ANHARMONIC VIBRATIONAL SPECTROSCOPY ON METAL TRANSITION COMPLEXES

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Advances in hardware performance and the availability of efficient and reliable computational models have made possible the application of computational spectroscopy to ever larger molecular systems. The systematic interpretation of experimental data and the full characterization of complex molecules can then be facilitated. Focusing on vibrational spectroscopy, several approaches have been proposed to simulate spectra beyond the double harmonic approximation, so that more details become available. However, a routine use of such tools requires the preliminary definition of a valid protocol with the most appropriate combination of electronic structure and nuclear calculation models. Several benchmark of anharmonic calculations frequency have been realized on organic molecules. Nevertheless, benchmarks of organometallics or inorganic metal complexes at this level are strongly lacking despite the interest of these systems due to their strong emission and vibrational properties.

Herein we report the benchmark study realized with anharmonic calculations on simple metal complexes, along with some pilot applications on systems of direct technological or biological interest.