THE GROUND STATE ROTATIONAL SPECTRUM OF SO₂F₂.

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The analysis of the ground state rotational spectrum of SO₂F₂ has been performed with the Watson’s Hamiltonian up to sextic terms but shows some limits due to the \( A \) and \( S \) reductions. Since SO₂F₂ is a quasi-spherical top, it can also be regarded as derived from an hypothetical \( XY_4 \) molecule. Thus we have developed a new tensorial formalism in the \( O(3) \supset T_{d} \supset C_{2v} \) group chain. We test it on the ground state of this molecule using the same experimental data (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