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Supporting Information

Microsolvation of $LiBO_2$ in Water: Anion Photoelectron Spectroscopy and *ab initio* Calculations

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Table S1 Relative energies of the low energy isomers of $LiBO_2(H_2O)_n^-$ (n = 0-5) as well as the comparison of their theoretical VDEs and ADEs based on wB97XD to the experimental measurements. All energies are in eV.

Isomer		ΔE	ADE		VDE	
			Theo.	Expt.	Theo.	Expt.
$LiBO_2^-$	0A'	0.00	0.89	0.81	0.92	0.83
$LiBO_2(H_2O)^-$	1A'	0.00	0.44	0.46	0.46	0.53
	1B'	0.04	0.71	0.71	0.69	0.74
	1C'	0.21	1.04		1.09	
	1D'	0.32	0.29		0.38	
$LiBO_2(H_2O)_2^-$	2A'	0.00	0.45	0.80	0.86	0.86
	2B'	0.10	0.41	0.47	0.39	0.55
	2C'	0.39	0.29		0.40	
	2D'	0.40	0.81		0.80	
	2E'	0.42	0.45		0.72	
	2F'	0.45	0.21		0.28	
	2G'	0.55	0.13		0.48	
	2H'	0.58	0.29		0.71	
	2I'	0.59	0.07		1.24	
	2J'	0.60	0.06		0.63	
$LiBO_2(H_2O)_3^-$	3A'	0.00	0.19	0.38	0.44	0.50
	3B'	0.02	0.20		0.64	
	3C'	0.15	-0.06		0.18	
	3D'	0.35	-0.10		1.19	
	3E'	0.41	0.23		0.37	
	3F'	0.50	0.23		0.50	
	3G'	0.54	0.19		0.63	
	3H'	0.58	0.09	0.73	0.76	0.92
	3I'	0.61	0.03		0.85	
$LiBO_2(H_2O)_4^-$	4A'	0.00	0.25	0.42	0.47	0.57
	4B'	0.44	-0.29		0.49	
	4C'	0.61	0.21		0.37	
	4D'	0.63	0.03		0.09	
	4E'	0.64	0.20		0.34	
	4F'	0.70	0.06		0.55	
	4G'	0.74	0.13		0.63	
	4H'	0.75	0.04		0.85	
	4I'	0.75	0.37		0.59	
	4J'	0.75	0.65	0.74	0.73	0.79
	4K'	0.77	0.41		0.76	
	4L'	0.79	0.27		0.59	
	4M'	0.86	0.21		0.32	
$LiBO_2(H_2O)_5^-$	5A'	0.00	-0.11	0.33	0.38	0.55
	5B'	0.32	0.27		0.63	
	5C'	0.41	0.26		0.40	
	5D'	0.43	0.23		0.52	
	5E'	0.46	0.11		0.23	
	5F'	0.46	0.03		0.12	
	5G'	0.47	0.26		0.40	
	5H'	0.54	-0.06		0.60	
	5I'	0.57	0.07		0.64	
	5J'	0.58	-0.09		0.93	
	5K'	0.58	-0.12		0.54	
	5L'	0.59	-0.04		0.88	
	5M'	0.62	-0.13		0.43	
	5N'	0.63	-0.03		0.77	
	5O'	0.65	0.13		1.08	

Table S2 Relative energies of the low energy isomers of $LiBO_2(H_2O)_n^-$ (n = 0-5) as well as the comparison of their theoretical VDEs and ADEs based on CCSD(T) // B3LYP/6-311++G(d,p) to the experimental measurements. All energies are in eV.

Isomer		ΔE	ADE		VDE	
			Theo.	Expt.	Theo.	Expt.
$LiBO_2^-$	0A	0.00	0.85	0.83	0.86	0.83
$LiBO_2(H_2O)^-$	1A	0.00	0.72	0.71	0.69	0.74
	1B	0.13	0.42	0.46	0.43	0.53
	1C	0.26	0.34		0.40	
	1D	0.28	0.99		1.04	
$LiBO_2(H_2O)_2^-$	2A	0.00	0.43	0.47	0.40	0.55
	2B	0.01	0.48	0.80	0.83	0.86
	2C	0.12	0.35		0.42	
	2D	0.14	0.51		0.67	
	2E	0.23	0.81		0.81	
	2F	0.28	0.25		0.29	
	2G	0.39	0.35		0.49	
	2H	0.40	0.12		0.61	
	2I	0.45	0.56		0.69	
$LiBO_2(H_2O)_3^-$	3A	0.00	0.31	0.38	0.65	0.50
	3B	0.21	0.29		0.40	
	3C	0.24	-0.16		0.39	
	3D	0.30	0.47		0.53	
	3E	0.37	0.72	0.73	0.72	0.92
	3F	0.38	0.64		0.61	
	3G	0.40	0.10		0.78	
$LiBO_2(H_2O)_4^-$	4A	0.00	0.46	0.42	0.50	0.57
	4B	0.42	0.30		0.38	
	4C	0.47	0.27		0.40	
	4D	0.49	0.09		0.12	
	4E	0.50	0.38		0.64	
	4F	0.50	0.01		0.54	
	4G	0.54	0.50	0.74	0.76	0.79
	4H	0.58	0.20		0.61	
	4I	0.60	0.19		0.64	
	4J	0.60	0.13		0.82	
	4K	0.63	0.69		0.74	
	4L	0.63	0.32		0.57	
	4M	0.89	0.19		0.23	
$LiBO_2(H_2O)_5^-$	5A	0.00	0.17	0.33	0.58	0.56
	5B	0.18	0.02		0.41	
	5C	0.41	0.23		0.29	
	5D	0.48	0.45		0.50	
	5E	0.53	0.11		0.18	
	5F	0.53	0.34		0.49	
	5G	0.55	0.12		0.78	
	5H	0.55	0.16		0.69	
	5I	0.56	0.09		0.81	
	5J	0.57	0.35		0.44	
	5K	0.57	0.09		0.88	
	5L	0.57	0.18		0.71	
	5M	0.59	0.04		0.62	
	5N	0.60	0.27		0.40	
	5O	0.61	0.28		1.01	

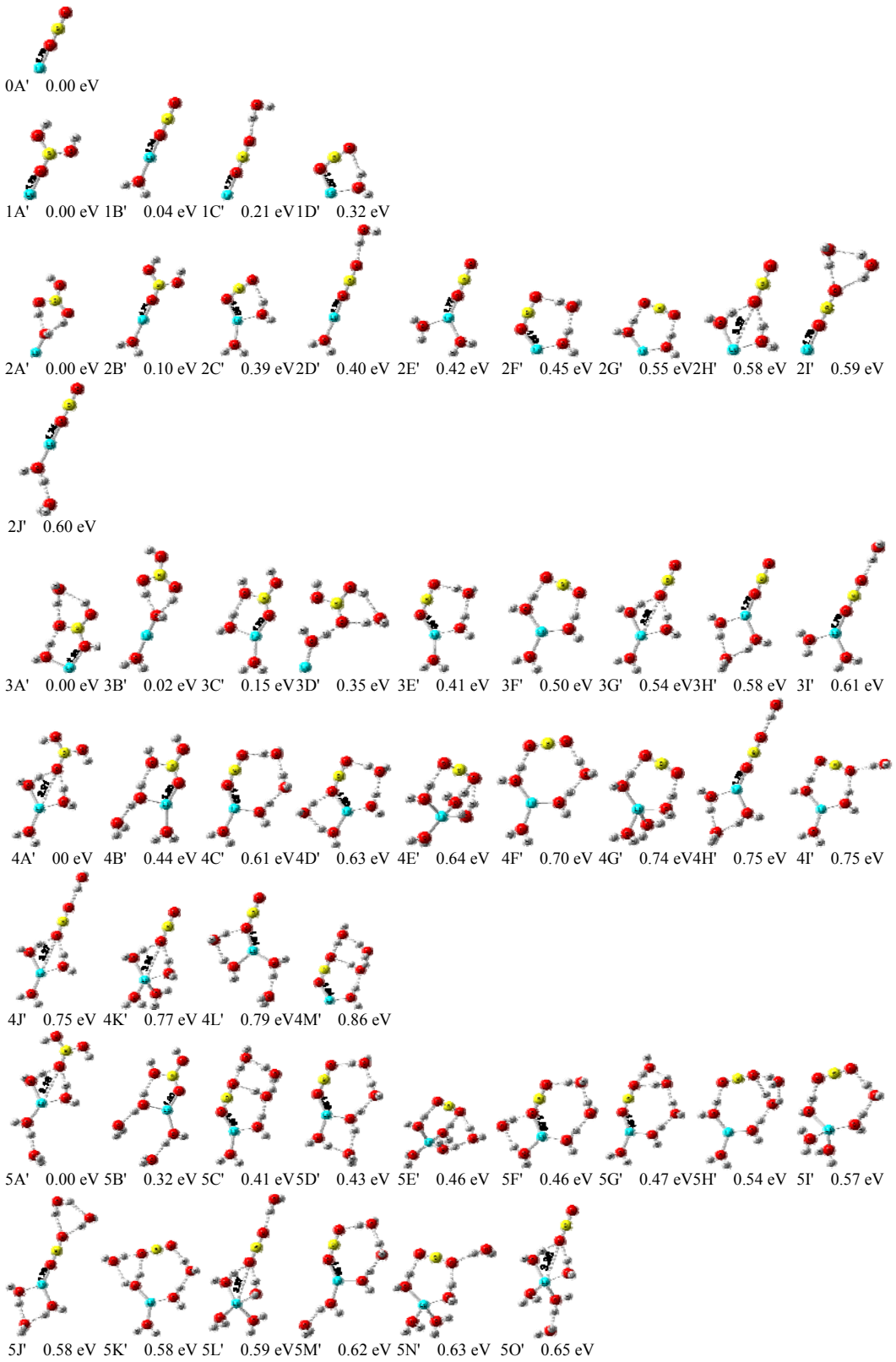

Figure S1 Optimized geometries of the typical low-lying isomers of $LiBO_2(H2O)_n^-$ (n = 0-5) based on wB97XD functional and 6-31++G(d,p) basis set. Relative energies and Li-O bond lengths (in Å) are indicated.

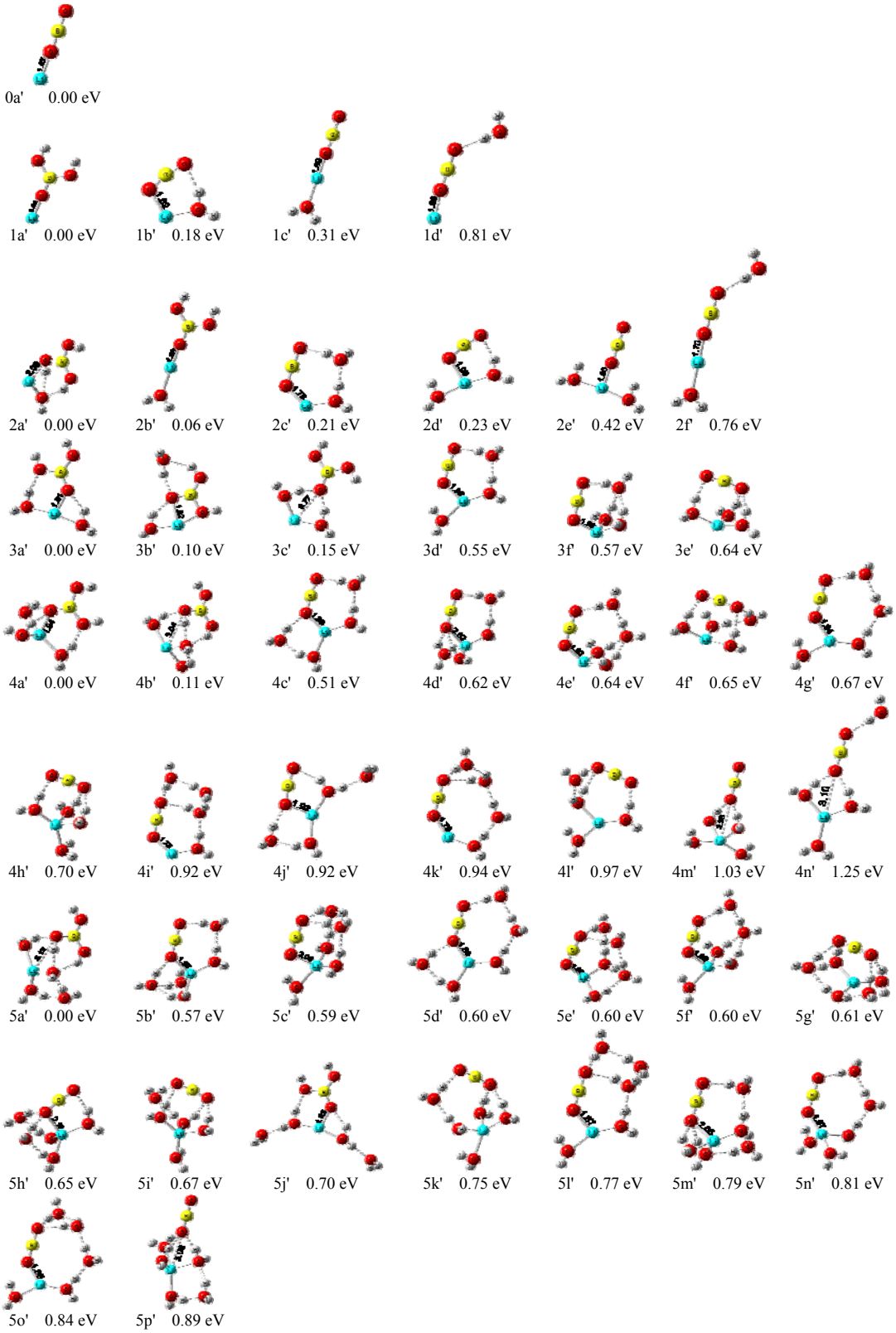

Figure S2 Optimized geometries of the typical low-lying isomers of $LiBO_2(H2O)_n$ (n = 0-5) neutral clusters based on wB97XD functional and 6-31++G(d,p) basis set. Relative energies and Li-O bond lengths (in Å) are indicated.

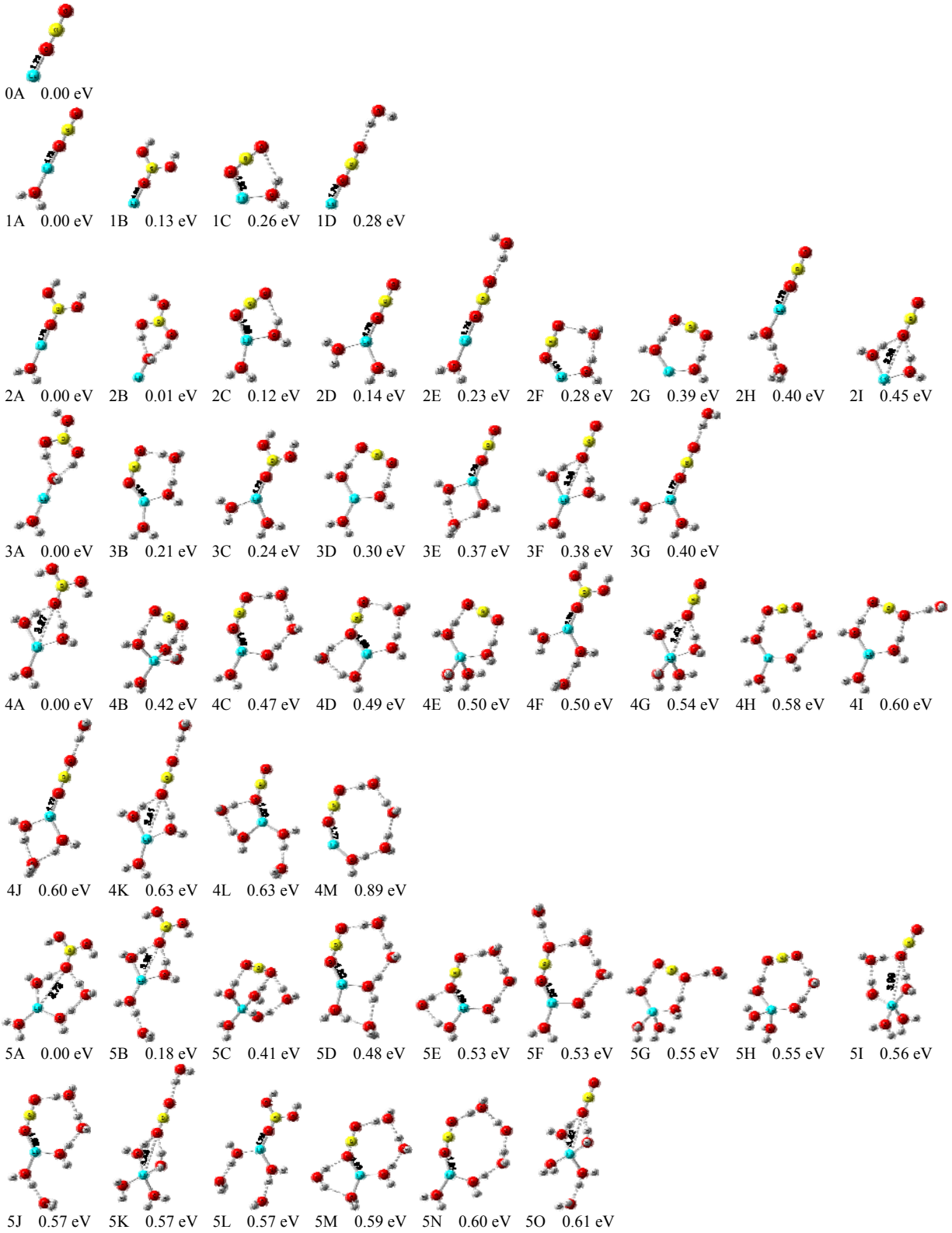

Figure S3 Optimized geometries of the typical low-lying isomers of $LiBO_2(H_2O)_n^-$ (n = 0-5) based on CCSD(T) // B3LYP/6-311++G(d,p). Relative energies and Li-O bond lengths (in Å) are indicated.

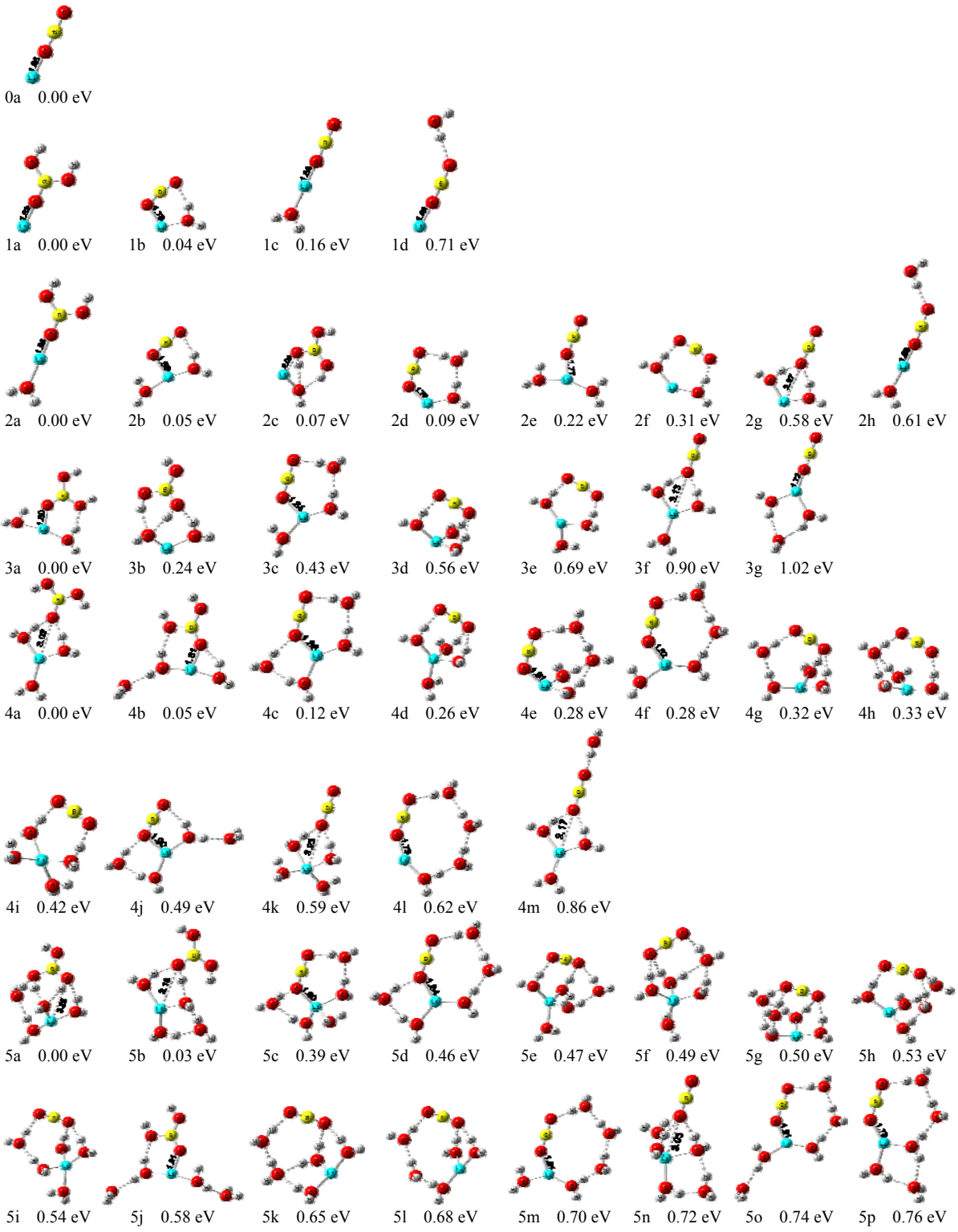

Figure S4 Optimized geometries of the typical low-lying isomers of $LiBO_2(H_2O)_n$ (n = 0-5) neutral clusters based on CCSD(T) // B3LYP/6-311++G(d,p). Relative energies and Li-O bond lengths (in Å) are indicated.