Calculating of UV-Vis Absorbance/Fluorescence Spectra of Indole and Tryptophan

Elijah B. Kofke, Kristine M. Vorwerk, William W. Kennerly
Department of Chemistry
Skidmore College
Saratoga Springs, NY

We are characterizing the UV-Vis absorption and fluorescence spectra of gaseous indole and tryptophan, using quantum computational modelling methods available in Gaussian 09. We have settled on using time-dependent density functional theory (TD-DFT), after initially attempting to use complete active space (CAS) calculations. Using DFT at the B3LYP/aug-cc-pVTZ level of theory, we calculated optimized ground-state geometries for both indole and tryptophan. We then used these geometries to calculate vertical excitation data using a variety of basis sets and functionals. The CAM-B3LYP and ωB97XD functionals showed a high degree of consistency, across a variety of augmented and polarized basis sets (both double and triple split valence). In both indole and tryptophan, the S_1 and S_2 states are nearly degenerate. Gaussian has struggled to distinguish their minimum energy geometries, converging the second excited state geometry to that of the first. Our predicted vertical absorption energies at the ωB97XD/6-31+G(d) level of theory are 5.08 eV (S_1) and 5.13 eV (S_2) for indole, and 4.98 eV (S_1) and 5.08 eV (S_2) for tryptophan. Our predicted vertical fluorescence energy (from S_1) for indole and tryptophan is 4.50 eV and 4.30 eV, respectively. We were partially successful characterizing indole using smaller basis sets in CAS calculations, but were unable to generate results for larger basis sets or for tryptophan. With successful characterization, we hope to move on to investigating tryptophan in solvated environments, and for protein-embedded tryptophan moieties.