ROTATIONAL SPECTROSCOPY MEETS THEORY

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Rotational spectroscopy is known to be a technique widely used to infer information on molecular structure and dynamics. In the last decades, its role in the field of atmospheric and astrophysical investigations has rapidly grown up. However, several are the challenging aspects in rotational spectroscopy, since the detection and analysis of spectra as well as interpretation of obtained results are not at all straightforward. Quantum chemistry has reached such an accuracy that can be used to disentangle these challenging situations by guiding the experimental investigation, assisting in the determination of the spectroscopic parameters, and extracting information of chemical interest. This presentation provides an overview of the theoretical background and computational requirements needed for the accurate evaluation of the spectroscopic parameters of relevance to rotational spectroscopy. The role of theory in guiding and supporting experiment is detailed through a few examples and the interplay of experiment and theory is discussed in terms of the information of physical and chemical interest that can be derived.