TWO-PHOTON SPECTROSCOPIC STUDY OF QUADRUPLY BONDED DIMERS: EVIDENCE OF ZWITTERIONIC STATES

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Through the use of two-photon spectroscopy it has been possible to locate and identify "hidden" electronic excited states of quadruply bonded metal dimers.[a] The existence of these hidden states and the values of their energies provide information about the electronic character of all of the electronic states of the δ-δ* manifold, which can be described using a model that predicts two pairs of states. The lowest energy pair can be described as diradical states and the highest energy pair can be described as zwitterionic states. The relative disposition within each pair of states can provide valuable information about where a molecule lies on the potential energy surface that describes the electronic overlap.[b] We have obtained two-photon excitation spectra of a series of molecules having the general formula $Mo_2X_4(PMe_3)_4$ (X = Cl, Br, I) and related congeners. The energy gap between the zwitterionic states will be compared with the value obtained for the corresponding diradical states by NMR[c] and SQUID[d] measurements.

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