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2-(1*H*-1,2,3-Benzotriazol-1-yl)-acetonitrile

Xiong-Bin Xu and Qiong Ye*

Ordered Matter Science Research Center, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: yeqiong@seu.edu.cn

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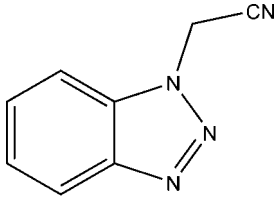
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.137; data-to-parameter ratio = 15.5.

The title compound, $C_8H_6N_4$, crystallizes with two molecules in the asymmetric unit. The two conformers have distinctive orientations of the CCN groups with respect to the benzotriazole planes are 67.0 (10) and 85.8 (8)°. C—H···N interactions are present in the crystal structure.

Related literature

For related literature, see: Danan *et al.* (1997).



Experimental

Crystal data

$C_8H_6N_4$
M_r = 158.17
Triclinic, $P\overline{1}$
a = 8.2423 (16) Å
b = 9.833 (2) Å
c = 10.631 (2) Å
α = 88.13 (3)°
β = 72.07 (3)°
γ = 71.90 (3)°
V = 777.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.20 × 0.15 × 0.10 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.805, T_{max} = 1.000
(expected range = 0.797–0.991)
8053 measured reflections
3559 independent reflections
2183 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.137
S = 1.01
3559 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···N6^{i}	0.97	2.51	3.475 (3)	176
C11—H11A···N4^{ii}	0.97	2.62	3.468 (3)	145
C11—H11B···N2^{iii}	0.97	2.61	3.412 (3)	140
C1—H1A···N6^{iv}	0.97	2.75	3.544 (3)	140
C1—H1A···N7^{iv}	0.97	2.68	3.609 (3)	161
C2—H2A···N5^{iv}	0.93	2.75	3.537 (3)	143

Symmetry codes: (i) $x+1, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z$.

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* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by a start-up grant from Southeast University (to QY).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2142).

References

Danan, A., Charon, D., Kirkiacharian, S., Bories, C. & Loiseau, P. M. (1997). *Farmaco*, **52**, 227–229.
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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.

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supplementary materials

Acta Cryst. (2007). E**63**, o4607 [**doi:10.1107/S1600536807055547**]

2-(1*H*-1,2,3-Benzotriazol-1-yl)acetonitrile

X.-B. Xu and Q. Ye

Comment

The title compound is obtained with high yield through the gentle reation of benzoletriazole and bromo acetonitrile in the presence of K_2CO_3 as catalyst. Colourless crystals of the title compound are obtained at room temperature after 3 days. The molecular structure with two molecules in the asymmetric unit (Fig. 1) shows almost linear acetonitrile moieties [bonding angles are 178.0 (2) and 179.3 (3) °]. The crystal packing is dominated by C—H···N interactions (Fig. 2, Table 1).

Experimental

To a solution of benzotriazole in 40 ml acetone, K_2CO_3 (3.5 g, 25 mmol) was added and the mixture was stirred at room temperature. A solution of bromo acetonitrile (7.2 g, 60 mmol) in acetone 20 ml was dropped slowly into the mixture. After stirring for 5 h, the mixture was filtered. A filtrate was evaporated to dryness under reduced pressure. The solid residue obtained was flash- chromatographed on silica gel (eluent: light petroleum-acetic ester 7:1) affording in sequence: 2-(*2H*-benzotriazol-2-yl)acetonitrile (0.39 g, 5.1%), m.p. 351–352 K (Danan *et al.* (1997): m.p. 351 K), a 1:1 mixture of isomers 2-(*2H*-benzotriazol-2-yl)acetonitrile and 2-(*1H*benzotriazol-1-yl)acetonitrile (0.19 g, 2.3%) and then 2-(*1H*benzotriazol-1-yl)acetonitrile (6.71 g, 85.1%), m.p. 359–360 K (Danan *et al.* (1997): m.p. 360 K). The suitable crystal of the title compound for X-ray diffraction are obtained in ethanol solution after standing at room temperature for several days.

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 U_{iso}(H) = 1.2Ueq.

Figures

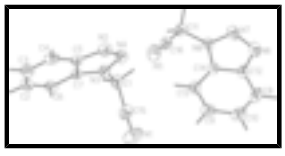

Fig. 1. The molecular structure of (I). Displacement ellipsoids were drawn at the 30% probability level.

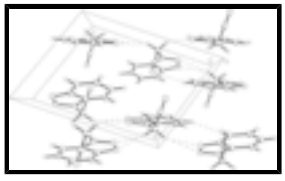

Fig. 2. The crystal packing of (I).

2-(1*H*-Benzo[*d*]-1,2,3-triazol-1-yl)acetonitrile

Crystal data

$C_8H_6N_4$	$Z = 4$
$M_r = 158.17$	$F_{000} = 328$
Triclinic, $P\overline{1}$	$D_x = 1.352$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.2423$ (16) Å	Cell parameters from 6664 reflections
$b = 9.833$ (2) Å	$\theta = 3.1$–28.8º
$c = 10.631$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 88.13$ (3)º	$T = 293$ (2) K
$\beta = 72.07$ (3)º	Prism, colourless
$\gamma = 71.90$ (3)º	0.20 × 0.15 × 0.10 mm
$V = 777.3$ (3) Å^3	

Data collection

Rigaku Mercury2 (2x2 bin mode) diffractometer	2183 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.038$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 293(2)$ K	$\theta_{min} = 3.1$º
CCD Profile fitting' scans	$h = -10\rightarrow10$
Absorption correction: Multi-scan (CrystalClear; Rigaku, 2005)	$k = -12\rightarrow12$
$T_{min} = 0.805$, $T_{max} = 1.000$	$l = -13\rightarrow13$
8053 measured reflections	Standard reflections: ?
3559 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.0638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3559 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
229 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
N1	0.5499 (4)	1.0795 (3)	0.1618 (3)	0.1058 (9)
N2	0.8556 (2)	0.5781 (2)	0.28482 (16)	0.0602 (5)
N3	0.8417 (2)	0.74294 (17)	0.14567 (15)	0.0489 (4)
N4	0.8779 (2)	0.7030 (2)	0.26055 (16)	0.0606 (5)
C1	0.8566 (3)	0.8776 (2)	0.0939 (2)	0.0565 (5)
H1A	0.9052	0.8652	−0.0020	0.075 (7)*
H1B	0.9397	0.9060	0.1267	0.084 (8)*
C2	0.7116 (3)	0.5057 (2)	−0.0368 (2)	0.0567 (5)
H2A	0.6810	0.4925	−0.1117	0.070 (7)*
C3	0.7191 (3)	0.3982 (2)	0.0533 (2)	0.0635 (6)
H3A	0.6932	0.3163	0.0366	0.072 (7)*
C4	0.7633 (3)	0.4109 (2)	0.1645 (2)	0.0593 (6)
H4A	0.7666	0.3400	0.2245	0.066 (6)*
C5	0.8036 (2)	0.5350 (2)	0.18505 (18)	0.0461 (5)
C6	0.7475 (3)	0.6286 (2)	−0.01844 (18)	0.0488 (5)
H6A	0.7410	0.7000	−0.0780	0.045 (5)*
C7	0.7945 (2)	0.64060 (19)	0.09500 (17)	0.0408 (4)
C15	0.6831 (4)	0.9913 (3)	0.1317 (2)	0.0659 (6)
N5	0.3078 (3)	0.4137 (2)	0.3596 (2)	0.0753 (6)
N6	0.1370 (3)	−0.0085 (2)	0.22156 (17)	0.0616 (5)
N7	0.0731 (2)	0.1280 (2)	0.25838 (17)	0.0597 (5)
N8	0.1134 (2)	0.14813 (15)	0.36958 (14)	0.0439 (4)
C8	0.3127 (3)	−0.2251 (2)	0.3148 (2)	0.0632 (6)
H8A	0.3244	−0.2940	0.2518	0.071 (7)*
C9	0.3674 (3)	−0.1588 (2)	0.5105 (2)	0.0603 (6)
H9A	0.4180	−0.1885	0.5778	0.074 (7)*
C10	0.3832 (3)	−0.2615 (2)	0.4160 (2)	0.0655 (6)
H10A	0.4432	−0.3573	0.4225	0.079 (7)*
C11	0.0597 (3)	0.2907 (2)	0.4319 (2)	0.0520 (5)
H11A	0.0265	0.2851	0.5273	0.068 (6)*
H11B	−0.0455	0.3505	0.4110	0.075 (7)*
C12	0.2222 (3)	−0.0796 (2)	0.30924 (18)	0.0461 (5)
C13	0.2805 (3)	−0.0164 (2)	0.50763 (19)	0.0500 (5)

H13A	0.2700	0.0517	0.5708	0.055 (6)*
C14	0.2082 (2)	0.02065 (18)	0.40414 (16)	0.0387 (4)
C16	0.2010 (3)	0.3579 (2)	0.38981 (19)	0.0510 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.1034 (19)	0.0616 (15)	0.122 (2)	−0.0069 (14)	−0.0132 (16)	0.0147 (14)
N2	0.0671 (12)	0.0624 (12)	0.0425 (10)	−0.0067 (9)	−0.0194 (9)	0.0081 (8)
N3	0.0574 (10)	0.0486 (10)	0.0394 (9)	−0.0118 (8)	−0.0184 (8)	0.0033 (7)
N4	0.0756 (13)	0.0607 (12)	0.0436 (10)	−0.0100 (9)	−0.0275 (9)	0.0012 (8)
C1	0.0684 (14)	0.0537 (13)	0.0537 (13)	−0.0253 (11)	−0.0218 (11)	0.0055 (10)
C2	0.0528 (13)	0.0629 (14)	0.0608 (13)	−0.0213 (11)	−0.0234 (11)	0.0024 (11)
C3	0.0571 (13)	0.0528 (13)	0.0880 (17)	−0.0217 (11)	−0.0289 (13)	0.0072 (12)
C4	0.0503 (12)	0.0494 (13)	0.0713 (15)	−0.0116 (10)	−0.0154 (11)	0.0199 (11)
C5	0.0404 (10)	0.0479 (12)	0.0394 (10)	−0.0033 (9)	−0.0087 (9)	0.0058 (8)
C6	0.0501 (11)	0.0576 (13)	0.0417 (11)	−0.0182 (9)	−0.0181 (9)	0.0113 (9)
C7	0.0380 (10)	0.0405 (10)	0.0397 (10)	−0.0085 (8)	−0.0101 (8)	0.0021 (8)
C15	0.0824 (17)	0.0453 (14)	0.0673 (15)	−0.0194 (12)	−0.0205 (13)	0.0071 (11)
N5	0.0905 (15)	0.0630 (13)	0.0790 (14)	−0.0374 (12)	−0.0224 (12)	0.0048 (10)
N6	0.0786 (13)	0.0679 (13)	0.0506 (10)	−0.0314 (10)	−0.0286 (10)	0.0002 (9)
N7	0.0709 (12)	0.0662 (12)	0.0538 (11)	−0.0270 (10)	−0.0314 (10)	0.0129 (9)
N8	0.0534 (9)	0.0409 (9)	0.0420 (9)	−0.0159 (7)	−0.0205 (8)	0.0052 (7)
C8	0.0680 (15)	0.0441 (13)	0.0694 (15)	−0.0219 (11)	−0.0041 (12)	−0.0145 (11)
C9	0.0589 (13)	0.0544 (14)	0.0688 (15)	−0.0150 (10)	−0.0259 (12)	0.0174 (11)
C10	0.0593 (14)	0.0394 (13)	0.0856 (17)	−0.0079 (10)	−0.0135 (13)	0.0048 (11)
C11	0.0578 (13)	0.0408 (11)	0.0527 (13)	−0.0109 (10)	−0.0155 (11)	0.0038 (9)
C12	0.0515 (11)	0.0459 (11)	0.0434 (11)	−0.0221 (9)	−0.0108 (9)	−0.0029 (9)
C13	0.0579 (12)	0.0469 (12)	0.0490 (11)	−0.0174 (9)	−0.0213 (10)	0.0056 (9)
C14	0.0413 (10)	0.0361 (10)	0.0389 (10)	−0.0156 (8)	−0.0097 (8)	0.0060 (7)
C16	0.0706 (14)	0.0352 (11)	0.0484 (12)	−0.0137 (10)	−0.0237 (11)	0.0066 (9)

Geometric parameters (Å, °)

N1—C15	1.127 (3)	N5—C16	1.138 (3)
N2—N4	1.303 (2)	N6—N7	1.304 (2)
N2—C5	1.382 (2)	N6—C12	1.380 (3)
N3—N4	1.362 (2)	N7—N8	1.358 (2)
N3—C7	1.365 (2)	N8—C14	1.362 (2)
N3—C1	1.443 (2)	N8—C11	1.447 (2)
C1—C15	1.463 (3)	C8—C10	1.362 (3)
C1—H1A	0.9700	C8—C12	1.402 (3)
C1—H1B	0.9700	C8—H8A	0.9301
C2—C6	1.364 (3)	C9—C13	1.365 (3)
C2—C3	1.402 (3)	C9—C10	1.396 (3)
C2—H2A	0.9301	C9—H9A	0.9300
C3—C4	1.359 (3)	C10—H10A	0.9300
C3—H3A	0.9301	C11—C16	1.460 (3)
C4—C5	1.400 (3)	C11—H11A	0.9700

C4—H4A	0.9300	C11—H11B	0.9700
C5—C7	1.390 (2)	C12—C14	1.388 (2)
C6—C7	1.394 (2)	C13—C14	1.393 (2)
C6—H6A	0.9300	C13—H13A	0.9299
N4—N2—C5	108.73 (16)	N7—N6—C12	108.47 (15)
N4—N3—C7	110.57 (16)	N6—N7—N8	108.51 (16)
N4—N3—C1	120.34 (16)	N7—N8—C14	110.26 (15)
C7—N3—C1	129.09 (16)	N7—N8—C11	120.45 (16)
N2—N4—N3	108.19 (16)	C14—N8—C11	129.27 (15)
N3—C1—C15	112.06 (18)	C10—C8—C12	117.2 (2)
N3—C1—H1A	109.2	C10—C8—H8A	121.4
C15—C1—H1A	109.2	C12—C8—H8A	121.4
N3—C1—H1B	109.2	C13—C9—C10	122.3 (2)
C15—C1—H1B	109.2	C13—C9—H9A	118.8
H1A—C1—H1B	107.9	C10—C9—H9A	118.8
C6—C2—C3	122.4 (2)	C8—C10—C9	121.8 (2)
C6—C2—H2A	118.9	C8—C10—H10A	119.1
C3—C2—H2A	118.8	C9—C10—H10A	119.1
C4—C3—C2	121.6 (2)	N8—C11—C16	112.93 (17)
C4—C3—H3A	119.2	N8—C11—H11A	109.0
C2—C3—H3A	119.2	C16—C11—H11A	109.0
C3—C4—C5	117.40 (19)	N8—C11—H11B	109.0
C3—C4—H4A	121.3	C16—C11—H11B	109.0
C5—C4—H4A	121.3	H11A—C11—H11B	107.8
N2—C5—C7	108.42 (17)	N6—C12—C14	108.33 (17)
N2—C5—C4	131.43 (19)	N6—C12—C8	131.67 (19)
C7—C5—C4	120.16 (18)	C14—C12—C8	120.00 (19)
C2—C6—C7	115.86 (19)	C9—C13—C14	115.83 (19)
C2—C6—H6A	122.0	C9—C13—H13A	122.1
C7—C6—H6A	122.1	C14—C13—H13A	122.1
N3—C7—C5	104.10 (16)	N8—C14—C12	104.42 (16)
N3—C7—C6	133.29 (17)	N8—C14—C13	132.78 (17)
C5—C7—C6	122.61 (18)	C12—C14—C13	122.80 (17)
N1—C15—C1	179.3 (3)	N5—C16—C11	178.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1B···N6^{i}	0.97	2.51	3.475 (3)	176
C11—H11A···N4^{ii}	0.97	2.62	3.468 (3)	145
C11—H11B···N2^{iii}	0.97	2.61	3.412 (3)	140
C1—H1A···N6^{iv}	0.97	2.75	3.544 (3)	140
C1—H1A···N7^{iv}	0.97	2.68	3.609 (3)	161
C2—H2A···N5^{iv}	0.93	2.75	3.537 (3)	143

Symmetry codes: (i) *x*+1, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*+1, −*z*.

Fig. 1

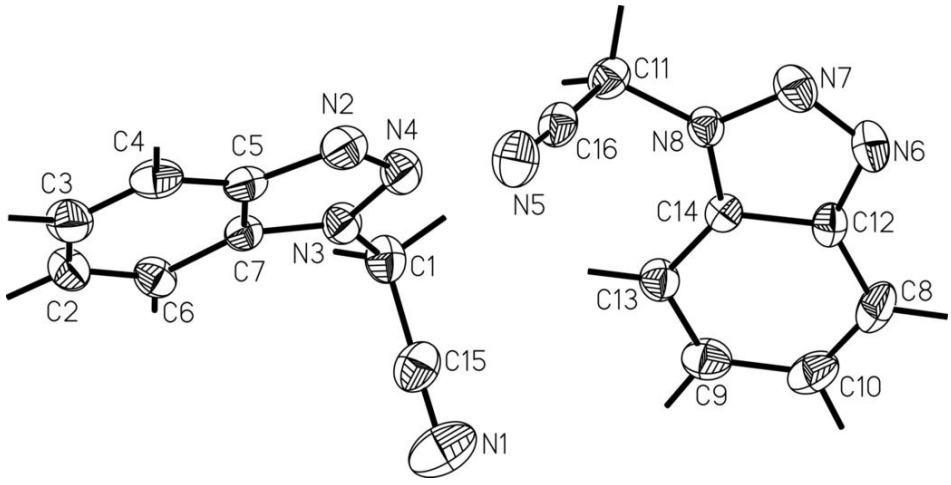
C11
N7
N2
N4
C4
C5
C16
N8
N6
C3
N5
C14
C12
N3
C1
C7
C13
C8
C2
C6
C15
C9
C10
N1

Fig. 2