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A comparative DFT study of interactions of Au and small gold clusters Au_n ($n=2-4$) with CH_3S and CH_2 radicals

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Abstract

We compare DFT binding energies (BEs) of Au and small gold clusters interacting with CH_3S and CH_2 ligands (Au_n-L complexes, $n=1-4$). The spin state and the binding mechanism in Au_n-L varies with the participation of singly occupied non-bonding orbitals or doubly occupied lone-pair orbitals of a ligand and on the number of atoms (even or odd) of Au_n . The highest BE, 354 kJ/mol, exhibits the Au_3-CH_2 complex with the covalent bond in which participate two singly occupied orbitals of the triplet state of CH_2 . With CH_3S the highest BE (277 kJ/mol) is calculated for Au_3-SCH_3 with the single Au-S bond.

Keywords: gold clusters, methylene, methylthiolate, binding energy, open shell complexes, thermochemistry, DFT, CCSD(T)

1. INTRODUCTION

The methylthio radical CH_3S interacting with a metallic atom is the smallest species which may serve as a model for understanding the binding characteristics in the important class of species, Self-Assembled Monolayers (SAMs), created most frequently on the gold surfaces. Most important SAMs, based on the family of thiolate containing ligands¹⁻⁴ are considered in material science, catalysis and nanotechnologies. Since both CH_3S and the Au atom are doublets in their ground state (X^2E and 2S , respectively), their interaction leads to either closed shell singlet or to the triplet state product⁵. The structure and stability of the closed shell $Au-SCH_3$ complex ($^1A'$, assuming simplified C_{3v} structure of CH_3S) is determined by quite strong Au-S covalent bond

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