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N-Benzylidene-4-(ferrocenyl)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazol-2-amine

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Key indicators

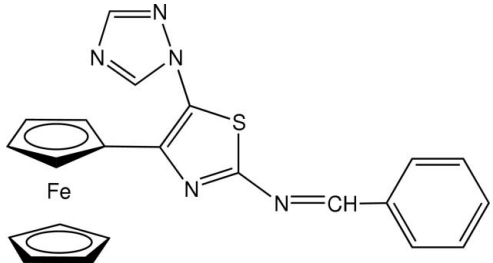
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.038
wR factor = 0.103
Data-to-parameter ratio = 13.0

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

In search of potent fungicidal agents, the title compound, $[Fe(C_5H_5)(C_{17}H_{12}N_5S)]$, has been synthesized and its crystal structure determined. The dihedral angles between the planes of the phenyl and thiazole rings and between the thiazole and triazole rings are 42.19 (13) and 81.15 (12)°, respectively.

Comment

Ferrocene-containing organic compounds often exhibit biological activity (Biot *et al.*, 2000; Fang *et al.*, 2003*a*,*b*). Thiazoles and their derivatives are found to be associated with various biological activities, such as antibacterial, antifungal and anti-inflammatory activities (Gusmeroli *et al.*, 2003; Wilson *et al.*, 2001). Triazole antifungals are known as potent inhibitors of cytochrome P450 monooxygenase in the process of fungal biosynthesis of ergosterol, which is an important constituent of fungal cell membranes (Miyauchi *et al.*, 1995). In order to discover more biologically active thiazole compounds, the title compound, (I), was synthesized and its crystal structure determined (Fig. 1).



(I)

Three planar rings in the title compound are (i) the phenyl ring C17–C22; (ii) the thiazole ring C11/C12/S1/C15/N4; (iii) the triazole ring N1/C13/N3/N2/C14. The dihedral angles between planes i and ii, and between planes ii and iii are 42.19 (13) and 81.15 (12)°, respectively.

Experimental

2-Amino-4-(ferrocenyl)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazole (Shao *et al.*, 2004) (0.7 g, 2 mmol) and benzaldehyde (0.21 g, 2 mmol) were dissolved in benzene (10 ml). One drop of piperidine was added. The solution was heated and refluxed in a 50 ml flask equipped with a Dean–Stark trap condenser until no water appeared (*ca* 1 h). The solution was then concentrated and purified by silica column chromatography (eluent: ethyl acetate–petroleum ether, 1:1). Single crystals were obtained by evaporation of the solvent (m.p. 438–439 K; yield 88%). Analysis calculated for $C_{22}H_{17}FeN_5S$: C 60.15, H 3.90, N 15.94%; found: C 60.27, H 4.04, N 16.03%. ^{1}H NMR ($CDCl_3$): δ 9.02 (*s*, 1H), 8.30 (*s*, 1H), 8.25 (*s*, 1H), 7.63–7.51(*m*, 5H), 4.27 (*s*, 2H), 4.26 (*s*, 2H), 4.12 (*s*, 5H).

Crystal data

$[Fe(C_5H_5)(C_{17}H_{12}N_5S)]$	$Z = 2$
$M_r = 439.32$	$D_x = 1.495$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 8.826$ (4) Å	Cell parameters from 1939 reflections
$b = 10.608$ (5) Å	$\theta = 2.30$–$22.20°$
$c = 11.619$ (5) Å	$\mu = 0.90$ mm^{-1}
$\alpha = 64.982$ (7)°	$T = 294$ (2) K
$\beta = 83.064$ (8)°	Plate, orange
$\gamma = 83.425$ (7)°	0.22 × 0.20 × 0.18 mm
$V = 976.0$ (8) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3425 independent reflections
	2557 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.025$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -10 \rightarrow 8$
$T_{min} = 0.817$, $T_{max} = 0.851$	$k = -12 \rightarrow 12$
4998 measured reflections	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.1365P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
3425 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
263 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.057 (3)

Table 1
Selected geometric parameters (Å, °).

S1—C12	1.729 (3)	N3—C13	1.337 (4)
S1—C15	1.743 (3)	N4—C15	1.299 (4)
N1—C13	1.310 (4)	N4—C11	1.379 (3)
N1—C14	1.343 (6)	N5—C16	1.249 (4)
N2—C14	1.317 (5)	N5—C15	1.386 (4)
N2—N3	1.368 (4)		
C13—N1—C14	102.3 (3)	N3—C12—S1	121.2 (2)
C14—N2—N3	100.1 (3)	N1—C13—N3	110.2 (3)
C13—N3—N2	110.4 (3)	N2—C14—N1	116.9 (4)
C15—N4—C11	111.3 (2)	N4—C15—S1	115.4 (2)
C16—N5—C15	121.4 (3)	N5—C15—S1	123.2 (2)
C11—C12—S1	111.8 (2)	N5—C16—C17	122.5 (3)

All H atoms were placed in calculated positions, with C—H = 0.93 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

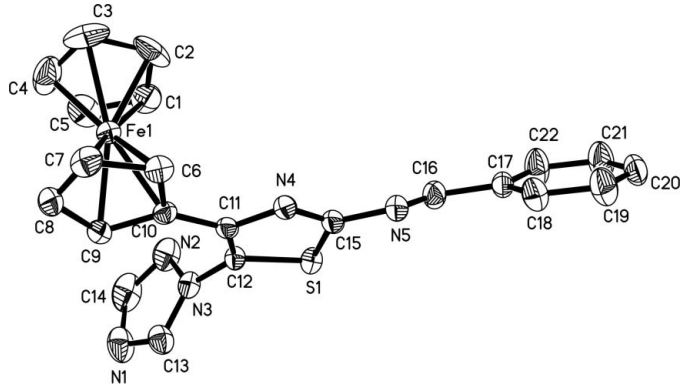


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted.

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