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# 5-Phenyl-1,2,4-triazolo[3,4-*b*]benzothiazole

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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 = 0.128
Data-to-parameter ratio = 13.0

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



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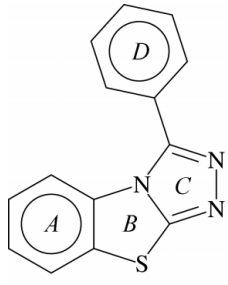
In the title compound, $C_{14}H_9N_3S$, the triazole and benzothiazole moieties are coplanar. The dihedral angle between the fused triazole–benzothiazole fragment and the phenyl ring is 39.20 (5)°. The structure is stabilized by C—H···N intermolecular interactions.

## Comment

The triazole moiety possesses many pharmacological properties, such as acting as an antimicrobial (Habib *et al.*, 1997), antiviral (Ergen *et al.*, 1996), anti-HIV-1 (Invidiata *et al.*, 1996), antifungal, antimycobacterial and anticonvulsant (Gülerman *et al.*, 1997) agent. It is also a highly potent eosinophilia inhibitor (Naito *et al.*, 1996) and is used as fungicide (Crofton, 1996) and herbicide (Tada *et al.*, 1995). Some triazole derivatives have been evaluated for their antibacterial activity against both Gram-positive and Gram-negative bacteria (Bs *et al.*, 1996). Benzothiazoles are extremely important heterocycles from industrial and agricultural points of view. They are also used as antineoplastic agents and show antinociceptive, anti-inflammatory and antitumor activities (Bradshaw *et al.*, 1998; Dögruer *et al.*, 1998). The fused benzothiazole–triazole fragment may have useful medicinal properties. Some Schiff bases derived from thiazole and benzothiazoles (Dash *et al.*, 1980) and several derivatives of the styrylbenzothiazoles have shown biological activity (Cox *et al.*, 1982). In view of these features associated with the benzothiazole and triazole moieties, the structure determination of 5-phenyl-1,2,4-triazolo[3,4-*b*]benzothiazole, (I), incorporating both these units, was undertaken.




(I)

Bond distances and angles observed for (I) are similar to those found in the structures of related compounds, namely, 7-methyl-3-(2-methylphenyl)-1,2,4-triazolo[3,4-*b*]benzothiazole and 7-methyl-3-(4-methylphenyl)-1,2,4-triazolo[3,4-*b*]-benzothiazole (Puviarasan *et al.*, 1999). The large size of the S atom compared with N results in a reduction of the C1—S1—

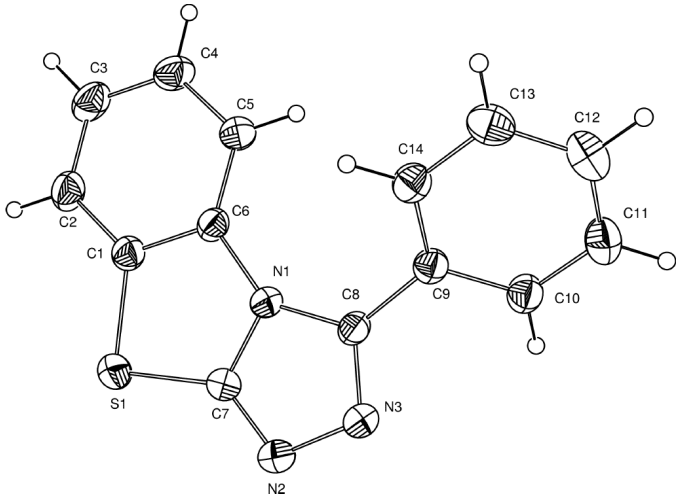



**Figure 1**
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

C7 angle [89.0 (1)°] compared with the C7—N1—C6 angle [113.5 (2)°] in thiazole ring. This suggests that the S atom might be using unhybridized *p* orbitals for bonding (Muir *et al.*, 1987). As a result of the fusion of the benzothiazole and triazole moieties, the ring-junction endocyclic bond angles are larger than normal values. The title compound is non-planar, with a dihedral angle of 39.20 (5)° between the 1,2,4-triazolo[3,4-*b*]benzothiazole moiety and the phenyl ring. The geometry of the benzothiazole moiety is essentially planar, with no atom deviating from the plane by more than 0.051 (2) Å [$\chi^2$ = 12.6]. The dihedral angle between the mean planes of the rings *A*, *B*, *C* are *A*/*B* 3.78 (6)°, *A*/*C* 6.59 (8)° and *B*/*C* 2.81 (7)°. The structure is stabilized by van der Waals interactions and C—H···N-type intermolecular interactions [H10···N3$^{i}$ = 2.61 Å, C10···N3$^{i}$ = 3.520 (4) Å and angle at C10—H10···N3$^{i}$ = 167.0°; symmetry code: (i) $-x$, $-y$, $-z$+1].

## Experimental

The title compound, (I), was obtained from the photolysis of 4-(2-chlorophenyl)-5-phenyl-1,2,4-triazole-3-thione (0.7 g, 0.0024 mol) in absolute methanol (150 ml). It was flushed with nitrogen for 1 h and irradiated for 1.5 h in a thin-film reactor (equipped with one lamp) at 254 nm. After completion of the reaction, the solvent was removed and the residue, on chromatographic purification using an ethyl acetate–petroleum ether mixture (1:6), afforded a yellow solid (m.p. 417–419 K) (Jayanthi *et al.*, 1997). Crystals suitable for an X-ray diffraction study were grown by slow evaporation from ethyl acetate–petroleum ether (1:6) mixture.

*Crystal data*

$C_{14}H_9N_3S$
$M_r$ = 251.30
Monoclinic, $P2_1/c$
$a$ = 8.702 (1) Å
$b$ = 15.000 (2) Å
$c$ = 9.799 (1) Å
$\beta$ = 113.70 (1)°
$V$ = 1171.2 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.425 Mg m$^{-3}$
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 14–30°
$\mu$ = 2.31 mm$^{-1}$
$T$ = 293 (2) K
Needle, yellow
0.35 × 0.13 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$–2$\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.924, $T_{max}$ = 0.998
2277 measured reflections
2128 independent reflections
1936 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
$\theta_{max}$ = 69.9°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 18$
$l = -11 \rightarrow 10$
3 standard reflections
frequency: 120 min
intensity decay: <1%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
$S$ = 1.09
2128 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 0.27P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0126 (12)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *SDP* (Frenz, 1978); data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Farrugia, 1997); software used to prepare material for publication: *PARST*97 (Nardelli, 1995).

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