# Investigating the Electrochemical Behavior of Dihydropyrrolopyroles for Use as Anodically Coloring Electrochromes

Perry Skiouris
*Kennesaw State University*

Ally Kisiel
*Kennesaw State University*

Valentino Sorto
*Kennesaw State University*

Julia Mauro
*Kennesaw State University*

Graham Collier
*Kennesaw State University*

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Abstract:

Electrochromic materials have found widespread use in consumer electronics, energy saving windows, and military applications. They contain unique electronic properties allowing them to undergo a color change in a redox reaction. One classification of these molecules is known as anodically coloring electrochromes (ACEs). When in solution, these compounds are transmissive in the neutral (ground) state and absorb visible light upon oxidation, by the formation of a radical cation, thus making them colored. The focus of this study is the electronic transitions of this radical cation and how chemical modifications to the structures produce a variable color profile. To design prospective molecules that behave as ACEs, time-dependent density functional theory (TDDFT) calculations were used to generate theoretical UV-vis absorbance spectra, where a preliminary understanding of structure, connectivity, and functionality is achieved. The goal here is to vary the low-energy absorption in the oxidized state while maintaining UV-absorption as a neutral molecule. Two molecules were synthesized, one containing an electron-donating group (PS-7) and the other containing an electron-withdrawing group (PS-11). The impact on altering chemical substituents was elucidated by UV-vis and NMR spectroscopies, and the experimental data compared with our calculations. Further experiments were done using cyclic voltammetry and differential pulse voltammetry, showing a relatively low onset of oxidation (0.7 V vs Ag/AgCl). This data shows an improvement to traditionally used electrochromes, resulting in a more defined absorbance across the visible spectrum, maximizing the performance of these materials.