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

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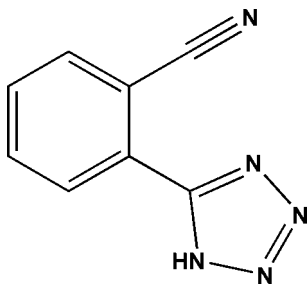
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.055; wR factor = 0.138; data-to-parameter ratio = 12.7.

The title compound, $\text{C}_8\text{H}_5\text{N}_5$, was synthesized from phthalonitrile. The benzonitrile and tetrazole rings are inclined at a dihedral angle of 37.14 (11)°. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds link the tetrazole rings of adjacent molecules, forming chains along the a axis.

Related literature

For background to the chemistry of tetrazoles, see: Bekhit *et al.* (2004); Aykut İközler & 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

$\text{C}_8\text{H}_5\text{N}_5$
 $M_r = 171.17$
 Monoclinic, $P2_1/n$
 $a = 4.9281$ (10) Å

$b = 6.5420$ (13) Å
 $c = 24.867$ (5) Å
 $\beta = 95.27$ (3)°
 $V = 798.3$ (3) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹

$T = 293$ (2) K
 $0.25 \times 0.07 \times 0.07$ mm

Data collection

Rigaku SCXmini diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.993$, $T_{\max} = 0.996$

6844 measured reflections
 1553 independent reflections
 1167 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.138$
 $S = 1.10$
 1553 reflections
 122 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|----------|-------------|-------------|---------------|
| $\text{N2}-\text{H2}\cdots\text{N5}^i$ | 0.92 (3) | 1.91 (3) | 2.820 (2) | 172 (2) |
| $\text{N2}-\text{H2}\cdots\text{N4}^i$ | 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*.

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

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supporting information

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2-(1*H*-Tetrazol-5-yl)benzotrile**Zheng Xing, Guang-Fan Han, Wei-Feng Zhu and Yu-Yuan Zhao****S1. 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 İközler & 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*-tetrazol-5-yl)benzotrile, Fig 1 with its crystal packing shown in Figure 2, Table 1.

S2. 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.

S3. 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$

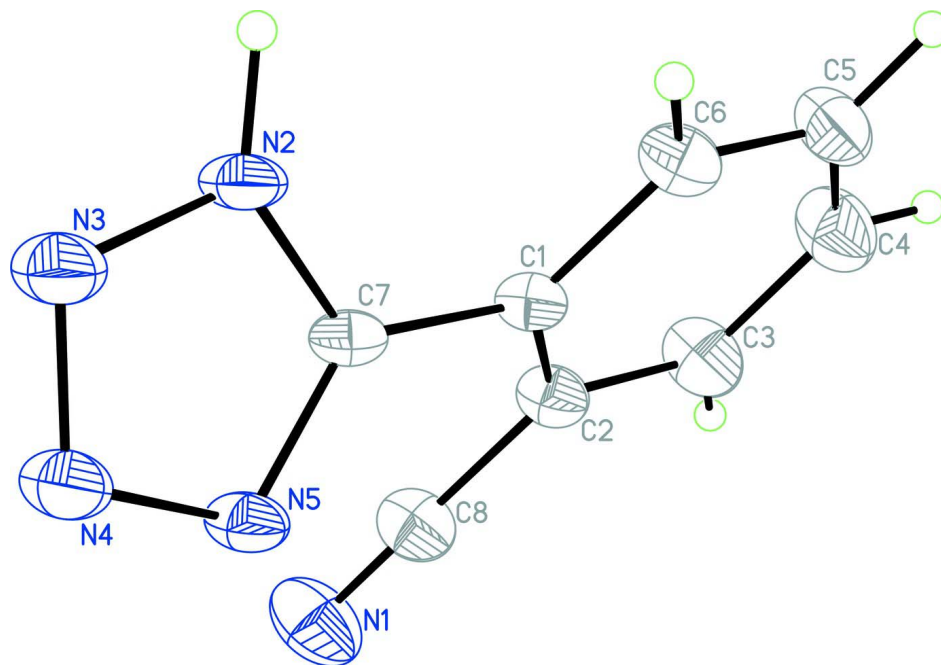


Figure 1

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

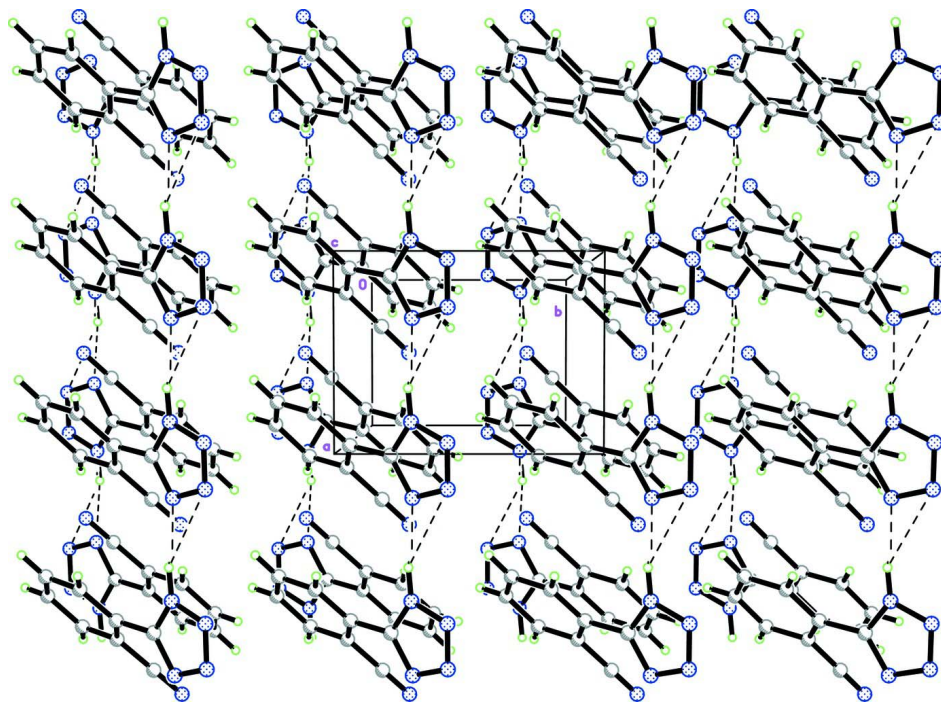


Figure 2

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

(I)

*Crystal data*C₈H₅N₅ $M_r = 171.17$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 4.9281 (10) \text{ \AA}$ $b = 6.5420 (13) \text{ \AA}$ $c = 24.867 (5) \text{ \AA}$ $\beta = 95.27 (3)^\circ$ $V = 798.3 (3) \text{ \AA}^3$ $Z = 4$ $F(000) = 352$ $D_x = 1.424 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 6584 reflections

 $\theta = 3.1\text{--}28.8^\circ$ $\mu = 0.10 \text{ mm}^{-1}$ $T = 293 \text{ K}$

Prism, colorless

 $0.25 \times 0.07 \times 0.07 \text{ mm}$ *Data collection*

Rigaku SCXmini

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 13.6612 pixels mm^{-1} ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku, 2005)

 $T_{\min} = 0.993$, $T_{\max} = 0.996$

6844 measured reflections

1553 independent reflections

1167 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.061$ $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.2^\circ$ $h = -6 \rightarrow 6$ $k = -8 \rightarrow 8$ $l = -30 \rightarrow 30$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.138$ $S = 1.10$

1553 reflections

122 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

 $w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.1285P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL*

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 $F^2 > \sigma(F^2)$ 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|------------|------------|-------------|----------------------------------|
| 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 (Å²)

| | 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 (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------|----------|-------------|-------------|---------------|
| N2—H2 \cdots N5 ⁱ | 0.92 (3) | 1.91 (3) | 2.820 (2) | 172 (2) |
| N2—H2 \cdots N4 ⁱ | 0.92 (3) | 2.60 (3) | 3.374 (2) | 142 (2) |

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