VIBRATIONAL SPECTROSCOPY OF BINARY METAL OXIDE CLUSTERS

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Cerium oxide is one of the most reactive rare earth metal oxides and is commonly used as a support material for metals and metal oxides in heterogeneous catalysis. In many cases it is not chemically inert, but directly participates in the catalytic process. The well-known difficulty of quantum chemical approaches for f-element containing molecules remains unresolved. In order to investigate the electronic and geometric structure and deliver benchmark vibrational frequencies for testing the accuracy of density functional theory calculations, infrared photodissociation spectra of rare gas tagged binary $(CeO_2)(VO_2)^+$, $(CeO_2)(VO_2)_2^+$ and $(Ce_2O_3)(VO_2)^+$ clusters are measured in the 400 to 1200 wave number range. The first cluster contains no electron in either the Ce-f or V-d orbitals. As the number of valence electrons is increased, the question arises, which orbital the additional electrons prefers, i.e., which atom is preferentially reduced. The present results are compared to the previously determined structures of the respective monometalic oxide clusters.