Electronic supplementary information

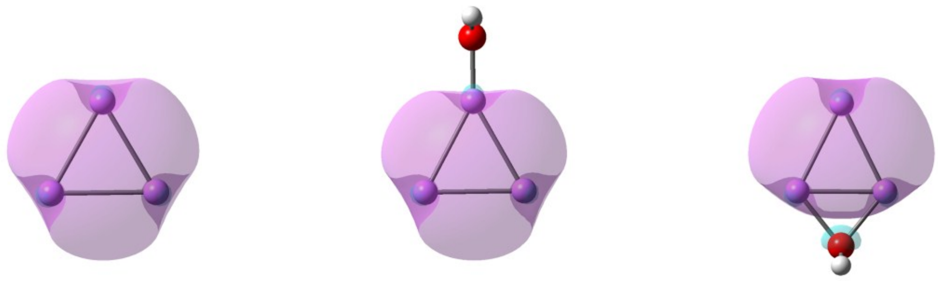
Hydration effect on electronic structure and stability of superalkali cation Li_3^+

Jia-Huan Hou, Di Wu, Jia-Yuan Liu, Si-Yi Li, Dan Yu, Ying Li*

Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, P. R. China

* Corresponding author.

Email address: liyingedu@jlu.edu.cn



$Li_3^+(D_{3h})$ I-1(C_{2v}) I-2(C_{2v})

Fig. S1 The highest occupied molecular orbitals (HOMOs) of Li_3^+ and $Li_3^+(H_2O)$.

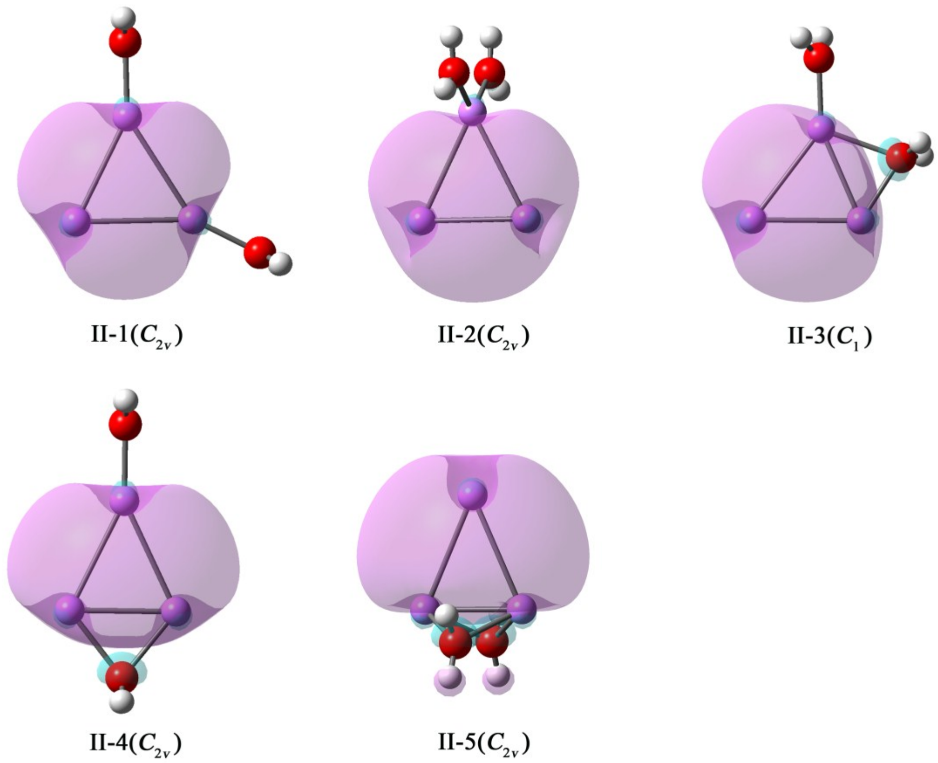


Fig. S2 The highest occupied molecular orbitals (HOMOs) of $Li_3^+(H_2O)_2$.

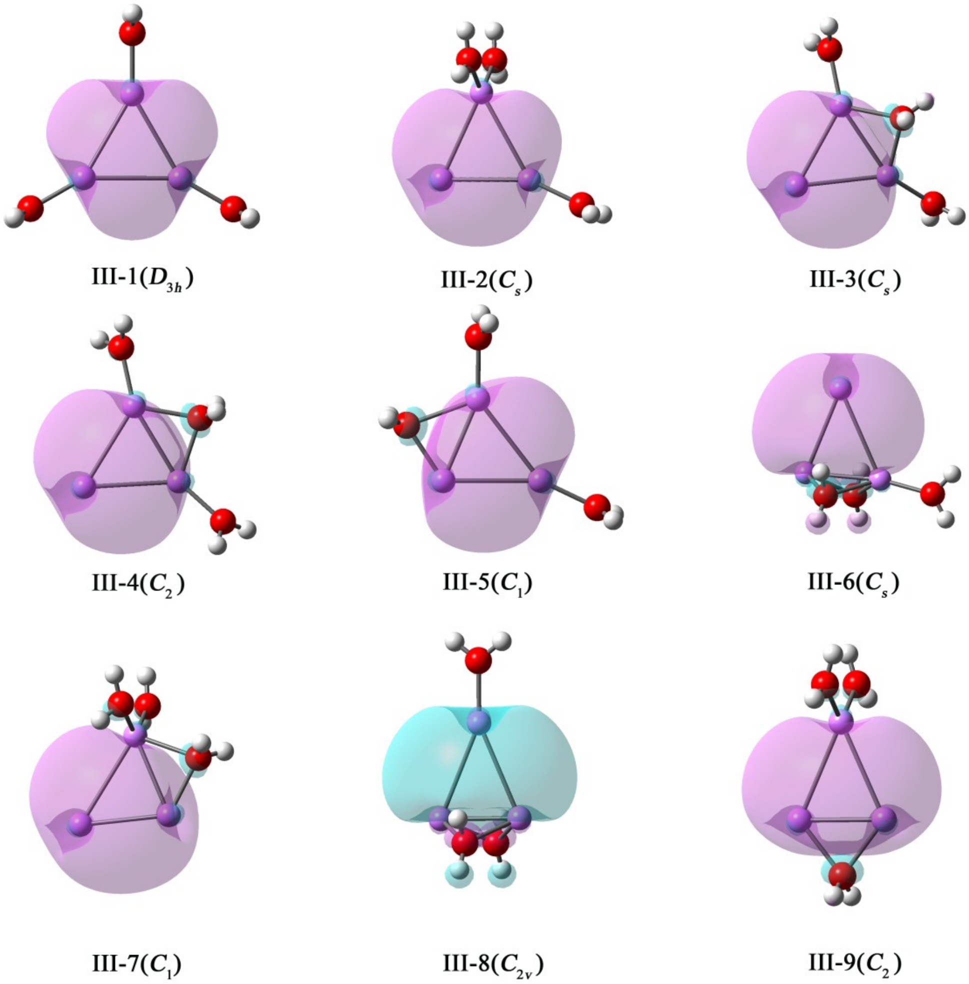


Fig. S3 The highest occupied molecular orbitals (HOMOs) of $Li_3^+(H_2O)_3$.

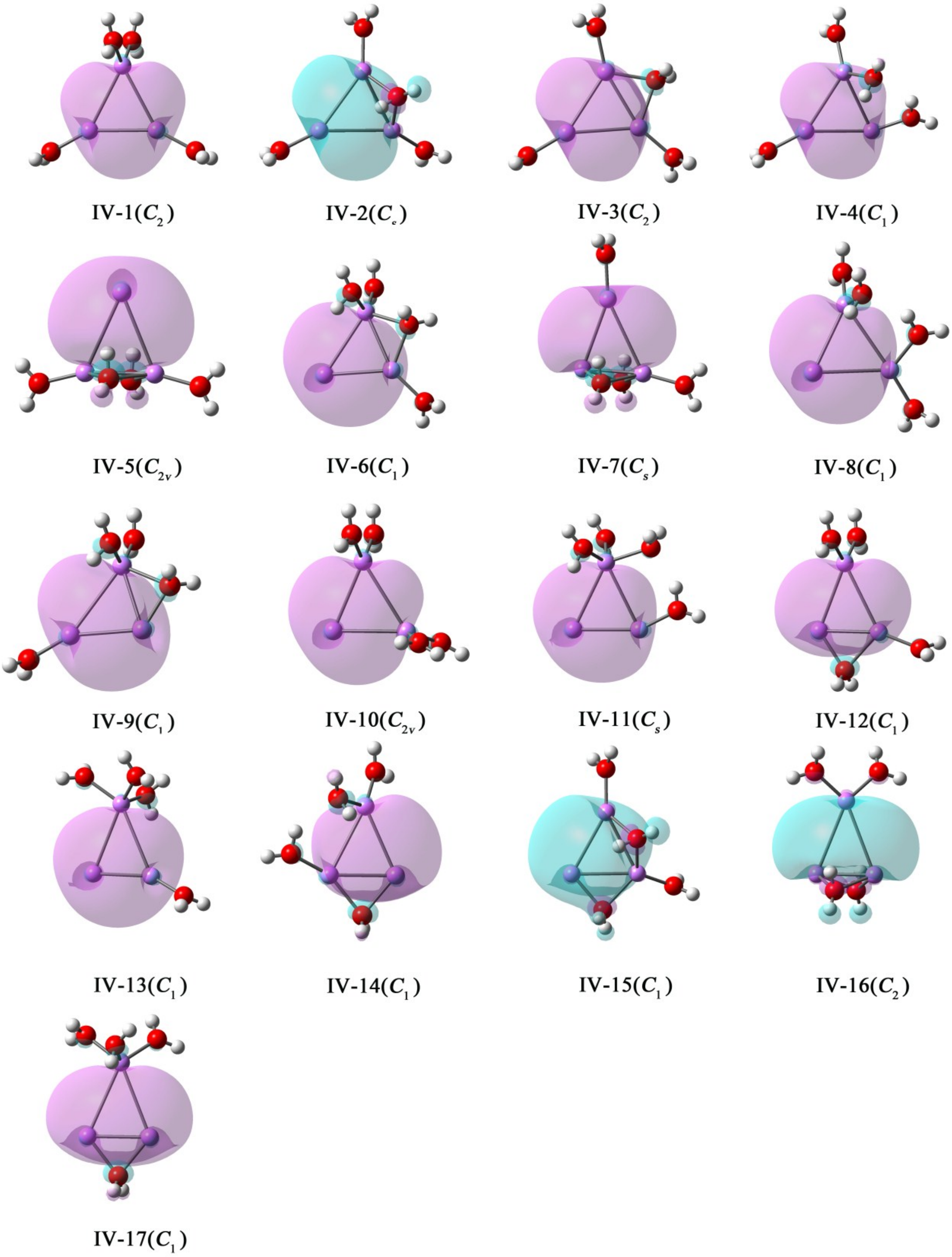


Fig. S4 The highest occupied molecular orbitals (HOMOs) of $Li_3^+(H_2O)_4$.

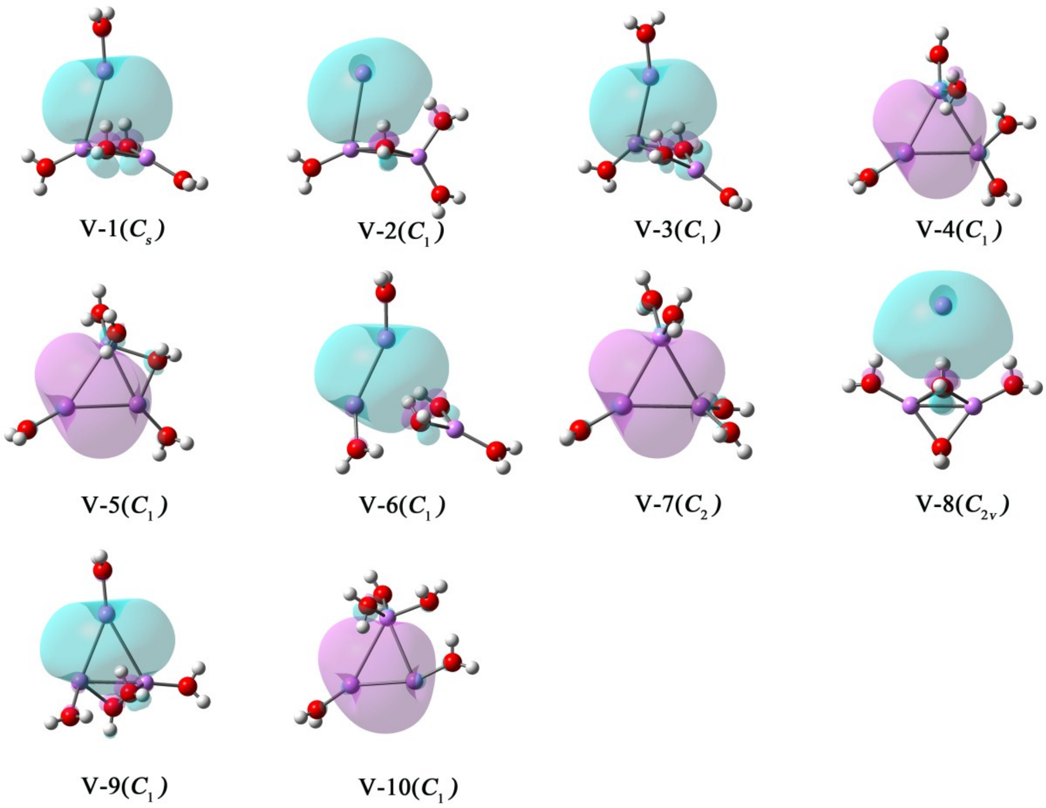


Fig. S5 The highest occupied molecular orbitals (HOMOs) of $Li_3^+(H_2O)_5$.

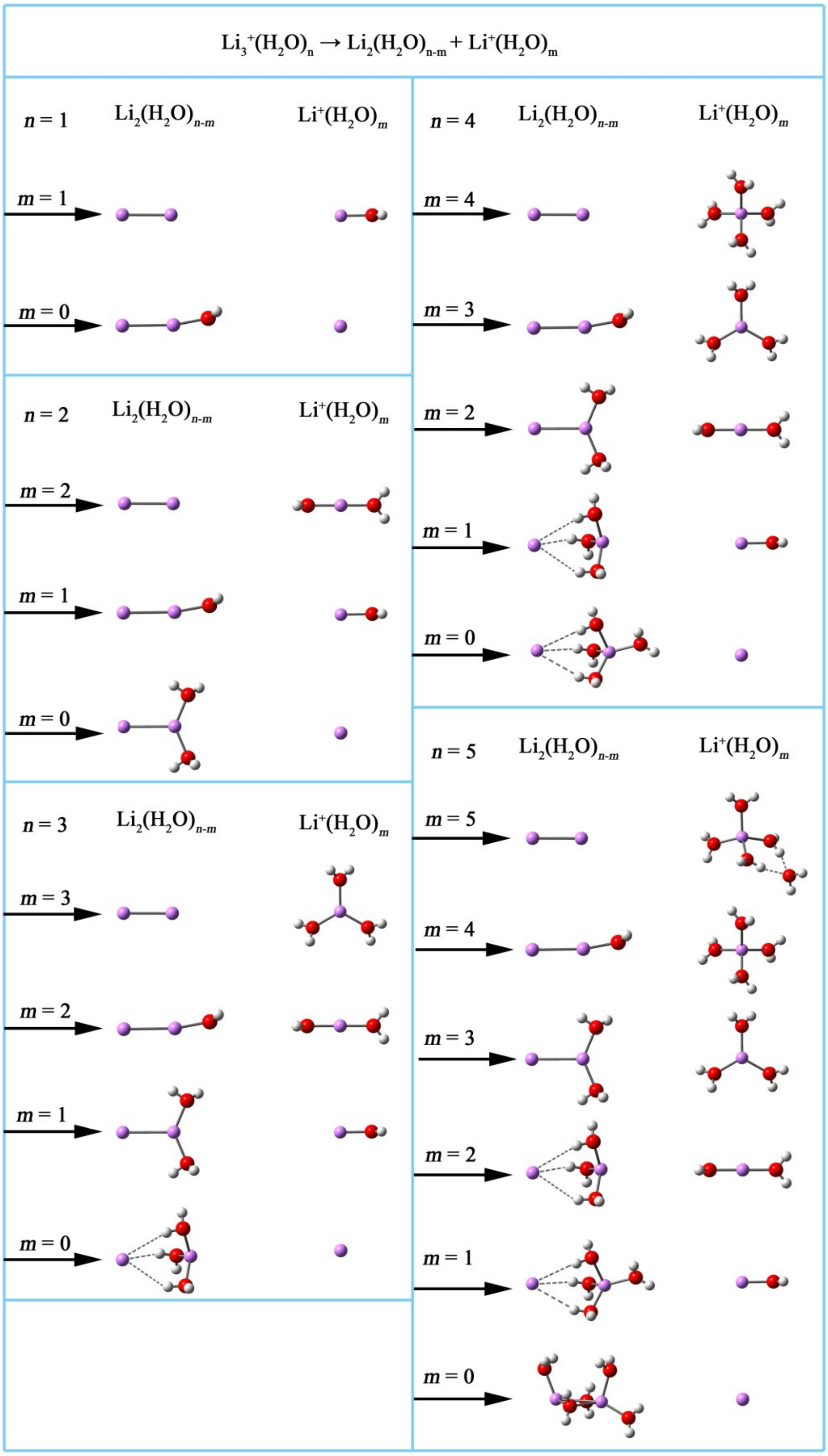


Fig. S6 Equilibrium structures of the products for the $Li_3^+(H_2O)_n \rightarrow Li_2(H_2O)_{n-m} + Li^+(H_2O)_m$ reaction (channel 1).

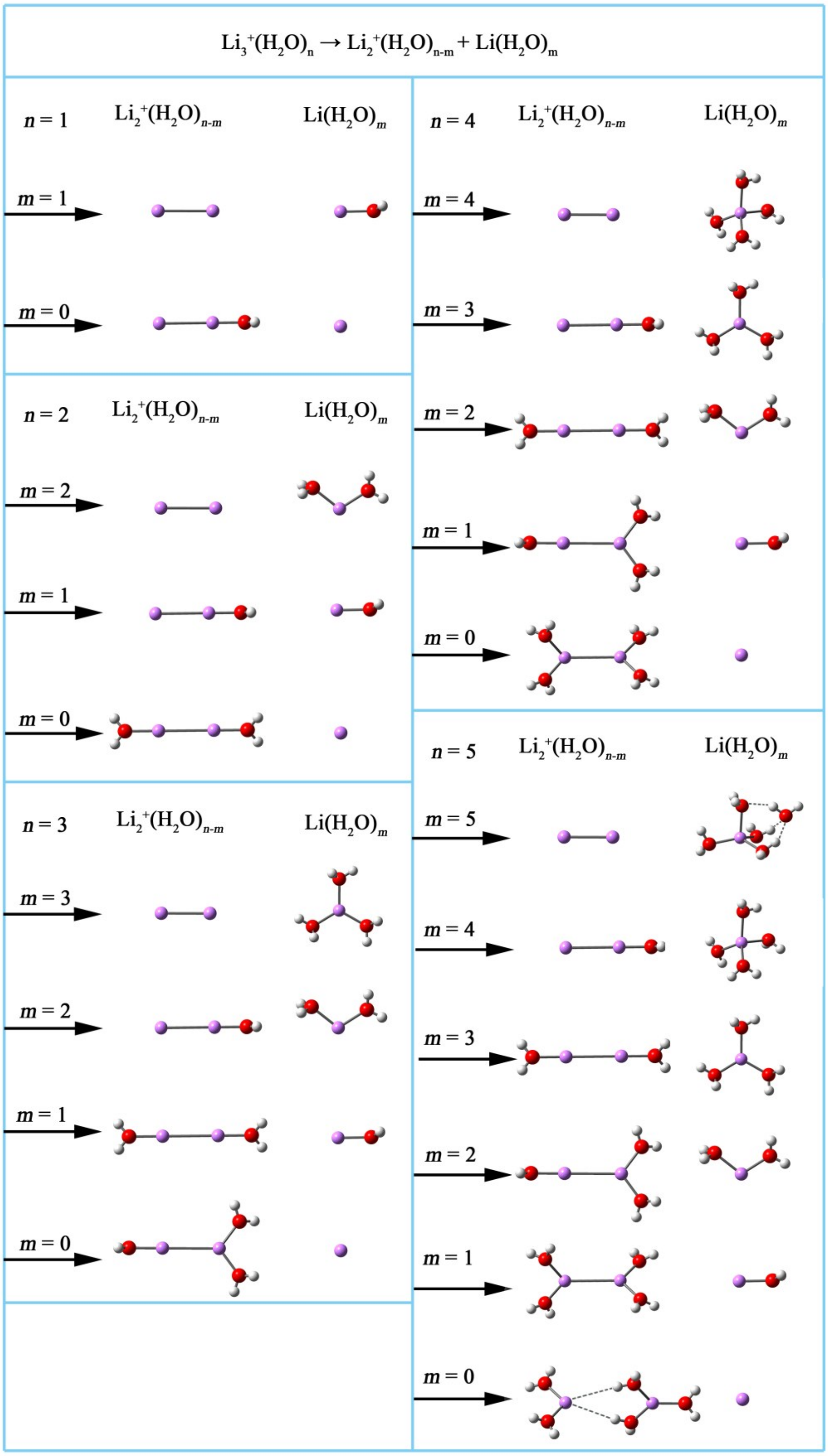


Fig. S7 Equilibrium structures of the products for the $Li_3^+(H_2O)_n \rightarrow Li_2^+(H_2O)_{n-m} + Li(H_2O)_m$ reaction (channel 2).

Table S1 NPA charges on the three Li atoms (Q_1, Q_2, Q_3, in |e|), total NPA charge on Li_3^+ (Q_{tot}, in |e|), the average Li-O distances when the H_2O molecules occupy on-top ($T_{Li\text{-}O}$) and bridge ($B_{Li\text{-}O}$) sites, respectively, and the VEA values of low-lying isomers of the $Li_3^+(H_2O)_n$ (n = 1-4) clusters.

isomer	Q_1	Q_2	Q_3	Q_{tot}	VEA (eV)	$T_{Li\text{-}O}$ (Å)	$B_{Li\text{-}O}$ (Å)
I-2	0.316	0.316	0.316	0.948	3.313	—	2.139
II-2	0.355	0.267	0.267	0.889	2.937	1.925	—
II-3	0.293	0.290	0.299	0.882	3.088	1.924	2.171
II-4	0.280	0.323	0.323	0.926	2.955	1.911	2.136
II-5	0.233	0.342	0.342	0.917	3.087	—	2.089
III-2	0.351	0.258	0.232	0.841	2.498	1.923	—
III-3	0.286	0.286	0.243	0.815	2.528	1.925	2.125
III-4	0.285	0.285	0.243	0.813	2.586	1.929	2.132
III-5	0.302	0.261	0.276	0.839	2.579	1.923	2.322
III-6	0.149	0.357	0.305	0.811	2.832	1.917	2.078
III-7	0.324	0.263	0.215	0.802	2.678	1.951	2.124
III-8	0.196	0.327	0.327	0.850	2.781	1.917	2.075
III-9	0.309	0.270	0.270	0.849	2.758	1.935	2.125
IV-2	0.322	0.322	0.183	0.827	2.244	1.917	2.067
IV-3	0.266	0.266	0.238	0.770	2.371	1.931	2.128
IV-4	0.299	0.311	0.191	0.801	2.420	1.936	—
IV-5	-0.007	0.428	0.428	0.849	2.594	1.916	2.047
IV-6	0.306	0.299	0.134	0.739	2.642	1.953	2.109
IV-7	0.107	0.407	0.308	0.822	2.107	1.919	2.054
IV-8	0.278	0.381	0.138	0.797	2.493	1.946	—
IV-9	0.328	0.248	0.187	0.763	2.604	1.944	2.124
IV-10	0.336	0.336	0.113	0.785	2.270	1.933	—
IV-11	0.316	0.312	0.143	0.771	2.620	1.980	—
IV-12	0.289	0.185	0.312	0.786	2.497	1.932	2.140
IV-13	0.405	0.205	0.164	0.774	2.366	1.964	—
IV-14	0.269	0.373	0.157	0.799	2.391	1.944	2.139
IV-15	0.300	0.346	0.173	0.819	2.621	1.922	2.119
IV-16	0.226	0.296	0.296	0.818	2.619	1.949	2.058
IV-17	0.362	0.205	0.219	0.786	2.745	1.981	2.105