GLOBAL TREATMENT OF TORSIONAL EXCITED STATES OF NON-EQUIVALENT CH3 TOPS: TEST WITH 2-PROPANIMINE

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Understanding the torsional excited states is an important topic in high resolution spectroscopy. Accurately modeling these states not only improves our understanding of the internal motion of molecules, but also provides accurate transition frequencies and partition functions for atmospheric and astrophysical applications. Due to the complexity of the model, however, the global treatment of ground state and torsional excited states of internal rotors, particularly those with two coupled internal rotors, remains a challenge. To our knowledge, only very few examples, such as acetone[1,2] and dimethylsulfide[3], which are equivalent two-tops, exist for such global treatment.

In this study, we initiate the global treatment of the ground state and torsional excited states of 2-propanimine using the "BELGI-2Top-Cs" model, valid for nonequivalent two-top internal rotors. It is the first time for this model to treat such a challenging problem. 2-propanimine ($(CH_3)_2C{=}NH$) is a tentative interstellar molecule with a structure resembling acetone. The millimeter-wave spectrum of 2-propanimine was recorded in PhLAM, Lille, and its ground state lines have been sucessfully assigned and modeled using local models ERHAM and XIAM[4], revealing its V_3 barriers to internal rotation of 2-propanimine to be 532 cm^{-1} and 465 cm^{-1}, respectively. According to anharmonic vibrational frequency calculations, at least three torsional excited states below 300 cm^{-1}, and therefore populated in the room temperature spectrum. These states will give rise to several spectral components with symmetry species A1, A2, E1, E2, E3, and E4 in the G9 permutation-inversion group, with similar splittings due to their similar barrier to internal rotation. To correctly identify and pair these components with their respective states, we start our analysis using the "BELGI-Cs" model. We search for the series of lines that can form valid A-E state pairs as if they were from an individual molecule. Then, our goal is to combine these series into the "BELGI-2Top-Cs" model that can simultaneously fit all assigned series and reveal the remaining coupled components. The latest progress of this project will be presented.

References: [1] I. A. Armieieva et al., Radio Phys. Radio Astron. **21**, 37–47 (2016). [2] V. V. Ilyushin et al., J. Mol. Spectrosc. **363**, 111169 (2019). [3] V. V. Ilyushin et al., J. Mol. Struct. **1200**, 127114 (2020). [4] L. Zou et al., MNRAS **520**, 4089–4102 (2023).

p-number: p018 **Submitted on Mon, 29 May 2023 11:57:07 +0200**