Structures of scandium oxide cluster cations studied by ion mobility-mass spectrometry

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Scandium oxide nanostructures can be used as catalysts in some reactions, such as the selective reduction of nitric oxides with methane.[1] In previous studies, theoretical calculations have been performed to calculate the structures and properties of scandium oxide clusters Sc_nO_m with small numbers of n (n = 1-3).[2] However, experiments and theoretical calculations on scandium oxide cluster cations are rarely reported. In order to study the stable components of scandium oxide cluster cations ($Sc_nO_m^+$, n = 3-8) and their structures, ion mobility-mass spectrometry (IM-MS) experiments and quantum chemical calculations have been performed. Collision induced dissociation (CID) in the ion drift tube for ion mobility measurement indicated that the most stable components of $Sc_nO_m^+$ have the stoichiometric composition of $ScO(Sc_2O_3)_x^+$. The experimental values of collision cross sections (CCSs) of each component of $Sc_nO_m^+$ with He buffer gas have been derived from the arrival time distributions of the IM-MS experiments. The structures and CCSs of the observed stable components have also been obtained by applying quantum chemical calculations using the Gaussian 16 and MOBCAL programs, and their CCSs have been compared with the experimental values. For $Sc_nO_m^+$ with n = 5-8, similar structures of $Sc_nO_{m+1}^+$ clusters with one more oxygen atom than $Sc_nO_m^+$ clusters have been obtained for $Sc_nO_m^+$ clusters of $ScO(Sc_2O_3)_x^+$ and $(Sc_2O_3)_x^+$. In addition, for $Sc_nO_m^+$ with n = 4-7, the energetically stable components contain $Sc_3O_4^+$-like units as shown in Fig. 1. Both features may be caused by a sequence of oxidations from smaller sized clusters.

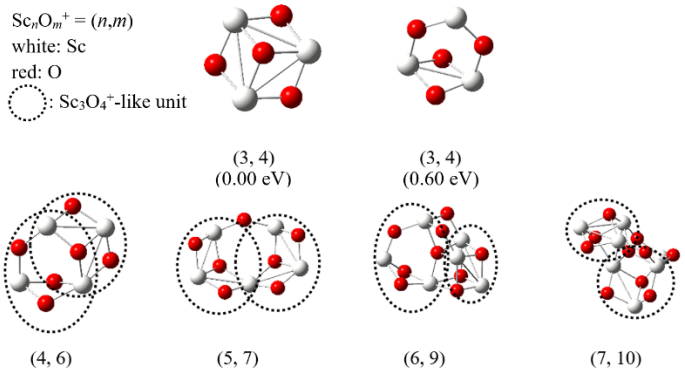

Fig. 1 Structures of $Sc_3O_4^+$ clusters and some larger clusters with $Sc_3O_4^+$-like units

1) M. Fokema, and J. Ying, *Applied Catalysis B: Environmental*, **18**, 71 (1998).

2) Y. Yang, H. Liu, and P. Zhang, *Phys. Rev. B*, **84**, 205430 (2011).