RAMAN SPECTROSCOPY OF THE ν_1 AND $2\nu_1 - \nu_1$ REGIONS OF $^{32}SF_6$ AND $^{34}SF_6$. EXPERIMENTAL DETERMINATION OF THE EQUILIBRIUM BOND LENGTH OF SULFUR HEXAFLUORIDE

V. BOUDON, *Laboratoire de Physique de l'Université de Bourgogne, CNRS UMR 5027, 9, Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France*; J. L. DOMENECH and D. BERMEJO, *Instituto de Estructura de la Materia, CSIC Serrano 123, 28006 Madrid, Spain*; H. WILLNER, *Fachbereich 9 – Anorganische Chemie, Bergische Universität Wuppertal, D-42097 Wuppertal, Germany*.

The ν_1 region of $^{32}SF_6$ and $^{34}SF_6$ has been studied by stimulated Raman spectroscopy. For both isotopomers, a detailed analysis has been performed. Several hot bands ($\nu_1+\nu_6-\nu_6$, $\nu_1+2\nu_6-2\nu_6$, $\nu_1+\nu_5-\nu_5$) have been taken into account to calculate synthetic spectra that satisfactorily reproduce the experimental data. These results, together with the previous studies of the other fundamental bands have allowed us to determine the equilibrium bond length of sulfur hexafluoride as $r_e = 1.5560(1)$ Å, in very good agreement with recent *ab initio* calculations[a]. The $2\nu_1 - \nu_1$ band has also been studied for both isotopomers by Raman-Raman double resonance spectroscopy and the resulting spectra have been analyzed. In this case, a striking difference is observed between the two isotopomers, since the $2\nu_1 - \nu_1$ band of $^{34}SF_6$ appears to have a very narrow structure that could not be rotationally resolved under the present experimental conditions. All analyses have been performed thanks to the HTDS program suite (http://www.u-bourgogne.fr/LPUB/hTDS.html)[b] dedicated to octahedral XY_6 molecules.

[a] I. V. Kochikov, Y. I. Tarasov, V. P. Spiridonov, G. M. Kuramshina, A. S. Saakjan, A. G. Yagola, *J. Mol. Struct.*, **550–551**, 429–438 (2000).
[b] C. Wenger, V. Boudon, J.-P. Champion, G. Pierre, *J. Quant. Spectrosc. Radiat. Transfer*, **66**, 1–16 (2000).