# N′-Cyclopentylidenepyridine-4-carbo-hydrazide

## Andreas Lemmerer,[a]* Joel Bernstein[b] and Volker Kahlenberg[c]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, PO Wits 2050, South Africa, [b]Faculty of Science, NYU Abu Dhabi, PO Box 129188, Abu Dhabi, United Arab Emirates, and [c]Institute of Mineralogy and Petrography, University of Innsbruck, Innsbruck 6020, Austria

Correspondence e-mail: andreas.lemmerer@wits.ac.za

The title compound, $C_{11}H_{13}N_3O$, is a derivative of the antituberculosis drug isoniazid [systematic name: pyridine-4-carbohydrazide]. The crystal structure consists of repeating hydrogen-bonded chains parallel to the b axis. Adjacent molecules in the chains are linked by bifurcated N—H···(O,N) hydrogen bonds, which form an $R_1^2(5)$ ring motif.

## Related literature

For hydrogen-bond motifs, see: Bernstein et al. (1995).
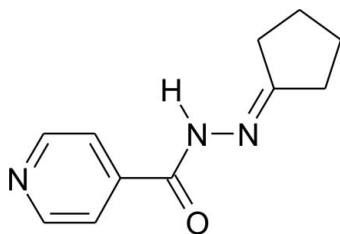


## Experimental

### Crystal data

| | |
|---|---|
| $C_{11}H_{13}N_3O$ | $V = 2048.3$ (7) Å$^3$ |
| $M_r = 203.24$ | $Z = 8$ |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a = 15.762$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $b = 8.1144$ (16) Å | $T = 173$ K |
| $c = 16.015$ (3) Å | $0.35 \times 0.22 \times 0.2$ mm |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur Gemini R diffractometer | 11794 measured reflections |
| Absorption correction: multi-scan (ABSPACK in CrysAlis PRO; Oxford Diffraction, 2006) | 1884 independent reflections |
| | 1420 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.970$, $T_{max} = 0.983$ | $R_{int} = 0.034$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.081$ | |
| $S = 0.96$ | |
| 1884 reflections | $\Delta\rho_{max} = 0.14$ e Å$^{-3}$ |
| 140 parameters | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|---|---|---|---|
| N1—H1···N3$^i$ | 0.889 (15) | 2.303 (15) | 3.1155 (16) | 151.9 (12) |
| N1—H1···O1$^i$ | 0.889 (15) | 2.607 (15) | 3.3368 (14) | 140.0 (11) |

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

Data collection: CrysAlis PRO (Oxford Diffraction, 2006); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and DIAMOND (Brandenburg, 1999); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON (Spek, 2009).

## References

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Sheldrick, G. M. (2008). Acta Cryst. A**64**, 112–122.
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# *N*′-Cyclopentylidenepyridine-4-carbohydrazide

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## Comment

Fig. 1 shows the atomic numbering scheme of the title compound. The amide functional groups form a torsion angle of -39.73 (17)° (C5—C1—C6—O1) with the pyridine ring. Fig. 2 shows the $R^2_1(5)$ (Bernstein *et al.*, 1995) hydrogen bonded ring formed with adjacent amide functional groups, leading to a chain along the *b*-axis.

## Experimental

A stoichiometric amount in the ratio of 1:1 of isonicotinic acid hydrazide (0.200 g, 1.46 mmol) to cyclopentanone (0.129 g) was dissolved in 5 ml of methanol. The solution was refluxed for a few hours, and left to cool to room temperature. Colourless, block-like crystals were harvested after slow evaporation over a few days at ambient conditions.

## Refinement

The C-bound H atoms were geometrically placed (C—H bond lengths of 0.95 (aromatic CH) and 0.99 (methylene CH$_2$) Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound H atoms were located in the difference map and coordinates refined freely together with their isotropic thermal parameters.

## Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2006); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).
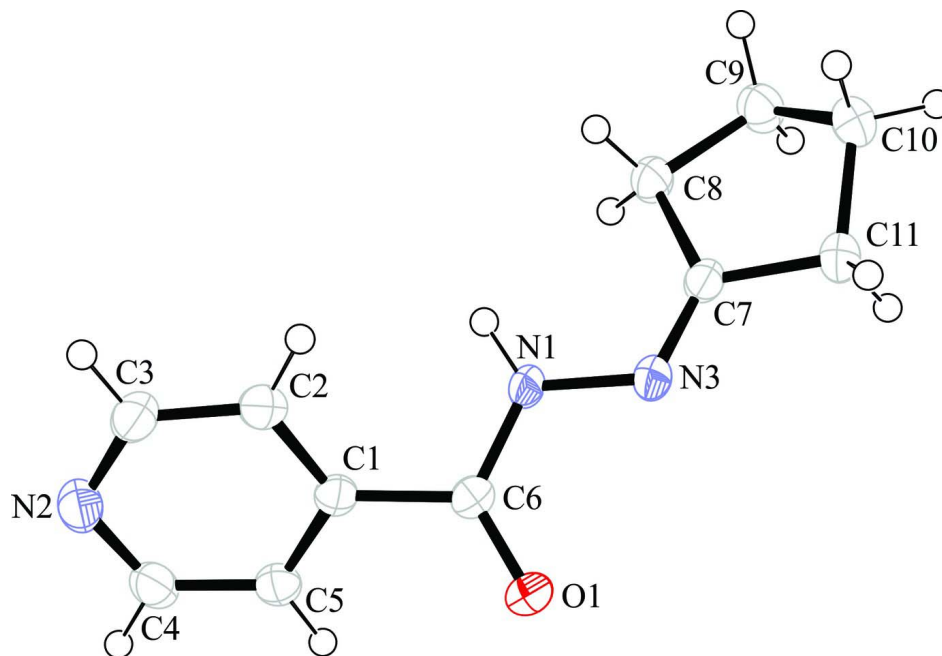
**Figure 1**

The asymmetric unit of (I) showing the atom numbering scheme. Displacement ellipsoids are shown at the 50% probability level.
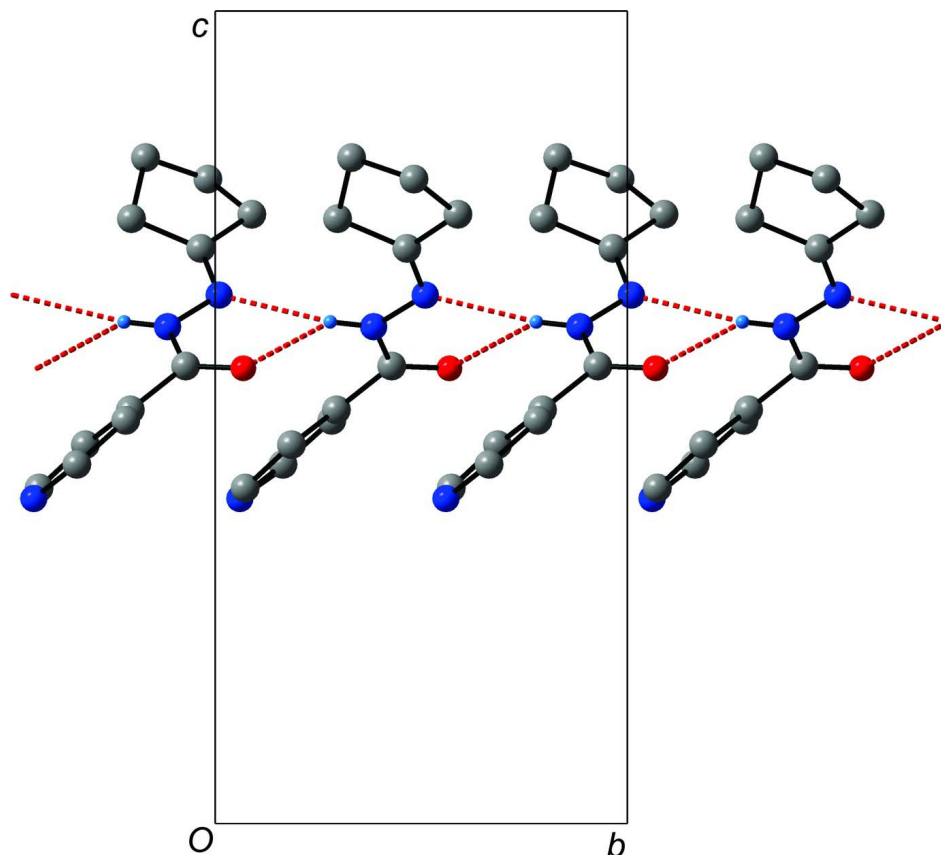
**Figure 2**

Hydrogen bonding chain showing the ring shaped hydrogen bonding motif. Intermolecular N—H···O and N—-H···N hydrogen bonds are shown as dashed red lines.

***N′*-Cyclopentylidenepyridine-4-carbohydrazide**

*Crystal data*

| | |
|---|---|
| $C_{11}H_{13}N_3O$ | $F(000) = 864$ |
| $M_r = 203.24$ | $D_x = 1.318$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *Kα* radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 5050 reflections |
| $a = 15.762$ (3) Å | $\theta = 2.9$–28.5° |
| $b = 8.1144$ (16) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 16.015$ (3) Å | $T = 173$ K |
| $V = 2048.3$ (7) Å$^3$ | Block, colourless |
| $Z = 8$ | 0.35 × 0.22 × 0.2 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Gemini R diffractometer | 1884 independent reflections |
| | 1420 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.034$ |
| Absorption correction: multi-scan (ABSPACK in *CrysAlis PRO*; Oxford Diffraction, 2006) | $\theta_{max} = 25.5°$, $\theta_{min} = 3.1°$ |
| | $h = -17 \rightarrow 18$ |
| | $k = -9 \rightarrow 9$ |
| $T_{min} = 0.970$, $T_{max} = 0.983$ | $l = -19 \rightarrow 14$ |
| 11794 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H atoms treated by a mixture of independent |
| Least-squares matrix: full | and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | $w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ |
| $wR(F^2) = 0.081$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.96$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1884 reflections | $\Delta\rho_{max} = 0.14$ e Å$^{-3}$ |
| 140 parameters | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |
| 0 restraints | |

*Special details*

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

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

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.63373 (8) | 0.29380 (15) | 0.50919 (7) | 0.0229 (3) |
| C2 | 0.68605 (8) | 0.18488 (16) | 0.46629 (8) | 0.0300 (3) |
| H2 | 0.7458 | 0.1879 | 0.4736 | 0.036* |
| C3 | 0.64926 (9) | 0.07249 (17) | 0.41303 (9) | 0.0362 (3) |
| H3 | 0.6856 | −0.0007 | 0.3836 | 0.043* |
| C4 | 0.51676 (9) | 0.16426 (16) | 0.44216 (8) | 0.0330 (3) |
| H4 | 0.4571 | 0.1569 | 0.4345 | 0.04* |
| C5 | 0.54713 (8) | 0.28276 (16) | 0.49627 (7) | 0.0265 (3) |
| H5 | 0.5093 | 0.3554 | 0.5241 | 0.032* |
| C6 | 0.66894 (7) | 0.42811 (15) | 0.56313 (7) | 0.0223 (3) |
| C7 | 0.83244 (7) | 0.46470 (15) | 0.70795 (8) | 0.0238 (3) |
| C8 | 0.84781 (8) | 0.29668 (16) | 0.74453 (8) | 0.0284 (3) |
| H8A | 0.8763 | 0.2236 | 0.7037 | 0.034* |
| H8B | 0.7939 | 0.245 | 0.7624 | 0.034* |
| C9 | 0.90543 (8) | 0.33071 (17) | 0.81972 (9) | 0.0322 (3) |
| H9A | 0.8715 | 0.3536 | 0.8705 | 0.039* |
| H9B | 0.9435 | 0.2361 | 0.8307 | 0.039* |
| C10 | 0.95583 (8) | 0.48203 (16) | 0.79324 (8) | 0.0302 (3) |
| H10A | 1.0022 | 0.4519 | 0.7544 | 0.036* |
| H10B | 0.9803 | 0.5393 | 0.8422 | 0.036* |
| C11 | 0.88949 (8) | 0.58868 (17) | 0.74995 (9) | 0.0328 (3) |
| H11A | 0.8576 | 0.6558 | 0.7909 | 0.039* |
| H11B | 0.9161 | 0.6629 | 0.7085 | 0.039* |
| N1 | 0.73514 (6) | 0.38419 (14) | 0.61158 (6) | 0.0247 (3) |
| H1 | 0.7496 (8) | 0.2789 (19) | 0.6174 (9) | 0.036 (4)* |
| N2 | 0.56579 (8) | 0.05969 (14) | 0.40008 (7) | 0.0377 (3) |
| N3 | 0.78134 (6) | 0.50934 (12) | 0.65045 (6) | 0.0251 (3) |
| O1 | 0.63990 (5) | 0.56802 (10) | 0.56036 (5) | 0.0298 (2) |

*Atomic displacement parameters (Å²)*

|      | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$       | $U^{23}$       |
| ---- | ----------- | ----------- | ----------- | ------------ | ------------- | ------------- |
| C1   | 0.0297 (7)  | 0.0192 (6)  | 0.0197 (6)  | 0.0008 (5)   | −0.0020 (5)   | 0.0038 (5)    |
| C2   | 0.0304 (7)  | 0.0305 (7)  | 0.0292 (7)  | 0.0059 (6)   | −0.0038 (5)   | −0.0017 (6)   |
| C3   | 0.0478 (9)  | 0.0292 (8)  | 0.0316 (7)  | 0.0092 (7)   | −0.0051 (6)   | −0.0063 (6)   |
| C4   | 0.0349 (7)  | 0.0283 (7)  | 0.0359 (8)  | −0.0032 (6)  | −0.0117 (6)   | 0.0051 (6)    |
| C5   | 0.0295 (7)  | 0.0238 (7)  | 0.0260 (7)  | 0.0008 (6)   | −0.0024 (5)   | 0.0041 (5)    |
| C6   | 0.0232 (6)  | 0.0207 (7)  | 0.0230 (6)  | 0.0000 (5)   | 0.0028 (5)    | 0.0013 (5)    |
| C7   | 0.0260 (7)  | 0.0200 (7)  | 0.0253 (7)  | 0.0003 (5)   | 0.0004 (5)    | −0.0029 (5)   |
| C8   | 0.0322 (7)  | 0.0218 (7)  | 0.0312 (7)  | −0.0027 (6)  | −0.0053 (5)   | 0.0016 (6)    |
| C9   | 0.0335 (8)  | 0.0330 (8)  | 0.0299 (7)  | −0.0018 (6)  | −0.0052 (5)   | 0.0016 (6)    |
| C10  | 0.0296 (7)  | 0.0332 (8)  | 0.0279 (7)  | −0.0029 (6)  | −0.0047 (5)   | −0.0027 (6)   |
| C11  | 0.0349 (8)  | 0.0244 (7)  | 0.0390 (8)  | −0.0033 (6)  | −0.0091 (6)   | −0.0044 (6)   |
| N1   | 0.0319 (6)  | 0.0146 (6)  | 0.0277 (6)  | −0.0010 (5)  | −0.0073 (4)   | −0.0016 (5)   |
| N2   | 0.0499 (8)  | 0.0289 (7)  | 0.0343 (6)  | −0.0009 (6)  | −0.0141 (5)   | −0.0026 (5)   |
| N3   | 0.0284 (6)  | 0.0189 (6)  | 0.0281 (6)  | −0.0021 (4)  | −0.0041 (4)   | −0.0023 (5)   |
| O1   | 0.0298 (5)  | 0.0221 (5)  | 0.0374 (5)  | 0.0048 (4)   | −0.0036 (4)   | −0.0022 (4)   |

*Geometric parameters (Å, º)*

| | | | |
| --- | --- | --- | --- |
| C1—C5   | 1.3836 (18) | C7—C11     | 1.5076 (17) |
| C1—C2   | 1.3904 (18) | C8—C9      | 1.5333 (18) |
| C1—C6   | 1.4973 (17) | C8—H8A     | 0.99        |
| C2—C3   | 1.3768 (19) | C8—H8B     | 0.99        |
| C2—H2   | 0.95        | C9—C10     | 1.5227 (19) |
| C3—N2   | 1.3360 (19) | C9—H9A     | 0.99        |
| C3—H3   | 0.95        | C9—H9B     | 0.99        |
| C4—N2   | 1.3309 (18) | C10—C11    | 1.5243 (18) |
| C4—C5   | 1.3801 (18) | C10—H10A   | 0.99        |
| C4—H4   | 0.95        | C10—H10B   | 0.99        |
| C5—H5   | 0.95        | C11—H11A   | 0.99        |
| C6—O1   | 1.2249 (14) | C11—H11B   | 0.99        |
| C6—N1   | 1.3484 (16) | N1—N3      | 1.3961 (14) |
| C7—N3   | 1.2759 (15) | N1—H1      | 0.889 (15)  |
| C7—C8   | 1.5035 (17) |            |             |
| | | | |
| C5—C1—C2 | 118.04 (11) | C9—C8—H8B     | 111         |
| C5—C1—C6 | 119.94 (11) | H8A—C8—H8B    | 109         |
| C2—C1—C6 | 121.87 (11) | C10—C9—C8     | 103.63 (10) |
| C3—C2—C1 | 118.51 (12) | C10—C9—H9A    | 111         |
| C3—C2—H2 | 120.7       | C8—C9—H9A     | 111         |
| C1—C2—H2 | 120.7       | C10—C9—H9B    | 111         |
| N2—C3—C2 | 124.23 (13) | C8—C9—H9B     | 111         |
| N2—C3—H3 | 117.9       | H9A—C9—H9B    | 109         |
| C2—C3—H3 | 117.9       | C9—C10—C11    | 103.09 (10) |
| N2—C4—C5 | 124.11 (13) | C9—C10—H10A   | 111.1       |
| N2—C4—H4 | 117.9       | C11—C10—H10A  | 111.1       |
| C5—C4—H4 | 117.9       | C9—C10—H10B   | 111.1       |
| C4—C5—C1 | 118.76 (12) | C11—C10—H10B  | 111.1       |

| | | | |
|---|---|---|---|
| C4—C5—H5 | 120.6 | H10A—C10—H10B | 109.1 |
| C1—C5—H5 | 120.6 | C7—C11—C10 | 103.49 (10) |
| O1—C6—N1 | 123.71 (11) | C7—C11—H11A | 111.1 |
| O1—C6—C1 | 121.01 (11) | C10—C11—H11A | 111.1 |
| N1—C6—C1 | 115.24 (10) | C7—C11—H11B | 111.1 |
| N3—C7—C8 | 129.82 (11) | C10—C11—H11B | 111.1 |
| N3—C7—C11 | 120.59 (11) | H11A—C11—H11B | 109 |
| C8—C7—C11 | 109.59 (10) | C6—N1—N3 | 117.90 (10) |
| C7—C8—C9 | 103.78 (10) | C6—N1—H1 | 120.9 (9) |
| C7—C8—H8A | 111 | N3—N1—H1 | 121.2 (9) |
| C9—C8—H8A | 111 | C4—N2—C3 | 116.34 (11) |
| C7—C8—H8B | 111 | C7—N3—N1 | 116.39 (10) |
| | | | |
| C5—C1—C2—C3 | 0.30 (18) | C7—C8—C9—C10 | −30.69 (13) |
| C6—C1—C2—C3 | −175.20 (12) | C8—C9—C10—C11 | 40.97 (13) |
| C1—C2—C3—N2 | −0.6 (2) | N3—C7—C11—C10 | −163.83 (11) |
| N2—C4—C5—C1 | −0.92 (19) | C8—C7—C11—C10 | 15.97 (14) |
| C2—C1—C5—C4 | 0.40 (17) | C9—C10—C11—C7 | −34.78 (13) |
| C6—C1—C5—C4 | 175.99 (11) | O1—C6—N1—N3 | −10.45 (17) |
| C5—C1—C6—O1 | −39.73 (17) | C1—C6—N1—N3 | 167.52 (9) |
| C2—C1—C6—O1 | 135.69 (13) | C5—C4—N2—C3 | 0.65 (19) |
| C5—C1—C6—N1 | 142.25 (11) | C2—C3—N2—C4 | 0.1 (2) |
| C2—C1—C6—N1 | −42.34 (16) | C8—C7—N3—N1 | −3.79 (18) |
| N3—C7—C8—C9 | −171.14 (12) | C11—C7—N3—N1 | 175.96 (10) |
| C11—C7—C8—C9 | 9.09 (14) | C6—N1—N3—C7 | 166.86 (11) |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1—H1···N3[i] | 0.889 (15) | 2.303 (15) | 3.1155 (16) | 151.9 (12) |
| N1—H1···O1[i] | 0.889 (15) | 2.607 (15) | 3.3368 (14) | 140.0 (11) |

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