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2-(Benzenesulfonyl)-1-(4-bromophenyl)ethyne

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.069
Data-to-parameter ratio = 9.3

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

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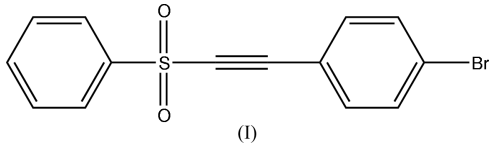
The title compound, $C_{14}H_9BrO_2S$, contains benzenesulfonyl and 4-bromophenyl moieties linked by an acetylene fragment. The crystal packing is stabilized by weak van der Waals interactions and intermolecular π–π stacking interactions.

Comment

The chemistry of acetylenic sulfones has been extensively studied and widely exploited in organic synthesis for several years (Back & Wehrli, 1995).



(I)

The molecular structure of the title compound, (I), is built up from benzenesulfonyl and 4-bromophenyl moieties linked by an acetylene fragment. The C1≡C2 triple bond is nearly in the plane of the 4-bromophenyl moiety; however, the acetylenic bond is not collinear with atom S1 as shown by the C2—C1—S1 angle of 171.3 (3)°. The cohesion of the crystal structure is governed by van der Waals and weak π–π stacking interactions (Fig. 2).

Experimental

(*Z*)-1-(4-Bromophenyl)-1-iodo-2-(benzenesulfonyl)ethene (4.49 g, 10 mmol) was dissolved in 25 ml anhydrous acetone and 3.45 g

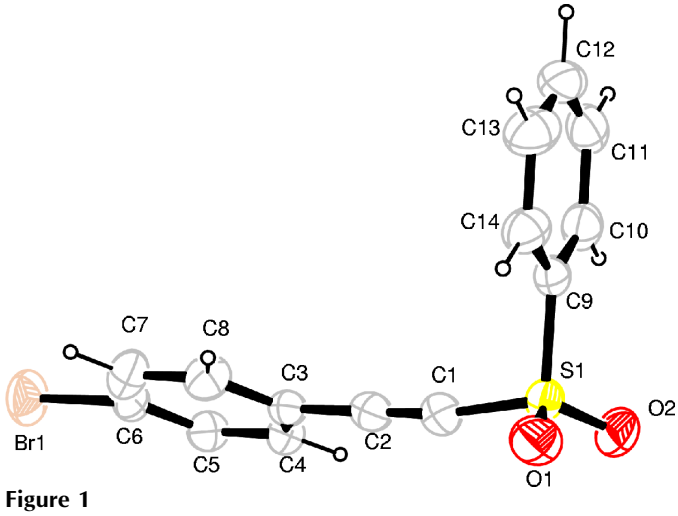


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids.

K_2CO_3 (25 mmol) was added to the mixture. The mixture was stirred at room temperature for 2 h. The resulting solution was extracted with CH_2Cl_2, dried with anhydrous $MgSO_4$ and recrystallized from ethanol, producing crystals of (I) (Back & Krishna, 1987).

Crystal data

$C_{14}H_9BrO_2S$	D_x = 1.626 Mg m^{-3}
M_r = 321.19	Mo Kα radiation
Monoclinic, $P2_1/n$	Cell parameters from 7173 reflections
a = 5.8032 (3) Å	θ = 1.9–27.4°
b = 21.161 (1) Å	μ = 3.29 mm^{-1}
c = 10.6863 (5) Å	T = 293 (1) K
β = 90.748 (1)°	Chunk, yellow
V = 1312.2 (1) Å^3	0.53 × 0.49 × 0.33 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3001 independent reflections
ω scans	1509 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.055
T_{min} = 0.194, T_{max} = 0.338	θ_{max} = 27.5°
12268 measured reflections	$h = -6 \rightarrow 7$
	$k = -27 \rightarrow 27$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[0.0005F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.069	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
1509 reflections	Extinction correction: Larson (1970)
163 parameters	
H-atom parameters constrained	Extinction coefficient: 73 (9)

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.708 (3)	C2—C3	1.433 (5)
C1—C2	1.187 (5)		
S1—C1—C2	171.4 (3)	C1—C2—C3	178.8 (4)

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

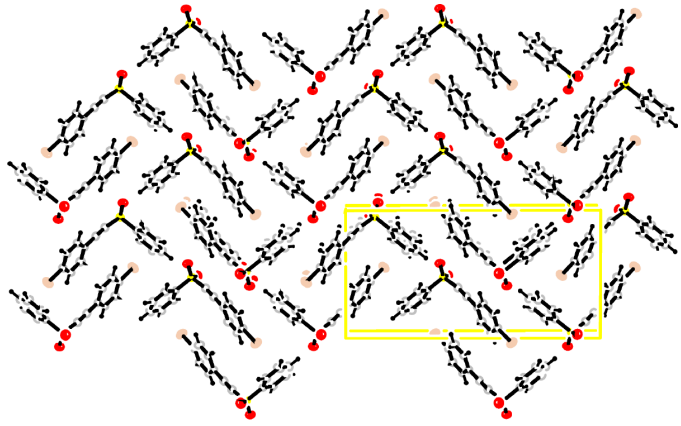


Figure 2
The crystal packing of (I) viewed along the *b* axis.

Data collection: *PROCESS-AUTO* (Rigaku/1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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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