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3-Cyclohexyl-4-(3-methyl-3-phenylcyclobutyl)-1,3-thiazole-2(3*H*)-thione

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The cyclohexyl ring of the title compound, $C_{20}H_{25}NS_2$, has a chair conformation. The dihedral angle between the thiazole and phenyl rings is 89.70 (2)°. The crystal structure involves two weak intramolecular C—H···S hydrogen-bond contacts.

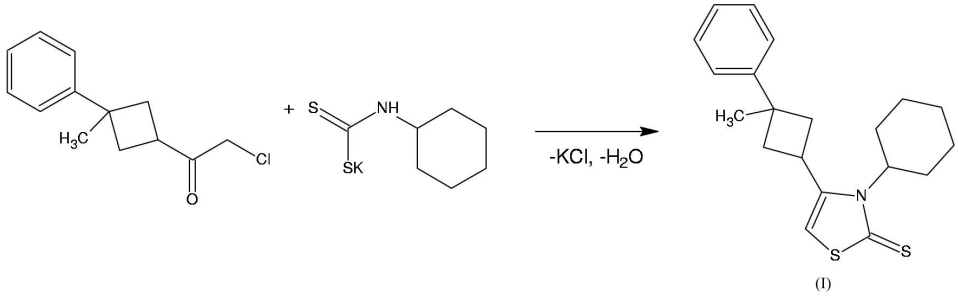
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.070
Data-to-parameter ratio = 15.2

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

Comment

The title compound, (I) (Fig. 1), was synthesized and characterized as part of our ongoing studies (Kırılmış *et al.*, 2005, and references therein) of 1,3-thiazole-2(3*H*)-thione derivatives. We report here the crystal structure of (I).



(I)

Compound (I) exhibits normal geometrical parameters (Allen *et al.*, 1987; Özdemir *et al.*, 2004; Yüksektepe *et al.*, 2004). The cyclohexyl ring has a chair conformation [puckering parameters (Cremer & Pople, 1975); Q_T = 0.587 (2) Å, θ = 179.2 (2)° and φ = 198.6°]. The thiazolethione system is essentially planar, with a maximum deviation from planarity of 0.0309 (2) Å for atom N1. The dihedral angle between the thiazole and phenyl rings is 89.70 (2)°. In the cyclobutane ring, the C10/C11/C9 plane forms a dihedral angle of 23.82 (3)° with

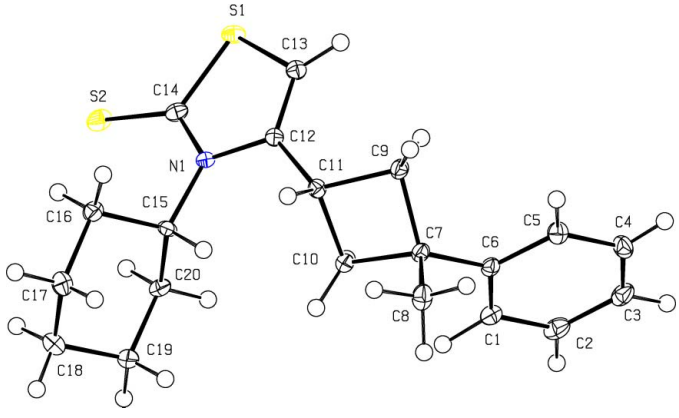


Figure 1
The structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms are shown as small circles of arbitrary radii.

the C9/C7/C10 plane. This agrees with the angle of 23.5 (4)° reported for a hexafluorocyclobutane (Swenson *et al.*, 1997).

The crystal structure has two weak intramolecular C—H···S hydrogen contacts (Table 1). The C···S distances of 3.433 (2) and 3.427 (2) Å are longer than that [3.132 (2) Å] observed in another thiazoline compound (Kırılmış *et al.*, 2005).

Experimental

The title compound was prepared according to the method of Ahmedzade *et al.* (2003).

Crystal data

$C_{20}H_{25}NS_2$
M_r = 343.53
Orthorhombic, $P2_12_12_1$
a = 9.9686 (8) Å
b = 12.2843 (8) Å
c = 14.7707 (3) Å
V = 1808.8 (2) Å^3
Z = 4
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 264 reflections
θ = 6.0–20.0°
μ = 0.29 mm^{-1}
T = 100 (2) K
Block, colourless
0.30 × 0.28 × 0.23 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.916, T_{max} = 0.935
27385 measured reflections
4306 independent reflections
3828 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.9°
$h = -13 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.070
S = 1.06
4306 reflections
283 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1856 Freidel pairs
Flack parameter = −0.02 (5)

Table 1
Selected geometric parameters (Å, °).

S1—C13	1.725 (2)	S2—C14	1.677 (2)
S1—C14	1.734 (2)		
C13—S1—C14	92.34 (8)	N1—C14—S1	109.1 (1)
C12—C13—S1	111.5 (1)	S2—C14—S1	121.4 (1)
N1—C14—S2	129.6 (1)		

H atoms were located in a difference map and only the H-atom coordinates were refined [C—H = 0.91 (2)–1.05 (2)]; the U_{iso} values were fixed at 0.040 Å^2.

Data collection: *COLLECT* (Bruker–Nonius, 2002); cell refinement: *EVALCCD* (Bruker–Nonius, 2002); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

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