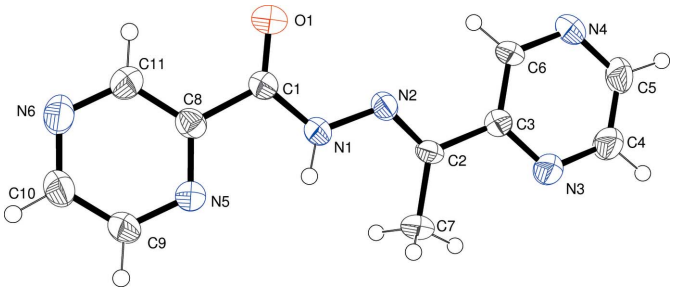



**Figure 1**
The title compound showing displacement ellipsoids drawn at the 50% probability level.

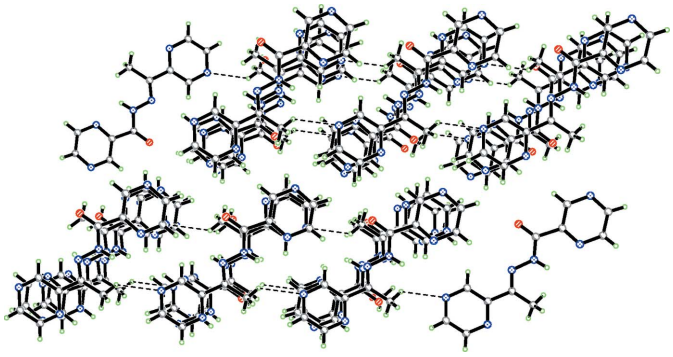


**Figure 2**
Crystal packing viewed along the *b*-axis direction.

## Synthesis and crystallization

The title molecule was prepared by the condensation reaction of pyrazine-2-carbohydrazide (1.38 g, 10 mmol) with 2-acetylpyrazine (1.22 g, 10 mmol) in 50 ml of refluxing ethanol for 16 h, resulting in a transparent light-yellow solution. After one night, colourless crystals suitable for X-ray analysis had formed.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Funding information

The author would like to thank the major cultivation project of Chongqing University of Arts and Sciences (No. P2017CH10) for financial support.

## References

Albelda, M. T., Frias, J. C., Garcia-Espana, E. & Schneider, H. J. (2012). *Chem. Soc. Rev.* **41**, 3859–3877.

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N5 | 0.86 | 2.28 | 2.671 (7) | 108 |
| C7—H7$C$···N4$^{i}$ | 0.96 | 2.57 | 3.247 (8) | 127 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{11}H_{10}N_6O$ |
| $M_r$ | 242.25 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 296 |
| $a, b, c$ (Å) | 7.247 (8), 8.066 (9), 9.77 (1) |
| $\alpha, \beta, \gamma$ (°) | 79.706 (14), 79.526 (15), 89.518 (14) |
| $V$ (Å$^3$) | 552.4 (10) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.10 |
| Crystal size (mm) | 0.2 × 0.17 × 0.12 |
| | |
| Data collection | |
| Diffractometer | Bruker P4 |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.598, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 1918, 1918, 1155 |
| $R_{int}$ | 0.037 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.087, 0.268, 1.08 |
| No. of reflections | 1918 |
| No. of parameters | 165 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.36, −0.33 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Anwar, M. U., Al-Harrasi, A., Gavey, E. L., Pilkington, M., Rawson, J. M. & Thompson, L. K. (2018). *Dalton Trans.* **47**, 2511–2521.
Bruker (2014). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Coskun, A., Banaszak, M., Astumian, R. D., Stoddart, J. F. & Grzybowski, B. A. (2012). *Chem. Soc. Rev.* **41**, 19–30.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Hou, X.-F., Zhao, X.-L., Zhang, L., Wu, W.-N. & Wang, Y. (2018). *Chin. J. Inorg. Chem.* **34**, 201–205.
Li, C.-R., Liao, Z.-C., Qin, J.-C., Wang, B.-D. & Yang, Z.-Y. (2015). *J. Lumin.* **168**, 330–333.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Stadler, A. M. & Harrowfield, J. (2009). *Inorg. Chim. Acta*, **362**, 4298–4314.

# full crystallographic data

*IUCrData* (2018). **3**, x181146 [https://doi.org/10.1107/S2414314618011460X]

## *N*′-[1-(Pyrazin-2-yl)ethylidene]pyrazine-2-carbohydrazide

**Zhaodong Wang**

### *N*′-[1-(Pyrazin-2-yl)ethylidene]pyrazine-2-carbohydrazide

*Crystal data*

$C_{11}H_{10}N_6O$
$M_r = 242.25$
Triclinic, $P\overline{1}$
$a = 7.247$ (8) Å
$b = 8.066$ (9) Å
$c = 9.77$ (1) Å
$\alpha = 79.706$ (14)°
$\beta = 79.526$ (15)°
$\gamma = 89.518$ (14)°
$V = 552.4$ (10) Å$^3$
$Z = 2$
$F(000) = 252$
$D_x = 1.456$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1331 reflections
$\theta = 2.6$–$27.8$°
$\mu = 0.10$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.2 × 0.17 × 0.12 mm

*Data collection*

Bruker P4 diffractometer
$\omega$ scan
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.598$, $T_{max} = 0.746$
1918 measured reflections
1918 independent reflections
1155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -11 \rightarrow 11$
1 standard reflections every 20 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.087$
$wR(F^2) = 0.268$
$S = 1.08$
1918 reflections
165 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2 + 1.0907P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.33$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refined as a 2-component twin.
The $U_{iso}$ values of all C(H) groups and all N(H) groups were set to 1.2$U_{eq}$(C). The $U_{iso}$ values of all C(H,H,H)groups were set to 1.5$U_{eq}$(C) Aromatic/amide H refined with riding coordinates: N1(H1), C6(H6), C4(H4), C11(H11), C9(H9), C10(H10), C5(H5) Idealized Me refined as rotating group: C7(H7A,H7B,H7C)

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.6785 (7) | 1.0992 (5) | −0.2460 (4) | 0.0522 (13) |
| N1 | 0.7251 (7) | 0.9311 (5) | −0.0408 (4) | 0.0346 (12) |
| H1 | 0.727205 | 0.829179 | 0.003733 | 0.042* |
| N2 | 0.7598 (6) | 1.0627 (5) | 0.0231 (4) | 0.0315 (11) |
| N3 | 0.8448 (8) | 1.1337 (6) | 0.3525 (5) | 0.0436 (14) |
| N4 | 0.8932 (8) | 1.4608 (6) | 0.1988 (5) | 0.0454 (14) |
| N5 | 0.6503 (7) | 0.6541 (6) | −0.1374 (5) | 0.0375 (12) |
| N6 | 0.6035 (8) | 0.6692 (7) | −0.4173 (5) | 0.0510 (15) |
| C1 | 0.6874 (8) | 0.9607 (7) | −0.1745 (6) | 0.0329 (14) |
| C2 | 0.7991 (7) | 1.0232 (6) | 0.1484 (5) | 0.0278 (13) |
| C3 | 0.8373 (8) | 1.1694 (6) | 0.2138 (6) | 0.0320 (13) |
| C4 | 0.8768 (10) | 1.2648 (7) | 0.4115 (6) | 0.0479 (17) |
| H4 | 0.885694 | 1.246186 | 0.506743 | 0.057* |
| C5 | 0.8969 (9) | 1.4251 (8) | 0.3369 (7) | 0.0469 (17) |
| H5 | 0.913865 | 1.512815 | 0.383846 | 0.056* |
| C6 | 0.8640 (9) | 1.3318 (6) | 0.1381 (6) | 0.0381 (15) |
| H6 | 0.861439 | 1.351038 | 0.041703 | 0.046* |
| C7 | 0.8116 (10) | 0.8504 (7) | 0.2285 (6) | 0.0473 (17) |
| H7A | 0.688201 | 0.799464 | 0.257749 | 0.071* |
| H7B | 0.865746 | 0.855539 | 0.310357 | 0.071* |
| H7C | 0.888978 | 0.784256 | 0.169222 | 0.071* |
| C8 | 0.6552 (8) | 0.8001 (6) | −0.2275 (6) | 0.0325 (13) |
| C9 | 0.6244 (9) | 0.5172 (7) | −0.1905 (6) | 0.0439 (16) |
| H9 | 0.623360 | 0.412256 | −0.132576 | 0.053* |
| C10 | 0.5992 (9) | 0.5243 (8) | −0.3272 (6) | 0.0455 (16) |
| H10 | 0.578353 | 0.424432 | −0.357767 | 0.055* |
| C11 | 0.6329 (9) | 0.8077 (8) | −0.3658 (6) | 0.0435 (16) |
| H11 | 0.638494 | 0.912245 | −0.424953 | 0.052* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.082 (4) | 0.032 (2) | 0.043 (3) | 0.001 (2) | −0.016 (2) | 0.0002 (19) |
| N1 | 0.045 (3) | 0.026 (2) | 0.032 (3) | −0.006 (2) | −0.006 (2) | −0.006 (2) |
| N2 | 0.036 (3) | 0.026 (2) | 0.032 (3) | −0.002 (2) | −0.003 (2) | −0.008 (2) |
| N3 | 0.057 (4) | 0.040 (3) | 0.034 (3) | −0.006 (2) | −0.008 (3) | −0.007 (2) |
| N4 | 0.065 (4) | 0.026 (2) | 0.046 (3) | −0.005 (2) | −0.008 (3) | −0.009 (2) |
| N5 | 0.046 (3) | 0.033 (3) | 0.032 (3) | −0.004 (2) | −0.006 (2) | −0.005 (2) |
| N6 | 0.064 (4) | 0.054 (3) | 0.037 (3) | −0.011 (3) | −0.010 (3) | −0.015 (3) |
| C1 | 0.038 (4) | 0.028 (3) | 0.032 (3) | −0.001 (2) | −0.005 (3) | −0.005 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.030 (3) | 0.020 (2) | 0.031 (3) | 0.000 (2) | −0.003 (3) | −0.001 (2) |
| C3 | 0.035 (3) | 0.030 (3) | 0.030 (3) | 0.001 (2) | −0.004 (3) | −0.005 (2) |
| C4 | 0.066 (5) | 0.045 (4) | 0.034 (3) | −0.009 (3) | −0.011 (3) | −0.009 (3) |
| C5 | 0.060 (4) | 0.044 (4) | 0.042 (4) | −0.006 (3) | −0.011 (3) | −0.020 (3) |
| C6 | 0.058 (4) | 0.021 (3) | 0.035 (3) | −0.002 (3) | −0.010 (3) | −0.002 (2) |
| C7 | 0.072 (5) | 0.027 (3) | 0.039 (3) | −0.007 (3) | −0.009 (3) | 0.003 (3) |
| C8 | 0.030 (3) | 0.030 (3) | 0.036 (3) | −0.003 (2) | −0.002 (3) | −0.006 (2) |
| C9 | 0.056 (4) | 0.033 (3) | 0.041 (3) | −0.014 (3) | −0.004 (3) | −0.005 (3) |
| C10 | 0.054 (4) | 0.040 (3) | 0.045 (4) | −0.009 (3) | −0.009 (3) | −0.014 (3) |
| C11 | 0.055 (4) | 0.043 (3) | 0.031 (3) | −0.005 (3) | −0.006 (3) | −0.004 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.215 (6) | C2—C7 | 1.482 (7) |
| N1—H1 | 0.8600 | C3—C6 | 1.381 (7) |
| N1—N2 | 1.371 (6) | C4—H4 | 0.9300 |
| N1—C1 | 1.362 (7) | C4—C5 | 1.361 (8) |
| N2—C2 | 1.291 (7) | C5—H5 | 0.9300 |
| N3—C3 | 1.345 (7) | C6—H6 | 0.9300 |
| N3—C4 | 1.332 (7) | C7—H7A | 0.9600 |
| N4—C5 | 1.333 (8) | C7—H7B | 0.9600 |
| N4—C6 | 1.323 (7) | C7—H7C | 0.9600 |
| N5—C8 | 1.335 (7) | C8—C11 | 1.380 (8) |
| N5—C9 | 1.329 (7) | C9—H9 | 0.9300 |
| N6—C10 | 1.329 (8) | C9—C10 | 1.372 (8) |
| N6—C11 | 1.339 (7) | C10—H10 | 0.9300 |
| C1—C8 | 1.514 (7) | C11—H11 | 0.9300 |
| C2—C3 | 1.487 (7) | | |
| | | | |
| N2—N1—H1 | 119.8 | C4—C5—H5 | 118.8 |
| C1—N1—H1 | 119.8 | N4—C6—C3 | 121.8 (5) |
| C1—N1—N2 | 120.4 (4) | N4—C6—H6 | 119.1 |
| C2—N2—N1 | 116.3 (4) | C3—C6—H6 | 119.1 |
| C4—N3—C3 | 115.7 (5) | C2—C7—H7A | 109.5 |
| C6—N4—C5 | 116.3 (5) | C2—C7—H7B | 109.5 |
| C9—N5—C8 | 115.4 (5) | C2—C7—H7C | 109.5 |
| C10—N6—C11 | 115.6 (5) | H7A—C7—H7B | 109.5 |
| O1—C1—N1 | 125.2 (5) | H7A—C7—H7C | 109.5 |
| O1—C1—C8 | 122.1 (5) | H7B—C7—H7C | 109.5 |
| N1—C1—C8 | 112.7 (5) | N5—C8—C1 | 118.1 (5) |
| N2—C2—C3 | 114.7 (4) | N5—C8—C11 | 122.1 (5) |
| N2—C2—C7 | 126.4 (5) | C11—C8—C1 | 119.8 (5) |
| C7—C2—C3 | 118.9 (5) | N5—C9—H9 | 118.6 |
| N3—C3—C2 | 115.7 (5) | N5—C9—C10 | 122.8 (6) |
| N3—C3—C6 | 121.6 (5) | C10—C9—H9 | 118.6 |
| C6—C3—C2 | 122.7 (5) | N6—C10—C9 | 122.1 (5) |
| N3—C4—H4 | 118.9 | N6—C10—H10 | 118.9 |
| N3—C4—C5 | 122.2 (6) | C9—C10—H10 | 118.9 |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 118.9 | N6—C11—C8 | 122.0 (5) |
| N4—C5—C4 | 122.3 (5) | N6—C11—H11 | 119.0 |
| N4—C5—H5 | 118.8 | C8—C11—H11 | 119.0 |
| | | | |
| O1—C1—C8—N5 | −173.8 (5) | C1—C8—C11—N6 | −179.8 (6) |
| O1—C1—C8—C11 | 6.5 (9) | C2—C3—C6—N4 | 178.3 (6) |
| N1—N2—C2—C3 | 179.5 (5) | C3—N3—C4—C5 | 1.3 (9) |
| N1—N2—C2—C7 | 0.5 (8) | C4—N3—C3—C2 | −179.3 (6) |
| N1—C1—C8—N5 | 5.8 (7) | C4—N3—C3—C6 | 0.9 (9) |
| N1—C1—C8—C11 | −173.9 (5) | C5—N4—C6—C3 | 0.5 (9) |
| N2—N1—C1—O1 | −1.1 (9) | C6—N4—C5—C4 | 1.7 (10) |
| N2—N1—C1—C8 | 179.4 (5) | C7—C2—C3—N3 | −12.5 (8) |
| N2—C2—C3—N3 | 168.4 (5) | C7—C2—C3—C6 | 167.4 (6) |
| N2—C2—C3—C6 | −11.8 (8) | C8—N5—C9—C10 | −1.7 (9) |
| N3—C3—C6—N4 | −1.8 (10) | C9—N5—C8—C1 | −179.0 (5) |
| N3—C4—C5—N4 | −2.7 (11) | C9—N5—C8—C11 | 0.6 (8) |
| N5—C8—C11—N6 | 0.6 (10) | C10—N6—C11—C8 | −0.7 (9) |
| N5—C9—C10—N6 | 1.7 (10) | C11—N6—C10—C9 | −0.4 (10) |
| C1—N1—N2—C2 | −178.2 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N5 | 0.86 | 2.28 | 2.671 (7) | 108 |
| C7—H7*C*···N4$^{i}$ | 0.96 | 2.57 | 3.247 (8) | 127 |

Symmetry code: (i) *x*, *y*−1, *z*.