THEORETICAL SPECTROSCOPIC STUDY OF ISOPROPYL ALCOHOL ($CH_3 - CHOH - CH_3$)

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Isopropyl alcohol ($CH_3 - CHOH - CH_3$) is a non-rigid species of atmospheric and astrophysical interest. We present highly correlated ab initio calculations (CCSD(T)-F12/CVTZ-F12) performed for the study of the FIR region of the spectrum. The molecule can be classified in the MSG G_{18}. It shows three interacting internal rotations corresponding to the two methyl groups and the OH alcoholic group. Torsional energy levels and subcomponents are determined variationally from a three-dimensional potential energy surface. For the classification of the computed levels, we apply symmetry considerations. Final torsional wave-functions denote the relevance of the interactions on the results. Perturbation theory is also used to determine the vibrational corrections of rotational constants. This project has received funding from the European Unionś Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 872081.