organic compounds

4-[(2H-Tetrazol-2-yl)methyl]benzonitrile

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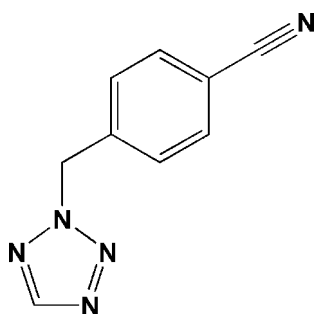Correspondence e-mail: quzr@seu.edu.cn

The title compound, $C_9H_7N_5$, was synthesized by reaction of 4-(bromomethyl)benzonitrile and 2H-tetrazole in the presence of KOH. The relative orientation of the planar tetrazole ring and the methylbenzonitrile moiety is (−)-anticlinal. The crystal packing is dominated by van der Waals interactions.

Related literature

For the chemisty of tetrazoles, see: Bethel *et al.* (1999); Wu *et al.* (2005); Zhang *et al.* (2006); Jin *et al.* (1994).

Experimental

Crystal data

$C_9H_7N_5$	γ = 72.600 (5)°
M_r = 185.20	V = 448.64 (10) Å^3
Triclinic, $P\bar{1}$	Z = 2
a = 5.7514 (8) Å	Mo $K\alpha$ radiation
b = 7.4029 (10) Å	μ = 0.09 mm^{-1}
c = 11.3511 (12) Å	T = 293 (2) K
α = 81.088 (3)°	$0.20 \times 0.12 \times 0.02$ mm
β = 77.844 (3)°	

Data collection

Rigaku Mercury2 diffractometer	4114 measured reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	1720 independent reflections
T_{min} = 0.980, T_{max} = 0.996	923 reflections with $I > 2\sigma(I)$
	R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.156	
S = 0.92	
1720 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
132 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

References

Bethel, P. A., Hill, M. S., Mahon, M. F. & Molloy, K. C. (1999). *J. Chem. Soc. Perkin Trans. 1*, pp. 3507–3514.
Jin, Z., Nolan, K., McArthur, C. R., Lever, A. B. P. & Leznoff, C. C. (1994). *J. Organomet. Chem.* **468**, 205–212.
Rigaku (2005). *CrystalClear*. Version 1.4.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wu, T., Yi, B. H. & Li, D. (2005). *Inorg. Chem.* **44**, 4130–4132.
Zhang, X. M., Zhao, Y. F., Wu, H. S., Batten, S. R. & Ng, S. W. (2006). *Dalton Trans.* pp. 3170–3178.

supplementary materials

4-[(2*H*-Tetrazol-2-yl)methyl]benzonitrile

Z. Xing and Z.-R. Qu

Comment

Tetrazoles has been the subject of investigations during the last 20 years (Bethel *et al.*, 1999). In recent years, tetrazoles have found a wide range of applications in coordination chemistry due to their role as mono- or bidentate ligands and strong networking ability (Wu *et al.*, 2005; Zhang *et al.*, 2006). Nitrile derivatives have found many industrial applications. For example, phthalonitriles have been used as starting materials for phthalocyanines (Jin *et al.*, 1994). The title compound, is a new tetrazole derivative. We now report the synthesis and crystal structure analysis of 4-((2*H*-tetrazol-2-yl)methyl)benzonitrile (Fig. 1). The overall molecular conformation is defined by the torsion angle N1—N4—C8—C5 of −92.05 (10)°.

Experimental

The ligand 4-((2*H*-tetrazol-2-yl)methyl)benzonitrile was synthesized by reaction of 4-(bromomethyl)benzonitrile (1.95 g, 0.01 mol) and 2*H*-tetrazole (0.7 g, 0.01 mol) and KOH (0.56 g, 0.01 mol) in methanol (20 ml) reacted at 353 K with stirring for 24 h. A mixture of 4-((2*H*-tetrazol-2-yl)methyl)benzonitrile (18.5 mg, 0.1 mmol) and water (15 ml) and ethanol (15 ml) sealed in a glass were maintained at 293 K. Crystals suitable for X-ray ananlysis were obtained after 2 d.

Refinement

H atoms were included at calculated positions and constrained to an ideal geometry, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Figures
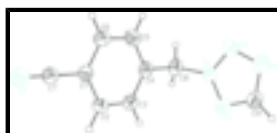
Fig. 1. A view of the compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

4-[(2*H*-Tetrazol-2-yl)methyl]benzonitrile

Crystal data

$C_9H_7N_5$	$Z = 2$
$M_r = 185.20$	$F_{000} = 192$
Triclinic, $P\bar{1}$	$D_x = 1.371$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.7514$ (8) Å	Cell parameters from 655 reflections
$b = 7.4029$ (10) Å	$\theta = 3.3$–27.4º

$c = 11.3511\ (12)$ Å

$\alpha = 81.088\ (3)°$

$\beta = 77.844\ (3)°$

$\gamma = 72.600\ (5)°$

$V = 448.64\ (10)$ Å^3

$\mu = 0.09$ mm^{-1}

$T = 293\ (2)$ K

Block, colourless

$0.20 \times 0.12 \times 0.02$ mm

Data collection

Rigaku Mercury2 diffractometer	1720 independent reflections
Radiation source: fine-focus sealed tube	923 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 26.0°$
$T = 293(2)$ K	$\theta_{min} = 3.3°$
CCD_Profile_fitting scans	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	$k = -9 \rightarrow 9$
$T_{min} = 0.980$, $T_{max} = 0.996$	$l = -13 \rightarrow 13$
4114 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o{}^2) + (0.0718P)^2]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$
$wR(F^2) = 0.156$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.92$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
1720 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
132 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.044 (14)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
N2	1.0618 (5)	0.2439 (4)	0.4265 (2)	0.0821 (8)
C1	0.3315 (4)	0.9248 (4)	0.9005 (2)	0.0554 (6)
C2	0.4374 (4)	0.7403 (3)	0.8573 (2)	0.0502 (6)
C3	0.6613 (4)	0.6272 (3)	0.8855 (2)	0.0547 (7)
H3	0.7445	0.6703	0.9324	0.066*
C4	0.7606 (4)	0.4506 (3)	0.8438 (2)	0.0560 (7)
H4	0.9121	0.3749	0.8622	0.067*
C5	0.6377 (4)	0.3841 (3)	0.7748 (2)	0.0525 (6)
C6	0.4133 (5)	0.4976 (4)	0.7479 (2)	0.0621 (7)
H6	0.3292	0.4541	0.7018	0.075*
C7	0.3128 (5)	0.6752 (4)	0.7891 (2)	0.0606 (7)
H7	0.1613	0.7510	0.7708	0.073*
C8	0.7485 (5)	0.1932 (3)	0.7266 (2)	0.0611 (7)
H8A	0.8329	0.1040	0.7865	0.073*
H8B	0.6176	0.1460	0.7124	0.073*
N1	0.8605 (4)	0.2339 (4)	0.5064 (2)	0.0764 (7)
C9	1.2358 (6)	0.2213 (5)	0.4920 (3)	0.0730 (9)
N3	1.1596 (4)	0.1945 (3)	0.6083 (2)	0.0703 (7)
N4	0.9239 (4)	0.2044 (3)	0.61371 (17)	0.0550 (6)
N5	0.2481 (4)	1.0719 (3)	0.9343 (2)	0.0770 (8)
H9	1.385 (6)	0.208 (5)	0.462 (3)	0.116 (13)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0782 (17)	0.103 (2)	0.0630 (15)	−0.0277 (15)	−0.0037 (14)	−0.0081 (13)
C1	0.0509 (14)	0.0546 (15)	0.0616 (16)	−0.0117 (13)	−0.0132 (12)	−0.0098 (13)
C2	0.0510 (14)	0.0511 (14)	0.0485 (13)	−0.0148 (12)	−0.0083 (11)	−0.0038 (11)
C3	0.0527 (15)	0.0602 (16)	0.0554 (15)	−0.0151 (12)	−0.0162 (12)	−0.0101 (12)
C4	0.0481 (14)	0.0594 (15)	0.0569 (15)	−0.0083 (12)	−0.0081 (12)	−0.0091 (12)
C5	0.0569 (15)	0.0506 (14)	0.0493 (14)	−0.0184 (12)	−0.0030 (12)	−0.0045 (11)
C6	0.0635 (17)	0.0629 (17)	0.0672 (17)	−0.0183 (14)	−0.0200 (13)	−0.0144 (13)
C7	0.0489 (14)	0.0657 (17)	0.0690 (17)	−0.0118 (12)	−0.0165 (12)	−0.0113 (13)
C8	0.0634 (16)	0.0532 (15)	0.0625 (15)	−0.0163 (13)	0.0032 (13)	−0.0118 (12)
N1	0.0705 (16)	0.0940 (18)	0.0654 (15)	−0.0193 (14)	−0.0167 (13)	−0.0102 (13)
C9	0.063 (2)	0.087 (2)	0.070 (2)	−0.0270 (17)	0.0022 (17)	−0.0190 (16)
N3	0.0574 (14)	0.0879 (17)	0.0730 (16)	−0.0225 (12)	−0.0144 (12)	−0.0204 (13)
N4	0.0550 (13)	0.0549 (12)	0.0575 (13)	−0.0148 (10)	−0.0104 (10)	−0.0124 (10)
N5	0.0703 (16)	0.0659 (16)	0.0962 (18)	−0.0046 (13)	−0.0285 (13)	−0.0211 (13)

Geometric parameters (Å, °)

N2—C9	1.326 (4)	C5—C8	1.502 (3)
N2—N1	1.325 (3)	C6—C7	1.380 (3)
C1—N5	1.141 (3)	C6—H6	0.9300

C1—C2	1.436 (3)	C7—H7	0.9300
C2—C7	1.379 (3)	C8—N4	1.463 (3)
C2—C3	1.381 (3)	C8—H8A	0.9700
C3—C4	1.375 (3)	C8—H8B	0.9700
C3—H3	0.9300	N1—N4	1.312 (3)
C4—C5	1.384 (3)	C9—N3	1.304 (3)
C4—H4	0.9300	C9—H9	0.84 (3)
C5—C6	1.379 (3)	N3—N4	1.324 (3)
C9—N2—N1	105.1 (2)	C2—C7—C6	119.9 (2)
N5—C1—C2	179.6 (3)	C2—C7—H7	120.0
C7—C2—C3	120.1 (2)	C6—C7—H7	120.0
C7—C2—C1	119.7 (2)	N4—C8—C5	111.39 (19)
C3—C2—C1	120.2 (2)	N4—C8—H8A	109.4
C4—C3—C2	119.6 (2)	C5—C8—H8A	109.4
C4—C3—H3	120.2	N4—C8—H8B	109.4
C2—C3—H3	120.2	C5—C8—H8B	109.4
C3—C4—C5	120.8 (2)	H8A—C8—H8B	108.0
C3—C4—H4	119.6	N4—N1—N2	106.5 (2)
C5—C4—H4	119.6	N3—C9—N2	113.6 (3)
C6—C5—C4	119.2 (2)	N3—C9—H9	122 (3)
C6—C5—C8	120.0 (2)	N2—C9—H9	124 (2)
C4—C5—C8	120.9 (2)	C9—N3—N4	102.1 (2)
C5—C6—C7	120.5 (2)	N1—N4—N3	112.7 (2)
C5—C6—H6	119.8	N1—N4—C8	123.1 (2)
C7—C6—H6	119.8	N3—N4—C8	124.1 (2)
C7—C2—C3—C4	0.8 (4)	C4—C5—C8—N4	−83.5 (3)
C1—C2—C3—C4	179.9 (2)	C9—N2—N1—N4	−0.6 (3)
C2—C3—C4—C5	−0.6 (4)	N1—N2—C9—N3	1.0 (3)
C3—C4—C5—C6	0.1 (4)	N2—C9—N3—N4	−1.0 (3)
C3—C4—C5—C8	178.5 (2)	N2—N1—N4—N3	0.0 (3)
C4—C5—C6—C7	0.1 (4)	N2—N1—N4—C8	177.3 (2)
C8—C5—C6—C7	−178.3 (2)	C9—N3—N4—N1	0.6 (3)
C3—C2—C7—C6	−0.6 (4)	C9—N3—N4—C8	−176.6 (2)
C1—C2—C7—C6	−179.7 (2)	C5—C8—N4—N1	−92.0 (3)
C5—C6—C7—C2	0.1 (4)	C5—C8—N4—N3	84.9 (3)
C6—C5—C8—N4	94.9 (3)		

Fig. 1