

Abstract

Geminally diaurated complexes are important intermediates involved in some of the gold catalyzed reactions and therefore they have become a subject of the current research. The aim of this thesis was to assess the influence of electronic structure of an aryl ligand on the stability of gold complexes with three-center-two-electron interaction Au_2C . A series of geminally diaurated complexes was obtained by a reaction of gold complex $[(IPr)Au(NCMe)]BF_4$ (IPr = 1,3-bis(2,6-di-iso-propylphenyl)imidazol-2-ylidene) with arylboronic acids $ArB(OH)_2$ bearing different substituents at the aryl group (Ar = *para*- $O_2NC_6H_4$, *para*- NCC_6H_4 , *para*- ClC_6H_4 , C_6H_5 , *para*- $H_3CC_6H_4$, *para*- $H_3COC_6H_4$, *meta*- $O_2NC_6H_4$, *meta*- NCC_6H_4 , *meta*- $H_3CC_6H_4$, *ortho*- $O_2NC_6H_4$, *ortho*- NCC_6H_4 , *ortho*- $H_3CC_6H_4$).

Mass spectrometry (MS) was used as the main experimental method in this study. Appearance energies (AE) for the fragmentation of geminally diaurated complexes were estimated by the methods MS/MS. The obtained energies were plotted against the corresponding Hammett σ -constants to assess the correlation between the electronic structure of a given aryl ligand and the stability of the Au_2C bond.

It was found that structures of gold complexes derived from the cyanophenylboronic acids do not correspond to the geminally diaurated complexes but to the C,N-digold complexes that do not contain the Au_2C bond.

Key words: *gold catalysis, aurophilicity, arylboronic acid, reaction intermediates, geminal diauration, electrospray ionization, mass spectrometry*