

Supporting Information for:

“An Experimental and Theoretical Investigation of the Charge Separation Energies of Hydrated Zinc (II): Redefinition of the Critical Size” by Theresa Cooper and P. B. Armentrout

Figure Captions:

Figure S1. Zero pressure extrapolated cross sections for the CID of $\text{Zn}^{2+}(\text{H}_2\text{O})_8$ with Xe. Solid lines show the best fit to both the primary and secondary water loss and the competing charge separation product ion using eq 3 convoluted over the kinetic and internal energy distributions of the neutral and ion i.e. reactants. Dashed lines show the models in the absence of experimental kinetic energy broadening for reactants with an internal energy of 0 K.

Figure S2: Optimized GSs of the $n = 5$ and 8 charge separation products $\text{ZnOH}^+(\text{H}_2\text{O})_m + \text{H}^+(\text{H}_2\text{O})_{n-m-1}$, where $m = 2$ and 4 and $n-m-1 = 2$ and 3 for parts a and b, respectively, calculated at the B3LYP/6-311+G(d,p) level of theory.

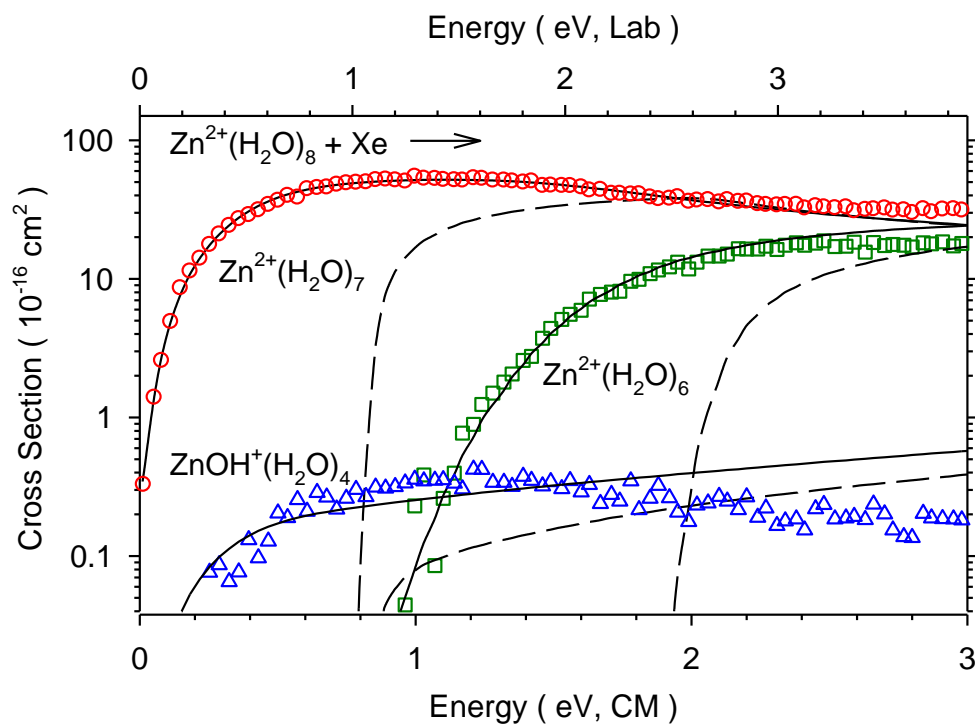
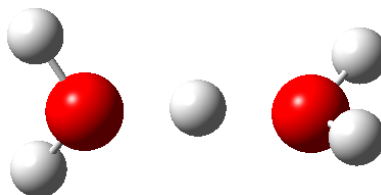
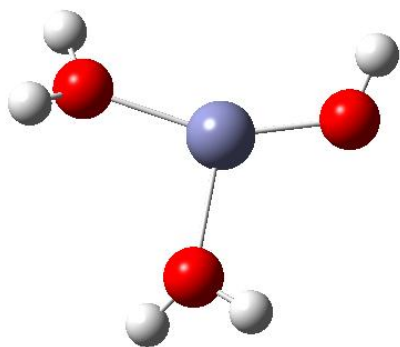


Figure S1

a)



b)

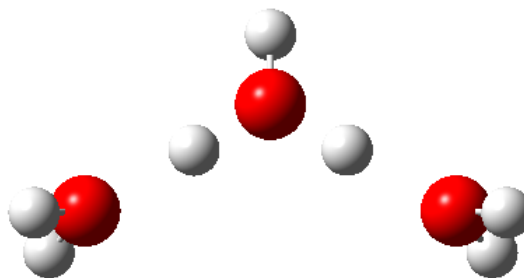
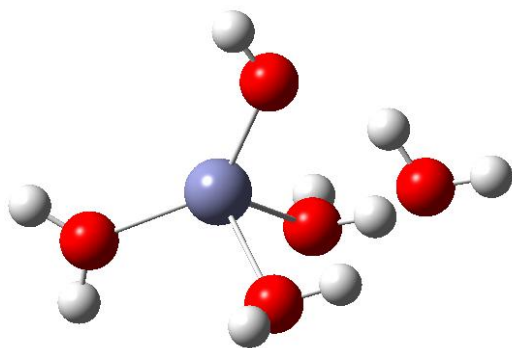


Figure S2