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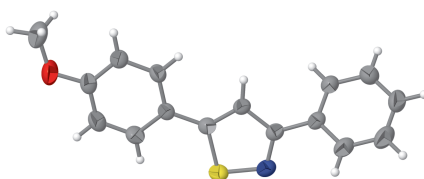
5-(4-Methoxyphenyl)-3-phenylisothiazole

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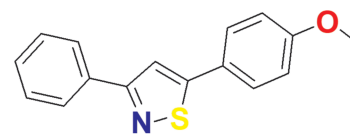
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In the title compound, C₁₆H₁₃NOS, the dihedral angles between the central isothiazole ring and pendant phenyl and *p*-methoxyphenyl rings are 41.57 (15) and 4.63 (13)°, respectively. In the extended structure, weak C—H··· π interactions may help to consolidate the packing.

3D view



Chemical scheme



Structure description

The title compound, C₁₆H₁₃NOS (**2**), crystallizes with one molecule in the asymmetric unit (Fig. 1) in space group *P*2₁. The dihedral angles between the central C1—C3/N1/S1 isothiazole ring and pendant C4—C9 phenyl and C10—C15 *p*-methoxybenzene rings are 41.57 (15) and 4.63 (13)°, respectively. This suggests the possibility of enhanced conjugation between the C1 and C10 rings, but the C1—C10 and C3—C4 bond lengths of 1.471 (3) and 1.474 (4) Å, respectively, are almost identical. A short intramolecular C11—H11···S1 contact (Table 1) occurs. Otherwise, the bond lengths and angles of **2** are within the ranges reported for related structures in the literature (Akkurt *et al.*, 2015; Sreenatha *et al.*, 2018, 2021; Sukhonosova *et al.*, 2016; Meundaeng *et al.*, 2019).

In the extended structure of **2**, weak C—H··· π interactions (Table 1) may help to establish the packing (Fig. 2), with each ring accepting one such interaction.

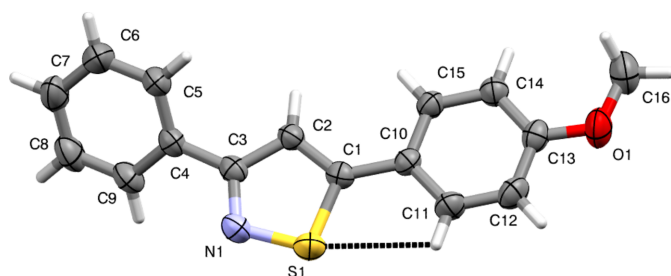
Synthesis and crystallization

The title compound was prepared by the literature method (Fig. 3) (Zhang *et al.* 2021) and 0.5 g of it was dissolved in 5 ml of *N,N*-dimethylformamide and was allowed to undergo slow evaporation to form colourless blocks of **2**.



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**Figure 1**

The molecular structure of **2** with displacement ellipsoids drawn at the 50% probability level. The short C—H...S contact is shown as a dashed line.

Refinement

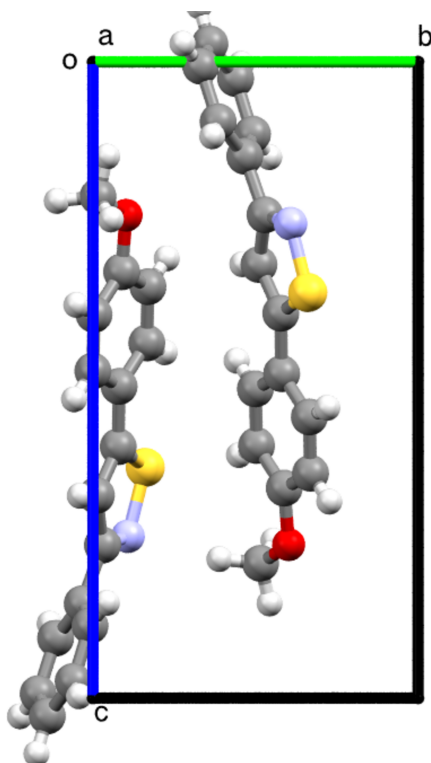
Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank BMSIT&M, Bengaluru and Govt. Engineering College, Chamarajanagara, for laboratory support.

References

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**Figure 2**

The packing of **2** viewed along the crystallographic *a* axis.

Table 1

Hydrogen-bond geometry (Å, °).

Cg1, Cg2 and Cg3 are the centroids of the C1–C3/N1/S1, C4–C9 and C10–C15 rings, respectively.

<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>
C11—H11...S1	0.93	2.73	3.137 (3)	107
C8—H8...Cg2 ⁱ	0.93	2.82	3.503 (4)	132
C12—H12...Cg1 ⁱⁱ	0.93	2.88	3.542 (4)	129
C15—H15...Cg3 ⁱⁱⁱ	0.93	2.92	3.688 (3)	140

Symmetry codes: (i) $-x, y - \frac{1}{2}, -z$; (ii) $-x, y + \frac{1}{2}, -z + 1$; (iii) $-x + 1, y - \frac{1}{2}, -z + 1$.

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₃ NOS
<i>M_r</i>	267.33
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.0239 (2), 7.4924 (2), 14.7003 (5)
β (°)	92.779 (1)
<i>V</i> (Å ³)	662.70 (4)
<i>Z</i>	2
Radiation type	Mo Kα
μ (mm ^{−1})	0.23
Crystal size (mm)	0.31 × 0.28 × 0.23
Data collection	
Diffractionmeter	Bruker SMART APEX
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	40942, 4059, 3351
<i>R</i> _{int}	0.103
(sin θ/λ) _{max} (Å ^{−1})	0.715
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.047, 0.130, 1.01
No. of reflections	4059
No. of parameters	173
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.34, −0.23
Absolute structure	Flack <i>x</i> determined using 1295 quotients [(<i>I</i> ⁺ − <i>I</i> [−])/(<i>I</i> ⁺ + <i>I</i> [−])] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.13 (5)

Computer programs: *APEX* and *SAINT* (Bruker, 2012), *SHELXT2014/4* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

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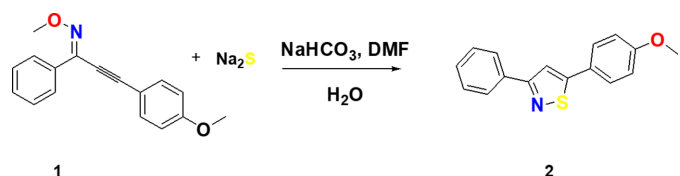
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**Figure 3**

Synthesis scheme of the title compound.

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full crystallographic data

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5-(4-Methoxyphenyl)-3-phenylisothiazole

Crystal data

$C_{16}H_{13}NOS$

$M_r = 267.33$

Monoclinic, $P2_1$

$a = 6.0239$ (2) Å

$b = 7.4924$ (2) Å

$c = 14.7003$ (5) Å

$\beta = 92.779$ (1)°

$V = 662.70$ (4) Å³

$Z = 2$

$F(000) = 280$

$D_x = 1.340$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 40942 reflections

$\theta = 3.1\text{--}30.5^\circ$

$\mu = 0.23$ mm⁻¹

$T = 298$ K

Block, colourless

$0.31 \times 0.28 \times 0.23$ mm

Data collection

Bruker SMART APEX

diffractometer

Radiation source: graphite

40942 measured reflections

4059 independent reflections

3351 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.103$

$\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -8 \rightarrow 8$

$k = -10 \rightarrow 10$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.130$

$S = 1.01$

4059 reflections

173 parameters

1 restraint

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.34$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Absolute structure: Flack x determined using

1295 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et*

al., 2013)

Absolute structure parameter: 0.13 (5)

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. Hydrogen atoms were placed in the calculated positions and refined as riding: C—H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms and C—H = 0.96 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.4874 (4)	0.6019 (3)	0.75885 (14)	0.0623 (6)
S1	−0.10260 (11)	0.66085 (10)	0.36254 (5)	0.0505 (2)
N1	−0.0930 (4)	0.6076 (4)	0.25432 (17)	0.0473 (6)
C1	0.1545 (4)	0.5777 (3)	0.39509 (17)	0.0355 (5)
C2	0.2470 (4)	0.5106 (3)	0.31860 (17)	0.0369 (5)
C3	0.1002 (4)	0.5291 (3)	0.24041 (17)	0.0375 (5)
C4	0.1477 (4)	0.4669 (3)	0.14826 (17)	0.0391 (5)
C5	0.3554 (5)	0.4910 (5)	0.11364 (19)	0.0482 (6)
C6	0.3930 (6)	0.4388 (6)	0.0261 (2)	0.0627 (9)
C7	0.2257 (6)	0.3597 (5)	−0.0282 (2)	0.0643 (10)
C8	0.0206 (6)	0.3312 (5)	0.0068 (3)	0.0598 (8)
C9	−0.0196 (5)	0.3850 (4)	0.0941 (2)	0.0490 (7)
C10	0.2439 (4)	0.5804 (3)	0.49001 (17)	0.0351 (5)
C11	0.1298 (5)	0.6657 (4)	0.55817 (19)	0.0461 (6)
C12	0.2156 (5)	0.6693 (5)	0.64660 (19)	0.0503 (6)
C13	0.4162 (5)	0.5883 (4)	0.66996 (18)	0.0430 (6)
C14	0.5328 (5)	0.5032 (4)	0.60302 (18)	0.0427 (6)
C15	0.4457 (5)	0.4996 (4)	0.51409 (18)	0.0403 (5)
C16	0.6838 (8)	0.5155 (6)	0.7883 (2)	0.0706 (10)
H2	0.387587	0.459462	0.318032	0.044*
H5	0.469362	0.542442	0.149633	0.058*
H6	0.532215	0.456678	0.002941	0.075*
H7	0.251766	0.326248	−0.087616	0.077*
H8	−0.091138	0.275419	−0.028633	0.072*
H9	−0.158997	0.366739	0.117046	0.059*
H11	−0.005761	0.720686	0.543607	0.055*
H12	0.137634	0.726921	0.691119	0.060*
H14	0.668691	0.449069	0.617911	0.051*
H15	0.523906	0.441921	0.469656	0.048*
H16A	0.665401	0.388862	0.781437	0.106*
H16B	0.717252	0.543204	0.851271	0.106*
H16C	0.803493	0.555074	0.752536	0.106*

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

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0806 (16)	0.0688 (15)	0.0369 (10)	0.0052 (13)	−0.0040 (10)	−0.0104 (10)
S1	0.0416 (3)	0.0599 (4)	0.0499 (4)	0.0159 (3)	0.0029 (3)	−0.0015 (3)
N1	0.0395 (12)	0.0548 (14)	0.0470 (13)	0.0073 (10)	−0.0044 (10)	0.0051 (10)
C1	0.0358 (11)	0.0307 (11)	0.0401 (12)	0.0005 (9)	0.0014 (9)	0.0026 (10)
C2	0.0332 (11)	0.0390 (12)	0.0382 (12)	0.0029 (9)	−0.0017 (9)	−0.0004 (10)
C3	0.0361 (12)	0.0353 (11)	0.0408 (13)	−0.0026 (9)	−0.0020 (10)	0.0030 (9)
C4	0.0394 (13)	0.0386 (12)	0.0387 (13)	0.0019 (10)	−0.0059 (10)	0.0020 (9)
C5	0.0391 (14)	0.0637 (17)	0.0414 (14)	0.0005 (12)	−0.0032 (11)	−0.0032 (13)
C6	0.0483 (18)	0.091 (3)	0.0487 (17)	0.0113 (17)	0.0045 (14)	−0.0061 (16)

C7	0.067 (2)	0.082 (2)	0.0428 (16)	0.0203 (18)	−0.0066 (14)	−0.0188 (16)
C8	0.0622 (19)	0.0598 (19)	0.0552 (17)	0.0033 (16)	−0.0200 (15)	−0.0146 (15)
C9	0.0443 (15)	0.0497 (15)	0.0518 (16)	−0.0033 (12)	−0.0106 (12)	−0.0038 (12)
C10	0.0373 (12)	0.0319 (10)	0.0364 (11)	−0.0007 (9)	0.0048 (9)	−0.0018 (9)
C11	0.0453 (13)	0.0452 (13)	0.0480 (14)	0.0094 (13)	0.0048 (10)	−0.0081 (12)
C12	0.0567 (16)	0.0499 (15)	0.0453 (14)	0.0038 (15)	0.0111 (12)	−0.0114 (13)
C13	0.0538 (15)	0.0388 (12)	0.0366 (12)	−0.0044 (11)	0.0049 (11)	−0.0038 (10)
C14	0.0434 (14)	0.0435 (13)	0.0412 (13)	0.0047 (11)	0.0009 (11)	−0.0016 (11)
C15	0.0426 (14)	0.0428 (13)	0.0361 (12)	0.0045 (11)	0.0062 (10)	−0.0037 (10)
C16	0.087 (3)	0.078 (2)	0.0453 (17)	0.003 (2)	−0.0114 (17)	0.0013 (17)

Geometric parameters (Å, °)

S1—N1	1.644 (3)	C15—H15	0.9300
S1—C1	1.716 (2)	C14—H14	0.9300
O1—C13	1.359 (3)	C12—H12	0.9300
O1—C16	1.399 (5)	C5—C4	1.385 (4)
N1—C3	1.329 (4)	C5—C6	1.374 (5)
C1—C2	1.374 (4)	C5—H5	0.9300
C1—C10	1.471 (3)	C4—C9	1.396 (4)
C3—C2	1.423 (3)	C9—C8	1.378 (5)
C3—C4	1.474 (4)	C9—H9	0.9300
C10—C15	1.389 (4)	C7—C8	1.378 (6)
C10—C11	1.397 (4)	C7—C6	1.387 (5)
C2—H2	0.9300	C7—H7	0.9300
C11—C12	1.376 (4)	C6—H6	0.9300
C11—H11	0.9300	C8—H8	0.9300
C13—C12	1.381 (4)	C16—H16A	0.9600
C13—C14	1.391 (4)	C16—H16B	0.9600
C15—C14	1.385 (4)	C16—H16C	0.9600
N1—S1—C1	96.22 (12)	C13—C12—C11	120.7 (3)
C13—O1—C16	119.1 (3)	C13—C12—H12	119.6
C3—N1—S1	109.17 (18)	C11—C12—H12	119.6
C2—C1—C10	129.6 (2)	C4—C5—C6	120.0 (3)
C2—C1—S1	107.52 (18)	C4—C5—H5	120.0
C10—C1—S1	122.92 (19)	C6—C5—H5	120.0
N1—C3—C2	115.7 (2)	C5—C4—C9	119.2 (3)
N1—C3—C4	119.5 (2)	C5—C4—C3	121.1 (2)
C2—C3—C4	124.8 (2)	C9—C4—C3	119.7 (3)
C15—C10—C11	118.2 (2)	C8—C9—C4	120.3 (3)
C15—C10—C1	120.7 (2)	C8—C9—H9	119.8
C11—C10—C1	121.1 (2)	C4—C9—H9	119.8
C1—C2—C3	111.4 (2)	C8—C7—C6	119.4 (3)
C1—C2—H2	124.3	C8—C7—H7	120.3
C3—C2—H2	124.3	C6—C7—H7	120.3
C12—C11—C10	120.7 (3)	C5—C6—C7	120.8 (3)
C12—C11—H11	119.6	C5—C6—H6	119.6

C10—C11—H11	119.6	C7—C6—H6	119.6
O1—C13—C12	115.9 (3)	C9—C8—C7	120.2 (3)
O1—C13—C14	124.6 (3)	C9—C8—H8	119.9
C12—C13—C14	119.4 (2)	C7—C8—H8	119.9
C10—C15—C14	121.3 (2)	O1—C16—H16A	109.5
C10—C15—H15	119.4	O1—C16—H16B	109.5
C14—C15—H15	119.4	H16A—C16—H16B	109.5
C13—C14—C15	119.7 (3)	O1—C16—H16C	109.5
C13—C14—H14	120.1	H16A—C16—H16C	109.5
C15—C14—H14	120.1	H16B—C16—H16C	109.5
C1—S1—N1—C3	−0.5 (2)	O1—C13—C14—C15	−179.1 (3)
N1—S1—C1—C2	0.9 (2)	C12—C13—C14—C15	−0.5 (4)
N1—S1—C1—C10	−177.9 (2)	C10—C15—C14—C13	0.4 (4)
S1—N1—C3—C2	−0.1 (3)	O1—C13—C12—C11	179.1 (3)
S1—N1—C3—C4	179.4 (2)	C14—C13—C12—C11	0.4 (5)
C2—C1—C10—C15	−3.4 (4)	C10—C11—C12—C13	−0.2 (5)
S1—C1—C10—C15	175.1 (2)	C6—C5—C4—C9	1.7 (5)
C2—C1—C10—C11	175.9 (3)	C6—C5—C4—C3	−177.2 (3)
S1—C1—C10—C11	−5.5 (4)	N1—C3—C4—C5	138.5 (3)
C10—C1—C2—C3	177.7 (2)	C2—C3—C4—C5	−42.1 (4)
S1—C1—C2—C3	−1.1 (3)	N1—C3—C4—C9	−40.4 (4)
N1—C3—C2—C1	0.8 (3)	C2—C3—C4—C9	139.0 (3)
C4—C3—C2—C1	−178.6 (2)	C5—C4—C9—C8	−0.9 (4)
C15—C10—C11—C12	0.0 (5)	C3—C4—C9—C8	178.0 (3)
C1—C10—C11—C12	−179.3 (3)	C4—C5—C6—C7	−0.8 (6)
C16—O1—C13—C12	176.8 (3)	C8—C7—C6—C5	−0.9 (6)
C16—O1—C13—C14	−4.6 (5)	C4—C9—C8—C7	−0.8 (5)
C11—C10—C15—C14	−0.2 (4)	C6—C7—C8—C9	1.7 (6)
C1—C10—C15—C14	179.2 (2)		

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

Cg1, Cg2 and Cg3 are the centroids of the C1—C3/N1/S1, C4—C9 and C10—C15 rings, respectively.

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C11—H11 $\cdots$ S1	0.93	2.73	3.137 (3)	107
C8—H8 $\cdots$ Cg2 ⁱ	0.93	2.82	3.503 (4)	132
C12—H12 $\cdots$ Cg1 ⁱⁱ	0.93	2.88	3.542 (4)	129
C15—H15 $\cdots$ Cg3 ⁱⁱⁱ	0.93	2.92	3.688 (3)	140

Symmetry codes: (i) $-x, y-1/2, -z$; (ii) $-x, y+1/2, -z+1$; (iii) $-x+1, y-1/2, -z+1$.