COMPUTATIONAL MODELING OF ELECTRONIC SPECTROSCOPY OF 3-PHENYL-2-PROPYNENITRILE

CLAUDIA I VIQUEZ ROJAS, KHADIJA M. JAWAD, TIMOTHY S. ZWIER, LYUDMILA V SLIPCHENKO, *Department of Chemistry, Purdue University, West Lafayette, IN, USA*.

3-phenyl-2-propynenitrile (PPN) is a potentially important component of Titan's atmosphere. This molecule exhibits intriguing patterns in high-resolved absorption and fluorescence spectra. To better understand PPN's photochemistry, we employ computational tools to examine its electronic structure and excited states. The presence of vibronic coupling is evaluated by mapping potential energy surfaces of the first four electronic excitations along different vibrational modes. The parameters that describe the interactions between vibrational and electronic states are used to build the vibronic Hamiltonian and predict the absorption and emission spectra of PPN with the multi configuration time dependent Hartree (MCTDH) algorithm.