# HIGH RESOLUTION SPECTROSCOPY OF INTERNAL ROTORS: FROM MOLECULAR STRUCTURE TO ASTROPHYSICS

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The topic of my talk will concern molecules with one or two methyl ($CH_3$) internal rotors. Internal rotors are present everywhere in our environment, and they are important indicators of the physico-chemical conditions which exist in it. They are also excellent "sensors" for molecular structure determinations. The high resolution microwave, millimeter and infrared spectra of those molecules cannot be treated by traditional Hamiltonian methods[a]. Dedicated theoretical methods and codes have been developed to calculate the energy levels, and then to fit the observed line positions for internal rotors. First I will briefly review those approaches. Following this strategy reliable predictions of line positions and intensities for astrophysical molecules containing one internal rotor $CH_3$ or two-top molecules can be provided[b]. I will present several internal rotors of interstellar interest as well as the latest results obtained with a code dealing with one Large-Amplitude Rotatory Motion and one Large-Amplitude Oscillatory Motion[c]. Internal rotation can be also used to acquire knowledge on structural properties for small organic molecules or biomimetic molecules, which can serve as benchmark, and be compared to quantum chemical calculations. In this talk, I will show results for internal rotors, which are prototype for odorant molecules, phytohormones or bee pheromones. Recent results obtained on methyl and dimethyl derivatives of five or six-membered nitrogen aromatic rings of biological interest will be also presented[d].

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[a] C. Lin and J. D. Swalen, Rev. Mod. Phys., 1959, 31, 841-892.

[b] I. Kleiner, ACS Earth and Space Chemistry, 2019, 3, 1812-1842.

[c] I. Kleiner and J. T. Hougen, J. Mol. Spectrosc., 2020, 368, 111255.

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