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

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We shall discuss the computational issues and the state-of-the-art in *ab initio* and empirically optimized initio potential energy (PES) and dipole moment surfaces (DMS) as well as variational and pertirbative calculations from three-to-six atomic molecules (ozone, phosphine, methane, germane, ethylene ... and isotopic species) in terms of accuracy and completeness, particularly with the examples of complementary methods currently in progress in Reims GSMA PMT group*) in collaboration with Universities of Tomsk and of Central Florida [1-9]. Theoretical predictions of excited molecular states and transitions together with extensive rotationally resolved line lists using ab initio PESs and DMSs have recently become available for small and medium size molecular systems (as collected for example the TheoReTS database[7] with 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. 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 [5,6] of astrophysical objects. Minimum energy path models [1] for the molecular PES , the role of the potential barriers in the transition state channels [8] towards the dissociation threshold, metastable states and their lifetimes [9], the impact of symmetry breaking isotopic substitutions on the resonance coupling and intensity borrowing, qualitative changes of highly excited vibrational modes and prospective for future studies will be discussed.

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