THE EXOTIC EXCITED STATE BEHAVIOR OF 3-PHENYL-2-PROPYNENITRILE

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

3-phenyl-2-propynenitrile (Ph-C≡C-C≡N) is of interest to the study of Titan's atmosphere as it is a likely product of the photochemical reaction between two known species in that environment: benzene and cyanoacetylene. The gas phase jet-cooled resonant two-photon ionization, laser induced fluorescence, and preliminary dispersed fluorescence spectra were previously reported without firm assignments due to the scarcity of totally symmetric vibrations and the prevalence of strong bands of b2 and b1 symmetry vibrations. These had called into question the identity and geometry of the excited state(s) involved in the transitions. We will here present the completed set of dispersed fluorescence data along with an analysis of the potential energy surfaces and vibronic coupling characteristic of the close-lying excited states in this intriguing molecule.