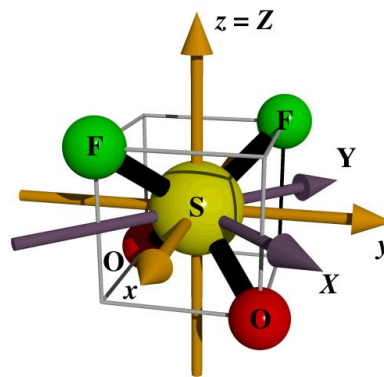


## THE GROUND STATE ROTATIONAL SPECTRUM OF SO<sub>2</sub>F<sub>2</sub>.

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The analysis of the ground state rotational spectrum of SO<sub>2</sub>F<sub>2</sub><sup>a</sup> has been performed with the Watson's Hamiltonian up to sextic terms but shows some limits due to the *A* and *S* reductions. Since SO<sub>2</sub>F<sub>2</sub> is a quasi-spherical top, it can also be regarded as derived from an hypothetical XY<sub>4</sub> molecule. Thus we have developed a new tensorial formalism in the  $O(3) \supset T_d \supset C_{2v}$  group chain<sup>b</sup>. We test it on the ground state of this molecule using the same experimental data<sup>c</sup> (0–1 THz region, *J* up to 99). Both fits are comparable even if the formalisms are slightly different. This talk intends to establish a link between the classical approach and the tensorial formalism. In particular, our tensorial parameters at a given order of the development are related to the usual ones. Programs for spectrum simulation and fit using these methods are named *C*<sub>2v</sub>TDS. They are freely available at the URL:

<http://www.u-bourgogne.fr/LPUB/c2vTDS.html>



<sup>a</sup>K. Sarka, J. Demaison, L. Margulès, I. Merke, N. Heineking, H. Bürger and H. Ruland, *J. Mol. Spectrosc.*, **200**, 55-64, (2000).

<sup>b</sup>M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.*, **216**, 297-307, (2002).

<sup>c</sup>M. Rotger, V. Boudon, M. Loëte, L. Margulès, J. Demaison, H. Mäder, G. Winnewisser and H.S.P. Müller, *J. Mol. Spectrosc.*, in preparation, (2003).