VMS-ROT: A NEW MODULE OF THE VIRTUAL MULTIFREQUENCY SPECTROMETER FOR SIMULATION, INTERPRETATION, AND FITTING OF ROTATIONAL SPECTRA

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The Virtual Multifrequency Spectrometer (VMS) is a tool that aims at integrating a wide range of computational and experimental spectroscopic techniques with the final goal of disclosing the static and dynamic physical-chemical properties "hidden" in molecular spectra. VMS is composed of two parts, namely, VMS-Comp, which provides access to the latest developments in the field of computational spectroscopy, and VMS-Draw, which provides a powerful graphical user interface (GUI) for an intuitive interpretation of theoretical outcomes and a direct comparison to experiment. In the present work, we introduce VMS-ROT, a new module of VMS that has been specifically designed to deal with rotational spectroscopy. This module offers an integrated environment for the analysis of rotational spectra: from the assignment of spectral transitions to the refinement of spectroscopic parameters and the simulation of the spectrum. While bridging theoretical and experimental rotational spectroscopy, VMS-ROT is strongly integrated with quantum-chemical calculations, and it is composed of four independent, yet interacting units: (1) the computational engine for the calculation of the spectroscopic parameters that are employed as a starting point for guiding experiments and for the spectral interpretation, (2) the fitting-prediction engine for the refinement of the molecular parameters on the basis of the assigned transitions and the prediction of the rotational spectrum of the target molecule, (3) the GUI module that offers a powerful set of tools for a vis-a-vis comparison between experimental and simulated spectra, and (4) the new assignment tool for the assignment of experimental transitions in terms of quantum numbers upon comparison with the simulated ones. The implementation and the main features of VMS-ROT are presented, and the software is validated by means of selected test cases ranging from isolated molecules of different sizes to molecular complexes. VMS-ROT offers an integrated environment for the analysis of the rotational spectra, with the innovative perspective of an intimate connection to quantum-chemical calculations that can be exploited at different levels of refinement, as an invaluable support and complement for experimental studies.