Theoretical study of the closed-shell d10-d10 Au(I)-Cu(I) attraction in complexes in extended unsupported chains

Rodríguez-Castillo, María

Monge, Miguel

López-de-Luzuriaga, José M.

Olmos, M. Elena

Laguna, Antonio

Mendizabal, Fernando

Model compounds are used to study the metallophilic attraction between gold and copper atoms. Ab initio calculations on dimers and tetramers in different distributions of the simplified units are analyzed. An attraction is found for all models and there is a reasonable agreement between the experimental and theoretical geometries.