ANION PHOTOELECTRON SPECTROSCOPY OF Mo-V BINARY TRANSITION METAL SUBOXIDE CLUSTERS

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Vibrationally-resolved photoelectron spectra of molybdenum vanadium oxo cluster anions with 2 to 5 oxygen atoms and measured using 2.33 eV, 3.49 eV and 4.66 eV photon energies generally exhibit broad and overlapping electronic states. The adiabatic electron affinities for the series are 1.68(3) eV, 1.73(3) eV, 2.89(1) eV, and 3.4(1) eV for two through five oxygen atoms, respectively. Vibrational structure observed in the spectra can be reconciled with the lowest energy structural isomers of the anions determined in DFT calculations: The lowest energy isomers have low symmetry, with the Mo center in a higher oxidation state than the V center, and high spin states are favored.