1114-15-311 **Patrick Cassam-Chenaï*** (cassam@unice.fr), Lab. J. A. Dieudonné, Parc Valrose, UNS, 06100 NICE, France. *Algebraic problems from ab initio computational molecular spectroscopy.*

Computational molecular spectroscopy is gradually taking a larger part in the prediction of molecular spectra. Recent methods to find approximate solutions of the nuclear-motion Schrödinger eq. of molecules, have demonstrated unprecedented abilities to predict high temperature spectra relevant to exoplanet atmospheres, with better reliability than what can be achieved by using spectroscopic databases.

The main accuracy limitation of ab initio quantum calculations lies in the resolution of the Schrödinger eq. for the electrons of the molecule, whose solution provides the potential energy operator (PEO) for the nuclei, in the so-called Born-Oppenheimer approach. The electrons being Fermions their wave function is element of an exterior algebra, which can be endowed with a coproduct to turn into a Hopf algebra. We present a new method making use of Hopf algebra techniques to solve the electronic Schrödinger eq., along with open problems to reduce its computational complexity.

Finally, assuming that the PEO and other observables for the nuclei can be calculated to sufficient accuracy, we explain how to take advantage of integrity basis for modules of polynomial covariants adapted to the molecular symmetry, and state another open problem standing for linear molecules. (Received August 31, 2015)