

Abstract Submitted
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Anion Photoelectron Spectroscopy of the Homogenous 2-Hydroxypyridine Dimer Electron Induced Proton Transfer System¹

ALEXANDRA VLK, SARAH STOKES, Towson University, YI WANG, ZACHARY HICKS, XINXING ZHANG, NICOLAS BLANDO, Johns Hopkins University, ANDREW FROCK, Baltimore Polytechnic Institute, SARA MARQUEZ, KIT BOWEN², Johns Hopkins University, BOWEN LAB JHU TEAM — Anion photoelectron spectroscopic (PES) and density functional theory (DFT) studies on the dimer anion of (2-hydroxypyridine)₂⁻ are reported. The experimentally measured vertical detachment energy (VDE) of 1.21eV compares well with the theoretically predicted values. The 2-hydroxypyridine anionic dimer system was investigated because of its resemblance to the nitrogenous heterocyclic pyrimidine nucleobases. Experimental and theoretical results show electron induced proton transfer (EIPT) in both the lactim and lactam homogeneous dimers. Upon electron attachment, the anion can serve as the intermediate between the two neutral dimers. A possible double proton transfer process can occur from the neutral (2-hydroxypyridine)₂ to (2-pyridone)₂ through the dimer anion. This potentially suggests an electron catalyzed double proton transfer mechanism of tautomerization.

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