

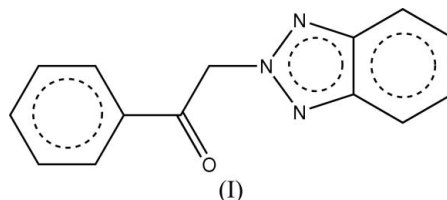
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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.097  
Data-to-parameter ratio = 9.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2-(2*H*-Benzotriazol-2-yl)-1-phenylethanoneThe molecule of the title compound,  $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$ , is non-  
planar, with a dihedral angle of  $72.06(9)^\circ$  between the  
benzene and benzotriazole planes. Molecules are linked into  
two-dimensional layers *via* weak  $\text{C}-\text{H}\cdots\text{N}$  and  $\text{C}-\text{H}\cdots\text{O}$   
interactions.

## Comment

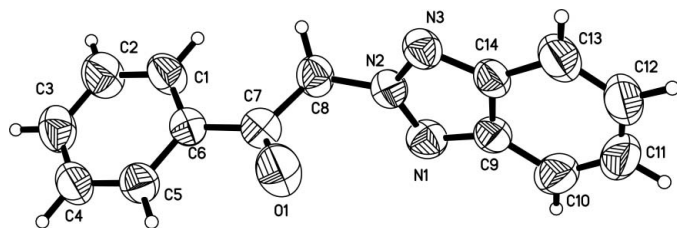
In recent years, benzotriazoles, especially, those substituted at  
the 2-position of the heterocycle, have attracted special  
attention (Voronkov *et al.*, 2003). A variety of benzotriazoles  
exhibit growth-inhibiting activities against some microorgan-  
isms and other derivatives are endowed with anti-inflamma-  
tory properties (Zelnik & Strehlau, 1971). We report here the  
structure of a 2-substituted benzotriazole compound, (I).The bond lengths and angles are within normal ranges  
(Allen *et al.*, 1987), and the bonds in the benzotriazole group  
show a characteristic intermediate length between single and  
double bonds because of the conjugated  $\pi$  system (Table 1).  
The C9–C14 benzene and triazole rings are essentially  
coplanar, with a dihedral angle of  $0.7(1)^\circ$  between these two  
rings, while the benzotriazole plane and the phenyl ring twist  
 $72.06(9)^\circ$  from each other. In the crystal structure, molecules  
are linked into two-dimensional layers *via*  $\text{C}-\text{H}\cdots\text{N}$  and  
 $\text{C}-\text{H}\cdots\text{O}$  interactions (Table 2 and Fig. 2).

## Experimental

To a solution of 2-(2*H*-bromine-2-yl)-1-phenylethanone (20 g,  
0.1 mol) in acetone (80 ml) was added 1,2,3-benzotriazole (11.9 g,  
0.1 mol). The mixture was heated under reflux for 1 h, yielding a  
copious precipitate. Colorless single crystals suitable for X-ray  
diffraction were obtained by slow evaporation of an ethyl acetate and  
petroleum ether (1:1 *v/v*) solution over a period of one week.

## Crystal data

 $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$   
 $M_r = 237.26$   
Tetragonal,  $P4_32_12$   
 $a = 8.1925(3)$  Å  
 $c = 35.462(3)$  Å  
 $V = 2380.1(2)$  Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.324$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation  
Cell parameters from 2708  
reflections  
 $\theta = 2.5\text{--}20.7^\circ$   
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 293(2)$  K  
Block, colorless  
 $0.35 \times 0.11 \times 0.08$  mmReceived 25 October 2005  
Accepted 2 November 2005  
Online 10 November 2005



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

#### Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.970$ ,  $T_{\max} = 0.993$   
14062 measured reflections

1477 independent reflections  
1277 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.039$   
 $\theta_{\text{max}} = 26.0^\circ$   
 $h = -10 \rightarrow 9$   
 $k = -10 \rightarrow 10$   
 $l = -43 \rightarrow 30$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.098$   
 $S = 1.20$   
1477 reflections  
163 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.1331P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.14 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.12 \text{ e } \text{\AA}^{-3}$

**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

O1—C7	1.196 (3)	N2—N3	1.323 (2)
N1—N2	1.319 (2)	N2—C8	1.449 (3)
N1—C9	1.348 (3)	N3—C14	1.347 (3)

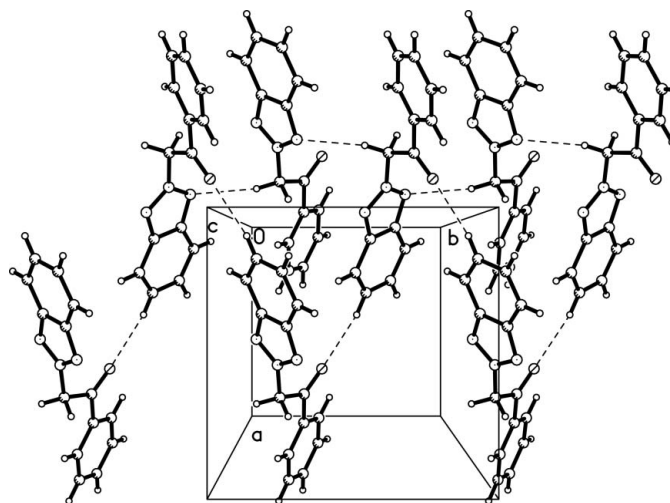
**Table 2**

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A $\cdots$ N3 <sup>i</sup>	0.97	2.54	3.471 (3)	160
C11—H11A $\cdots$ O1 <sup>ii</sup>	0.93	2.52	3.439 (3)	170

Symmetry codes: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{4}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, -z + \frac{1}{4}$ .

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with  $C-H = 0.93$  or  $0.97 \text{ \AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . The Friedel pairs were merged before



**Figure 2**  
A packing view down the  $c$  axis. Hydrogen bonds are indicated by dashed lines.

the final refinement because of the absence of significant anomalous scattering effects.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; 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).

This project was supported by the Program for New Century Excellent Talents in Universities (No. NCET-04-0649) and the Project of Educational Administration of Shandong Province (No. J04B12).

#### 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.  
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 *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
Voronkov, M. G., Trofimova, O. M., Bolgova, Yu. I., Larina, L. I., Albanov, A. I., Pestunovich, V. A., Chernov, N. F. & Petrusenko, K. B. (2003). *Chem. Heterocycl. Comp.* **39**, 1639–1644.  
Zelnik, R. & Strehlau, F. (1971). *Ann. Acad. Bras. Cienc.* **43**, 385–388.