Crystal structure of 5-amino-4H-1,2,4-triazol-1-ium pyrazine-2-carboxylate: an unexpected salt arising from the decarboxylation of both precursors

José A. Fernandes, Bing Liu, João P. C. Tomé, Luís Cunha-Silva and Filipe A. Almeida Paz

Received 13 June 2015
Accepted 17 June 2015

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

Keywords: crystal structure; ionothermal synthesis; decarboxylation; triazolium salt; hydrogen bonding; π-π stacking interactions

CCDC reference: 1407396
Supporting information: this article has supporting information at journals.iucr.org/e

Both the 3-amino-2H,4H-1,2,4-triazolium cation and the pyrazine-2-carboxylato anion in the title salt, C₇H₇N₅⁺·C₅H₃N₂O₂⁻, were formed by an unexpected decarboxylation reaction, from 5-amino-1H-1,2,4-triazole-3-carboxylic acid and pyrazine-2,3-dicarboxylic acid, respectively. The dihedral angle between the pyrazine ring (r.m.s. deviation = 0.008 Å) and the carboxylate group in the anion is 3.7 (3)°. The extended structure of the salt contains a supramolecular zigzag tape in which cations and anions are engaged in strong and highly directional N-H···O hydrogen bonds, forming R₂²(8) and R₂²(9) graph-set motifs. The packing between the tapes is mediated by π-π stacking interactions between the triazole and pyrazine rings.

1. Chemical context

A remarkable feature of ionothermal synthesis is the fact that ionic liquids (ILs) can act simultaneously as sustainable solvents and structure-directing agents (also known as templates). This has been widely demonstrated by their potential in the discovery of unprecedented crystalline materials (Xu et al., 2013). Following our interest in the design and preparation of new types of metal-organic frameworks (MOFs), we have been exploring the use of 5-amino-1H-1,2,4-triazole-3-carboxylic acid (H₂atrc) and pyrazine-2,3-dicarboxylic acid (H₂Pzdc) as a double-ligand system in the presence of transition metal centers using ionothermal synthetic conditions. In the presence of AgNO₃, the obtained product revealed, however, to be an unexpected organic salt (Bond, 2007) composed of the 3-amino-2H,4H(+)-1,2,4-triazolium cation and the pyrazine-2-carboxylato anion.

2. Structural commentary

The title compound is a product of decomposition of the H₂atrc and H₂Pzdc organic molecules by way of decarboxylation leading to, respectively, 3-amino-2H,4H-1,2,4-triazolium
[(C$_2$H$_5$N$_4$)$_+^+$] and pyrazine-2-carboxylate [(C$_5$H$_3$N$_2$O$_2$)$^-_-$]. The asymmetric unit is composed of one of each of these moieties, as depicted in both the chemical diagram and in Fig. 1.

3. Supramolecular features

The cation present in the title compound is rich in groups capable of forming strong N $\cdots$ N,O hydrogen-bonding interactions (see Table 1 for further geometrical details), many highly directional with the observed $<(D$ $\cdots$ $A)$ interaction angles being above 165$^\circ$. These supramolecular contacts are the main driving force which mediate the crystal packing features of the title compound. Indeed, the donation of hydrogen atoms from the cation to the carboxylate group of an adjacent anion (N6 $\cdots$ O2 and N5 $\cdots$ O1) forms the known structurally robust $R^2_2(8)$ graph-set motif (dashed pink lines in Fig. 2) (Grell et al., 1999). This graph-set motif has already been found in salts containing the title compound cation and carboxylic acids (see Database survey below). Two other interactions, N6 $\cdots$ H6A$\cdots$N1 (dashed aqua lines) and N4 $\cdots$ H4A$\cdots$O2, describe a second $R^2_2(9)$ hydrogen-bond motif. In contrast to the previous graph-set motif, the $R^2_2(9)$ ring has not been observed in structures containing the title-compound cation. The zigzag alternation of these two graph-set motifs leads to the formation of a highly coplanar supramolecular tape running parallel to the [010] direction of the unit cell (Fig. 2). Adjacent tapes interact by way of weak $\pi$ $\cdots$ $\pi$ stacking contacts between triazole and pyrazine rings, with the inter-centroid distance being 3.75 (3) Å (dashed orange lines in Fig. 2).

4. Database survey

Triazole molecules have been extensively used in the preparation of organic co-crystals (Kastelic et al., 2011; Remenar et al., 2003), and a survey of the Cambridge Structural Database (Groom & Allen, 2014) revealed the existence of about a dozen of crystallographic reports of co-crystals of the title compound cation (Byriel et al., 1992; Essid et al., 2013; research communications Acta Cryst. (2015). E71, 840–843 Fernandes et al. • C$_2$H$_5$N$_4$$^+$C$_5$H$_3$N$_2$O$_2$ 841

![Figure 1](image1.png)

Figure 1
The asymmetric unit of the title salt. Non H atoms are represented as displacement ellipsoids drawn at the 50% probability level, while H atoms are depicted as small spheres with arbitrary radii. The atomic labelling scheme for all non H atoms is provided. Hydrogen bonds are represented as dashed lines.

![Figure 2](image2.png)

Figure 2
Supramolecular tape running parallel to the [010] direction of the unit cell. N $\cdots$ N and N $\cdots$ N hydrogen bonds are depicted as dashed aqua and pink lines, respectively. Graph set motifs present in the structure are highlighted. For geometric details of the represented supramolecular contacts, see Table 1. $\pi$ $\cdots$ $\pi$ stacking interactions between two adjacent supramolecular tapes are shown as orange dashed lines.

| Table 1 | Hydrogen bond geometry (Å, $^\circ$). |
|---------|-------------------------------------|
| D $\cdot$ $\cdots$ $\cdot$ A | D $\cdot$ $\cdots$ $\cdot$ A |
| N4 $\cdots$ H4A$\cdots$O2 | 0.90 (1) | 1.77 (1) | 2.655 (3) | 166 (3) |
| N5 $\cdots$ H5$\cdots$O1 | 0.90 (1) | 1.73 (1) | 2.632 (3) | 176 (3) |
| N6 $\cdots$ H6B$\cdots$O2 | 0.90 (1) | 1.97 (1) | 2.853 (3) | 169 (3) |
| N6 $\cdots$ H6A$\cdots$N1 | 0.90 (1) | 2.21 (1) | 3.099 (3) | 169 (3) |

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

| Crystal data | Chemical formula | C\textsubscript{2}H\textsubscript{5}N\textsubscript{4}\textsuperscript{+}-C\textsubscript{5}H\textsubscript{4}N\textsubscript{2}O\textsubscript{2} | M\textsubscript{r} | 208.19 |
| Crystal system, space group | Monoclinic, P2\textsubscript{1}/c | Temperature (K) | 296 |
| a, b, c (Å) | 7.0599 (5), 12.1868 (8), 10.8385 (6) | β (°) | 103.593 (4) |
| V (Å\textsuperscript{3}) | 906.40 (10) | Z | 4 |
| Radiation type | Mo Kα | μ (mm\textsuperscript{-1}) | 0.12 |
| Crystal size (mm) | 0.09 × 0.04 × 0.03 |

Data collection

| Diffractometer | Bruker X8 Kappa CCD APEXII |
| Absorption correction | Multi-scan (SAINT: Sheldrick, 1998) |
| T\text{min}, T\text{max} | 0.989, 0.997 |
| No. of measured, independent and observed reflections | 12089, 1858, 1037 |
| R\text{int}, \Deltaρ_{max}, Δρ_{min} (e Å\textsuperscript{-1}) | 0.077, 0.19, 0.20 |

Joo et al., 2013; Luo et al., 2013; Lynch et al., 1992, 1998, 1999; Lynch, Smith, Byriel & Kennard, 1994; Lynch, Smith, Byriel, Kennard et al., 1994; Matulková et al., 2007; Smith et al., 1996). The only compounds known with both of the title compound entities present is a bimetallic complex also containing Cd\textsuperscript{2+} and NO\textsubscript{3}\textsuperscript{-} ions (Chen et al., 2009).

5. Synthesis and crystallization

5-Amino-1H-1,2,4-triazole-3-carboxylic acid (H\textsubscript{2}atrc, 98% purity), pyrazine-2,3-dicarboxylic acid (H\textsubscript{2}Pzdc, 97% purity), 1-methylimidazole (99% purity), 1-bromobutane (99% purity), N-(1-bromomethyl)imidazole (99% purity) and AgNO\textsubscript{3} (99% purity) were purchased from Sigma Aldrich and were used as received without further purification. 1-Butyl-3-methylimidazolium bromide ([BMM][Br]) was prepared according to the literature method (Parnham & Morris, 2006) and was isolated as a pale-yellow oil (yield of ca 78%). AgNO\textsubscript{3} (0.0687 g; 0.400 mmol), H\textsubscript{2}atrc (0.0510 g; 0.400 mmol) and H\textsubscript{2}Pzdc (0.0607 g; 0.361 mmol) were mixed with 0.49 g of [BMM][Br] and 0.3 mL of distilled water in a ca 25 mL Teflon-lined stainless-steel reaction vessel. The resulting mixture was heated to 383 K for 7 days. The vessel was then allowed to cool to ambient temperature at a rate of ca 1 K h\textsuperscript{-1}. Small colourless crystals of the title compound were directly isolated from the vessel contents.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms bound to carbon were placed at idealized positions with C - H = 0.95 Å, and included in the final structural model in a riding-motion approximation with the isotropic thermal displacement parameters fixed at 1.2U\text{eq} of the carbon atom to which they are attached. Hydrogen atoms associated with nitrogen atoms were located directly from difference Fourier maps and were included in the model with the N - H and H⋯H (only for the NH\textsubscript{2} groups) distances restrained to 0.90 (1) and 1.55 (1) Å, respectively, in order to ensure a chemically reasonable environment for these groups. These hydrogen atoms were modelled with the isotropic thermal displacement parameters fixed at 1.5U\text{eq}(N).

Acknowledgements

Funding Sources and Entities: The Fundação para a Ciência e a Tecnologia (FCT, Portugal), the European Union, QREN, FEDER through Programa Operacional Factores de Competitividade (COMPETE), CICECO-Aveiro Institute of Materials (Ref. FCT UID/CTM/50011/2013), REQUIMTE/LAQV (Ref. FCT UID/QUI/50006/2013) financed by national funds through the FCT/MEC and when applicable co-financed by FEDER under the PT2020 Partnership Agreement.

Projects and Individual grants: We wish to thank the FCT for funding the R&D projects FCOMP-01 0124-FEDER-041282 (Ref. FCT EXPL/CTM-NAN/0013/2013) and FCOMP-01 0124-FEDER-041445 (Ref. FCT EXPL/OEQ-QUI/0199/2013), and also CICECO for specific funding towards the purchase of the single-crystal diffractometer. The FCT is gratefully acknowledged for the post-doctoral research grants Nos. SFRH/BPD/63736/2009 and SFRH/BPD/47566/2008 (to JAF and BL, respectively).

References

Bond, A. D. (2007). CrystEngComm, 9, 833 834.
Brandenburg, K. (2009). DIAMOND. Crystal Impact GbR, Bonn, Germany.
Bruker (2005). SAINT Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). SAINT Plus. Bruker AXS, Delft, The Netherlands.
Byriel, K. A., Kennard, C. H. L., Lynch, D. E., Smith, G. & Thompson, J. G. (1992). Aust. J. Chem. 45, 969.
Chen, L. F., Qin, Y. Y., Li, Z. J. & Yao, Y. G. (2009). Chin. J. Struct. Chem. 28, 223 227.
Essid, M., Marouani, H., Al Deyab, S. S. & Rzaigui, M. (2013). Acta Cryst. E69, o1279.
Grell, J., Bernstein, J. & Tinhofer, G. (1999). Acta Cryst. B55, 1030 1043.
Groom, C. R. & Allen, F. H. (2014). Angew. Chem. Int. Ed. 53, 662 671.
Joo, Y. H., Chung, J. H., Cho, S. G. & Goh, E. M. (2013). New J. Chem. 37, 1180 1188.
Kastelic, J., Lah, N., Kikeli, D. & Leban, I. (2011). Acta Cryst. C67, o370 o372.
Luo, Y. H., Xu, B. & Sun, B. W. (2013). J. Cryst. Growth, 374, 88 98.
Lynch, D. E., Dougall, T., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1999). J. Chem. Crystallogr. 29, 67 73.
Lynch, D. E., Latif, T., Smith, G., Byriel, K. A., Kennard, C. H. L. & Parsons, S. (1998). Aust. J. Chem. 51, 403 408.
Lynch, D. E., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1992). Acta Cryst. C48, 1265 1267.
Lynch, D. E., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1994). Acta Cryst. C50, 1291 1294.
Lynch, D. E., Smith, G., Byriel, K. A., Kennard, C. H. L. & Whittaker, A. K. (1994). Aust. J. Chem. 47, 309 319.
Matulková, I., Němec, I., Císařová, I., Němec, P. & Mička, Z. (2007). J. Mol. Struct. 834 836, 328 335.

Parnham, E. R. & Morris, R. E. (2006). Chem. Mater. 18, 4882 4887.
Remenar, J. F., Morissette, S. L., Peterson, M. L., Moulton, B., MacPhee, J. M., Guzmán, H. R. & Almarsson, O. (2003). J. Am. Chem. Soc. 125, 8456 8457.
Sheldrick, G. M. (1998). SADABS. University of Gottingen, Germany.
Sheldrick, G. M. (2008). Acta Cryst. A64, 112 122.
Sheldrick, G. M. (2015). Acta Cryst. C71, 3 8.
Smith, G., Lynch, D. E., Byriel, K. A. & Kennard, C. H. L. (1996). Acta Cryst. C52, 231 235.
Xu, L., Kwon, Y. U., Castro, B. & Cunha Silva, L. (2013). Cryst. Growth Des. 13, 1260 1266.
Crystal structure of 5-amino-4H-1,2,4-triazol-1-ium pyrazine-2-carboxylate: an unexpected salt arising from the decarboxylation of both precursors

José A. Fernandes, Bing Liu, João P. C. Tomé, Luís Cunha-Silva and Filipe A. Almeida Paz

Computing details
Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT-Plus (Bruker, 2005); data reduction: SAINT-Plus (Bruker, 2005); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: DIAMOND (Brandenburg, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

5-Amino-4H-1,2,4-triazol-1-ium pyrazine-2-carboxylate

Crystal data
C₂H₅N₄⁺·C₅H₃N₂O₂
Mr = 208.19
Monoclinic, P2₁/c
a = 7.0599 (5) Å
b = 12.1868 (8) Å
b = 10.8385 (6) Å
β = 103.593 (4)°
V = 906.40 (10) Å³
Z = 4

F(000) = 432
Dₐ = 1.526 Mg m⁻³
Mo Kα radiation, λ = 0.71073 Å
Cell parameters from 1298 reflections
θ = 2.6°–19.7°
μ = 0.12 mm⁻¹
T = 296 K
Block, colourless

0.09 × 0.04 × 0.03 mm

Data collection
Bruker X8 Kappa CCD APEXII diffractometer
Radiation source: fine-focus sealed tube
ω / φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)
Tmin = 0.989, Tmax = 0.997
12089 measured reflections
1858 independent reflections
1037 reflections with I > 2σ(I)
Refinement
Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.059
wR(F²) = 0.133
S = 1.01
1858 reflections
148 parameters
5 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
w = 1/[σ²(Fo²) + (0.0599P)²]
where P = (Fo² + 2Fc²)/3
(Δ/σ)max < 0.001
Δρmax = 0.19 e Å⁻³
Δρmin = −0.20 e Å⁻³
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 (Å²)

| Atom | x     | y     | z     | Uiso*/Ueq |
|------|-------|-------|-------|-----------|
| N1   | 0.2890 (3) | 0.79063 (17) | 0.49872 (19) | 0.0389 (6) |
| N2   | 0.0664 (3) | 0.79145 (18) | 0.2472 (2) | 0.0468 (6) |
| C1   | 0.2177 (4) | 0.8840 (2) | 0.4404 (2) | 0.0334 (6) |
| C2   | 0.1066 (4) | 0.8815 (2) | 0.3165 (2) | 0.0412 (7) |
| H2   | 0.0571 | 0.9476 | 0.2797 | 0.049* |
| C3   | 0.1381 (4) | 0.6995 (2) | 0.3059 (2) | 0.0448 (7) |
| H3   | 0.1147 | 0.6334 | 0.2623 | 0.054* |
| C4   | 0.2461 (4) | 0.6993 (2) | 0.4297 (3) | 0.0442 (7) |
| H4   | 0.2912 | 0.6326 | 0.4668 | 0.053* |
| C5   | 0.2560 (4) | 0.9921 (2) | 0.5101 (2) | 0.0378 (7) |
| O1   | 0.1745 (3) | 1.07442 (14) | 0.45075 (15) | 0.0481 (6) |
| O2   | 0.3628 (3) | 0.99415 (14) | 0.61986 (16) | 0.0543 (6) |
| N3   | 0.7128 (4) | 0.94320 (19) | 0.8957 (2) | 0.0622 (8) |
| N4   | 0.6167 (4) | 0.88117 (19) | 0.7929 (2) | 0.0476 (6) |
| H4A  | 0.535 (3) | 0.912 (2) | 0.7253 (18) | 0.071* |
| N5   | 0.7480 (3) | 0.76575 (18) | 0.93596 (19) | 0.0417 (6) |
| C6   | 0.778 (4) | 0.6996 (2) | 0.972 (2) | 0.063* |
| N6   | 0.6528 (4) | 0.6942 (2) | 0.7405 (2) | 0.0540 (7) |
| H6A  | 0.473 (3) | 0.714 (2) | 0.6709 (19) | 0.081* |
| H6B  | 0.585 (5) | 0.6271 (13) | 0.775 (3) | 0.081* |
| C7   | 0.6369 (4) | 0.7751 (2) | 0.8181 (2) | 0.0365 (7) |
| C7   | 0.7892 (5) | 0.8695 (2) | 0.9782 (3) | 0.0553 (8) |
| H7   | 0.8649 | 0.8861 | 1.0584 | 0.066* |

Atomic displacement parameters (Å²)

|       | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   |
|-------|-------|-------|-------|-------|-------|-------|
| N1    | 0.0450 (14) | 0.0290 (13) | 0.0400 (12) | −0.0006 (11) | 0.0049 (10) | 0.0005 (10) |
| N2    | 0.0557 (16) | 0.0387 (14) | 0.0406 (12) | 0.0008 (12) | 0.0005 (11) | −0.0086 (12) |
| C1    | 0.0331 (15) | 0.0309 (15) | 0.0355 (13) | −0.0004 (13) | 0.0067 (11) | 0.0022 (12) |
| C2    | 0.0495 (18) | 0.0320 (16) | 0.0367 (14) | 0.0061 (14) | −0.0007 (13) | 0.0020 (12) |
| C3    | 0.0487 (19) | 0.0352 (17) | 0.0478 (16) | −0.0016 (15) | 0.0059 (14) | −0.0099 (13) |
| C4    | 0.0499 (18) | 0.0299 (16) | 0.0497 (16) | 0.0036 (14) | 0.0056 (14) | 0.0028 (13) |
| C5    | 0.0420 (17) | 0.0344 (16) | 0.0330 (13) | 0.0001 (14) | 0.0006 (12) | 0.0036 (12) |
| O1    | 0.0625 (14) | 0.0319 (11) | 0.0402 (10) | 0.0058 (9) | −0.0074 (9) | 0.0021 (8) |
| O2    | 0.0708 (14) | 0.0375 (12) | 0.0399 (10) | 0.0067 (10) | −0.0165 (10) | −0.0025 (9) |
| N3    | 0.089 (2)  | 0.0419 (15) | 0.0461 (14) | 0.0029 (15) | −0.0032 (13) | 0.0024 (12) |
| N4    | 0.0625 (18) | 0.0367 (15) | 0.0386 (13) | 0.0037 (13) | 0.0019 (12) | 0.0061 (11) |
| N5    | 0.0480 (14) | 0.0362 (15) | 0.0359 (12) | 0.0025 (12) | −0.0004 (11) | 0.0083 (11) |

Acta Cryst. (2015). E71, 840–843
### Geometric parameters (Å, °)

|       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| N1—C4 | 1.335 (3) | N3—C7 | 1.293 (3) |       |       |       |       |       |       |
| N1—C1 | 1.341 (3) | N3—N4 | 1.384 (3) |       |       |       |       |       |       |
| N2—C2 | 1.323 (3) | N4—C6 | 1.322 (3) |       |       |       |       |       |       |
| N2—C3 | 1.328 (3) | N4—H4A | 0.902 (10) |       |       |       |       |       |       |
| C1—C2 | 1.387 (3) | N5—C6 | 1.338 (3) |       |       |       |       |       |       |
| C1—C5 | 1.512 (3) | N5—C7 | 1.353 (3) |       |       |       |       |       |       |
| C2—H2 | 0.9300 | N5—H5 | 0.901 (10) |       |       |       |       |       |       |
| C3—C4 | 1.379 (4) | N6—C6 | 1.321 (3) |       |       |       |       |       |       |
| C3—H3 | 0.9300 | N6—H6A | 0.899 (10) |       |       |       |       |       |       |
| C4—H4 | 0.9300 | N6—H6B | 0.896 (10) |       |       |       |       |       |       |
| C5—O2 | 1.250 (2) | C7—H7 | 0.9300 |       |       |       |       |       |       |
| C5—O1 | 1.256 (3) |       |       |       |       |       |       |       |       |

### Selected bond lengths (Å)

| Atom | Atom | Distance |
|------|------|----------|
| N6   | C6   | 0.0607 (18) |
| C6   | C7   | 0.074 (2) |
| C7   | C4   | 0.0440 (16) |
| C4   | C3   | 0.0491 (15) |
| C4   | N1   | −0.0005 (15) |
| C4   | N2   | −0.0038 (13) |
| C4   | O2   | 0.0020 (17) |
| N1   | C1   | −0.0026 (15) |
| N1   | C5   | 0.0030 (13) |
| C1   | C2   | 0.0068 (12) |
| C1   | C3   | 0.0057 (12) |
| C1   | C5   | 0.0030 (13) |
| C2   | C1   | 0.0068 (12) |
| C2   | C3   | 0.0057 (12) |
| C3   | C4   | 0.0030 (13) |
| C3   | N2   | −0.0026 (15) |
| C3   | O2   | 0.0030 (13) |
| C4   | N1   | −0.0005 (15) |
| C4   | N2   | −0.0038 (13) |
| C4   | O2   | 0.0020 (17) |
| N1   | C1   | −0.0026 (15) |
| N1   | C5   | 0.0030 (13) |
| C1   | C2   | 0.0068 (12) |
| C1   | C3   | 0.0057 (12) |
| C1   | C5   | 0.0030 (13) |
| C2   | C1   | 0.0068 (12) |
| C2   | C3   | 0.0057 (12) |
| C3   | C4   | 0.0030 (13) |
| C3   | N2   | −0.0026 (15) |
| C3   | O2   | 0.0030 (13) |
| C4   | N1   | −0.0005 (15) |
| C4   | N2   | −0.0038 (13) |
| C4   | O2   | 0.0020 (17) |
| N1   | C1   | −0.0026 (15) |
| N1   | C5   | 0.0030 (13) |
| C1   | C2   | 0.0068 (12) |
| C1   | C3   | 0.0057 (12) |
| C1   | C5   | 0.0030 (13) |
Hydrogen bond geometry (Å, °)  

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N4—H4A···O2 | 0.90 (1) | 1.77 (1) | 2.655 (3) | 166 (3) |
| N5—H5···O1i | 0.90 (1) | 1.73 (1) | 2.632 (3) | 176 (3) |
| N6—H6B···O2i | 0.90 (1) | 1.97 (1) | 2.853 (3) | 169 (3) |
| N6—H6A···N1 | 0.90 (1) | 2.21 (1) | 3.099 (3) | 169 (3) |

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