

Photophysical and Structural Insights into BODIPY-Imidazolium Salts and an NHC-Silver Complex

Miguel A. Rosero-Mafla^{a,c}, Manuel N. Chaur^b, Renso R. Visbal^a, M. Concepción Gimeno^c

^a Grupo de Investigación en Síntesis Organometálica y Catálisis, Universidad del Valle, Colombia

^b Síntesis y Mecanismos de Reacción en Química Orgánica, Universidad del Valle, Colombia

^c Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC, Universidad de Zaragoza, España.
miguelrosero@unizar.es

This study explores the photophysical and structural properties of novel imidazolium salts and a silver organometallic complex. To understand the fundamental interactions influencing the photophysical behavior of water-soluble BODIPY derivatives, four imidazolium salts were synthesized via S_NAr reactions using a chlorinated BODIPY and four imidazole derivatives. The stability of one imidazolium salt was assessed through 1H NMR spectroscopy, revealing relatively low stability, which was further investigated through synthetic analogs and DFT-level computational calculations. Fluorescence and UV-Vis experiments showed classical BODIPY behavior photophysical properties in these imidazolium salts.

In parallel, leveraging the notable electrochemical and photophysical properties of *p*-benzoquinone derivatives and NHC-ligand complexes, a silver organometallic complex (Ag(I)-NHC) was synthesized using a quinobis(imidazolium) salt as a ligand precursor and Ag_2O as the metal source. Characterization of the highly insoluble complex was carried out by solid-state ^{13}C NMR and MALDI-TOF, with *m/z* fragments suggesting oligomer formation. The obtained complex exhibited an emission maximum at 588 nm. Cyclic voltammetry displayed a pseudoreversible redox pattern associated with the *p*-benzoquinone component, providing insights into its electrochemical behavior. TGA analysis showed a decomposition temperature around 355 °C, indicating notable thermal stability.

