THE GROUND STATE ROTATIONAL SPECTRUM OF $SO_2F_2$.

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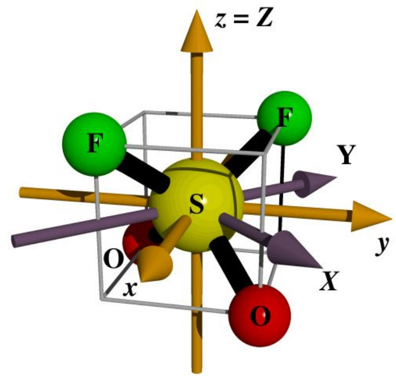
The analysis of the ground state rotational spectrum of $SO_2F_2$[a] has been performed with the Watson's Hamiltonian up to sextic terms but shows some limits due to the $A$ and $S$ reductions. Since $SO_2F_2$ is a quasi-spherical top, it can also be regarded as derived from an hypothetical $XY_4$ molecule. Thus we have developped a new tensorial formalism in the $\mathbf{O(3)} \supset \mathbf{T_d} \supset \mathbf{C_{2v}}$ group chain[b]. We test it on the ground state of this molecule using the same experimental data[c] (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 $C_{2v}$TDS. They are freely available at the URL:
`http://www.u-bourgogne.fr/LPUB/c2vTDS.html`

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