

Electronic Supplementary Information

Probing the potential of halogen-free superhalogen anions forming effective electrolyte of Li-ion battery. A theoretical prospect from combined *ab initio* and DFT study

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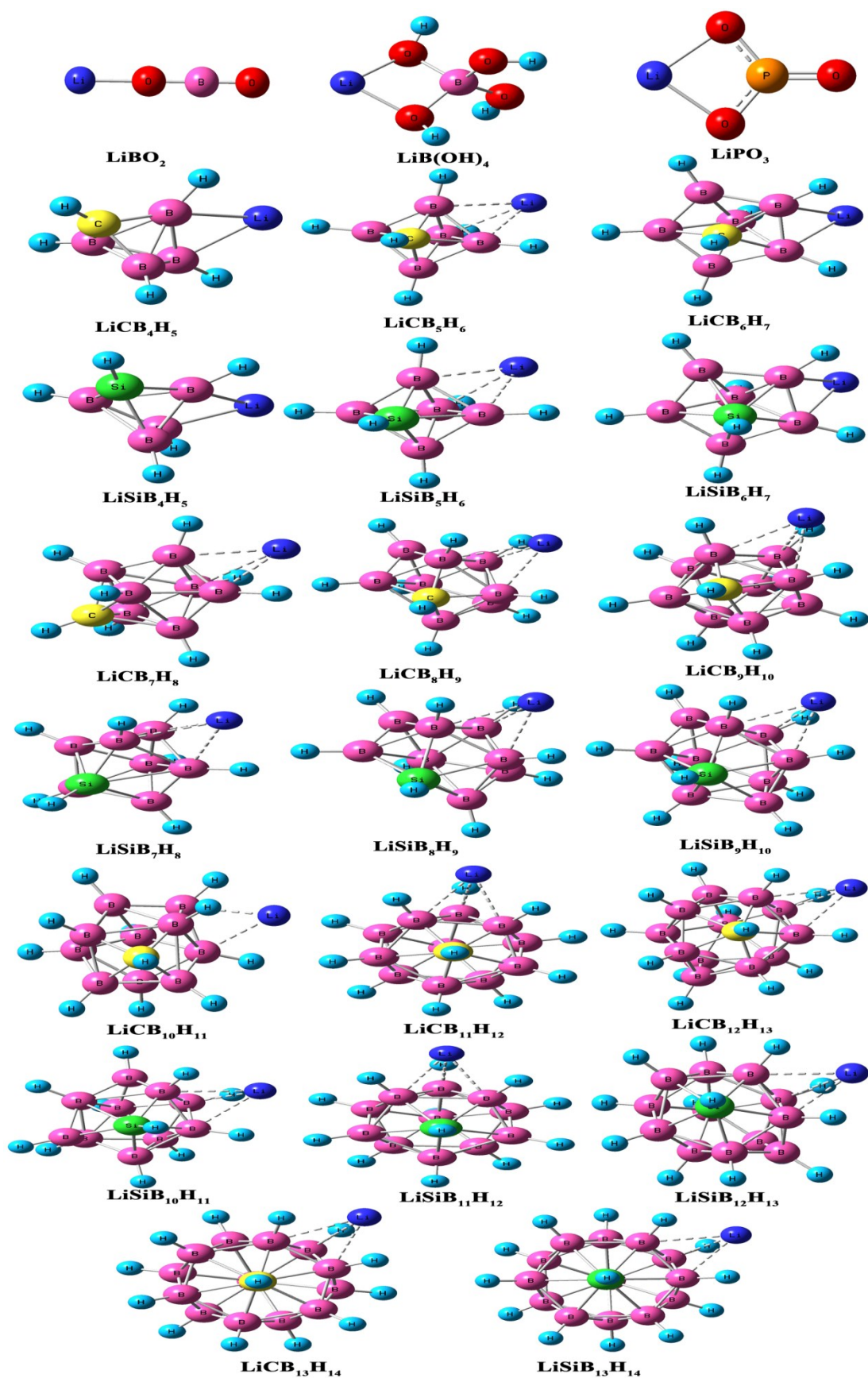


Fig. S1 Optimized geometries of different Li-salts containing new potential electrolytes in Li-ion batteries under study at $\omega\text{B97XD/6-311+G}^*$ level.

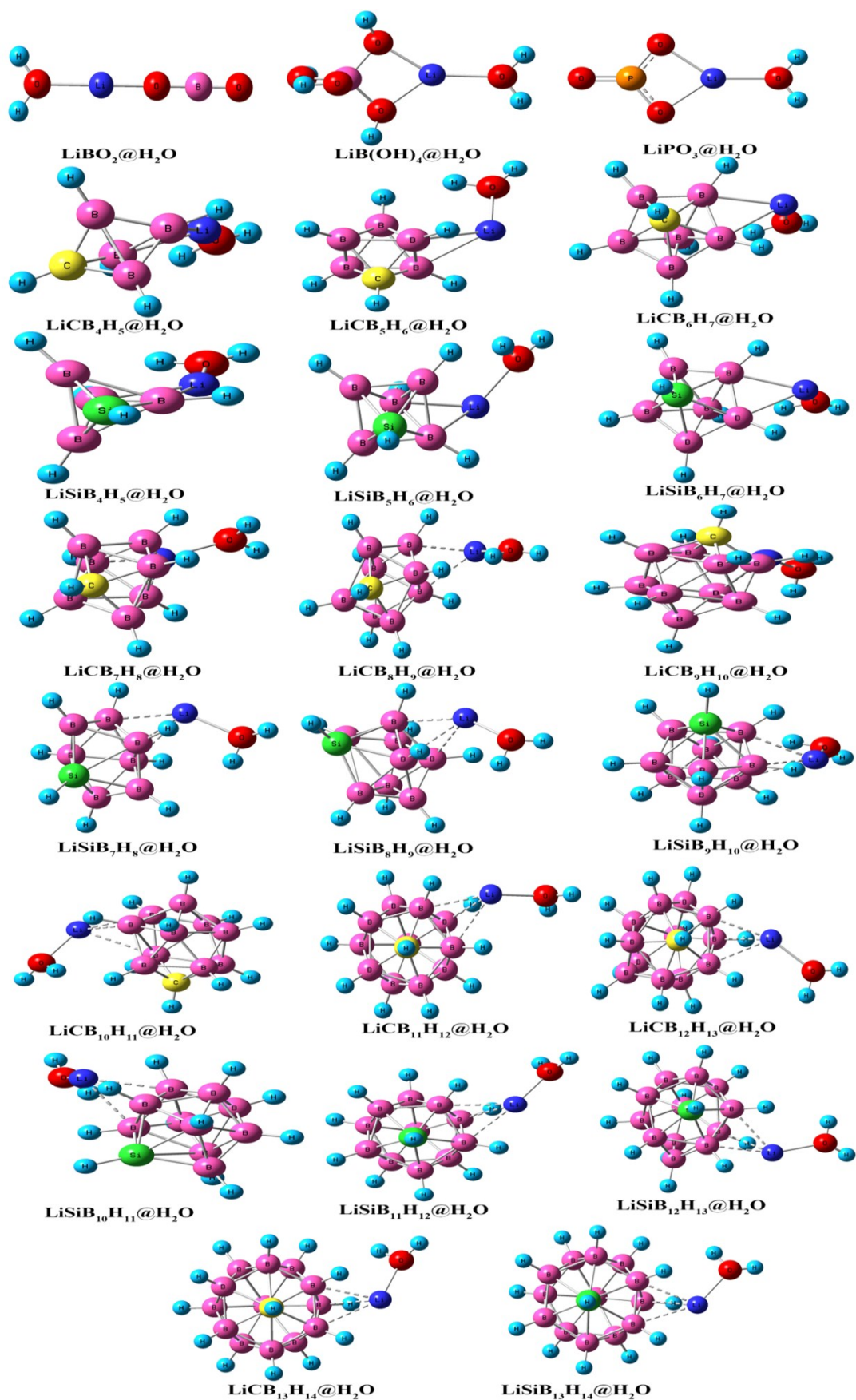


Fig. S2 Optimized geometries of Li-salts interacting with H_2O under study at $\omega B97XD/6-311+G^*$ level.

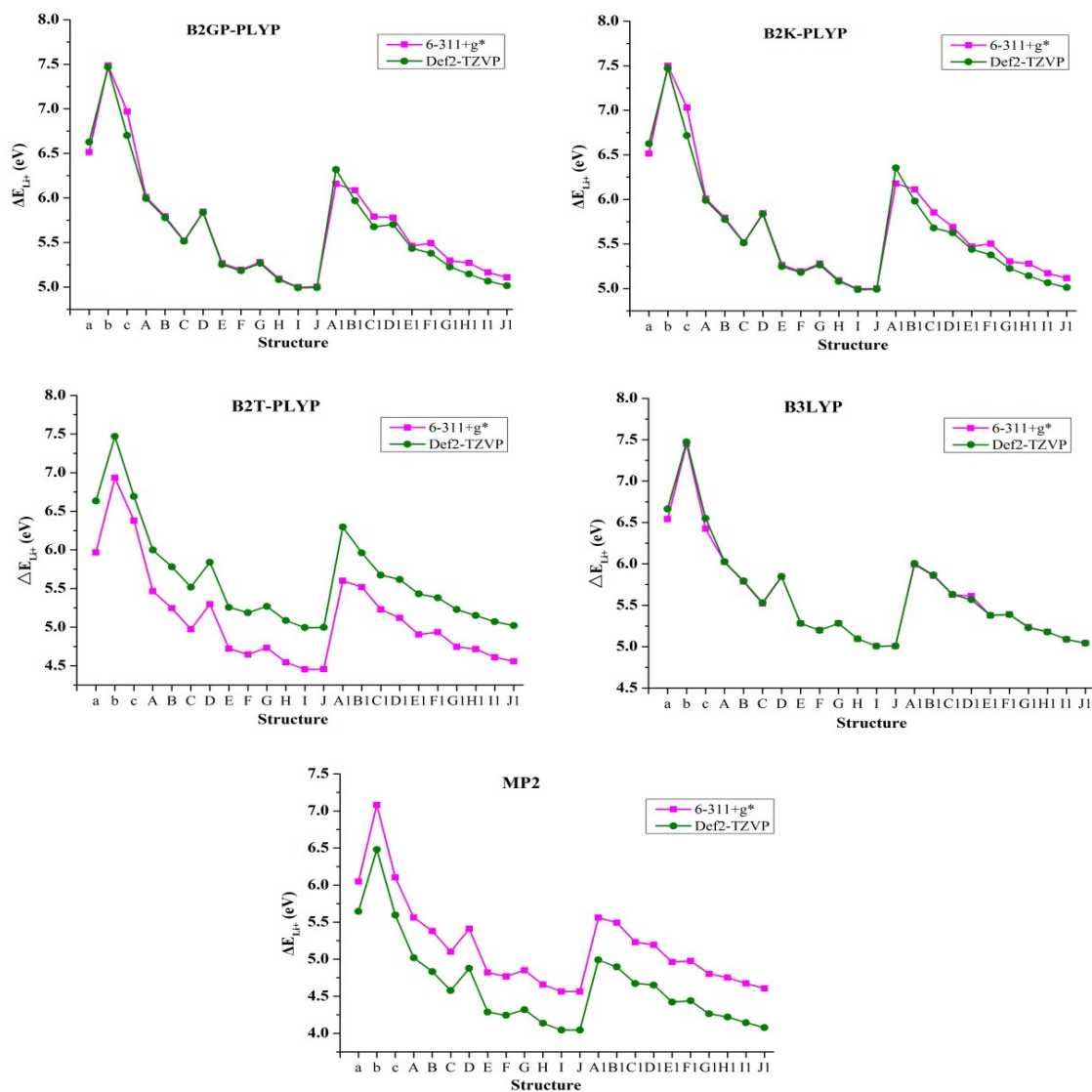


Fig. S3 The variations of Li^+ Binding Energy (ΔE_{Li^+}) of twenty-three potential new electrolytes (**a-JI**) at various functionals levels with different basis sets.

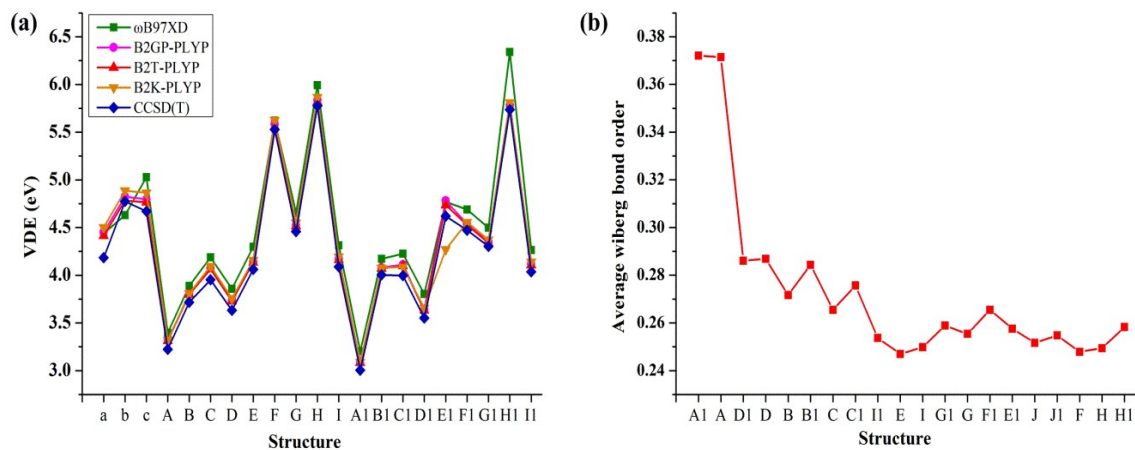


Fig. S4 (a) The variations of VDE of anion (**a-I1**) at various functionals and CCSD(T) levels with 6-311+G* basis set; (b) The Li-B average wiberg bond order of the corresponding Li-salt with increasing VDE of anion (**A-J1**) at the ω B97XD/6-311+G* level.

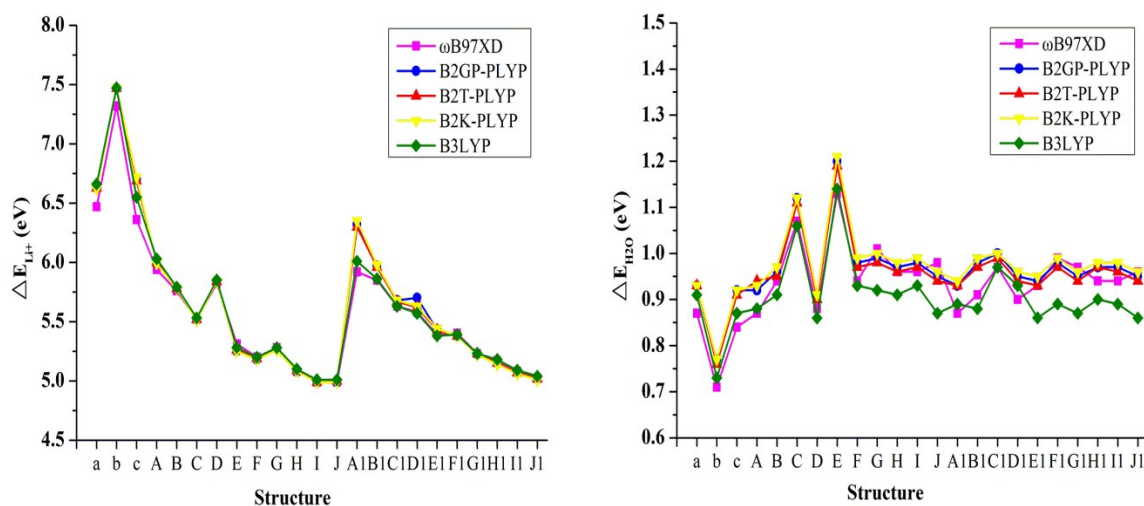


Fig. S(5) The variations of Li⁺(a) and H₂O(b) binding energy (ΔE_{Li^+} , ΔE_{H_2O}) of the structure (**a-J1**) at various functional level with Def2-TZVP basis set.

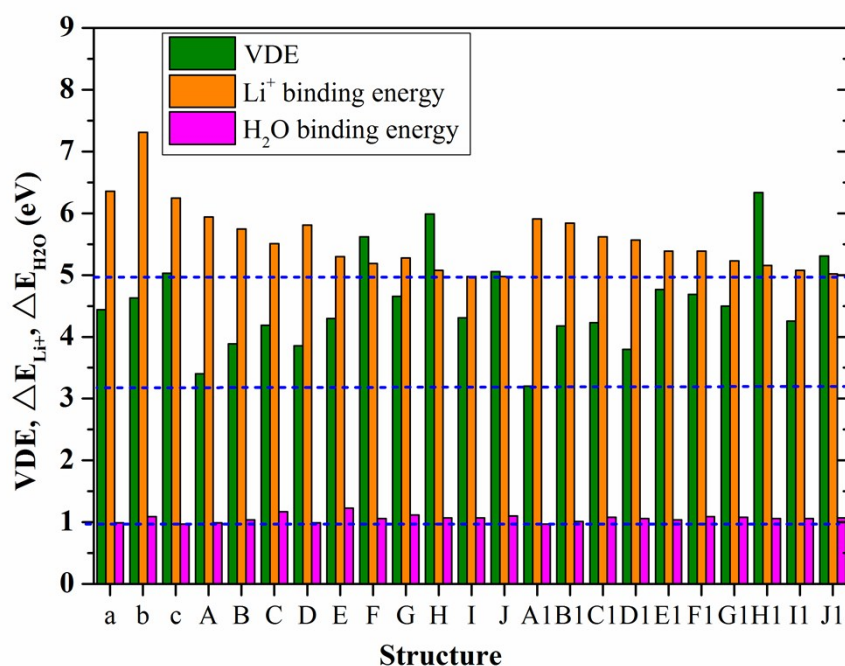


Fig. S(6) Comparison between VDEs and binding energies of Li⁺ and H₂O in proposed new halogen-free electrolytes at ω B97XD/6-311+G* level.

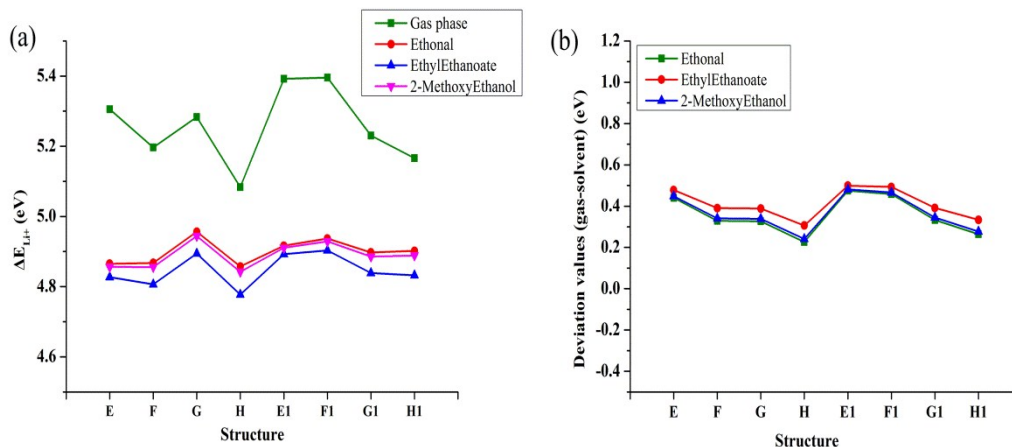


Fig. S6 The variations of Li^+ binding energy (ΔE_{Li^+}) (a) values and the deviation values of the structure E,F,G,H, E1,F1,G1, H1 between the different solvent and gas-phase

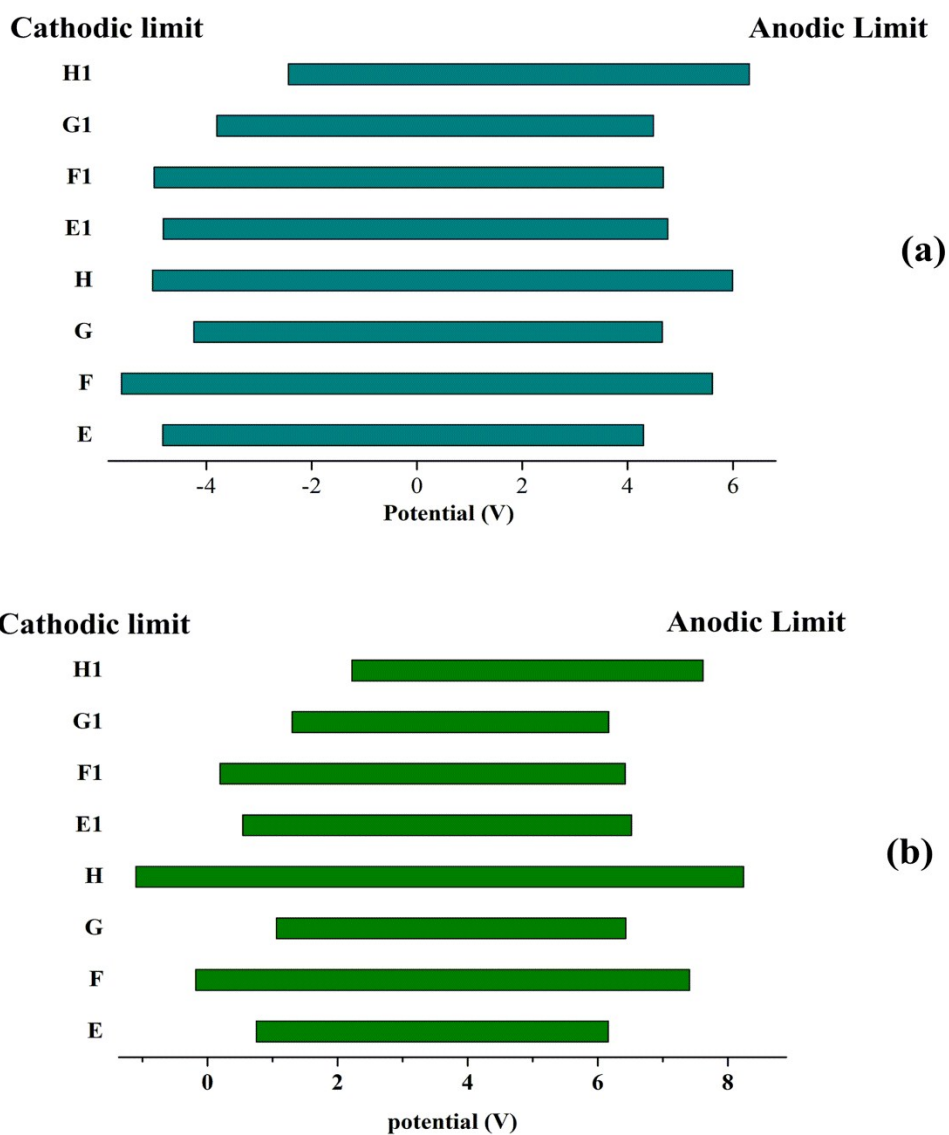


Fig. S7 The calculated V_{cl} , V_{al} and EW of selected electrolytes from both gas phase(a) and ethanol solvent calculations.

Table S1 Calculated ΔE_{Li^+} values of the potential new electrolytes for Li-ion battery under study at various theoretical levels (in eV)

	ω B97XD	B2GP-PLYP	B2T-PLYP	B2K-PLYP	B3LYP	MP2	CCSD(T)
a^a	6.36 ^b	6.51	5.97	6.51	6.54	6.05	6.02
b	7.31	7.49	6.93	7.50	7.45	7.08	7.02
c	6.25	6.97	6.38	7.03	6.42	6.10	6.07
A	5.94	6.01	5.47	6.01	6.02	5.56	5.53
B	5.75	5.79	5.25	5.79	5.79	5.38	5.33
C	5.51	5.52	4.97	5.52	5.52	5.10	5.04
D	5.81	5.84	5.30	5.84	5.84	5.41	5.36
E	5.30	5.27	4.72	5.26	5.28	4.82	4.79
F	5.19	5.19	4.65	5.19	5.20	4.77	4.71
G	5.28	5.28	4.73	5.28	5.28	4.85	4.80
H	5.08	5.09	4.55	5.09	5.10	4.65	4.60
I	4.98	5.00	4.45	5.00	5.01	4.56	4.50
J	4.98	5.00	4.46	5.00	5.01	4.56	4.50
A1	5.91	6.16	5.60	6.12	5.99	5.56	5.51
B1	5.84	6.09	5.52	6.11	5.86	5.49	5.44
C1	5.62	5.79	5.23	5.85	5.63	5.23	5.18
D1	5.57	5.78	5.22	5.80	5.61	5.19	5.14
E1	5.39	5.46	4.91	5.47	5.38	4.96	4.91
F1	5.39	5.49	4.94	5.50	5.39	4.98	4.92
G1	5.23	5.30	4.74	5.30	5.24	4.80	4.76
H1	5.16	5.27	4.72	5.28	5.18	4.75	4.70
I1	5.08	5.16	4.61	5.17	5.09	4.67	4.61
J1	5.02	5.11	4.56	5.12	5.04	4.61	4.55

^a Entry shows deviation values.

^b Results obtained with the 6-311+g* basis set.

Table S2 Calculated ΔE_{H_2O} values of the potential new electrolytes for Li-ion battery under study at various theoretical levels (in eV)

	ω B97XD	B2GP-PLYP	B2T-PLYP	B2K-PLYP	B3LYP	MP2	CCSD(T)
a^a	0.99 ^b	1.08	1.07	1.09	1.01	1.11	1.10
b	0.82	0.92	0.91	0.93	0.84	0.96	0.96
c	0.97	1.11	1.10	1.13	0.99	1.10	1.10
A	0.99	1.06	1.05	1.07	0.98	1.10	1.10
B	1.04	1.07	1.07	1.09	1.00	1.10	1.10
C	1.17	1.23	1.22	1.24	1.19	1.25	1.25
D	0.99	1.04	1.03	1.06	0.95	1.09	1.09
E	1.23	1.32	1.31	1.34	1.22	1.36	1.34
F	1.06	1.13	1.12	1.14	1.03	1.17	1.17
G	1.12	1.12	1.11	1.14	1.00	1.18	1.17
H	1.07	1.11	1.10	1.13	1.01	1.17	1.16

I	1.07	1.13	1.12	1.14	1.03	1.18	1.18
J	1.10	1.08	1.06	1.10	0.96	1.14	1.14
A1	0.98	1.05	1.04	1.07	0.97	1.09	1.09
B1	1.01	1.04	1.03	1.05	0.97	1.08	1.07
C1	1.08	1.11	1.11	1.12	1.06	1.16	1.16
D1	1.02	1.09	1.07	1.11	0.97	1.12	1.11
E1	1.04	1.07	1.06	1.09	0.95	1.11	1.11
F1	1.09	1.09	1.08	1.11	0.97	1.15	1.14
G1	1.08	1.07	1.05	1.09	0.96	1.14	1.13
H1	1.06	1.11	1.10	1.13	1.00	1.15	1.15
I1	1.06	1.10	1.09	1.12	0.99	1.15	1.15
J1	1.07	1.07	1.06	1.09	0.96	1.13	1.13

^a Entry shows deviation values.

^b Results obtained with the 6-311+G* basis set.

Table S3 The deviation of the ΔE_{Li^+} between CCSD(T) and DFT methods for the superhalogen structures(**a-J1**) (in eV).

	ωB97XD	B2GP-PLYP	B2T-PLYP	B2K-PLYP	B3LYP	MP2
a^a	0.92 ^b	1.08	1.08	1.08	1.11	0.10
b	0.95	1.10	1.10	1.10	1.10	0.11
c	0.86	1.21	1.20	1.22	1.06	0.10
A	1.02	1.07	1.07	1.06	1.10	0.09
B	1.04	1.05	1.06	1.05	1.07	0.11
C	1.06	1.05	1.06	1.05	1.07	0.12
D	1.06	1.07	1.07	1.07	1.08	0.11
E	1.11	1.05	1.06	1.05	1.08	0.09
F	1.07	1.06	1.06	1.06	1.07	0.12
G	1.08	1.06	1.06	1.06	1.07	0.11
H	1.07	1.06	1.07	1.06	1.08	0.12
I	1.07	1.07	1.07	1.07	1.09	0.12
J	1.06	1.07	1.07	1.07	1.09	0.12
A1	1.04	1.44	1.42	1.48	1.13	0.11
B1	1.06	1.18	1.18	1.20	1.08	0.11
C1	1.07	1.12	1.11	1.12	1.07	0.11
D1	1.05	1.17	1.17	1.18	1.04	0.12
E1	1.09	1.13	1.13	1.14	1.08	0.12
F1	1.08	1.06	1.06	1.06	1.07	0.12
G1	1.07	1.07	1.07	1.07	1.07	0.11
H1	1.06	1.04	1.05	1.04	1.08	0.12
I1	1.06	1.04	1.05	1.04	1.07	0.12
J1	1.06	1.06	1.06	1.05	1.08	0.12

^a Entry shows deviation values.

^b Results obtained with the Def2-TZVP basis set.

Table S4 The deviation of the $\Delta E_{\text{H}_2\text{O}}$ between CCSD(T) and DFT methods for the superhalogen structures(**a-J1**) (in eV).

	ωB97XD	B2GP-PLYP	B2T-PLYP	B2K-PLYP	B3LYP
a^a	-0.03 ^b	0.04	0.04	0.04	0.02
b	-0.04	0.02	0.02	0.03	-0.01
c	-0.02	0.05	0.05	0.06	0.01
A	-0.02	0.03	0.03	0.04	-0.01
B	0.01	0.02	0.02	0.03	-0.02
C	-0.02	0.03	0.02	0.04	-0.03
D	-0.01	0.02	0.01	0.02	-0.03
E	-0.05	0.03	0.02	0.04	-0.04
F	-0.01	0.03	0.02	0.03	-0.02
G	0.02	0	-0.01	0.01	-0.08
H	0	0.01	0.01	0.02	-0.04
I	-0.01	0.02	0.01	0.03	-0.04
J	0.03	0	-0.02	0.01	-0.09
A1	-0.02	0.05	0.04	0.05	0
B1	0	0.07	0.06	0.08	-0.03
C1	-0.02	0	0	0	-0.03
D1	-0.01	0.04	0.03	0.05	0.02
E1	0.01	0.02	0.01	0.03	-0.06
F1	0.02	0.01	0	0.02	-0.08
G1	0.02	0	-0.01	0.01	-0.08
H1	0	0.03	0.03	0.04	-0.04
I1	0	0.03	0.02	0.04	-0.05
J1	0.02	0.01	0	0.02	-0.08

^a Entry shows deviation values.

^bResults obtained with the Def2-TZVP basis set.

Table S5 Calculated VDEs, ΔE_{Li^+} , $\Delta E_{\text{H}_2\text{O}}$ and molar volume at the ω B97XD /6-311+G(d) level for potential new electrolytes in Li-ion battery.

	VDE [eV]	ΔE_{Li^+} [eV]	$\Delta E_{\text{H}_2\text{O}}$ [eV]
a	4.44	6.36	0.99
b	4.63	7.31	1.09
c	5.03	6.25	0.97
A	3.40	5.94	0.99
B	3.89	5.75	1.04
C	4.19	5.51	1.17
D	3.86	5.81	0.99
E	4.30	5.30	1.23
F	5.62	5.19	1.06
G	4.66	5.28	1.12
H	5.99	5.08	1.07
I	4.31	4.98	1.07
J	5.06	4.98	1.10
A1	3.20	5.91	0.97
B1	4.18	5.84	1.01
C1	4.23	5.62	1.08
D1	3.80	5.57	1.06
E1	4.77	5.39	1.04
F1	4.69	5.39	1.09
G1	4.50	5.23	1.08
H1	6.34	5.16	1.06
I1	4.26	5.08	1.06
J1	5.31	5.02	1.07

Table S6 The deviation of the VDE between CCSD(T) and DFT methods for the superhalogen structures(**a- c** , **A-I**, **A1-I1**) (in eV).

	ω B97XD	B2GP-PLYP	B2T-PLYP	B2K-PLYP
a^a	0.26 ^b	0.27	0.23	0.32
b	-0.14	0.05	0.01	0.11
c	0.36	0.13	0.09	0.19
A	0.17	0.10	0.09	0.10
B	0.17	0.09	0.08	0.10
C	0.24	0.12	0.11	0.14
D	0.23	0.10	0.10	0.12
E	0.24	0.08	0.08	0.10
F	0.09	0.06	0.03	0.10
G	0.20	0.07	0.06	0.10
H	0.22	0.06	0.04	0.09
I	0.23	0.09	0.08	0.11
A1	0.20	0.08	0.08	0.08
B1	0.17	0.07	0.07	0.07
C1	0.23	0.12	0.10	0.09
D1	0.25	0.09	0.08	0.11
E1	0.15	0.16	0.12	-0.35
F1	0.22	0.07	0.05	0.08
G1	0.20	0.05	0.04	0.07
H1	0.60	0.05	0.03	0.07
I1	0.23	0.08	0.07	0.10

^a Entry shows deviation values.

^b Results obtained with the 6-311+g* basis set.

Table S7 Calculated the ΔE_{Li^+} of the some potential new electrolytes for Li-ion battery under study at the ω B97XD /Def2-TZVP level (in eV)

	Gas-phase	Ethonal	EthylEthanoate	2-MethoxyEthanol
E	5.31	4.87(0.44) ^a	4.83(0.48) ^a	4.86(0.45) ^a
F	5.20	4.87(0.33)	4.81(0.39)	4.86(0.34)
G	5.28	4.96(0.32)	4.89(0.39)	4.94(0.34)
H	5.08	4.86(0.22)	4.78(0.30)	4.84(0.24)
E1	5.39	4.92(0.47)	4.89(0.50)	4.91(0.48)
F1	5.40	4.94(0.46)	4.90(0.50)	4.93(0.47)
G1	5.23	4.90(0.33)	4.84(0.39)	4.89(0.34)
H1	5.17	4.90(0.27)	4.83(0.34)	4.89(0.28)

^a the deviation of the ΔE_{Li^+} between the gas-phase and various solvents

Lowest normal mode frequencies and optimized coordinates at ω B97XD /6-311+G* level of the anions **a-c, A-J, A1-J1**

a

Lowest normal mode frequency: 608.4 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.26038200
O	0.00000000	0.00000000	-1.26038200

b

Lowest normal mode frequency: 189.94 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00000000	0.00000000	0.00000000
O	1.05071100	0.67588200	-0.79702200
H	1.67621500	-0.00558000	-1.04571800
O	-1.05071000	-0.67588300	-0.79702200
H	-1.67621400	0.00557900	-1.04571900
O	0.67588300	-1.05071000	0.79702300
H	-0.00558000	-1.67621400	1.04572000
O	-0.67588300	1.05071100	0.79702100
H	0.00557900	1.67621500	1.04571800

c

Lowest normal mode frequency: 467.47 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

O	-1.45764900	-0.32365400	0.00007300
O	1.00913100	-1.10044900	-0.00006400
O	0.44851900	1.42407000	-0.00000800
P	0.00000000	0.00001800	0.00000000

ALowest normal mode frequency: 522.7 cm⁻¹Optimized coordinates at ω B97XD /6-311+G* level:

B	0.01335000	-0.65415800	-0.83316300
B	0.01325800	-0.39448100	0.98307100
B	0.01331800	1.04862800	-0.14991700
B	1.30223100	0.00002900	0.00000200
H	-2.20323300	0.00001200	-0.00004700
H	-0.09041600	-0.84097300	2.09578900
H	-0.09054400	2.23549400	-0.31963400
H	-0.09049100	-1.39458400	-1.77615100
H	2.50150100	-0.00001200	0.00006000
C	-1.12293500	-0.00000400	0.00000200

BLowest normal mode frequency: 460.64 cm⁻¹Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00000400	-0.00027200	1.24531800
B	-0.98529200	-0.71154100	0.02105900
B	0.98529200	0.71153100	0.02136300
B	0.71153600	-0.98529600	0.02099300
B	-0.71153600	0.98528700	0.02142900
H	0.00000900	-0.00053500	2.44630300
H	-1.94756600	-1.40634500	-0.14236100
H	1.40637500	-1.94753500	-0.14249100
H	1.94756500	1.40640700	-0.14175900
H	-1.40637600	1.94759700	-0.14162900
C	-0.00000400	0.00023300	-1.06367900
H	-0.00000800	0.00047000	-2.14680400

C

Lowest normal mode frequency: 444.71 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.99368100	-0.97887900	0.02392200
B	1.23806500	0.64261400	0.02406800
B	-0.62394700	-1.24750600	0.02384100
B	-1.37932300	0.20790200	0.02400800
B	-0.22855000	1.37605900	0.02413200
H	-2.54897500	0.38413600	-0.17144000
H	-1.15304800	-2.30532200	-0.17170600
H	1.83630800	-1.80888800	-0.17163400
H	2.28798400	1.18737500	-0.17149300
H	-0.42239200	2.54291100	-0.17134300
C	0.00003100	0.00008900	-1.01320600
H	0.00008600	0.00018100	-2.10027300
B	0.00004900	-0.00029700	1.20577500
H	-0.00002200	-0.00038900	2.40839600

D

Lowest normal mode frequency: 295.43 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.28529200	-1.28120700	-0.00383600
B	1.34145500	0.80921100	0.02522900
B	0.29852100	-0.00001200	1.28904100
B	-1.31958200	-0.00001100	0.78824300
B	-0.28531300	1.28120800	-0.00382000
B	1.34146400	-0.80919800	0.02521900
H	-2.35283200	-0.00001900	1.39017100
H	-0.70858000	2.40259300	-0.06206500
H	2.25212200	-1.58934400	0.05377700
H	-0.70861000	-2.40257200	-0.06209700
H	2.25211700	1.58935200	0.05379900
H	0.56000000	-0.00002300	2.46258400
H	-1.98501700	0.00001100	-1.43494500
B	0.34445200	0.00000200	-1.24658200
H	0.52588300	-0.00000200	-2.43367500

C	-1.16893400	0.00000700	-0.72250300
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E

Lowest normal mode frequency: 18.68 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	1.00367400	0.55287600	-0.89068000
B	1.00367100	0.55287400	0.89068100
B	1.42617500	-0.82981400	-0.00000100
B	-1.00367100	0.55287400	0.89068100
B	0.00000000	-1.15007700	0.89176700
B	0.00000000	-1.15008000	-0.89176600
B	-1.00367400	0.55287600	-0.89068000
B	-1.42617500	-0.82981400	-0.00000100
H	1.66359700	1.09143100	-1.73130900
H	1.66359300	1.09142900	1.73131200
H	0.00000000	2.52606100	-0.00000100
H	2.46437400	-1.42322700	-0.00000100
H	-1.66359300	1.09142900	1.73131200
H	0.00000000	-1.98775000	1.74993700
H	0.00000000	-1.98775400	-1.74993500
H	-1.66359700	1.09143100	-1.73130900
H	-2.46437400	-1.42322600	-0.00000100
C	0.00000000	1.44526600	-0.00000100

F

Lowest normal mode frequency: 470.08 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00000000	0.00000000	-1.87044300
B	0.91835100	0.91835100	-0.77089700
B	-0.91835100	0.91835100	-0.77089700
B	-0.91835100	-0.91835100	-0.77089700
B	0.91835100	-0.91835100	-0.77089700
B	0.00000000	1.30197500	0.73741400
B	-1.30197500	0.00000000	0.73741400
B	0.00000000	-1.30197500	0.73741400
B	1.30197500	0.00000000	0.73741400
H	0.00000000	0.00000000	-3.06455100

H	0.00000000	0.00000000	2.75021900
H	1.71851600	1.71851600	-1.16746500
H	-1.71851600	1.71851600	-1.16746500
H	-1.71851600	-1.71851600	-1.16746500
H	1.71851600	-1.71851600	-1.16746500
H	0.00000000	2.38363900	1.24479300
H	-2.38363900	0.00000000	1.24479300
H	0.00000000	-2.38363900	1.24479300
H	2.38363900	0.00000000	1.24479300
C	0.00000000	0.00000000	1.67114800

G

Lowest normal mode frequency: 232.85 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.94713700	-1.33850900	-0.19119000
B	0.94724300	1.33835800	-0.19215900
B	-1.48804200	0.00038300	0.80939300
B	-0.91146200	1.33260500	-0.23342500
B	-0.02668300	0.91354400	1.23867700
B	1.69978300	-0.00029600	-0.85104400
B	-0.91162600	-1.33268300	-0.23229700
B	0.06729500	-0.00087900	-1.43937500
B	1.46105200	0.00029400	0.88075100
B	-0.02670500	-0.91255400	1.23938800
H	1.36496200	2.45038200	-0.35080800
H	-2.53089300	0.00061900	1.38978000
H	-1.43474500	2.37510100	-0.48844400
H	-0.06369300	1.63745600	2.19160500
H	2.65649400	-0.00049200	-1.56596200
H	-1.43484800	-2.37542500	-0.48641900
H	0.06329300	-0.00120500	-2.63602900
H	2.38162800	0.00054500	1.64819000
H	-0.06372700	-1.63570500	2.19289100
H	-2.32157900	-0.00049100	-1.51677300
H	1.36489600	-2.45063300	-0.34899900
C	-1.46195800	-0.00024400	-0.86210400

H

Lowest normal mode frequency: 525.77 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.09179000	1.50554200	-0.74035300
B	-1.46812100	0.38230200	-0.72265500
B	1.40196100	0.54387900	-0.74987100
B	0.94880100	-1.17394000	-0.73837400
B	-0.82493400	-1.27377300	-0.72155400
B	0.09251600	-1.51215400	0.77598500
B	1.47488300	-0.38381000	0.75843400
B	0.82878800	1.27955400	0.75706200
B	-1.40771900	-0.54613600	0.78574400
B	-0.95275000	1.17927600	0.77400700
H	-1.36883800	-2.11186500	-1.37356500
H	0.15814900	-2.59088700	1.28844500
H	2.52635700	-0.65777200	1.25834100
H	1.41943900	2.19204800	1.25613400
H	-1.63256900	2.02020600	1.28514500
H	-2.41214700	-0.93589100	1.30518500
H	-2.43471000	0.63290400	-1.37553300
H	-0.15371000	2.49447700	-1.40483000
H	2.32177400	0.90068000	-1.42067600
H	1.57083500	-1.94634900	-1.40154900
B	0.01575400	0.00739000	1.70248600
H	0.02684600	0.01252400	2.89927700
C	-0.01405100	-0.00658500	-1.51992400
H	-0.02406300	-0.01121300	-2.60137400

I

Lowest normal mode frequency: 146.44 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-2.12415100	0.03676300	-0.00000300
B	-1.26639500	1.41029700	0.00004700
B	-1.31890900	-1.36717300	-0.00004900
B	-0.84330800	0.01969100	1.35863600

B	0.28224700	1.50497900	0.87852900
B	0.21601700	-1.48364700	0.87994100
B	0.21600200	-1.48349100	-0.88016300
B	0.28227100	1.50512800	-0.87830200
B	0.96929200	-0.00161900	1.42384600
B	0.96930200	-0.00140600	-1.42384100
B	1.63988600	0.86237200	0.00006900
H	-1.86737100	2.44965800	0.00008400
H	-1.93068900	-2.40085400	-0.00008400
H	-1.33644800	0.01317300	2.44983500
H	-1.33643000	0.01356900	-2.44984200
H	2.75329800	1.28970900	0.00010400
H	2.40718400	-1.37106700	-0.00009600
H	0.42356200	-2.48219800	1.49848700
H	0.40470400	2.48308500	1.55479100
H	0.40477300	2.48334600	-1.55439400
H	0.42351300	-2.48194100	-1.49888400
H	1.62210800	-0.09944000	-2.41654700
H	1.62209300	-0.09979400	2.41654200
H	-3.31969800	0.05504000	-0.00000300
B	-0.84329500	0.01995200	-1.35863900
C	1.47243500	-0.82691900	-0.00005700

J

Lowest normal mode frequency: 209.89 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00004700	0.00004400	1.57885000
B	1.50984900	0.85914400	-0.73225700
B	0.01074900	1.73692200	-0.73233900
B	-1.49925100	0.87794400	-0.73197500
B	1.74384200	-0.01069100	0.76667800
B	0.86253200	-1.51559200	0.76661900
B	-0.86249100	1.51563200	0.76658700
B	0.88136300	1.50497600	0.76650300
H	-0.00008000	-0.00006900	-2.49739400
H	0.00008300	0.00007700	2.77457300
H	2.33879400	1.33084400	-1.44951200
H	0.01652900	2.69061700	-1.44965100
H	-2.32232200	1.36002900	-1.44909800

H	2.32227000	-1.36012900	-1.44914000
H	2.79848800	-0.01726000	1.32898900
H	1.38426400	-2.43223000	1.32881300
H	-1.38420200	2.43229300	1.32876200
H	1.41433300	2.41524800	1.32848500
B	1.49925700	-0.87801200	-0.73197300
B	-0.88131500	-1.50493600	0.76664100
B	-1.74379400	0.01073800	0.76678200
B	-0.01079400	-1.73691100	-0.73227800
B	-1.50993400	-0.85920800	-0.73208300
H	-2.33890600	-1.33093900	-1.44928500
H	-2.79840700	0.01735200	1.32915600
H	-1.41424000	-2.41518400	1.32870500
H	-0.01661400	-2.69066400	-1.44951700
C	-0.00004800	-0.00003900	-1.41377800

A1

Lowest normal mode frequency: 256.92 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.42554600	-0.71428500	-0.87945700
B	-0.42571600	1.11884700	-0.17875900
B	-0.42569600	-0.40454200	1.05833800
B	-1.63025100	0.00001600	0.00006000
H	2.65344100	0.00008200	0.00062000
H	-0.56309700	2.29827900	-0.36741200
H	-0.56293200	-0.83097100	2.17407500
H	-0.56327100	-1.46739000	-1.80648900
H	-2.82848100	-0.00016300	-0.00029100
Si	1.17145600	-0.00000100	-0.00010100

B1

Lowest normal mode frequency: 335.12 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-1.49043800	-0.00000100	-0.00002200
B	-0.35953600	0.97364600	-0.82610000
B	-0.35954800	-0.97362100	0.82611400
B	-0.35952100	-0.82612400	-0.97362300
B	-0.35954300	0.82609400	0.97363900
H	-2.68904800	-0.00000200	-0.00004100
H	-0.42720900	1.88612000	-1.60092600
H	-0.42719200	-1.60095000	-1.88609700
H	-0.42722100	-1.88609300	1.60094200
H	-0.42722400	1.60091700	1.88611500
Si	1.17048000	0.00000300	-0.00000600
H	2.65410900	-0.00000400	0.00005200

C1

Lowest normal mode frequency: 411.58 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.15022500	0.86427000	1.19951100
B	0.36363400	-1.38399800	-0.40148100
B	1.34292700	0.01191900	0.16182900
H	0.50034200	-2.52290900	-0.75103900
H	-2.62037500	-0.02318100	-0.31327300
H	0.11140800	1.57418400	2.16521200
H	2.53462000	0.02249600	0.30519600
H	0.13667600	-1.54414600	2.18530600
H	0.69944900	-0.01105300	-2.58664400
B	0.16405000	-0.84624200	1.21050100
H	0.45939800	2.52080100	-0.78354100
B	0.34119100	1.38441100	-0.41931400
B	0.47284100	-0.00526300	-1.40903200
Si	-1.14256100	-0.01012000	-0.13795000

D1

Lowest normal mode frequency: 220.93 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.54963500	0.04826800	1.31774100
B	0.54963500	0.04826800	-1.31774100
B	0.77713700	1.28838200	0.00000000
B	-0.78216000	1.07566000	0.83663000
B	-0.78216000	1.07566000	-0.83663000
B	1.69982600	-0.17471600	0.00000000
H	-1.43872500	1.71509600	1.60942100
H	-1.43872500	1.71509600	-1.60942100
H	2.89618600	-0.25470400	0.00000000
H	0.83292400	-0.08729600	2.47572800
H	0.83292400	-0.08729500	-2.47572800
H	1.32467100	2.35835500	0.00000000
H	-2.41472300	-1.45922700	0.00000000
B	0.70102300	-1.46354300	0.00000000
H	1.09004300	-2.59607400	0.00000000
Si	-1.08923300	-0.77098900	0.00000000

E1

Lowest normal mode frequency: 178.01 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.08546100	-0.94273100	1.03790300
B	-0.40737200	-1.41627600	-0.73899100
B	1.10537700	-1.44878400	-0.11601200
B	-0.40737200	1.41627600	-0.73899100
B	1.22062900	0.00000000	-1.05055100
B	1.45248100	0.00000000	0.76341100
B	-0.08546100	0.94273100	1.03790300
B	1.10537700	1.44878400	-0.11601200
H	-0.44051600	-1.54240400	2.01584100
H	-0.79703100	-2.32350600	-1.41591800
H	-2.99183000	0.00000000	0.35714200
H	1.82827200	-2.39963100	-0.19275100

H	-0.79703100	2.32350600	-1.41591800
H	1.91520700	0.00000000	-2.02925300
H	2.40726400	0.00000000	1.49164000
H	-0.44051500	1.54240400	2.01584100
H	1.82827200	2.39963100	-0.19275200
Si	-1.57164800	0.00000000	-0.07336900

F1

Lowest normal mode frequency: 353.34 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.69821200	1.70639500	0.00000000
B	0.11280100	0.70136500	1.34387400
B	-0.94593400	1.31228500	0.00000000
B	0.11280100	0.70136500	-1.34387400
B	-1.40690000	-0.17857800	0.91627000
B	-1.40690000	-0.17857800	-0.91627000
B	0.11280100	-1.17188600	-0.96604500
B	0.11280100	-1.17188600	0.96604500
H	1.21885600	2.77999500	0.00000000
H	-1.84994500	-2.61364700	0.00000000
H	0.27167200	1.04565900	2.47878400
H	-1.69853100	2.24398400	0.00000000
H	0.27167200	1.04565900	-2.47878400
H	2.96301400	-0.39128200	0.00000000
H	-2.29027500	-0.10779400	1.72332300
H	-2.29027500	-0.10779400	-1.72332300
H	0.57348200	-1.94085400	-1.76324100
H	0.57348200	-1.94085400	1.76324100
B	-1.21529400	-1.60257600	0.00000000
Si	1.52749300	-0.04304200	0.00000000

G1

Lowest normal mode frequency: 209.59 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.34308800	0.22130600	-1.43907400
B	-1.48835400	-0.77428100	0.78861600
B	0.93844500	0.98253600	0.95494400
B	0.21473100	-0.67459600	1.31459800
B	-0.79639500	0.80083100	1.25760500

B	-1.60124400	-0.83880100	-0.96341700
B	1.23714900	1.07290300	-0.89608200
B	-0.23353000	-1.51473100	-0.27512500
B	-1.77290200	0.66880300	-0.22183700
B	-0.22375400	1.62872000	-0.21576000
H	-2.26936100	-1.34637300	1.49419100
H	1.63769600	1.57498800	1.72491500
H	0.55962400	-1.30387800	2.27429000
H	-1.22110800	1.37626100	2.21694500
H	-2.35635700	-1.41962400	-1.68342600
H	1.88640000	1.82879300	-1.55165100
H	0.00967500	-2.66038500	-0.55083400
H	-2.75689800	1.33976500	-0.34981300
H	-0.42870400	2.77856700	-0.47579400
H	2.82602200	-1.47276500	0.06768600
H	-0.28795400	0.25683200	-2.63525300
Si	1.62469100	-0.62968700	-0.14668500

H1

Lowest normal mode frequency: 421.41 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	-0.49759900	-0.94305400	-1.28345900
B	-0.49757400	0.92919100	-1.29357600
B	-0.49762300	-1.51211100	0.50031000
B	-0.49770200	0.00861400	1.59268800
B	-0.49763000	1.51743400	0.48395200
B	0.99196000	0.90040400	1.22534900
B	0.99199000	-0.88713800	1.23499700
B	0.99203800	-1.44865300	-0.46207900
B	0.99201500	1.44359100	-0.47766000
B	0.99207800	-0.00821400	-1.52048500
H	-1.00809900	2.54903500	0.81292400
H	1.52551700	1.53441800	2.08820200
H	1.52561600	-1.51181100	2.10460100
H	1.52568300	-2.46872200	-0.78745700
H	1.52573200	-0.01402400	-2.59117500
H	1.52561200	2.46011300	-0.81402800
H	-1.00800200	1.56088000	-2.17302100
H	-1.00797400	-1.58422200	-2.15604000
H	-1.00800400	-2.54012900	0.84043200
H	-1.00818000	0.01447400	2.67545600

Si	-1.74374500	-0.00003600	-0.00003100
H	-3.21687100	0.00000900	-0.00008300
B	1.91423000	0.00003000	0.00006400
H	3.11049400	0.00001500	0.00012400

I1

Lowest normal mode frequency: 154.52 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	2.19886100	-0.74128200	-0.00000300
B	1.90468500	0.85470900	0.00000200
B	0.94506000	-1.76076300	-0.00000500
B	1.01570000	-0.25951600	-1.35700800
B	0.52044100	1.53654200	-0.88381800
B	-0.50423700	-1.31971000	-0.92706800
B	-0.50424300	-1.31972600	0.92704300
B	0.52044000	1.53652300	0.88384400
B	-0.66873900	0.41043800	-1.49342300
B	-0.66874100	0.41041200	1.49342800
B	-0.98151500	1.53567800	0.00001200
H	2.85702500	1.58480600	0.00000500
H	1.14637500	-2.94487300	-0.00000900
H	1.48897100	-0.44755800	-2.44077400
H	1.48896300	-0.44760400	2.44076800
H	-1.72660000	2.47219300	0.00002000
H	-3.35858800	-0.46297400	-0.00000600
H	-0.91623900	-2.21391400	-1.60837700
H	0.80419700	2.49063400	-1.54676100
H	0.80419900	2.49060000	1.54680800
H	-0.91625100	-2.21394000	1.60833500
H	-1.17185800	0.61183400	2.56010900
H	-1.17185400	0.61187700	-2.56010200
H	3.32454400	-1.14419900	-0.00000600
B	1.01569400	-0.25954700	1.35700300
Si	-1.90142200	-0.25040500	-0.00000400

J1

Lowest normal mode frequency: 365.42 cm⁻¹

Optimized coordinates at ω B97XD /6-311+G* level:

B	0.00004700	0.00005100	-1.74266600
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B	0.86337000	1.60500100	0.55461700
B	1.82173300	0.05469900	0.55465400
B	0.95833300	-1.55031100	0.55438400
B	-0.05237500	1.74346100	-0.94119600
B	-1.53613600	0.82632400	-0.94124400
B	1.53618700	-0.82626900	-0.94120900
B	1.48380900	0.91724400	-0.94099500
H	-0.00008400	-0.00009100	3.09388900
H	0.00008000	0.00008700	-2.93819300
H	1.36210600	2.53229000	1.12056800
H	2.87425500	0.08637300	1.12043600
H	1.51182200	-2.44602500	1.12029100
H	-1.51188500	2.44596300	1.12035600
H	-0.08334700	2.77476500	-1.54405300
H	-2.44472200	1.31509900	-1.54420200
H	2.44480300	-1.31501200	-1.54414700
H	2.36144500	1.45967400	-1.54391000
B	-0.95836800	1.55028600	0.55441900
B	-1.48375800	-0.91718900	-0.94113000
B	0.05242600	-1.74340500	-0.94129600
B	-1.82175400	-0.05473200	0.55455500
B	-0.86340500	-1.60504200	0.55447100
H	-1.36216900	-2.53236000	1.12034800
H	0.08343700	-2.77467300	-1.54421200
H	-2.36136400	-1.45957800	-1.54412500
H	-2.87431200	-0.08643900	1.12027100
Si	-0.00004400	-0.00004800	1.62141900