VIBRONIC SPECTROSCOPY OF A STRUCTURAL ISOMER OF QUINOLINE: (Z)-PHENYLVINYLNITRILE

DEEPALI N. MEHTA-HURT, JOSEPH A. KORN, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084 U.S.A.*.

This talk will present results of a gas phase, jet-cooled vibronic spectroscopy study of (Z)-phenylvinylnitrile ((Z)-C_6H_5-CH=CH-C=N, (Z)-PVN). With a substituent locked into a cis conformation with respect to the aromatic ring, (Z)-PVN is postulated to be a molecule with an ideal functionality to isomerize to quinoline upon photoexcitation. As such, (Z)-PVN is particularly relevant to Titan's nitrile-containing atmosphere, where much of the chemistry is photochemically driven. As a first step towards such photochemical studies, a fluorescence excitation spectrum of a mixture of (E)- and (Z)-PVN was collected spanning the range 33,300-35,580 cm^{-1} (300.0-281.0 nm). Previous investigations in the Zwier group pertaining to the vibronic spectroscopy of (E)-PVN allowed for the identification of peaks in the (E)- and (Z)-PVN composite spectrum that were solely due to (Z)-PVN, and the S_0-S_1 origin of (Z)-PVN was identified as a dominant band that occurs at 33,706 cm^{-1}. For additional confirmation, ultraviolet depletion spectroscopy (UVD) was used to obtain an isomer specific spectrum of (Z)-PVN as well as search for non-radiative transitions. Dispersed fluorescence spectra that characterize the vibronic activity have also been acquired. A comparison between the vibronic spectroscopy of (Z)-PVN with both (E)-PVN and (Z)-phenylvinylacetylene ((Z)-PVA), the hydrocarbon analog of (Z)-PVN, will be made in this talk.