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5-(Pyridin-2-yl)-3,3′-bi(1*H*-1,2,4-triazole)

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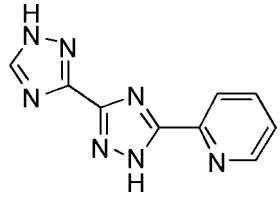
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.156; data-to-parameter ratio = 11.9.

In the title molecule, $C_9H_7N_7$, the two triazole rings are twisted by an angle of 3.8 (5)°; the central triazole ring is twisted by 32.3 (6)° with respect to the pyridyl ring. The crystal packing consists of layers generated by intermolecular N—H···N hydrogen bonds.

Related literature

For related structures, see: Mai *et al.* (2009); Zhang *et al.* (2010). For the synthesis, see: Potts (1960); Wiley & Hart (1953).



Experimental

Crystal data

$C_9H_7N_7$
M_r = 213.22
Monoclinic, $P2_1/c$
a = 12.372 (3) Å
b = 7.5361 (15) Å
c = 10.007 (2) Å
β = 93.670 (4)°
V = 931.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.24 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.979
5150 measured reflections
1832 independent reflections
1072 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.156
S = 0.94
1832 reflections
154 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H1···N4^{i}	0.98 (4)	1.93 (4)	2.891 (3)	165 (3)
N2—H2···N3^{ii}	0.99 (3)	1.90 (4)	2.878 (3)	167 (3)

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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: NG5195).

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supporting information

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5-(Pyridin-2-yl)-3,3′-bi(1*H*-1,2,4-triazole)

Zhouqing Xu, Xinping Zhao and Qiang Wang

S1. Comment

During the past decads, copounds containling trazole subunits have been intensively studied due to their diverse biological activities, such as fungicide, herbicide, medicine, *etc*., and have become a central focus in the sudy of agricultural, medicinal and material chemicals. Furthermore, the study on crystal structures and properties of the new metal-organic frameworks (MOFs) of N-containing ligands have attracted considerable attentions during the past years for the their potential applications in polymeric materials, catalytic materials, biological materials optical materials and so on (Zhang, *et al.*, 2010). Therefore, in search for new multidentate ligands, we have synthesized the title compound and determined its structure.

The molecule structure of title compound was shown in the Fig.1, the lengths and angles are within normal ranges. In triazol ring, the average C—N bond length is 1.336 (5) Å, which is shorter than C—N (mean 1.461 (2) Å) (Zhang, *et al.*, 2010), but longer than C=N (mean 1.269 (3) Å) (Mai, *et al.*, 2009). This is caused probably by electron delocalization in heterocyclic systems. In the crystal structure, the two triazole rings are almost coplanar, they are twisted by an angle of 3.8 (5)°. the central triazole ring form dihedral angles of 32.3 (6)° with the pyridyl ring. The crystal packing (Fig. 2) consists of two-dimensional infinite plane along the *b* axis generated by intermolecular interactions of N—H···N hydrogen bonds.

S2. Experimental

5-(Pyridin-2-yl)-1H,1′H-3,3′-bi(1,2,4-triazole)was prepared according to Wiley & Hart (1953) and Potts *et al.* (1960). The crystals suitable for crystallographic analysis were grown by recrystallization from DMF and ethanol solution as colorless block.

S3. Refinement

N-bound H-atoms were located in a difference map and refined freely. C-bound H atoms were positioned geometrically (C—H = 0.94 Å) and were constrained in a riding motion approximation with U_{iso}(H) = 1.2U_{eq}(C).

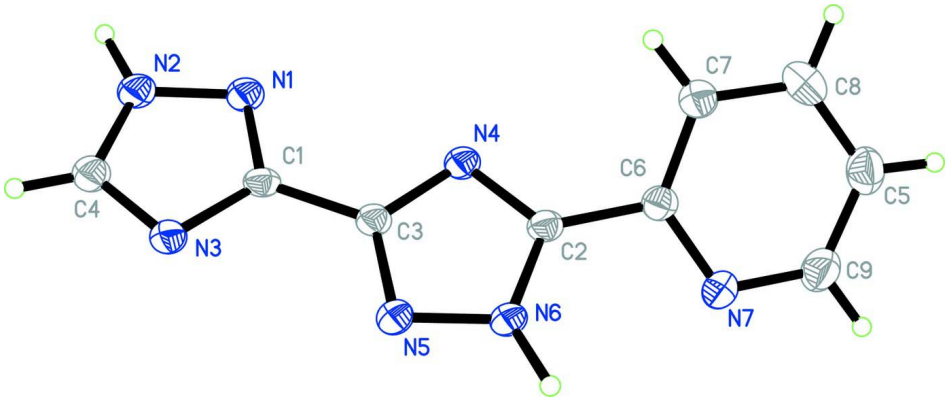

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

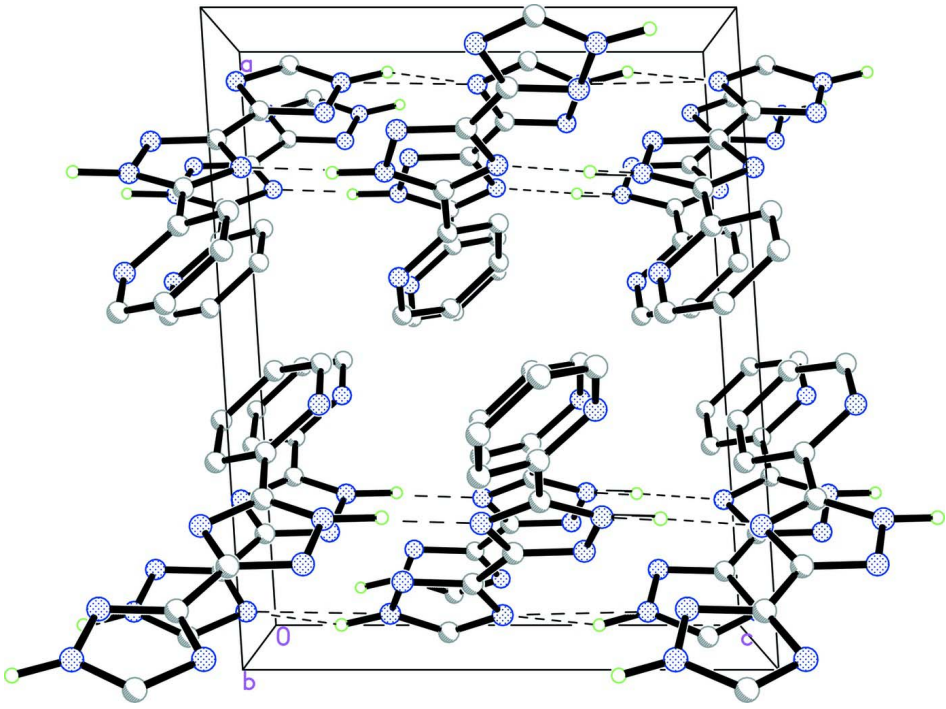

Figure 2

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines, viewed down the *b* axis.

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Crystal data

$C_9H_7N_7$
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$c = 10.007$ (2) Å
$\beta = 93.670$ (4)°
$V = 931.1$ (3) Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.521$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6322 reflections
$\theta = 2.0$–27.9°

μ = 0.11 mm^{-1}
T = 296 K

Block, colourless
0.24 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.979

5150 measured reflections
1832 independent reflections
1072 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 26.0°, θ_{min} = 1.7°
h = −15→12
k = −9→9
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.156
S = 0.94
1832 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.0843P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (5)

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}
N4	0.22980 (16)	0.2080 (3)	0.46400 (19)	0.0342 (6)
N6	0.23958 (18)	0.2161 (3)	0.6818 (2)	0.0370 (6)
N2	0.07056 (18)	−0.2247 (3)	0.2744 (2)	0.0394 (6)
N3	0.06963 (16)	−0.2067 (3)	0.4914 (2)	0.0367 (6)
N5	0.18243 (17)	0.0672 (3)	0.6502 (2)	0.0372 (6)
C1	0.1252 (2)	−0.0720 (3)	0.4381 (2)	0.0311 (6)
N1	0.12802 (17)	−0.0763 (3)	0.3067 (2)	0.0387 (6)
C2	0.26642 (19)	0.2993 (3)	0.5708 (2)	0.0329 (6)
C3	0.1792 (2)	0.0682 (3)	0.5182 (2)	0.0324 (6)
C4	0.0376 (2)	−0.2994 (3)	0.3838 (3)	0.0388 (7)
H4	−0.0028	−0.4034	0.3851	0.047*
N7	0.40073 (18)	0.4877 (3)	0.6744 (2)	0.0446 (6)

C5	0.4476 (2)	0.7649 (4)	0.5774 (3)	0.0543 (8)
H5	0.4900	0.8669	0.5828	0.065*
C6	0.3285 (2)	0.4650 (3)	0.5701 (2)	0.0343 (6)
C7	0.3123 (2)	0.5856 (3)	0.4680 (3)	0.0417 (7)
H7	0.2620	0.5636	0.3969	0.050*
C8	0.3724 (2)	0.7401 (4)	0.4729 (3)	0.0531 (8)
H8	0.3618	0.8257	0.4064	0.064*
C9	0.4592 (2)	0.6366 (4)	0.6738 (3)	0.0547 (8)
H9	0.5113	0.6543	0.7437	0.066*
H1	0.249 (2)	0.252 (4)	0.776 (4)	0.088 (11)*
H2	0.062 (2)	−0.262 (4)	0.179 (3)	0.081 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N4	0.0456 (13)	0.0338 (12)	0.0232 (11)	0.0004 (10)	0.0025 (9)	−0.0019 (9)
N6	0.0522 (14)	0.0363 (13)	0.0222 (12)	−0.0021 (11)	0.0009 (10)	−0.0032 (10)
N2	0.0552 (15)	0.0364 (13)	0.0262 (13)	0.0000 (11)	−0.0009 (10)	−0.0045 (10)
N3	0.0461 (13)	0.0346 (13)	0.0291 (12)	−0.0022 (10)	−0.0010 (10)	0.0007 (9)
N5	0.0483 (14)	0.0354 (13)	0.0276 (12)	−0.0030 (10)	−0.0001 (10)	−0.0029 (9)
C1	0.0411 (15)	0.0302 (14)	0.0220 (13)	0.0052 (11)	0.0015 (11)	0.0005 (11)
N1	0.0539 (15)	0.0371 (13)	0.0248 (12)	−0.0014 (11)	0.0011 (10)	−0.0023 (9)
C2	0.0402 (15)	0.0325 (15)	0.0257 (14)	0.0036 (12)	0.0003 (11)	−0.0006 (11)
C3	0.0422 (15)	0.0304 (14)	0.0246 (13)	0.0019 (11)	0.0022 (11)	−0.0009 (11)
C4	0.0485 (17)	0.0348 (15)	0.0329 (15)	0.0001 (12)	−0.0002 (12)	−0.0018 (12)
N7	0.0514 (14)	0.0434 (14)	0.0379 (14)	−0.0093 (12)	−0.0042 (11)	−0.0014 (11)
C5	0.061 (2)	0.0467 (19)	0.056 (2)	−0.0133 (15)	0.0099 (16)	−0.0040 (16)
C6	0.0399 (15)	0.0334 (15)	0.0299 (14)	0.0039 (12)	0.0041 (11)	−0.0020 (11)
C7	0.0461 (17)	0.0409 (16)	0.0380 (16)	0.0001 (13)	0.0017 (12)	0.0001 (13)
C8	0.057 (2)	0.0426 (17)	0.060 (2)	0.0022 (15)	0.0098 (16)	0.0114 (16)
C9	0.057 (2)	0.058 (2)	0.0487 (19)	−0.0165 (16)	−0.0029 (15)	−0.0037 (16)

Geometric parameters (Å, º)

N4—C2	1.326 (3)	C2—C6	1.467 (3)
N4—C3	1.356 (3)	C4—H4	0.9300
N6—C2	1.336 (3)	N7—C9	1.336 (3)
N6—N5	1.353 (3)	N7—C6	1.341 (3)
N6—H1	0.98 (4)	C5—C9	1.366 (4)
N2—C4	1.319 (3)	C5—C8	1.368 (4)
N2—N1	1.353 (3)	C5—H5	0.9300
N2—H2	0.99 (3)	C6—C7	1.372 (4)
N3—C4	1.322 (3)	C7—C8	1.380 (4)
N3—C1	1.354 (3)	C7—H7	0.9300
N5—C3	1.319 (3)	C8—H8	0.9300
C1—N1	1.318 (3)	C9—H9	0.9300
C1—C3	1.461 (3)		

C2—N4—C3	102.9 (2)	N2—C4—N3	111.0 (2)
C2—N6—N5	110.4 (2)	N2—C4—H4	124.5
C2—N6—H1	131 (2)	N3—C4—H4	124.5
N5—N6—H1	119 (2)	C9—N7—C6	115.9 (2)
C4—N2—N1	109.8 (2)	C9—C5—C8	118.6 (3)
C4—N2—H2	131.2 (19)	C9—C5—H5	120.7
N1—N2—H2	118.9 (19)	C8—C5—H5	120.7
C4—N3—C1	102.0 (2)	N7—C6—C7	123.6 (2)
C3—N5—N6	102.2 (2)	N7—C6—C2	115.3 (2)
N1—C1—N3	114.9 (2)	C7—C6—C2	121.1 (2)
N1—C1—C3	121.6 (2)	C6—C7—C8	118.7 (3)
N3—C1—C3	123.5 (2)	C6—C7—H7	120.7
C1—N1—N2	102.3 (2)	C8—C7—H7	120.7
N4—C2—N6	109.7 (2)	C5—C8—C7	118.7 (3)
N4—C2—C6	126.1 (2)	C5—C8—H8	120.6
N6—C2—C6	124.2 (2)	C7—C8—H8	120.6
N5—C3—N4	114.8 (2)	N7—C9—C5	124.5 (3)
N5—C3—C1	121.9 (2)	N7—C9—H9	117.8
N4—C3—C1	123.3 (2)	C5—C9—H9	117.8

C2—N6—N5—C3	0.7 (3)	N1—C1—C3—N4	4.1 (4)
C4—N3—C1—N1	0.6 (3)	N3—C1—C3—N4	−176.4 (2)
C4—N3—C1—C3	−179.1 (2)	N1—N2—C4—N3	0.5 (3)
N3—C1—N1—N2	−0.3 (3)	C1—N3—C4—N2	−0.6 (3)
C3—C1—N1—N2	179.4 (2)	C9—N7—C6—C7	−0.9 (4)
C4—N2—N1—C1	−0.2 (3)	C9—N7—C6—C2	178.9 (2)
C3—N4—C2—N6	0.6 (3)	N4—C2—C6—N7	−147.8 (3)
C3—N4—C2—C6	179.8 (2)	N6—C2—C6—N7	31.2 (3)
N5—N6—C2—N4	−0.9 (3)	N4—C2—C6—C7	32.0 (4)
N5—N6—C2—C6	180.0 (2)	N6—C2—C6—C7	−149.0 (2)
N6—N5—C3—N4	−0.3 (3)	N7—C6—C7—C8	−0.8 (4)
N6—N5—C3—C1	179.4 (2)	C2—C6—C7—C8	179.5 (2)
C2—N4—C3—N5	−0.2 (3)	C9—C5—C8—C7	−0.9 (5)
C2—N4—C3—C1	−179.9 (2)	C6—C7—C8—C5	1.7 (4)
N1—C1—C3—N5	−175.6 (2)	C6—N7—C9—C5	1.7 (4)
N3—C1—C3—N5	3.9 (4)	C8—C5—C9—N7	−0.9 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H1···N4^{i}	0.98 (4)	1.93 (4)	2.891 (3)	165 (3)
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