

ANALYSIS OF THE $\nu_3/\nu_7/\nu_9$ BENDING TRIAD OF THE QUASI-SPHERICAL TOP MOLECULE SO_2F_2

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The analysis of the $\nu_3/\nu_7/\nu_9$ bending triad of SO_2F_2 was previously performed using Watson's Hamiltonian up to octic terms employing 79 rovibrational parameters^a. Since SO_2F_2 is a quasi-spherical top, it can also be regarded as a slightly distorted SO_4^{2-} sulfate ion. Thus we have developed a new tensorial formalism in the $\mathbf{O}(3) \supset \mathbf{T}_d \supset \mathbf{C}_{2v}$ group chain^b. In a first step, we tested the tensorial formalism for the ground state of this molecule^c. 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 $C_{2v}\text{TDS}^d$ has been used for this analysis and is freely available at the URL:

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

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