A RAPID METHOD FOR THE EVALUATION OF CHIROPTICAL VIBRATIONAL SPECTRA OF LARGE MOLECULES

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An accurate first-principles evaluation of chiroptic spectroscopic properties of large molecules is a challenge in electronic structure theory. The Molecules-in-Molecules (MIM) fragment-based method is an efficient and widely applicable model to study the structure and energetics of large molecules. Recently, the MIM method has been adapted for the accurate evaluation of the infrared (IR), Raman, vibrational circular dichroism (VCD) and Raman optical activity (ROA) spectra for large molecules. The relevant higher energy derivatives from smaller fragments are used to build the property tensors of the parent molecule in our approach. Further, the fragment tensor components are evaluated in the global coordinate framework, and the link atom tensor components projected onto the corresponding host and supporting atoms through the Jacobian projection method in our rigorous implementation. Our methods have been benchmarked on a set of peptide and carbohydrate molecules, and the vibrational frequencies and chiroptic spectral intensities are accurately reproduced relative to the full, unfragmented, results for these systems. In this talk, I will be presenting the details of the theory, implementation and performance of the MIM model for evaluating the VCD and ROA spectra of large molecules.