FTIR STUDY OF THE REACTIVITY OF HETERONUCLEAR SMALL TRANSITION METAL CLUSTER WITH CARBON MONOXIDE

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Bimetallic catalysts have attracted great research efforts in the past decades due to their chemical and physical properties different from the individual pure metals and promising applications in chemical conversion, energy technology and environmental protection. Numerous experimental and theoretical investigations have been focused on the reactions of transition metal atoms and small clusters with CO, and a variety of transition-metal carbonyl complexes have been characterized in gas phase and in solid argon. Since they are a very few studies on the transition metal heteronuclear dimer, we have studied in solid argon the reactivity of carbon monoxide with the heterodimer PdTi by infrared spectroscopy (FTIR). Heteronuclear cluster carbonyls, $\mathrm{PdTi(CO)}_n$ (n=1-3) and $\mathrm{Pd_2Ti(CO)_2}$, have been characterized on the basis of the isotopic substitution and irradiation effect. DFT calculations of the geometrical and electronic properties are also presented, and compared with the experimental values. An irradiation in visible leads to conversion between the isomers Pd-Ti-CO and Ti-Pd-CO distinguished by a large shift of the stretching frequency of the diatomic CO.