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(*E*)-3-(3-Methylthiophen-2-yl)-1-*p*-tolylprop-2-en-1-one

S. Naveen,[a] Helmi Muhammed Al-Maqtari,[b] Joazaizulfazli Jamalis,[b] Hasnah Mohd Sirat,[b] N. K. Lokanath[c]* and Muneer Abdoh[d]*

[a]Institution of Excellence, University of Mysore, Manasagangotri, Mysuru 570 006, India, [b]Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Skudai Johor, Malaysia, [c]Department of Studies in Physics, University of Mysore, Manasagangotri, Mysuru 570 006, India, and [d]Department of Physics, Science College, An-Najah National University, PO Box 7, Nablus, West Bank, Palestinian Territories. *Correspondence e-mail: lokanath@physics.uni-mysore.ac.in, muneer@najah.edu

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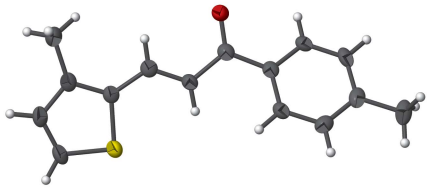
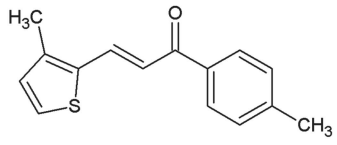
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{15}H_{14}OS$, the dihedral angle between the thiophene and benzene rings is 31.34 (13)°. The thiophene S atom and enone C═O group are approximately in an *anti* orientation. In the crystal, molecules are linked *via* pairs of very weak C—H···O hydrogen bonds, forming inversion dimers with $R_2^2(16)$ ring motifs.

3D view



Chemical scheme



Structure description

Chalcones and heterocyclic chalcone derivatives play important roles against diverse human diseases due to their anti-inflammatory, anti-leishmanial (Aponte *et al.*, 2010) and other properties. As part of our ongoing studies of such molecules (Tejkiran *et al.*, 2016; Karthik *et al.*, 2016), we report herein the synthesis and crystal structure of the title compound (Fig. 1).

The molecule is non-planar, with a dihedral angle of 31.34 (13)° between the methylthiophene and the *p*-toluene rings that are bridged by the enone group. This value is larger than the 19.13 (15)° reported earlier between the aromatic rings in the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Naveen *et al.*, 2016).

The thiophene ring is affected by π conjugation. This can be explained by the longer C—S bond lengths of 1.738 (3) Å and 1.704 (3) Å for C11—S1 and C14—S1, respectively. The bond angles about C8 [119.7 (3), 121.3 (3) and 119.0 (3) for O1—C8—C6, O1—C8—C9 and C9—C8—C6, respectively] indicate that this carbon atom is in a distorted trigonal planar conformation, which may be due to the steric bulk of the oxygen atom.

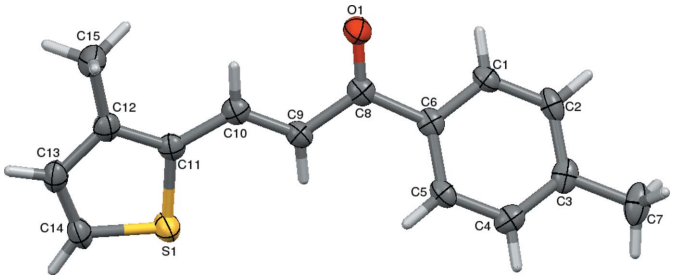


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

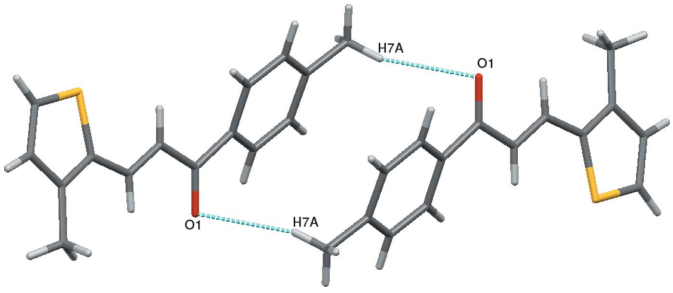


Figure 2
C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif.

In the crystal, the molecules are linked *via* pairs of very weak C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif (Table 1, Fig. 2).

Synthesis and crystallization

A mixture of 3-methyl-2-thiophenecarboxaldehyde (1 mol) with 4-methylacetophenone (1 mol) was dissolved in methanol (25 ml) and aqueous potassium hydroxide (15 ml) was added drop wise. The reaction mixture was stirred overnight at room temperature. The solid product obtained was separated, filtered and washed with cold methanol. Pure yellow crystals of the title compound were obtained by recrystallization from methanol solution (yield 78%, m.p. 350–353 K).

Refinement

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

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1^{i}	0.96	2.63	3.554 (4)	163

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{14}OS$
M_r	242.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	6.9231 (4), 27.7148 (16), 7.1228 (5)
β (°)	114.774 (4)
V (Å^3)	1240.89 (14)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.14
Crystal size (mm)	0.30 × 0.25 × 0.14
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.566, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8610, 2031, 1598
R_{int}	0.070
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.174, 1.03
No. of reflections	2031
No. of parameters	156
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.30

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2017). **2**, x170234 [https://doi.org/10.1107/S2414314617002346]

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Crystal data

$C_{15}H_{14}OS$
M_r = 242.33
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.9231 (4) Å
b = 27.7148 (16) Å
c = 7.1228 (5) Å
β = 114.774 (4)°
V = 1240.89 (14) Å^3
Z = 4
$F(000)$ = 512
D_x = 1.297 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 1598 reflections
θ = 7.0–64.7°
μ = 2.14 mm^{-1}
T = 296 K
Prism, yellow
0.30 × 0.25 × 0.14 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.566, T_{max} = 0.754
8610 measured reflections
2031 independent reflections
1598 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 64.7°, θ_{min} = 7.0°
h = −8→7
k = −32→30
l = −7→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.174
S = 1.03
2031 reflections
156 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1125P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Experimental. IR (cm^{-1}): 3116 (C-H-sp^2 stretching of aromatic ring), 2919 (CH-sp^3) 1646 (C═O), 1565, 1423 (C═C aromatic Ring).
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.40 (s, 3H, H-7′) , 2.45 (s, 3H, H-6), 6.94 (d, 1H, H-4, J = 5.20 Hz), 7.28-7.36 (m, 4H, H-5, H-α, H-3′, H-5′), 7.95 (d, 2H, H-2′, H-6′, J = 8.40 Hz), 8.07(d, 1H, H-β, J = 14.80 Hz).
^{13}C NMR (75 MHz, $CDCl_3$): δ 14.33, 21.70, 119.79, 127.14, 128.52, 129.31, 131.44, 134.64, 135.21, 135.69, 142.63, 143.54, 189.35.

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.16726 (11)	0.78110 (3)	0.19824 (12)	0.0348 (3)
O1	0.7151 (3)	0.63224 (7)	0.3438 (3)	0.0352 (7)
C1	0.4738 (4)	0.54657 (10)	0.2368 (4)	0.0283 (9)
C2	0.3694 (5)	0.50372 (10)	0.2248 (4)	0.0313 (9)
C3	0.1868 (5)	0.50153 (10)	0.2602 (4)	0.0303 (9)
C4	0.1105 (5)	0.54441 (11)	0.3021 (4)	0.0316 (10)
C5	0.2131 (4)	0.58790 (10)	0.3123 (4)	0.0273 (9)
C6	0.3991 (4)	0.58970 (10)	0.2829 (4)	0.0250 (8)
C7	0.0761 (6)	0.45430 (11)	0.2523 (5)	0.0426 (11)
C8	0.5255 (4)	0.63491 (10)	0.3072 (4)	0.0279 (9)
C9	0.4192 (5)	0.68178 (10)	0.2859 (4)	0.0276 (9)
C10	0.5260 (5)	0.72348 (10)	0.3183 (4)	0.0286 (9)
C11	0.4400 (4)	0.77137 (10)	0.2968 (4)	0.0269 (9)
C12	0.5471 (5)	0.81482 (10)	0.3461 (4)	0.0309 (10)
C13	0.4087 (5)	0.85438 (11)	0.3060 (5)	0.0335 (10)
C14	0.2008 (5)	0.84200 (11)	0.2269 (4)	0.0343 (10)
C15	0.7838 (5)	0.81953 (11)	0.4367 (6)	0.0474 (13)
H1	0.59650	0.54680	0.21390	0.0340*
H2	0.42210	0.47560	0.19230	0.0380*
H4	−0.01280	0.54400	0.32400	0.0380*
H5	0.15690	0.61620	0.33920	0.0330*
H7A	0.16060	0.43520	0.37080	0.0640*
H7B	0.05750	0.43720	0.12860	0.0640*
H7C	−0.06030	0.46040	0.25240	0.0640*
H9	0.27350	0.68250	0.24870	0.0330*
H10	0.67210	0.72120	0.35930	0.0340*
H13	0.45570	0.88620	0.33140	0.0400*
H14	0.08970	0.86400	0.19240	0.0410*
H15A	0.83880	0.81980	0.58480	0.0710*
H15B	0.82160	0.84910	0.39000	0.0710*

H15C	0.84320	0.79270	0.39350	0.0710*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0330 (5)	0.0269 (5)	0.0420 (5)	0.0017 (3)	0.0132 (4)	−0.0031 (3)
O1	0.0274 (12)	0.0299 (12)	0.0449 (13)	0.0026 (9)	0.0117 (9)	0.0026 (9)
C1	0.0265 (15)	0.0290 (16)	0.0274 (16)	0.0063 (12)	0.0094 (12)	0.0009 (11)
C2	0.0406 (18)	0.0225 (15)	0.0236 (15)	0.0071 (13)	0.0063 (13)	0.0001 (11)
C3	0.0353 (17)	0.0294 (16)	0.0168 (14)	−0.0041 (13)	0.0018 (12)	0.0028 (11)
C4	0.0291 (15)	0.0389 (19)	0.0255 (16)	−0.0042 (13)	0.0101 (12)	0.0012 (12)
C5	0.0290 (15)	0.0270 (16)	0.0223 (15)	0.0052 (12)	0.0072 (12)	−0.0022 (11)
C6	0.0265 (14)	0.0282 (16)	0.0144 (13)	0.0024 (12)	0.0028 (11)	0.0005 (10)
C7	0.055 (2)	0.0318 (18)	0.0275 (17)	−0.0094 (15)	0.0039 (15)	0.0044 (12)
C8	0.0309 (16)	0.0305 (17)	0.0203 (14)	0.0023 (13)	0.0089 (12)	0.0002 (11)
C9	0.0285 (15)	0.0268 (16)	0.0273 (15)	0.0034 (12)	0.0115 (12)	−0.0013 (11)
C10	0.0326 (16)	0.0312 (17)	0.0229 (15)	0.0005 (13)	0.0126 (13)	−0.0007 (11)
C11	0.0333 (16)	0.0279 (15)	0.0224 (15)	0.0007 (12)	0.0145 (13)	−0.0008 (11)
C12	0.0405 (18)	0.0284 (17)	0.0286 (16)	−0.0006 (13)	0.0193 (13)	0.0012 (11)
C13	0.0474 (19)	0.0242 (16)	0.0343 (17)	−0.0019 (14)	0.0224 (14)	0.0009 (12)
C14	0.046 (2)	0.0234 (16)	0.0367 (17)	0.0071 (13)	0.0204 (15)	0.0041 (12)
C15	0.042 (2)	0.0305 (18)	0.073 (3)	−0.0043 (15)	0.0273 (18)	0.0001 (16)

Geometric parameters (Å, º)

S1—C11	1.738 (3)	C12—C15	1.494 (5)
S1—C14	1.704 (3)	C13—C14	1.352 (5)
O1—C8	1.229 (4)	C1—H1	0.9300
C1—C2	1.374 (4)	C2—H2	0.9300
C1—C6	1.395 (4)	C4—H4	0.9300
C2—C3	1.390 (5)	C5—H5	0.9300
C3—C4	1.383 (4)	C7—H7A	0.9600
C3—C7	1.506 (5)	C7—H7B	0.9600
C4—C5	1.385 (4)	C7—H7C	0.9600
C5—C6	1.389 (4)	C9—H9	0.9300
C6—C8	1.496 (4)	C10—H10	0.9300
C8—C9	1.469 (4)	C13—H13	0.9300
C9—C10	1.339 (4)	C14—H14	0.9300
C10—C11	1.436 (4)	C15—H15A	0.9600
C11—C12	1.380 (4)	C15—H15B	0.9600
C12—C13	1.404 (5)	C15—H15C	0.9600
C11—S1—C14	92.00 (15)	C1—C2—H2	119.00
C2—C1—C6	121.2 (3)	C3—C2—H2	119.00
C1—C2—C3	121.4 (3)	C3—C4—H4	119.00
C2—C3—C4	117.4 (3)	C5—C4—H4	119.00
C2—C3—C7	121.2 (3)	C4—C5—H5	120.00
C4—C3—C7	121.4 (3)	C6—C5—H5	120.00

C3—C4—C5	121.7 (3)	C3—C7—H7A	109.00
C4—C5—C6	120.7 (3)	C3—C7—H7B	109.00
C1—C6—C5	117.6 (3)	C3—C7—H7C	109.00
C1—C6—C8	119.2 (3)	H7A—C7—H7B	109.00
C5—C6—C8	123.1 (3)	H7A—C7—H7C	110.00
O1—C8—C6	119.7 (3)	H7B—C7—H7C	110.00
O1—C8—C9	121.3 (3)	C8—C9—H9	119.00
C6—C8—C9	119.0 (3)	C10—C9—H9	119.00
C8—C9—C10	121.9 (3)	C9—C10—H10	116.00
C9—C10—C11	127.2 (3)	C11—C10—H10	116.00
S1—C11—C10	121.2 (2)	C12—C13—H13	123.00
S1—C11—C12	110.1 (2)	C14—C13—H13	123.00
C10—C11—C12	128.7 (3)	S1—C14—H14	124.00
C11—C12—C13	112.4 (3)	C13—C14—H14	124.00
C11—C12—C15	124.1 (3)	C12—C15—H15A	109.00
C13—C12—C15	123.4 (3)	C12—C15—H15B	109.00
C12—C13—C14	113.8 (3)	C12—C15—H15C	109.00
S1—C14—C13	111.7 (2)	H15A—C15—H15B	109.00
C2—C1—H1	119.00	H15A—C15—H15C	109.00
C6—C1—H1	119.00	H15B—C15—H15C	110.00

C14—S1—C11—C10	179.2 (2)	C5—C6—C8—O1	157.1 (3)
C14—S1—C11—C12	−0.6 (2)	C5—C6—C8—C9	−23.1 (4)
C11—S1—C14—C13	0.4 (2)	O1—C8—C9—C10	−4.4 (4)
C6—C1—C2—C3	−0.7 (4)	C6—C8—C9—C10	175.8 (3)
C2—C1—C6—C5	−1.2 (4)	C8—C9—C10—C11	178.1 (3)
C2—C1—C6—C8	176.2 (2)	C9—C10—C11—S1	−6.1 (4)
C1—C2—C3—C4	1.8 (4)	C9—C10—C11—C12	173.7 (3)
C1—C2—C3—C7	−178.4 (3)	S1—C11—C12—C13	0.7 (3)
C2—C3—C4—C5	−1.1 (4)	S1—C11—C12—C15	179.3 (3)
C7—C3—C4—C5	179.1 (3)	C10—C11—C12—C13	−179.2 (3)
C3—C4—C5—C6	−0.8 (4)	C10—C11—C12—C15	−0.5 (5)
C4—C5—C6—C1	1.9 (4)	C11—C12—C13—C14	−0.4 (4)
C4—C5—C6—C8	−175.4 (2)	C15—C12—C13—C14	−179.0 (3)
C1—C6—C8—O1	−20.2 (4)	C12—C13—C14—S1	−0.1 (4)
C1—C6—C8—C9	159.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O1^{i}	0.96	2.63	3.554 (4)	163

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.