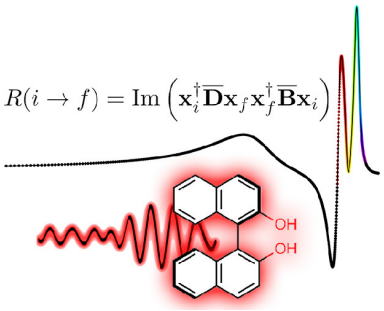
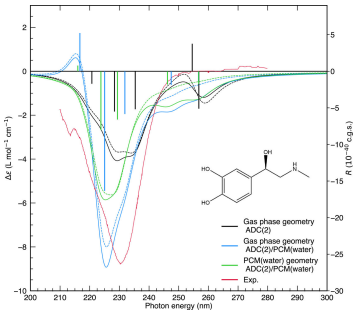
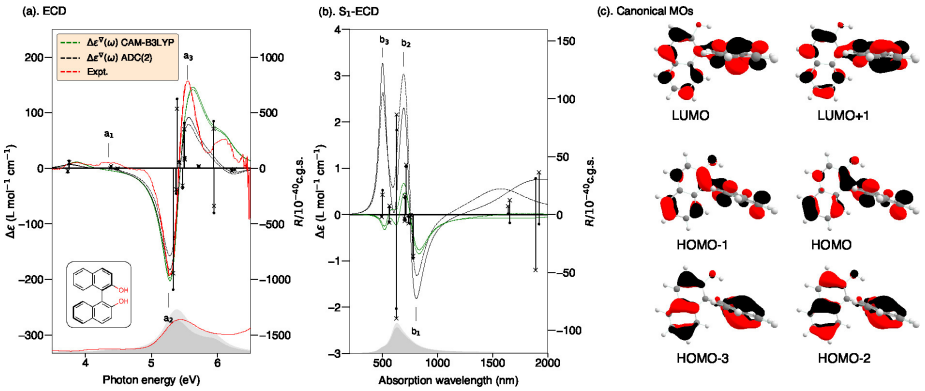
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Simulating ECD Spectra Using the ADC Schemes of the Polarization Propagator





- The algebraic diagrammatic construction (ADC) scheme for the polarization propagator provides a family of many-body Green's function methods for excited states.
- Electronic circular dichroism (ECD) spectroscopy is a widely used technique to study chiral molecules.
- ADC provides size-consistent, Hermitian, compact and accurate correlation methods for calculating ECD spectra. The accuracies of ADC methods are comparable to those of coupled cluster methods.
- With Q-Chem, one can run ADC calculations truncated at different orders of perturbation to simulate the ECD spectra of molecules in gas or solution phases (PCM model).
- Molecular ECD spectroscopy can be simulated for ground or excited states, in order to study time-resolved pump-probe experiments or chiral chemical reaction paths.
- All calculations can be done in velocity gauge and thus are origin-independent.



(a) ADC(2) (black) and CAM-B3LYP (green) simulated and experimental ECD (top) and UV-vis spectrum (bottom) and (b) ADC simulated excited state ECD (top) and excited state absorption spectra (bottom) of of (R)-binol in length (solid) and velocity (dashed) gauges; (c) canonical MOs.

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