This thesis consists of a computational study done on group VI transition metal hexacarbonyl complexes to determine the structure, infrared spectroscopy and thermodynamics. The hexacarbonyl complexes were broken into fragments and analyzed by how the missing ligand affected their geometry. The CO stretching frequencies were examined for the various complexes. These studies were repeated with a single pyridine inserted into each of the coordinatively unsaturated complexes. The results suggest that the octahedral symmetry is the most stable and that removing a ligand results in a less stable complex. The most stable geometries were found to be the octahedral complexes with Tungsten being the most stable out of the three transition metals. For the coordination numbers 2-6, the singlet state was observed to be the most stable spin except when looking at Chromium, the square planar triplet state was found to be the most stable. For monocarbonyls, the septet state was observed to be the most stable spin. Adding the pyridine to the coordination site doesn’t change any of the results. The same energy patterns are still observed.