Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-Cyano-*N*′-[1-(pyridin-2-yl)ethylidene]-acetohydrazide

**Xiao-Yi Zhang,[a] Xiao-Lin Han[b] and Zhi-Bin Qian[c]***

[a]School of Pharmacy, Xinxiang Medical University, Xinxiang Henan 453003, People's Republic of China, [b]The Hematology Department of the First Affiliated Hospital of Xinxiang Medical University, Weihui Henan 453100, People's Republic of China, and [c]School of Basic Medical Sciences, Xinxiang Medical University, Xinxiang Henan 453003, People's Republic of China
Correspondence e-mail: qianzhibin2012@163.com

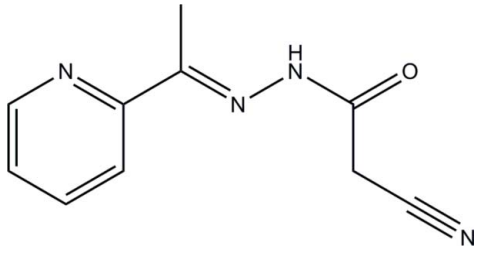
Received 7 October 2012; accepted 13 October 2012

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.064; $wR$ factor = 0.143; data-to-parameter ratio = 15.9.

In the title compound, $C_{10}H_{10}N_4O$, the dihedral angle between the pyridine ring and the –C=O($CH_2$)CN group is 24.08 (12)°. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops.

## Related literature

For the biological activity of hydrazone compounds, see: Rauf *et al.* (2008); Zhang *et al.* (2012). For related structures, see: Taha *et al.* (2012); Kargar *et al.* (2012); Rassem *et al.* (2012).




## Experimental

### Crystal data

$C_{10}H_{10}N_4O$
$M_r$ = 202.22
Monoclinic, $P2_1/c$
$a$ = 8.192 (2) Å
$b$ = 14.520 (2) Å
$c$ = 8.7340 (17) Å
$\beta$ = 98.466 (2)°
$V$ = 1027.6 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.17 × 0.13 × 0.12 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.985, $T_{max}$ = 0.989
6189 measured reflections
2222 independent reflections
1128 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.143
$S$ = 1.03
2222 reflections
140 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···O1$^{i}$ | 0.90 (1) | 2.05 (1) | 2.929 (2) | 167 (2) |

Symmetry code: (i) $-x+2, -y, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The intensity data were collected by Xiao-Lin Han under the guidance of Mr Yanglu Zhu at Dalian Institute of Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6969).

## References

Bruker (1998). *SMART* and *SAINT* . Bruker AXS Inc., Madison, Wisconsin, USA.
Kargar, H., Kia, R. & Tahir, M. N. (2012). *Acta Cryst.* E**68**, o2118–o2119.
Rassem, H. H., Salhin, A., Bin Salleh, B., Rosli, M. M. & Fun, H.-K. (2012). *Acta Cryst.* E**68**, o2279.
Rauf, A., Banday, M. R. & Mattoo, R. H. (2008). *Acta Chim. Slov.* **55**, 448-452.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Taha, M., Naz, H., Rahman, A. A., Ismail, N. H. & Yousuf, S. (2012). *Acta Cryst.* E**68**, o2846.
Zhang, M., Xian, D.-M., Li, H.-H., Zhang, J.-C. & You, Z.-L. (2012). *Aust. J. Chem.* **65**, 343–350.

# supporting information

*Acta Cryst.* (2012). E**68**, o3203 [doi:10.1107/S1600536812042869]

## 2-Cyano-*N*′-[1-(pyridin-2-yl)ethylidene]acetohydrazide

**Xiao-Yi Zhang, Xiao-Lin Han and Zhi-Bin Qian**

### S1. Comment

Hydrazone compounds bearing biological active functional groups -C(O)-NH-N=CH- are readily prepared by the condensation reactions of hydrazines with various aldehydes (e.g. Rauf *et al.*, 2008; Zhang *et al.*, 2012). In the present work, the title new hydrazone compound, derived from 2-acetylpyridine and cyanoacetohydrazide, is reported.

The molecule of the compound adopts a *trans* conformation about the C6=N2 double bond (Fig. 1). The torsion angles of C6-N2-N3-C8, N2-N3-C8-C9, and N3-C8-C9-C10 are 4.8 (3), 5.1 (3), and 6.5 (3)°, respectively. The bond lengths are comparable to those in similar compounds (Taha *et al.*, 2012; Kargar *et al.*, 2012; Rassem *et al.*, 2012). The crystal structure of the compound features N—H···O hydrogen bonds (Table 1), generating dimers (Fig. 2).

### S2. Experimental

2-Acetylpyridine (1.0 mmol, 0.121 g) and cyanoacetohydrazide (1.0 mmol, 0.991 g) were mixed and stirred in methanol (50 mL) at room temperature for 1 h. Colorless block-shaped single crystals were obtained after slow evaporation of the solution in air for a few days.

### S3. Refinement

H3A attached to N3 was located in a difference Fourier map and was refined isotropically, with N—H distance of 0.90 (1) Å. The remaining hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å for aromatic and $CH_2$ and 0.96 Å for $CH_3$. The $U_{iso}$ values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl group.

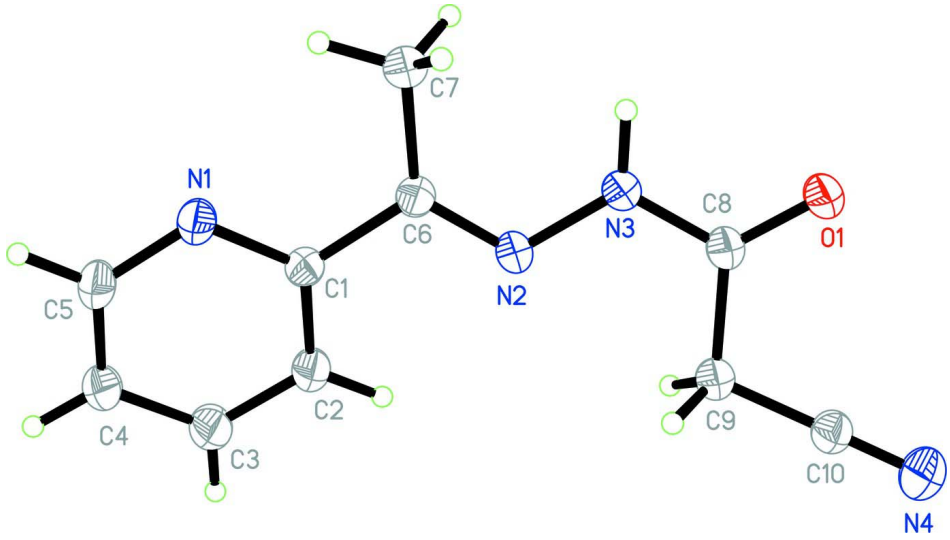



**Figure 1**

Molecular structure of the title compound with 30% thermal ellipsoids.

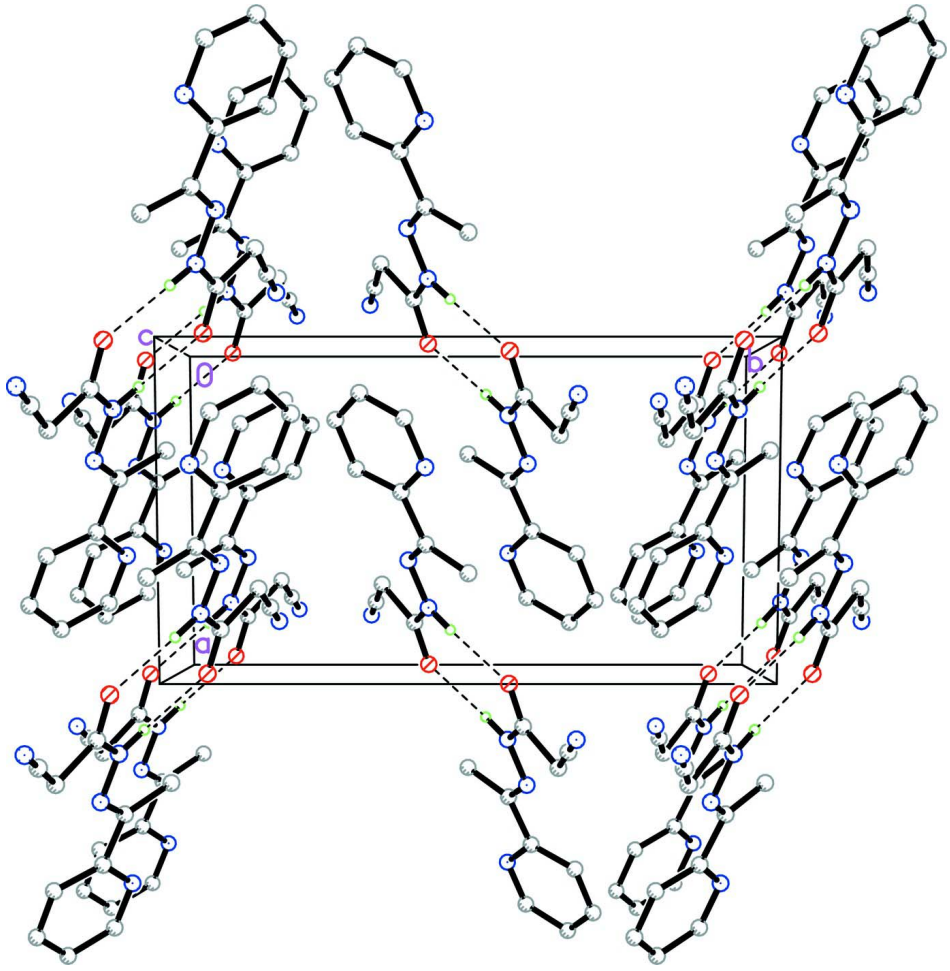


**Figure 2**

Molecular packing diagram of the title compound, viewed down the *c* axis. Hydrogen bonds are drawn as dashed lines.

**2-Cyano-*N*′-[1-(pyridin-2-yl)ethylidene]acetohydrazide**

*Crystal data*

$C_{10}H_{10}N_4O$
$M_r = 202.22$
Monoclinic, $P2_1/c$
$a = 8.192$ (2) Å
$b = 14.520$ (2) Å
$c = 8.7340$ (17) Å
$\beta = 98.466$ (2)°
$V = 1027.6$ (4) Å$^3$
$Z = 4$
$F(000) = 424$
$D_x = 1.307$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1009 reflections
$\theta = 2.7$–$24.5°$
$\mu = 0.09$ mm$^{-1}$
$T = 298$ K
Block, colorless
0.17 × 0.13 × 0.12 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.985$, $T_{max} = 0.989$
6189 measured reflections
2222 independent reflections
1128 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.7°$
$h = -9 \rightarrow 10$
$k = -18 \rightarrow 12$
$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.143$
$S = 1.03$
2222 reflections
140 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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.0523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ 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**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2$sigma($F^2$) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.3684 (2) | 0.07074 (13) | 0.3032 (2) | 0.0623 (6) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.6478 (2) | 0.10204 (13) | 0.0382 (2) | 0.0537 (5) |
| N3 | 0.7946 (2) | 0.06818 (13) | 0.0033 (2) | 0.0583 (5) |
| N4 | 0.8363 (3) | 0.17583 (17) | −0.4976 (3) | 0.0901 (8) |
| O1 | 0.97937 (19) | 0.06914 (12) | −0.16256 (18) | 0.0727 (5) |
| C1 | 0.4400 (3) | 0.11185 (15) | 0.1938 (2) | 0.0504 (6) |
| C2 | 0.3705 (3) | 0.18833 (17) | 0.1157 (3) | 0.0667 (7) |
| H2 | 0.4223 | 0.2167 | 0.0404 | 0.080* |
| C3 | 0.2244 (3) | 0.22169 (19) | 0.1506 (3) | 0.0805 (9) |
| H3 | 0.1764 | 0.2733 | 0.0993 | 0.097* |
| C4 | 0.1494 (3) | 0.17926 (19) | 0.2605 (3) | 0.0714 (7) |
| H4 | 0.0494 | 0.2006 | 0.2851 | 0.086* |
| C5 | 0.2256 (3) | 0.10466 (18) | 0.3330 (3) | 0.0686 (7) |
| H5 | 0.1747 | 0.0755 | 0.4082 | 0.082* |
| C6 | 0.5976 (3) | 0.07141 (15) | 0.1606 (2) | 0.0512 (6) |
| C7 | 0.6822 (3) | −0.00024 (17) | 0.2651 (3) | 0.0675 (7) |
| H7A | 0.6830 | −0.0574 | 0.2098 | 0.101* |
| H7B | 0.6246 | −0.0083 | 0.3522 | 0.101* |
| H7C | 0.7936 | 0.0187 | 0.3006 | 0.101* |
| C8 | 0.8458 (3) | 0.09339 (15) | −0.1295 (3) | 0.0554 (6) |
| C9 | 0.7285 (3) | 0.15165 (16) | −0.2381 (2) | 0.0587 (6) |
| H9A | 0.6215 | 0.1218 | −0.2570 | 0.070* |
| H9B | 0.7146 | 0.2109 | −0.1904 | 0.070* |
| C10 | 0.7896 (3) | 0.16532 (16) | −0.3836 (3) | 0.0594 (6) |
| H3A | 0.860 (2) | 0.0304 (13) | 0.066 (2) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0625 (14) | 0.0709 (13) | 0.0578 (12) | 0.0094 (11) | 0.0226 (10) | 0.0093 (10) |
| N2 | 0.0449 (11) | 0.0645 (13) | 0.0536 (11) | 0.0050 (9) | 0.0137 (9) | 0.0024 (9) |
| N3 | 0.0490 (13) | 0.0724 (14) | 0.0548 (12) | 0.0110 (10) | 0.0125 (9) | 0.0116 (10) |
| N4 | 0.0921 (18) | 0.1099 (19) | 0.0729 (15) | 0.0051 (14) | 0.0278 (13) | 0.0163 (14) |
| O1 | 0.0543 (11) | 0.0962 (13) | 0.0717 (11) | 0.0180 (9) | 0.0226 (9) | 0.0185 (9) |
| C1 | 0.0485 (14) | 0.0581 (14) | 0.0448 (12) | −0.0002 (12) | 0.0069 (10) | −0.0003 (11) |
| C2 | 0.0622 (17) | 0.0784 (18) | 0.0631 (15) | 0.0105 (14) | 0.0215 (13) | 0.0169 (13) |
| C3 | 0.0741 (19) | 0.091 (2) | 0.0809 (19) | 0.0283 (16) | 0.0261 (16) | 0.0236 (16) |
| C4 | 0.0623 (17) | 0.0910 (19) | 0.0649 (16) | 0.0209 (15) | 0.0232 (14) | 0.0064 (15) |
| C5 | 0.0664 (17) | 0.0843 (19) | 0.0610 (15) | 0.0076 (15) | 0.0291 (13) | 0.0074 (14) |
| C6 | 0.0486 (14) | 0.0581 (14) | 0.0471 (12) | −0.0015 (11) | 0.0081 (11) | 0.0011 (11) |
| C7 | 0.0607 (17) | 0.0816 (17) | 0.0616 (15) | 0.0133 (14) | 0.0131 (12) | 0.0181 (13) |
| C8 | 0.0481 (15) | 0.0633 (16) | 0.0568 (14) | 0.0015 (12) | 0.0143 (12) | 0.0027 (12) |
| C9 | 0.0536 (15) | 0.0676 (16) | 0.0564 (13) | 0.0062 (12) | 0.0132 (11) | 0.0058 (12) |
| C10 | 0.0594 (16) | 0.0618 (15) | 0.0583 (14) | 0.0026 (12) | 0.0131 (13) | 0.0045 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C5 | 1.331 (3) | C3—H3 | 0.9300 |
| N1—C1 | 1.333 (2) | C4—C5 | 1.359 (3) |

| | | | |
|---|---|---|---|
| N2—C6 | 1.280 (2) | C4—H4 | 0.9300 |
| N2—N3 | 1.374 (2) | C5—H5 | 0.9300 |
| N3—C8 | 1.341 (3) | C6—C7 | 1.486 (3) |
| N3—H3A | 0.899 (10) | C7—H7A | 0.9600 |
| N4—C10 | 1.128 (3) | C7—H7B | 0.9600 |
| O1—C8 | 1.224 (2) | C7—H7C | 0.9600 |
| C1—C2 | 1.382 (3) | C8—C9 | 1.506 (3) |
| C1—C6 | 1.486 (3) | C9—C10 | 1.446 (3) |
| C2—C3 | 1.366 (3) | C9—H9A | 0.9700 |
| C2—H2 | 0.9300 | C9—H9B | 0.9700 |
| C3—C4 | 1.361 (3) | | |

| | | | |
|---|---|---|---|
| C5—N1—C1 | 117.8 (2) | N2—C6—C1 | 114.9 (2) |
| C6—N2—N3 | 117.41 (19) | N2—C6—C7 | 125.31 (19) |
| C8—N3—N2 | 119.3 (2) | C1—C6—C7 | 119.78 (18) |
| C8—N3—H3A | 117.5 (15) | C6—C7—H7A | 109.5 |
| N2—N3—H3A | 123.2 (15) | C6—C7—H7B | 109.5 |
| N1—C1—C2 | 121.4 (2) | H7A—C7—H7B | 109.5 |
| N1—C1—C6 | 116.7 (2) | C6—C7—H7C | 109.5 |
| C2—C1—C6 | 121.88 (19) | H7A—C7—H7C | 109.5 |
| C3—C2—C1 | 119.1 (2) | H7B—C7—H7C | 109.5 |
| C3—C2—H2 | 120.5 | O1—C8—N3 | 122.0 (2) |
| C1—C2—H2 | 120.5 | O1—C8—C9 | 121.5 (2) |
| C4—C3—C2 | 119.9 (2) | N3—C8—C9 | 116.48 (19) |
| C4—C3—H3 | 120.1 | C10—C9—C8 | 111.03 (18) |
| C2—C3—H3 | 120.1 | C10—C9—H9A | 109.4 |
| C5—C4—C3 | 117.7 (2) | C8—C9—H9A | 109.4 |
| C5—C4—H4 | 121.1 | C10—C9—H9B | 109.4 |
| C3—C4—H4 | 121.1 | C8—C9—H9B | 109.4 |
| N1—C5—C4 | 124.1 (2) | H9A—C9—H9B | 108.0 |
| N1—C5—H5 | 118.0 | N4—C10—C9 | 179.6 (3) |
| C4—C5—H5 | 118.0 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···O1$^{i}$ | 0.90 (1) | 2.05 (1) | 2.929 (2) | 167 (2) |

Symmetry code: (i) −*x*+2, −*y*, −*z*.