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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.055
 wR factor = 0.138
Data-to-parameter ratio = 8.2

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

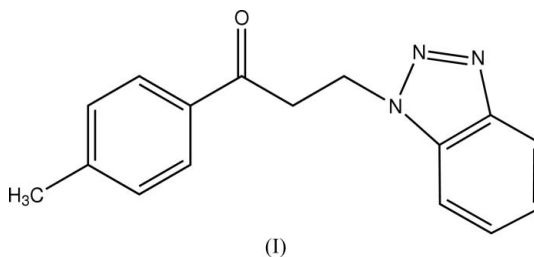
3-(Benzotriazol-1-yl)-1-*p*-tolylpropan-1-one

In the molecule of the title compound, $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}$, the benzotriazole system is planar. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into chains. The packing is further stabilized by $\text{C}-\text{H}\cdots\pi$ interactions.

Received 2 August 2006
Accepted 2 August 2006

Comment

1*H*-Benzotriazoles are an important class of compounds because of their wide use in synthetic organic chemistry and pharmaceutical sciences. They are also found to exhibit a broad spectrum of pharmacological activities such as anti-fungal, antitumor and antineoplastic activities (Chen *et al.*, 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.



In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). All the bonds show a characteristic length intermediate between those of single and double bonds.

Rings *A* (atoms N1–N3/C10/C11), *B* (C10–C15) and *C* (C1–C6) are, of course, planar. The benzotriazole system is also planar, having a total puckering amplitude, Q_T , of 0.0193 (3) Å (Cremer & Pople, 1975). The dihedral angle between rings *A* and *B* is 0.6 (2)°, while that between the benzotriazole system and ring *C* is 78.3 (2)°.

As can be seen from the packing diagram (Fig. 2), intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1) link the molecules into chains. The packing is further stabilized by $\text{C}-\text{H}\cdots\pi$ interactions (Table 1).

Experimental

To a solution of Mannich base 3-(dimethylamino)-1-*p*-tolylpropan-1-one (1.9 g, 0.01 mol) in water (50 ml) was added benzotriazole (1.19 g, 0.01 mol). The mixture was heated under reflux for 4 h. The resulting precipitate was purified by recrystallization from ethyl acetate–petroleum ether (1:2 *v/v*). Colorless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of an

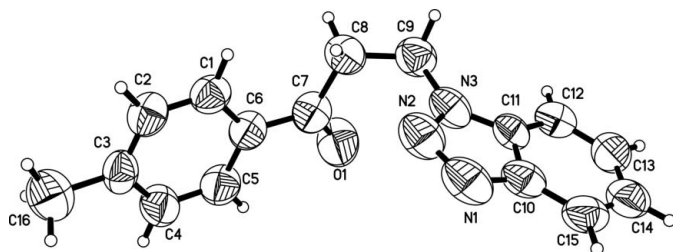


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

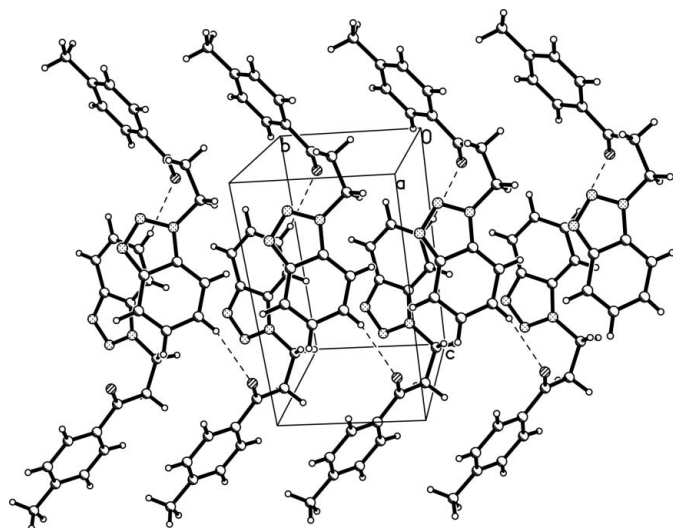


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

acetone–ethanol (1:2) solution at room temperature over a period of several days.

Crystal data

$C_{16}H_{15}N_3O$	$Z = 2$
$M_r = 265.31$	$D_x = 1.279 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 11.565 (4) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 5.7481 (18) \text{ \AA}$	$T = 294 (2) \text{ K}$
$c = 11.666 (4) \text{ \AA}$	Needle, colorless
$\beta = 117.309 (5)^\circ$	$0.47 \times 0.11 \times 0.08 \text{ mm}$
$V = 689.1 (4) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3769 measured reflections
ω scans	1492 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1031 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.962$, $T_{\max} = 0.993$	$R_{\text{int}} = 0.028$
	$\theta_{\text{max}} = 26.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.138$
 $S = 1.03$
 1492 reflections
 181 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.1105P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.020$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.11 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2A\cdots Cg1^i$	0.93	2.86	3.428	121
$C8-H8A\cdots Cg2^{ii}$	0.97	2.99	3.930	165
$C12-H12A\cdots Cg3^{iii}$	0.93	2.86	3.534	130
$C13-H13A\cdots O1^{iii}$	0.93	2.54	3.435 (5)	161

Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z$; (ii) $x, y - 1, z$; (iii) $-x + 1, y - \frac{1}{2}, -z - 1$. $Cg1$, $Cg2$ and $Cg3$ denote the centroids of the A, C and B rings, respectively

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with $C-H = 0.93, 0.97$ and 0.96 \AA for aromatic, methylene and methyl H atoms, respectively, and with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); 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 (grant No. 05-2-JC-80) and the Outstanding Adult-Young Scientific Research Encouraging Foundation of Shandong Province (grant No. 2005BS04007).

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