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(*Z*)-1-Methoxy-1-phenyl-2-(4-toluenesulfonyl)ethene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.143
Data-to-parameter ratio = 9.2

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

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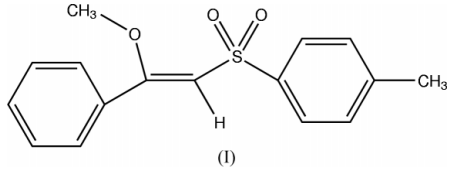
In the title compound, $C_{16}H_{16}O_3S$, the methoxy group and sulfonyl moiety are *cis* with respect to the olefinic bond. The two benzene rings, located *trans* with respect to the olefin bond, are almost perpendicular to each other, forming a dihedral angle of 75.81 (11)°.

Comment

Vinyl sulfones have now become generally accepted useful intermediates in organic synthesis, where they can serve efficiently as both Michael acceptors and π partners in cycloaddition reaction (Fuchs & Braish, 1986).



(I)

In the title compound, (I), the olefin group is in the *cis* configuration and the two benzene rings are located in *trans* positions (Fig. 1). The dihedral angle between these benzene rings is 75.81 (11)°, indicating that they are almost perpendicular to each other. Intermolecular π–π stacking is observed in the crystal structure (Fig. 2). Adjacent toluene moieties are nearly parallel to each other and the C10···C13^{i} distance [symmetry code: (i) $1-x, y, \frac{3}{2}-z$] is 3.93 (7) Å. Furthermore, the C10···H14^{i} distance is 2.87 Å, where H14 is one of the H atoms bonded to C16.

Experimental

(*Z*)-1-Iodo-1-phenyl-2-(4-toluenesulfonyl)ethene (3.84 g, 10 mmol) was dissolved in methanol (25 ml). To the mixture was added K_2CO_3 (3.45 g, 25 mmol) in 20 ml water. The mixture was stirred at room

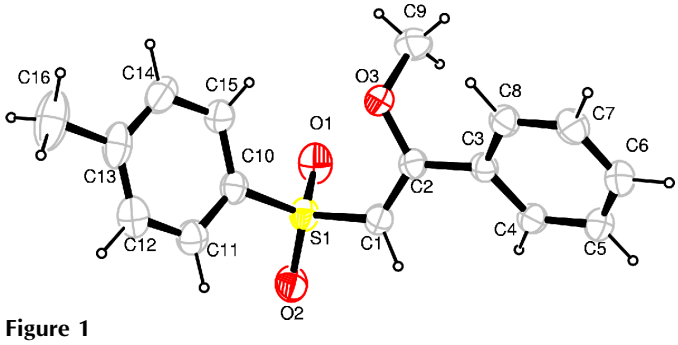


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids.

temperature for 24 h, then extracted with CH_2Cl_2; the product was dried with anhydrous $MgSO_4$ and recrystallized from ethanol to obtain the title compound (yield 77%; Back & Krishna, 1987).

Crystal data

$C_{16}H_{16}O_3S$
M_r = 288.36
Orthorhombic, *Pbcn*
a = 29.7459 (6) Å
b = 11.2443 (2) Å
c = 8.8337 (2) Å
V = 2954.6 (1) Å^3
Z = 8
D_x = 1.296 Mg m^{-3}
Mo Kα radiation
Cell parameters from 29 982 reflections
θ = 1.4–27.4°
μ = 0.22 mm^{-1}
T = 293 (1) K
Chunk, colorless
0.51 × 0.40 × 0.31 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.821, T_{max} = 0.933
21 953 measured reflections
3356 independent reflections
1815 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.040
θ_{max} = 27.5°
$h = -38 \rightarrow 38$
$k = -14 \rightarrow 14$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.143
S = 1.00
1815 reflections
198 parameters
H-atom parameters constrained
$w = 1/[0.0035F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 1.31 (6) × 10^2

H atoms were placed in calculated positions, with C—H = 0.96–0.98 Å, and included in the final cycles of refinement as riding, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms.

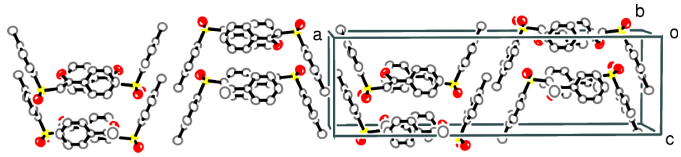


Figure 2
The crystal structure of (I).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2004); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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