

**(2*E*,2'*E*)-1,1'-Bis(2,5-dimethyl-3-thienyl)-3,3'-(*p*-phenylene)diprop-2-en-1-one**

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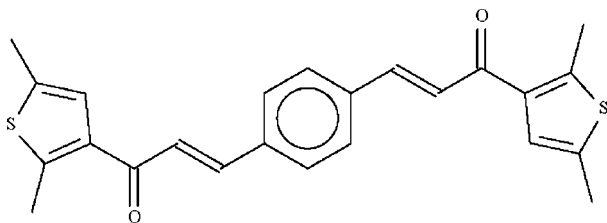
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Key indicators: single-crystal X-ray study; *T* = 140 K; mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$ ; *R* factor = 0.052; *wR* factor = 0.125; data-to-parameter ratio = 13.8.

In the title bis-chalcone,  $\text{C}_{24}\text{H}_{22}\text{O}_2\text{S}_2$ , the  $-\text{C}(\text{O})\text{CH}=\text{CH}-\text{C}_6\text{H}_4-\text{CH}=\text{CHC}(\text{O})-$  portion is planar (r.m.s. deviation = 0.04  $\text{Å}$ ); one thienyl ring is aligned at 8.8 (1)° with respect to this fragment, whereas the other is aligned at 21.3 (1)°.

**Related literature**

Chalcones possess anti-bacterial, anti-fungal and anti-inflammatory properties, see: Yarishkin *et al.* (2008); such properties are dramatically enhanced in bis-chalcones. For the crystal structures of some bis-chalcones, see: Harrison *et al.* (2007*a,b,c*); Prajapati *et al.* (2008).



**Experimental**

*Crystal data*

$\text{C}_{24}\text{H}_{22}\text{O}_2\text{S}_2$   
 $M_r = 406.54$   
 Monoclinic,  $P2_1/c$   
 $a = 15.6120 (12) \text{ \AA}$   
 $b = 7.5600 (6) \text{ \AA}$   
 $c = 18.2863 (14) \text{ \AA}$   
 $\beta = 111.305 (4)^\circ$

$V = 2010.8 (3) \text{ \AA}^3$   
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.28 \text{ mm}^{-1}$   
 $T = 140 \text{ K}$   
 $0.40 \times 0.10 \times 0.01 \text{ mm}$

*Data collection*

Bruker SMART APEX diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.896, T_{\text{max}} = 0.997$

10889 measured reflections  
 3537 independent reflections  
 2102 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.098$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.125$   
 $S = 0.97$   
 3537 reflections

257 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2486).

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**supplementary materials**

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**(2*E*,2'*E*)-1,1'-Bis(2,5-dimethyl-3-thienyl)-3,3'-(*p*-phenylene)diprop-2-en-1-one**

**A. M. Asiri, S. A. Khan and S. W. Ng**

**Experimental**

A solution of 3-acetyl-2,5-dimethylthiophene (3.13 ml, 0.0074 mol) and terephthaldehyde (2 g, 0.0074 mol) in ethanolic sodium hydroxide (60%) was stirred for 20 h at room temperature. The solution was poured into ice-cold water and the pH of the mixture was adjusted to 2 by the addition of concentrated hydrochloric acid. The solid that separated was dissolved in dichloromethane and then washed with saturated sodium bicarbonate. The residual obtained upon removal of the solvent was recrystallized from a methanol–chloroform (1/1) mixture in 80% yield; m.p. 467–468 K.

**Refinement**

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation with  $U(\text{H})$  fixed at  $1.2\text{--}1.5U_{\text{eq}}(\text{C})$ .

**Figures**

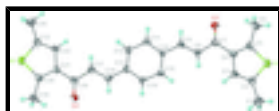


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of  $\text{C}_{24}\text{H}_{22}\text{O}_2\text{S}_2$  at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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*Crystal data*

$\text{C}_{24}\text{H}_{22}\text{O}_2\text{S}_2$	$F_{000} = 856$
$M_r = 406.54$	$D_x = 1.343 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-P 2_1/c$	Cell parameters from 765 reflections
$a = 15.6120 (12) \text{ \AA}$	$\theta = 2.8\text{--}19.6^\circ$
$b = 7.5600 (6) \text{ \AA}$	$\mu = 0.28 \text{ mm}^{-1}$
$c = 18.2863 (14) \text{ \AA}$	$T = 140 \text{ K}$
$\beta = 111.305 (4)^\circ$	Plate, yellow
$V = 2010.8 (3) \text{ \AA}^3$	$0.40 \times 0.10 \times 0.01 \text{ mm}$
$Z = 4$	

*Data collection*

Bruker SMART APEX diffractometer	3537 independent reflections
Radiation source: fine-focus sealed tube	2102 reflections with $I > 2\sigma(I)$

# supplementary materials

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Monochromator: graphite  
 $T = 140$  K  
 $\omega$  scans  
Absorption correction: Multi-scan  
(SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.896$ ,  $T_{\max} = 0.997$   
10889 measured reflections

$R_{\text{int}} = 0.098$   
 $\theta_{\max} = 25.0^\circ$   
 $\theta_{\min} = 1.4^\circ$   
 $h = -18 \rightarrow 18$   
 $k = -8 \rightarrow 8$   
 $l = -21 \rightarrow 21$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.125$   
 $S = 0.97$   
3537 reflections  
257 parameters  
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map  
Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0496P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$   
Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.05024 (6)	0.83736 (12)	0.17666 (5)	0.0311 (3)
S2	0.83487 (6)	-0.22707 (12)	0.99588 (5)	0.0309 (3)
O1	0.27593 (18)	0.9170 (3)	0.41549 (14)	0.0387 (7)
O2	0.64980 (17)	-0.3043 (3)	0.73797 (14)	0.0377 (7)
C1	0.0397 (3)	0.4820 (5)	0.1280 (2)	0.0389 (10)
H1A	0.0806	0.3799	0.1347	0.058*
H1B	0.0250	0.5316	0.0753	0.058*
H1C	-0.0171	0.4443	0.1346	0.058*
C2	0.0865 (2)	0.6196 (5)	0.1881 (2)	0.0284 (9)
C3	0.1587 (2)	0.6012 (5)	0.2562 (2)	0.0295 (9)
H3	0.1891	0.4915	0.2731	0.035*
C4	0.1860 (2)	0.7622 (5)	0.3013 (2)	0.0264 (8)
C5	0.1326 (2)	0.9034 (5)	0.2631 (2)	0.0272 (9)
C6	0.1384 (3)	1.0950 (4)	0.2861 (2)	0.0358 (10)
H6A	0.1373	1.1054	0.3391	0.054*
H6B	0.0860	1.1591	0.2491	0.054*
H6C	0.1958	1.1455	0.2851	0.054*
C7	0.2590 (2)	0.7752 (5)	0.3798 (2)	0.0268 (8)
C8	0.3077 (2)	0.6124 (4)	0.4165 (2)	0.0262 (9)
H8	0.3004	0.5090	0.3853	0.031*
C9	0.3615 (2)	0.6057 (4)	0.4917 (2)	0.0253 (8)
H9	0.3682	0.7128	0.5205	0.030*
C10	0.4115 (2)	0.4536 (4)	0.53522 (19)	0.0214 (8)

C11	0.4739 (2)	0.4748 (5)	0.61117 (19)	0.0249 (8)
H11	0.4832	0.5891	0.6344	0.030*
C12	0.5228 (2)	0.3329 (5)	0.6538 (2)	0.0270 (9)
H12	0.5657	0.3513	0.7056	0.032*
C13	0.5099 (2)	0.1626 (4)	0.6218 (2)	0.0242 (8)
C14	0.4463 (2)	0.1415 (5)	0.5455 (2)	0.0253 (8)
H14	0.4363	0.0269	0.5227	0.030*
C15	0.3978 (2)	0.2827 (4)	0.50260 (19)	0.0243 (8)
H15	0.3549	0.2645	0.4508	0.029*
C16	0.5607 (2)	0.0092 (5)	0.66412 (19)	0.0264 (9)
H16	0.5522	-0.0976	0.6350	0.032*
C17	0.6172 (2)	0.0010 (5)	0.7384 (2)	0.0272 (9)
H17	0.6275	0.1049	0.7696	0.033*
C18	0.6650 (2)	-0.1639 (5)	0.7744 (2)	0.0265 (9)
C19	0.7270 (2)	-0.4819 (4)	0.8930 (2)	0.0322 (9)
H19A	0.6629	-0.4868	0.8568	0.048*
H19B	0.7321	-0.5351	0.9433	0.048*
H19C	0.7658	-0.5473	0.8706	0.048*
C20	0.7578 (2)	-0.2932 (4)	0.9058 (2)	0.0256 (8)
C21	0.7327 (2)	-0.1511 (4)	0.8555 (2)	0.0229 (8)
C22	0.7768 (2)	0.0090 (5)	0.8912 (2)	0.0274 (9)
H22	0.7658	0.1194	0.8646	0.033*
C23	0.8357 (2)	-0.0104 (4)	0.9663 (2)	0.0276 (9)
C24	0.8943 (2)	0.1272 (5)	1.0203 (2)	0.0373 (10)
H24A	0.8767	0.2445	0.9968	0.056*
H24B	0.9591	0.1050	1.0287	0.056*
H24C	0.8856	0.1224	1.0707	0.056*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0305 (5)	0.0267 (5)	0.0311 (6)	0.0034 (4)	0.0052 (4)	0.0043 (4)
S2	0.0339 (6)	0.0282 (6)	0.0260 (5)	0.0042 (4)	0.0055 (4)	0.0039 (4)
O1	0.0514 (17)	0.0216 (15)	0.0339 (15)	0.0018 (13)	0.0046 (13)	-0.0036 (13)
O2	0.0467 (17)	0.0211 (15)	0.0347 (16)	0.0028 (12)	0.0020 (13)	-0.0040 (13)
C1	0.040 (2)	0.034 (2)	0.035 (2)	0.002 (2)	0.0059 (19)	-0.006 (2)
C2	0.033 (2)	0.024 (2)	0.027 (2)	0.0048 (17)	0.0091 (18)	0.0001 (17)
C3	0.033 (2)	0.017 (2)	0.033 (2)	0.0030 (17)	0.0068 (18)	-0.0027 (17)
C4	0.030 (2)	0.023 (2)	0.029 (2)	0.0000 (17)	0.0133 (17)	0.0014 (18)
C5	0.028 (2)	0.023 (2)	0.031 (2)	-0.0021 (17)	0.0122 (17)	0.0001 (18)
C6	0.040 (2)	0.024 (2)	0.042 (2)	0.0027 (19)	0.012 (2)	0.0004 (19)
C7	0.032 (2)	0.022 (2)	0.027 (2)	-0.0032 (17)	0.0113 (17)	-0.0004 (18)
C8	0.031 (2)	0.018 (2)	0.026 (2)	0.0015 (16)	0.0057 (17)	-0.0010 (16)
C9	0.028 (2)	0.020 (2)	0.025 (2)	-0.0017 (16)	0.0062 (17)	-0.0029 (17)
C10	0.0234 (19)	0.018 (2)	0.0199 (19)	-0.0017 (15)	0.0046 (15)	0.0008 (15)
C11	0.028 (2)	0.020 (2)	0.026 (2)	-0.0042 (16)	0.0091 (16)	-0.0046 (17)
C12	0.027 (2)	0.029 (2)	0.0200 (19)	-0.0022 (17)	0.0021 (16)	0.0012 (17)
C13	0.0280 (19)	0.021 (2)	0.024 (2)	0.0010 (17)	0.0091 (16)	0.0021 (17)

## supplementary materials

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C14	0.029 (2)	0.021 (2)	0.025 (2)	-0.0014 (16)	0.0085 (17)	-0.0040 (17)
C15	0.0236 (19)	0.024 (2)	0.0221 (19)	-0.0033 (16)	0.0041 (16)	-0.0017 (17)
C16	0.0256 (19)	0.023 (2)	0.028 (2)	-0.0041 (17)	0.0065 (17)	-0.0040 (17)
C17	0.032 (2)	0.020 (2)	0.028 (2)	0.0012 (17)	0.0101 (17)	-0.0016 (17)
C18	0.027 (2)	0.024 (2)	0.029 (2)	0.0014 (17)	0.0101 (17)	0.0018 (18)
C19	0.036 (2)	0.023 (2)	0.038 (2)	0.0039 (17)	0.0137 (18)	0.0047 (18)
C20	0.0252 (19)	0.022 (2)	0.029 (2)	0.0046 (16)	0.0082 (16)	0.0006 (17)
C21	0.0240 (18)	0.022 (2)	0.0227 (19)	0.0032 (16)	0.0081 (15)	0.0026 (17)
C22	0.032 (2)	0.021 (2)	0.027 (2)	0.0033 (17)	0.0079 (17)	0.0025 (17)
C23	0.028 (2)	0.024 (2)	0.030 (2)	0.0069 (17)	0.0090 (17)	0.0010 (18)
C24	0.036 (2)	0.029 (2)	0.040 (2)	-0.0009 (18)	0.0046 (19)	-0.0024 (19)

### Geometric parameters (Å, °)

S1—C5	1.710 (4)	C11—C12	1.382 (4)
S1—C2	1.729 (3)	C11—H11	0.9500
S2—C23	1.726 (4)	C12—C13	1.398 (5)
S2—C20	1.723 (3)	C12—H12	0.9500
O1—C7	1.233 (4)	C13—C14	1.396 (5)
O2—C18	1.230 (4)	C13—C16	1.458 (4)
C1—C2	1.497 (5)	C14—C15	1.378 (4)
C1—H1A	0.9800	C14—H14	0.9500
C1—H1B	0.9800	C15—H15	0.9500
C1—H1C	0.9800	C16—C17	1.325 (4)
C2—C3	1.348 (5)	C16—H16	0.9500
C3—C4	1.445 (5)	C17—C18	1.479 (5)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.378 (5)	C18—C21	1.479 (5)
C4—C7	1.475 (5)	C19—C20	1.497 (4)
C5—C6	1.502 (5)	C19—H19A	0.9800
C6—H6A	0.9800	C19—H19B	0.9800
C6—H6B	0.9800	C19—H19C	0.9800
C6—H6C	0.9800	C20—C21	1.375 (4)
C7—C8	1.474 (5)	C21—C22	1.428 (5)
C8—C9	1.327 (5)	C22—C23	1.355 (5)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.453 (4)	C23—C24	1.496 (5)
C9—H9	0.9500	C24—H24A	0.9800
C10—C11	1.386 (4)	C24—H24B	0.9800
C10—C15	1.407 (4)	C24—H24C	0.9800
C5—S1—C2	93.59 (17)	C13—C12—H12	119.6
C23—S2—C20	93.32 (16)	C14—C13—C12	117.7 (3)
C2—C1—H1A	109.5	C14—C13—C16	119.4 (3)
C2—C1—H1B	109.5	C12—C13—C16	122.8 (3)
H1A—C1—H1B	109.5	C15—C14—C13	121.7 (3)
C2—C1—H1C	109.5	C15—C14—H14	119.2
H1A—C1—H1C	109.5	C13—C14—H14	119.2
H1B—C1—H1C	109.5	C14—C15—C10	120.2 (3)
C3—C2—C1	128.9 (3)	C14—C15—H15	119.9

C3—C2—S1	109.7 (3)	C10—C15—H15	119.9
C1—C2—S1	121.4 (3)	C17—C16—C13	127.7 (3)
C2—C3—C4	114.5 (3)	C17—C16—H16	116.1
C2—C3—H3	122.7	C13—C16—H16	116.1
C4—C3—H3	122.7	C16—C17—C18	122.5 (3)
C5—C4—C3	111.3 (3)	C16—C17—H17	118.8
C5—C4—C7	123.6 (3)	C18—C17—H17	118.8
C3—C4—C7	125.0 (3)	O2—C18—C17	121.2 (3)
C4—C5—C6	129.9 (3)	O2—C18—C21	121.8 (3)
C4—C5—S1	110.9 (3)	C17—C18—C21	116.9 (3)
C6—C5—S1	119.3 (3)	C20—C19—H19A	109.5
C5—C6—H6A	109.5	C20—C19—H19B	109.5
C5—C6—H6B	109.5	H19A—C19—H19B	109.5
H6A—C6—H6B	109.5	C20—C19—H19C	109.5
C5—C6—H6C	109.5	H19A—C19—H19C	109.5
H6A—C6—H6C	109.5	H19B—C19—H19C	109.5
H6B—C6—H6C	109.5	C21—C20—C19	130.0 (3)
O1—C7—C8	120.6 (3)	C21—C20—S2	110.1 (3)
O1—C7—C4	120.9 (3)	C19—C20—S2	119.9 (3)
C8—C7—C4	118.4 (3)	C20—C21—C22	112.6 (3)
C9—C8—C7	122.1 (3)	C20—C21—C18	123.1 (3)
C9—C8—H8	118.9	C22—C21—C18	124.3 (3)
C7—C8—H8	118.9	C23—C22—C21	114.1 (3)
C8—C9—C10	127.5 (3)	C23—C22—H22	123.0
C8—C9—H9	116.2	C21—C22—H22	123.0
C10—C9—H9	116.2	C22—C23—C24	128.3 (3)
C11—C10—C15	118.3 (3)	C22—C23—S2	109.9 (3)
C11—C10—C9	120.0 (3)	C24—C23—S2	121.7 (3)
C15—C10—C9	121.7 (3)	C23—C24—H24A	109.5
C12—C11—C10	121.3 (3)	C23—C24—H24B	109.5
C12—C11—H11	119.4	H24A—C24—H24B	109.5
C10—C11—H11	119.4	C23—C24—H24C	109.5
C11—C12—C13	120.8 (3)	H24A—C24—H24C	109.5
C11—C12—H12	119.6	H24B—C24—H24C	109.5
C5—S1—C2—C3	0.4 (3)	C12—C13—C14—C15	0.2 (5)
C5—S1—C2—C1	-179.9 (3)	C16—C13—C14—C15	-178.9 (3)
C1—C2—C3—C4	-179.1 (3)	C13—C14—C15—C10	0.0 (5)
S1—C2—C3—C4	0.6 (4)	C11—C10—C15—C14	-0.6 (5)
C2—C3—C4—C5	-1.6 (5)	C9—C10—C15—C14	180.0 (3)
C2—C3—C4—C7	176.2 (3)	C14—C13—C16—C17	-173.7 (3)
C3—C4—C5—C6	-177.4 (4)	C12—C13—C16—C17	7.2 (6)
C7—C4—C5—C6	4.8 (6)	C13—C16—C17—C18	-179.8 (3)
C3—C4—C5—S1	1.8 (4)	C16—C17—C18—O2	-4.4 (5)
C7—C4—C5—S1	-176.0 (3)	C16—C17—C18—C21	174.5 (3)
C2—S1—C5—C4	-1.3 (3)	C23—S2—C20—C21	-1.1 (3)
C2—S1—C5—C6	178.0 (3)	C23—S2—C20—C19	-179.8 (3)
C5—C4—C7—O1	0.0 (5)	C19—C20—C21—C22	178.7 (3)
C3—C4—C7—O1	-177.6 (3)	S2—C20—C21—C22	0.1 (4)
C5—C4—C7—C8	176.5 (3)	C19—C20—C21—C18	0.6 (6)

## supplementary materials

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C3—C4—C7—C8	-1.0 (5)	S2—C20—C21—C18	-178.0 (3)
O1—C7—C8—C9	9.4 (5)	O2—C18—C21—C20	-24.7 (5)
C4—C7—C8—C9	-167.2 (3)	C17—C18—C21—C20	156.4 (3)
C7—C8—C9—C10	178.5 (3)	O2—C18—C21—C22	157.4 (3)
C8—C9—C10—C11	171.8 (3)	C17—C18—C21—C22	-21.5 (5)
C8—C9—C10—C15	-8.8 (6)	C20—C21—C22—C23	1.3 (4)
C15—C10—C11—C12	1.0 (5)	C18—C21—C22—C23	179.3 (3)
C9—C10—C11—C12	-179.6 (3)	C21—C22—C23—C24	178.6 (3)
C10—C11—C12—C13	-0.8 (5)	C21—C22—C23—S2	-2.0 (4)
C11—C12—C13—C14	0.2 (5)	C20—S2—C23—C22	1.8 (3)
C11—C12—C13—C16	179.2 (3)	C20—S2—C23—C24	-178.8 (3)



Fig. 1

