EXPERIMENTAL AND THEORETICAL STUDIES OF $Mn_2(CO)_{10}$

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Ground state resonance Raman spectroscopy, Fenske-Hall molecular orbital calculations, and density functional theory were utilized to study the photochemistry of $Mn_2(CO)_{10}$ in an attemt to understand better the photochemical reaction pathways of dinuclear transition metal organometallic complexes. In this work, resonance enhancement of the e_3 Mn-C-O bending mode, the e_3 C-O stretching vibration and the a_1 Mn-Mn bond stretch are found to play an important role in the resonance Raman spectra of $Mn_2(CO)_{10}$. These data, together with the theoretical calculations, are consistent with the proposal that the photochemical intermediate $Mn_2(CO)_9$ contains a linear semi-bridging CO.