

The structure of the title compound was solved by direct methods and refined by full-matrix least-squares calculations using *CRYSTAN-GM* (Gilmore & Brown, 1988). H atoms attached to *tert*-butanol O atoms were found from the difference Fourier map and fixed in the refinement. Other H atoms were placed at geometrically idealized positions with N—H and C—H distances of 0.96 Å, and were restricted to their parent atoms with the corresponding equivalent isotropic displacement parameters. The absolute configuration was assigned to agree with the known chirality at the C(6) and C(27) atoms arising from L-tryptophan methyl ester.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry, including contact distances, have been deposited with the IUCr (Reference: TA1063). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## 5-Cyclohexylamino-2-phenyl-4-thiazole-carbonitrile

MADIHA KAMMOUN, BÉCHIR HAJJEM, TAHAR JOUINI AND BELGACEM BACCAR

*Département de Chimie, Faculté des Sciences, Campus Universitaire, 1060 Tunis, Tunisia. E-mail: jouini@stardent.cck.tn*

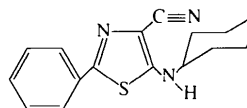
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## Abstract

C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>S contains a planar thiazole ring. The C—S bond length is shorter than that found in the tetrahydrothiophene [Allen, Kennard, Watson, Brammer, Orpen & Taylor (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19]. The phenyl and the thiazole rings are conjugated.

## Comment

The title compound (I) was synthesized by the treatment of methyl *N*-cyanomethylbenzimidate with lithium diisopropylamine at 203 K followed by the action of cyclohexylisothiocyanate (Kammoun, Hajjem & Baccar, 1996). Theoretically, the reaction could lead to the formation of imidazole or to thiazole derivatives. Single-crystal X-ray diffraction allowed the determination of the molecular structure. The thiazole ring is planar,



(I)

as shown by the torsion angles C7—S—C9—C8 = 1.4(2) and C9—S—C7—N1 = -1.2(2)°. The C—S bond lengths in the thiazole ring [C9—S 1.729(2) Å, C7—S 1.761(2) Å] are similar to the C—S bond distances in the thiophene ring (Allen *et al.*, 1987) indicating a partial  $\pi$ -bond character. This results from the delocalization of the negative density charge through the thiazole ring. The phenyl-ring plane is twisted about 7.9(2)° out of the thiazole ring. The low value of this twist angle and the short C1—C7 distance [1.468(3) Å] could explain the conjugation between the two rings.

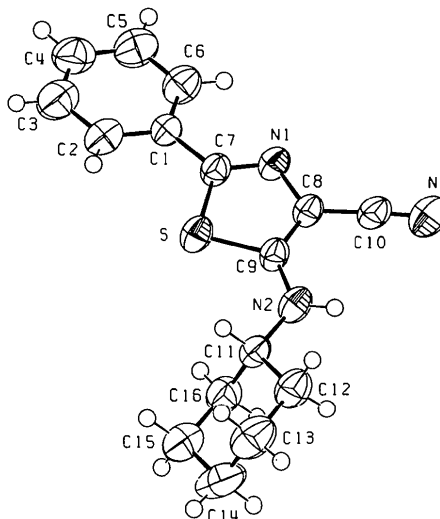


Fig. 1. ORTEP (Johnson, 1976) view of C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>S showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

## Experimental

The title compound was synthesized according to Kammoun, Hajjem & Baccar (1996) (see *Comment*).

## Crystal data

C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>S  
*M<sub>r</sub>* = 283.393  
 Monoclinic  
*P*2<sub>1</sub>/*n*  
*a* = 9.199 (1) Å  
*b* = 5.731 (3) Å  
*c* = 28.812 (6) Å  
 $\beta$  = 95.08 (1)°  
*V* = 1513.0 (9) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.244 Mg m<sup>-3</sup>

## Data collection

CAD-4 diffractometer  
 $\omega$  scans  
 Absorption correction:  
 none  
 2826 measured reflections  
 2649 independent reflections  
 2114 observed reflections  
 $[I > 2\sigma(I)]$

*R*<sub>int</sub> = 0.0096  
 $\theta_{\max}$  = 24.96°  
*h* = 0 → 10  
*k* = 0 → 6  
*l* = -34 → 34  
 2 standard reflections  
 frequency: 120 min  
 intensity decay: 0.11%

## Refinement

Refinement on *F*<sup>2</sup>  
 $R[F^2 > 2\sigma(F^2)] = 0.0401$   
 $wR(F^2) = 0.0955$   
*S* = 1.179  
 2649 reflections  
 250 parameters  
 All H-atom parameters  
 refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 0.6124P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = -0.186$

$\Delta\rho_{\max} = 0.174 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.160 \text{ e } \text{Å}^{-3}$   
 Extinction correction:  
*SHELXL93* (Sheldrick,  
 1993)  
 Extinction coefficient:  
 0.015 (1)  
 Atomic scattering factors  
 from *International Tables*  
 for *Crystallography* (1992,  
 Vol. C, Tables 4.2.6.8 and  
 6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)
$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub>
S	0.11796 (6)	-0.0161 (1)	0.14102 (2)	0.0549 (2)
C1	0.3725 (2)	0.1255 (4)	0.19470 (7)	0.0494 (5)
C2	0.3638 (3)	-0.0694 (5)	0.22202 (9)	0.0675 (7)
C3	0.4599 (3)	-0.1010 (6)	0.26111 (10)	0.0815 (9)
C4	0.5649 (3)	0.0612 (6)	0.27318 (10)	0.0814 (9)
C5	0.5753 (3)	0.2556 (6)	0.24627 (10)	0.0824 (9)
C6	0.4806 (3)	0.2885 (5)	0.20714 (9)	0.0680 (7)
C7	0.2701 (2)	0.1670 (4)	0.15350 (7)	0.0480 (5)
C8	0.1601 (2)	0.3404 (4)	0.09181 (7)	0.0479 (5)
C9	0.0594 (2)	0.1624 (4)	0.09470 (6)	0.0471 (5)
C10	0.1463 (2)	0.5155 (4)	0.05697 (7)	0.0523 (5)
C11	-0.1690 (2)	-0.0592 (4)	0.07586 (7)	0.0487 (5)
C12	-0.2669 (3)	-0.0995 (6)	0.03159 (9)	0.0678 (7)
C13	-0.3788 (4)	-0.2887 (6)	0.0386 (1)	0.090 (1)
C14	-0.4660 (3)	-0.2368 (8)	0.0790 (1)	0.101 (1)
C15	-0.3668 (3)	-0.1958 (7)	0.1230 (1)	0.0844 (9)
C16	-0.2587 (3)	-0.0005 (5)	0.1161 (1)	0.0683 (7)
N1	0.2771 (2)	0.3404 (3)	0.12529 (6)	0.0512 (5)
N2	-0.0641 (2)	0.1235 (4)	0.06743 (6)	0.0563 (5)
N3	0.1297 (2)	0.6496 (4)	0.02770 (7)	0.0720 (6)

Table 2. Geometric parameters (Å, °)

S—C9	1.729 (2)	C8—C9	1.386 (3)
S—C7	1.761 (2)	C8—C10	1.417 (3)
C1—C2	1.373 (3)	C9—N2	1.342 (3)
C1—C6	1.388 (3)	C10—N3	1.141 (3)
C1—C7	1.468 (3)	C11—N2	1.459 (3)
C2—C3	1.380 (4)	C11—C12	1.512 (3)
C3—C4	1.363 (4)	C11—C16	1.518 (3)
C4—C5	1.366 (4)	C12—C13	1.521 (4)
C5—C6	1.376 (4)	C13—C14	1.501 (5)
C7—N1	1.289 (3)	C14—C15	1.512 (5)
C8—N1	1.380 (2)	C15—C16	1.522 (4)
C9—S—C7	89.6 (1)	N2—C9—C8	128.5 (2)
C2—C1—C6	118.5 (2)	N2—C9—S	122.9 (2)
C2—C1—C7	122.0 (2)	C8—C9—S	108.5 (1)
C6—C1—C7	119.6 (2)	N3—C10—C8	176.5 (2)
C1—C2—C3	120.6 (3)	N2—C11—C12	108.8 (2)
C4—C3—C2	120.4 (3)	N2—C11—C16	112.4 (2)
C3—C4—C5	119.7 (3)	C12—C11—C16	110.7 (2)
C4—C5—C6	120.4 (3)	C11—C12—C13	110.8 (2)
C5—C6—C1	120.4 (3)	C14—C13—C12	112.1 (3)
N1—C7—C1	124.8 (2)	C13—C14—C15	110.8 (3)
N1—C7—S	114.4 (1)	C14—C15—C16	111.0 (3)
C1—C7—S	120.7 (2)	C11—C16—C15	110.0 (2)
N1—C8—C9	116.2 (2)	C7—N1—C8	111.2 (2)
N1—C8—C10	120.7 (2)	C9—N2—C11	124.1 (2)
C9—C8—C10	123.1 (2)		

The  $\omega$ -scan angle was  $(0.78 + 1.50 \tan \theta)^\circ$  and the background was measured by the usual scan on each side of the reflection. The structure was solved by direct methods (*SHELXS86*; Sheldrick, 1985) and refinement was by full-matrix least-squares methods (*SHELXL93*; Sheldrick, 1993).

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS86*. Program(s) used to refine structure: *SHELXL93*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, torsion angles and complete geometry have been deposited with the IUCr (Reference: DU1133). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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