Theoretical study in [C2H4-Tl]+ and [C2H2-Tl]+ complexes

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We studied the attraction between [C2Hn] and Tl(I) in the hypothetical [C2Hn-Tl]+ complexes (n = 2,4) using ab initio methodology. We found that the changes around the equilibrium distance C-Tl and in the interaction energies are sensitive to the electron correlation potential. We evaluated these effects using several levels of theory, including Hartree-Fock (HF), second-order Møller-Plesset (MP2), MP4, coupled cluster singles and doubles CCSD(T), and local density approximation augmented by nonlocal corrections for exchange and correlation due to Becke and Perdew (LDA/BP). The obtained interaction energies differences at the equilibrium distance Re (C-Tl) range from 33 and 46 kJ/mol at the different levels used. These results indicate that the interaction between olefinic systems and Tl(I) are a real minimum on the potential energy surfaces (PES). We can predict that these new complexes are viable for synthesizing. At long distances, the behavior of the [C2Hn]-Tl+ interaction may be r