

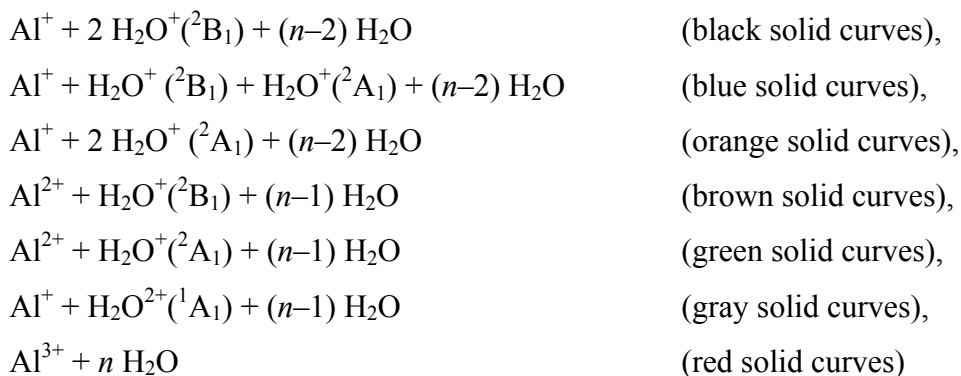
Supporting Information

Elucidating the mechanism behind the stabilization of multi-charged metal cations in water: A case study of the electronic states of microhydrated Mg^{2+} , Ca^{2+} and Al^{3+}

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Figures S1-S4. The $[\text{Al} - (\text{H}_2\text{O})_n]^{3+}$, $n=2, 4, 5, 6$ PECs of the singlet electronic states of ^1A symmetry as a function of the $R(\text{Al}-\text{O})$ distance for the approach of the water molecules to the metal center. The states arising from the various adiabatic fragments viz.



are shown. The black dashed line denotes the reference energy of the $\text{Al}^+ + 2 \text{H}_2\text{O}^+(^2\text{B}_1) + (n-2) \text{H}_2\text{O}$ asymptotic limit, while the red dashed line the one for $\text{Al}^{3+} + n \text{H}_2\text{O}$.

