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Key indicators

Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
Disorder in main residue
 R factor = 0.054
 wR factor = 0.155
Data-to-parameter ratio = 31.5

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1-(4-Methylphenyl)-3-(2-thienyl)prop-2-en-1-one

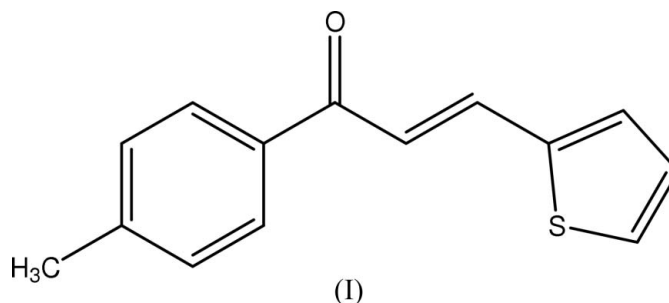
The title compound, $\text{C}_{14}\text{H}_{12}\text{OS}$, crystallizes with the two independent molecules in the asymmetric unit. All bond lengths and angles in both molecules show normal values. No intermolecular hydrogen bonds or short contacts are found in the crystal structure.

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Comment

Some chalcone derivatives crystallize as non-centrosymmetric structures and display significant non-linear optical (NLO) properties (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Zhang *et al.*, 1990; Zhao *et al.*, 2000). The title compound, (I), was prepared as part of our ongoing studies in this area (Patil *et al.*, 2006a,b).



The asymmetric unit of (I) contains two independent molecules, *A* and *B* (Fig. 1). The bond lengths and angles in both molecules have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Patil *et al.*, 2006a,b; Teh *et al.*, 2006). The thiophene ring in molecule *B* is disordered over two orientations (Fig. 1) with respect to the $\text{C}9\text{B}-\text{C}10\text{B}$ bond. The dihedral angle between the benzene and the thiophene rings is $46.55(6)^\circ$ in molecule *A*. In molecule *B*, the dihedral angles for the two orientations of the thiophene ring are $44.33(19)$ and $44.5(3)^\circ$.

Weak intramolecular $\text{C}-\text{H}\cdots\text{S}$ interactions are observed in both molecules (Table 1). No intermolecular hydrogen bonds or short contacts are found in the crystal structure.

Experimental

2-Thiophenecarbaldehyde (0.1 mol) and 4-methylacetophenone (0.1 mol) were stirred in 100 ml of ethanol at 298 K. An NaOH aqueous solution (10 g, 10%) was added and the mixture was stirred for 2 h. The resulting precipitate was filtered off, washed with water and dried. The crude product obtained was recrystallized twice from acetone. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Crystal data

C₁₄H₁₂OS
M_r = 228.30
 Monoclinic, *P*2₁/*c*
a = 11.7905 (1) Å
b = 13.6465 (2) Å
c = 17.3792 (2) Å
 β = 126.369 (1)°
V = 2251.62 (5) Å³

Z = 8
D_x = 1.347 Mg m⁻³
 Mo *K*α radiation
 μ = 0.26 mm⁻¹
T = 100.0 (1) K
 Block, yellow
 0.42 × 0.40 × 0.31 mm

Data collection

Bruker SMART APEX2 CCD area-
 detector diffractometer
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
T_{min} = 0.837, *T_{max}* = 0.923

64366 measured reflections
 9867 independent reflections
 7748 reflections with *I* > 2σ(*I*)
R_{int} = 0.046
 θ_{\max} = 35.0°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.054
wR(*F*²) = 0.156
S = 1.05
 9867 reflections
 313 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.9811P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.13 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{Å}^{-3}$

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>
C8A—H8AA...S1A	0.93	2.78	3.165 (2)	105
C8B—H8BA...S1B	0.93	2.75	3.141 (2)	106

H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, and refined as riding, with *U*_{iso}(H) = 1.5*U*_{eq}(C) for the methyl H atoms and 1.2*U*_{eq} for the remaining H atoms. The thiophene ring in molecule *B* was treated as disordered over two orientations with refined occupancies of 0.624 (2) and 0.376 (2). Restraints for similarity of displacement parameters and rigid-bond approximations were used in the refinement of the disordered thiophene ring. The highest residual peak is situated 0.44 Å from atom H11A.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINTE* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

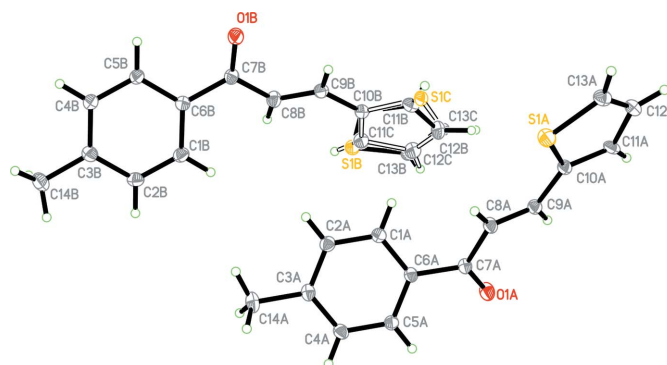


Figure 1

The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Both disorder components are shown.

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