

THE RENAISSANCE OF ROTATIONAL SPECTROSCOPY: THEORY MEETS EXPERIMENT FOR NEW CHALLENGES

CRISTINA PUZZARINI, *Dep. Chemistry 'Giacomo Ciamician', University of Bologna, Bologna, Italy.*

Among different spectroscopic techniques, rotational spectroscopy, given its intrinsic high resolution and high sensitivity, is one of the most powerful tools for investigating the structure and dynamics of molecules and supramolecular systems in the gas phase. Rotational spectra contain a wealth of accurate information on structural, molecular, and spectroscopic parameters that are difficult or impossible to obtain by other experimental techniques. However, the task of extracting information from the analysis of the spectral features is challenging, time-consuming, and prone to errors. In the last decade, rotational spectroscopy has experienced huge technological improvements that have led to a revitalization of the field, also due to parallel advancements in theoretical methods and computational resources.

Given these advances, the interplay of theory and experiment in rotational spectroscopy is discussed by means of representative examples that vividly illustrate what can be accomplished with theory and experiment brought together in this field. In particular, it will be shown how such an interplay can be exploited to address new challenges, exemplified by studying the nature of weak interactions in molecular adducts where the bonding pairs are made up of non-hydrogen atoms. Another fascinating challenge is offered by the open issues posed by astrochemistry. Astronomical observations of rotational spectroscopy signatures provide the unequivocal proof of the presence of chemical species in the astronomical source under consideration, and the talk will also explore the degree to which rotational spectroscopy can assist in going beyond the “simple” identification of interstellar species.