

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-(N-Cyanoguanyl)-3,5-dimethyl-1,2,4-triazole

Xiang-Xia Wu^{a*} and Zhen-Duo Guo^b^aLaboratory and Equipment Managing Department, Tianjin Normal University, Tianjin 300387, People's Republic of China, and ^bDepartment of Chemistry, Tianjin Normal University, Tianjin 300387, People's Republic of China

Correspondence e-mail: wuxiangxia@mail.nankai.edu.cn

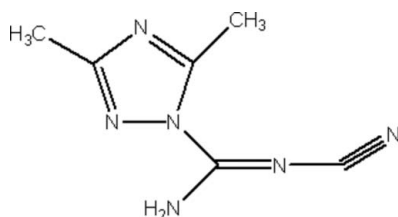
Received 15 October 2007; accepted 12 November 2007

Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.046; wR factor = 0.114; data-to-parameter ratio = 13.0.

The title compound, $\text{C}_6\text{H}_8\text{N}_6$, is of interest because it contains $-\text{CN}$, $-\text{NH}_2$ and triazole functional groups that can potentially bind metal(II) ions to form coordination polymers. In the crystal structure, $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds assemble the molecules into a two-dimensional sheet structure. There are also $\pi-\pi$ interactions between the sheets, with distances of 3.726 (1) Å between the triazole rings.

Related literature

For related literature, see: Guethner (1992); Haasnoot (2000); Kahn & Martinez (1998); Boga *et al.* (1999).



Experimental

Crystal data

$\text{C}_6\text{H}_8\text{N}_6$
 $M_r = 164.18$

Monoclinic, $C2/c$
 $a = 19.785$ (6) Å

$b = 7.5085$ (17) Å
 $c = 14.458$ (4) Å
 $\beta = 132.266$ (4)°
 $V = 1589.5$ (8) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 223$ (2) K
 $0.60 \times 0.32 \times 0.10$ mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 1999)
 $T_{\min} = 0.913$, $T_{\max} = 0.990$

7476 measured reflections
1451 independent reflections
1287 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.114$
 $S = 1.15$
1451 reflections

112 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N4}-\text{H4A}\cdots\text{N3}^i$	0.87	2.10	2.937 (2)	162
$\text{N4}-\text{H4B}\cdots\text{N6}^{ii}$	0.87	2.39	3.047 (2)	133

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

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

This work was supported financially by Tianjin Normal University (grant No. 5RL055).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2172).

References

- Boga, C., Forlani, L., Silvestroni, C., Corradi, A. B. & Sgarabotto, P. (1999). *J. Chem. Soc. Perkin Trans. 1*, pp. 1363–1368.
Guethner, T. (1992). UK Patent Application GB 2 247 237 No. 19 910 820.
Haasnoot, J. G. (2000). *Coord. Chem. Rev.* **131–135**, 200–248.
Kahn, O. & Martinez, C. J. (1998). *Science*, **279**, 44–48.
Rigaku, (1999). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E63, o4747 [doi:10.1107/S1600536807057972]

1-(*N*-Cyanoguanyl)-3,5-dimethyl-1,2,4-triazole

X.-X. Wu and Z.-D. Guo

Comment

Nowadays 1,2,4-triazole and its derivatives have attracted great interest because they combine the coordination modes of pyrazole and imidazole. They can bind different metal(II) ions forming a number of coordination polymers that exhibit diverse properties. For example, some iron(II) complexes containing 1,2,4-triazole ligands have spin-crossover properties, which could be used in molecular-based memory devices, displays and optical switches. (Kahn & Martinez, 1998) A comprehensive review of 1,2,4-triazole and its derivatives has been published (Haasnoot, 2000). However, triazole derivatives such as the title compound, (I), have not been well studied and from the viewpoint of coordination chemistry, it can be seen as a new ligand.

The molecular structure of (I) is shown in Fig. 1. The triazole ring is almost perfectly planar [maximum deviation from the least-squares plane is 0.002 (6) Å]. The distribution of bond lengths in the triazole ring vary from 1.311 (1)–1.377 (3) Å, which all fall in the intermediate range between 1.47 Å for a C—N single bond and 1.29 Å for a C=N double bond (Boga *et al.*, 1999). The result suggests a high degree of pi-delocalization over the whole triazole ring. Examination of the crystal structure with *PLATON* (Spek, 2003) shows that there are no solvent-accessible voids in the crystal structure. In the crystal N—H...N hydrogen bonds assemble the molecules into a two-dimensional sheet structure parallel to the *ab* plane. There are also pi-pi interactions between the sheets with distances of 3.726 (1) Å between the triazole rings.

Experimental

The title compound was synthesized according to a method described previously (Guethner, 1992). 0.2 mmol 1-(*N*-cyanoguanyl)-3,5-dimethyl-1,2,4-triazole was placed in 10 ml water medium and stirred for half an hour at room temperature. The resulting solution was filtrated and evaporated. After a few weeks, colorless block crystals of the title compound were obtained.

Refinement

The H atoms were placed at calculated positions and treated as riding atoms (N—H 0.87 Å; C—H 0.97 Å), with a displacement parameter U_{iso} set equal to 1.2 (NH) or 1.5 (CH3) times U_{eq} of the parent atom.

Figures

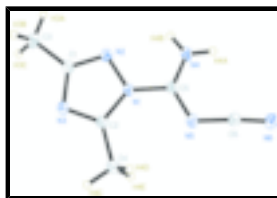


Fig. 1. The molecular structure and atom-labeling scheme of (I). Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. A two-dimensional supramolecular sheet structure of the title compound. The purple dashed lines represent the pi-pi interactions

112 parameters

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.51254 (9)	0.2511 (2)	0.51554 (13)	0.0268 (4)
N2	0.50709 (10)	0.1760 (2)	0.42335 (13)	0.0309 (4)
N3	0.36702 (10)	0.2194 (2)	0.35514 (13)	0.0299 (4)
N4	0.66908 (10)	0.2420 (2)	0.64689 (15)	0.0358 (4)
H4A	0.7243	0.2662	0.7161	0.043*
H4B	0.6606	0.1824	0.5882	0.043*
N5	0.59810 (9)	0.3847 (2)	0.70749 (13)	0.0322 (4)
N6	0.74386 (11)	0.4863 (2)	0.91092 (15)	0.0414 (5)
C1	0.41881 (12)	0.1611 (2)	0.32928 (16)	0.0293 (4)
C2	0.42647 (11)	0.2752 (2)	0.47144 (16)	0.0267 (4)
C3	0.37763 (13)	0.0909 (3)	0.20509 (17)	0.0410 (5)
H3A	0.4257	0.0523	0.2077	0.062*
H3B	0.3419	0.1838	0.1428	0.062*
H3C	0.3383	-0.0092	0.1836	0.062*
C4	0.40302 (13)	0.3484 (3)	0.54191 (18)	0.0381 (5)
H4C	0.3373	0.3447	0.4899	0.057*
H4D	0.4240	0.4706	0.5654	0.057*
H4E	0.4323	0.2777	0.6166	0.057*
C5	0.59893 (11)	0.2951 (2)	0.63111 (16)	0.0267 (4)
C6	0.67833 (12)	0.4345 (3)	0.81600 (16)	0.0310 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0182 (7)	0.0361 (9)	0.0198 (7)	-0.0006 (6)	0.0102 (6)	-0.0031 (6)
N2	0.0247 (8)	0.0407 (9)	0.0251 (8)	0.0001 (7)	0.0158 (7)	-0.0059 (7)
N3	0.0216 (8)	0.0396 (9)	0.0221 (8)	-0.0016 (6)	0.0121 (7)	-0.0004 (6)
N4	0.0180 (7)	0.0537 (10)	0.0258 (8)	-0.0005 (7)	0.0107 (7)	-0.0085 (7)
N5	0.0228 (8)	0.0433 (9)	0.0240 (8)	-0.0043 (7)	0.0131 (7)	-0.0066 (7)
N6	0.0356 (9)	0.0566 (11)	0.0273 (9)	-0.0093 (8)	0.0192 (8)	-0.0086 (8)
C1	0.0229 (9)	0.0361 (10)	0.0240 (9)	-0.0015 (7)	0.0138 (8)	-0.0022 (8)

supplementary materials

C2	0.0197 (9)	0.0321 (10)	0.0235 (9)	-0.0010 (7)	0.0125 (8)	0.0017 (7)
C3	0.0335 (10)	0.0542 (13)	0.0277 (10)	-0.0046 (9)	0.0174 (9)	-0.0094 (9)
C4	0.0261 (9)	0.0567 (13)	0.0314 (10)	-0.0018 (9)	0.0193 (9)	-0.0049 (9)
C5	0.0200 (9)	0.0325 (10)	0.0213 (9)	-0.0008 (7)	0.0113 (8)	0.0019 (7)
C6	0.0291 (10)	0.0386 (10)	0.0255 (10)	-0.0015 (8)	0.0185 (9)	-0.0013 (8)

Geometric parameters (Å, °)

N1—C2	1.371 (2)	N6—C6	1.150 (2)
N1—N2	1.383 (2)	C1—C3	1.483 (3)
N1—C5	1.407 (2)	C2—C4	1.480 (3)
N2—C1	1.311 (2)	C3—H3A	0.9700
N3—C2	1.314 (2)	C3—H3B	0.9700
N3—C1	1.377 (2)	C3—H3C	0.9700
N4—C5	1.308 (2)	C4—H4C	0.9700
N4—H4A	0.8700	C4—H4D	0.9700
N4—H4B	0.8700	C4—H4E	0.9700
N5—C5	1.303 (2)		
C2—N1—N2	109.78 (14)	C1—C3—H3B	109.5
C2—N1—C5	131.16 (15)	H3A—C3—H3B	109.5
N2—N1—C5	119.01 (15)	C1—C3—H3C	109.5
C1—N2—N1	102.74 (14)	H3A—C3—H3C	109.5
C2—N3—C1	105.05 (14)	H3B—C3—H3C	109.5
C5—N4—H4A	120.0	C2—C4—H4C	109.5
C5—N4—H4B	120.0	C2—C4—H4D	109.5
H4A—N4—H4B	120.0	H4C—C4—H4D	109.5
C5—N5—C6	117.34 (16)	C2—C4—H4E	109.5
N2—C1—N3	114.01 (16)	H4C—C4—H4E	109.5
N2—C1—C3	123.39 (17)	H4D—C4—H4E	109.5
N3—C1—C3	122.59 (16)	N5—C5—N4	128.79 (16)
N3—C2—N1	108.42 (15)	N5—C5—N1	115.46 (16)
N3—C2—C4	125.03 (16)	N4—C5—N1	115.75 (16)
N1—C2—C4	126.54 (16)	N6—C6—N5	174.5 (2)
C1—C3—H3A	109.5		
C2—N1—N2—C1	0.66 (19)	C5—N1—C2—N3	177.03 (17)
C5—N1—N2—C1	-177.05 (15)	N2—N1—C2—C4	178.65 (17)
N1—N2—C1—N3	-0.8 (2)	C5—N1—C2—C4	-4.0 (3)
N1—N2—C1—C3	178.20 (17)	C6—N5—C5—N4	1.7 (3)
C2—N3—C1—N2	0.6 (2)	C6—N5—C5—N1	-177.64 (16)
C2—N3—C1—C3	-178.36 (18)	C2—N1—C5—N5	-5.2 (3)
C1—N3—C2—N1	-0.2 (2)	N2—N1—C5—N5	171.93 (15)
C1—N3—C2—C4	-179.15 (18)	C2—N1—C5—N4	175.38 (18)
N2—N1—C2—N3	-0.3 (2)	N2—N1—C5—N4	-7.5 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N4—H4A \cdots N3 ⁱ	0.87	2.10	2.937 (2)	162

N4—H4B···N6ⁱⁱ

0.87

2.39

3.047 (2)

133

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

Fig. 1

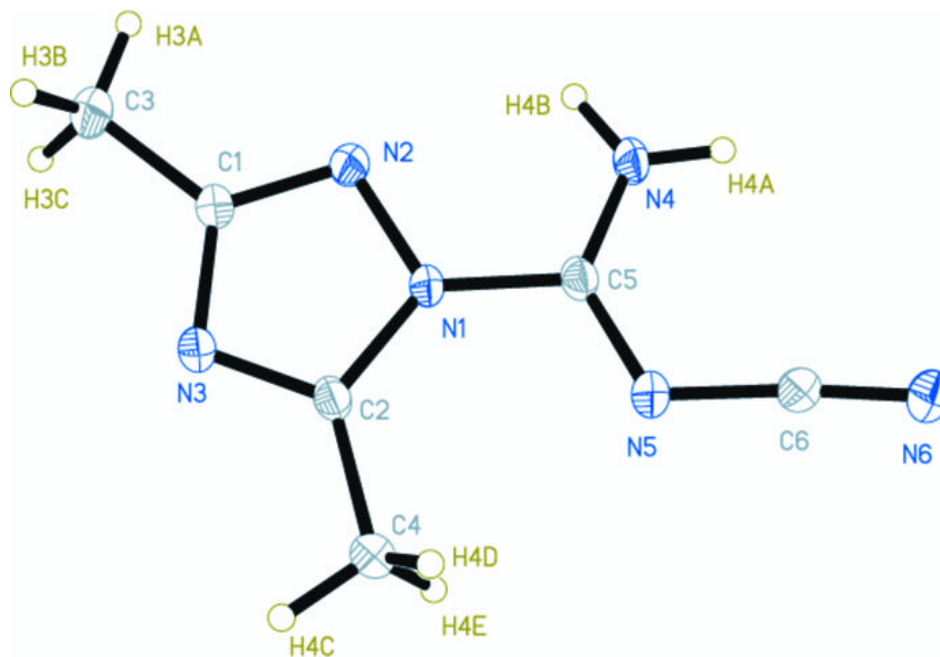


Fig. 2

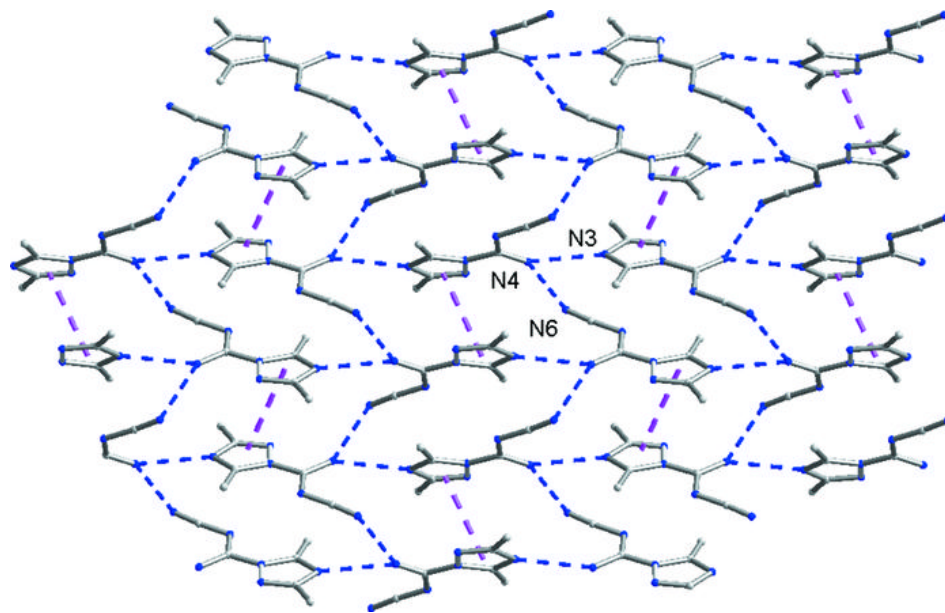


Fig. 3

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N4-H4A \cdots N3^i$	0.870	2.096	2.936(9)	162
$N4-H4B \cdots N6^{\#}$	0.870	2.389	3.047(4)	133

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