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CO Oxidation on Copper Oxide Cluster Ions
MASAHIKO ICHIHASHI, Toyota Technological Institute, SHINICHI HIRABAYASHI, Genesis Research Institute, Inc., YOSHIYUKI KAWAZOE, Tohoku University — We investigated the reaction of CO and O_2 on size-selected copper cluster ions, Cu_n^+ (n=4–18) and Cu_n^- (n=4–11), by use of a tandem mass-spectrometer equipped with octopole ion guides. A coadsorbing product, $Cu_nO_2(CO)^+$, was observed in the reaction of $Cu_nO_2^+$ with CO, and it was found that CO adsorbs onto $Cu_nO_2^+$ more efficiently than onto Cu_n^+ in $n \geq 9$. This shows the cooperative coadsorption of O_2 and CO. On the other hand, in the reaction of $Cu_nO_2^-$ with CO, a reduced product, Cu_nO^-, was obtained instead of the coadsorbing product, $Cu_nO_2(CO)^-$. In particular, $Cu_5O_2^-$ and $Cu_9O_2^-$ have relatively high efficiency for the production of Cu_nO^-. This result suggests the production of CO_2 by the oxidation of CO on $Cu_nO_2^-$. The DFT calculation indicates that the activation energy in the reaction of $Cu_5O_2(CO)^- \rightarrow Cu_5O(CO_2)^-$ is only 0.79 eV while that of the corresponding cation is 1.79 eV. The structure of Cu_n^- is more flexible than that of Cu_n^+ probably because of its excess electron. It is concluded that the stabilization of the transition state and the decrease of the activation energy make the CO oxidation proceed on $Cu_nO_2^-$.

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