

Theoretical study of the interaction d_{10-s_2} between Pt(0) and metals on the $[\text{Pt}(\text{PH}_3)_3\text{M}]$ complexes (M = Hg(0), Au(-I))

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We studied the attraction between $[\text{Pt}(\text{PH}_3)_3]$ and the metals (Hg(0) and Au(-I)) in the hypothetical $[\text{Pt}(\text{PH}_3)_3\text{M}]$ isoelectronic complexes using ab initio methodology. We found that the changes around the equilibrium distance Pt-M and in the interaction energies are sensitive to the electron correlation potential. This effect was evaluated using several levels of theory, including HF, MPn (n = 2-4), CCSD and CCSD(T). In the $[\text{Pt}(\text{PH}_3)_3\text{Hg}]$ complex, at the different methodology levels are obtained interaction energies at the equilibrium distance R_e (Pt-Hg) range from 10 to 42 kJ/mol. Such magnitude are in the order of a metallophilic interaction. On the other hand, in the $[\text{Pt}(\text{PH}_3)_3\text{Au}]^-$ complex, the interaction energies Au-Pt are range from 35 to 129 kJ/mol, beyond the metallophilic interaction. At long-distances, the behaviour of the $[\text{Pt}(\text{PH}_3)_3\text{-M}]$ interaction may be related mainly to electrostatic, charge-induced dipole and dispersion terms, involving the individual properties of $[\text{Pt}(\text{PH}_3)_3]$ and