

“That’s Not Coming Off of There”; An Exploration of Ligand Liability in Carbon Tetrachloride Dechlorination Technologies

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Carbon Tetrachloride (CT) is a carcinogenic industrial solvent, and known environmental contaminant. The Department of Energy’s Hanford Site has been identified as a Superfund Site. CT, is just one of the many environmental concerns. Environmentally CT dechlorinates in a stepwise manner forming lesser chlorinated intermediate complexes that pose a health threat to humans. $[\text{Cu}(\text{PDTC})\text{L}]$ is a small coordination compound capable of dechlorinating CT into less harmless decomposition products: CO_2 and Cl^- . In this study we draw a correlation between the dechlorination kinetics of CT of $[\text{Cu}(\text{PDTC})\text{L}]$ and the ligand liability of the L ligand. We use P K-edge X-Ray Absorption Spectroscopy to quantitate the phosphorus covalency of a series of PR_3 transition metal ligands $[\text{Cu}(\text{PDTC})\text{L}]$ (L= PPh_3 , and PCy_3). Our results show that there is no correlation between the covalent character of Cu-P bonds and the kinetics of dechlorination. Instead, we propose that the correlation has a greater correlation with the solubility of a ligand in a given solvent system.