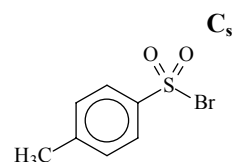


791 C₇H₇BrO₂SED, *ab initio*
calculations**4-Methylbenzenesulfonyl bromide***p*-Methylbenzenesulfonyl bromide

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–S	1.758(6)	C–C–S	120 ^{b)}
S–Br	2.234(5)	C–S–Br	99.9(3)
S=O	1.417(3)	C–S=O(1)	110.1(5)
C–C (phenyl)	1.399(4)	Br–S=O(1)	105.1(3)
C–H (phenyl)	1.105(25)	O=S=O	123.6(8)
C(phenyl)–C(methyl)	1.509(19)	C–C–C (phenyl)	120 ^{b)}
C(methyl)–H	1.121(37)	C(methyl)–C–C	120 ^{b)}
		C–C–H (phenyl)	120 ^{b)}
		C–C(methyl)–H(1)	107.4(44)
		H(1)–C(methyl)–H(2)	111.4(41)
		τ_1 ^{c)}	90.6(24)
		τ_2 ^{d)}	90 ^{e)}

Local D_{6h} symmetry was assumed for the benzene ring.
The nozzle temperature was 339...341(2) K.

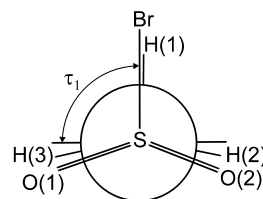
^{a)} 2.5 times the estimated standard errors
including a systematic error.

^{b)} Assumed.

^{c)} Br–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.



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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
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