HIGHLY EXCITED MOLECULAR STATES: CHALLENGE FOR SPECTROSCOPY, DYNAMICS AND ASTROPHYSICS

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Theoretical predictions of excited molecular states and transitions together with extensive rotationally resolved line listes using ab initio potential energy (PES) and dipole moment surfaces have recently become available for small and medium size molecular systems (Refs.[1,2,3,4] and Refs. therein). The high density with the increasing energy makes these calculations challenging but mandatory for analyses of new spectroscopic and dynamics experiments at various temperature and excitation conditions. The state of art in ab initio and empirically optimised surfaces, variational and pertirbative calculations from three-to-six atomic molecules (ozone, phosphine, methane, ethylene ... and isotopic species) as well as accuracy and completeness issues will be discussed, particularly for complementary methods currently in progress in Reims and Tomsk groups[3,4,5,6,7,8,9,10]. Various applications imply an access to high-energy levels: numerous weak transitions responsible for the opacity in planetary transparency windows at long optical path or an interpretation of high-temperature spectra[4] of astrophysical objects. Minimum energy path models[9] for the molecular PES , the role of the potential barriers in the transition state channels[10] towards the dissociation threshold, the impact of symmetry breaking isotopic substitutions on the resonance coupling and intensity borrowing, qualitative changes of highly excited vibrational modes and prospectives for future studies will be discussed. The work is partly supported by French-Russian LIA SAMIA and Tomsk State University Mendeleev program.

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