ANALYSIS OF THE $\nu_3/\nu_7/\nu_9$ BENDING TRIAD OF THE QUASI-SPERICAL TOP MOLECULE SO$_2$F$_2$

M. ROTGER, V. BOUDON, M. LOETE, Laboratoire de Physique de l’Université de Bourgogne, CNRS UMR 5027, 9, Avenue Alain Savary, B.P. 47 870, F-21078 Dijon Cedex, France; L. MARGULES, J. DEMAISON, Laboratoire de Physique des Lasers, Atomes et Molécules, UMR CNRS 8253, Université de Lille 1, F-59655 Villeneuve d’Ascq, France; F. HEGELUND, Department of Chemistry, University of Aarhus, DK-8000 Aarhus C, Denmark; I. MERKE, Institut für Physikalische Chemie, RWTH Aachen, D-52056 Aachen, Germany; H. BURGER, FBC, Anorganische Chemie, Universität, D-42097 Wuppertal, Germany.

The analysis of the $\nu_3/\nu_7/\nu_9$ bending triad of SO$_2$F$_2$ was previously performed using Watson’s Hamiltonian up to octic terms employing 79 rovibrational parameters. Since SO$_2$F$_2$ is a quasi-spherical top, it can also be regarded as a slightly distorted SO$_2^{2-}$ sulfate ion. Thus we have developed a new tensorial formalism in the $O(3) \supset T_d \supset C_{2v}$ group chain. In a first step, we tested the tensorial formalism for the ground state of this molecule. Now, we apply it to the bending triad with the same set of microwave assignments and almost the same set of IR assignments as in Ref. ?? Our analysis leads to a lower order (6) of the development and less parameters to be adjusted but involves more interaction terms. We also present some links between the classical (Watson) approach and the tensorial one mainly for the parameters and state labels. A set of programs for spectrum calculations and fits named $C_{2v}$TDS has been used for this analysis and is freely available at the URL: http://www.u-bourgogne.fr/LPUB/c2vTDS.html

---