

Aurophilic attraction in binuclear complexes with Au(i) and Au(iii). A theoretical study

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Model compounds are used to study the aurophilic attraction among gold atoms in the different oxidation states Au(i)-Au(i), Au(i)-Au(iii) and Au(iii)-Au(iii). An attraction is found for all models and there is a reasonable agreement between the experimental and theoretical geometries at the MP2 level. The dispersion, induction and electrostatic multipole components to this attraction are analyzed using intermolecular models. © the Owner Societies. © the Owner Societies.