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Environmental and Structural Effects on Intramolecular Charge Transfer Exhibited by 4-Aminobenzoic Acid and its Derivatives
MITCHELL THAYER[1], Ohio Northern University, SARAH SCHMIDTKE[2], College of Wooster — This study inspected intramolecular charge transfer in a variety of conditions by methodically adjusting the parent compound structure and solvent properties under spectroscopic analysis. 4-aminobenzoic acid and its derivatives were analyzed in three buffers of varying pH (2, 7, 10). The various compounds were used to study structural effects, while the placement in buffers allowed control of the protonation states of the molecules. The samples were each scanned for absorbance to determine excitation wavelengths which were used for subsequent fluorescent spectroscopic analysis. The charge transfer, when exhibited, is recognized by dual fluorescence. Varying the temperature of the scans allowed analysis of the thermodynamic driving forces for the reaction while the particular solvent-solute combinations that exhibited the phenomenon lend insight to the conditions conducive to charge transfer. To study what controlled the extent of the phenomenon, titrations were carried out to determine the amine pKa and computational models were generated to inspect hybridization and its influence on photophysical behavior.

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