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On the reactivity of neutral metal oxide clusters in the gas phase: Detection through 118 nm single photon ionization SHENG-GUI HE, YAN XIE, ELLIOT BERNSTEIN, Department of Chemistry, Colorado State University — Single photon ionization by a vacuum ultra-violet (VUV, 118 nm) laser is successfully employed for the study of reactions of *neutral* metal oxide clusters (Ti_mO_n, Fe_mO_n, Co_mO_n) with various simple molecules (CO, NO, SO_2, H_2O) in the gas phase. Neutral clusters are generated by reaction of laser ablation generated metal plasma with O_2 in a supersonic expansion. Clusters are reacted with reactant gases in a flow tube reactor. Detection of neutral clusters and products is through ionization with 118 nm laser radiation and time of flight mass spectroscopy. Rich neutral cluster chemistry is observed: (1) Ti_mO_{2m} and Ti_mO_{2m+1} absorb one or more H_2O molecules for $m \geq 2$ and $m \geq 1$, respectively; (2) FeO_2, FeO_3, and possibly FeO are reactive with CO while Fe_2O_4 and Fe_2O_5 are less reactive; (3) Fe_2O_5 is reactive with NO and SO_2, but FeO_2 is much less reactive with them; and (4) small Co_mO_n clusters ($m \leq 4$ and $n \leq 6$) are more reactive than large clusters ($6 \leq m \leq 12$ and $8 \leq n \leq 17$) with CO, and among these small clusters, Co_3O_4 is particularly reactive. A detailed quantum chemistry study of Fe_mO_n reactions with CO is in progress. Preliminary calculations indicate that reactions of FeO and FeO_2 with CO to produce CO_2 are overall barrierless, in agreement with the experimental observations.

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