

204 **F₆S****Sulfur hexafluoride****O_h**
SF₆ED, vibrational
spectroscopy, *ab initio*
and DFT calculations

$r_e^a)$	$\text{\AA}^b)$
S–F	1.557

Empirically scaled quadratic and cubic force constants from *ab initio* and DFT calculations were used in a regularizing algorithm for the effective interaction of ED [1] and vibrational spectroscopic data. It was observed that the use of both rectilinear and curvilinear presentations of internal coordinates does not affect much the quality of cubic constant scaling scheme.

^{a)} Using force constants from different quantum chemical calculations (HF/6-31G*, HF/6-311+G*, MP2/6-31G* or B3LYP/6-31G*).

^{b)} Though no uncertainty was given in the original paper, the agreement of various reported values based on different sources and approaches indicate that it is *ca.* 0.001 Å.

Kochikov, I.V., Tarasov, Y.I., Spiridonov, V.P., Kuramshina, G.M., Saakjan, A.S., Yagola, A.G.: J. Mol. Struct. **550-551** (2000) 429.

[1] Kelley, M.N., Fink, M.: J. Chem. Phys. **77** (1982) 1813.

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