

Ya-Wei Sun, Gui-Yun Duan,
Jun-Zhi Liu, Li-Juan Meng and
Jian-Wu Wang*School of Chemistry and Chemical Engineering,
Shandong University, Jinan 250100, People's
Republic of ChinaCorrespondence e-mail:
yugp2005@yahoo.com.cn

Key indicators

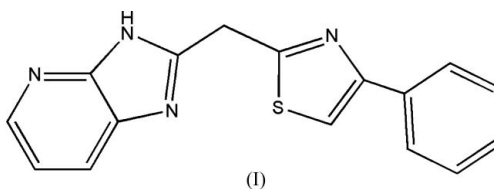
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.064
 wR factor = 0.146
Data-to-parameter ratio = 13.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-[(4,5-Dihydro-4-phenylthiazol-2-yl)methyl]-
3H-imidazo[4,5-*b*]pyridine

In the title compound, $\text{C}_{16}\text{H}_{12}\text{N}_4\text{S}$, the dihedral angles formed by the phenyl and the 3*H*-imidazo[4,5-*b*]pyridine ring systems with the thiazole ring are 9.14 (3) and 75.79 (6)°, respectively. There are some intra- and intermolecular hydrogen-bond interactions in the crystal structure, providing stabilization.

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Comment

Recently, (3*H*-imidazo[4,5-*b*]pyridine)(4-phenylthiazol-2-yl)-methane and its derivatives have been the focus of increasing attention due to their bioactivities, such as antitubercular (Bukowski, 2001), anticonvulsant (Tomczuk *et al.*, 1991), anxiolytic (Tomczuk *et al.*, 1991), and antiproliferative activity (Liszkiewicz *et al.*, 2003). These compounds are also employed as ligands (Abbotto *et al.*, 2002). In this paper, we report the crystal structure of the title compound, (I).



Bond lengths and angles of the 3*H*-imidazo[4,5-*b*]pyridine and thiazole ring systems (Table 1) are in agreement with the values quoted in previous reports (Rodier *et al.*, 1993; Rodriguez de Barbarín *et al.*, 2003). The dihedral angles formed by the phenyl (C3–C8) and the 3*H*-imidazo[4,5-*b*]pyridine (N1/N2/N3/C11–C16) ring systems with the thiazole (S1/N4/C1/C2/C9) ring are 9.14 (3) and 75.79 (6)°, respectively. The crystal structure is stabilized by intra- and intermolecular hydrogen-bond interactions (Table 2 and Fig. 2).

Experimental

Ethyl 2-(4-phenylthiazol-2-yl)acetate (10 mmol) and 2,3-diaminopyridine (10 mmol) were mixed and reacted at 453–473 K under solvent-free conditions for 1 h. Purification was achieved by recrystallization from methanol (yield 90%). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a methanol solution at room temperature for two weeks.

Crystal data

$\text{C}_{16}\text{H}_{12}\text{N}_4\text{S}$
 $M_r = 292.37$
Monoclinic, $P2_1/c$
 $a = 12.685$ (6) Å
 $b = 5.277$ (2) Å
 $c = 21.389$ (9) Å
 $\beta = 100.577$ (6)°
 $V = 1407.5$ (11) Å³
 $Z = 4$

$D_x = 1.375$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 2273
reflections
 $\theta = 2.3$ – 26.3 °
 $\mu = 0.23$ mm⁻¹
 $T = 293$ (2) K
Block, colourless
 $0.35 \times 0.21 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.925$, $T_{\max} = 0.973$
 6901 measured reflections

2509 independent reflections
 2210 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 25.2^\circ$
 $h = -15 \rightarrow 15$
 $k = -5 \rightarrow 6$
 $l = -23 \rightarrow 25$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.146$
 $S = 1.18$
 2509 reflections
 190 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.6991P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1—C2	1.349 (4)	C11—N2	1.351 (3)
C1—S1	1.700 (4)	C12—N3	1.392 (3)
C9—N4	1.298 (3)	C15—N1	1.338 (4)
C9—S1	1.725 (3)	C16—N1	1.333 (3)
C11—N3	1.307 (3)	C16—N2	1.370 (3)
C11—C10—C9	110.3 (2)	C1—S1—C9	89.08 (15)
C9—N4—C2	111.1 (2)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots N1 ⁱ	0.86	2.01	2.863 (3)	170
C8—H8 \cdots N4	0.93	2.57	2.884 (4)	100

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 \AA and N—H = 0.86 \AA , and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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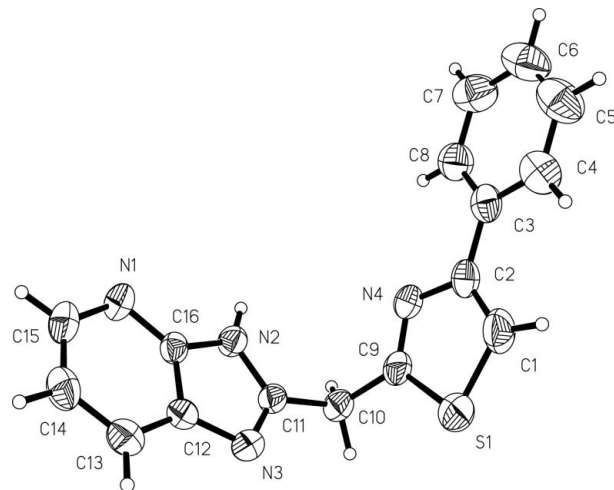


Figure 1

View of the title compound, with displacement ellipsoids drawn at the 40% probability level.

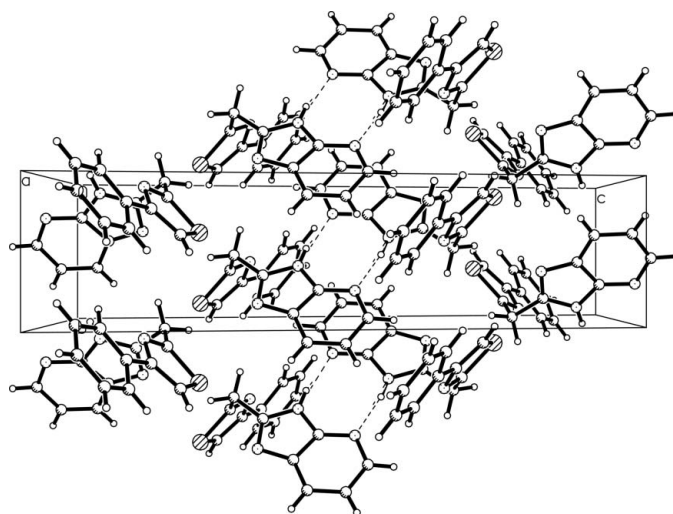


Figure 2

A packing diagram of the title compound, viewed down the a axis. Hydrogen bonds are shown as dashed lines.

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