JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(15), 3560-3570, DOI:10.1021/ja972726+

Table S1. Optimized Geometrical Parameters (Å and degrees) [a] and Total Binding Energies, $\Delta E(n)$ (kcal/mol), of $Li(H_2O)_n$ (n = 1–2) Calculated at Various Levels. Imaginary Frequencies (cm^{-1}) and Symmetry of Imaginary Modes are Given if Exist.

Symbol [b]	Level [c]	R_{Li-O1}	θ	R_{Li-O2}	∠O1LiO2	R_{H1-O2}	$\Delta E(n)$ [d]	Imag. freq. (sym)
$Li(H_2O)$								
I*a* 1+0 (C_{2v})	A	1.909					12.5	181*i* (B_1)
	B	1.903	0.0				12.2	122*i* (B_1)
	C	1.917	0.0				*10.6* (12.2)	
I*b* 1+0 (C_s)	A	1.918	29.3				*12.6*	
	B	1.910	27.1				*12.3*	
$Li(H_2O)_2$								
II*a* 2+0 (C_{2v})	A	1.917			142.9		25.8	77*i* (A_2), 66*i* (B_1)
	B	1.871			174.3		*26.8*	
	C	1.934			123.7		20.2	119*i* (A_2), 62*i* (B_2)
II*b* 2+0 (C_2)	A	1.917			119.0		26.2	12*i* (B)
	C	1.935			107.7		*21.1* (25.9)	
II*g* 2+0 (C_s)	A	1.909			127.4		26.1	26*i* (A")
	C	1.924			117.6		20.5	123*i* (A")
II*c* 2+0 (C_s)	A	1.937		1.903	104.7		26.1	188*i* (A")
	B	1.942		1.882	95.5		*26.2*	
	C	1.956		1.918	105.3		21.0	64*i* (A")
II*d* 2+0 (C_1)	A	1.924		1.919	113.0		*26.2*	
II*e* 1+1 (C_s)	A	1.884				1.776	22.5	77*i* (A")
	B	1.869				1.774	*22.7*	
	C	1.888				1.883	*19.2* (22.4)	
II*f* 1+1 (C_1)	A	1.890				1.778	*22.5*	

[a] Parameters are shown in Figure S1. [b] Corresponds to structures in Figure S1. [c] A: MP2/6-311++G(d,p). B: MP2/6-31++G(d,p). C: HF/6-31++G(d,p). [d] $-\Delta E(n) = E[Li(H_2O)_n] - E[Li] - nE[H_2O]$ (without CPC). Values for potential minima are in italic. Values in parentheses are at MP2/6–31++G(d,p) // HF/6–31++G(d,p).

Table S2. Optimized Geometrical Parameters (Å and degrees)[a] and Total Binding Energies, ΔE (kcal/mol), of $Li(H_2O)_3$ Calculated at Various Levels. Imaginary Frequencies (cm^{-1}) and Symmetry of Imaginary Modes are Presented if Exist.

Symbol[b]	Level[c]	R_{Li-O1}	R_{Li-O2}	R_{Li-O3}	∠O1LiO2	∠O2LiO3	∠O1LiO3	R_{H1-O3}	R_{H2-O2}	ΔE[d]	Imag. freq. (sym.)
III*a* 3+0 (C_{2v})	A	1.902	1.913		117.3					42.3	161*i* (B_1), 17*i* (B_2)
	B	1.885	1.886		113.0					43.5	66*i* (B_2), 57*i* (B_1)
	C	1.915	1.910		115.6					*33.2* (42.8)	
III*k* 3+0 (C_s)	A	1.909	1.913		117.0	125.3				42.3	1*i* (A")
	B	1.891	1.885		112.7	133.4				43.5	51*i* (A")
III*l* 3+0 (C_s)	A	1.903	1.918	1.912		125.0	127.0			42.3	150*i* (A")
	B	1.865	1.932	1.874		126.7	140.7			44.0	41*i* (A")
III*b* 3+0 (C_1)	A	1.909	1.913	1.913	117.4	125.3	116.7			*42.3*	
III*c* 3+0 (C_1)	B	1.859	1.930	1.860	118.3	92.5	149.2			*44.1*	
III*d* 3+0 (C_3)	A	1.907			119.6					*42.4*	
	B	1.880			117.5					*44.0*	
	C	1.912			119.9					*33.3* (40.2)	
III*e* 2+1 (C_s)	A	1.880	1.971		107.7			1.798	2.030	37.8	314*i* (A"), 114*i* (A")
	B	1.850	1.928		113.5			1.796	1.988	*40.5*	
	C	1.891	2.008		106.7			1.914	2.178	30.1	73*i* (A")

(Continues to next page.)

(Table S2 continued.)

Symbol[b]	Level[c]	R_{Li-O1}	R_{Li-O2}	R_{Li-O3}	∠O1LiO2	∠O2LiO3	∠O1LiO3	R_{H1-O3}	RH2-O2	ΔE^d	Imag. freq. (sym.)
III*f* 2+1 (C_1)	A	1.884	1.975		106.6			1.773	2.014	*38.3*	
	C	1.890	2.010		106.0			1.912	2.174	*30.1* (39.0)	
III*g* 2+1 (C_s)	A	1.921			103.2			1.994		*36.4*	
	B	1.888			111.2			1.994		*38.2*	
	C	1.931			99.7			2.126		*29.1* (34.7)	
III*h* 1+2 (C_{2v})	A	1.862						1.829		31.0	15*i* (B_1)
	B	1.842						1.825		31.5	47*i* (B_2)
	C	1.863						1.929		*26.4* (31.2)	
III*i* 1+2 (Cs)	A	1.863						1.829		*31.0*	
	B	1.836						1.838		31.7	63*i* (A")
III*j* 1+2 (C_1)	B	1.830						1.823	1.844	*31.7*	

[a] Parameters are shown in Figure 1. [b] Corresponds to structures in Figure 1. [c] A: MP2/6-311++G(d,p). B: MP2/6-31++G(d,p). C: HF/6-31++G(d,p). [d] $-\Delta E(n) = E[Li(H_2O)_n] - E[Li] - n\,E[H_2O]$ (without CPC). Values for potential minima are in italic. Values in parentheses are at MP2/6–31++G(d,p)//HF/6–31++G(d,p).

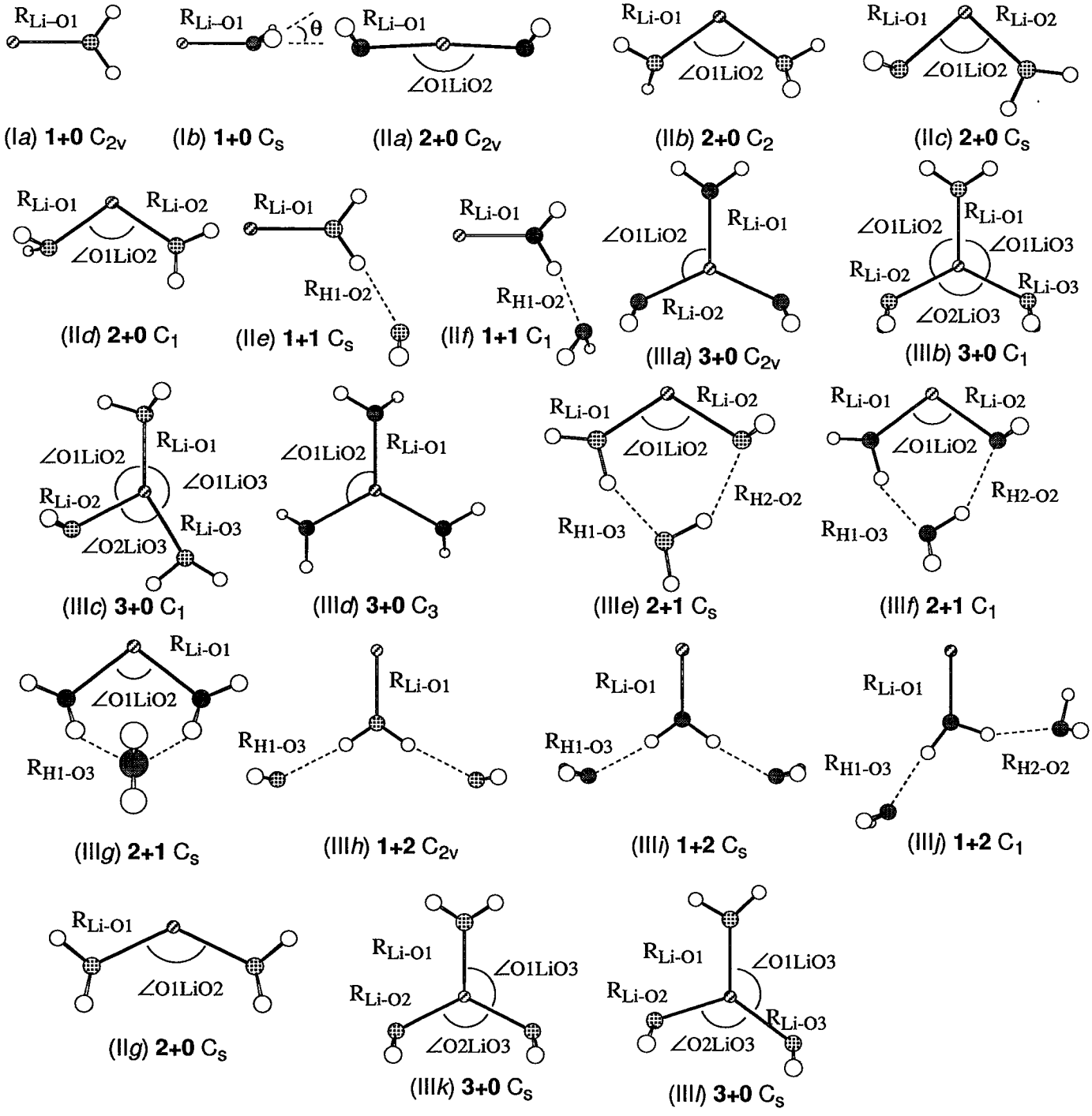
Table S3. Mulliken Total Gross Population in Li s Basis Functions in $Li(H_2O)_n$ Clusters by HF/6-31++G(d,p) Method.

		Li s basis function			
n	structure [a]	inner	outer	diffuse	total
0		0.32	0.60	0.03	0.96
1	I*a*	0.21	0.69	0.08	0.98
2	II*b*	0.17	0.59	0.14	0.90
3	III*a*	0.18	0.29	0.33	0.79
4	IV*a*	0.22	0.17	0.36	0.74
5	V*a*	0.21	0.10	0.28	0.59
6	VI*a*	0.21	0.10	0.21	0.52
8	VIII*a*	0.20	0.17	0.15	0.52

[a] Indicates the structures in Figures 1 and 2.

K. Hashimoto

Supporting Information
(4/5)



K. Hashimoto Fig. S1

Supporting Information (5/5)