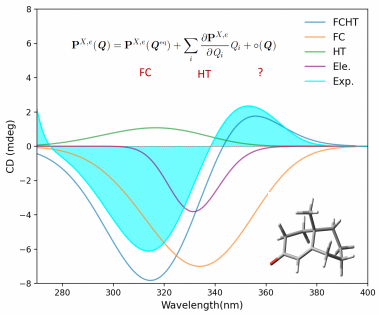
IS THE HERZBERG-TELLER EFFECT SUFFICIENT TO SIMULATE ONE PHOTON ABSORPTION SPECTRA?

QIN YANG, *Institute of Organic Chemistry and Biochemistry, Czech Academy of Science, Prague, Czechia*; TAO WU, *Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czechia*; LI LI, *Department of Synthetic Medicinal Chemistry, Institute of Materia Medica , Beijing, China*; JULIEN BLOINO, *Scuola Normale Superiore, Scuola Normale Superiore, Pisa, Italy*; PETR BOUR, *Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague, Czechia*.

UV-vis absorption and circular dichroism spectra play a significant role in probing excited-state molecular properties. They developed to become routine tools used in a variety of fields, such as pharmacology, chemical analysis, and environmental monitoring. With the advances of instrumentation and broader applications, spectral simulations face increasing challenges. Theoretical methods including vibrational effects have replaced cruder models based purely on electronic transitions. With a better balance of computational cost and accuracy, such simulations are becoming routine.



An important aspect of vibronic simulations is the treatment of the transition dipole moments. The usual Franck-Condon approximation may not be adequate for weak or forbidden electronic transitions and the first order expansion (Herzberg-Teller, HT) term must be considered. For several organic molecules we show the importance of the HT effects for understanding the spectra. A family of porphyrin molecules not only exhibits the HT effects, but also hints at the need for higher-order terms to be included.