MODELLING OF PLANETARY ATMOSPHERES FROM ACCURATE MOLECULAR LINE LISTS: PERSPECTIVES IN QUANTUM-CHEMICAL AND NUCLEAR-MOTION CALCULATIONS

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The study of various planetary objects, including the modelling of Earth atmosphere, remains an active field of research and demonstrates how having access to accurate molecular line lists is of primary importance. In this poster, we propose a general recipe for the construction of future line lists for different families of semi-rigid and nonrigid molecules (including short-lived radicals) up to a dozen atoms as well as for small van der Waals (vdW) complexes for which the knowledge of intra- and intermolecular states is of great interest. Due to their constant progress, we deeply think that *ab initio* calculation will be inseparable from high-resolution spectroscopy in a near future, by providing complementary information to the ordinary effective perturbative models. To this end, we intend using existing quantum chemistry methods as efficiently as possible.

– In this poster, we will briefly explain how to gradually increase accuracy of the *ab initio* surfaces from suitable corrections and basis-set extrapolations for applications requiring (or not) sub-percent accuracy for the line intensities. With the increase in the computer capabilities, it is now reasonable to obtain ~ 0.1 cm^{-1} of accuracy for the energy levels, and even less for the pure *ab initio* transitions, before applying a refinement procedure.

– In parallel, we will show how the methodology we adopted these past few years, including efficient algorithms for solving the time-independent Schrödinger equation and mathematical tools designed to spectroscopists, will be of great help for constructing suitable tailor-made Hamiltonian (polyad) models adapted to the low, medium and high resolution.

Among the molecules of planetary interest that could be potentially studied in short-, medium- and long-term, we can mention the medium-sized rigid and non-rigid systems H_2O_2, HONO, HOCO, HCOOH, HNO_3, CH_3CN, C_2H_2O, CH_3OH or CH_3NH_2 and larger systems as C_5H_6, C_6H_6 or $C_4H_4O_2N_2$.

A potential list of vdW molecules could include the water clusters (dimers: H_2O-HX, H_2O-O_3, H_2O-CO_2, H_2O-H_2O, trimers), $(HF)_3$ but also other species like CH_4-

N_2 or CH_4-O_2. In a general manner, nuclear motion calculations of vdW complexes beyond the rigid-monomer approximations will be considered.

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