

*trans*-2,3-Bis(methylsulfonyl)indane

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## Key indicators

Single-crystal X-ray study  
 T = 170 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
 R factor = 0.042  
 wR factor = 0.134  
 Data-to-parameter ratio = 13.6

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

In the structure of the title compound,  $\text{C}_{11}\text{H}_{14}\text{O}_4\text{S}_2$ , two sulfonyl groups are *trans*-fused to the five-membered ring of indane that adopts an envelope conformation. The  $\text{S}-\text{C}_{\text{methyl}}$  and  $\text{S}-\text{C}_{\text{indyl}}$  distances, with average values of 1.752 (3) and 1.792 (5) Å, respectively, are significantly different from each other. The molecules lie in pairs about inversion centers, with indyl moieties parallel to each other, forming a hydrocarbon zone in the middle of the unit cell.

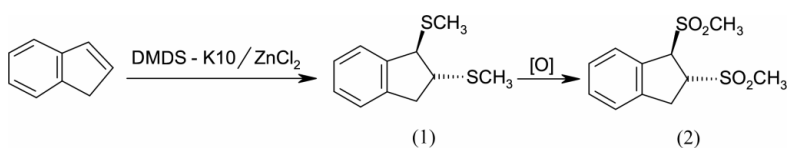
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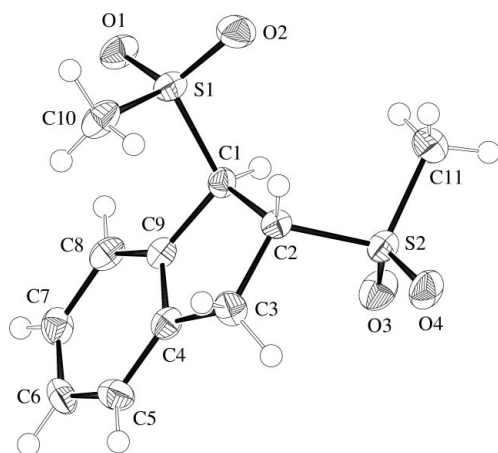
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## Comment

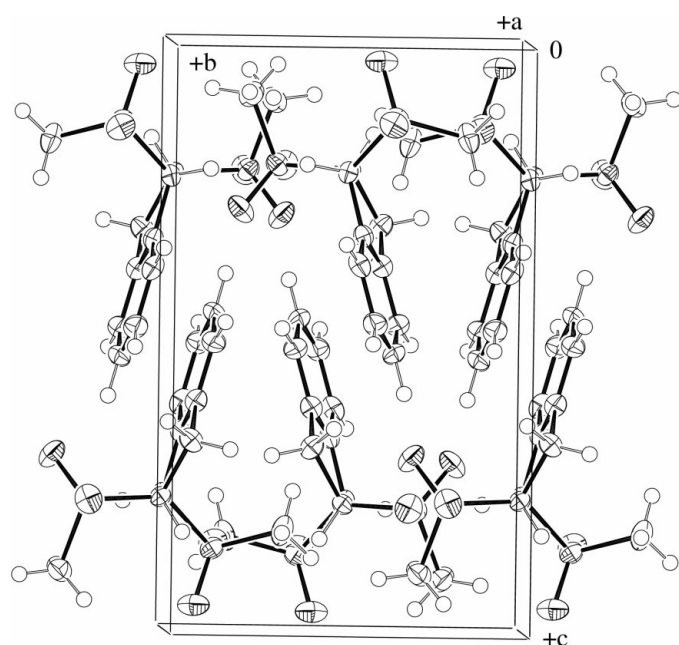
Compounds with extended delocalization of  $\pi$ -electrons through sulfur-containing structures, such as tetrathiafulvalene, become electrical conductors at low temperatures when present in crystalline arrays with electron-accepting systems. These observations have resulted in considerable research aimed at producing organic conductors. Synthesis of these systems requires precursors containing vicinal sulfur substitution. In this paper, we report the facile synthesis of such a precursor, derived from a diene which was prepared in a one-step reaction of indene with dimethyl disulfide (DMDS) in the presence of a zinc-promoted montmorillonite clay. Since the stereochemistry of the oily 1,2-di-SCH<sub>3</sub> adduct, (1), could not be determined unequivocally using NMR spectroscopy, (1) was oxidized to the crystalline disulfone, *trans*-2,3-bis(methylsulfonyl)indane, (2), for characterization using X-ray diffraction methods.



The crystal structure is composed of discrete molecules of (2) (Fig. 1), separated by normal van der Waals distances. The two sulfonyl groups are *trans*-fused to the five-membered indane ring. The C1/C2/C3/C4/C9 five-membered ring adopts a C2-envelope conformation, with C2 0.224 (8) Å out of the plane formed by the rest of the atoms in the ring; the maximum deviation of any atom from this plane is 0.001 (3) Å. The molecular dimensions in (2) are in agreement with values reported in the literature for the corresponding dimensions (Orpen *et al.*, 1994). It is interesting to note that the S–C distances involving the terminal methyl groups are significantly shorter [average 1.752 (3) Å] than the S–C bonds involving the indyl group [average 1.792 (5) Å]. The molecules of (2) lie in pairs about inversion centers, with indyl moieties parallel to each other, as shown in Fig. 2, thus forming a hydrocarbon zone in the middle of the unit cell along the *b* axis.



**Figure 1**  
ORTEPII (Johnson, 1976) drawing of (2), with displacement ellipsoids drawn at the 50% probability level.



**Figure 2**  
Unit-cell packing diagram of (2).

## Experimental

A solution of indene (2.92 ml, 25 mmol) in 1,2-dichloroethane was added dropwise to a stirred suspension of  $K_{10}/ZnCl_2$  (15.92 g) (Clark *et al.*, 1994) and DMDS (2.25 ml, 25 mmol) in dichloroethane (35 ml). After the mixture had been stirred for 3 h, the clay catalyst was removed by filtration and the filtrate was washed with aqueous EDTA ( $2 \times 100$  ml) to remove traces of  $ZnCl_2$  from the organic phase. The organic solution was then washed with water ( $1 \times 100$  ml) and was dried over anhydrous  $MgSO_4$ . Evaporation of the solvents and excess DMDS left an oil which, on distillation under high vacuum, yielded the dithio adduct (1) as a pale yellow oil (2.14 g, 41%, b.p. 379 K at 0.01 mm Hg). Oxidation of this product (Aitken *et al.*, 1994) gave the disulfone (2) in quantitative yield as colorless crystals (m.p. 415 K).

## Crystal data

$C_{11}H_{14}O_4S_2$   
 $M_r = 274.34$   
Monoclinic,  $P2_1/a$   
 $a = 11.138$  (6) Å  
 $b = 8.102$  (2) Å  
 $c = 13.307$  (2) Å  
 $\beta = 91.82$  (2)°  
 $V = 1200.2$  (7) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.518$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 12 reflections  
 $\theta = 15.0$ – $30.0^\circ$   
 $\mu = 0.44$  mm<sup>-1</sup>  
 $T = 170$  (2) K  
Plate, colorless  
 $0.40 \times 0.30 \times 0.07$  mm

## Data collection

Rigaku AFC-6S diffractometer  
 $\omega/2\theta$  scans  
Absorption correction:  $\psi$  scan  
(North *et al.*, 1968)  
 $T_{min} = 0.843$ ,  $T_{max} = 0.970$   
2249 measured reflections  
2128 independent reflections  
1034 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.042$   
 $\theta_{max} = 25.1^\circ$   
 $h = 0 \rightarrow 13$   
 $k = 0 \rightarrow 9$   
 $l = -15 \rightarrow 15$   
3 standard reflections  
every 200 reflections  
intensity decay: 1.4%

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.134$   
 $S = 0.98$   
2128 reflections  
156 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.402P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.34$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

S1–O2	1.448 (3)	S2–O3	1.436 (3)
S1–O1	1.448 (3)	S2–O4	1.450 (3)
S1–C10	1.749 (5)	S2–C11	1.755 (5)
S1–C1	1.797 (5)	S2–C2	1.786 (5)
O2–S1–O1	117.4 (2)	O3–S2–O4	118.1 (2)
O2–S1–C10	109.2 (2)	O3–S2–C11	109.3 (2)
O1–S1–C10	108.5 (2)	O4–S2–C11	108.4 (2)
O2–S1–C1	107.1 (2)	O3–S2–C2	108.7 (2)
O1–S1–C1	108.3 (2)	O4–S2–C2	106.7 (2)
C10–S1–C1	105.7 (2)	C11–S2–C2	104.7 (2)

The H atoms were located in a difference Fourier map and were included in the refinement at idealized positions, with isotropic displacement parameters 1.5 (CH<sub>3</sub>) and 1.2 (CH and CH<sub>2</sub>) times  $U_{eq}(C)$ , with C–H distances in the range 0.98–1.00 Å.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1994); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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