Supporting Information for

A Comprehensive Guide for Accurate Conformational Energies of Microsolvated Li^+ Clusters with Organic Carbonates

Arseniy A. Otlyotov,[1] *Andrey D. Moshchenkov,*[1] *Timofey P. Rozov,*[1,2] *Anna A. Tuma,* [1,2] *Alexander S. Ryzhako*[1,3] *and Yury Minenkov*[1]*

[1] N.N. Semenov Federal Research Center for Chemical Physics RAS, Kosygina Street 4, 119991, Moscow, Russian Federation

[2] Department of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia

[3] Dmitry Mendeleev University of Chemical Technology of Russia, Miusskaya sq. 9, 125047, Moscow, Russian Federation

Corresponding Author e-mail: Yury.Minenkov@chph.ras.ru

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Additional statistical data for the LICARBCONF806 database

Table S1. Numbers of conformers, maximum and average conformational energies (in kcal mol^{-1}) and Pearson correlation coefficients obtained for individual $Li^+(S)_n$ clusters using standard and composite DFT methods. Reference conformational energies were calculated at RI-SCS-MP2/CBS level of theory.

	N[a]	ΔE_{max}[b]	ΔE_{avg}[b]	ωB97M-V[c]	B3LYP-D4[c]	PBE0-D4[c]	r^2SCAN-D4[c]	B97-3c	PBEh-3c	r^2SCAN-3c	PBE-D3(BJ)[d]
$Li^+(BC)_2$	24	27.2	12.4	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$Li^+(BC)_3$	22	14.4	2.4	0.99	1.00	1.00	1.00	1.00	1.00	0.98	0.95
$Li^+(BC)_4$	33	2.6	1.6	0.80	0.86	0.95	0.88	0.94	0.84	0.80	0.55
$Li^+(BC)_5$	31	7.1	3.7	0.99	0.98	0.99	0.99	0.99	0.97	0.99	0.94
$Li^+(BC)_6$	34	15.1	7.9	0.98	0.98	0.99	0.99	0.99	0.98	0.98	0.93
$Li^+(DMC)_3$	13	5.4	1.9	1.00	1.00	1.00	1.00	0.98	1.00	0.99	0.99
$Li^+(DMC)_4$	30	12.1	4.3	0.98	0.97	0.98	0.99	0.99	0.99	0.98	0.98
$Li^+(DMC)_5$	32	18.3	3.5	0.98	0.99	0.99	0.99	0.98	0.99	0.99	0.97
$Li^+(DMC)_6$	29	9.0	4.2	0.95	0.96	0.97	0.96	0.96	0.96	0.94	0.87
$Li^+(EMC)_2$	16	7.2	2.9	0.98	0.98	0.97	0.97	0.98	0.98	0.98	0.97
$Li^+(EMC)_3$	32	6.2	2.3	0.97	0.96	0.95	0.97	0.95	0.98	0.96	0.94
$Li^+(EMC)_4$	33	8.9	3.4	0.97	0.99	0.98	0.98	0.98	0.98	0.98	0.96
$Li^+(EMC)_5$	34	29.7	5.6	0.99	1.00	1.00	1.00	1.00	0.99	1.00	0.99
$Li^+(EMC)_6$	31	29.5	7.1	0.99	0.99	0.99	0.99	1.00	0.99	0.99	0.96
$Li^+(DEC)_2$	28	7.5	3.8	0.97	0.96	0.95	0.96	0.95	0.95	0.98	0.97
$Li^+(DEC)_3$	33	7.5	3.4	0.95	0.94	0.92	0.94	0.97	0.97	0.95	0.92
$Li^+(DEC)_4$	33	7.2	3.5	0.97	0.98	0.97	0.97	0.97	0.96	0.97	0.90
$Li^+(DEC)_5$	33	10.9	3.6	0.97	0.98	0.98	0.98	0.98	0.96	0.97	0.87
$Li^+(DEC)_6$	30	9.0	3.8	0.97	0.97	0.97	0.97	0.95	0.85	0.98	0.81
$Li^+(VC)_4$	12	49.2	21.4	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

$Li^+(VC)_5$	27	54.6	9.2	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$Li^+(VC)_6$	31	26.6	6.6	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99
$Li^+(EC)_4$	18	20.4	8.7	0.99	0.99	1.00	1.00	1.00	1.00	0.99	0.98
$Li^+(EC)_5$	28	11.5	4.8	0.98	0.98	0.99	0.99	1.00	0.99	0.98	0.94
$Li^+(EC)_6$	31	16.3	5.5	0.99	0.99	1.00	0.99	0.99	0.99	0.98	0.97
$Li^+(PC)_3$	18	38.8	17.7	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$Li^+(PC)_4$	31	44.8	13.0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99
$Li^+(PC)_5$	32	50.8	13.9	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99
$Li^+(PC)_6$	27	51.5	14.9	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99
minimum				0.80	0.86	0.92	0.88	0.94	0.84	0.80	0.55
Q_1				0.97	0.98	0.97	0.97	0.98	0.97	0.98	0.94
median				0.99	0.99	0.99	0.99	0.99	0.99	0.98	0.97
Q_3				1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99
maximum				1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
average				0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.94

[a] Number of conformers.
[b] Maximum and average conformational energies at RI-SCS-MP2/CBS level of theory.
[c] in conjunction with Complete Basis Set (CBS, TZ/QZ) extrapolation.
[d] in conjunction with def2-SVP basis set.

Table S2. Numbers of conformers, maximum and average conformational energies (in kcal mol^{-1}) and Pearson correlation coefficients obtained for individual $Li^+(S)_n$ clusters using semi-empirical approximations. Reference conformational energies were calculated at RI-SCS-MP2/CBS level of theory.

	N[a]	ΔE_{max}[b]	ΔE_{avg}[b]	QM3	GFN1-xTB	GFN2-xTB	AM1	PM3	PM6	PM6-D3	PM6-D3H4	PM7
$Li^+(BC)_2$	24	27.2	12.4	1.00	1.00	1.00	0.99	0.98	0.99	0.96	0.97	1.00
$Li^+(BC)_3$	22	14.4	2.4	0.99	0.98	0.97	0.76	0.73	0.78	0.30	0.41	0.71
$Li^+(BC)_4$	33	2.6	1.6	0.37	0.57	0.48	0.25	–0.18	0.33	0.34	0.48	0.30

$Li^+(BC)_5$	31	7.1	3.7	0.93	0.83	0.86	0.40	0.29	0.04	0.20	0.15	–0.02
$Li^+(BC)_6$	34	15.1	7.9	0.87	0.90	0.86	0.18	–0.08	0.05	0.44	0.44	0.39
$Li^+(DMC)_3$	13	5.4	1.9	0.96	0.94	0.97	0.98	0.04	0.96	0.96	0.95	0.94
$Li^+(DMC)_4$	30	12.1	4.3	0.81	0.96	0.96	0.66	0.71	0.53	0.57	0.57	0.76
$Li^+(DMC)_5$	32	18.3	3.5	0.76	0.95	0.89	0.66	0.53	0.56	0.68	0.66	0.71
$Li^+(DMC)_6$	29	9.0	4.2	0.67	0.56	0.74	0.26	–0.07	0.14	0.28	0.27	0.41
$Li^+(EMC)_2$	16	7.2	2.9	0.99	0.84	0.90	0.96	0.52	0.98	0.96	0.96	0.97
$Li^+(EMC)_3$	32	6.2	2.3	0.94	0.82	0.87	0.92	–0.06	0.89	0.86	0.87	0.86
$Li^+(EMC)_4$	33	8.9	3.4	0.91	0.88	0.90	0.92	0.77	0.80	0.75	0.78	0.85
$Li^+(EMC)_5$	34	29.7	5.6	0.95	0.96	0.95	0.64	0.51	0.63	0.76	0.74	0.83
$Li^+(EMC)_6$	31	29.5	7.1	0.89	0.89	0.92	0.56	0.41	0.39	0.55	0.55	0.75
$Li^+(DEC)_2$	28	7.5	3.8	0.97	0.59	0.90	0.88	0.15	0.95	0.92	0.91	0.93
$Li^+(DEC)_3$	33	7.5	3.4	0.94	0.83	0.84	0.91	0.61	0.73	0.68	0.66	0.70
$Li^+(DEC)_4$	33	7.2	3.5	0.86	0.75	0.79	0.87	0.74	0.52	0.29	0.33	0.57
$Li^+(DEC)_5$	33	10.9	3.6	0.78	0.73	0.68	0.70	0.57	0.33	0.20	0.24	0.43
$Li^+(DEC)_6$	30	9.0	3.8	0.62	0.33	0.25	0.56	0.52	0.08	0.06	0.11	0.34
$Li^+(VC)_4$	12	49.2	21.4	0.99	1.00	1.00	0.97	0.96	0.98	0.98	0.98	1.00
$Li^+(VC)_5$	27	54.6	9.2	0.94	0.99	0.99	0.77	0.67	0.90	0.93	0.94	0.97
$Li^+(VC)_6$	31	26.6	6.6	0.89	0.96	0.98	0.08	–0.22	0.57	0.81	0.81	0.89
$Li^+(EC)_4$	18	20.4	8.7	0.92	0.99	0.99	0.92	0.83	0.91	0.44	0.60	0.96
$Li^+(EC)_5$	28	11.5	4.8	0.87	0.98	0.94	0.13	–0.30	0.66	0.79	0.82	0.92
$Li^+(EC)_6$	31	16.3	5.5	0.95	0.98	0.90	0.09	–0.36	0.48	0.82	0.82	0.78
$Li^+(PC)_3$	18	38.8	17.7	0.99	1.00	1.00	0.99	0.97	0.98	0.96	0.97	1.00
$Li^+(PC)_4$	31	44.8	13.0	0.98	1.00	1.00	0.95	0.90	0.98	0.94	0.95	0.99
$Li^+(PC)_5$	32	50.8	13.9	0.95	1.00	0.99	0.92	0.80	0.95	0.86	0.89	0.97
$Li^+(PC)_6$	27	51.5	14.9	0.94	1.00	0.99	0.93	0.77	0.96	0.90	0.93	0.97
minimum				0.37	0.33	0.25	0.08	–0.36	0.04	0.06	0.11	–0.02
Q_1				0.87	0.83	0.86	0.56	0.04	0.48	0.44	0.48	0.70
median				0.94	0.95	0.92	0.77	0.53	0.73	0.76	0.78	0.85
Q_3				0.96	0.99	0.99	0.92	0.77	0.95	0.92	0.93	0.97
maximum				1.00	1.00	1.00	0.99	0.98	0.99	0.98	0.98	1.00
average				0.88	0.87	0.88	0.68	0.44	0.66	0.66	0.68	0.75

[a] Number of conformers.
[b] Maximum and average conformational energies at RI-SCS-MP2/CBS level of theory.

Table S3. Numbers of conformers, maximum and average conformational energies (in kcal mol^{-1}) and mean unsigned errors (MUEs, kcal mol^{-1}) obtained for individual $Li^+(S)_n$ clusters using standard and composite DFT methods. Reference conformational energies were calculated at RI-SCS-MP2/CBS level of theory.

	N[a]	ΔE_{max}[b]	ΔE_{avg}[b]	ωB97M-V[c]	B3LYP-D4[c]	PBE0-D4[c]	r^{2}SCAN-D4[c]	B97-3c	PBEh-3c	r^{2}SCAN-3c	PBE-D3(BJ)[d]
$Li^+(BC)_2$	24	27.2	12.4	0.22	0.67	0.57	0.35	0.68	2.17	0.53	1.10
$Li^+(BC)_3$	22	14.4	2.4	0.42	0.16	0.18	0.26	0.20	0.56	0.45	0.98
$Li^+(BC)_4$	33	2.6	1.6	0.49	0.25	0.15	0.37	0.16	0.40	0.72	1.27
$Li^+(BC)_5$	31	7.1	3.7	0.49	1.00	0.61	0.26	0.26	0.49	0.31	1.21
$Li^+(BC)_6$	34	15.1	7.9	1.59	2.26	1.03	0.67	0.41	1.10	1.16	1.98
$Li^+(DMC)_3$	13	5.4	1.9	0.30	0.13	0.24	0.30	0.48	0.33	0.31	0.17
$Li^+(DMC)_4$	30	12.1	4.3	0.60	0.78	0.66	0.52	0.48	0.86	0.62	0.65
$Li^+(DMC)_5$	32	18.3	3.5	0.79	0.55	0.55	0.75	1.11	0.52	0.89	1.07
$Li^+(DMC)_6$	29	9.0	4.2	1.51	1.22	0.56	0.78	0.49	1.29	0.88	1.23
$Li^+(EMC)_2$	16	7.2	2.9	0.40	0.37	0.45	0.42	0.45	0.50	0.40	0.98
$Li^+(EMC)_3$	32	6.2	2.3	0.41	0.29	0.49	0.37	0.72	0.26	0.38	0.53
$Li^+(EMC)_4$	33	8.9	3.4	0.52	0.47	0.46	0.40	0.71	0.69	0.40	0.58
$Li^+(EMC)_5$	34	29.7	5.6	0.60	0.51	0.48	0.53	0.77	0.85	0.54	0.91
$Li^+(EMC)_6$	31	29.5	7.1	1.23	0.82	0.52	0.75	0.62	2.66	0.85	1.32
$Li^+(DEC)_2$	28	7.5	3.8	0.58	0.51	0.66	0.65	0.69	0.68	0.66	1.33
$Li^+(DEC)_3$	33	7.5	3.4	0.85	1.27	1.14	0.93	0.55	0.51	1.09	0.62
$Li^+(DEC)_4$	33	7.2	3.5	0.49	0.35	0.50	0.48	1.11	0.57	0.43	0.92
$Li^+(DEC)_5$	33	10.9	3.6	0.62	0.57	0.55	0.53	0.74	0.72	0.57	0.95
$Li^+(DEC)_6$	30	9.0	3.8	0.59	0.80	0.48	0.55	0.60	1.10	0.52	1.84

$Li^+(VC)_4$	12	49.2	21.4	0.47	0.79	0.66	0.31	0.51	4.02	0.62	2.25
$Li^+(VC)_5$	27	54.6	9.2	1.47	1.01	0.43	1.28	0.45	1.96	1.68	1.78
$Li^+(VC)_6$	31	26.6	6.6	1.56	1.03	0.46	1.00	1.00	1.42	1.38	2.08
$Li^+(EC)_4$	18	20.4	8.7	1.01	1.05	0.53	0.63	0.23	2.41	0.97	1.51
$Li^+(EC)_5$	28	11.5	4.8	0.83	0.67	0.34	0.50	0.22	0.85	0.81	1.95
$Li^+(EC)_6$	31	16.3	5.5	1.41	1.33	0.52	0.87	0.35	0.90	1.14	3.04
$Li^+(PC)_3$	18	38.8	17.7	0.36	0.74	0.74	0.28	0.72	3.84	0.42	1.93
$Li^+(PC)_4$	31	44.8	13.0	0.60	0.57	0.49	0.43	0.42	3.35	0.58	2.33
$Li^+(PC)_5$	32	50.8	13.9	0.91	0.81	0.58	0.66	0.41	3.26	0.78	2.43
$Li^+(PC)_6$	27	51.5	14.9	1.23	1.18	0.74	0.71	0.41	3.53	1.05	3.17
minimum				0.22	0.13	0.15	0.26	0.16	0.26	0.31	0.17
Q_1				0.49	0.51	0.46	0.37	0.41	0.56	0.45	0.95
median				0.60	0.74	0.52	0.53	0.49	0.86	0.62	1.27
Q_3				1.01	1.01	0.61	0.71	0.71	2.17	0.89	1.95
maximum				1.59	2.26	1.14	1.28	1.11	4.02	1.68	3.17
average				0.78	0.76	0.54	0.57	0.55	1.44	0.73	1.45

[a] Number of conformers.
[b] Maximum and average conformational energies at RI-SCS-MP2/CBS level of theory.
[c] in conjunction with Complete Basis Set (CBS, TZ/QZ) extrapolation.
[d] in conjunction with def2-SVP basis set.

Table S4. Numbers of conformers, maximum and average conformational energies (in kcal mol^{-1}) and mean unsigned errors (MUEs, kcal mol^{-1}) obtained for individual $Li^+(S)_n$ clusters using semi-empirical approximations. Reference conformational energies were calculated at RI-SCS-MP2/CBS level of theory.

	N[a]	ΔE_{max}[b]	ΔE_{avg}[b]	QM3	GFN1-xTB	GFN2-xTB	AM1	PM3	PM6	PM6-D3	PM6-D3H4	PM7
$Li^+(BC)_2$	24	27.2	12.4	2.32	2.14	1.85	5.49	3.05	7.43	8.29	7.93	5.48
$Li^+(BC)_3$	22	14.4	2.4	1.25	1.63	0.57	1.90	5.96	1.38	2.47	2.49	2.00
$Li^+(BC)_4$	33	2.6	1.6	1.80	1.14	2.15	1.06	4.74	0.88	1.32	0.97	0.76

$Li^+(BC)_5$	31	7.1	3.7	4.34	1.23	1.84	1.88	3.22	2.54	2.37	2.37	2.39
$Li^+(BC)_6$	34	15.1	7.9	7.26	1.42	2.74	4.24	13.23	4.41	3.22	3.16	3.32
$Li^+(DMC)_3$	13	5.4	1.9	2.96	0.48	0.82	2.31	1.56	4.73	4.58	4.80	3.45
$Li^+(DMC)_4$	30	12.1	4.3	3.67	2.10	0.86	3.91	7.35	3.73	2.96	3.10	2.64
$Li^+(DMC)_5$	32	18.3	3.5	4.87	1.37	1.82	3.01	6.76	2.92	2.70	2.61	2.69
$Li^+(DMC)_6$	29	9.0	4.2	4.22	1.71	3.11	3.20	9.03	3.69	4.56	4.39	3.11
$Li^+(EMC)_2$	16	7.2	2.9	1.68	1.43	1.04	2.25	1.65	3.52	2.86	3.00	1.86
$Li^+(EMC)_3$	32	6.2	2.3	4.30	0.90	1.24	2.87	2.89	6.24	6.23	6.42	5.73
$Li^+(EMC)_4$	33	8.9	3.4	4.89	1.72	1.04	4.39	6.65	6.59	4.52	4.68	2.46
$Li^+(EMC)_5$	34	29.7	5.6	2.59	1.69	1.84	3.55	7.22	4.08	3.49	3.55	3.84
$Li^+(EMC)_6$	31	29.5	7.1	7.52	2.28	2.13	5.64	10.62	6.18	6.71	6.42	3.57
$Li^+(DEC)_2$	28	7.5	3.8	2.53	1.82	1.73	2.94	3.30	4.19	3.76	4.05	2.69
$Li^+(DEC)_3$	33	7.5	3.4	5.07	0.94	0.98	6.37	5.90	5.47	5.17	5.66	2.98
$Li^+(DEC)_4$	33	7.2	3.5	2.96	1.26	1.07	3.89	6.45	2.89	2.56	2.89	2.67
$Li^+(DEC)_5$	33	10.9	3.6	5.05	1.48	2.06	5.78	13.53	5.36	4.91	5.27	3.45
$Li^+(DEC)_6$	30	9.0	3.8	6.54	2.36	2.86	4.95	11.78	5.48	6.60	6.43	3.95
$Li^+(VC)_4$	12	49.2	21.4	2.67	3.75	2.79	10.74	5.95	11.49	12.29	11.73	7.59
$Li^+(VC)_5$	27	54.6	9.2	6.72	1.64	5.62	5.58	7.32	4.36	4.36	4.11	3.49
$Li^+(VC)_6$	31	26.6	6.6	10.00	1.49	6.05	6.95	11.29	4.44	3.39	3.36	2.89
$Li^+(EC)_4$	18	20.4	8.7	4.24	1.13	1.81	4.81	5.39	5.33	6.54	6.19	3.49
$Li^+(EC)_5$	28	11.5	4.8	4.77	1.13	2.38	3.53	9.42	2.79	1.63	1.56	0.99
$Li^+(EC)_6$	31	16.3	5.5	7.03	1.76	4.26	4.42	19.79	3.76	2.40	2.18	2.28
$Li^+(PC)_3$	18	38.8	17.7	2.43	2.58	2.70	9.33	4.04	11.14	12.38	11.78	7.84
$Li^+(PC)_4$	31	44.8	13.0	5.39	2.09	4.34	7.98	5.83	7.89	7.89	7.48	4.88
$Li^+(PC)_5$	32	50.8	13.9	4.74	2.73	4.35	7.50	7.62	7.93	7.33	7.10	4.99
$Li^+(PC)_6$	27	51.5	14.9	9.83	1.92	6.28	7.52	8.21	7.88	7.56	7.23	4.86
minimum				1.25	0.48	0.57	1.06	1.56	0.88	1.32	0.97	0.76
Q_1				2.67	1.26	1.24	3.01	4.74	3.69	2.86	3.00	2.64
median				4.34	1.64	2.06	4.39	6.65	4.44	4.52	4.39	3.32
Q_3				5.39	2.09	2.86	5.78	9.03	6.24	6.60	6.42	3.95
maximum				10.00	3.75	6.28	10.74	19.79	11.49	12.38	11.78	7.84
average				4.61	1.70	2.49	4.76	7.23	5.13	5.00	4.93	3.53

[a] Number of conformers.
[b] Maximum and average conformational energies at RI-SCS-MP2/CBS level of theory.

Table S5. Total times (in s) required for 1 SCF iteration for the individual $Li^+(S)_n$ clusters using different DFT methods. In all cases the lowest energy (according to the reference RI-SCS-MP2/CBS energies) conformer was considered.

	B3LYP-D4/TZ[a]	B97-3c	PBE-D3/DZ[b]	PBE0-D4/TZ[a]	PBEh-3c	r^{2}SCAN-3c	r^{2}SCAN-D4/TZ[a]	ωB97M-V/TZ[a]
$Li^+(BC)_2$	21.5	6.2	5.8	21.9	10.4	7.0	10.8	31.9
$Li^+(BC)_3$	46.2	10.5	9.4	46.7	19.3	12.3	16.6	72.3
$Li^+(BC)_4$	84.6	16.8	14.2	86.8	31.3	19.0	25.2	138.7
$Li^+(BC)_5$	141.4	24.5	19.3	142.9	48.2	27.3	37.7	237.2
$Li^+(BC)_6$	219.5	36.0	26.2	223.4	69.2	38.6	56.0	367.9
$Li^+(DEC)_2$	23.6	6.8	6.2	24.3	11.7	7.6	9.7	35.2
$Li^+(DEC)_3$	53.8	12.0	14.0	54.6	21.6	13.6	18.7	90.1
$Li^+(DEC)_4$	101.3	19.3	15.6	100.8	36.5	21.9	28.7	167.7
$Li^+(DEC)_5$	163.0	28.0	22.9	164.1	54.8	30.6	43.0	284.7
$Li^+(DEC)_6$	264.6	38.4	28.6	248.1	76.5	41.8	62.6	424.6
$Li^+(DMC)_2$	13.3	4.5	4.3	13.2	10.1	5.0	5.9	18.7
$Li^+(DMC)_3$	26.8	7.7	6.8	26.7	13.0	8.3	10.5	40.1
$Li^+(DMC)_4$	50.5	11.4	10.0	51.8	21.4	12.8	16.4	76.8
$Li^+(DMC)_5$	87.6	17.7	13.5	81.5	32.0	18.9	23.4	135.4
$Li^+(DMC)_6$	111.9	21.8	17.0	122.6	39.6	24.2	31.2	210.3
$Li^+(EC)_2$	11.6	4.1	3.8	11.7	6.8	4.6	5.3	16.2
$Li^+(EC)_3$	23.5	6.4	5.9	22.5	11.0	7.2	17.7	33.0
$Li^+(EC)_4$	39.3	10.1	8.1	40.1	18.1	11.3	14.2	61.8
$Li^+(EC)_5$	56.8	13.1	10.8	56.0	23.0	14.5	17.9	87.8
$Li^+(EC)_6$	101.1	20.1	14.5	100.6	35.1	21.9	28.9	164.3
$Li^+(EMC)_2$	19.0	5.5	5.1	18.0	13.8	6.2	7.6	26.7

$Li^+(EMC)_3$	39.5	9.5	8.6	39.7	16.7	11.2	14.0	61.8
$Li^+(EMC)_4$	73.4	15.2	12.6	72.9	27.3	17.4	22.1	119.1
$Li^+(EMC)_5$	120.4	22.8	17.6	121.6	42.2	25.3	33.6	201.8
$Li^+(EMC)_6$	184.5	34.5	22.6	178.5	57.3	32.9	46.0	300.2
$Li^+(VC)_2$	16.4	5.0	4.8	17.3	8.4	5.9	7.1	23.3
$Li^+(VC)_3$	33.7	8.5	7.7	36.4	14.7	10.0	12.2	54.9
$Li^+(VC)_4$	59.3	13.2	11.1	60.4	24.2	14.7	18.9	93.6
$Li^+(VC)_5$	101.9	19.5	15.4	102.8	40.6	21.9	29.3	168.4
$Li^+(VC)_6$	138.9	24.6	18.9	152.7	50.3	27.3	37.2	229.8
$Li^+(PC)_2$	10.5	3.6	3.3	10.3	5.8	4.1	4.8	14.0
$Li^+(PC)_3$	32.1	5.9	5.3	20.2	9.5	6.4	7.8	27.7
$Li^+(PC)_4$	33.7	8.7	7.2	34.0	14.6	9.8	12.1	50.9
$Li^+(PC)_5$	47.0	11.4	23.9	47.2	19.6	12.7	15.8	72.4
$Li^+(PC)_6$	76.4	16.4	11.8	77.4	28.4	18.1	22.6	125.5

[a] TZ denotes def2-TZVP basis set.
[b] DZ denotes def2-SVP basis set.

Table S6. Numbers of conformers and Pearson correlation coefficients obtained for conformational Gibbs energies (ΔG_{conf}) of the individual $Li^+(S)_n$ clusters using different vibrational thermochemistry and/or continuum solvation models. Conformational electronic energies (ΔE_{conf}) calculated at RI-SCS-MP2/CBS level of theory were used as reference values.

	N[a]	PCM	Solv	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO
				gas			+PCM			+Solv		
$Li^+(BC)_2$	24	0.99	1.00	1.00	1.00	0.99	1.00	1.00	1.00	0.99	0.99	0.98
$Li^+(BC)_3$	22	0.80	0.99	0.96	0.95	0.89	0.92	0.93	0.96	0.93	0.91	0.85
$Li^+(BC)_4$	33	0.40	0.74	0.63	0.55	0.30	0.13	0.08	–0.03	0.36	0.31	0.16
$Li^+(BC)_5$	31	0.53	0.84	0.96	0.96	0.89	0.33	0.35	0.25	0.68	0.69	0.56
$Li^+(BC)_6$	34	0.72	0.68	0.95	0.93	0.77	0.49	0.48	0.23	0.31	0.28	0.08

$Li^+(DMC)_3$	13	0.35	0.86	0.98	0.98	0.94	0.43	0.42	0.48	0.91	0.91	0.86
$Li^+(DMC)_4$	30	0.94	0.98	0.98	0.97	0.93	0.95	0.94	0.94	0.96	0.95	0.91
$Li^+(DMC)_5$	32	0.93	0.98	0.98	0.97	0.93	0.91	0.89	0.86	0.94	0.91	0.84
$Li^+(DMC)_6$	29	0.86	0.85	0.84	0.76	0.53	0.65	0.55	0.32	0.48	0.38	0.18
$Li^+(EMC)_2$	16	0.87	0.93	0.97	0.96	0.90	0.63	0.48	0.31	0.76	0.72	0.60
$Li^+(EMC)_3$	32	0.35	0.81	0.95	0.93	0.88	0.22	0.16	0.22	0.64	0.60	0.55
$Li^+(EMC)_4$	33	0.90	0.98	0.97	0.96	0.91	0.86	0.83	0.77	0.93	0.91	0.85
$Li^+(EMC)_5$	34	0.99	0.99	0.99	0.99	0.97	0.98	0.98	0.97	0.97	0.96	0.93
$Li^+(EMC)_6$	31	0.97	0.93	0.98	0.97	0.92	0.97	0.96	0.92	0.86	0.85	0.76
$Li^+(DEC)_2$	28	0.87	0.81	0.96	0.96	0.91	0.74	0.69	0.57	0.58	0.55	0.49
$Li^+(DEC)_3$	33	0.84	0.91	0.95	0.93	0.88	0.56	0.48	0.42	0.79	0.75	0.69
$Li^+(DEC)_4$	33	0.93	0.97	0.98	0.97	0.95	0.91	0.89	0.88	0.94	0.93	0.91
$Li^+(DEC)_5$	33	0.93	0.94	0.98	0.97	0.93	0.87	0.85	0.81	0.90	0.89	0.84
$Li^+(DEC)_6$	30	0.90	0.89	0.96	0.95	0.89	0.85	0.83	0.77	0.85	0.83	0.75
$Li^+(VC)_4$	12	0.99	0.99	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.97	0.96
$Li^+(VC)_5$	27	0.98	0.98	0.99	0.99	0.96	0.98	0.97	0.95	0.93	0.92	0.85
$Li^+(VC)_6$	31	0.95	0.98	0.97	0.96	0.82	0.94	0.94	0.89	0.86	0.83	0.48
$Li^+(EC)_4$	18	0.98	0.98	0.98	0.97	0.93	0.97	0.97	0.94	0.92	0.92	0.87
$Li^+(EC)_5$	28	0.90	0.86	0.87	0.82	0.47	0.74	0.70	0.44	0.48	0.41	0.12
$Li^+(EC)_6$	31	0.90	0.84	0.84	0.77	0.20	0.65	0.54	–0.09	–0.02	–0.13	–0.43
$Li^+(PC)_3$	18	1.00	0.99	1.00	1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.97
$Li^+(PC)_4$	31	0.99	0.99	1.00	0.99	0.99	0.99	0.99	0.98	0.98	0.98	0.96
$Li^+(PC)_5$	32	0.98	0.97	0.99	0.99	0.97	0.98	0.97	0.95	0.93	0.92	0.87
$Li^+(PC)_6$	27	0.98	0.98	1.00	0.99	0.98	0.98	0.97	0.97	0.96	0.95	0.92
minimum		0.35	0.68	0.63	0.55	0.20	0.13	0.08	–0.09	–0.02	–0.13	–0.43
Q_1		0.86	0.86	0.96	0.95	0.88	0.65	0.54	0.42	0.68	0.69	0.55
median		0.93	0.97	0.98	0.97	0.92	0.91	0.89	0.86	0.91	0.91	0.84
Q_3		0.98	0.98	0.99	0.99	0.96	0.98	0.97	0.95	0.94	0.93	0.91
maximum		1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.99	0.99	0.98
average		0.85	0.92	0.95	0.94	0.85	0.78	0.75	0.68	0.79	0.76	0.67

[a] Number of conformers.

Table S7. Numbers of conformers and mean unsigned errors (MUEs, kcal mol^{-1}) obtained for conformational Gibbs energies (ΔG_{conf}) of the individual $Li^+(S)_n$ clusters using different vibrational thermochemistry and/or continuum solvation models. Conformational electronic energies (ΔE_{conf}) calculated at RI-SCS-MP2/CBS level of theory were used as reference values.

	N[a]	PCM	Solv	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO
				gas			+PCM			+Solv		
$Li^+(BC)_2$	24	4.32	4.30	1.46	1.51	2.69	3.46	3.44	2.91	4.13	4.22	3.90
$Li^+(BC)_3$	22	1.82	0.29	1.29	1.44	2.56	1.23	1.11	0.81	1.47	1.61	2.44
$Li^+(BC)_4$	33	0.77	0.47	0.74	0.69	0.94	0.78	0.83	1.13	0.80	0.91	1.33
$Li^+(BC)_5$	31	1.75	1.11	0.47	0.53	0.94	1.84	1.84	1.95	1.52	1.56	1.87
$Li^+(BC)_6$	34	4.08	3.32	1.23	1.32	2.06	4.68	4.47	3.94	3.41	3.47	4.61
$Li^+(DMC)_3$	13	1.27	0.82	0.44	0.44	1.06	1.41	1.40	1.19	0.77	0.78	0.83
$Li^+(DMC)_4$	30	1.17	0.59	1.26	1.43	2.40	1.05	1.10	1.60	1.05	1.22	2.07
$Li^+(DMC)_5$	32	1.05	0.77	0.63	0.80	1.15	1.37	1.51	1.67	1.18	1.35	1.71
$Li^+(DMC)_6$	29	0.76	0.99	1.55	1.52	1.43	1.96	2.08	1.52	1.83	1.67	1.95
$Li^+(EMC)_2$	16	1.96	0.97	0.67	0.74	1.52	1.76	1.83	1.55	1.12	1.20	1.49
$Li^+(EMC)_3$	32	1.53	0.86	0.51	0.53	0.88	1.38	1.39	1.40	0.94	0.98	1.16
$Li^+(EMC)_4$	33	1.53	0.63	0.54	0.56	0.87	1.18	1.16	1.21	0.76	0.83	1.08
$Li^+(EMC)_5$	34	0.75	0.99	0.72	0.87	1.28	1.20	1.32	1.62	1.45	1.58	1.93
$Li^+(EMC)_6$	31	1.10	1.37	0.99	1.15	1.94	1.19	1.27	1.71	2.14	2.28	3.00
$Li^+(DEC)_2$	28	2.69	0.95	0.55	0.49	1.10	2.19	2.38	1.71	1.23	1.27	1.54
$Li^+(DEC)_3$	33	2.00	0.82	0.52	0.59	0.96	1.65	1.64	1.59	1.22	1.32	1.92
$Li^+(DEC)_4$	33	0.86	0.57	0.91	0.91	1.40	0.76	0.81	1.00	1.36	1.36	1.83
$Li^+(DEC)_5$	33	0.73	0.57	0.50	0.67	1.63	1.74	2.06	3.06	1.68	2.02	3.07
$Li^+(DEC)_6$	30	0.72	0.87	0.76	0.92	1.29	1.21	1.34	1.75	1.46	1.51	2.03
$Li^+(VC)_4$	12	4.80	6.86	1.01	1.23	1.89	4.96	5.10	5.12	7.44	7.64	7.23
$Li^+(VC)_5$	27	2.04	2.81	1.75	1.83	2.89	2.16	2.32	2.96	3.62	3.73	4.87

$Li^+(VC)_6$	31	2.06	2.14	2.36	2.54	3.23	2.18	2.34	3.18	3.18	3.19	4.81
$Li^+(EC)_4$	18	2.60	1.35	1.49	1.67	2.81	2.93	3.02	3.88	2.70	2.89	3.99
$Li^+(EC)_5$	28	1.38	1.45	1.71	1.94	3.15	2.14	2.48	4.58	3.52	3.88	6.30
$Li^+(EC)_6$	31	1.72	2.61	2.06	2.46	5.57	3.23	3.48	5.25	5.03	5.70	11.56
$Li^+(PC)_3$	18	3.29	4.94	0.80	0.93	1.75	3.36	3.46	3.22	5.21	5.33	5.10
$Li^+(PC)_4$	31	2.78	3.27	1.11	1.25	2.37	3.16	3.25	3.50	4.08	4.22	4.63
$Li^+(PC)_5$	32	2.09	3.22	1.43	1.60	2.67	2.55	2.67	3.53	4.24	4.38	6.10
$Li^+(PC)_6$	27	3.13	4.80	1.66	1.87	2.44	3.93	4.01	4.05	4.65	4.85	5.38
minimum		0.72	0.29	0.44	0.44	0.87	0.76	0.81	0.81	0.76	0.78	0.83
Q_1		1.10	0.82	0.63	0.69	1.15	1.23	1.34	1.55	1.22	1.32	1.83
median		1.75	0.99	0.99	1.15	1.75	1.84	2.06	1.75	1.68	1.67	2.44
Q_3		2.60	2.81	1.46	1.52	2.56	2.93	3.02	3.50	3.62	3.88	4.81
maximum		4.80	6.86	2.36	2.54	5.57	4.96	5.10	5.25	7.44	7.64	11.56
average		1.96	1.89	1.07	1.19	1.96	2.16	2.25	2.50	2.52	2.65	3.44

[a] Number of conformers.

Table S8. Maximum conformational electronic (ΔE_{max}) and Gibbs (ΔG_{max}) energies obtained for individual $Li^+(S)_n$ clusters using different vibrational thermochemistry and/or continuum solvation models. All values are given in kcal mol^{-1}.

	ΔE_{max}	ΔG_{max}										
	gas	PCM	Solv	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO	msRRHO (100,4,0)	msRRHO (100,4,1)	sRRHO
				gas			+PCM			+Solv		
$Li^+(BC)_2$	27.24	18.86	17.36	29.10	29.09	30.79	19.62	19.61	21.31	19.22	19.21	20.91
$Li^+(BC)_3$	14.41	14.58	12.11	14.35	14.34	15.08	12.89	12.94	13.67	12.16	12.15	12.60
$Li^+(BC)_4$	2.56	2.23	2.45	2.93	3.28	4.86	3.61	3.98	5.36	4.25	4.60	6.18
$Li^+(BC)_5$	7.06	5.11	6.55	6.93	7.14	8.26	6.15	6.13	6.83	7.62	7.83	8.95
$Li^+(BC)_6$	15.06	13.48	12.21	12.62	12.39	12.21	11.56	11.54	11.33	12.60	12.81	15.90

$Li^+(DMC)_3$	5.39	1.93	3.17	5.69	5.70	6.34	1.32	1.36	1.81	2.76	2.75	3.54
$Li^+(DMC)_4$	12.09	11.96	10.28	12.95	12.95	14.13	10.78	10.82	11.72	10.89	10.96	12.37
$Li^+(DMC)_5$	18.29	16.14	15.46	16.45	16.08	15.28	14.31	13.93	13.14	13.62	13.25	12.45
$Li^+(DMC)_6$	9.01	7.27	6.15	6.01	6.68	8.58	5.08	4.88	5.98	4.94	5.86	8.54
$Li^+(EMC)_2$	7.15	2.22	4.33	6.92	6.94	8.11	2.58	2.60	3.77	4.60	4.63	5.87
$Li^+(EMC)_3$	6.21	2.03	4.04	6.08	6.03	7.26	2.81	2.96	3.35	4.46	4.62	5.74
$Li^+(EMC)_4$	8.93	5.93	8.40	8.99	9.63	10.77	6.83	7.13	8.20	8.84	9.31	10.45
$Li^+(EMC)_5$	29.69	26.95	24.06	27.28	26.79	25.86	24.44	23.95	23.02	22.10	21.78	21.02
$Li^+(EMC)_6$	29.52	27.17	25.94	28.19	28.12	27.52	25.84	25.77	25.48	24.91	24.94	25.96
$Li^+(DEC)_2$	7.45	2.72	5.77	8.06	7.86	8.75	2.84	2.59	3.56	6.38	6.18	7.08
$Li^+(DEC)_3$	7.46	3.39	6.56	7.74	7.54	8.49	3.80	3.78	4.78	8.01	7.98	9.28
$Li^+(DEC)_4$	7.23	5.81	7.31	8.77	8.72	9.72	7.45	7.40	8.40	8.95	8.90	9.90
$Li^+(DEC)_5$	10.87	7.88	10.01	11.07	11.33	12.96	9.61	10.05	11.68	11.73	12.17	13.80
$Li^+(DEC)_6$	9.03	9.75	11.82	9.61	10.05	10.45	10.36	10.77	11.26	12.65	12.90	13.55
$Li^+(VC)_4$	49.20	39.01	31.46	48.55	48.09	50.26	36.96	36.48	38.10	30.80	30.34	32.01
$Li^+(VC)_5$	54.55	43.89	31.50	50.18	49.56	50.36	39.25	38.33	37.66	28.68	28.06	28.86
$Li^+(VC)_6$	26.64	28.58	19.60	22.91	22.52	24.24	22.26	21.81	21.29	17.92	17.96	19.80
$Li^+(EC)_4$	20.37	22.82	19.39	21.95	22.34	25.42	23.11	23.50	26.58	22.77	23.16	26.24
$Li^+(EC)_5$	11.52	12.82	11.09	12.28	12.24	17.05	12.08	12.69	17.50	16.33	16.94	21.75
$Li^+(EC)_6$	16.30	16.79	10.28	10.19	9.90	17.41	10.63	10.69	14.14	14.31	15.53	23.56
$Li^+(PC)_3$	38.79	30.69	26.38	38.44	38.48	41.22	30.57	30.64	33.38	27.90	27.97	30.71
$Li^+(PC)_4$	44.82	39.39	34.16	45.08	44.86	47.20	39.39	39.23	40.89	34.98	34.76	37.10
$Li^+(PC)_5$	50.76	41.23	34.25	47.87	47.49	48.60	38.86	38.59	40.34	34.76	34.80	40.49
$Li^+(PC)_6$	51.50	41.83	34.72	49.39	48.94	49.95	40.03	39.80	41.35	36.32	36.18	39.52
minimum	2.56	1.93	2.45	2.93	3.28	4.86	1.32	1.36	1.81	2.76	2.75	3.54
Q_1	7.46	5.81	6.56	8.06	7.86	8.75	6.15	6.13	6.83	8.01	7.98	9.28
median	14.41	13.48	11.82	12.62	12.39	15.08	11.56	11.54	13.14	12.65	12.90	13.80
Q_3	29.52	27.17	24.06	28.19	28.12	27.52	24.44	23.95	25.48	22.77	23.16	25.96
maximum	54.55	43.89	34.72	50.18	49.56	50.36	40.03	39.80	41.35	36.32	36.18	40.49
average	20.66	17.33	15.41	19.88	19.83	21.28	16.38	16.34	17.44	16.05	16.16	18.07

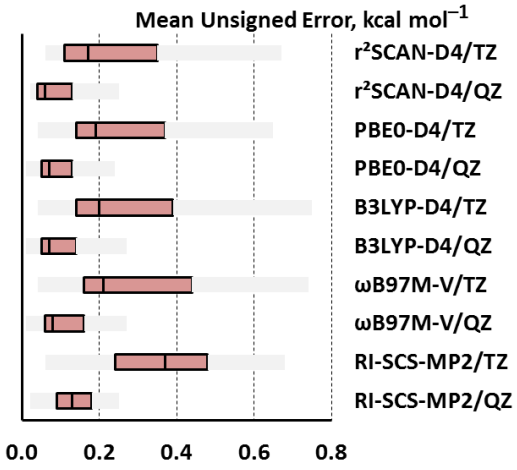


Figure S1. Mean unsigned errors (MUEs) for the conformational energies obtained using DFT and RI-SCS-MP2 approximations with TZ and QZ basis sets calculated versus their CBS-extrapolated counterparts. The left/right sides of the rectangles correspond to the first ($Q1$) and third ($Q3$) quartiles, respectively. The vertical bold line inside each rectangle shows the median value. The left/right sides of the gray boxes display the lowest/largest values for each method.

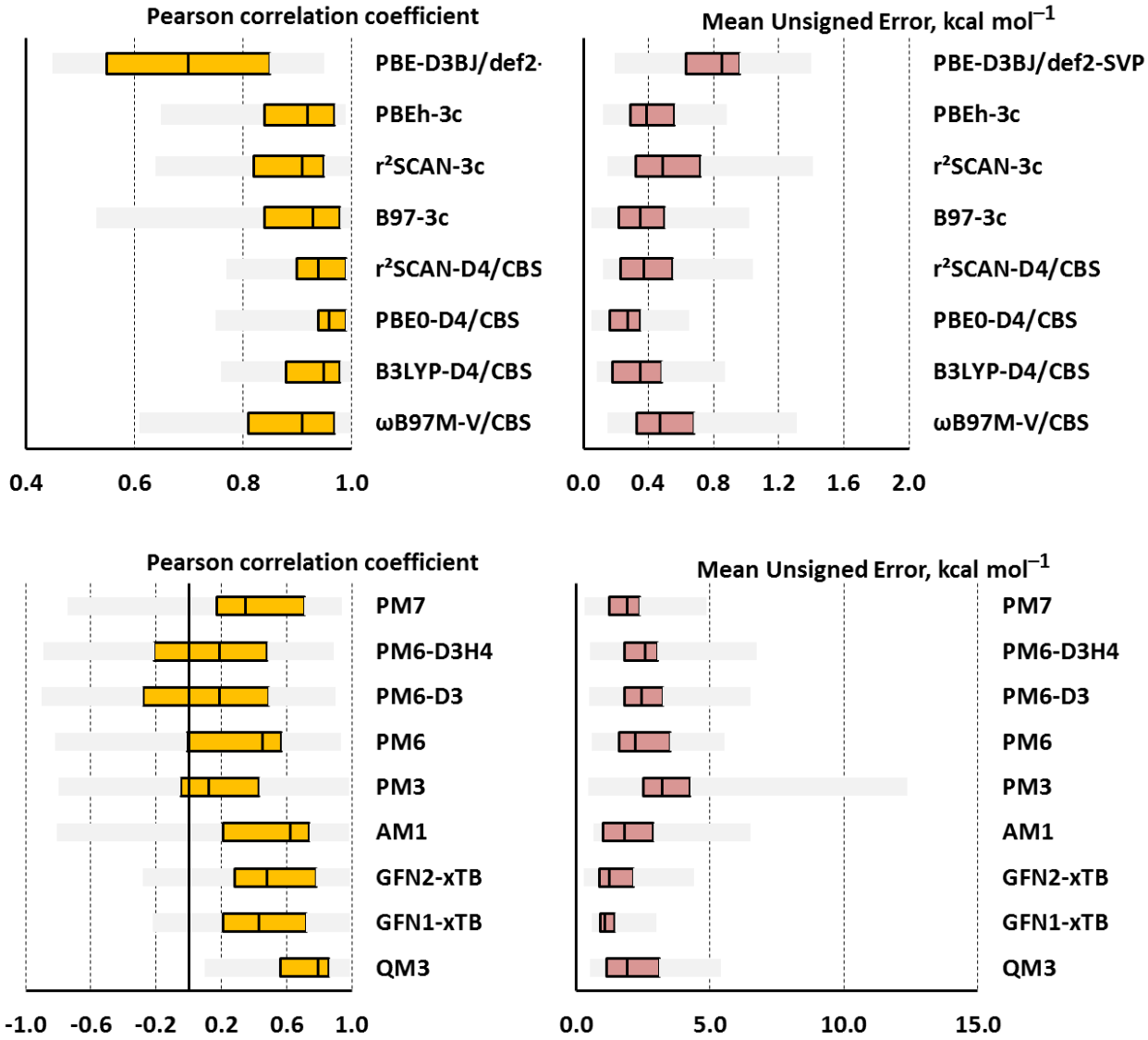


Figure S2. Pearson correlation coefficients and mean unsigned errors (MUEs) for the DFT and semi-empirical methods considered in this work with respect to the reference RI-SCS-MP2/CBS approximation obtained for the subset of **LICARBCONF806** database containing only the conformers with relative energies below 3 kcal mol^{-1} at RI-SCS-MP2/CBS level of theory. The left/right sides of the rectangles correspond to the first (*Q*1) and third (*Q*3) quartiles, respectively. The vertical bold line inside each rectangle shows the median value. The left/right sides of the gray boxes display the lowest/largest values for each method.

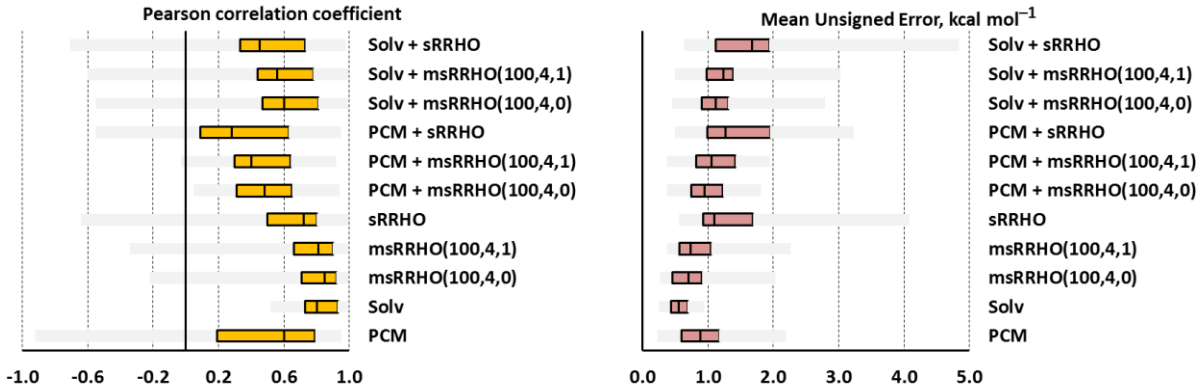
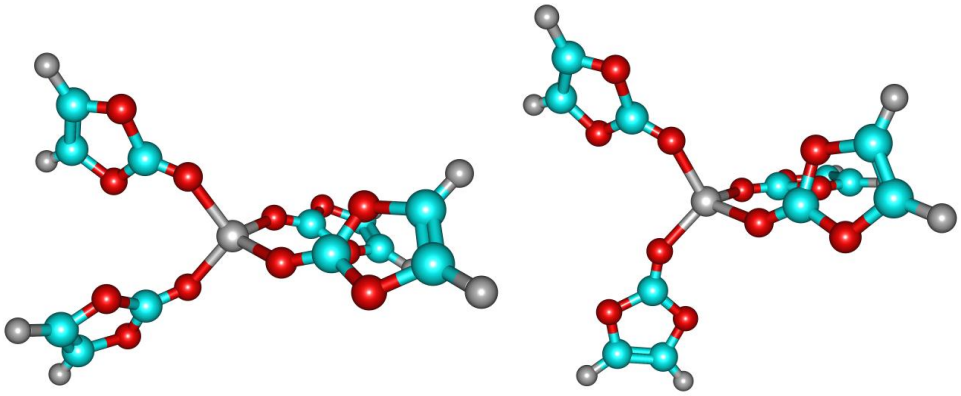


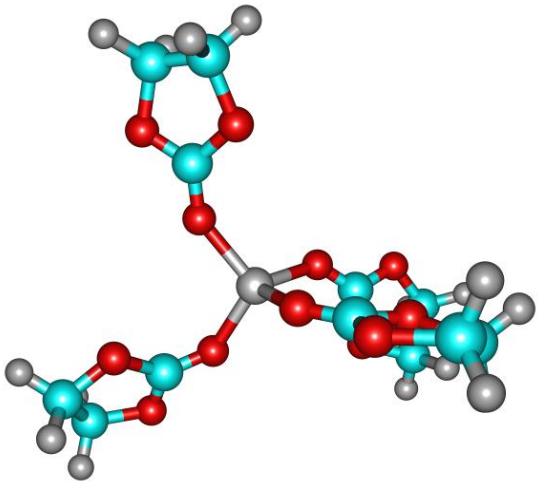
Figure S3. Pearson correlation coefficients and mean unsigned errors (MUEs) for the different models for vibrational thermostatistical corrections (sRRHO and msRRHO) and continuum solvation models (PCM and Solv) obtained for the subset of **LICARBCONF806** database containing only the conformers with relative energies below 3 kcal mol^{-1}. Both statistical measures are computed versus reference gas-phase RI-SCS-MP2/CBS conformational energies. Detailed description of the models is given in Section 2.4. The left/right sides of the rectangles correspond to the first ($Q1$) and third ($Q3$) quartiles, respectively. The vertical bold line inside each rectangle shows the median value. The left/right sides of the gray boxes display the lowest/largest values for each method.

Lowest energy conformers of $Li^+(S)_4$ clusters according to the conformational electronic and Gibbs free energies



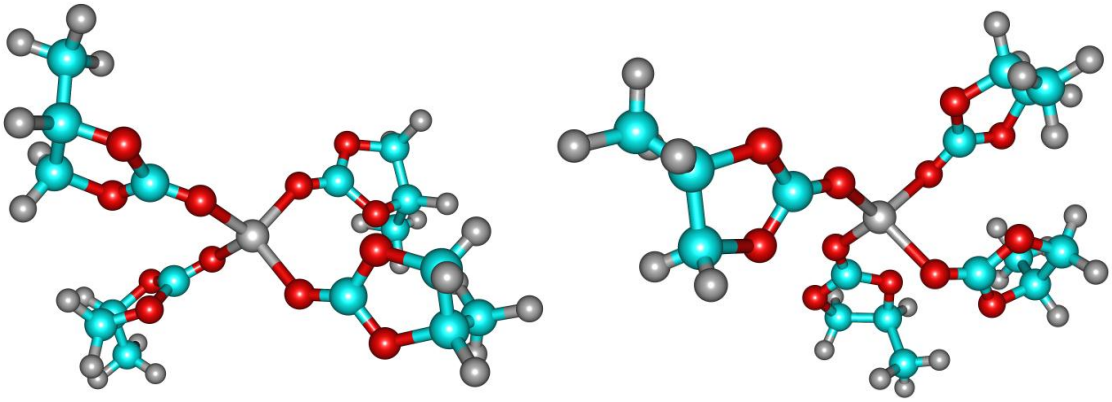
ΔE_{conf}	+0.4	0.0
ΔG_{conf}		
• (HO/msRRHO + PCM)	0.0	+0.3/+0.4
• (HO/msRRHO + Solv)	+0.04/+0.10	0.0

Figure S4. Lowest energy spatial structures of $Li^+(VC)_4$ cluster. Conformational energies are given in kcal mol^{-1}. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).



ΔE_{conf}	0.0
ΔG_{conf}	0.0

Figure S5. Lowest energy spatial structure of $Li^+(EC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).



ΔE_{conf}	+0.2	0.0
ΔG_{conf}	0.0	+2.7/+4.5

Figure S6. Lowest energy spatial structures of $Li^{+}(PC)_4$ cluster. Conformational energies are given in kcal mol^{-1}. The spread in ΔG_{conf} refers to the influence of a particular combination of the continuum solvation model (PCM or Solv) and thermostatistical correction (HO, msRRHO(100,4,0), msRRHO(100,4,1). Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

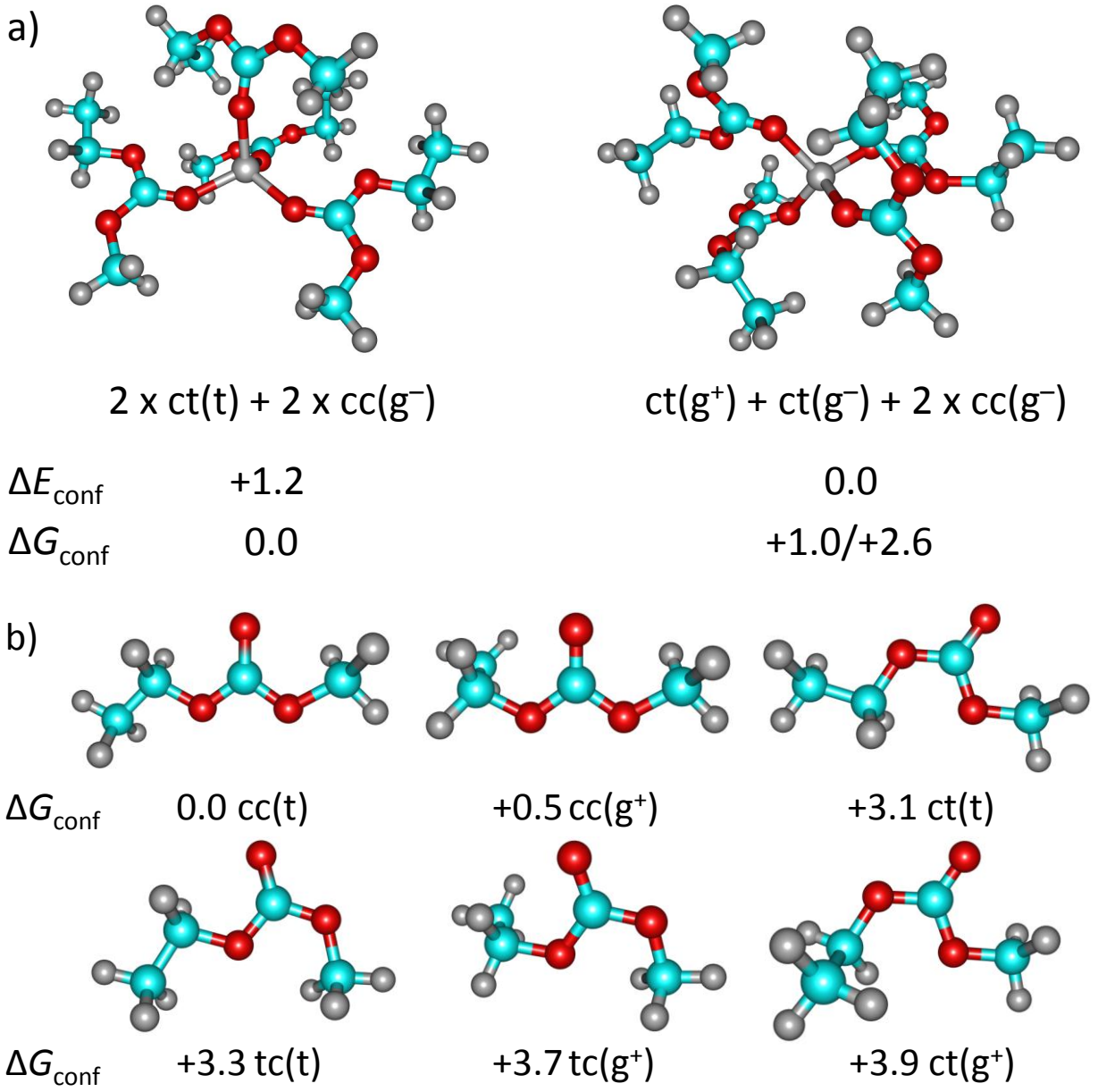


Figure S7. a) Lowest energy spatial structures of $Li^+(EMC)_4$ cluster and b) conformers of Ethylmethyl carbonate (EMC). Conformational energies are given in kcal mol^{-1}. The spread in ΔG_{conf} for $Li^+(EMC)_4$ refers to the influence of a particular combination of the continuum solvation model (PCM or Solv) and thermostatistical correction (HO, msRRHO(100,4,0), msRRHO(100,4,1). Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

Generation of conformers of flexible carbonates (BC, EMC, DEC) with *uniconf* program

In order to obtain the conformers of EMC and DEC molecules, the systematic conformational search was performed with *uniconf* program. Starting structures of g^- conformer of BC, cc(t) conformer of EMC and cc(tt) conformer of DEC were optimized at B97-3c level of theory with subsequent calculation of CHELPG atomic charges. Cartesian coordinates of the optimized structures and the respective sets of atomic charges were used as input data for the *uniconf* program. The torsional angles about the following rotatable bonds were systematically changed to obtain possible conformations of the molecules (see Figure S8):

- BC: C6–C9, in the range of 330 degrees with a step of 30 degrees;
- EMC: C1–O2 and C1–O3 in the range of 180 degrees with a step of 180 degrees (i.e., only cis-cis and cis-trans arrangements of the anomeric carbons were considered) and O3–C5 in the range of 300 degrees with a step of 60 degrees;
- DEC: C1–O2 and C1–O3 in the range of 180 degrees with a step of 180 degrees, O2–C12 in the range of 180 degrees with a step of 60 degrees; O3–C5 in the range of 300 degrees with a step of 60 degrees.

All obtained structures were pre-optimized at B97-3c level of theory and duplicates were removed. Finally, all the unique structures were re-optimized at PBE0-D3(BJ)/def2-TZVP level of theory followed by calculations of vibrational frequencies. Reference single-point energies of the optimized structures were obtained at RI-SCS-MP2/CBS {def2-TZVPP/def2-QZVPP}level of theory. Thermostatistical corrections were computed using msRRHO(100,4,1) approximation with a scale factor of 0.983.

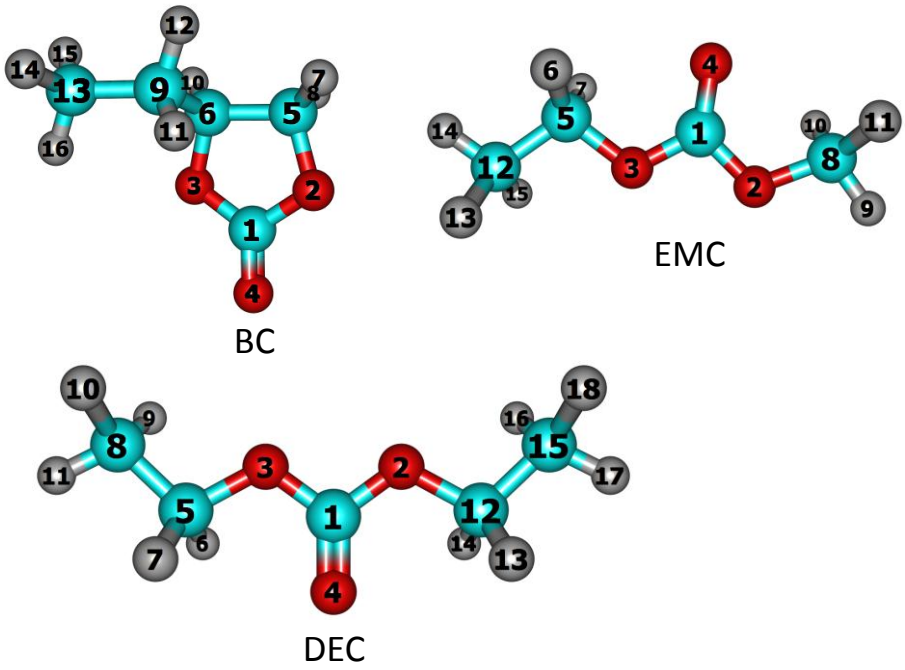


Figure S8. Molecular models flexible organic carbonates used as starting structures for the conformer generation with *uniconf* program. Internal operational atomic numbering is used. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray).

Spatial structures of the lowest energy conformers of $Li^+(S)_n$ clusters according to the msRRHO(100,4,1) + Solv conformational Gibbs energies

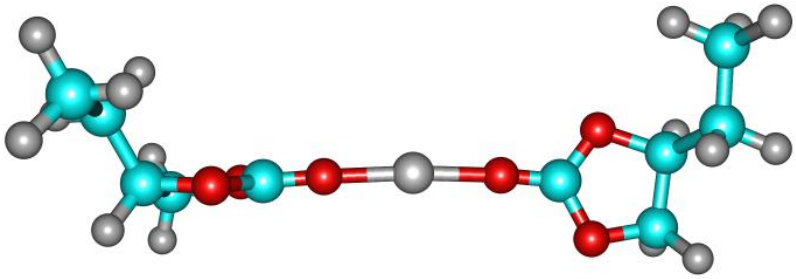


Figure S9. Molecular model of $Li^+(BC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

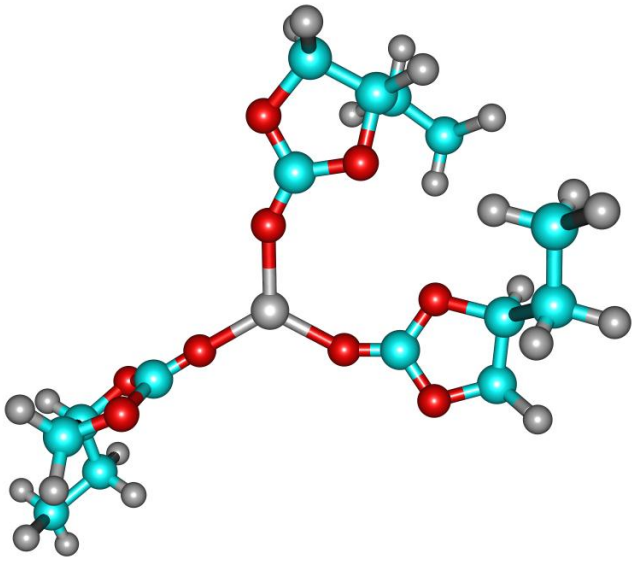


Figure S10. Molecular model of $Li^+(BC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

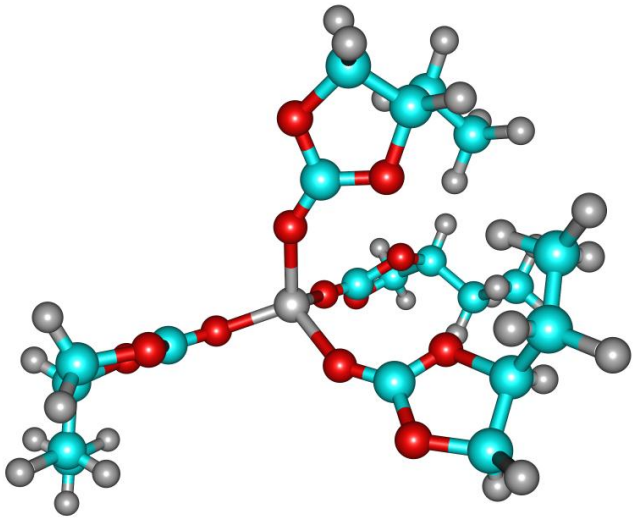


Figure S11. Molecular model of $Li^+(BC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

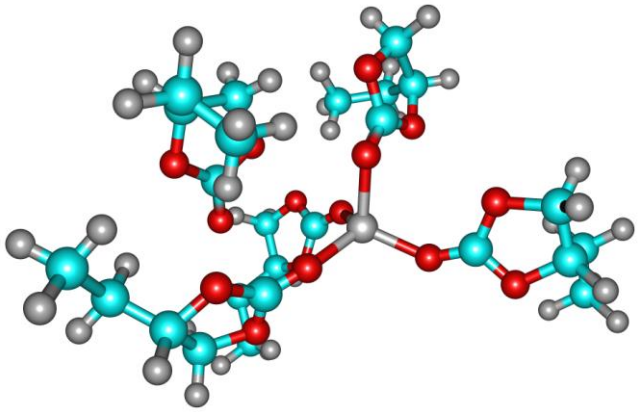


Figure S12. Molecular model of $Li^+(BC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

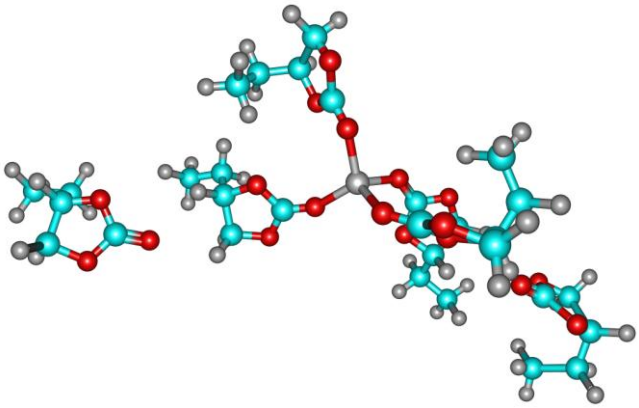


Figure S13. Molecular model of $Li^+(BC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

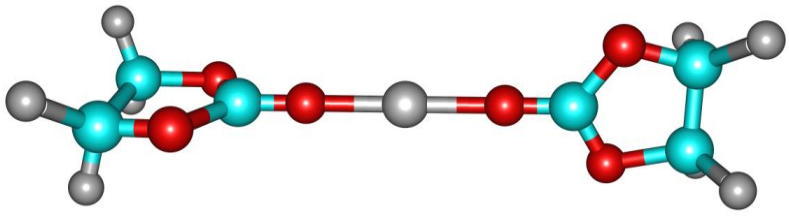


Figure S14. Molecular model of $Li^+(EC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

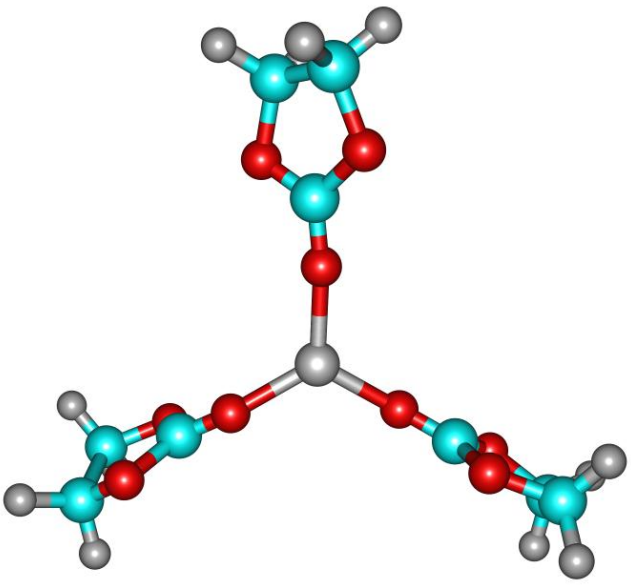


Figure S15. Molecular model of $Li^+(EC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

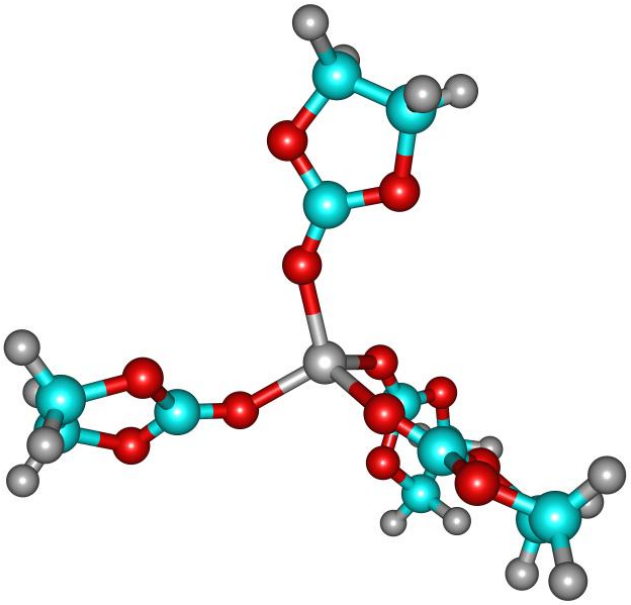


Figure S16. Molecular model of $Li^+(EC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

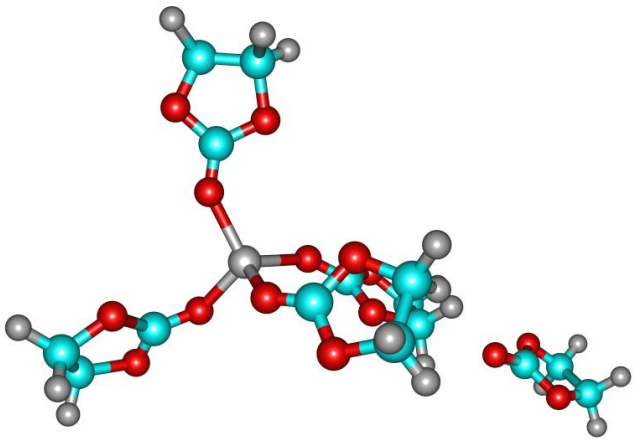


Figure S17. Molecular model of $Li^+(EC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

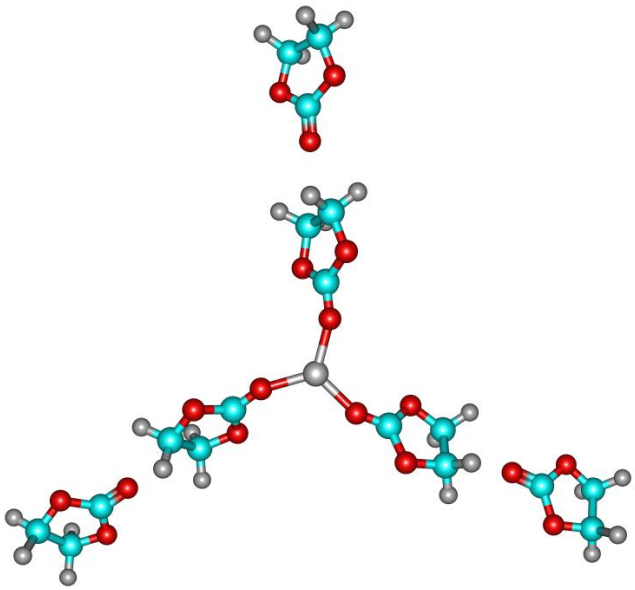


Figure S18. Molecular model of $Li^+(EC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

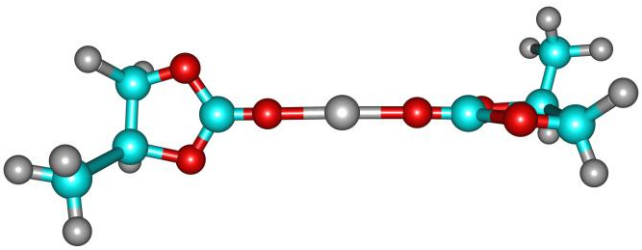


Figure S19. Molecular model of $Li^+(PC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

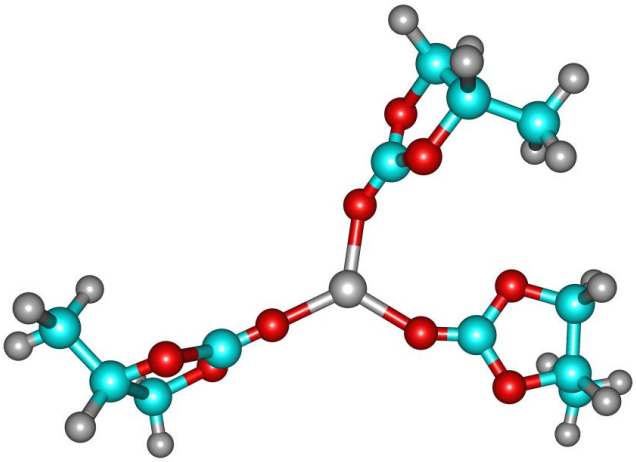


Figure S20. Molecular model of $Li^+(PC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

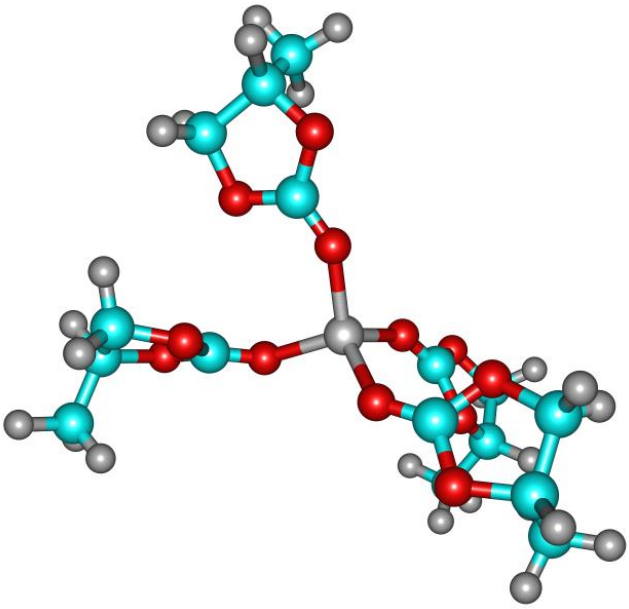


Figure S21. Molecular model of $Li^+(PC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

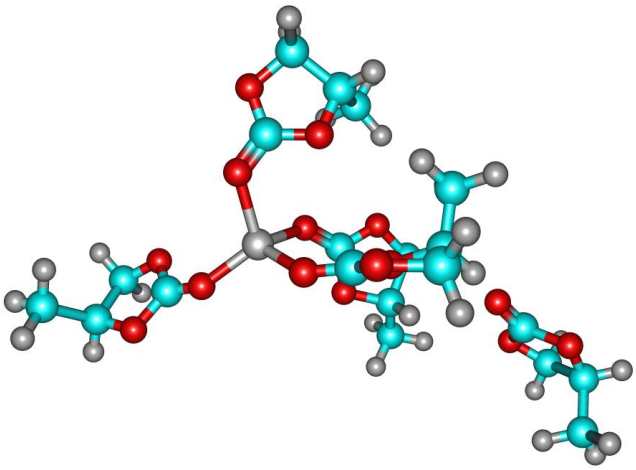


Figure S22. Molecular model of $Li^+(PC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

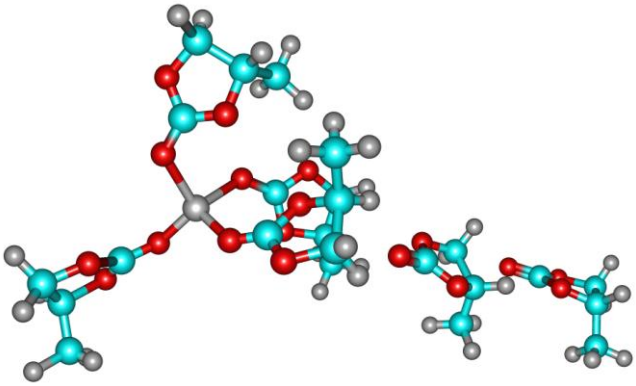


Figure S23. Molecular model of $Li^+(PC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

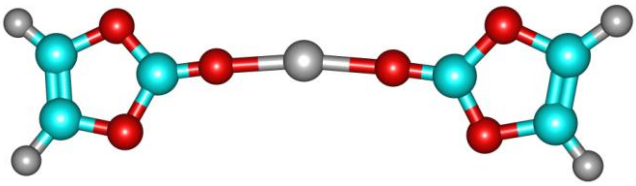


Figure S24. Molecular model of $Li^+(VC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

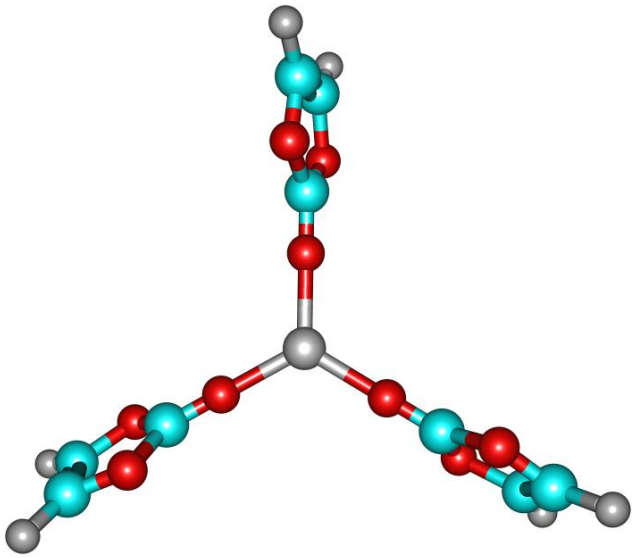


Figure S25. Molecular model of $Li^+(VC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

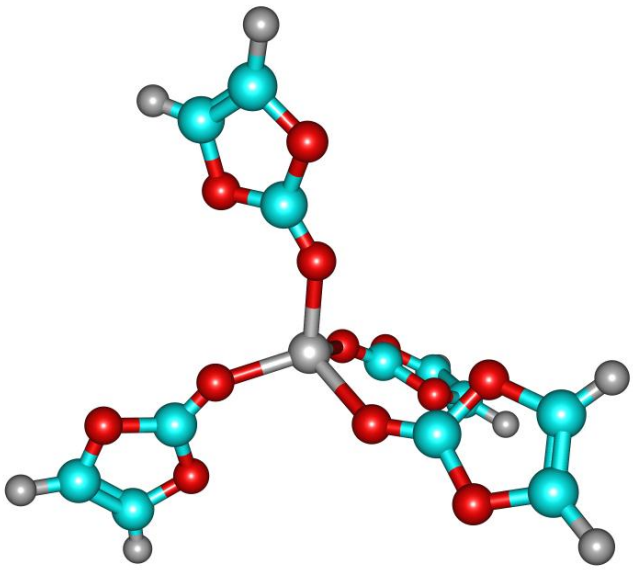


Figure S26. Molecular model of $Li^+(VC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

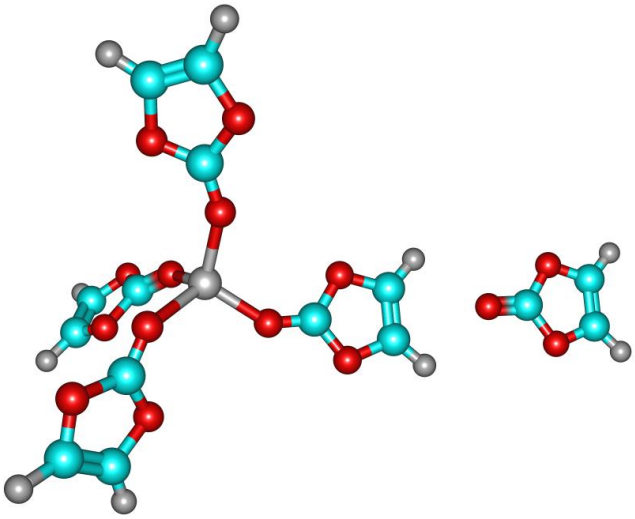


Figure S27. Molecular model of $Li^+(VC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

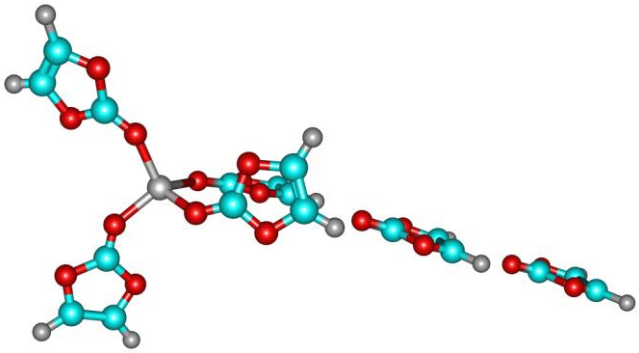


Figure S28. Molecular model of $Li^+(VC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

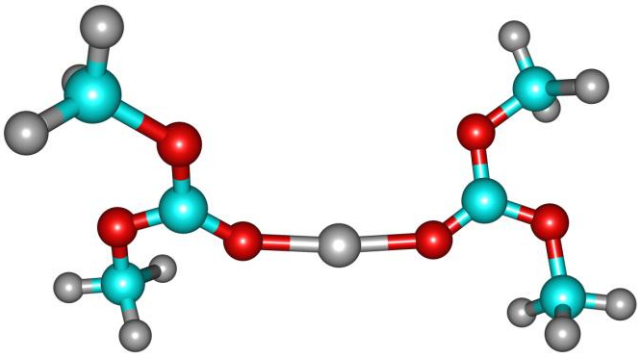


Figure S29. Molecular model of $Li^+(DMC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

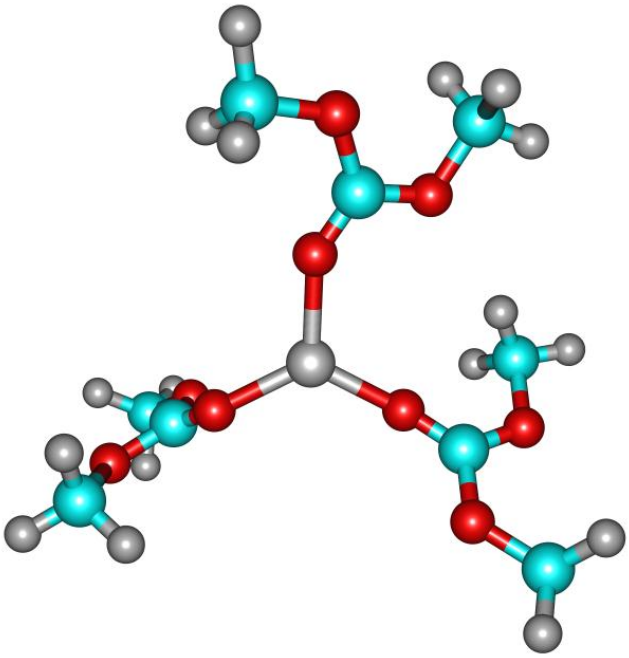


Figure S30. Molecular model of $Li^+(DMC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

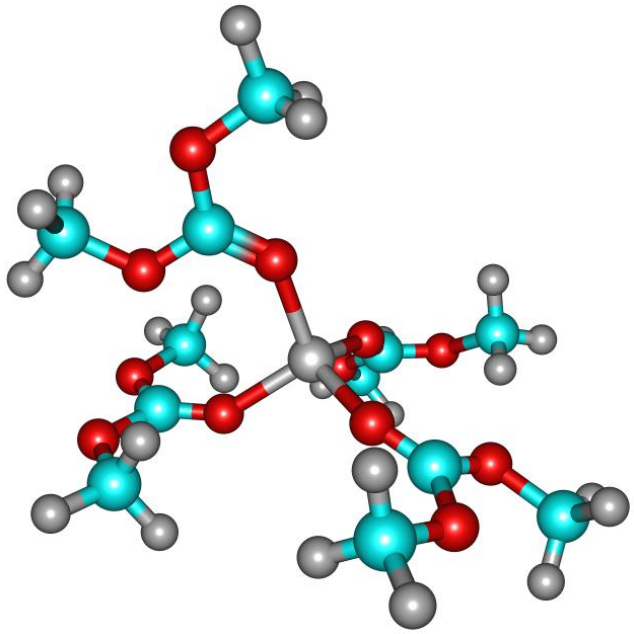


Figure S31. Molecular model of $Li^+(DMC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

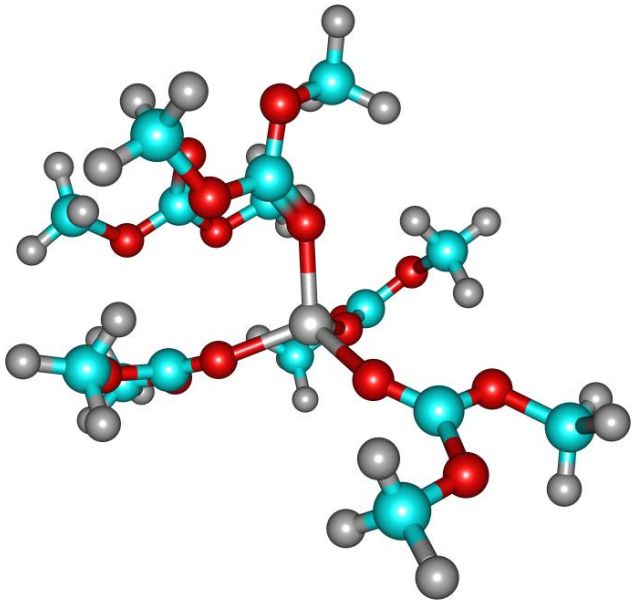


Figure S32. Molecular model of $Li^+(DMC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

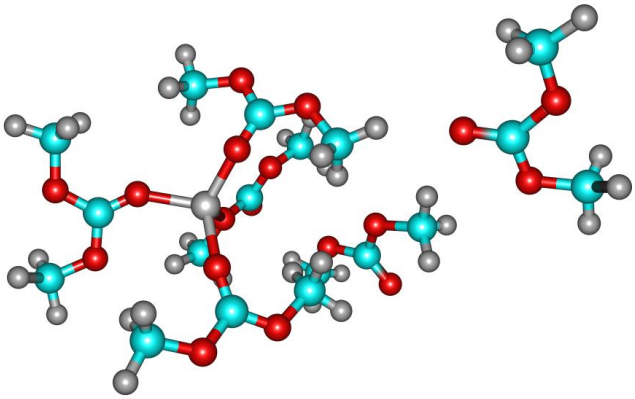


Figure S33. Molecular model of $Li^{+}(DMC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

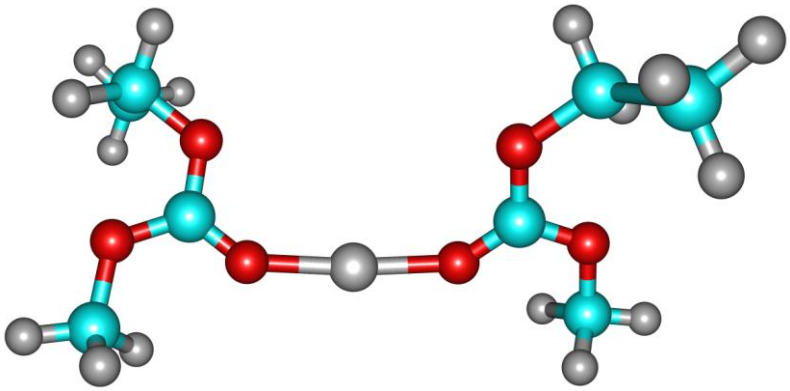


Figure S34. Molecular model of $Li^{+}(EMC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

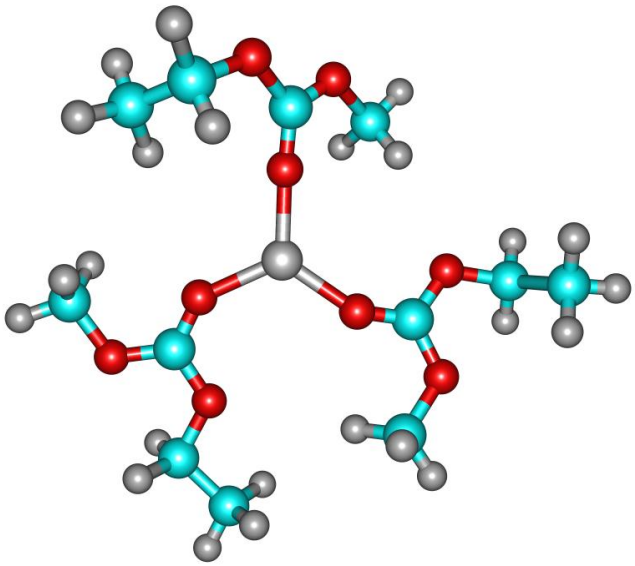


Figure S35. Molecular model of $Li^{+}(EMC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

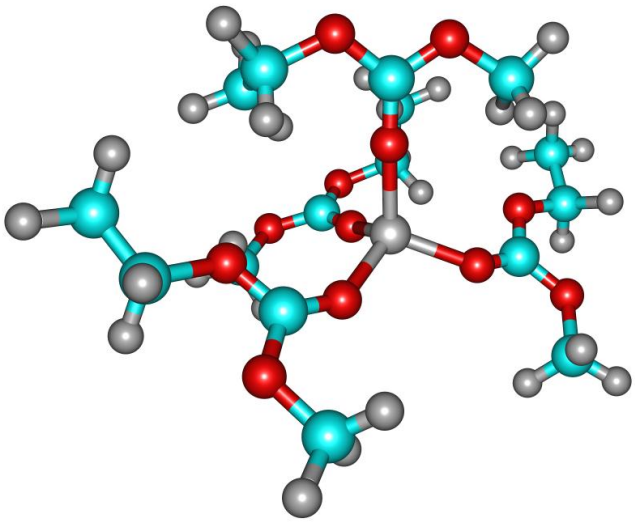


Figure S36. Molecular model of $Li^{+}(EMC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

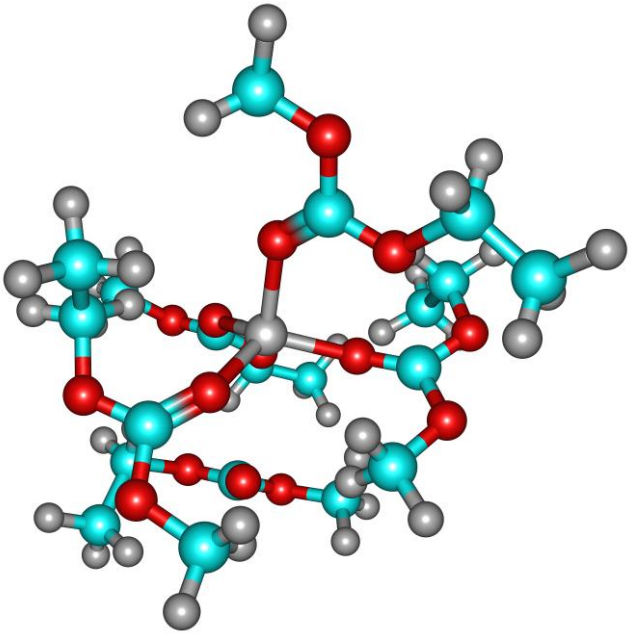


Figure S37. Molecular model of $Li^{+}(EMC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

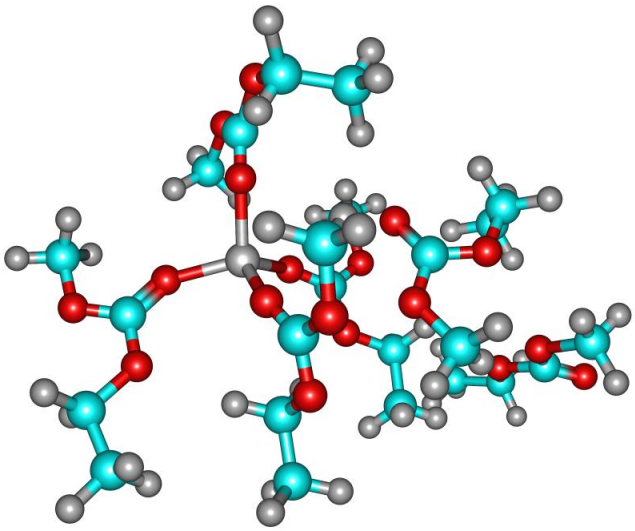


Figure S38. Molecular model of $Li^+(EMC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

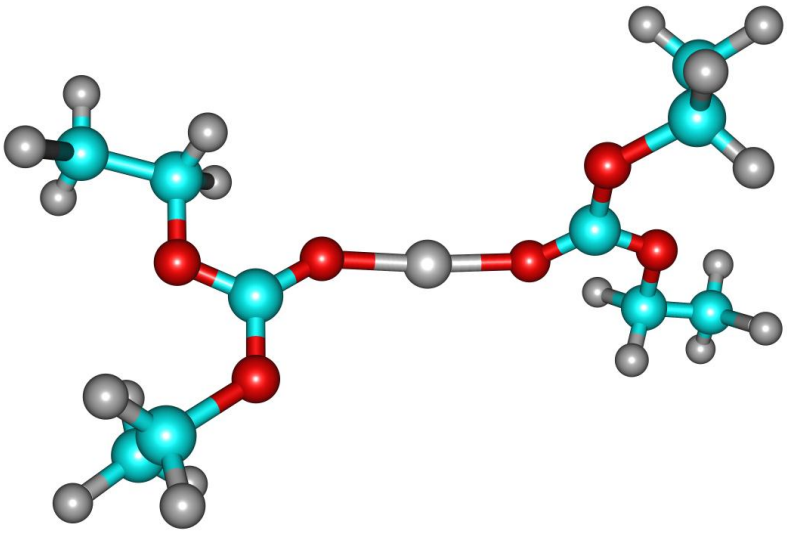


Figure S39. Molecular model of $Li^+(DEC)_2$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

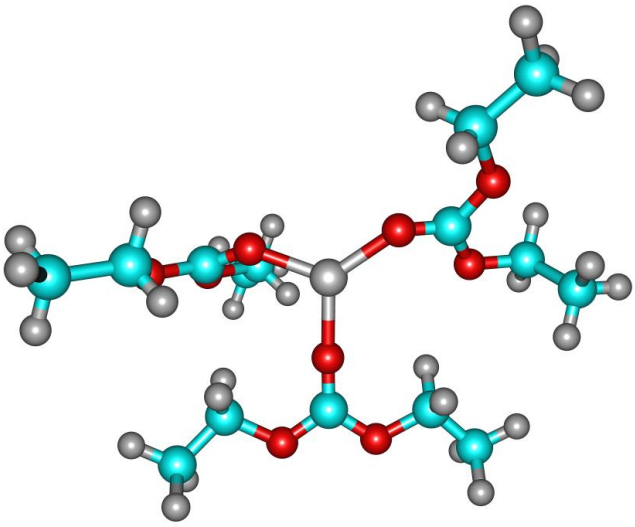


Figure S40. Molecular model of $Li^{+}(DEC)_3$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

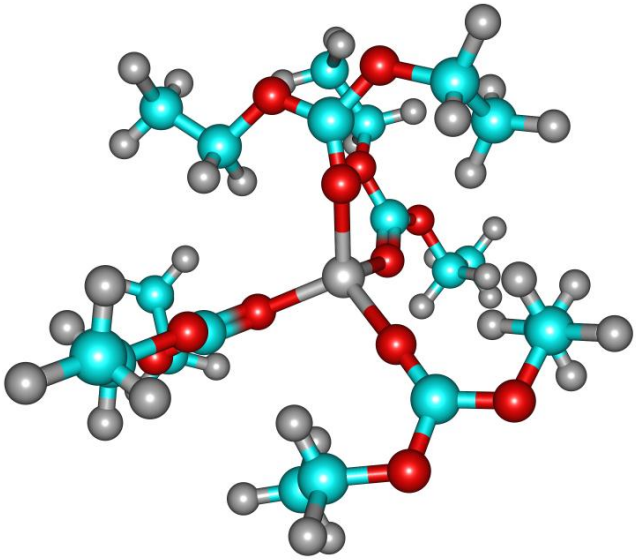


Figure S41. Molecular model of $Li^{+}(DEC)_4$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

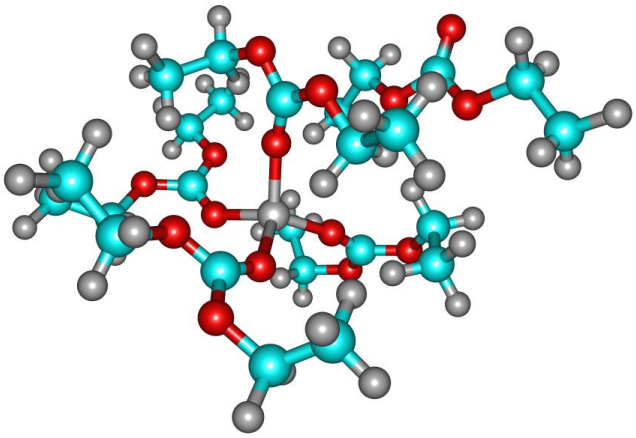


Figure S42. Molecular model of $Li^{+}(DEC)_5$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).

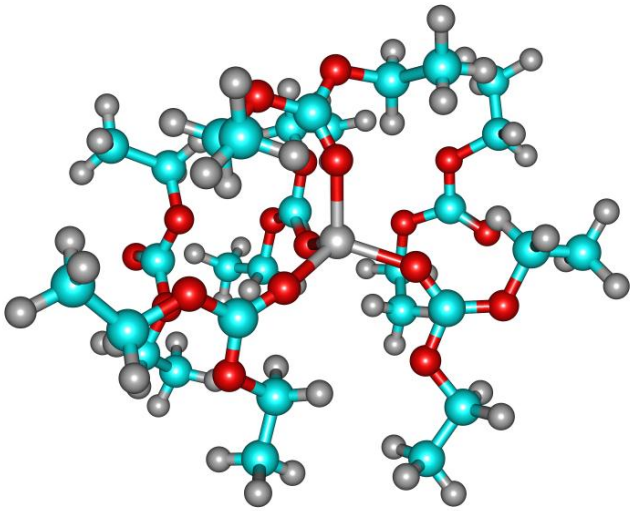


Figure S43. Molecular model of $Li^{+}(DEC)_6$ cluster. Atom color coding: carbon (turquoise), oxygen (red), hydrogen (gray), lithium (gray).