Proton-coupled Electron Transfer in $[C_5H_5N \cdot (H_2O)_n]^-$ Clusters <u>Kaye A. Archer¹</u> and Kenneth D. Jordan¹ ¹Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260

Pyridine-water cluster anions, $[C_5H_5N \cdot (H_2O)_{n=3,4}]^-$ are of interest because three types of diabatic states can exist. They include $C_5H_5N^- \cdot (H_2O)_n$, $C_5H_5N \cdot (H_2O)_n^-$ and $C_5H_6N \cdot (OH^-) \cdot (H_2O)_{n-1}$. One-dimensional potential energy curves along the proton transfer coordinate are calculated at EOMEA-CCSD(2)/aug-cc-pVDZ+7*s*7*p* level of theory, for the *n* = 3 and 4 cases. We show that there is an avoided crossing between the dipole-bound and valence-bound diabatic states along this coordinate and that the zero point vibrational level of the OH stretch in the case of the *n* =3, samples these two diabatic states.