ROVIBRATIONAL SPECTROSCOPY OF SULFUR HEXAFLUORIDE: A REVIEW

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Some new interests in sulfur hexafluoride studies appeared recently, since this compound has proved to be a species of growing importance in the field of atmospheric physics and chemistry. As a matter of fact, it is now recognized as a pollutant that can contribute to the greenhouse effect. SF_6 concentration in the Earth's atmosphere is presently small but increases at a rate of about 7 % per year due to industrial emissions[a]. Moreover, its lifetime in the atmosphere is very long, reaching 3200 years or maybe even more. For this reason, correct quantitative measurements and monitoring of SF_6 are necessary.

However, the spectroscopy of this molecule, whose knowledge is essential for such quantitative measurements, has still not been extensively studied. The present knowledge about SF_6 high-resolution spectroscopy is very limited compared to methane, for instance. In particular, the region of the ν_3 fundamental near $948\ \mathrm{cm}^{-1}$ is of great importance since its very strong absorption is responsible for the huge greenhouse capabilities of SF_6. Nevertheless, if the $v_3 = 1$ level itself has been analyzed at extremely high resolution, the hot bands in this region which largely contribute to the absorption (the ground state population is only 30 % at 300 K) are very poorly known.

We intend to present here the most recent results concerning the high-resolution (infrared and Raman) rovibrational spectroscopy of SF_6[b,c]. The simulated spectra and the effective Hamiltonian parameter sets for all the bands that where studied up to now will be presented and discussed. The analyses where carried out using the tensorial formalism[d] and HTDS software[e] developed in the Dijon group[f] for spherical-top studies.

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