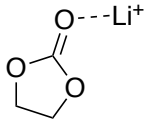
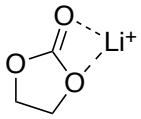
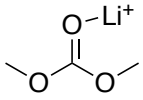
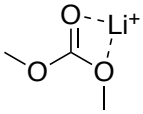
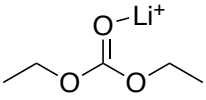
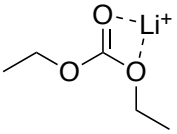
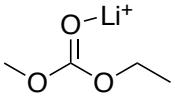
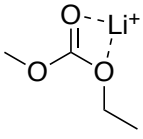
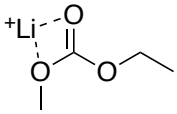
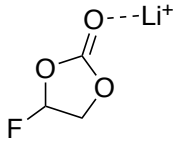
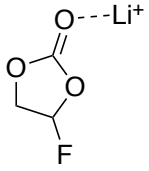
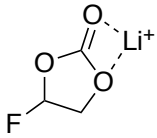
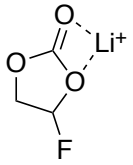
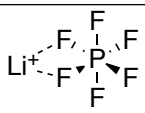
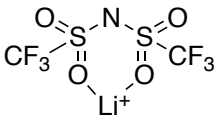
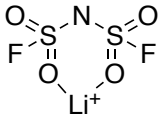
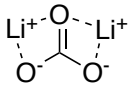
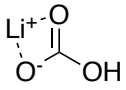
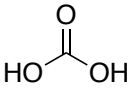
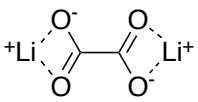
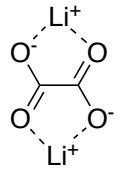
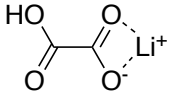
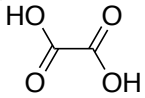
Supplementary Table 1 for:
Quantum chemical calculations of lithium-ion battery electrolyte and interphase species

Molecule Number	**Structure**	**Fragmentation Steps**
1		MAX
2		MAX
3		MAX
4		MAX
5		MAX
6		MAX
7		MAX
8		MAX
9		MAX

10		MAX
11		MAX
12		MAX
13		MAX
14		MAX
15		MAX
16		MAX
17		MAX
18		MAX
19		MAX
20		MAX

21		MAX
22		MAX
23		MAX
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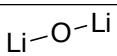
25		MAX
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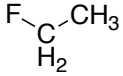
32		MAX
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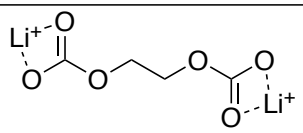
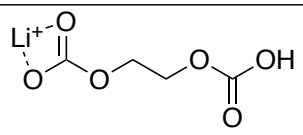
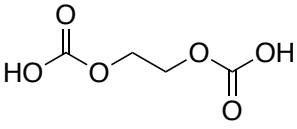
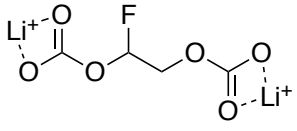
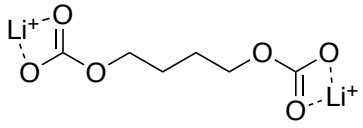
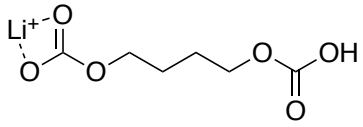
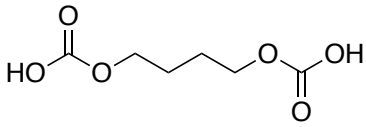
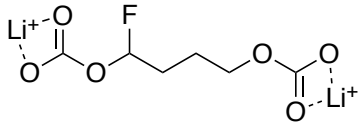
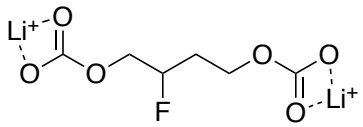
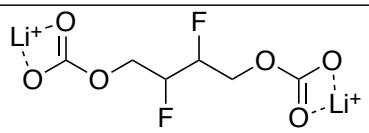
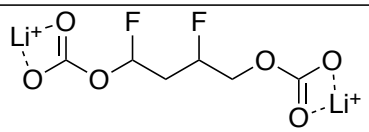
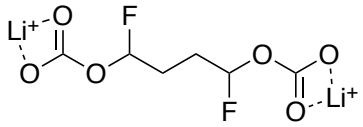
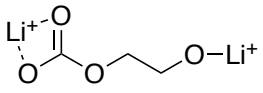
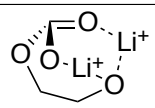
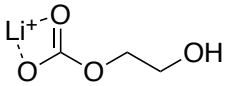
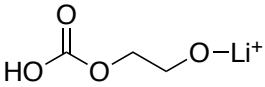
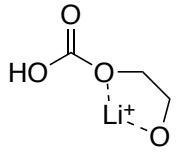
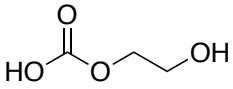
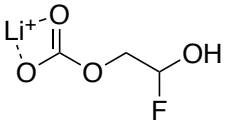
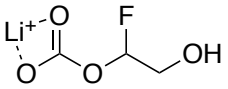
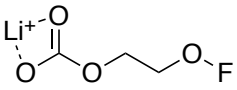
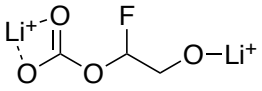
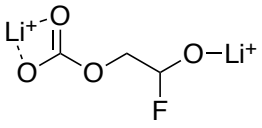
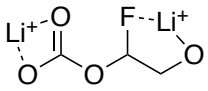
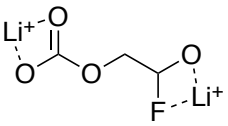
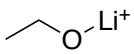
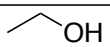
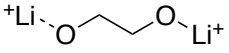
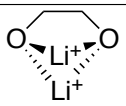
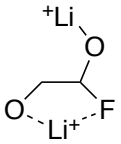
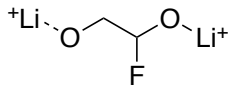
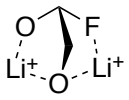
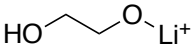
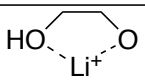
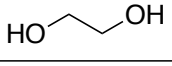
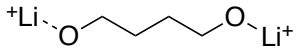
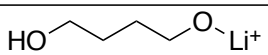
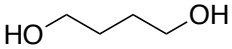
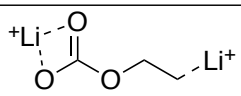
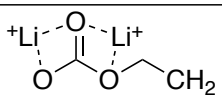
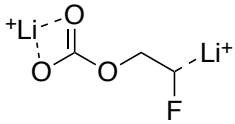
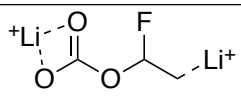
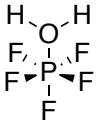
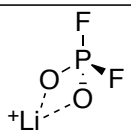
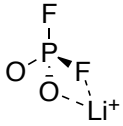
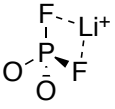
36		MAX
37		MAX
38		MAX
39		MAX

40		3
41		3
42		3
43		2
44		2
45		2
46		2
47		2
48		MAX
49		MAX
50		MAX
51		MAX

52		MAX
53		MAX
54		MAX
55		MAX
56		MAX
57		MAX
58		MAX
59		MAX
60		MAX
61		MAX
62		MAX
63		MAX
64		MAX
65		MAX

66		MAX
67		MAX
68		MAX
69		MAX
70		MAX
71		MAX
72		MAX
73		MAX
74		MAX
75		MAX
76		MAX
77		MAX
78		MAX
79		MAX
80		MAX
81		MAX

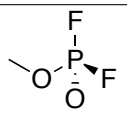
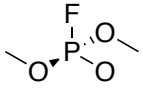
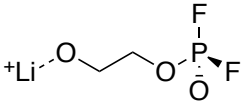
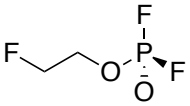
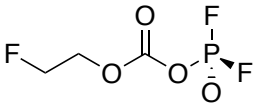
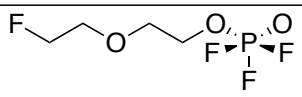
82		MAX
83		MAX
84		MAX
85		MAX
86		MAX
87		4

Table 1: Principal molecules used for fragmentation, including depth of fragmentation. A fragmentation depth of "MAX" indicates that all possible combinations of bonds were broken during fragmentation.