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3-(1*H*-Benzotriazol-1-yl)-1-(4-chlorophenyl)-propan-1-one

Jun Wan,[a] Wu-Lan Zeng,[b] Yue-Qin Yu,[a] Sai Bi[a] and Shu-Sheng Zhang[a]*

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

Correspondence e-mail: shushzhang@126.com

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Key indicators

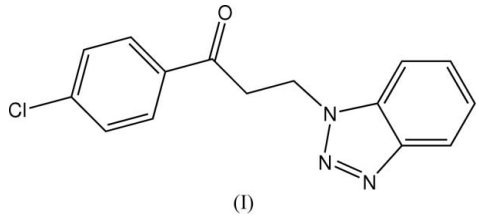
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.115
Data-to-parameter ratio = 14.9

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

In the molecule of the title compound, $C_{15}H_{12}ClN_3O$, the dihedral angle between the benzotriazole ring system and the chlorobenzene ring is 63.06 (1)°. π–π Interactions stabilize the crystal structure.

Comment

1*H*-Benzotriazoles are an important class of compounds because of their wide use in synthetic organic chemistry and pharmaceutical sciences. They are found to exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). As part of a search for new benzotriazole compounds with higher bioactivity, the title compound, (I), was synthesized and its structure is presented here.



(I)

In the molecule of the title compound, (I) (Fig. 1), the 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 1.62 (1)° between the N1–N3/C10/C15 and C10–C15 rings. The mean planes through the benzotriazole ring system and the C1–C6 benzene ring make a dihedral angle of 63.06 (1)°.

The crystal packing is stabilized by π–π interactions involving the benzotriazole rings, with a $Cg1\cdots Cg2^{i}$ [symmetry code: (i) $-x, 1-y, -z$] distance of 3.789 (2) Å, where *Cg*1 and *Cg*2 denote the centroids of the N1–N3/C10/C15 and C10–C15 rings, respectively.

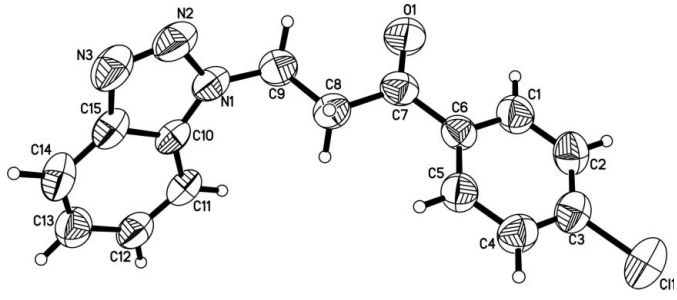


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

To a solution of 1-(4-chlorophenyl)-3-(dimethylamino)propan-1-one (10.58 g, 0.05 mol) in water (25 ml) was added benzotriazole (7.1 g, 0.06 mol). The mixture was heated under reflux for 6 h, yielding a copious precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane–cyclohexane (1:2 *v*/*v*) solution at room temperature over a period of 5 d.

Crystal data

$C_{15}H_{12}ClN_3O$
M_r = 285.73
Monoclinic, $C2/c$
a = 22.183 (7) Å
b = 10.444 (3) Å
c = 12.326 (4) Å
β = 106.705 (5)°
V = 2735.2 (15) Å^3
Z = 8
D_x = 1.388 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 (2) K
Plate, colourless
0.28 × 0.21 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.926, T_{max} = 0.973
7533 measured reflections
2694 independent reflections
1874 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.02
2694 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.759P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

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

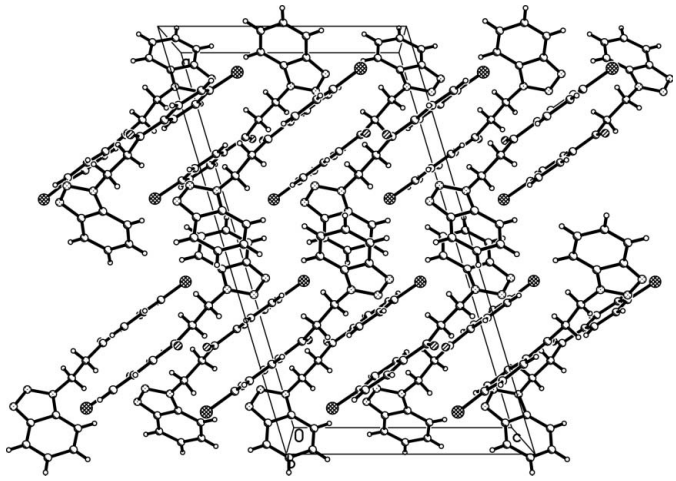


Figure 2
A packing diagram of (I), viewed down the *b* axis, showing the stacking of the benzotriazole rings.

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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.
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). *SHELXTL*. Version 5.1. 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.