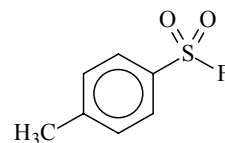


795 **C₇H₇FO₂S**ED, *ab initio*
calculations**4-Methylbenzenesulfonyl fluoride***p*-Methylbenzenesulfonyl fluoride**C_s**

r_a	\AA^a	θ_a	deg^a
C–S	1.753(7)	C–C–S	120 ^b
S–F	1.546(10)	C–S–F	94.9(9)
S=O	1.407(6)	C–S=O(1)	108.3(4)
C–C (phenyl)	1.397(5)	F–S=O(1)	109.0(5)
C–H (phenyl)	1.095(25)	O=S=O	123.6(15)
C(phenyl)–C(methyl)	1.505(26)	C–C–C (phenyl)	120 ^b
C(methyl)–H	1.115(30)	C(methyl)–C–C	120 ^b
		C–C–H (phenyl)	120 ^b
		C–C(methyl)–H(1)	108.7(48)
		H(1)–C(methyl)–H(2)	110.2(48)
		τ_1^c	89.5(27)
		τ_2^d	90 ^e

Local D_{6h} symmetry was assumed for the benzene ring.
The nozzle temperature was 350(2) K.

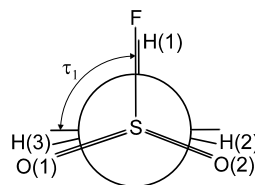
^a) 2.5 times the estimated standard errors including
a systematic error.

^b) Assumed.

^c) F–S–C–C torsional angle, see figure.

^d) H(1)–C(methyl)–C–C torsional angle.

^e) Uncertainty was not given in the original paper.



Petrov, V.M., Petrova, V.N., Kislov, V.V., Ivanov, S.N., Noskov, S.Yu., Krasnov, A.V.,
Bylova, Z.M.: Zh. Strukt. Khim. **41** No.6 (2000) 1137; J. Struct. Chem. (Engl. Transl.)
41 (2000) 939.

See also: Kislov, V.V., Petrov, V.M., Noskov, S.Y., Petrova, V.N., Ivanov, S.N.: Internet
J. Chem. **2** (1999) 1.