organic compounds

2-(1H-Tetrazol-5-yl)benzonitrile

Zheng Xing, Guang-Fan Han,* Wei-Feng Zhu and Yu-Yuan Zhao

School of Materials Science and Engineering, Jiangsu University of Science, and Technology, Zhenjiang, Jiangsu 212003, People's Republic of China

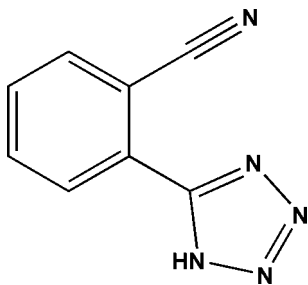Correspondence e-mail: gf552002@yahoo.com.cn

The title compound, $C_8H_5N_5$, was synthesized from phthalonitrile. The benzonitrile and tetrazole rings are inclined at a dihedral angle of 37.14 (11)°. In the crystal structure, intermolecular N—H···N hydrogen bonds link the tetrazole rings of adjacent molecules, forming chains along the a axis.

Related literature

For background to the chemisty of tetrazoles, see: Bekhit *et al.* (2004); Aykut İkizler & Sancak (1992, 1995, 1998); Rajasekaran & Thampi (2004); Satyanarayana *et al.* (2006); Schmidt & Schieffer (2003); Upadhayaya *et al.* (2004); Wexler *et al.* (1996).

Experimental

Crystal data

$C_8H_5N_5$	$b = 6.5420$ (13) Å
$M_r = 171.17$	$c = 24.867$ (5) Å
Monoclinic, $P2_1/n$	$\beta = 95.27$ (3)°
$a = 4.9281$ (10) Å	$V = 798.3$ (3) Å^3

$Z = 4$	$T = 293$ (2) K
Mo $K\alpha$ radiation	$0.25 \times 0.07 \times 0.07$ mm
$\mu = 0.10$ mm^{-1}	

Data collection

Rigaku SCXmini diffractometer	6844 measured reflections
Absorption correction: multi-scan	1553 independent reflections
(*CrystalClear*; Rigaku, 2005)	1167 reflections with $I > 2\sigma(I)$
$T_{min} = 0.993$, $T_{max} = 0.996$	$R_{int} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$	H atoms treated by a mixture of
$wR(F^2) = 0.138$	independent and constrained
$S = 1.10$	refinement
1553 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
122 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N5^i	0.92 (3)	1.91 (3)	2.820 (2)	172 (2)
N2—H2···N4^i	0.92 (3)	2.60 (3)	3.374 (2)	142 (2)

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2471).

References

Aykut İkizler, A. & Sancak, K. (1992). *Monatsh. Chem.* **123**, 257–263.
Aykut İkizler, A. & Sancak, K. (1995). *Collect. Czech. Chem. Commun.* **60**, 903–909.
Aykut İkizler, A. & Sancak, K. (1998). *Rev. Roum. Chim.* **43**, 133–138.
Bekhit, A. A., El-Sayed, O. A., Aboulmagd, E. & Park, J. Y. (2004). *Eur. J. Med. Chem.* **39**, 249–255.
Rajasekaran, A. & Thampi, P. P. (2004). *Eur. J. Med. Chem.* **39**, 273–279.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Satyanarayana, B., Sumalatha, Y., Sridhar, C., Venkatraman, S. & Reddy, P. P. (2006). *Synth. Commun.* **36**, 2079–2086.
Schmidt, B. & Schieffer, B. (2003). *J. Med. Chem.* **46**, 2261–2270.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Upadhayaya, R. S., Jain, S., Sinha, N., Kishore, N., Chandra, R. & Arora, S. K. (2004). *Eur. J. Med. Chem.* **39**, 579–592.
Wexler, R. R., Greenlee, W. J., Irvin, J. D., Goldberg, M. R., Prendergast, K., Smith, R. D. & Timmermans, P. B. M. W. (1996). *J. Med. Chem.* **39**, 625–656.

supplementary materials

2-(1*H*-Tetrazol-5-yl)benzonitrile

Z. Xing, G.-F. Han, W.-F. Zhu and Y.-Y. Zhao

Comment

Nitriles are close relatives of azoles and hydrazones and are parent compounds for the preparation of various functional organic materials having triazole, imidazole or tetrazole rings (Aykut İkizler & Sancak, 1992, 1995, 1998). Tetrazoles find wide application in the synthesis of medicinal products such as antihypertensive agents (Wexler *et al.*, 1996; Schmidt & Schieffer, 2003; Satyanarayana *et al.*, 2006), resolvents (Bekhit *et al.*, 2004), anaesthetics (Rajasekaran & Thampi, 2004) and antifungal agents (Upadhayaya *et al.*, 2004). We report herein the crystal structure of the title compound, 2-(1*H*-tet-razol-5-yl)benzonitrile, Fig 1 with its crystal packing shown in Figure 2, Table 1.

Experimental

Phthalonitrile (1.28 g, 0.01 mol), sodium azide (0.975 g, 0.015 mol), ammonium chloride (0.605 g, 0.011 mol) and DMF (15 ml) were added in a flask and reacted at 120 °C with stirring for 24 h. A mass of white solid was collected after solvents removed. The crude product was recrystallized by slowly evaporating a mixed solution of ethanol and water (2:1) to yield colorless prism-like crystals, suitable for X-ray analysis.

Refinement

The H2 atom bound to N2 was located in a difference map and was refined freely. Other H atoms were placed in calculated positions, with C—H = 0.93 Å and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2 U_{eq}$
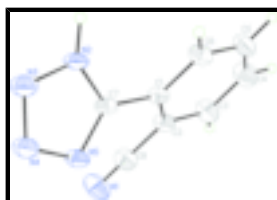
Figures

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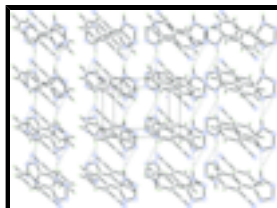

Fig. 2. The crystal packing of the title compound viewed along the *c* axis. Hydrogen bonds are drawn as dashed lines.

(I)

Crystal data

$C_8H_5N_5$	$F_{000} = 352$
$M_r = 171.17$	$D_x = 1.424$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 6584 reflections
$a = 4.9281$ (10) Å	$\theta = 3.1–28.8°$
$b = 6.5420$ (13) Å	$\mu = 0.10$ mm^{-1}
$c = 24.867$ (5) Å	$T = 293$ (2) K
$\beta = 95.27$ (3)°	Prism, colorless
$V = 798.3$ (3) Å^3	$0.25 \times 0.07 \times 0.07$ mm
$Z = 4$	

Data collection

Rigaku SCXmini diffractometer	1553 independent reflections
Radiation source: fine-focus sealed tube	1167 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 26.0°$
$T = 293(2)$ K	$\theta_{min} = 3.2°$
ω scans	$h = -6 \rightarrow 6$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	$k = -8 \rightarrow 8$
$T_{min} = 0.993$, $T_{max} = 0.996$	$l = -30 \rightarrow 30$
6844 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
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.1285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.138$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
1553 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
122 parameters	Extinction correction: SHELXL
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.044 (14)
Secondary atom site location: difference Fourier map	

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}
C1	0.5249 (4)	0.5054 (3)	0.13602 (8)	0.0345 (5)
C2	0.6569 (4)	0.5277 (3)	0.08892 (8)	0.0403 (5)
C3	0.6021 (5)	0.6960 (4)	0.05536 (10)	0.0548 (7)
H3	0.6925	0.7116	0.0244	0.066*
C4	0.4141 (5)	0.8390 (4)	0.06821 (11)	0.0608 (7)
H4	0.3762	0.9509	0.0457	0.073*
C5	0.2821 (5)	0.8174 (4)	0.11410 (11)	0.0539 (6)
H5	0.1537	0.9140	0.1223	0.065*
C6	0.3384 (4)	0.6532 (3)	0.14819 (9)	0.0441 (6)
H6	0.2504	0.6416	0.1796	0.053*
C7	0.5736 (4)	0.3299 (3)	0.17202 (8)	0.0323 (5)
C8	0.8482 (5)	0.3773 (4)	0.07280 (9)	0.0476 (6)
N1	0.9990 (5)	0.2612 (4)	0.05847 (9)	0.0701 (7)
N2	0.3814 (3)	0.2405 (3)	0.19806 (7)	0.0399 (5)
N3	0.4920 (3)	0.0893 (3)	0.22916 (8)	0.0480 (5)
N4	0.7498 (3)	0.0881 (3)	0.22217 (7)	0.0458 (5)
N5	0.8068 (3)	0.2363 (3)	0.18650 (7)	0.0380 (5)
H2	0.195 (6)	0.253 (4)	0.1939 (10)	0.072 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0263 (10)	0.0405 (11)	0.0363 (11)	0.0019 (9)	0.0016 (8)	0.0010 (9)
C2	0.0345 (12)	0.0463 (12)	0.0407 (12)	0.0040 (10)	0.0062 (9)	0.0018 (10)
C3	0.0598 (16)	0.0595 (15)	0.0473 (14)	0.0110 (12)	0.0171 (12)	0.0137 (12)
C4	0.0658 (17)	0.0558 (15)	0.0611 (17)	0.0139 (13)	0.0072 (14)	0.0187 (13)
C5	0.0491 (14)	0.0480 (14)	0.0642 (16)	0.0144 (11)	0.0041 (12)	−0.0003 (12)
C6	0.0397 (12)	0.0507 (13)	0.0425 (13)	0.0070 (10)	0.0069 (10)	−0.0014 (10)
C7	0.0221 (9)	0.0434 (11)	0.0319 (11)	0.0004 (8)	0.0055 (8)	−0.0021 (9)
C8	0.0476 (13)	0.0573 (15)	0.0395 (13)	0.0069 (12)	0.0127 (10)	0.0069 (11)
N1	0.0705 (15)	0.0809 (15)	0.0623 (15)	0.0288 (13)	0.0242 (12)	0.0062 (12)
N2	0.0203 (9)	0.0531 (11)	0.0468 (11)	0.0024 (8)	0.0058 (8)	0.0107 (8)

N3	0.0306 (9)	0.0600 (12)	0.0540 (12)	0.0029 (9)	0.0074 (8)	0.0166 (10)
N4	0.0296 (9)	0.0583 (12)	0.0494 (11)	0.0047 (8)	0.0042 (8)	0.0139 (9)
N5	0.0238 (8)	0.0510 (10)	0.0400 (10)	0.0035 (8)	0.0065 (7)	0.0070 (8)

Geometric parameters (Å, °)

C1—C6	1.386 (3)	C5—H5	0.9300
C1—C2	1.399 (3)	C6—H6	0.9300
C1—C7	1.462 (3)	C7—N5	1.323 (2)
C2—C3	1.393 (3)	C7—N2	1.331 (2)
C2—C8	1.445 (3)	C8—N1	1.142 (3)
C3—C4	1.375 (3)	N2—N3	1.340 (2)
C3—H3	0.9300	N2—H2	0.92 (3)
C4—C5	1.372 (3)	N3—N4	1.298 (2)
C4—H4	0.9300	N4—N5	1.361 (2)
C5—C6	1.381 (3)		
C6—C1—C2	118.61 (19)	C6—C5—H5	119.8
C6—C1—C7	119.24 (18)	C5—C6—C1	120.5 (2)
C2—C1—C7	122.13 (17)	C5—C6—H6	119.7
C3—C2—C1	120.31 (19)	C1—C6—H6	119.7
C3—C2—C8	117.86 (19)	N5—C7—N2	107.65 (17)
C1—C2—C8	121.81 (19)	N5—C7—C1	128.31 (17)
C4—C3—C2	119.7 (2)	N2—C7—C1	123.99 (17)
C4—C3—H3	120.1	N1—C8—C2	177.8 (2)
C2—C3—H3	120.1	C7—N2—N3	109.61 (16)
C5—C4—C3	120.3 (2)	C7—N2—H2	130.9 (16)
C5—C4—H4	119.9	N3—N2—H2	118.7 (16)
C3—C4—H4	119.9	N4—N3—N2	106.16 (16)
C4—C5—C6	120.5 (2)	N3—N4—N5	110.25 (16)
C4—C5—H5	119.8	C7—N5—N4	106.33 (15)
C6—C1—C2—C3	0.4 (3)	C6—C1—C7—N5	−141.7 (2)
C7—C1—C2—C3	179.22 (19)	C2—C1—C7—N5	39.5 (3)
C6—C1—C2—C8	−178.3 (2)	C6—C1—C7—N2	35.6 (3)
C7—C1—C2—C8	0.5 (3)	C2—C1—C7—N2	−143.2 (2)
C1—C2—C3—C4	−1.1 (4)	N5—C7—N2—N3	−0.1 (2)
C8—C2—C3—C4	177.7 (2)	C1—C7—N2—N3	−177.85 (18)
C2—C3—C4—C5	0.5 (4)	C7—N2—N3—N4	0.3 (2)
C3—C4—C5—C6	0.7 (4)	N2—N3—N4—N5	−0.4 (2)
C4—C5—C6—C1	−1.3 (4)	N2—C7—N5—N4	−0.2 (2)
C2—C1—C6—C5	0.8 (3)	C1—C7—N5—N4	177.48 (19)
C7—C1—C6—C5	−178.05 (19)	N3—N4—N5—C7	0.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N5[i]	0.92 (3)	1.91 (3)	2.820 (2)	172 (2)
N2—H2···N4[i]	0.92 (3)	2.60 (3)	3.374 (2)	142 (2)

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

Fig. 2