

THE VIBRATIONAL SPECTRA OF TRANSITION METAL MONOCARBONYLS MOLECULES

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The infrared spectrum of MCO molecules (M=Co, Ni, Pd, Pt, and Cu) isolated in solid argon has been reinvestigated. Various isotopic data ($^{12}\text{C}/^{13}\text{C}$, $^{16}\text{O}/^{18}\text{O}$, natural isotopes for the metal) on ν_1 , ν_2 , ν_3 and number of two quantum transitions have been measured in the near- and far-infrared regions. This enables a complete harmonic force-field calculation based on calculated geometry can be estimated. Comparisons of spectroscopic parameters for the Ni-, Pd-, PtCO and Co-, Ni-, CuCO series, experimental binding energies and the latest ab initio predictions are also presented. The bond force constants can be compared and the results show that the perturbations of the CO ligand are very unreliable indicators of the evolution of the binding energies, contrary to the metal-carbon force constant.