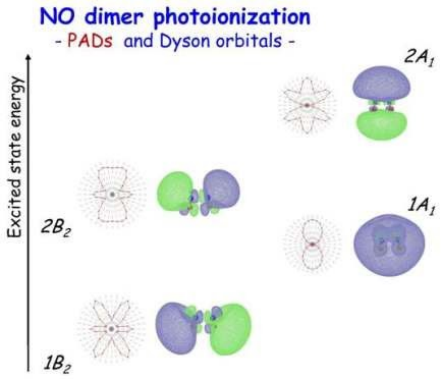
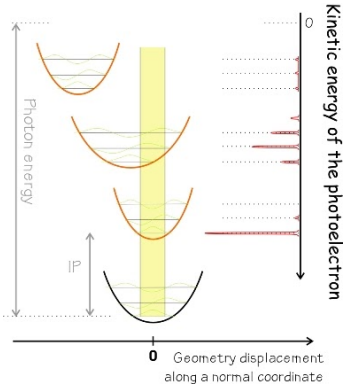
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

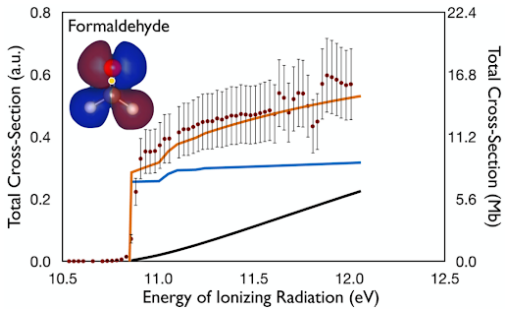
Simulating Electronic Spectroscopy using ezSpectra Suite



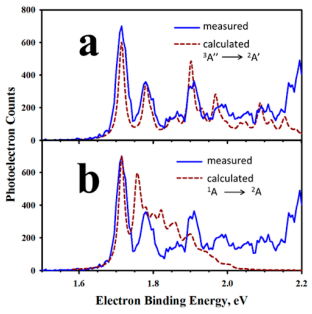


ezFCF and ezDyson post-processing tools compute vibrational progressions for electronic transitions and photoionization cross sections using Q-Chem's outputs:

- Q-Chem: determines relevant electronic states and their optimized geometries, vibrational frequencies, normal modes, and Dyson orbitals (for photoionization).
- ezFCF: computes Franck-Condon factors (within the double-harmonic approximation) to obtain vibrational structure; Duschinsky rotations can be included.
- ezDyson: computes photoelectron dipole matrix elements between Dyson orbitals and outgoing photoelectron wavefunction (treated either as a plane wave or a Coulomb wave). The total and differential photoionization cross sections, photoelectron angular distributions (PAD), and anisotropy parameters can be computed.
- Can be combined with different quantum-chemistry methods.



(a) Formaldehyde photoionization cross section



(b) Photoelectron spectra of quinoniminyl radicals

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