Molecular Geometries of Transition Metal Complexes Influenced by Metal-Sulfur Interactions

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In pursuit of 'deactivatable' transition metal complexes for catalysis, a new ligand was prepared with a presumablytriggerable disulfide moiety incorporated into the scaffold. The reactivity between this ligand and late first-row transition metal halides was explored, producing eight coordination compounds. The crystal structures of all eight compounds show variable metal-sulfur interactions that directly influence the molecular geometries. While the choice of halide does not appear to influence the molecular geometries, solvent has a drastic effect on the solvated structures. The metal-sulfur interactions do not appear to affect the disulfide bond, as evidenced by X-ray crystallography and Raman spectroscopy. From this investigation, two isomorphous solvate series, and a kryptoracemate, were obtained. Although chemically-identical, the enantiomeric pair in the kryptoracemic structure possess two strikingly different metal-sulfur distances. The crystallographic and structural analyses of this investigation will be discussed.