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## Structure Reports

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# 4-[(1*H*-Benzotriazol-1-yl)methyl]benzotrile

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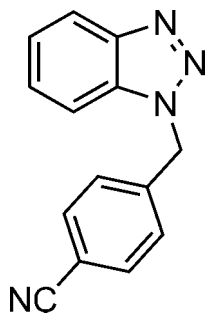
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.067;  $wR$  factor = 0.182; data-to-parameter ratio = 16.7.

In the molecule of the title compound,  $\text{C}_{14}\text{H}_{10}\text{N}_4$ , which was prepared by reaction of benzotriazole with 4-(bromomethyl)benzonitrile in alkaline solution, the dihedral angle between the benzotriazole and benzene ring systems is  $69.03(6)^\circ$ .

## Related literature

For the application of benzotriazole compounds in industry, see: Pillard *et al.* (2001); Kopanska *et al.* (2004); Gruden *et al.* (2001). For the structure of a related compound, see: Selvanayagam *et al.* (2002).



## Experimental

## Crystal data

$\text{C}_{14}\text{H}_{10}\text{N}_4$	$V = 1193.0(2) \text{ \AA}^3$
$M_r = 234.26$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.1912(13) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 19.0520(9) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 8.6610(6) \text{ \AA}$	$0.50 \times 0.40 \times 0.40 \text{ mm}$
$\beta = 118.0390(10)^\circ$	

## Data collection

Rigaku Mercury2 diffractometer	11866 measured reflections
Absorption correction: multi-scan ( <i>CrystalClear</i> ; Rigaku, 2005)	2715 independent reflections
$T_{\min} = 0.960$ , $T_{\max} = 0.969$	1903 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.047$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$	163 parameters
$wR(F^2) = 0.182$	H-atom parameters constrained
$S = 1.09$	$\Delta\rho_{\max} = 0.34 \text{ e \AA}^{-3}$
2715 reflections	$\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2206).

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## supporting information

*Acta Cryst.* (2008). E64, o975 [doi:10.1107/S1600536808010969]

**4-[(1*H*-Benzotriazol-1-yl)methyl]benzonitrile****Wen-Xiang Wang and Hong Zhao****S1. Comment**

Benzotriazole and its derivatives comprise an important class of corrosion inhibitors, typically used as trace additives in industrial chemical mixtures, such as coolants, cutting fluids and hydraulic fluid (Pillard *et al.*, 2001). These derivatives are also used as inhibitors of *Acanthamoeba castellanii* (Kopanska *et al.*, 2004) and are responsible for toxicity to bacteria (Gruden *et al.*, 2001). In this paper the crystal structure of the title compound is reported.

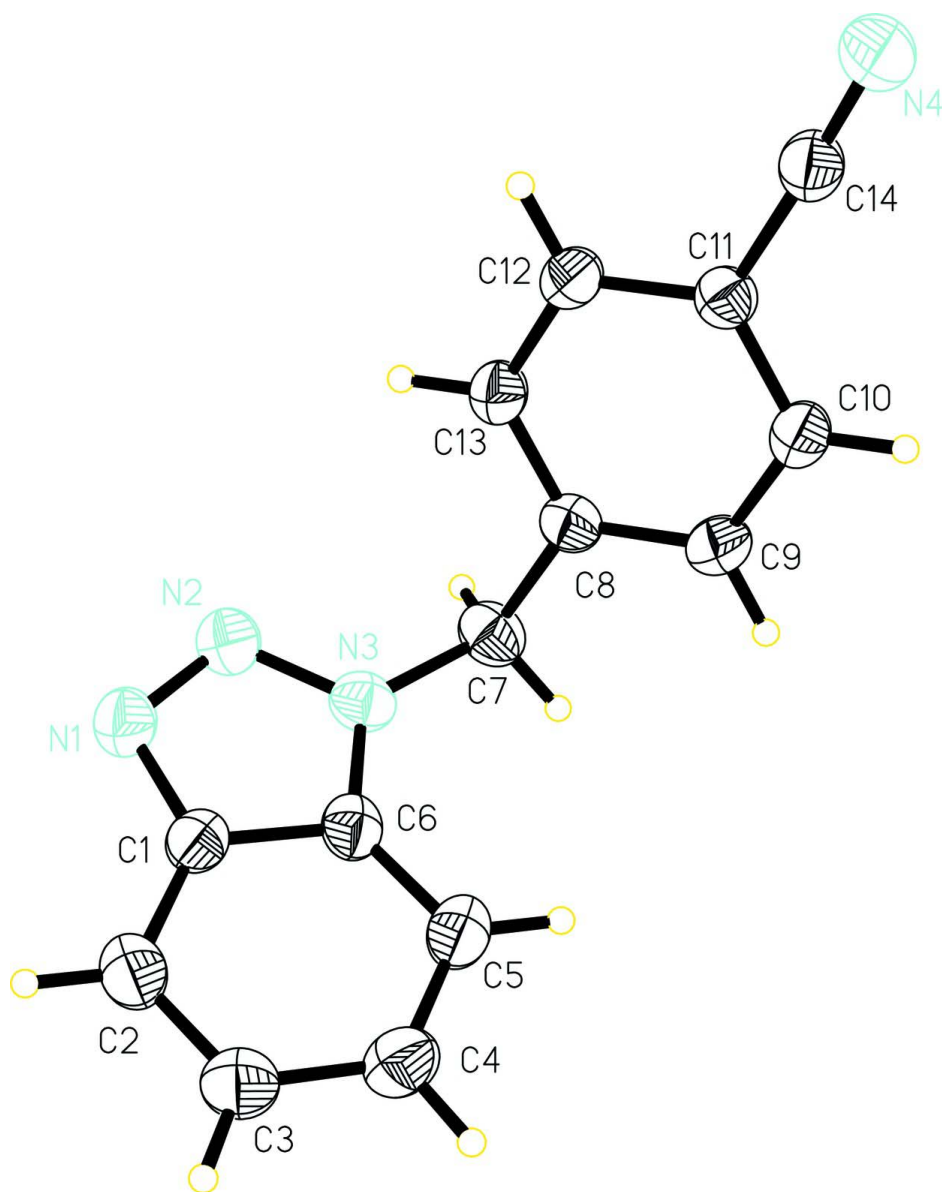
In the title compound, bond lengths and angles observed in the benzotriazole ring system are comparable with those reported in other benzotriazole compounds (Selvanayagam *et al.*, 2002). The dihedral angle between benzotriazole and benzene rings is 69.03 (6)°. The crystal structure is stabilized only by van der Waals contacts.

**S2. Experimental**

A mixture of benzotriazole (0.01 mol) and KOH (0.56 g) in methanol (20 ml) was stirred for 10 min. 4-(Bromomethyl)-benzonitrile (0.01 mol) was then added and the solution refluxed for 24 h. After completion of the reaction, the reaction mixture was evaporated under vacuum. Yellow crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution after 3 days.

**S3. Refinement**

All H atoms were calculated geometrically and were refined using the riding-model approximation, with C—H = 0.93–0.87 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Figure 1**

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

**4-[(1*H*-Benzotriazol-1-yl)methyl]benzonitrile***Crystal data* $C_{14}H_{10}N_4$  $M_r = 234.26$ Monoclinic,  $P2_1/n$ Hall symbol:  $-P\ 2_1/n$  $a = 8.1912(13)\ \text{\AA}$  $b = 19.0520(9)\ \text{\AA}$  $c = 8.6610(6)\ \text{\AA}$  $\beta = 118.039(1)^\circ$  $V = 1193.0(2)\ \text{\AA}^3$  $Z = 4$  $F(000) = 488$  $D_x = 1.304\ \text{Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$ 

Cell parameters from 2264 reflections

 $\theta = 3.0\text{--}27.4^\circ$  $\mu = 0.08\ \text{mm}^{-1}$

$T = 293$  K  
Block, yellow

$0.50 \times 0.40 \times 0.40$  mm

*Data collection*

Rigaku Mercury2  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
Detector resolution:  $13.6612$  pixels  $\text{mm}^{-1}$   
CCD Profile fitting scans  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2005)  
 $T_{\min} = 0.960$ ,  $T_{\max} = 0.969$

11866 measured reflections  
2715 independent reflections  
1903 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.0^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -24 \rightarrow 24$   
 $l = -11 \rightarrow 11$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.067$   
 $wR(F^2) = 0.182$   
 $S = 1.09$   
2715 reflections  
163 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 0.2728P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7006 (4)	0.10232 (14)	0.9067 (4)	0.0662 (7)
H1A	0.6891	0.1496	0.8769	0.079*
C2	0.8443 (4)	0.07658 (15)	1.0621 (4)	0.0714 (7)
H2B	0.9320	0.1081	1.1380	0.086*
C3	0.8630 (4)	0.00549 (15)	1.1096 (4)	0.0706 (7)
C4	0.7387 (4)	-0.04391 (14)	1.0033 (4)	0.0674 (7)
H4A	0.7493	-0.0911	1.0344	0.081*
C5	0.5915 (3)	-0.01855 (12)	0.8418 (3)	0.0554 (6)
C6	0.5771 (3)	0.05233 (12)	0.8006 (3)	0.0546 (6)
C7	0.3403 (4)	0.11817 (13)	0.5272 (3)	0.0631 (6)
H7A	0.2790	0.1033	0.4058	0.076*
H7B	0.4372	0.1510	0.5420	0.076*
C8	0.2010 (3)	0.15545 (12)	0.5681 (3)	0.0513 (5)
C9	0.2298 (3)	0.22412 (12)	0.6302 (3)	0.0626 (6)

H9A	0.3379	0.2474	0.6504	0.075*
C10	0.0989 (3)	0.25833 (13)	0.6624 (3)	0.0616 (6)
H10A	0.1182	0.3044	0.7026	0.074*
C11	-0.0614 (3)	0.22289 (11)	0.6339 (3)	0.0515 (5)
C12	-0.0901 (3)	0.15394 (12)	0.5744 (3)	0.0583 (6)
H12A	-0.1967	0.1302	0.5566	0.070*
C13	0.0408 (3)	0.12081 (12)	0.5417 (3)	0.0574 (6)
H13A	0.0212	0.0747	0.5015	0.069*
C14	-0.2037 (4)	0.25735 (12)	0.6617 (3)	0.0621 (6)
N1	0.4254 (3)	0.05596 (10)	0.6402 (3)	0.0574 (5)
N2	0.3499 (3)	-0.00893 (11)	0.5862 (3)	0.0684 (6)
N3	0.4492 (3)	-0.05515 (11)	0.7082 (3)	0.0688 (6)
N4	-0.3207 (3)	0.28251 (13)	0.6795 (4)	0.0841 (8)
H3B	0.9617	-0.0085	1.2151	0.101*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0730 (16)	0.0558 (14)	0.0776 (18)	-0.0081 (12)	0.0417 (14)	-0.0063 (12)
C2	0.0659 (16)	0.0753 (18)	0.0646 (17)	-0.0119 (13)	0.0238 (13)	-0.0063 (13)
C3	0.0653 (16)	0.0776 (18)	0.0631 (16)	-0.0004 (13)	0.0253 (13)	-0.0002 (13)
C4	0.0726 (17)	0.0598 (15)	0.0774 (18)	0.0070 (12)	0.0417 (15)	0.0072 (13)
C5	0.0539 (13)	0.0533 (13)	0.0677 (15)	-0.0040 (10)	0.0358 (12)	-0.0103 (11)
C6	0.0604 (14)	0.0511 (12)	0.0641 (14)	0.0022 (10)	0.0390 (12)	-0.0023 (10)
C7	0.0645 (15)	0.0679 (15)	0.0641 (15)	0.0104 (12)	0.0361 (12)	0.0075 (12)
C8	0.0492 (12)	0.0554 (13)	0.0497 (12)	0.0039 (9)	0.0235 (10)	0.0039 (10)
C9	0.0508 (13)	0.0606 (15)	0.0791 (17)	-0.0085 (10)	0.0327 (12)	-0.0035 (12)
C10	0.0604 (14)	0.0509 (13)	0.0748 (16)	-0.0079 (11)	0.0328 (12)	-0.0098 (11)
C11	0.0509 (12)	0.0520 (12)	0.0526 (13)	0.0003 (9)	0.0252 (10)	-0.0016 (10)
C12	0.0527 (13)	0.0531 (13)	0.0713 (15)	-0.0084 (10)	0.0310 (12)	-0.0083 (11)
C13	0.0583 (14)	0.0478 (12)	0.0672 (15)	-0.0029 (10)	0.0303 (12)	-0.0084 (10)
C14	0.0659 (15)	0.0530 (13)	0.0762 (16)	-0.0044 (11)	0.0408 (13)	-0.0065 (12)
N1	0.0533 (11)	0.0651 (12)	0.0564 (12)	0.0047 (9)	0.0279 (9)	-0.0029 (9)
N2	0.0658 (13)	0.0603 (13)	0.0782 (15)	0.0012 (10)	0.0330 (11)	-0.0047 (11)
N3	0.0681 (13)	0.0547 (12)	0.0851 (15)	-0.0019 (10)	0.0373 (12)	-0.0069 (11)
N4	0.0786 (16)	0.0733 (15)	0.119 (2)	-0.0010 (12)	0.0622 (16)	-0.0153 (14)

*Geometric parameters (Å, °)*

C1—C6	1.379 (3)	C7—H7B	0.9700
C1—C2	1.396 (4)	C8—C13	1.388 (3)
C1—H1A	0.9301	C8—C9	1.392 (3)
C2—C3	1.403 (4)	C9—C10	1.391 (3)
C2—H2B	0.9300	C9—H9A	0.9299
C3—C4	1.374 (4)	C10—C11	1.391 (3)
C3—H3B	0.9299	C10—H10A	0.9300
C4—C5	1.435 (4)	C11—C12	1.390 (3)
C4—H4A	0.9300	C11—C14	1.453 (3)

C5—N3	1.384 (3)	C12—C13	1.383 (3)
C5—C6	1.387 (3)	C12—H12A	0.9299
C6—N1	1.362 (3)	C13—H13A	0.9300
C7—N1	1.486 (3)	C14—N4	1.145 (3)
C7—C8	1.521 (3)	N1—N2	1.363 (3)
C7—H7A	0.9700	N2—N3	1.321 (3)
C6—C1—C2	114.9 (2)	C13—C8—C9	119.1 (2)
C6—C1—H1A	122.5	C13—C8—C7	119.6 (2)
C2—C1—H1A	122.5	C9—C8—C7	121.3 (2)
C1—C2—C3	123.2 (2)	C10—C9—C8	120.7 (2)
C1—C2—H2B	118.4	C10—C9—H9A	119.6
C3—C2—H2B	118.4	C8—C9—H9A	119.6
C4—C3—C2	121.4 (2)	C11—C10—C9	119.3 (2)
C4—C3—H3B	119.4	C11—C10—H10A	120.4
C2—C3—H3B	119.3	C9—C10—H10A	120.4
C3—C4—C5	116.2 (2)	C12—C11—C10	120.4 (2)
C3—C4—H4A	121.9	C12—C11—C14	118.6 (2)
C5—C4—H4A	121.9	C10—C11—C14	121.0 (2)
N3—C5—C6	109.8 (2)	C13—C12—C11	119.7 (2)
N3—C5—C4	129.6 (2)	C13—C12—H12A	120.2
C6—C5—C4	120.6 (2)	C11—C12—H12A	120.2
N1—C6—C1	132.6 (2)	C12—C13—C8	120.8 (2)
N1—C6—C5	103.8 (2)	C12—C13—H13A	119.6
C1—C6—C5	123.6 (2)	C8—C13—H13A	119.6
N1—C7—C8	112.97 (18)	N4—C14—C11	177.3 (3)
N1—C7—H7A	109.0	C6—N1—N2	110.69 (19)
C8—C7—H7A	109.0	C6—N1—C7	129.3 (2)
N1—C7—H7B	109.0	N2—N1—C7	120.0 (2)
C8—C7—H7B	109.0	N3—N2—N1	108.7 (2)
H7A—C7—H7B	107.8	N2—N3—C5	107.0 (2)