Abstract

Gold catalysis has recently experienced a sustained upswing in interest from scientific community. The amount of new reactions catalysed by gold is so significant that little is known about mechanisms of most of these reactions. Research into mechanisms of (not only) gold catalysed reactions is therefore very significant area of interest and important to the continued improvement of gold catalysed reactions. Formation of cationic π-complexes is considered a first mechanistic step in reactions catalysed by gold(I). The bond dissociation energies of gas phase cationic π-complexes were investigated by mass spectrometry and theory calculations in this thesis. These complexes consisted of differently substituted unsaturated hydrocarbons (alkenes, alkynes, alkadienes and allenes) and complex cations of silver and gold containing second ligand (triphenylphosphine, acetonitrile). On the basis of the results obtained from this study, a possible origin of the "silver effect" in gold(I) catalysis is discussed.

Key words

catalysis, gold, silver, mass spectrometry, DFT calculations, reaction intermediates