Crystal structure of methylphenylsulfoxide, C_7H_8OS

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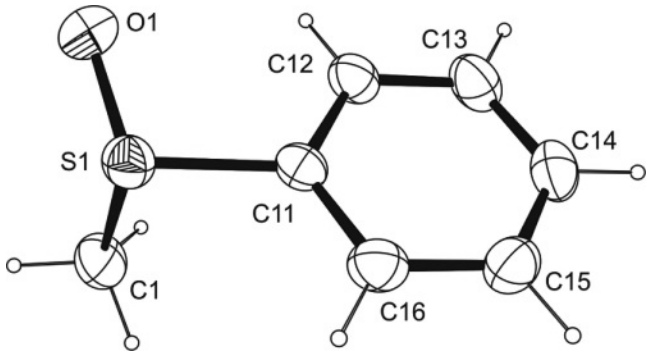

Abstract

C_7H_8OS, orthorhombic, $Pna2_1$ (no. 33), a = 8.2607(4) Å, b = 5.5020(3) Å, c = 15.3395(8) Å, V = 697.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.0241, $wR_{ref}(F^2)$ = 0.0633, T = 200 K.

Table 1. Data collection and handling.

Crystal:	colourless platelets, size 0.42×0.51×0.57 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.73 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω
$2\theta_{max}$:	56.54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9698, 1721
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1645
$N(param)_{refined}$:	83
Programs:	SHELX [11], WinGX [12], MERCURY [13], PLATON [14]

Source of material

The compound was obtained in analogy to the procedures described in references [3–7]. Crystals suitable for the diffraction study were obtained upon cooling the reaction product to 0 °C.

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The H atoms of the methyl group were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density (HFIX 137 in the SHELX program suite [11]), with U_{iso}(H) set to 1.5U_{eq}(C).

Discussion

The development and synthesis of powerful and targeted oxygenation catalysts to convert organic sulfides into sulfoxides and sulfones has been a focus of research in chemistry. The interest specifically stems from the potential application of such sulfur-containing entities in the process of preparing compounds of biological importance [1] as well as from potential applications in the desulfurization of crude oil in industrial-scale petrochemical industry processes [2]. A promising pathway in this context is research done on the field of polymer-bound oxidovanadium species [3–7]. In the wake of testing the effectiveness of one of our catalysts with oxidizing methylphenylsulfide, the title compound was obtained. To ascertain the chemical composition of the product and confirm the effected mono-oxidation, its crystal structure was determined. The compound is an asymmetric sulfoxide featuring a methyl and a phenyl group bonded to the sulfur atom. The S–O bond length of 1.4938(12) Å is in good agreement – although slightly towards smaller values – with other values reported for organic sulfoxides whose structural data was deposited with the Cambridge Structural Database [8]. The angles around the sulfur atom span a range of 97.40(7)–107.18(7)° with the smallest angle found in between the two organic substituents and the largest angle apparent in between the oxygen atom and the phenyl group. The least-squares planes as defined by the non-hydrogen atoms of the phenyl moiety on the one hand and the O=S–C_{ar} entity on the other hand intersect at an angle of 16.49(9)° only. In the crystal, intermolecular C–H···O contacts can be observed whose range falls invariably by more than 0.1 Å below the sum of van-der-Waals radii of the atoms participating in them. These are exclusively supported by hydrogen atoms of the methyl group. The oxygen atom serves as two-fold acceptor but could be discussed to be the end point of a third C–H···O contact, the latter one being an intramolecular one stemming from a hydrogen atom in *ortho* position on the aromatic substituent. This could explain the small torsional angle as mentioned above for the intersection of the least-suqares planes. In total, the molecules are connected to planes perpendicular to the crystallographic c axis. In terms of graph-set analysis [9, 10], the descriptor for these contacts is $S(5)C^1_1(4)C^1_1(4)$ on the unary level. The shortest intercentroid distance between two centers of gravity was found at 4.9447(10) Å ruling out any interactions.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1A)	4*a*	0.2509	1.0359	0.6594	0.061
H(1B)	4*a*	0.1231	1.0889	0.7354	0.061
H(1C)	4*a*	0.1377	1.2716	0.6546	0.061
H(12)	4*a*	0.2058	0.6608	0.5069	0.040
H(13)	4*a*	0.3121	0.7160	0.3667	0.049
H(14)	4*a*	0.2375	1.0541	0.2843	0.046
H(15)	4*a*	0.0590	1.3404	0.3415	0.046
H(16)	4*a*	–0.0434	1.2922	0.4832	0.043

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4*a*	–0.00597(4)	0.93030(6)	0.61519(4)	0.0303(2)	0.0323(2)	0.0331(2)	–0.0008(1)	0.0038(2)	–0.0022(2)
O(1)	4*a*	0.0218(2)	0.6705(2)	0.63916(7)	0.0569(7)	0.0317(6)	0.0448(8)	–0.0052(5)	0.0068(5)	0.0052(5)
C(1)	4*a*	0.1432(2)	1.1009(3)	0.6726(1)	0.0499(9)	0.0421(9)	0.0294(7)	–0.0083(7)	–0.0034(8)	–0.0057(6)
C(11)	4*a*	0.0745(2)	0.9731(3)	0.50783(9)	0.0265(6)	0.0275(7)	0.0293(6)	–0.0021(5)	–0.0026(6)	–0.0051(6)
C(12)	4*a*	0.1775(2)	0.8003(3)	0.4737(1)	0.0383(7)	0.0310(7)	0.0307(7)	0.0071(6)	–0.0047(6)	–0.0035(6)
C(13)	4*a*	0.2393(2)	0.8323(3)	0.3903(1)	0.0444(9)	0.0438(9)	0.0338(8)	0.0090(7)	0.0022(7)	–0.0088(7)
C(14)	4*a*	0.1952(2)	1.0333(3)	0.3414(1)	0.0412(8)	0.0473(9)	0.0260(7)	–0.0038(7)	–0.0025(6)	–0.0024(7)
C(15)	4*a*	0.0898(2)	1.2036(3)	0.3755(1)	0.0462(9)	0.0341(8)	0.0358(8)	–0.0014(7)	–0.0059(7)	0.0048(7)
C(16)	4*a*	0.0287(2)	1.1752(3)	0.4594(1)	0.0382(7)	0.0299(7)	0.0394(8)	0.0055(6)	–0.0015(7)	–0.0017(7)

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