Supplementary Information

Compositions and structures of niobium oxide cluster ions, $Nb_mO_n^{\pm}$, (m = 2−12) revealed with ion mobility mass spectrometry

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Section S1. Comparison of Experimental CCSs under different *E*/*N* conditions

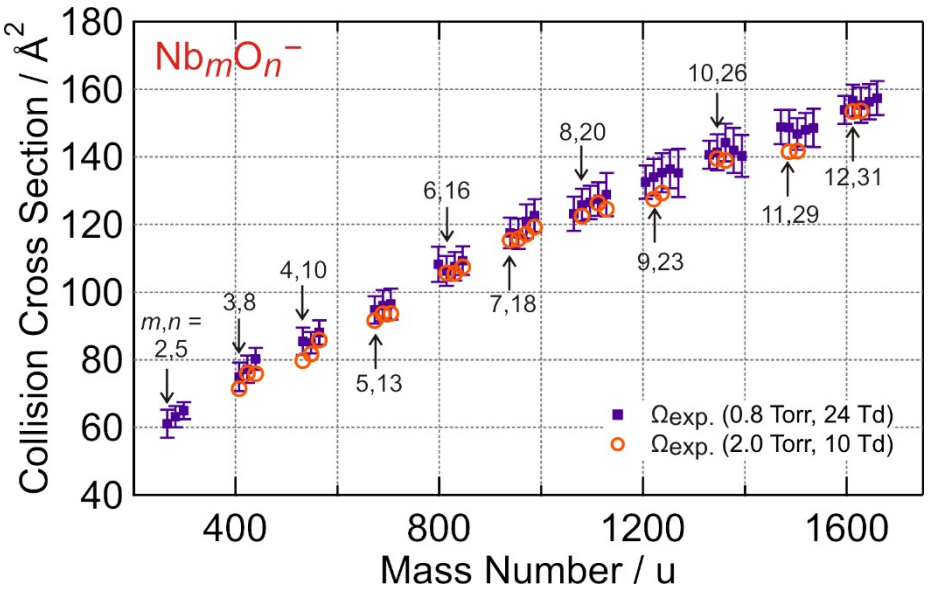

Figure S1. Experimental CCSs (Ω_{exp}) of niobium oxide cluster anions $Nb_mO_n^-$ obtained by ion mobility experiments under two different *E*/*N* conditions of 24 Td (purple squares) and 10 Td (red open circles). The two sets of CCSs shared the same experimental conditions such as injection energy of 50 eV, 180 K cell temperature, and 10 V/cm electrostatic field.

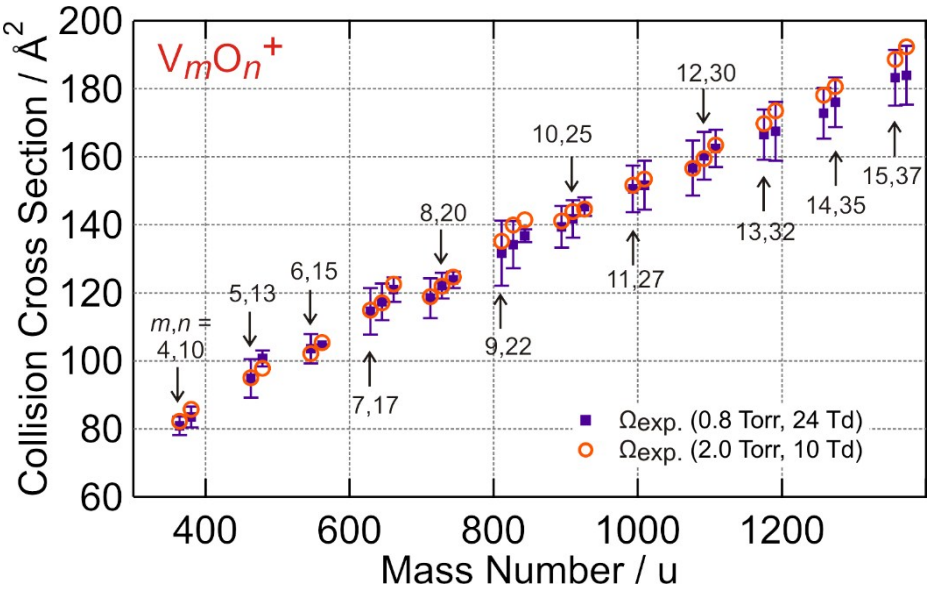

Figure S2. Experimental CCSs (Ω_{exp}) of vanadium oxide cluster cations $V_mO_n^+$ obtained by ion mobility experiments under two different *E*/*N* conditions of 24 Td (purple squares) and 10 Td (red open circles). The two sets of CCSs shared the same experimental conditions such as injection energy of 50 eV, 185 K cell temperature, and 10 V/cm electrostatic field. Part of the experimental CCSs taken under 24 Td (purple squares) were already reported in our past studies.[37,38]

Section S2. Mass and 2D Spectra of Niobium Oxide Cluster Ions

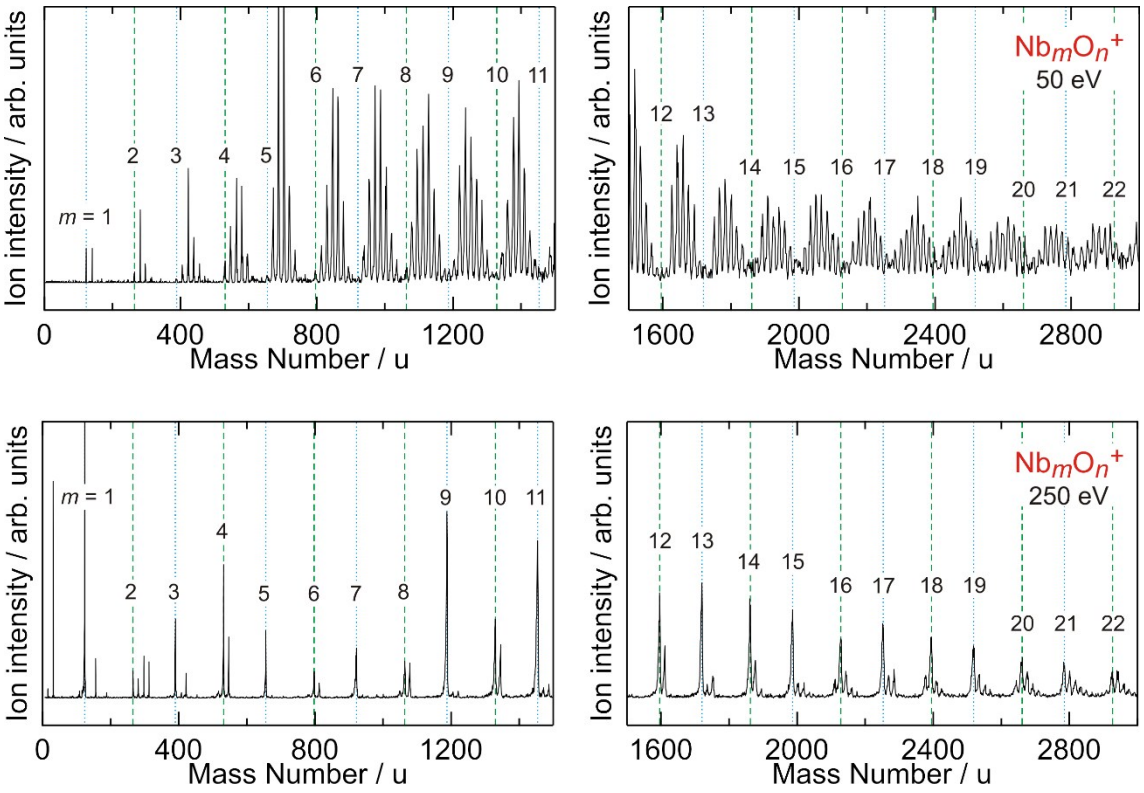

Figure S3. Mass spectra of $Nb_mO_n^+$ taken under injection energy of 50 eV shown in top two panels and 250 eV shown in bottom two panels. Experimental conditions such as cell temperature of 180 K, buffer gas pressure of 0.8 Torr, and oxygen carrier gas concentration of 10 % were kept constant for all data sets. The green dashed lines represent stable species with even number of niobium atom such as $(Nb_2O_5)_{m/2}^+$, and blue dotted lines represent stable species with odd number of niobium atoms such as $(NbO_2)(Nb_2O_5)_{(m-1)/2}^+$.

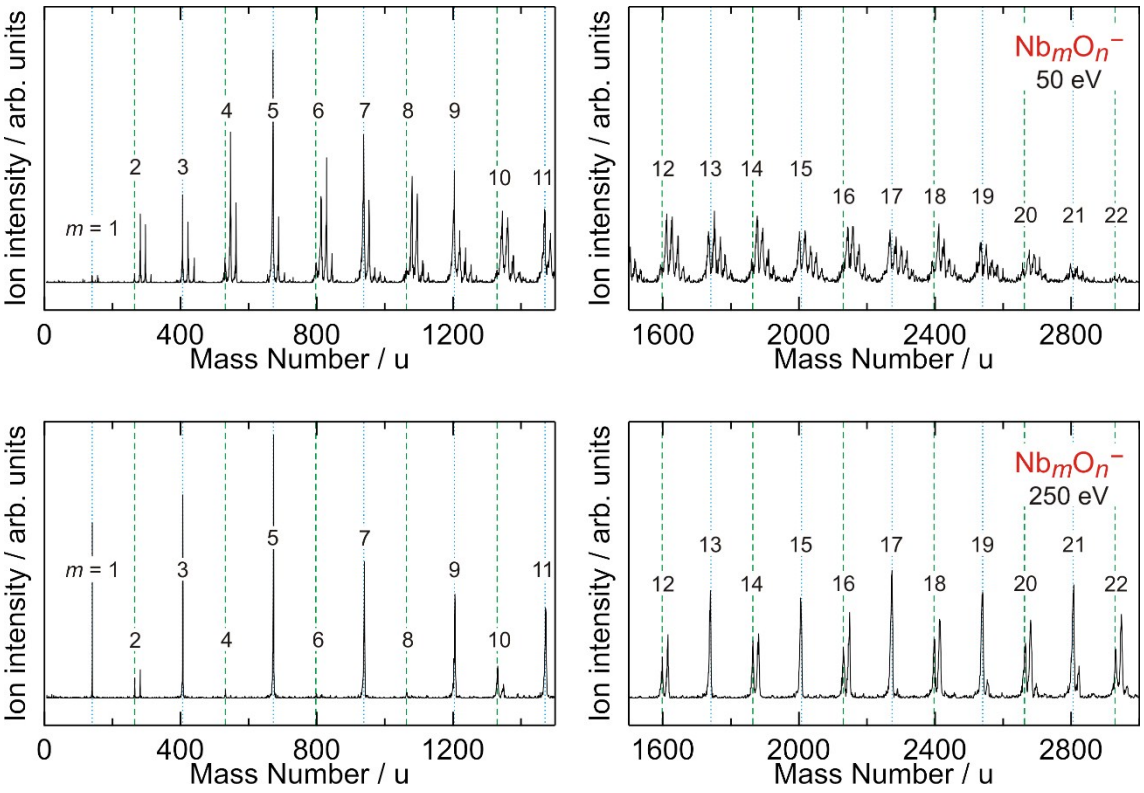

Figure S4. Mass spectra of $Nb_mO_n^-$ taken under injection energy of 50 eV shown in top two panels and 250 eV shown in bottom two panels. Experimental conditions such as cell temperature of 180 K, buffer gas pressure of 0.8 Torr, and oxygen carrier gas concentration of 10 % were kept constant for all data sets. The green dashed lines represent stable species with even number of niobium atom such as $(Nb_2O_5)_{m/2}^-$, and blue dotted lines represent stable species with odd number of niobium atoms such as $(NbO_3)(Nb_2O_5)_{(m-1)/2}^-$.

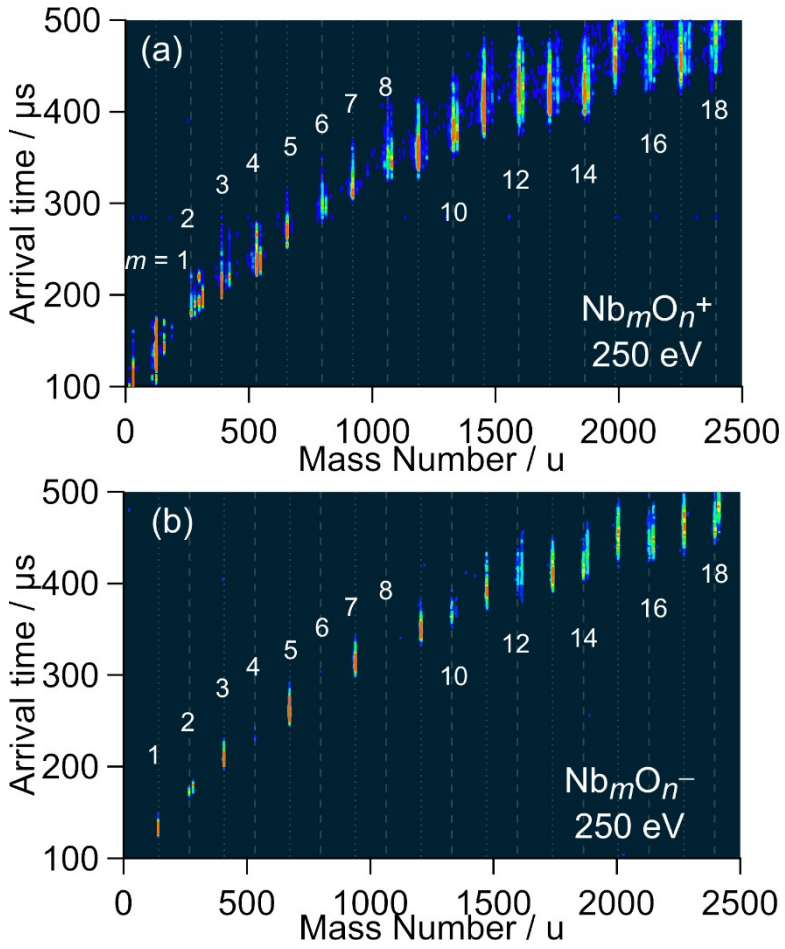

Figure S5. Arrival time vs. mass number 2D spectra taken under injection energy of 250 eV for niobium oxide cluster (a) cations and (b) anions. These 2D spectra correspond to the mass spectra shown in Figure 1c and 1d.

Section S3. Details on Calculation Results

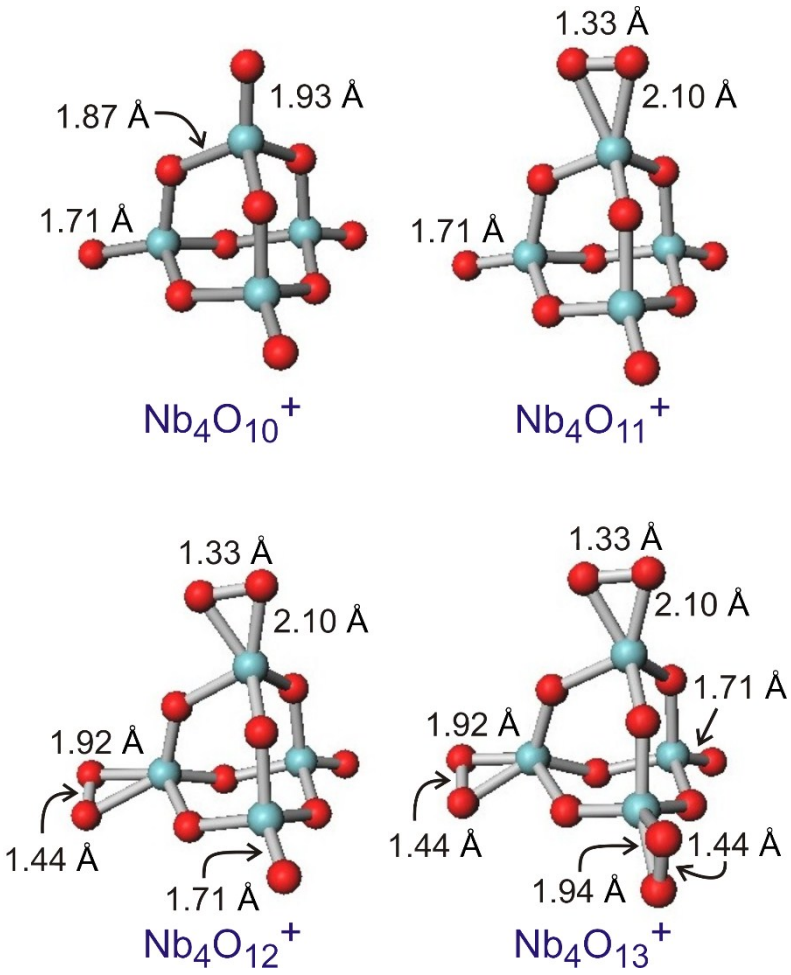

Figure S6. Specific bond lengths labeled for $Nb_4O_{10\text{-}13}^+$, including terminal and bridging Nb-O bonds. The O-O bonds on the terminal are also labeled.