Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1*H*-1,2,3-Benzotriazol-1-yl)methyl benzoate

Ting Guo,[a] Gang Cao[a]* and Sen Xu[b]

[a]Department of Stomatology, Nanjing Jinling Hospital, Nanjing University School of Medicine, 305, East Zhongshan Road, 210002 Nanjing, Jiangsu Province, People's Republic of China, and [b]Department of Applied Chemistry, School of Material Science and Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing, Jiangsu Province 210016, People's Republic of China
Correspondence e-mail: caogang69@163.com

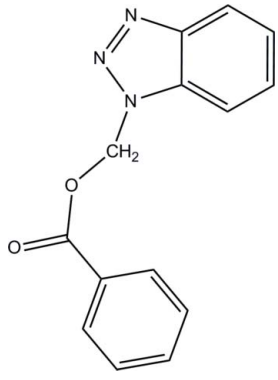
Received 26 March 2012; accepted 5 April 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.060; wR factor = 0.162; data-to-parameter ratio = 12.5.

In the title compound, $C_{14}H_{11}N_3O_2$, the dihedral angle between the phenyl ring and the benzotriazole ring system is 76.80 (19)° and the molecule has an L-shaped conformation. In the crystal, weak aromatic π–π stacking is observed, the closest centroid–centroid distance being 3.754 (2) Å.

Related literature

For related structures and the synthesis, see: Xu & Shen (2012); Zeng & Jian (2009). For applications of benzotriazole derivatives, see: Wan & Lv (2010).



Experimental

Crystal data

$C_{14}H_{11}N_3O_2$
M_r = 253.26
Monoclinic, $P2_1/c$
a = 10.7181 (4) Å
b = 6.4826 (2) Å
c = 18.7076 (7) Å
β = 96.773 (3)°
V = 1290.75 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.982, T_{max} = 0.984
9412 measured reflections
2268 independent reflections
1352 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.162
S = 1.06
2268 reflections
181 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was supported by the Surface Project Foundation of Nanjing Military Region (10MA095), the Jinling Hospital Foundation of Nanjing Province of China (2009Q021) and the Surface Project Foundation of Nanjing Military Region (11MA099).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6707).

References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wan, J. & Lv, P.-C. (2010). *J. Chem. Inf. Comput. Sci.* **122**, 597–606.
Xu, S. & Shen, Y. (2012). *Acta Cryst.* E**68**, o1066.
Zeng, W.-L. & Jian, F.-F. (2009). *Acta Cryst.* E**65**, o2165.

supplementary materials

Acta Cryst. (2012). E**68**, o1409 [doi:10.1107/S1600536812015140]

(1*H*-1,2,3-Benzotriazol-1-yl)methyl benzoate

Ting Guo, Gang Cao and Sen Xu

Comment

Benzotriazole derivatives have been broadly researched due to their potential applications (Wan & Lv, 2010). Herein, we have synthesized a new benzotriazole derivative(Fig. 1), $C_{12}H_{15}N_3O_2$. Bond lengths and angles are comparable to other reported benzotriazol-1-yl intermediate derivatives (Zeng & Jian, 2009; Xu & Shen, 2012). Furthermore, the dihedral angle between the mean planes of the phenyl and benzotriazole rings is 76.80 (19)°. In the crystal, π–π stacking is observed between the inversion related phenyl rings of benzotriazolyl, the closest centroid-centroid distance being 3.754 (2)Å.

Experimental

The title compound synthesis method is similar to that reported by Xu & Shen (2012), but methylene chloride was replaced by benzoyl chloride

Refinement

The H atoms on the CH_2 group were located by difference maps and freely refined without constraints. H atoms bonded to the remaining C atoms were included in calculated positions and treated as riding with C–H =0.93Å and U_{iso}(H)=1.2Ueq(aromatic C).

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

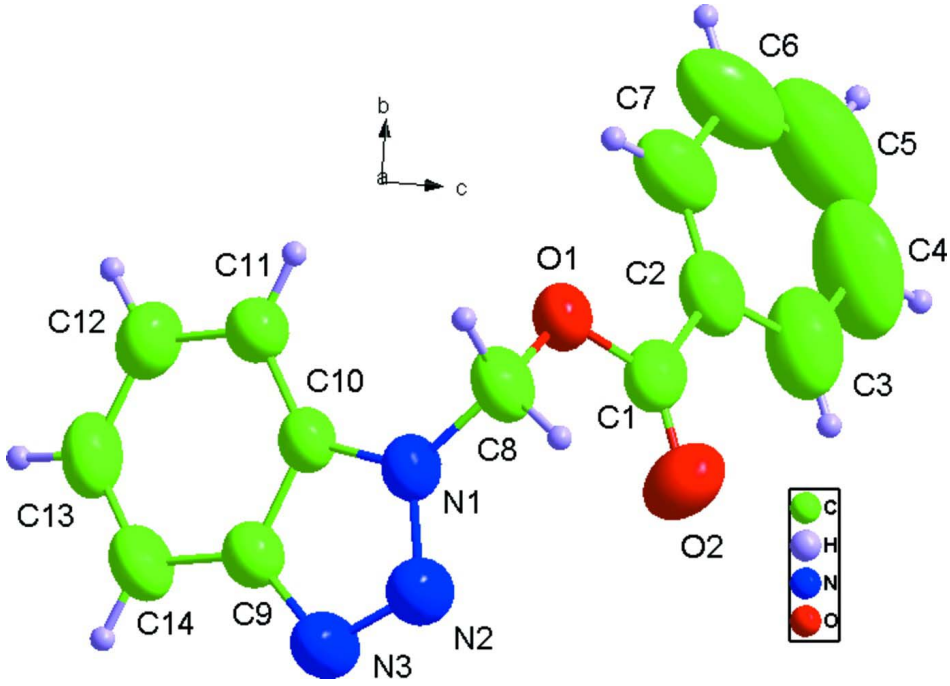


Figure 1

The molecular structure of the title compound with 50% probability displacement ellipsoids.

(1*H*-1,2,3-Benzotriazol-1-yl)methyl benzoate

Crystal data

$C_{14}H_{11}N_3O_2$
$M_r = 253.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.7181$ (4) Å
$b = 6.4826$ (2) Å
$c = 18.7076$ (7) Å
$\beta = 96.773$ (3)°
$V = 1290.75$ (8) Å^3
$Z = 4$

$F(000) = 528$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1419 reflections
$\theta = 2.7$–$21.6°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Block, colorless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.982$, $T_{max} = 0.984$

9412 measured reflections
2268 independent reflections
1352 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 12$
$k = -7 \rightarrow 7$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.162$
$S = 1.06$
2268 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.4539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0073 (18)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7169 (3)	0.5849 (5)	0.27655 (16)	0.0599 (8)
C2	0.8234 (3)	0.7177 (6)	0.30445 (18)	0.0672 (9)
C3	0.9100 (4)	0.6382 (8)	0.3586 (2)	0.1029 (14)
H3	0.8998	0.5062	0.3765	0.123*
C4	1.0110 (5)	0.7578 (13)	0.3853 (3)	0.145 (2)
H4	1.0696	0.7062	0.4215	0.174*
C5	1.0258 (6)	0.9545 (14)	0.3586 (4)	0.157 (3)
H5	1.0944	1.0342	0.3769	0.189*
C6	0.9397 (5)	1.0320 (8)	0.3054 (3)	0.1179 (18)
H6	0.9497	1.1645	0.2878	0.141*
C7	0.8391 (3)	0.9146 (6)	0.2781 (2)	0.0814 (11)
H7	0.7810	0.9671	0.2418	0.098*
C8	0.5351 (3)	0.5700 (6)	0.19118 (18)	0.0614 (9)
C9	0.6278 (3)	0.2459 (5)	0.05103 (16)	0.0564 (8)
C10	0.6200 (3)	0.4440 (4)	0.07805 (14)	0.0505 (7)
C11	0.6600 (3)	0.6164 (5)	0.04401 (16)	0.0608 (9)
H11	0.6543	0.7485	0.0628	0.073*
C12	0.7088 (3)	0.5800 (5)	−0.01930 (17)	0.0726 (10)
H12	0.7380	0.6911	−0.0441	0.087*
C13	0.7165 (3)	0.3815 (6)	−0.04810 (17)	0.0724 (10)
H13	0.7504	0.3649	−0.0913	0.087*
C14	0.6758 (3)	0.2130 (5)	−0.01465 (17)	0.0686 (9)
H14	0.6796	0.0817	−0.0343	0.082*
H1M	0.482 (3)	0.679 (5)	0.1671 (18)	0.078 (11)*

H2M	0.491 (3)	0.493 (5)	0.2271 (18)	0.087 (11)*
N1	0.5679 (2)	0.4166 (4)	0.14069 (12)	0.0571 (7)
N2	0.5446 (3)	0.2141 (4)	0.15102 (14)	0.0729 (8)
N3	0.5796 (3)	0.1092 (4)	0.09718 (15)	0.0752 (9)
O1	0.64454 (19)	0.6783 (3)	0.22152 (10)	0.0584 (6)
O2	0.6951 (2)	0.4154 (4)	0.29774 (13)	0.0830 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.065 (2)	0.067 (2)	0.0494 (17)	0.0088 (18)	0.0141 (16)	0.0005 (16)
C2	0.055 (2)	0.090 (3)	0.057 (2)	−0.0006 (19)	0.0115 (17)	−0.0160 (19)
C3	0.071 (3)	0.155 (4)	0.080 (3)	0.016 (3)	−0.003 (2)	−0.014 (3)
C4	0.075 (4)	0.240 (8)	0.114 (5)	0.002 (5)	−0.015 (3)	−0.043 (5)
C5	0.075 (4)	0.228 (8)	0.170 (7)	−0.039 (5)	0.018 (4)	−0.089 (7)
C6	0.085 (3)	0.125 (4)	0.152 (5)	−0.041 (3)	0.050 (3)	−0.057 (4)
C7	0.072 (3)	0.089 (3)	0.088 (3)	−0.018 (2)	0.030 (2)	−0.026 (2)
C8	0.061 (2)	0.070 (2)	0.0534 (19)	0.0043 (19)	0.0083 (18)	−0.0129 (18)
C9	0.064 (2)	0.0560 (17)	0.0497 (17)	0.0003 (15)	0.0079 (16)	−0.0034 (14)
C10	0.0551 (19)	0.0539 (17)	0.0423 (15)	0.0009 (14)	0.0045 (14)	−0.0016 (13)
C11	0.076 (2)	0.0547 (18)	0.0516 (17)	−0.0021 (16)	0.0078 (17)	−0.0012 (14)
C12	0.085 (3)	0.079 (2)	0.0553 (19)	−0.0057 (19)	0.0155 (19)	0.0080 (18)
C13	0.081 (3)	0.092 (3)	0.0465 (18)	0.006 (2)	0.0182 (17)	−0.0043 (18)
C14	0.081 (2)	0.070 (2)	0.0552 (19)	0.0090 (18)	0.0105 (18)	−0.0145 (17)
N1	0.0712 (18)	0.0564 (15)	0.0454 (13)	0.0007 (13)	0.0136 (13)	−0.0026 (12)
N2	0.103 (2)	0.0594 (17)	0.0583 (17)	−0.0114 (15)	0.0191 (16)	−0.0007 (14)
N3	0.110 (2)	0.0569 (16)	0.0611 (17)	−0.0071 (15)	0.0225 (17)	−0.0055 (14)
O1	0.0718 (15)	0.0583 (12)	0.0450 (11)	−0.0001 (11)	0.0064 (11)	−0.0033 (10)
O2	0.0905 (19)	0.0774 (16)	0.0804 (17)	0.0015 (13)	0.0077 (14)	0.0232 (13)

Geometric parameters (Å, º)

C1—O2	1.200 (3)	C8—H1M	0.98 (3)
C1—O1	1.356 (3)	C8—H2M	1.00 (3)
C1—C2	1.476 (5)	C9—N3	1.379 (4)
C2—C7	1.385 (5)	C9—C10	1.386 (4)
C2—C3	1.389 (5)	C9—C14	1.404 (4)
C3—C4	1.377 (7)	C10—N1	1.367 (3)
C3—H3	0.9300	C10—C11	1.380 (4)
C4—C5	1.385 (9)	C11—C12	1.371 (4)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.371 (8)	C12—C13	1.401 (4)
C5—H5	0.9300	C12—H12	0.9300
C6—C7	1.369 (6)	C13—C14	1.357 (4)
C6—H6	0.9300	C13—H13	0.9300
C7—H7	0.9300	C14—H14	0.9300
C8—O1	1.426 (4)	N1—N2	1.355 (3)
C8—N1	1.443 (4)	N2—N3	1.306 (3)
O2—C1—O1	122.9 (3)	H1M—C8—H2M	112 (3)

O2—C1—C2	126.1 (3)	N3—C9—C10	108.9 (3)
O1—C1—C2	111.0 (3)	N3—C9—C14	130.8 (3)
C7—C2—C3	120.2 (4)	C10—C9—C14	120.3 (3)
C7—C2—C1	122.2 (3)	N1—C10—C11	133.0 (3)
C3—C2—C1	117.6 (4)	N1—C10—C9	103.9 (2)
C4—C3—C2	119.0 (5)	C11—C10—C9	123.1 (3)
C4—C3—H3	120.5	C12—C11—C10	115.5 (3)
C2—C3—H3	120.5	C12—C11—H11	122.3
C3—C4—C5	120.4 (7)	C10—C11—H11	122.3
C3—C4—H4	119.8	C11—C12—C13	122.4 (3)
C5—C4—H4	119.8	C11—C12—H12	118.8
C6—C5—C4	120.2 (7)	C13—C12—H12	118.8
C6—C5—H5	119.9	C14—C13—C12	121.7 (3)
C4—C5—H5	119.9	C14—C13—H13	119.1
C7—C6—C5	120.0 (6)	C12—C13—H13	119.1
C7—C6—H6	120.0	C13—C14—C9	116.9 (3)
C5—C6—H6	120.0	C13—C14—H14	121.6
C6—C7—C2	120.2 (5)	C9—C14—H14	121.6
C6—C7—H7	119.9	N2—N1—C10	110.4 (2)
C2—C7—H7	119.9	N2—N1—C8	120.7 (3)
O1—C8—N1	110.3 (3)	C10—N1—C8	128.8 (3)
O1—C8—H1M	103.6 (18)	N3—N2—N1	108.6 (2)
N1—C8—H1M	111.5 (19)	N2—N3—C9	108.1 (2)
O1—C8—H2M	114.3 (19)	C1—O1—C8	116.9 (3)
N1—C8—H2M	105.7 (19)		

O2—C1—C2—C7	−177.9 (3)	C11—C12—C13—C14	−0.1 (6)
O1—C1—C2—C7	3.0 (4)	C12—C13—C14—C9	−1.2 (5)
O2—C1—C2—C3	2.5 (5)	N3—C9—C14—C13	179.8 (3)
O1—C1—C2—C3	−176.6 (3)	C10—C9—C14—C13	1.9 (5)
C7—C2—C3—C4	−0.1 (6)	C11—C10—N1—N2	−180.0 (3)
C1—C2—C3—C4	179.5 (4)	C9—C10—N1—N2	−0.4 (3)
C2—C3—C4—C5	0.1 (8)	C11—C10—N1—C8	1.9 (6)
C3—C4—C5—C6	0.1 (10)	C9—C10—N1—C8	−178.5 (3)
C4—C5—C6—C7	−0.4 (9)	O1—C8—N1—N2	119.7 (3)
C5—C6—C7—C2	0.4 (6)	O1—C8—N1—C10	−62.3 (4)
C3—C2—C7—C6	−0.1 (5)	C10—N1—N2—N3	−0.1 (4)
C1—C2—C7—C6	−179.7 (3)	C8—N1—N2—N3	178.3 (3)
N3—C9—C10—N1	0.7 (3)	N1—N2—N3—C9	0.5 (4)
C14—C9—C10—N1	179.0 (3)	C10—C9—N3—N2	−0.8 (4)
N3—C9—C10—C11	−179.7 (3)	C14—C9—N3—N2	−178.9 (3)
C14—C9—C10—C11	−1.3 (5)	O2—C1—O1—C8	3.2 (4)
N1—C10—C11—C12	179.6 (3)	C2—C1—O1—C8	−177.7 (2)
C9—C10—C11—C12	0.0 (5)	N1—C8—O1—C1	−81.1 (3)
C10—C11—C12—C13	0.7 (5)		