BREAKDOWN OF THE REDUCTION OF THE ROVIBRATIONAL HAMILTONIAN : THE CASE OF $S^{18}O_2F_2$

L. MARGULÈS, J. DEMAISON, *Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, Bat. P5, 59655 Villeneuve d'Ascq Cedex, France.*; A. PERRIN, *Laboratoire Inter Universitaire des Systemes Atmosphériques, CNRS UMR 7583, Université Paris 12, 61 Av du General de Gaulle, 94010 Créteil Cedex France.*; I. MERKE, *; Institute für Physikalische Chemie, RWTH Aachen, 52056 Aachen, Germany*; H. WILLNER, *Anorganische Chemie, FB C, Universität-GH Wuppertal, 42097 Wuppertal, Germany*; M. ROTGER, *Groupe de Spectromtrie Moléculaire et Atmosphrique, CNRS UMR 6089, Moulin de la Housse, BP 1039, Cases 16-17, 51687 Reims Cedex 2, France*; and V. BOUDON, *Institut Carnot de Bourgogne, UMR CNRS 5209, 9 avenue Alain Savary, BP 47870, 21078 Dijon Cedex, France*.

The ground state rotational spectrum of the near-spherical top molecule $S^{18}O_2F_2$ (sulfuryl fluoride) has been measured from 50 to 700 GHz. As for the parent isotopologue, $S^{16}O_2F_2$[a], it was necessary to use a non-reduced Hamiltonian in order to obtain a satisfactory fit. It was possible to determine six quartic centrifugal distortion constants (instead of five for a standard asymmetric top) and an additional sextic constant could also be determined. This ground state level has also been analysed thanks to a tensorial formalism developed in Dijon. Only two tensorial sextic constants are fixed to zero, all others have been adjusted. Although $S^{18}O_2F_2$ is less spherical than $S^{16}O_2F_2$, the analysis was more difficult. It is partly due to the fact that $S^{18}O_2F_2$ is oblate whereas $S^{16}O_2F_2$ is prolate. The experimental quartic centrifugal distortion constants were found in good agreement with those calculated from the force field, confirming the correctness of the analysis.

[a]K. Sarka, J. Demaison, L. Margulès, I. Merke, N. Heineking, H. Bürger, and H. Ruland, *J. Mol. Spectrosc.*, **200**, 55 (2000)