Supplementary Information: Mg(II) and Ca(II) Microsolvation by Ammonia: Born-Oppenheimer Molecular Dynamics Studies

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Figure S 1: Evolution of the total potential energy (a.u) as a function of time (fs) for the \([\text{Ca(NH}_3\text{)}_{27}]^{2+}\) at 300 K (top left), \([\text{Ca(NH}_3\text{)}_{27}]^{2+}\) at 220 K (top right), \([\text{Ca(NH}_3\text{)}_{20}]^{2+}\) at 3000 K (middle), \([\text{Mg(NH}_3\text{)}_{27}]^{2+}\) at 220 K systems (bottom left) and \([\text{Mg(NH}_3\text{)}_{20}]^{2+}\) at 220 K (bottom right) cluster systems. A slope of the linear fit of the order of \(10^{-7}\) was found for all the BOMD simulations done in this work.
Figure S 2: Average cation-N distance in $[\text{Mg(NH}_3\text{)}_n]^{2+}$ (top) and $[\text{Ca(NH}_3\text{)}_n]^{2+}$ (bottom) clusters. There are two types of possible coordination structures for $[\text{Ca(NH}_3\text{)}_8]^{2+}$, the 6+2 and 8+0 coordination, only the values for the former were plotted.
Figure S 3: Binding energies per ammonia molecule of the optimal \([\text{Mg(NH}_3\text{)}_n]^{2+}\) (top) and \([\text{Ca(NH}_3\text{)}_n]^{2+}\) (bottom) clusters. There are two types of possible coordination structures for \([\text{Ca(NH}_3\text{)}_8]^{2+}\), the 6+2 and 8+0 coordination, only the values for the former were plotted.
Figure S 4: Binding energies per ammonia molecule of the optimal \([\text{Mg(NH}_3\text{)}_n]^{2+}\) (top) and \([\text{Ca(NH}_3\text{)}_n]^{2+}\) (bottom) clusters with their respective analytical curve fitting (see main text).