IMPORTANCE OF THE VIBRONIC EFFECTS IN CHIROPTICAL SPECTRA

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Chirality is an important property of biosystems and can be found also in technologies such as 3D displays or energy storage. The chirality is reflected in the chiroptical signal. For a full understanding, it is important to know the link between the observed optical spectra and the structure. To this aim, computational spectroscopy plays a crucial role. However, common protocols, which rely on pure electronic transitions, have limited accuracy, and are generally insufficient to predict chiroptical properties, such as electronic circular dichroism or circularly polarized luminescence. Our previous studies have shown the importance of considering the vibrational contributions in simulations of UV-visible spectra of chiral molecules as well. However, the inclusion of vibronic contributions significantly increases the computational cost, and the underlying harmonic approximation is particularly problematic for flexible compounds.

We present a systematic approach to account for the vibronic effects in large chiral molecules. Starting from a prototypical molecule to highlight the importance of vibronic effects in chiroptical spectra, a general protocol is tested on Ir-complex molecules[1]. The procedure is then applied to a chiral boron dipyrromethene dye (BODIPY), which exhibits a variety of conformations and crossing of excited electronic states[2].

To analyze the results, graphical tools were developed and used. The data generated by the simulations and potential sources of inaccuracy can be overviewed more easily. These visualization techniques can provide new insights into the origin of the chiroptical signal and help design more efficient chiral molecules of technological interest.

[1] Yang, Q.; Fusé, M.; Bloino, J. et. al. *Spectrochim. Acta A* 2021, **254**, 119631.
[2] Yang, Q.; Fusé, M.; Bloino, J. *Front. Chem.* 2020, **801**.