SIMULATION OF HIGH RESOLUTION VIBRATIONAL AND ELECTRONIC SPECTRA WITH A MULTIFREQUENCY VIRTUAL SPECTROMETER

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Moving from the common practice of extracting numerical data from experiment to be compared with quantum mechanical (QM) results toward a direct *vis-à-vis* comparison of experimental and simulated spectra would strongly reduce any arbitrariness in analysis of complex experimental outcomes and allow a proper account of the information connected to both position and shape of spectral bands. The development of such "virtual *ab initio* spectrometers" for a wide range of wavelengths has been one of our major research goals in the last years [1,2]. Recent methodological advances from our group allow simulation of optical (IR, Raman, UV-vis, etc.) spectra line-shapes for medium-to-large closed- and open-shell molecular systems. Vibrational spectra are computed including anharmonicities through perturbative corrections while electronic spectra line-shapes are simulated accounting for the vibrational structure. Well resolved and accurate theoretical spectra provide data as close as possible to the results directly available from experiment allowing to avoid ambiguities in analysis of the latter. Several examples illustrating interpretation, assignment or revision of experimental spectra for prototypes of bio-molecular systems (phenyl radical, glycine, thymine, pyrimidine, anisole dimer) will be presented.

1. V. Barone, A. Baiardi, M. Biczysko, J. Bloino, C. Cappelli, F. Lipparini Phys. Chem. Chem. Phys, 14, 12404, 2012
2. M. Biczysko, J. Bloino, G. Brancato, et al. Theor. Chem. Acc. 113, 1201, 2012