

318	O₂S	Sulfur dioxide	C_{2v}
	ED, <i>ab initio</i> and DFT		SO ₂
	calculations		

$r_e^a)$	$\text{\AA}^b)$	$\theta_e^a)$	deg ^{b)}
S=O	1.4311(6)	O=S=O	119.4(4)

Equilibrium structure was derived from the experimental intensities obtained in [1] using the scaled cubic force constants estimated at several levels of quantum chemical calculations.

^{a)} One of the typical results obtained using scaled quadratic and cubic force constants from B3LYP/aug-cc-pVTZ calculations.

^{b)} No clear estimate of uncertainty was reported in the original paper. Variations in the reported structures based on different levels of calculations roughly range in the values in parentheses.

Kochikov, I.V., Tarasov, Yu.I., Spiridonov, V.P., Kuramshina, G.M., Saakyan, A.S., Pentin, Yu.A.: Zh. Fiz. Khim. **75** No.3 (2001) 461; Russ. J. Phys. Chem. (Engl. Transl.) **75** (2001) 395.

[1] Mawhorter, R.J., Fink, M.: J. Chem. Phys. **79** (1983) 3292.

See also: Tarasov, Yu.I., Tyulin, V.I., Spiridonov, V.P.: Vestn. Mosk. Univ., Ser. II, Khim. **38** (1997) 219; Mosc. Univ. Chem. Bull. (Engl. Transl.) **52** (1997) 11.

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