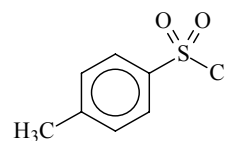


**792**      **C<sub>7</sub>H<sub>7</sub>ClO<sub>2</sub>S**  
ED, *ab initio*  
calculations

**4-Methylbenzenesulfonyl chloride**  
*p*-Methylbenzenesulfonyl chloride

essentially C<sub>s</sub>



$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–S	1.758(6)	C–C–S	120 <sup>b)</sup>
S–Cl	2.049(5)	C–S–Cl	101.3(6)
S=O	1.419(3)	C–S=O(1)	110.5(6)
C–C (phenyl)	1.403(7)	Cl–S=O(1)	106.9(3)
C–H (phenyl)	1.103(27)	O=S=O	120.5(9)
C(phenyl)–C(methyl)	1.512(25)	C–C–C (phenyl)	120 <sup>b)</sup>
C(methyl)–H	1.104(41)	C–C–C(methyl)	120 <sup>b)</sup>
		C–C–H (phenyl)	120 <sup>b)</sup>
		C–C(methyl)–H(1)	106.9(47)
		H(1)–C(methyl)–H(2)	111.9(40)
		$\tau_1$ <sup>c)</sup>	83 <sup>d)</sup>
		$\tau_2$ <sup>e)</sup>	90 <sup>d)</sup>

Local D<sub>6h</sub> symmetry was assumed for the benzene ring.

According to results of HF/6-311G\*\* calculations,  
the molecule has C<sub>s</sub> symmetry.

The nozzle temperature was 330(2) K.

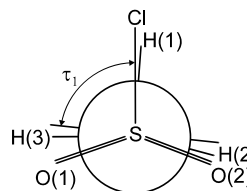
<sup>a)</sup> 2.5 times the estimated standard errors  
including a systematic error.

<sup>b)</sup> Assumed.

<sup>c)</sup> Torsional angle Cl–S–C–C, see figure.

<sup>d)</sup> Uncertainty was not given in the original paper.

<sup>e)</sup> H(1)–C(methyl)–C–C torsional angle.



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**2** (1999) 1.

See also: Petrov, V.M., Petrova, V.N., Kislov, V.V., Ivanov, S.N., Girichev, G.V.,  
Noskov, S.Yu., Krasnov, A.V.: Zh. Strukt. Khim. **40** No.4 (1999) 654; J. Struct. Chem.  
(Engl. Transl.) **40** (1999) 533.