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N-(1*H*-1,2,4-Triazol-5-yl)pyridine-2-carboxamide

Jing Miao, Maomao Jia, Xianlin Liu, Wei Xiong and Zilu Chen*

College of Chemistry and Chemical Engineering, Guangxi Normal University, Yucai Road 15, Guilin 541004, People's Republic of China
Correspondence e-mail: chenziluczl@yahoo.co.uk

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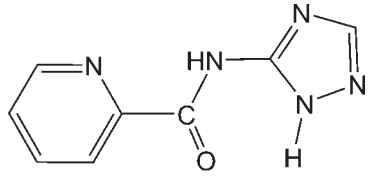
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.106; data-to-parameter ratio = 11.3.

In the structure of the title compound, $C_8H_7N_5O$, the pyridine ring and the imidazole ring are nearly coplanar, making a dihedral angle of 2.97 (15)°. An intramolecular N—H···O hydrogen bond occurs. In the crystal molecules are connected by intermolecular hydrogen bonds and π–π stacking interactions between neighboring imidazole rings [centroid–centroid distance = 3.5842 (5) Å and off-set angle = 21.77°], leading to the formation of a two-dimensional supramolecular sheet.

Related literature

For an alternative preparative method for the title compound, see: Browne & Polya (1968). For the potential bioinorganic applications of 1,2,4-triazole derivatives, see: Bohm & Karow (1981); Bahel *et al.* (1984).



Experimental

Crystal data

$C_8H_7N_5O$
M_r = 189.19
Monoclinic, $P2_1/n$
a = 8.6906 (17) Å
b = 5.2854 (10) Å
c = 17.880 (4) Å
β = 90.700 (3)°
V = 821.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 273 K
0.26 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.972, T_{max} = 0.980
3938 measured reflections
1443 independent reflections
961 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.106
S = 1.00
1443 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···N3^{i}	0.88	2.09	2.946 (2)	164
N4—H41···O1^{ii}	0.86	2.06	2.873 (2)	158
N4—H41···O1	0.86	2.17	2.629 (2)	113

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2185).

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supporting information

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S1. Comment

1,2,4-Triazoles derivatives represent an interesting class of heterocycles. They present various potential applications in bioinorganic chemistry (Bohm & Karow, 1981; Bahel, *et al.*, 1984). The preparation of the title compound has been reported previously (Browne & Polya, 1968), but its crystal structure has not yet been reported. Thus we report here the structure (Fig. 1) of the title compound obtained using an alternative method.

The pyridine ring and the imidazole ring are nearly co-planar with a dihedral angle of 2.97 (15)°. An intramolecular N—H···O hydrogen bond is present in the molecule. Adjacent molecules are connected alternatively by intermolecular N—H···N and N—H···O hydrogen bonds into one dimensional supramolecular chains (Fig. 2). The neighboring imidazole rings from adjacent one dimensional chains are parallel to each other with a perpendicular distance of 3.3285 (1) Å, a centroid-to-centroid distance of 3.5842 (5) Å and an off-set angle of 21.774° (calculated as the angle formed by the line through the two centroids of the two imidazole rings and the normal of the imidazole plane). This indicates the presence of a π–π stacking interaction between the neighboring imidazole rings from adjacent one dimensional chains, which leads to the construction of a two dimensional supramolecular sheet (Fig. 2).

S2. Experimental

A mixture of 1,2-di-2-pyridyl-ethane-dione (0.2122 g, 1 mmol), 5-amino-1,2,4-triazole (0.1682 g, 2 mmol) and methanol (20 ml) was refluxed at 343 K for three hours. It was then filtered and the filtrate was left at ambient temperature to evaporate for three days, yielding crystals of the product. The overall yield is 70%. Elemental analysis for $C_8H_7N_5$, calculated: C 55.48, H 4.07, N 40.44%; found: C 55.12, H 4.35, N 40.82%.

S3. Refinement

H atoms on the N atoms were located in an electron density map and and allowed to ride on the N atoms with U_{iso}(H) = 1.5U_{eq}(N). H atoms on the carbon atoms were placed at calculated positions (C–H = 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

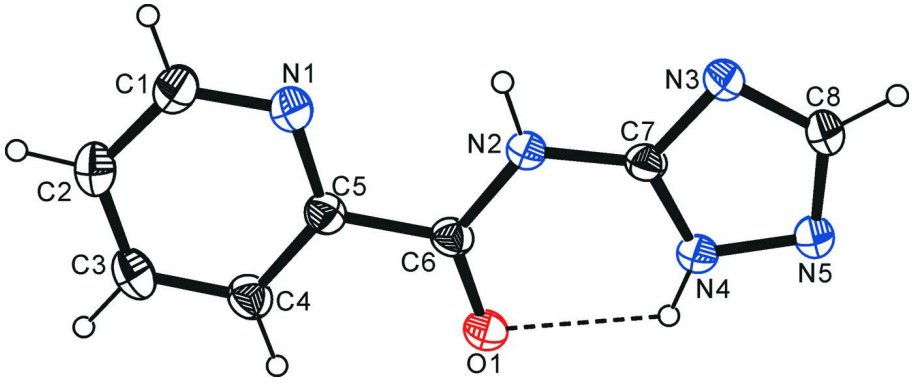

Figure 1

The molecular structure of the title compound with the atom-numbering scheme and 30% displacement ellipsoids.

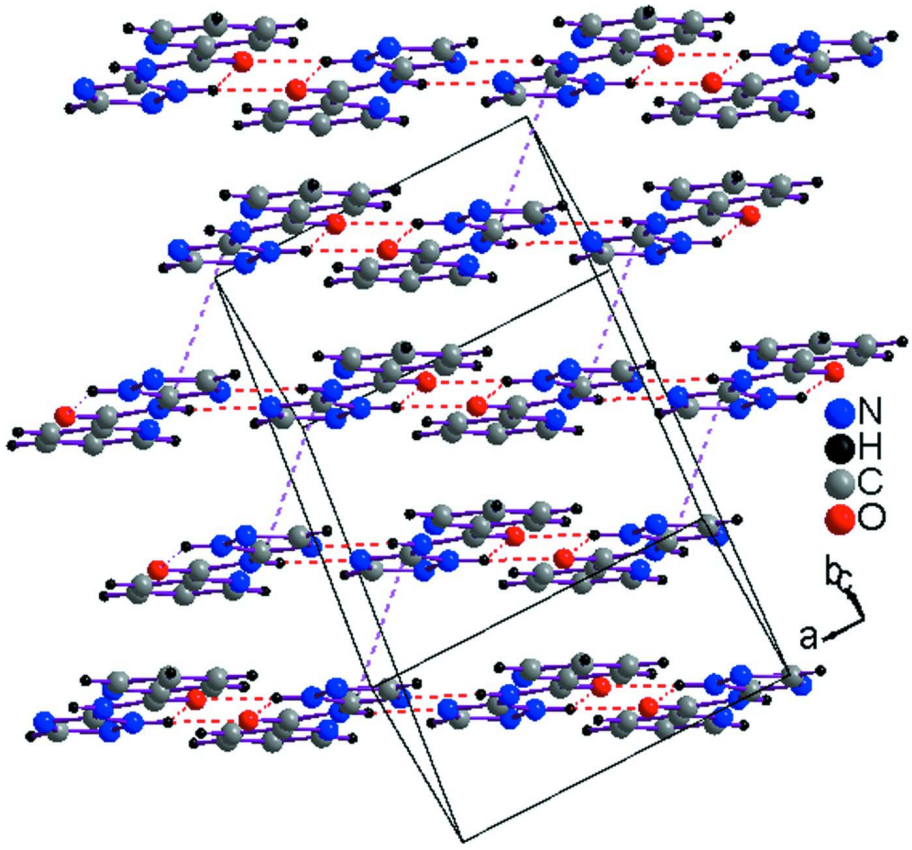

Figure 2

A view of the two-dimensional supramolecular sheet assembled by hydrogen bonds and π–π stacking interactions (indicated by dashed lines).

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Crystal data

$C_8H_7N_5O$
M_r = 189.19
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.6906 (17) Å
b = 5.2854 (10) Å

c = 17.880 (4) Å
β = 90.700 (3)°
V = 821.2 (3) Å^3
Z = 4
F(000) = 392
D_x = 1.530 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 1623 reflections
θ = 3.0–28.0°
μ = 0.11 mm^{-1}
T = 273 K
Block, colorless
0.26 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.972, T_{max} = 0.980

3938 measured reflections
1443 independent reflections
961 reflections with $I > 2\sigma(I)$
R_{int} = 0.095
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −8→10
k = −6→5
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.106
S = 1.00
1443 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.024 (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.

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 $F^2 > \sigma(F^2)$ 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	0.6956 (2)	0.7443 (3)	0.35815 (9)	0.0470 (5)
N2	0.77449 (17)	0.4023 (3)	0.46730 (8)	0.0410 (5)
H21	0.8406	0.5181	0.4539	0.061*
C5	0.5911 (2)	0.5707 (4)	0.37611 (10)	0.0389 (5)
C6	0.6318 (2)	0.3877 (4)	0.43697 (10)	0.0391 (5)
N4	0.74724 (18)	0.0445 (3)	0.54961 (8)	0.0438 (5)
H41	0.6579	−0.0130	0.5370	0.066*
N5	0.83128 (19)	−0.0771 (3)	0.60411 (9)	0.0481 (5)

N3	0.96153 (18)	0.2595 (3)	0.55752 (9)	0.0454 (5)
C3	0.4141 (3)	0.7178 (5)	0.28387 (12)	0.0529 (7)
H3	0.3198	0.7083	0.2589	0.063*
C4	0.4492 (2)	0.5512 (4)	0.34098 (11)	0.0478 (6)
H4	0.3789	0.4286	0.3555	0.057*
C1	0.6574 (3)	0.9042 (4)	0.30331 (12)	0.0547 (6)
H1	0.7281	1.0284	0.2905	0.066*
C7	0.8255 (2)	0.2395 (4)	0.52329 (11)	0.0380 (5)
C2	0.5196 (3)	0.8965 (5)	0.26449 (12)	0.0534 (7)
H2	0.4990	1.0104	0.2260	0.064*
C8	0.9568 (2)	0.0599 (4)	0.60561 (11)	0.0490 (6)
H8	1.0385	0.0229	0.6379	0.059*
O1	0.53795 (16)	0.2298 (3)	0.45747 (8)	0.0520 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0448 (11)	0.0521 (13)	0.0439 (10)	−0.0024 (9)	−0.0056 (8)	0.0052 (10)
N2	0.0348 (10)	0.0466 (12)	0.0414 (10)	−0.0067 (8)	−0.0051 (8)	0.0074 (9)
C5	0.0382 (12)	0.0424 (13)	0.0360 (11)	0.0004 (10)	−0.0015 (9)	−0.0021 (10)
C6	0.0346 (11)	0.0436 (14)	0.0390 (12)	−0.0060 (10)	−0.0031 (9)	−0.0033 (10)
N4	0.0371 (10)	0.0510 (13)	0.0431 (10)	−0.0086 (9)	−0.0042 (8)	0.0068 (9)
N5	0.0419 (10)	0.0541 (13)	0.0481 (10)	−0.0055 (10)	−0.0077 (8)	0.0132 (9)
N3	0.0391 (10)	0.0500 (12)	0.0469 (10)	−0.0077 (9)	−0.0092 (8)	0.0089 (9)
C3	0.0490 (14)	0.0611 (18)	0.0482 (13)	0.0082 (12)	−0.0150 (11)	−0.0033 (12)
C4	0.0438 (13)	0.0529 (15)	0.0465 (13)	−0.0028 (11)	−0.0065 (10)	−0.0015 (11)
C1	0.0580 (15)	0.0517 (16)	0.0542 (14)	−0.0055 (12)	−0.0027 (11)	0.0127 (12)
C7	0.0320 (11)	0.0441 (14)	0.0379 (11)	−0.0058 (10)	−0.0014 (9)	−0.0008 (10)
C2	0.0620 (16)	0.0542 (17)	0.0439 (12)	0.0088 (13)	−0.0074 (11)	0.0059 (12)
C8	0.0438 (13)	0.0582 (16)	0.0447 (13)	−0.0034 (12)	−0.0128 (10)	0.0109 (12)
O1	0.0390 (9)	0.0594 (11)	0.0574 (10)	−0.0141 (8)	−0.0100 (7)	0.0117 (8)

Geometric parameters (Å, º)

N1—C5	1.333 (2)	N5—C8	1.309 (3)
N1—C1	1.333 (3)	N3—C7	1.329 (2)
N2—C6	1.349 (2)	N3—C8	1.362 (2)
N2—C7	1.388 (2)	C3—C2	1.364 (3)
N2—H21	0.8751	C3—C4	1.379 (3)
C5—C4	1.381 (3)	C3—H3	0.9300
C5—C6	1.495 (3)	C4—H4	0.9300
C6—O1	1.226 (2)	C1—C2	1.377 (3)
N4—C7	1.324 (2)	C1—H1	0.9300
N4—N5	1.371 (2)	C2—H2	0.9300
N4—H41	0.8612	C8—H8	0.9300
C5—N1—C1	116.71 (19)	C4—C3—H3	120.4
C6—N2—C7	122.55 (17)	C3—C4—C5	118.5 (2)

C6—N2—H21	122.2	C3—C4—H4	120.7
C7—N2—H21	115.2	C5—C4—H4	120.7
N1—C5—C4	123.29 (19)	N1—C1—C2	124.0 (2)
N1—C5—C6	117.68 (18)	N1—C1—H1	118.0
C4—C5—C6	119.02 (19)	C2—C1—H1	118.0
O1—C6—N2	122.01 (19)	N4—C7—N3	110.85 (18)
O1—C6—C5	120.34 (18)	N4—C7—N2	125.30 (17)
N2—C6—C5	117.65 (18)	N3—C7—N2	123.85 (18)
C7—N4—N5	110.26 (16)	C3—C2—C1	118.4 (2)
C7—N4—H41	130.3	C3—C2—H2	120.8
N5—N4—H41	119.4	C1—C2—H2	120.8
C8—N5—N4	101.06 (17)	N5—C8—N3	116.56 (18)
C7—N3—C8	101.28 (17)	N5—C8—H8	121.7
C2—C3—C4	119.1 (2)	N3—C8—H8	121.7
C2—C3—H3	120.4		

C1—N1—C5—C4	0.0 (3)	C5—N1—C1—C2	−1.0 (3)
C1—N1—C5—C6	179.44 (19)	N5—N4—C7—N3	−0.1 (2)
C7—N2—C6—O1	0.4 (3)	N5—N4—C7—N2	179.57 (17)
C7—N2—C6—C5	−178.98 (17)	C8—N3—C7—N4	0.3 (2)
N1—C5—C6—O1	177.46 (18)	C8—N3—C7—N2	−179.40 (19)
C4—C5—C6—O1	−3.1 (3)	C6—N2—C7—N4	4.8 (3)
N1—C5—C6—N2	−3.1 (3)	C6—N2—C7—N3	−175.51 (19)
C4—C5—C6—N2	176.30 (17)	C4—C3—C2—C1	−0.4 (3)
C7—N4—N5—C8	−0.1 (2)	N1—C1—C2—C3	1.2 (4)
C2—C3—C4—C5	−0.5 (3)	N4—N5—C8—N3	0.3 (2)
N1—C5—C4—C3	0.7 (3)	C7—N3—C8—N5	−0.4 (2)
C6—C5—C4—C3	−178.68 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···N3^{i}	0.88	2.09	2.946 (2)	164
N4—H41···O1^{ii}	0.86	2.06	2.873 (2)	158
N4—H41···O1	0.86	2.17	2.629 (2)	113

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1.