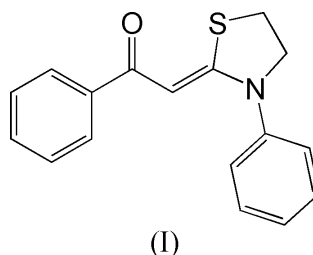


(Z)-1-Phenyl-2-(3-phenylthiazolidin-2-ylidene)-ethanoneLiang-Zhong Xu,^{a*} Hai-Zhen Xu,^b
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youquan_zhu@mail.nankai.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.035
 wR factor = 0.095
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_{17}\text{H}_{15}\text{NOS}$, crystallizes in space group $P\bar{1}$ with two independent molecules in the asymmetric unit. The dihedral angles between the two benzene rings and the heterocyclic five-membered mean ring in the two independent molecules are different: $35.62(7)$ and $58.80(7)^\circ$ in one molecule and $14.80(12)$ and $60.09(6)^\circ$ in the other.

Comment

Heterocyclic compounds possessing low toxicity can be highly efficient as fungicides (Shi *et al.*, 1995; Xu *et al.*, 2002). In this connection, studies of heterocyclic derivatives are mainly concentrated on compounds with triazole as the only active group. Many fungicidal heterocyclic compounds have been synthesized, including the title compound, (I) (Bogdanowicz-Szwed *et al.*, 1989). We report here the crystal structure of (I).



Compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1). All bond lengths and angles in both molecules are normal (Table 1) and comparable to those in published structures (Ciechanowicz-Rutkowska *et al.*, 1989, 1990; Bogdanowicz-Szwed *et al.*, 1994). The angles formed by the planes C6–C11 and C12–C17 with the hetero-ring plane (C1/C2/C3/N1/S1) are $35.62(7)$ and $58.80(7)^\circ$, respectively. In the second independent molecule, the planes C23–C28 and C29–C34 make angles of $14.80(12)$ and $60.09(6)^\circ$ with plane C18/C19/C20/N2/S2. This geometry is very similar to that found in the related compounds 3-phenyl-4-phenylamino-5-benzoyl-2,3-dihydro-2-phenylacylidene-thiazole (Bogdanowicz-Szwed *et al.*, 1994), 2-(*p*-methoxybenzoylmethylene)-3-phenyl-1,3-thiazolidine-4,5-dione (Ciechanowicz-Rutkowska *et al.*, 1990 and 2-(2-benzoylmethylene-4-oxo-3-phenyl-1,3-thiazolidin-5-ylidene)propanedinitrile (Ciechanowicz-Rutkowska *et al.*, 1989).

Experimental

The title compound was prepared by the reaction of acetophenone (0.01 mol), 1,2-dibromoethane (0.015 mol) and isothiocyanatobenzene (0.01 mol) at 313–318 K for 4 h. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

Received 10 December 2004

Accepted 20 January 2005

Online 29 January 2005

Crystal data

C₁₇H₁₅NOS
M_r = 281.37
 Triclinic, *P*1̄
a = 9.5998 (12) Å
b = 10.8872 (13) Å
c = 14.4903 (18) Å
 α = 79.303 (2)°
 β = 76.243 (2)°
 γ = 80.467 (2)°
V = 1433.7 (3) Å³

Z = 4
D_x = 1.304 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2755 reflections
 θ = 2.4–24.8°
 μ = 0.22 mm⁻¹
T = 293 (2) K
 Prism, colorless
 0.52 × 0.38 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.871, *T_{max}* = 0.959
 7858 measured reflections

5001 independent reflections
 3811 reflections with *I* > 2σ(*I*)
R_{int} = 0.017
 θ_{max} = 25.0°
h = -11 → 11
k = -12 → 12
l = -10 → 17

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.035
wR(*F*²) = 0.096
S = 1.03
 5001 reflections
 362 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.042*P*)² + 0.2564*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.20 e Å⁻³
 Δρ_{min} = -0.15 e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0143 (12)

Table 1

Selected geometric parameters (Å, °).

S1–C3	1.7442 (16)	O1–C5	1.2378 (19)
S1–C1	1.813 (2)	C1–C2	1.496 (3)
N1–C3	1.360 (2)	C3–C4	1.363 (2)
N1–C12	1.425 (2)	C4–C5	1.420 (2)
N1–C2	1.460 (2)	C5–C6	1.502 (2)
C3–S1–C1	91.58 (8)	N1–C3–S1	111.09 (12)
C3–N1–C12	122.70 (13)	C4–C3–S1	123.60 (13)
C3–N1–C2	114.95 (14)	O1–C5–C4	123.23 (16)
C12–N1–C2	119.87 (14)	O1–C5–C6	119.17 (15)
N1–C3–C4	125.31 (15)	C4–C5–C6	117.59 (15)
C12–N1–C2–C1	-165.56 (15)	O1–C5–C6–C7	-150.82 (17)
C2–N1–C3–C4	165.15 (17)	C4–C5–C6–C7	30.7 (2)
C12–N1–C3–S1	-176.16 (12)	O1–C5–C6–C11	27.7 (2)
N1–C3–C4–C5	178.60 (16)	C4–C5–C6–C11	-150.83 (17)
S1–C3–C4–C5	-2.2 (2)		

All H atoms were placed in calculated positions, with C–H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with *U_{iso}*(H) = 1.2*U_{eq}*(C).

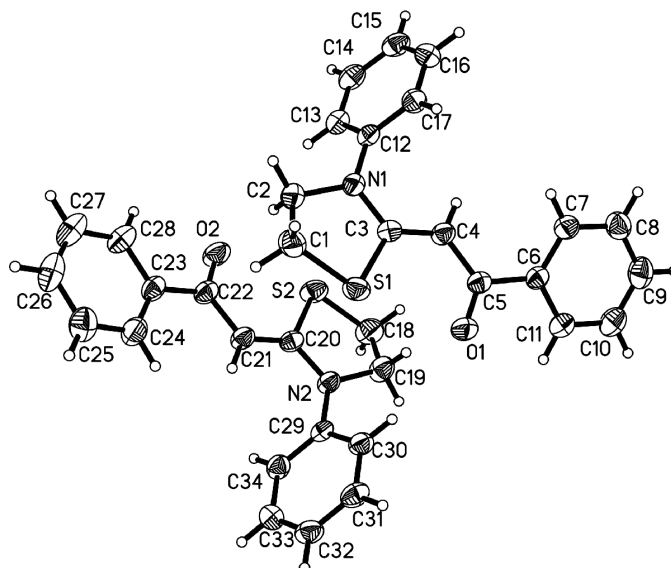


Figure 1

The asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

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, 1998); software used to prepare material for publication: SHELXTL.

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