

## (2E)-3-Phenylprop-2-en-1-yl thiocyanate

Ezzat Khan,<sup>a\*</sup> Adnan Shahzad,<sup>b</sup> M. Nawaz Tahir<sup>c</sup> and Muhammad Ateeq<sup>d</sup>

<sup>a</sup>Department of Chemistry, University of Malakand, Pakistan, <sup>b</sup>Institute of Chemical Sciences, University of Swat, Khyber Pakhtunkhwa, Pakistan, <sup>c</sup>Department of Physics, University of Sargodha, Sargodha, Pakistan, and <sup>d</sup>HEJ Research Institute, University of Karachi, Karachi, Pakistan. \*Correspondence e-mail: ekhan@uom.edu.pk

Received 21 March 2017

Accepted 11 April 2017

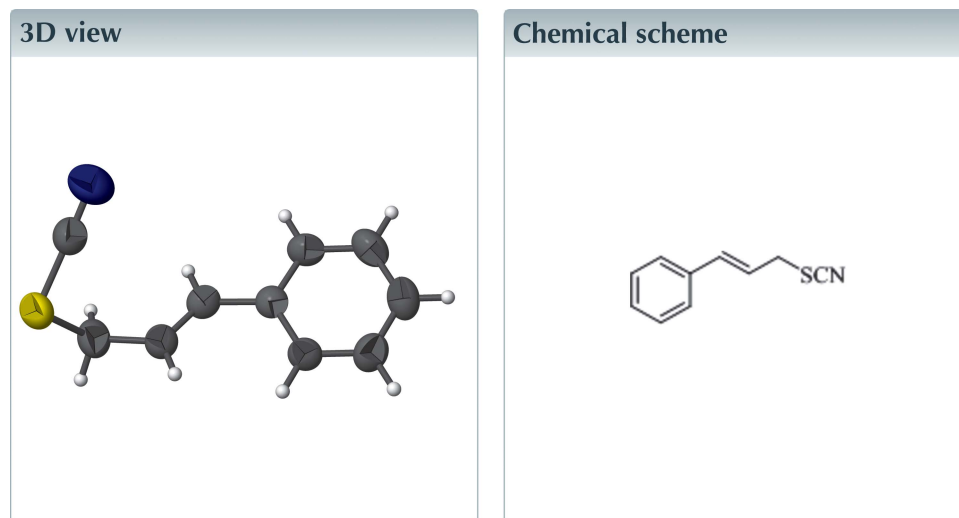
Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; cinammyl chloride; ammonium thiocyanate.

CCDC reference: 1543491

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>10</sub>H<sub>9</sub>NS, the C—S—C bond angle is 99.41 (9)° and the dihedral angle between the *trans*-alkene fragment and the benzene ring is 16.49 (19)°. In the crystal, inversion dimers linked by pairs of extremely weak C—H···N interactions occur, as does a short S···N contact [3.2258 (19) Å].



### Structure description

Alkyl thiocyanates are synthetic precursors for the preparation of sulfur-containing organic compounds such as disulfides (Lu *et al.*, 2014) and various heterocyclic compounds (Vikharev *et al.*, 2005; Batanero *et al.*, 2002). The title compound (Fig. 1) arose during our studies of unsymmetrical thiourea derivatives.

The C—S—C bond angle is 99.41 (9)° and the dihedral angle between the C2/C3/C4/C5 fragment and the benzene ring is 16.49 (19)°. A quantum-chemical calculation for this molecule (see Supporting information) gave a C—S—C angle of 160.0°. In the crystal, extremely weak C—H···N interactions (Table 1) generate inversion dimers with an *R*<sub>2</sub><sup>2</sup>(10) motif and short S···N contacts [3.2258 (19) Å, compared to a van der Waals radius sum of 3.35 Å] are also observed: these contacts link the dimers into [100] chains (Fig. 2).

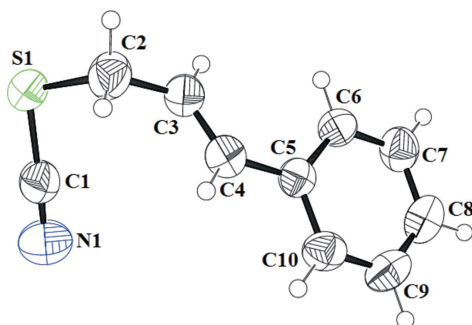
### Synthesis and crystallization

A round-bottom flask was charged with cinammyl chloride (1 ml, 7.2 mmol) in acetone. The solution was stirred vigorously and NH<sub>4</sub>SCN (0.5 g, 7.2 mmol) was added. The reaction mixture was heated to reflux for 30 min and then poured into crushed ice. The solid product was separated and dissolved in CH<sub>2</sub>Cl<sub>2</sub>. After 24 h, colorless prismatic crystals appeared in solution. Crystals of appropriate quality of the same compound were also obtained from *n*-hexane solution. A reaction scheme is given in Fig. 3.

**Table 1**  
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2B···N1 <sup>i</sup>	0.97	2.70	3.652 (2)	167

Symmetry code: (i)  $-x + 2, -y + 1, -z + 1$ .



**Figure 1**  
The molecular structure of the title compound, showing 50% displacement ellipsoids.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

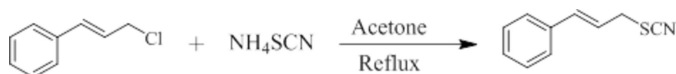
We are thankful to Professor Dr Muhammad Raza Shah for the EI-MS analysis of the title compound.

## Funding information

Funding for this research was provided by: Higher Education Commission Pakistan (Access to the Scientific Instrumentation project).

## References

- Batanero, B., Barba, F. & Martín, A. (2002). *J. Org. Chem.* **67**, 2369–2371.  
 Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.



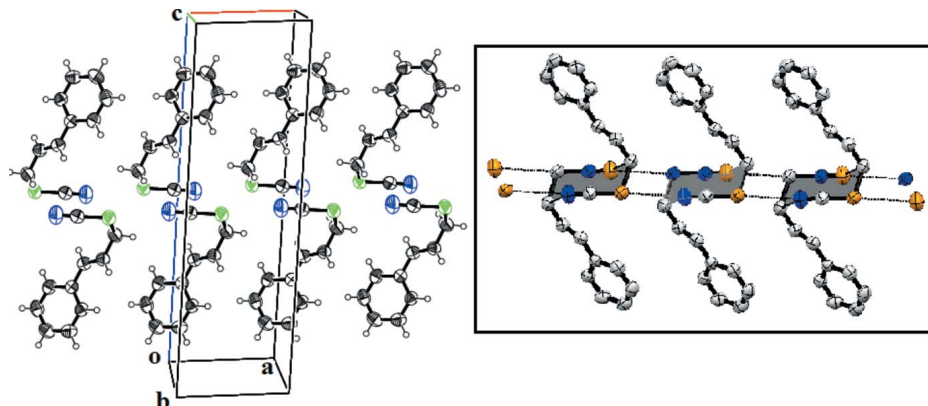
**Figure 3**  
Reaction scheme.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>10</sub> H <sub>9</sub> NS
<i>M<sub>r</sub></i>	175.24
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.0108 (5), 7.9243 (6), 19.8388 (16)
$\beta$ (°)	94.271 (4)
<i>V</i> (Å <sup>3</sup> )	942.33 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.29
Crystal size (mm)	0.37 × 0.27 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Sheldrick, 2005)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.902, 0.932
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	8591, 2319, 1697
<i>R<sub>int</sub></i>	0.022
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.668
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.043, 0.112, 1.05
No. of reflections	2319
No. of parameters	109
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.39, -0.39

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

- Lu, X., Wang, H. R., Gao, D., Sun, D. & Bi, X. (2014). *RSC Adv.* **4**, 28794–28797.  
 Sheldrick, G. M. (2005). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.  
 Vikharev, Y. B., Shklyayev, Y. V., Anikina, L., Kolla, V. & Tolstikov, A. (2005). *Pharm. Chem. J.* **39**, 405–408.



**Figure 2**  
Unit-cell packing diagram (left) and supramolecular chain (right insert) of the title compound showing the C—H···N hydrogen bonds and N—S interactions.

## full crystallographic data

*IUCrData* (2017). 2, x170549 [https://doi.org/10.1107/S2414314617005491]

(2*E*)-3-Phenylprop-2-en-1-yl thiocyanate

Ezzat Khan, Adnan Shahzad, M. Nawaz Tahir and Muhammad Ateeq

(2*E*)-3-Phenylprop-2-en-1-yl thiocyanate*Crystal data*

$C_{10}H_9NS$	$F(000) = 368$
$M_r = 175.24$	$D_x = 1.235 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.0108 (5) \text{ \AA}$	Cell parameters from 1697 reflections
$b = 7.9243 (6) \text{ \AA}$	$\theta = 2.8\text{--}28.4^\circ$
$c = 19.8388 (16) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$\beta = 94.271 (4)^\circ$	$T = 296 \text{ K}$
$V = 942.33 (13) \text{ \AA}^3$	Prism, colourless
$Z = 4$	$0.37 \times 0.27 \times 0.25 \text{ mm}$

*Data collection*

Bruker Kappa APEXII CCD diffractometer	8591 measured reflections
Radiation source: fine-focus sealed tube	2319 independent reflections
Graphite monochromator	1697 reflections with $I > 2\sigma(I)$
Detector resolution: $7.50 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.022$
$\omega$ scans	$\theta_{\text{max}} = 28.4^\circ$ , $\theta_{\text{min}} = 2.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2005)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.902$ , $T_{\text{max}} = 0.932$	$k = -9 \rightarrow 10$
	$l = -26 \rightarrow 24$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.2661P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
2319 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
109 parameters	$\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.66511 (8)	0.22408 (8)	0.47818 (3)	0.0691 (2)
N1	1.1334 (3)	0.2485 (3)	0.48932 (12)	0.0962 (7)
C1	0.9445 (3)	0.2408 (3)	0.48395 (10)	0.0633 (5)
C2	0.5958 (3)	0.3977 (3)	0.41956 (10)	0.0676 (5)
H2A	0.4348	0.4037	0.4114	0.081*
H2B	0.6457	0.5027	0.4408	0.081*
C3	0.6953 (3)	0.3822 (2)	0.35388 (9)	0.0564 (4)
H3	0.6398	0.3001	0.3236	0.068*
C4	0.8586 (3)	0.4791 (2)	0.33626 (9)	0.0522 (4)
H4	0.9140	0.5571	0.3683	0.063*
C5	0.9632 (3)	0.47826 (19)	0.27201 (8)	0.0465 (4)
C6	0.8665 (3)	0.3994 (2)	0.21446 (9)	0.0534 (4)
H6	0.7302	0.3447	0.2162	0.064*
C7	0.9699 (3)	0.4015 (2)	0.15505 (9)	0.0623 (5)
H7	0.9031	0.3484	0.1169	0.075*
C8	1.1715 (3)	0.4817 (2)	0.15159 (10)	0.0660 (5)
H8	1.2413	0.4825	0.1113	0.079*
C9	1.2691 (3)	0.5602 (2)	0.20754 (11)	0.0650 (5)
H9	1.4057	0.6143	0.2053	0.078*
C10	1.1658 (3)	0.5595 (2)	0.26705 (10)	0.0571 (4)
H10	1.2329	0.6145	0.3047	0.068*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0554 (3)	0.0917 (4)	0.0609 (3)	-0.0079 (2)	0.0080 (2)	0.0169 (3)
N1	0.0577 (11)	0.1294 (19)	0.1012 (16)	0.0042 (11)	0.0046 (10)	0.0073 (13)
C1	0.0601 (11)	0.0766 (13)	0.0537 (10)	0.0024 (9)	0.0081 (8)	-0.0006 (9)
C2	0.0608 (11)	0.0811 (14)	0.0625 (11)	0.0112 (10)	0.0148 (8)	0.0083 (10)
C3	0.0561 (10)	0.0601 (11)	0.0533 (10)	0.0004 (8)	0.0049 (7)	0.0036 (8)
C4	0.0591 (10)	0.0442 (9)	0.0529 (10)	0.0018 (7)	0.0015 (7)	-0.0023 (7)
C5	0.0516 (9)	0.0361 (8)	0.0516 (9)	0.0024 (6)	0.0022 (7)	0.0037 (7)
C6	0.0542 (9)	0.0490 (10)	0.0567 (10)	-0.0080 (7)	0.0026 (7)	0.0016 (8)
C7	0.0783 (12)	0.0558 (11)	0.0529 (10)	-0.0051 (9)	0.0046 (9)	-0.0020 (8)
C8	0.0779 (12)	0.0569 (12)	0.0658 (12)	0.0006 (9)	0.0235 (10)	0.0063 (9)
C9	0.0574 (10)	0.0531 (11)	0.0863 (14)	-0.0071 (8)	0.0177 (9)	0.0056 (10)
C10	0.0573 (10)	0.0462 (10)	0.0668 (11)	-0.0056 (8)	-0.0012 (8)	-0.0031 (8)

*Geometric parameters (Å, °)*

S1—C1	1.680 (2)	C5—C6	1.390 (2)
S1—C2	1.829 (2)	C6—C7	1.373 (2)
N1—C1	1.134 (2)	C6—H6	0.9300
C2—C3	1.479 (2)	C7—C8	1.374 (3)
C2—H2A	0.9700	C7—H7	0.9300
C2—H2B	0.9700	C8—C9	1.366 (3)
C3—C4	1.313 (2)	C8—H8	0.9300
C3—H3	0.9300	C9—C10	1.374 (3)
C4—C5	1.463 (2)	C9—H9	0.9300
C4—H4	0.9300	C10—H10	0.9300
C5—C10	1.388 (2)		
C1—S1—C2	99.41 (9)	C6—C5—C4	122.49 (15)
N1—C1—S1	178.0 (2)	C7—C6—C5	120.76 (16)
C3—C2—S1	114.20 (14)	C7—C6—H6	119.6
C3—C2—H2A	108.7	C5—C6—H6	119.6
S1—C2—H2A	108.7	C6—C7—C8	120.36 (18)
C3—C2—H2B	108.7	C6—C7—H7	119.8
S1—C2—H2B	108.7	C8—C7—H7	119.8
H2A—C2—H2B	107.6	C9—C8—C7	119.79 (18)
C4—C3—C2	123.06 (18)	C9—C8—H8	120.1
C4—C3—H3	118.5	C7—C8—H8	120.1
C2—C3—H3	118.5	C8—C9—C10	120.13 (17)
C3—C4—C5	127.41 (16)	C8—C9—H9	119.9
C3—C4—H4	116.3	C10—C9—H9	119.9
C5—C4—H4	116.3	C9—C10—C5	121.19 (17)
C10—C5—C6	117.75 (16)	C9—C10—H10	119.4
C10—C5—C4	119.76 (15)	C5—C10—H10	119.4
C1—S1—C2—C3	58.62 (17)	C5—C6—C7—C8	0.1 (3)
S1—C2—C3—C4	-108.73 (19)	C6—C7—C8—C9	-0.2 (3)
C2—C3—C4—C5	-177.71 (16)	C7—C8—C9—C10	-0.2 (3)
C3—C4—C5—C10	-164.85 (18)	C8—C9—C10—C5	0.7 (3)
C3—C4—C5—C6	15.7 (3)	C6—C5—C10—C9	-0.9 (3)
C10—C5—C6—C7	0.5 (2)	C4—C5—C10—C9	179.60 (16)
C4—C5—C6—C7	179.97 (16)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2B...N1 <sup>i</sup>	0.97	2.70	3.652 (2)	167

Symmetry code: (i)  $-x+2, -y+1, -z+1$ .