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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.055
 wR factor = 0.094
Data-to-parameter ratio = 12.7

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

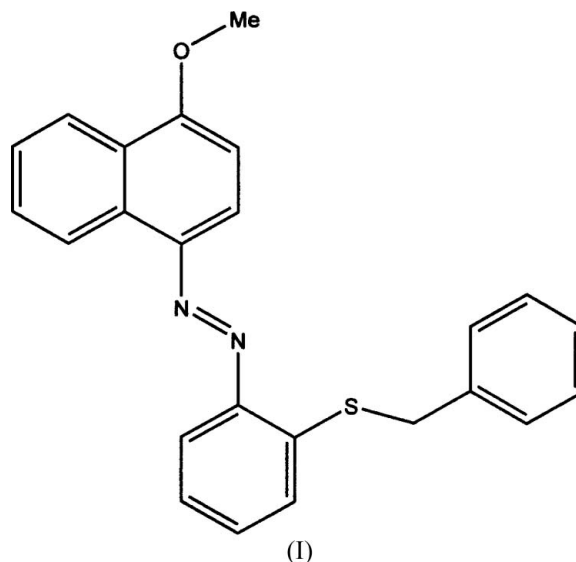
(*E*)-1-[2-(Benzylsulfanyl)phenyldiazenyl]-4-methoxynaphthalene

The title compound, $\text{C}_{24}\text{H}_{20}\text{N}_2\text{OS}$, contains an azo group ($-\text{N}=\text{N}-$), and the configuration around the $-\text{N}=\text{N}-$ double bond is *trans*. The dihedral angle between the naphthyl ring system and the benzene ring bearing the azo group is $32.40(10)^\circ$. There are intramolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ interactions and the crystal packing is stabilized by $\text{C}-\text{H}\cdots\pi$ interactions.

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Comment

Arylazo compounds have been extensively utilized as dyes and analytical reagents for decades (Campbell *et al.*, 1995; Betteridge & John, 1973). There is also current interest in arylazo compounds for their potential applications in liquid crystals and image storage devices (Ikeda & Tsutumi, 1995). Studies on *ortho*-mercaptoazoarenes or their derivatives are sparsely reported in the literature (Sanjib *et al.*, 2004; Chattopadhyay *et al.*, 1992). Against this background, we report here the crystal structure of (I).



The molecular structure of the title compound, (I), is shown in Fig. 1, with the atom-numbering scheme. The naphthyl and the benzene rings adopt a *trans* configuration about the azo functional group. Four planar fragments in the molecular structure of (I) may be identified: the naphthalene ring system (C1–C10) connected to N1 (A), the azo group along with C1 and C12 (B), the benzene ring (C12–C17) connected to N2 (C) and the benzene ring of the benzyl group (C19–C24) (D). The dihedral angles between the planes A/B, B/C, A/C and C/D are $14.97(30)$, $17.58(22)$, $32.40(10)$ and $79.78(7)^\circ$, respectively.

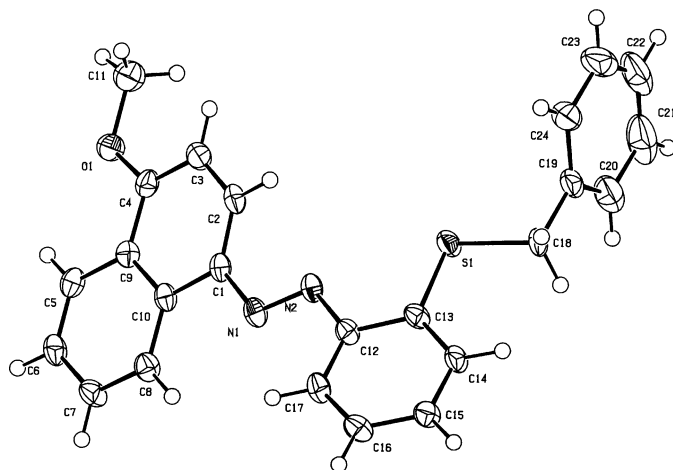


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

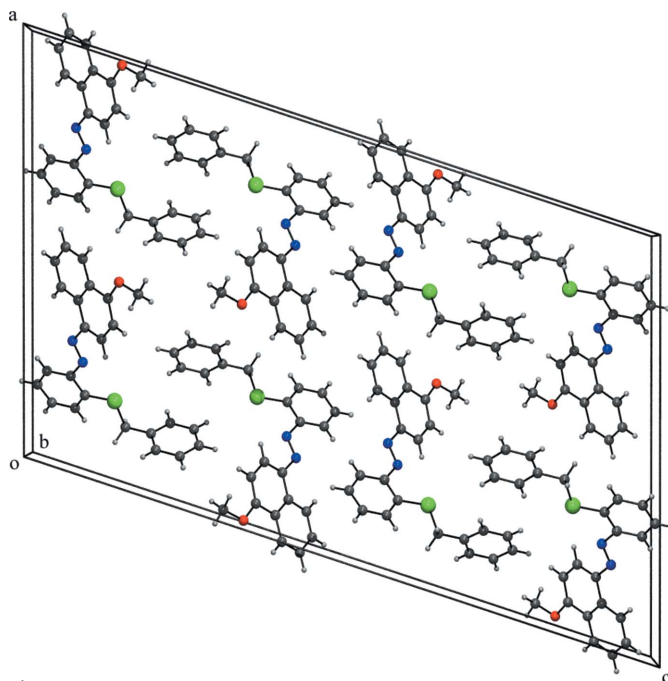


Figure 2
The packing of (I), projected on the *ac* plane.

Selected bond lengths, bond angles and torsion angles are listed in Table 1. The packing arrangement of (I) is shown in Fig. 2. The N1=N2 bond length is typical of *trans* azo compounds (Ersanlı *et al.*, 2005; Şahin *et al.*, 2005a,b). The bond distance N1–C1 (naphthyl) is almost same as that of N2–C12 (phenyl); the values are typical of *trans* azo compounds (Şahin *et al.*, 2005a,b; Karadayı *et al.*, 2006). The S–C bond distances are in agreement with the reported S–C distances under similar hybridization schemes of the bonded C atom (Li *et al.*, 2004; Moggach *et al.*, 2005). The O–C distance of the methoxy group is in good agreement with the literature values (Karadayı *et al.*, 2006). There are intramolecular C–H···O and C–H···N interactions (Table 2) in compound (I). An

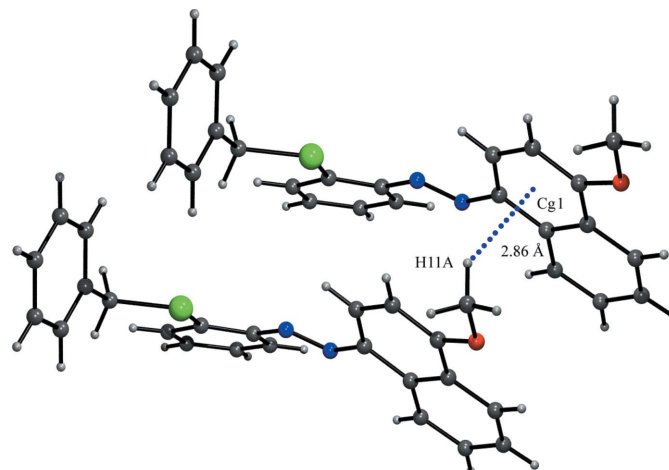


Figure 3
A representation of the intermolecular C–H··· π interaction of (I), indicated by a dotted line. [Symmetry code: (i) $x, 1 + y, z$]. *Cg1* is the centroid of atoms C1–C4, C9 and C10.

intermolecular C–H··· π interaction (Das *et al.*, 2005) (Table 2, Fig. 3) between the methyl H atom and the π electrons of one six-membered ring of the naphthyl system arranges molecules in a parallel fashion.

Experimental

1-[(2-Benzylsulfanylphenyl)diazenyl]-4-hydroxynaphthalene was prepared according to the literature method (Burawoy *et al.*, 1954), using 1-naphthol and 2-benzylthioaniline as starting materials. The title compound was obtained by methylation of 1-[(2-benzylsulfanylphenyl)diazenyl]-4-hydroxynaphthalene following a reported method (Lai *et al.*, 1992). The product was crystallized from ethanol (yield 70%; m.p. 388 K). Suitable crystals of (I) were obtained by slow diffusion of a dichloromethane solution into aqueous ethanol.

Crystal data

$C_{24}H_{20}N_2OS$
 $M_r = 384.48$
Monoclinic, $C2/c$
 $a = 21.891$ (4) Å
 $b = 5.1073$ (8) Å
 $c = 35.918$ (6) Å
 $\beta = 107.291$ (7)°
 $V = 3834.4$ (11) Å³

$Z = 8$
 $D_x = 1.332$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.19$ mm⁻¹
 $T = 293$ (2) K
Needle, yellow
 $0.35 \times 0.15 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.967$, $T_{max} = 0.983$

9087 measured reflections
3235 independent reflections
2115 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.083$
 $\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.094$
 $S = 0.99$
3235 reflections
254 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0263P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.24$ e Å⁻³
 $\Delta\rho_{min} = -0.20$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S1—C13	1.775 (3)	N1—N2	1.263 (3)
S1—C18	1.826 (2)	N1—C1	1.424 (3)
O1—C4	1.356 (3)	N2—C12	1.420 (3)
O1—C11	1.426 (3)		
C13—S1—C18	102.40 (12)	C2—C1—N1	124.0 (2)
N2—N1—C1	113.2 (2)	N1—C1—C10	116.3 (2)
N1—N2—C12	114.1 (2)	C17—C12—N2	125.1 (2)
C14—C13—S1	123.9 (2)	C13—C12—N2	115.2 (2)
C12—C13—S1	117.22 (19)		
C1—N1—N2—C12	179.39 (19)	N1—N2—C12—C17	−16.4 (3)
C18—S1—C13—C14	−2.2 (2)	S1—C18—C19—C20	−98.1 (3)
N2—N1—C1—C2	−16.7 (3)	S1—C18—C19—C24	82.0 (3)
C11—O1—C4—C3	2.2 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C5—H5...O1	0.93	2.43	2.744 (3)	100
C8—H8...N1	0.93	2.51	2.833 (3)	101
C11—H11A...Cg1 ⁱ	0.96	2.86	3.6255 (3)	137

Symmetry code: (i) $x, y + 1, z$. Cg1 is the centroid of atoms C1—C4, C9 and C10.

H atoms were included at calculated positions as riding atoms with C—H set to 0.93 Å for aromatic, 0.96 Å for CH₃ and 0.97 Å for CH₂ H atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ (1.5 U_{eq} for the methyl group). Some low-angle reflections were excluded from the refinement, as they were probably obscured by the beam stop.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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