The Orbit of Coordination: Synthesis and Geometries of Crown Jewel Complexes as a Foray to Medical Imaging Development Work

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The diaza-18-crown-6 macrocyclic ligand (D18CJ) used in our studies has never been studied from a coordination chemistry perspective. Characterized as a pincer ligand, D18CJ has biological value as evidenced from application in amino acid fluorescent detection; with its macrocyclic component, the ligand has additional potential to support diagnostic imaging agents. We will report the first examples of metal coordination with D18CJ. The intent of our studies was to survey interactions of D18CJ with different metals and understand bonding, resulting geometries, and metal-ligand coordination reaction kinetics. Kinetic data was collected using UV spectroscopy to follow Cu-D18CJ complex formation at room temperature. Electron paramagnetic resonance spectroscopy of the Cu-D18CJ complex showed a paramagnetic species with x-ray crystallographic studies providing secure characterization and a complete picture of the coordination chemistry. For Cu, a 4-coordinate species resulted but for Co-D18CJ the complex was found to be 7-coordinate. The results to date show D18CJ coordination to metal ions is dependent on the fullness of the metal's valence shell. More metal-ligand analogues need to be analyzed to fully study the coordination chemistry of D18CJ.

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