

INFRARED SPECTRA OF THE Pd_nCO (n=2-5) MOLECULES ISOLATED IN SOLID ARGON AND NEON BETWEEN 100 AND 4000 cm⁻¹

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The Pd+CO reaction has been reinvestigated using deposition of ground state reagents in solid argon and neon and the formation of Pd_nCO (n=2-5) is evidenced by strong absorption in the range 2015-1650 cm⁻¹. Various isotopic data (¹²C/¹³C, ¹⁶O/¹⁸O, natural isotopes for the palladium) and number of two quantum transitions have been measured in the near- and far-infrared regions. In argon, selective irradiation in visible leads to conversion between two Pd₂CO isomers distinguished by the stretching frequency of the diatomic CO: bridged T-shaped (ν_{CO} = 1856 cm⁻¹) and side on (ν_{CO} = 2015 cm⁻¹). DFT calculations of the geometrical and electronic properties of Pd_nCO complexes are also presented and compared to the experimental values.