Electronic Supplementary Material (ESI) for RSC Advances

Theoretical Study of the Reductive Decomposition of 1,3-Propane Sultone: SEI Forming Additive in Lithium-ion Batteries

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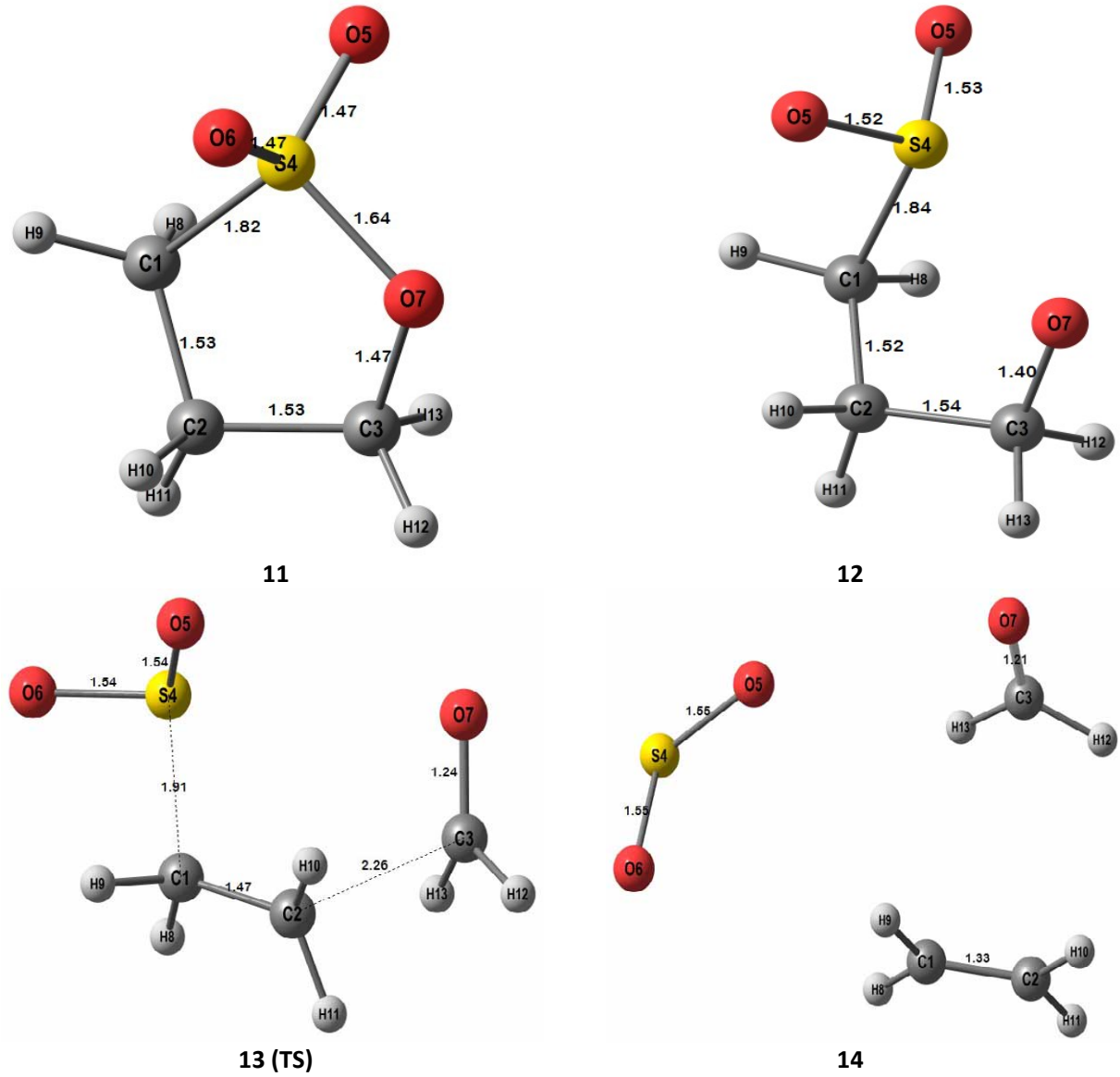


Figure S1. The optimized geometry of the reductive decomposition products of PS (bond length in Å)

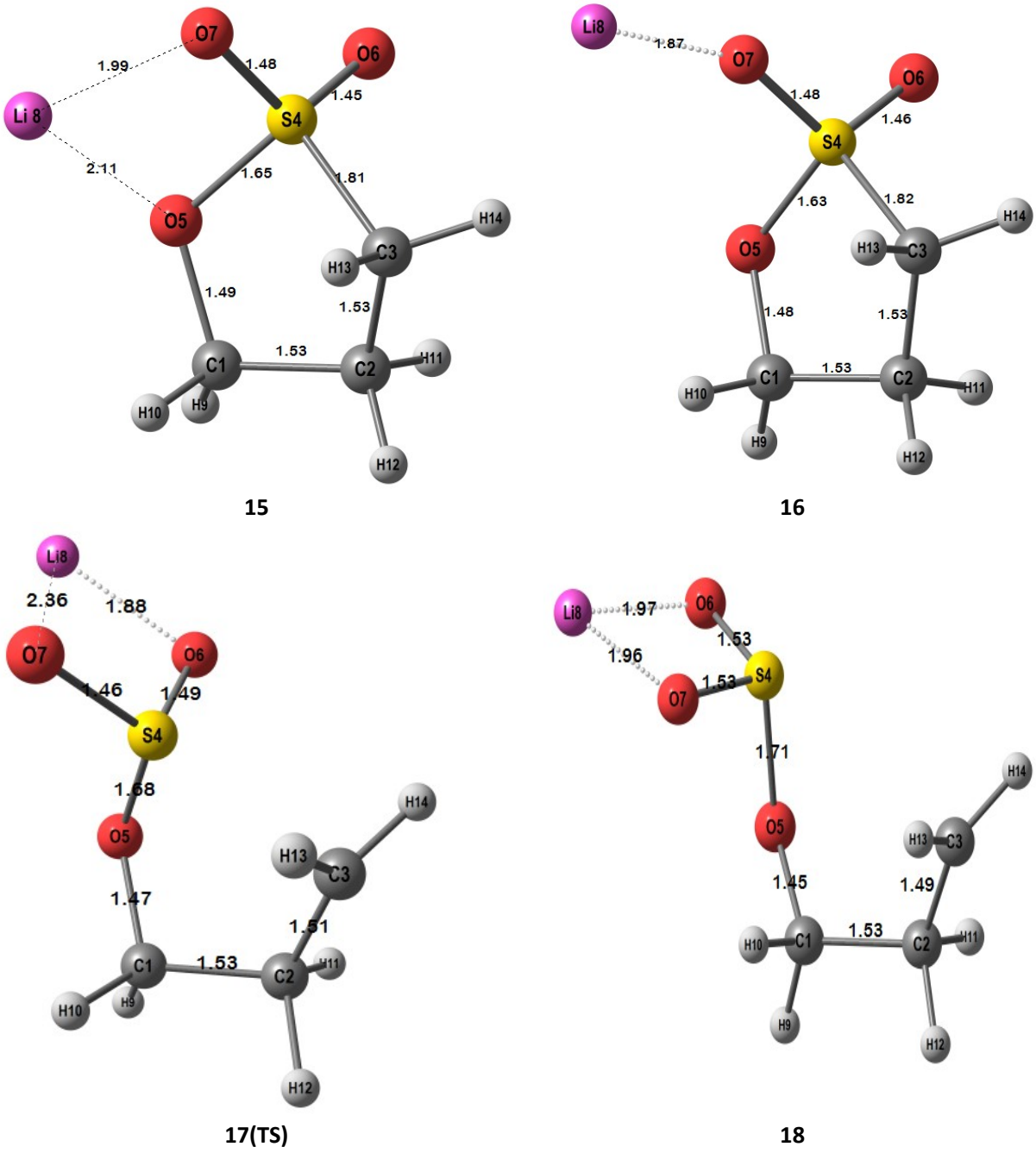
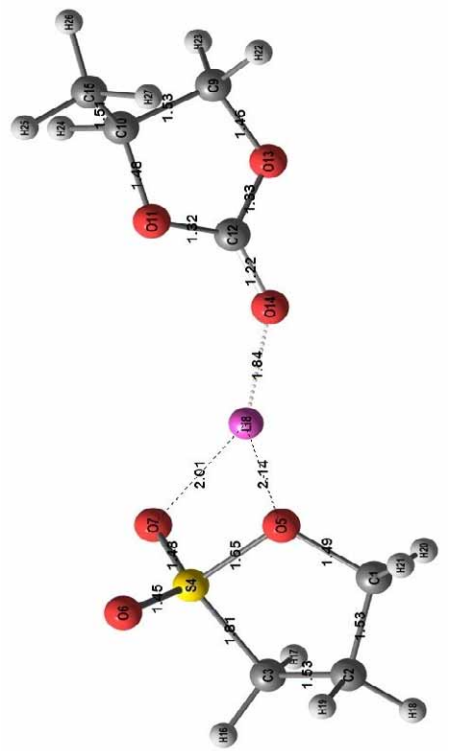


Figure S2. The optimized geometry of the reductive decomposition products of Li^+(PS) (bond length in Å)



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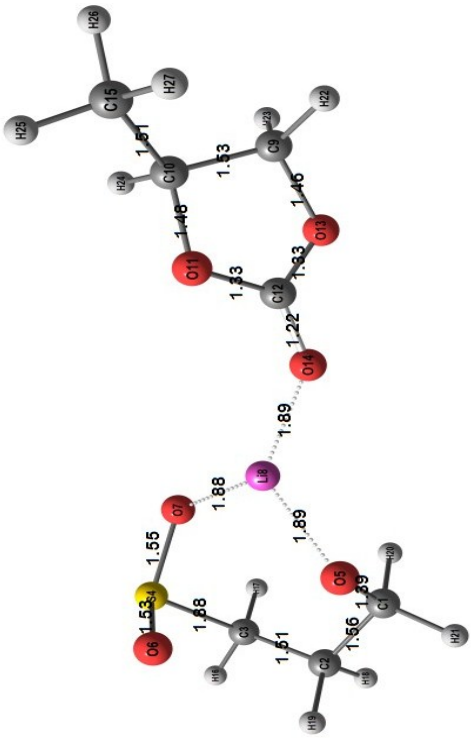

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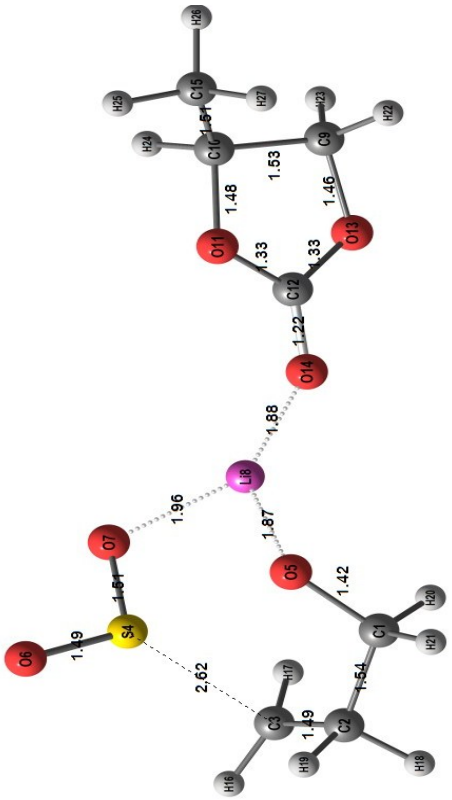

28(TS)

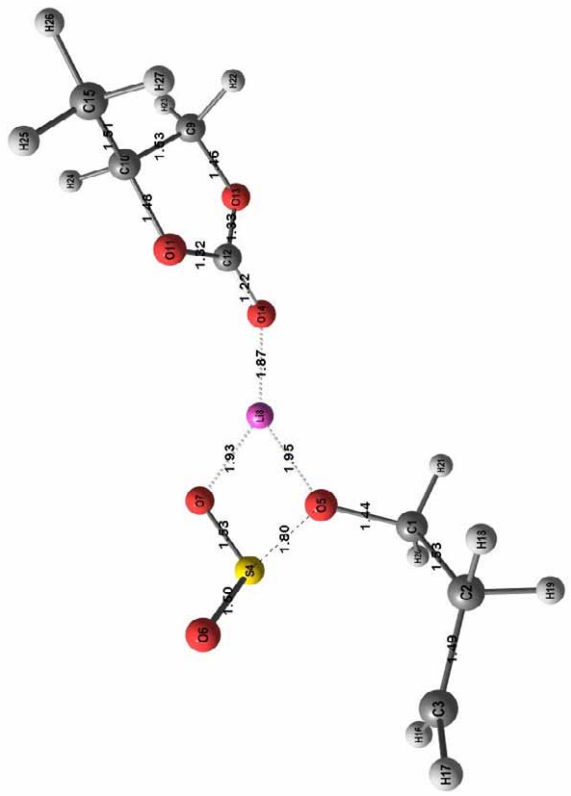

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Figure S3. The optimized geometry of the reductive decomposition products of (PC)Li^{+}(PS) (bond length in Å)

Table S1. Vibrational (harmonic approximation), $q_{vib,}$ electronic (q_{ele}), translational (q_{trans}), Rotational (q_{rot}) and calculated molecular partition functions ($Q = q_{vib}.q_{ele}.q_{trans}.q_{rot}$) per unit volume.

	q_{vib}	q_{ele}	q_{trans}	q_{rot}	Q
16	0.892×10^{16}	0.200×10^{1}	0.576×10^{8}	0.312×10^{6}	3.209×10^{29}
17 (TS)	0.327×10^{16}	0.200×10^{1}	0.576×10^{8}	0.328×10^{6}	1.231×10^{29}
12	0.122×10^{16}	0.200×10^{1}	0.530×10^{8}	0.281×10^{6}	3.647×10^{28}
13(TS)	0.120×10^{17}	0.200×10^{1}	0.530×10^{8}	0.364×10^{6}	4.236×10^{29}
27	0.111×10^{23}	0.200×10^{1}	0.138×10^{9}	0.401×10^{7}	1.235×10^{37}
28(TS)	0.237×10^{23}	0.200×10^{1}	0.138×10^{9}	0.445×10^{7}	2.912×10^{37}