2-[(2H-Tetrazol-2-yl)methyl]benzonitrile

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The title compound, $C_9H_7N_5$, is non-planar with a dihedral angle between the substituted benzene and tetrazole rings of 71.13 (9)°. Molecules are connected in centrosymmetric dimers by weak C—H···N interactions [C···N is 3.548 (5) Å]; these are the only interactions of significance in the crystal structure.

Related literature

For the applications of tetrazole derivatives as ligands in coordination chemistry, see: Huang *et al.* (2006); Fu & Zhao (2007); Hu *et al.* (2007).
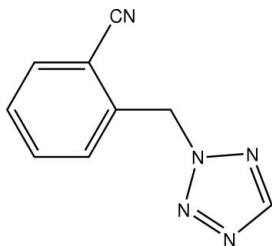
Experimental

Crystal data

$C_9H_7N_5$	V = 909.0 (15) Å^3
M_r = 185.20	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 12.213 (11) Å	μ = 0.09 mm^{-1}
b = 13.724 (13) Å	T = 293 (2) K
c = 5.549 (5) Å	0.22 × 0.15 × 0.1 mm
β = 102.24 (2)°	

Data collection

Rigaku SCXmini diffractometer	6450 measured reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	1493 independent reflections
T_{min} = 0.97, T_{max} = 1.00	1185 reflections with $I > 2\sigma(I)$
(expected range = 0.961–0.991)	R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059	127 parameters
$wR(F^2)$ = 0.187	H-atom parameters constrained
S = 1.05	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
1493 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

References

Fu, D.-W. & Zhao, H. (2007). *Acta Cryst.* E**63**, m1955.
Huang, X.-H., Sheng, T.-L., Xiang, S.-C., Fu, R.-B., Hu, S.-M., Li, Y.-M. & Wu, X.-T. (2006). *Inorg. Chem. Commun.* **9**, 1304–1307.
Hu, B., Xu, X.-B., Li, Y.-X. & Ye, H.-Y. (2007). *Acta Cryst.* E**63**, m2698.
Rigaku (2005). *CrystalClear*. Version 1.4.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

supporting information

2-[(2*H*-Tetrazol-2-yl)methyl]benzonitrile

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S1. Comment

Ligands containing tetrazole groups could serve as potential multidentate or bridging building blocks for the construction of polymeric structures as they possess several possible donor N atoms (Huang *et al.*,2006). The tetrazole functional group has found a wide range of applications in coordination chemistry as ligand in coordination chemistry, in medicinal chemistry as a metabolically stable surrogate for a carboxylic acid group, and in materials science as high density energy materials (Fu *et al.*, 2007). We originally attempted to synthesize complexes featuring Mn metal chains by reaction of the $MnCl_2.4H_2O$ with 2-(bromomethyl)benzonitrile and 2*H*-tetrazole ligand. Unfortunately, we obtained only the title compound and we report herein the crystal structure of the title compound, 2-[(2*H*-tetrazol-2-yl)methyl]benzonitrile (I) (Fig.1).

In the title molecule the bond lengths and angles are in normal ranges (Hu *et al.*, 2007). The phenyl ring is twisted away from coplanarity with the tetrazole ring and forms dihedral angles of 71.13 (9)°.

S2. Experimental

A mixture of 2-(bromomethyl)benzonitrile (39.2 mg, 0.2 mmol), 2*H*-tetrazole(14 mg, 0.2 mmol), KOH(11.2 mg, 0.2 mmol), $MnCl_2.4H_2O$ (20 mg, 0.1 mmol), 2 ml me thanol and 0.3 ml H_2O were placed in a thick Pyrex tube (*ca* 20 cm in length). The tube was frozen with liquid N_2, evacuated under vacuum and sealed by heat. The tube was then placed into oven at 75 °C for 3 days to give colorless block crystals of the title complex.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with d(C—H) = 0.93 and d(N—H) = 0.90Å and U_{iso}(H) = 1.2Ueq(C or N). In the absence of significant anomalous scattering effects, Friedel pairs were merged.
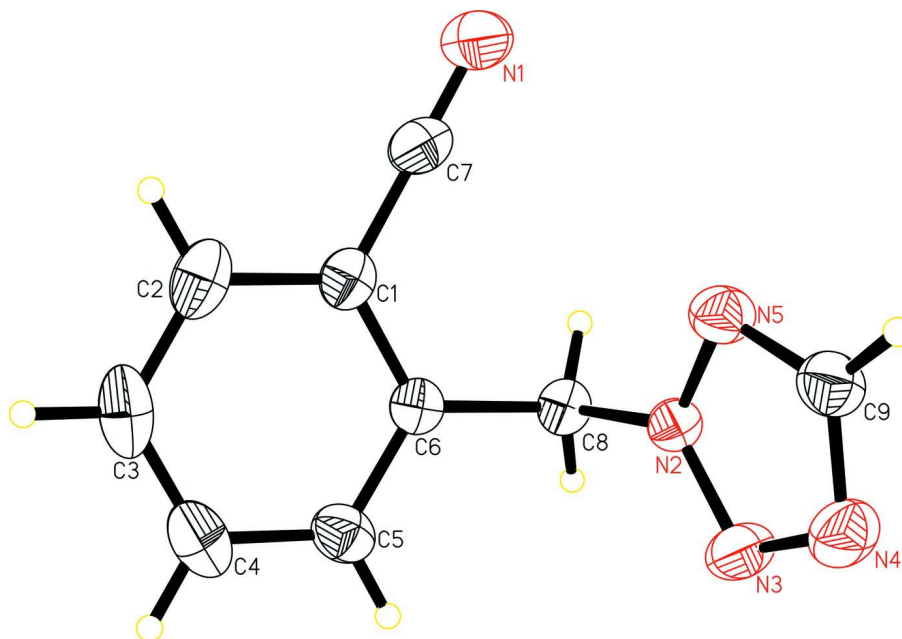
Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30%

probability level.

2-[(2H-Tetrazol-2-yl)methyl]benzonitrile

Crystal data

$C_9H_7N_5$	$F(000) = 384$
$M_r = 185.20$	$D_x = 1.353$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 356 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.213$ (11) Å	Cell parameters from 7893 reflections
$b = 13.724$ (13) Å	$\theta = 3.4$–27.5°
$c = 5.549$ (5) Å	$\mu = 0.09$ mm^{-1}
$\beta = 102.24$ (2)°	$T = 293$ K
$V = 909.0$ (15) Å^3	Block, colorless
$Z = 4$	$0.22 \times 0.15 \times 0.1$ mm

Data collection

Rigaku SCXmini diffractometer	6450 measured reflections
Radiation source: fine-focus sealed tube	1493 independent reflections
Graphite monochromator	1185 reflections with $I > 2\sigma(I)$
Detector resolution: 13.6612 pixels mm^{-1}	$R_{int} = 0.098$
ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan	$h = -14 \rightarrow 14$
(*CrystalClear*; Rigaku, 2005)	$k = -16 \rightarrow 16$
$T_{min} = 0.97$, $T_{max} = 1.00$	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.187$
$S = 1.05$
1493 reflections
127 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
$w = 1/[\sigma^2(F_o^2) + (0.1044P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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.

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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
C1	0.15609 (14)	0.47882 (13)	−0.0640 (4)	0.0489 (6)
C2	0.10185 (16)	0.56933 (17)	−0.1044 (5)	0.0666 (7)
H2A	0.0506	0.5814	−0.2510	0.080*
C3	0.1252 (2)	0.64046 (15)	0.0756 (6)	0.0744 (9)
H3A	0.0890	0.7004	0.0505	0.089*
C4	0.2020 (2)	0.62302 (15)	0.2925 (6)	0.0710 (7)
H4A	0.2181	0.6716	0.4117	0.085*
C5	0.25499 (16)	0.53387 (14)	0.3331 (4)	0.0569 (6)
H5A	0.3059	0.5226	0.4806	0.068*
C6	0.23325 (13)	0.46083 (12)	0.1566 (3)	0.0432 (5)
C7	0.12946 (15)	0.40397 (17)	−0.2487 (4)	0.0569 (6)
C8	0.29305 (15)	0.36441 (12)	0.2059 (4)	0.0465 (6)
H8A	0.3078	0.3507	0.3813	0.056*
H8B	0.2454	0.3130	0.1212	0.056*
C9	0.51482 (17)	0.36439 (14)	−0.0975 (4)	0.0587 (6)
H9A	0.5480	0.3608	−0.2334	0.070*
N1	0.10778 (17)	0.34457 (16)	−0.3975 (4)	0.0754 (7)
N2	0.39950 (12)	0.36529 (9)	0.1217 (3)	0.0433 (5)
N3	0.49695 (14)	0.37893 (13)	0.2704 (3)	0.0630 (6)
N4	0.57203 (15)	0.37836 (15)	0.1306 (4)	0.0678 (6)
N5	0.40562 (14)	0.35604 (12)	−0.1126 (3)	0.0552 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0428 (10)	0.0547 (11)	0.0522 (12)	0.0003 (8)	0.0167 (9)	0.0067 (8)
C2	0.0547 (13)	0.0700 (14)	0.0783 (15)	0.0112 (10)	0.0212 (12)	0.0261 (13)
C3	0.0700 (16)	0.0464 (12)	0.119 (2)	0.0109 (10)	0.0484 (17)	0.0138 (13)
C4	0.0750 (16)	0.0529 (12)	0.0948 (19)	−0.0049 (10)	0.0396 (15)	−0.0139 (12)
C5	0.0562 (13)	0.0592 (12)	0.0584 (13)	−0.0083 (9)	0.0191 (11)	−0.0097 (9)
C6	0.0407 (10)	0.0452 (9)	0.0463 (11)	−0.0036 (7)	0.0153 (9)	0.0037 (8)
C7	0.0463 (11)	0.0757 (14)	0.0472 (12)	−0.0005 (10)	0.0066 (10)	0.0048 (10)
C8	0.0457 (11)	0.0477 (11)	0.0480 (11)	−0.0004 (7)	0.0139 (9)	0.0058 (8)
C9	0.0521 (13)	0.0689 (14)	0.0585 (14)	−0.0083 (9)	0.0196 (11)	−0.0109 (10)
N1	0.0696 (13)	0.0911 (15)	0.0605 (13)	0.0000 (10)	0.0024 (11)	−0.0086 (11)
N2	0.0433 (9)	0.0448 (9)	0.0411 (9)	0.0003 (6)	0.0072 (7)	0.0010 (6)
N3	0.0460 (11)	0.0896 (13)	0.0505 (11)	−0.0045 (8)	0.0034 (9)	−0.0062 (9)
N4	0.0452 (10)	0.0904 (13)	0.0682 (13)	−0.0071 (8)	0.0133 (10)	−0.0068 (10)
N5	0.0523 (11)	0.0683 (11)	0.0455 (10)	−0.0045 (7)	0.0115 (8)	−0.0056 (8)

Geometric parameters (Å, °)

C1—C6	1.399 (3)	C6—C8	1.508 (3)
C1—C2	1.403 (3)	C7—N1	1.150 (3)
C1—C7	1.439 (3)	C8—N2	1.472 (3)
C2—C3	1.382 (4)	C8—H8A	0.9700
C2—H2A	0.9300	C8—H8B	0.9700
C3—C4	1.381 (4)	C9—N5	1.323 (3)
C3—H3A	0.9300	C9—N4	1.324 (3)
C4—C5	1.380 (3)	C9—H9A	0.9300
C4—H4A	0.9300	N2—N3	1.310 (2)
C5—C6	1.387 (3)	N2—N5	1.324 (3)
C5—H5A	0.9300	N3—N4	1.321 (3)
C6—C1—C2	120.24 (19)	C1—C6—C8	121.60 (17)
C6—C1—C7	120.39 (17)	N1—C7—C1	179.5 (2)
C2—C1—C7	119.35 (19)	N2—C8—C6	111.20 (14)
C3—C2—C1	119.4 (2)	N2—C8—H8A	109.4
C3—C2—H2A	120.3	C6—C8—H8A	109.4
C1—C2—H2A	120.3	N2—C8—H8B	109.4
C4—C3—C2	120.3 (2)	C6—C8—H8B	109.4
C4—C3—H3A	119.8	H8A—C8—H8B	108.0
C2—C3—H3A	119.8	N5—C9—N4	113.2 (2)
C5—C4—C3	120.3 (2)	N5—C9—H9A	123.4
C5—C4—H4A	119.9	N4—C9—H9A	123.4
C3—C4—H4A	119.9	N3—N2—N5	113.55 (16)
C4—C5—C6	120.8 (2)	N3—N2—C8	123.14 (17)
C4—C5—H5A	119.6	N5—N2—C8	123.26 (16)
C6—C5—H5A	119.6	N2—N3—N4	106.27 (18)
C5—C6—C1	118.86 (17)	N3—N4—C9	105.73 (18)

C5—C6—C8	119.54 (18)	C9—N5—N2	101.27 (16)
C6—C1—C2—C3	−0.1 (3)	C5—C6—C8—N2	−89.3 (2)
C7—C1—C2—C3	178.34 (18)	C1—C6—C8—N2	90.6 (2)
C1—C2—C3—C4	0.6 (3)	C6—C8—N2—N3	99.7 (2)
C2—C3—C4—C5	−0.9 (4)	C6—C8—N2—N5	−77.7 (2)
C3—C4—C5—C6	0.8 (3)	N5—N2—N3—N4	−0.3 (2)
C4—C5—C6—C1	−0.2 (3)	C8—N2—N3—N4	−177.94 (15)
C4—C5—C6—C8	179.64 (17)	N2—N3—N4—C9	0.1 (2)
C2—C1—C6—C5	−0.1 (3)	N5—C9—N4—N3	0.1 (3)
C7—C1—C6—C5	−178.51 (17)	N4—C9—N5—N2	−0.3 (2)
C2—C1—C6—C8	−179.96 (16)	N3—N2—N5—C9	0.38 (19)
C7—C1—C6—C8	1.6 (3)	C8—N2—N5—C9	178.00 (14)