
SYNTHESIS AND CHARACTERIZATION OF [Cu(PDTC)L] COORDINATION COMPOUND SERIES

Dr. Matt Queen *, Science, MSUB, Billings

Dr. Tom Lewis, Science, MSUB, Billings

Siana Wiles, Science, MSUB, Billings

Carbon Tetrachloride (CT) is a potential environmental contaminants in water, and soil. We are interested in studying potential CT environmental remediation technologies. Specially we are interested in 2,6-pyridinedithiocarboxylic (PDTC) and the dechlorination properties of its copper based coordination compounds, [Cu(PDTC)L]X. In the interest of creating better performing more soluble coordination compounds we seek to understand the link between coordination compound electronic structure and reactivity. With the ultimate goal in mind we present IR, UV-Vis, and NMR evidence for the successful synthesis of a series of [Cu(PDTC)_yL]X coordination compounds. Here L-Br, CN, PPh₃ as well as the dimer species [Cu(PDTC)₂]. These experimental spectra are compared to computational data calculated using DFT optimized structures utilizing a wide range of exchange and correlation density functionals.