EXPERIMENTALLY MAPPING OUT THE GROUND STATE POTENTIAL ENERGY SURFACE OF 5-PHENYL-1-PENTENE

NATHAN R. PILLSBURY and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

5-phenyl-1-pentene was previously studied by resonant two-photon ionization (R2PI) and UV-UV hole burning (UVHB) spectroscopies. These spectra revealed that five conformations were present in the free jet expansion. The isomers were also assigned to specific structures using structural calculations along with simulated and experimental rotational band contours. The current study utilizes stimulated emission pumping-population transfer spectroscopy (SEP-PTS) to place experimental bounds on the energy thresholds for isomerization between individual reactant/product isomer pairs. A comparison between experimental data and barriers predicted by density functional calculations will be made.