QUANTUM-CHEMICAL CALCULATIONS OF SPECTROSCOPIC PARAMETERS FOR ROTATIONAL SPECTROSCOPY: THE NEED OF THE INTERPLAY BETWEEN EXPERIMENT AND THEORY

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Quantum-chemical calculations are nowadays able to provide very accurate predictions of molecular and spectroscopic properties. The predictive capabilities of such computations take a fundamental role in the field of high-resolution spectroscopy: calculations allow to guide, support and/or challenge the experimental determinations. In the field of rotational spectroscopy, high-level calculations can provide reliable values for the corresponding spectroscopic parameters (mainly, rotational and centrifugal-distortion constants), thus significantly facilitating the assignment of unknown spectra and, if the case, for the hyperfine parameters (nuclear quadrupole-coupling constants, spin-rotation tensors, spin-spin couplings, etc.), essential for the analysis of complex hyperfine structures. Furthermore, calculations can be used to provide information which enable a rigorous interpretation of the obtained spectroscopic parameters. In the present contribution, it will be demonstrated how fruitful is to exploit the interplay of theory and experiment, and the power of such an interplay will be illustrated by a few significant examples.