Theoretical study of the interaction between Pt(0) and MPH3+ fragments in complexes of the [Pt3 (?-CO)3(PH3)3]-MPH3+ (M = Cu+, Au+, Ag+) type

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Ab initio calculations suggest that a series of complexes of the [Pt3(?-CO)3(PH3)3]-MPH3+ type (M = Cu, Au, Ag) are stable. We have studied these complexes at the HF, MP2, B3LYP, and PBE levels of theory. The magnitude of the interaction energies and Pt3-M distances indicate a substantial covalent character of the bond, the latter being confirmed by orbital diagrams. The chemical bond is sensitive to electron correlation effects. In addition, the Fukui index of nucleophilic attack and electrophilicity index on the metal were used to explore possible sites where chemical reactivity may play a role.