Abstract

Mass spectrometry with electrospray ionization is an excellent method for structural analysis of coordination compounds with outstanding sensitivity and selectivity. However, it fails to detect some low-polar rhenium complexes. This master thesis describes derivatization method of non-ionizable rhenium complexes with 1,2-dihydroxybenzene and 2,3-dihydroxytoluenene. Fragmentation mechanisms and structure of prepared complexes was studied using high resolution mass spectrometry and collision-induced dissociation (CID). Furthermore, density functional theory (DFT) computational method was used for prediction of bond cleavage based on bond lengthening.