Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(1*H*-Benzotriazol-1-yl)-1-(3-methoxyphenyl)-propan-1-one

Wu-Lan Zeng,[a] Sai Bi,[b] Hua Zhong[b] and Jun Wan[b]*

[a]Department of Chemistry and Chemical Engineering, Weifang University, 261061 Weifang, Shandong, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.131
Data-to-parameter ratio = 14.7

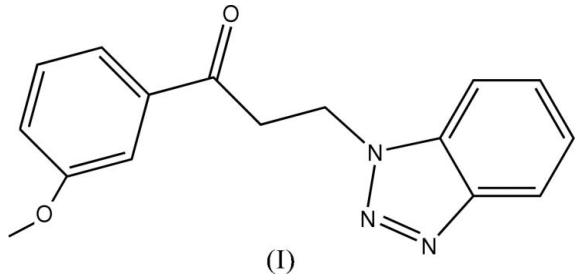
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 24 October 2006
Accepted 6 November 2006

In the title compound, $C_{16}H_{15}N_3O_2$, the dihedral angle between the benzotriazole unit and the other benzene ring is 79.06 (1)°. The crystal structure is stabilized by C—H···π interactions and van der Waals forces.

Comment

1*H*-Benzotriazole and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our ongoing studies on new benzotriazole compounds with higher bioactivity.



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 0.41 (1)° between the C10–C15 benzene and triazole (N1–N3/C10/C15) rings. The mean planes of the benzotriazole system and the other benzene ring (C1–C6) make a dihedral angle of 79.06 (1)°. The crystal structure (Fig. 2) is stabilized by C—H···π interactions (Table 1) and van der Waals forces.

Experimental

To a solution of 3-(dimethylamino)-1-(4-methoxyphenyl)propan-1-one (10.35 g, 0.05 mol) in water (25 ml) was added benzotriazole (7.1 g, 0.06 mol). The mixture was heated under reflux for 5 h, yielding a copious precipitate. Colourless single crystals of (I) suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane–cyclohexane (1:1 *v*/*v*) solution over a period of 6 d.

Crystal data

$C_{16}H_{15}N_3O_2$
M_r = 281.31
Monoclinic, $P2_1/c$
a = 10.000 (5) Å
b = 9.731 (4) Å
c = 14.407 (5) Å
V = 1401.9 (10) Å^3
Z = 4
D_x = 1.333 Mg m^{-3}
Mo *Kα* radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.25 × 0.19 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.996
7734 measured reflections
2783 independent reflections
1979 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.03
2783 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.141P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

Cg is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···$Cg3^{i}$	0.93	2.91	3.805	162
C9—H9B···$Cg3^{ii}$	0.97	2.98	3.663	128

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(methyl C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

This project was supported by the Special Project of Qingdao for Leadership of Science and Technology (No. 05–2-JC-80) and the Outstanding Adult-Young Scientific Research Encouraging Foundation of Shandong Province (No. 2005BS04007).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

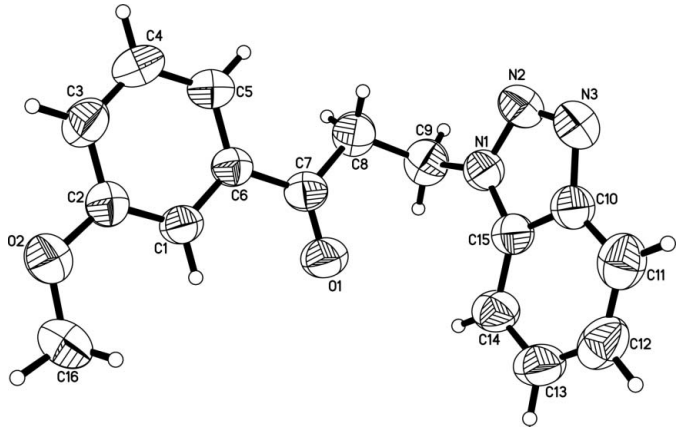


Figure 1
The molecular structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

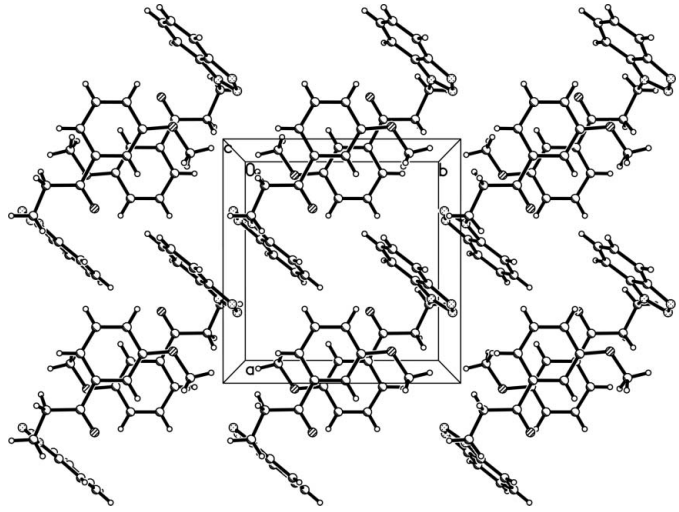


Figure 2
Packing diagram of (I), viewed down the *c* axis.

Chen, Z.-Y. & Wu, M.-J. (2005). *Org. Lett.* **7**, 475–477.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.