SYMMETRY-ADAPTED TENSORIAL FORMALISM FOR THE SPECTROSCOPY OF THE SO_2F_2 QUASI-SPHERICAL TOP: APPLICATION TO THE BENDING TRIAD

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The techniques of symmetry-adapted tensorial formalism and of vibrational extrapolation developed since many years by the Dijon group have proved their efficiency for the spectroscopy of spherical-top molecules (CH_4, SF_6, ...). We have extended these methods to the case of quasi-spherical tops such as SO_2F_2[a]. This model has been used recently to perform the analysis of the ground state of this molecule[b]. We present here a preliminary study concerning the analysis of the $\nu_3/\nu_7/\nu_9$ bending triad in the $550\ \mathrm{cm}^{-1}$ region. These results are compared to those obtained with the usual asymmetric-top approach[c] . A set of programs for spectrum calculations and fits named C_{2v}TDS has been used and is freely available at the URL:

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

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