

The present thesis deals with a study of the catalytically active species in carbon-carbon and carbon-heteroatom bond-forming reactions catalyzed by gold, palladium and copper.

In the case of the reactions catalyzed by gold salts (Au^+ and Au^{3+} , complexes Au^+ and Au nanoparticles), it was found that regardless of the gold source, the catalytically active species in some reactions are atomic clusters of gold between 2 to 9 atoms, and that, within this range, the reactions are sensitive to the number of gold atoms forming the cluster. These clusters have an unusually high catalytic activity for such reactions, reaching up to 10 million catalytic cycles per hour at room temperature. Furthermore, we have studied the stability of these clusters against anions and ligands in solution.

In the case of cross-coupling reactions catalyzed by palladium under Jeffery's conditions (without ligands, amide solvent, 130-140 °C), the formation of catalytically Pd clusters between 3 and 4 atoms has been observed for the Heck, Sonogashira, Stille and Suzuki coupling reactions. These clusters are stabilized in the presence of water or amines and exhibit high catalytic activity for aryl bromides and iodides.

Moreover, it has also been observed the formation of clusters of Cu in the coupling reactions between aryl iodides and various nucleophiles (amides, phenols, phosphines, thiols, alkynes) in the absence of diamine ligands. Furthermore, it has also been possible to establish the Cu atomicity, amount and formation mechanism of the Cu clusters formed.

Finally, we have compared the catalytic activity of gold clusters, palladium and copper catalysis in Lewis, redox and radical type reactions, relating the physicochemical nature of the clusters with their catalytic activity.