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## Structure Reports

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Methyl 1*H*-1,2,3-triazole-4-carboxylateK. Prabakaran,<sup>a</sup> T. Maiyalagan,<sup>a</sup> Venkatesha R. Hathwar,<sup>b</sup>  
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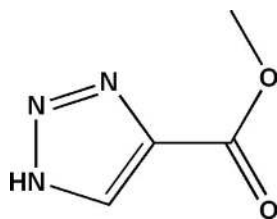
Received 6 January 2009; accepted 8 January 2009

Key indicators: single-crystal X-ray study;  $T = 290$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.039;  $wR$  factor = 0.116; data-to-parameter ratio = 12.1.

The title compound,  $\text{C}_4\text{H}_5\text{N}_3\text{O}_2$ , features an essentially planar molecule (r.m.s. deviation for all non-H atoms = 0.013 Å). The crystal structure is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\pi-\pi$  stacking interactions (centroid-centroid distance 3.882 Å).

## Related literature

For general background, see: Abu-Orabi *et al.* (1989); Fan & Katritzky (1996); Dehne (1994). For a related structure, see: Wang *et al.* (1998).



## Experimental

## Crystal data

$\text{C}_4\text{H}_5\text{N}_3\text{O}_2$   
 $M_r = 127.11$   
 Monoclinic,  $P2_1/n$   
 $a = 3.8823$  (7) Å  
 $b = 17.499$  (3) Å  
 $c = 8.8171$  (17) Å  
 $\beta = 100.938$  (3)°

$V = 588.12$  (19) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 290$  (2) K  
 $0.30 \times 0.23 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2004)  
 $T_{\min} = 0.956$ ,  $T_{\max} = 0.977$

4285 measured reflections  
 1098 independent reflections  
 917 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.116$   
 $S = 1.06$   
 1098 reflections  
 91 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.12$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N3}-\text{H3N}\cdots\text{O1}^i$	0.896 (19)	1.980 (19)	2.8659 (19)	169.56 (18)

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

Data collection: SMART (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: ORTEP-3 (Farrugia, 1999) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank the Department of Science and Technology, India, for use of the CCD facility set up under the IRHPA-DST program at IISc. We thank Prof T. N. Guru Row, IISc, Bangalore, for useful crystallographic discussions. FNK thanks the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2847).

## References

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## supporting information

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**Methyl 1*H*-1,2,3-triazole-4-carboxylate**

**K. Prabakaran, T. Maiyalagan, Venkatesha R. Hathwar, Canan Kazak and F. Nawaz Khan**

**S1. Comment**

Triazoles play an important role in pharmaceuticals, agrochemicals, dyes, photographic materials, and in corrosion inhibition (Fan & Katritzky, 1996; Dehne, 1994; Abu-Orabi *et al.*, 1989).

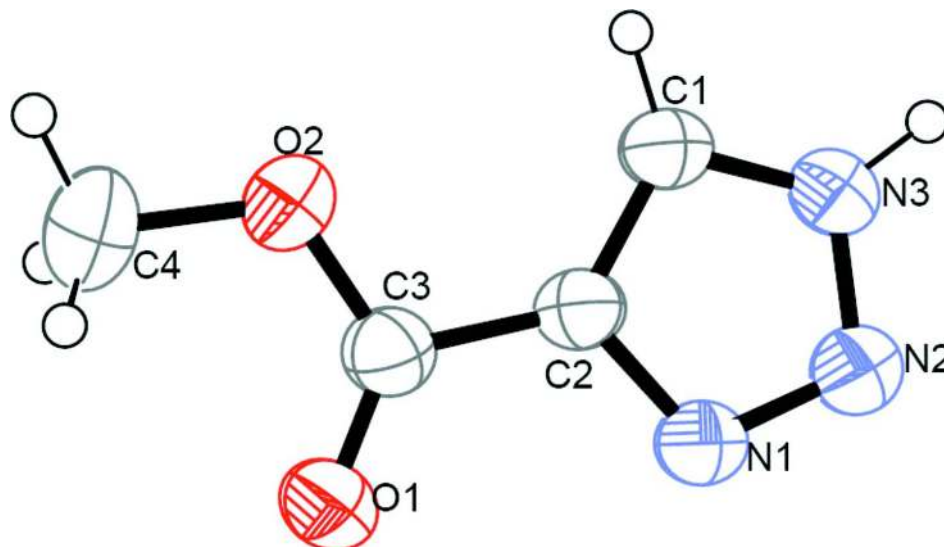
The crystal structure of the title compound is stabilized by intermolecular N—H···O hydrogen bonds and  $\pi$ – $\pi$  stacking interactions between the triazole rings at (symmetry operator 1+*X*,*Y*,*Z*; centroid-centroid distance 3.882 Å).

**S2. Experimental**

A mixture of methylpropiolate, 1 and trimethylsilylazide, 2 were heated at 100 °C till the completion of reaction, monitored by TLC. Then reaction mixture was cooled and methanol was added dropwise with cooling. The solid formed was allowed to stand for 30 min and filtered off, washed with ether, then with hexane. The product was then isolated as a colourless solid by column chromatography using 10% pet.ether/EtOAc. The single-crystal for X-ray structure analysis was obtained from ether solution by slow evaporation.

**S3. Refinement**

All the H atoms in (I) were positioned geometrically and refined using a riding model with C—H bond lengths of 0.93 Å and 0.97 Å for aromatic and for methyl H atoms respectively and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for all carbon bound H atoms.



**Figure 1**

ORTEP diagram of the asymmetric unit of the title compound with 50% probability displacement ellipsoids.

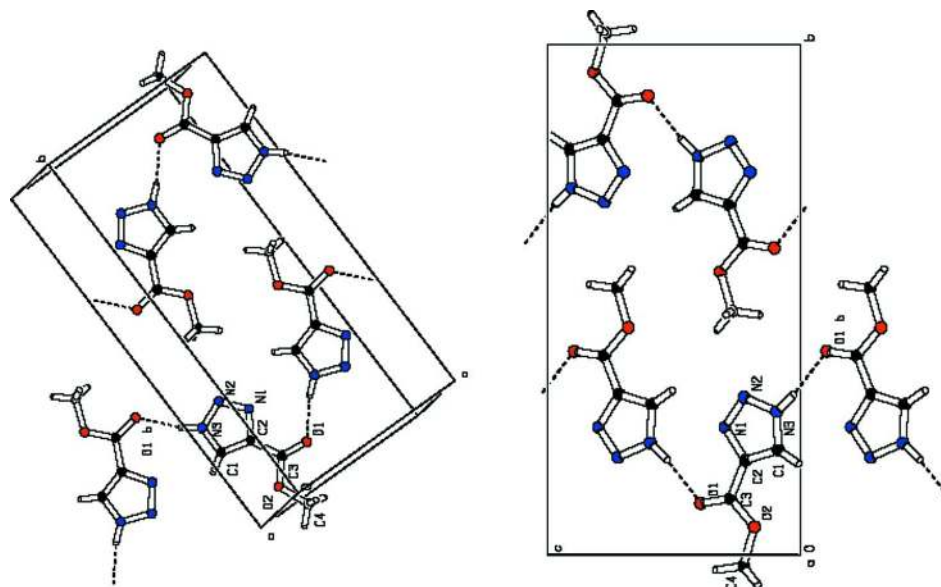


Figure 2

The crystal packing diagram of the title compound. The dotted lines indicate intermolecular N—H...O hydrogen bonds.

### Methyl 1*H*-1,2,3-triazole-4-carboxylate

#### Crystal data

$C_4H_5N_3O_2$

$M_r = 127.11$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1/n$

$a = 3.8823$  (7) Å

$b = 17.499$  (3) Å

$c = 8.8171$  (17) Å

$\beta = 100.938$  (3)°

$V = 588.12$  (19) Å<sup>3</sup>

$Z = 4$

$F(000) = 264$

$D_x = 1.436$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1804 reflections

$\theta = 2.4$ – $25.5$ °

$\mu = 0.12$  mm<sup>-1</sup>

$T = 290$  K

Block, pale yellow

$0.30 \times 0.23 \times 0.20$  mm

#### Data collection

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2004)

$T_{\min} = 0.956$ ,  $T_{\max} = 0.977$

4285 measured reflections

1098 independent reflections

917 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\max} = 25.5$ °,  $\theta_{\min} = 2.3$ °

$h = -4 \rightarrow 4$

$k = -21 \rightarrow 20$

$l = -10 \rightarrow 10$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.116$

$S = 1.06$

1098 reflections

91 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 atoms treated by a mixture of independent  
and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.085P]$   
where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.12 \text{ e } \text{\AA}^{-3}$

#### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
H3N	0.668 (5)	0.1865 (11)	0.529 (2)	0.069 (6)*
H1	0.630 (5)	0.3213 (10)	0.510 (2)	0.067 (5)*
O1	0.2633 (4)	0.39888 (6)	0.89548 (14)	0.0672 (4)
O2	0.4220 (4)	0.44536 (7)	0.68279 (14)	0.0670 (4)
C3	0.3702 (4)	0.38941 (9)	0.77686 (18)	0.0502 (4)
N3	0.5970 (4)	0.21920 (8)	0.59504 (15)	0.0520 (4)
C2	0.4540 (4)	0.31459 (8)	0.71907 (16)	0.0440 (4)
N2	0.5029 (4)	0.19156 (8)	0.72315 (16)	0.0577 (4)
C1	0.5704 (4)	0.29447 (9)	0.58856 (18)	0.0495 (4)
N1	0.4149 (4)	0.25012 (7)	0.79947 (15)	0.0541 (4)
C4	0.3391 (8)	0.52244 (11)	0.7273 (3)	0.0937 (8)
H4A	0.0894	0.5296	0.7056	0.141*
H4B	0.4472	0.5590	0.6700	0.141*
H4C	0.4261	0.5295	0.8358	0.141*

#### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0984 (10)	0.0524 (7)	0.0599 (8)	-0.0045 (6)	0.0379 (7)	-0.0077 (5)
O2	0.0959 (10)	0.0450 (7)	0.0671 (8)	0.0012 (6)	0.0330 (7)	0.0062 (5)
C3	0.0556 (9)	0.0481 (9)	0.0482 (9)	-0.0045 (7)	0.0137 (7)	-0.0012 (7)
N3	0.0643 (9)	0.0499 (8)	0.0443 (8)	0.0026 (6)	0.0167 (6)	-0.0038 (6)
C2	0.0478 (8)	0.0464 (8)	0.0384 (8)	-0.0034 (6)	0.0095 (6)	0.0015 (6)
N2	0.0754 (10)	0.0480 (8)	0.0532 (8)	0.0009 (6)	0.0213 (7)	0.0017 (6)
C1	0.0597 (10)	0.0499 (9)	0.0410 (9)	-0.0013 (7)	0.0152 (7)	0.0031 (7)
N1	0.0702 (9)	0.0480 (8)	0.0478 (8)	-0.0016 (6)	0.0207 (7)	0.0011 (5)
C4	0.134 (2)	0.0464 (11)	0.1117 (18)	0.0019 (11)	0.0499 (16)	0.0029 (11)

#### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O1—C3	1.2075 (19)	C2—N1	1.3561 (19)
O2—C3	1.3231 (19)	C2—C1	1.360 (2)
O2—C4	1.458 (2)	N2—N1	1.3065 (19)
C3—C2	1.464 (2)	C1—H1	0.906 (19)
N3—C1	1.322 (2)	C4—H4A	0.9600

N3—N2	1.3416 (19)	C4—H4B	0.9600
N3—H3N	0.90 (2)	C4—H4C	0.9600
C3—O2—C4	116.63 (15)	N3—C1—C2	104.91 (14)
O1—C3—O2	124.02 (15)	N3—C1—H1	121.4 (12)
O1—C3—C2	124.05 (14)	C2—C1—H1	133.7 (12)
O2—C3—C2	111.92 (13)	N2—N1—C2	108.49 (13)
C1—N3—N2	111.36 (14)	O2—C4—H4A	109.5
C1—N3—H3N	129.6 (12)	O2—C4—H4B	109.5
N2—N3—H3N	119.0 (12)	H4A—C4—H4B	109.5
N1—C2—C1	108.37 (14)	O2—C4—H4C	109.5
N1—C2—C3	120.51 (13)	H4A—C4—H4C	109.5
C1—C2—C3	131.12 (14)	H4B—C4—H4C	109.5
N1—N2—N3	106.88 (13)		
C4—O2—C3—O1	-0.7 (3)	N2—N3—C1—C2	0.00 (17)
C4—O2—C3—C2	178.67 (17)	N1—C2—C1—N3	-0.01 (17)
O1—C3—C2—N1	-0.2 (2)	C3—C2—C1—N3	-179.24 (16)
O2—C3—C2—N1	-179.54 (14)	N3—N2—N1—C2	-0.03 (18)
O1—C3—C2—C1	178.95 (17)	C1—C2—N1—N2	0.03 (18)
O2—C3—C2—C1	-0.4 (2)	C3—C2—N1—N2	179.35 (13)
C1—N3—N2—N1	0.02 (18)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3N...O1 <sup>i</sup>	0.896 (19)	1.980 (19)	2.8659 (19)	169.56 (18)

Symmetry code: (i)  $x+1/2, -y+1/2, z-1/2$ .