

## Electronic Supplementary Information

### **Lithiation of organic polysulfides: insight into embedding site preference and lithium storage capability from DFT calculations**

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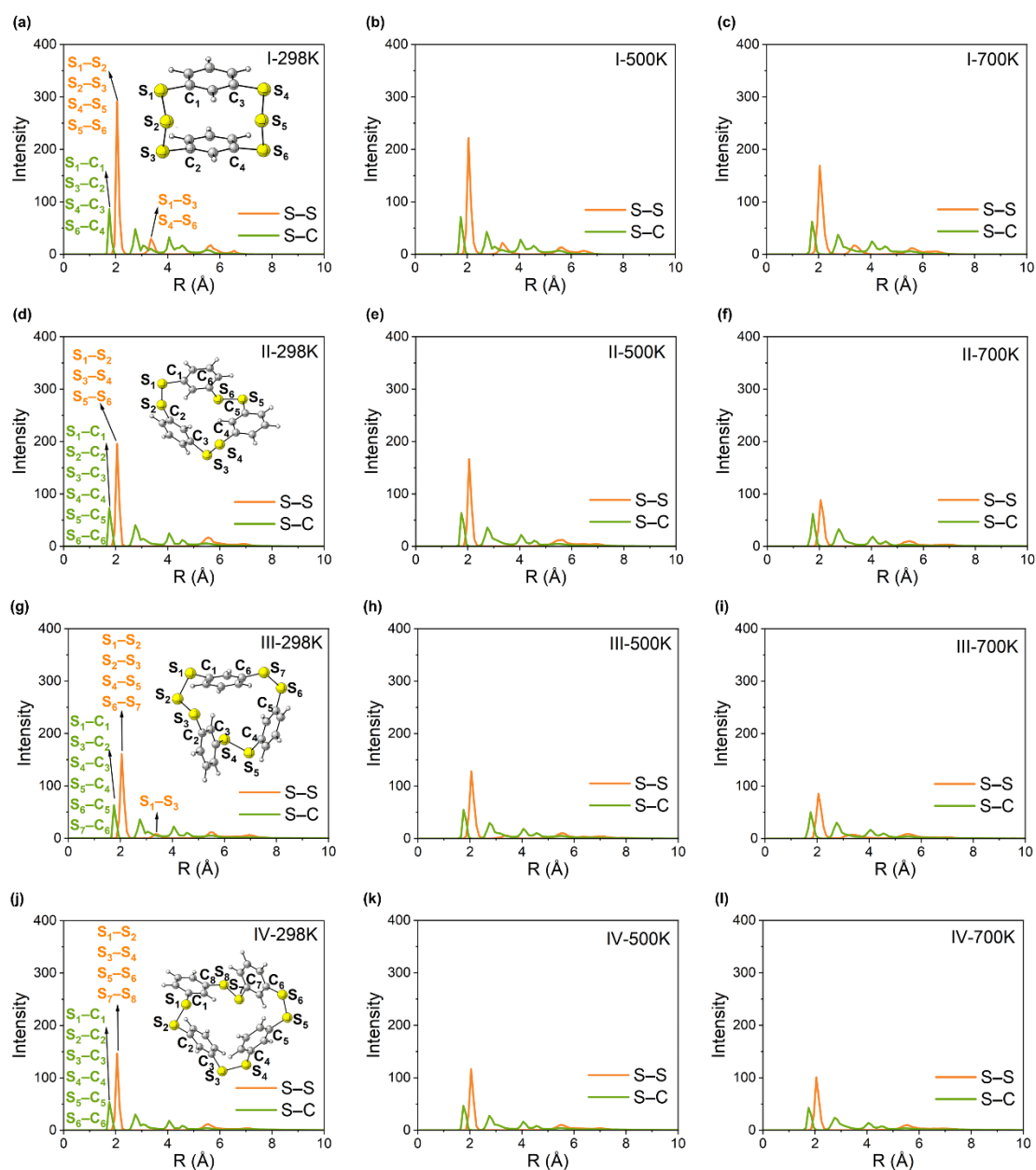
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## **AIMD simulations:**

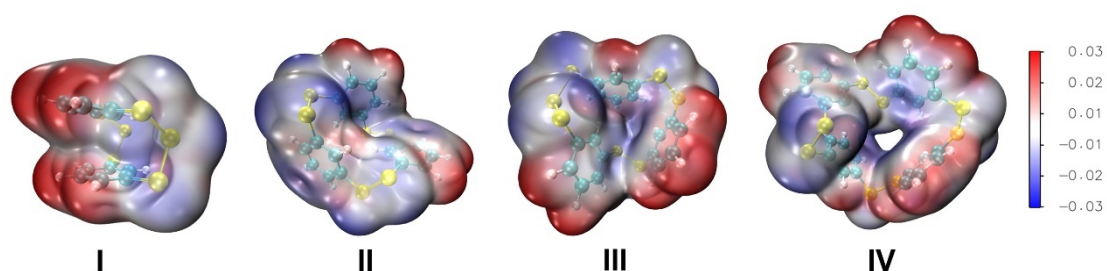
Ab initio molecular dynamics (AIMD) simulations were performed using the Vienna ab initio simulation package (VASP) to investigate the stability of cyclic OPSs (I~IV) at 298, 500 and 700 K.<sup>1, 2</sup> The cyclic OPSs (I~IV) molecules were confined within a cubic cell measuring  $20 \times 20 \times 20 \text{ \AA}$ , with a vacuum distance of over  $10 \text{ \AA}$  to avoid interactions between molecules in adjacent cells. In these simulations, the core electrons were described using the projector augmented wave (PAW)<sup>3</sup> method, while the valence electrons were treated by plane-wave basis sets of 500 eV cutoff kinetic energy. The exchange–correlation potential was treated using generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerh of (PBE).<sup>4</sup> The Brillouin-zone sampling was limited to the  $\Gamma$ -point. Atomic geometries were optimized using a conjugate gradient algorithm until the residual forces on atoms were reduced to less than  $0.02 \text{ eV \AA}^{-1}$ . These simulations utilized exact Hellmann–Feynman forces and applied the canonical ensemble statistics to the motion of atomic nuclei via a Nosé thermostat.<sup>5</sup> Newton's equations of motion were integrated using the Verlet algorithm, with a total simulation time of 10 ps and a time step of 1 fs.



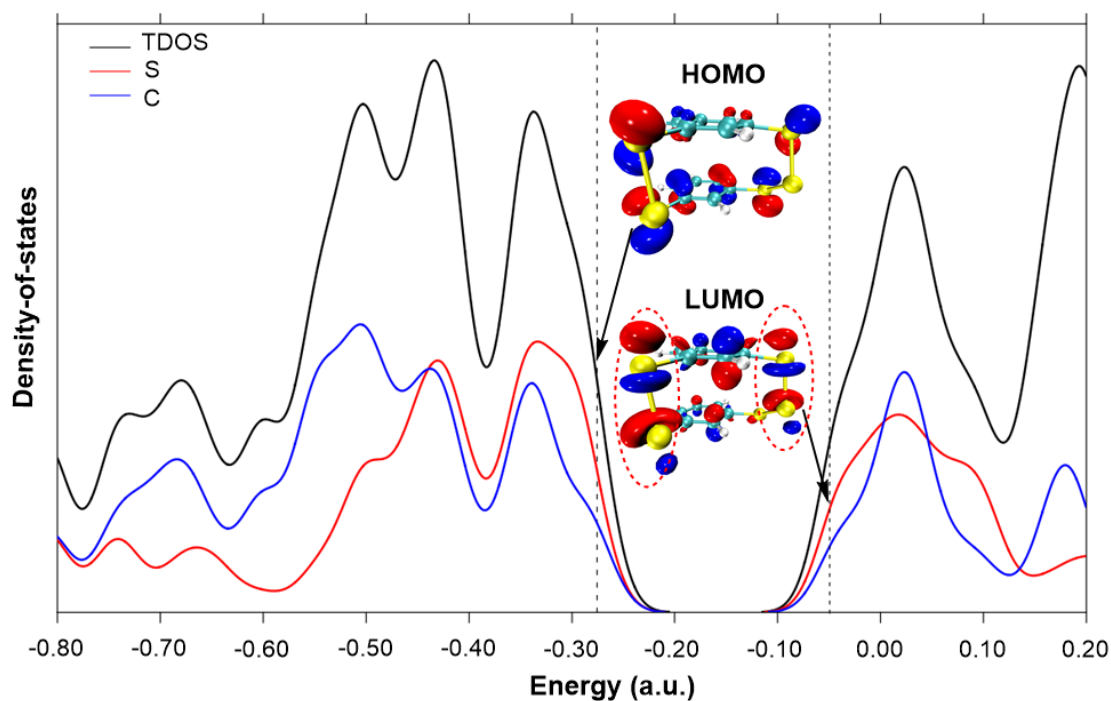
**Fig. S1** Radial distribution of selected interatomic distances for cyclic OPSs (I~IV) at 298, 500 and 700 K, respectively.

To investigate the structural stability of cyclic OPSs (I~IV), AIMD simulations were performed using VASP for 10 ps with a time step of 1 fs, at temperatures of 298, 500, and 700 K, respectively. The radial distribution of selected interatomic distances for cyclic OPSs (I~IV) is depicted in Fig. S1. During the AIMD simulations, the characteristic peaks of the main S–S and S–C bonds in OPSs (I~IV) remained nearly consistent across the temperatures

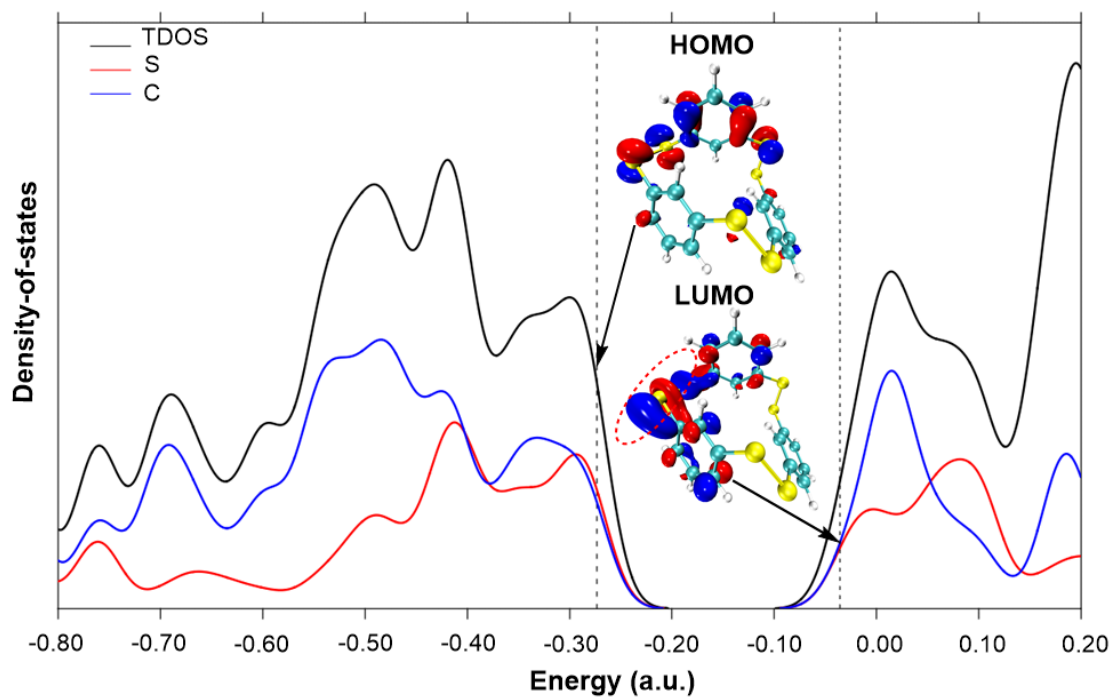
considered. Meanwhile, compared to 298 K, the intensity of the S–S bond peaks exhibits a slight decrease, attributed to the relatively larger changes in atomic distances at elevated temperatures (500 and 700 K). Overall, the AIMD simulations suggest that cyclic OPSs (I~IV) demonstrate a degree of kinetic and thermal stability.



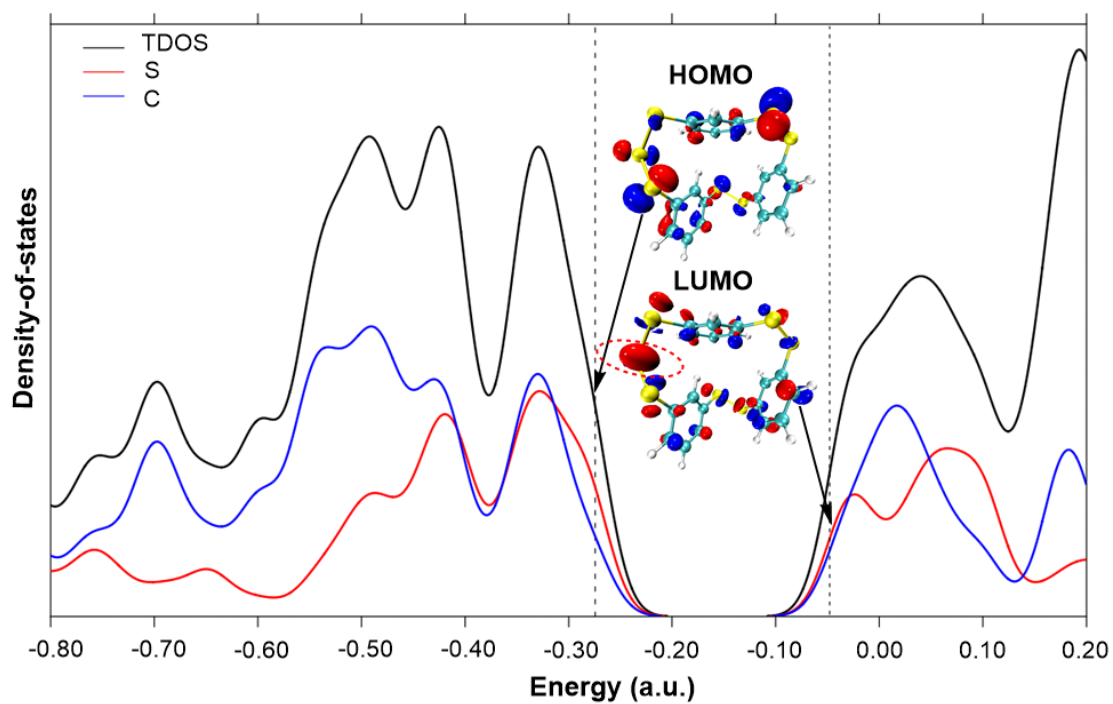
**Fig. S2** Molecular electrostatic potentials for the cyclic OPSs (I~IV). The red and blue isosurfaces (in a.u.) denote the positive and negative electrostatic potential regions, respectively.



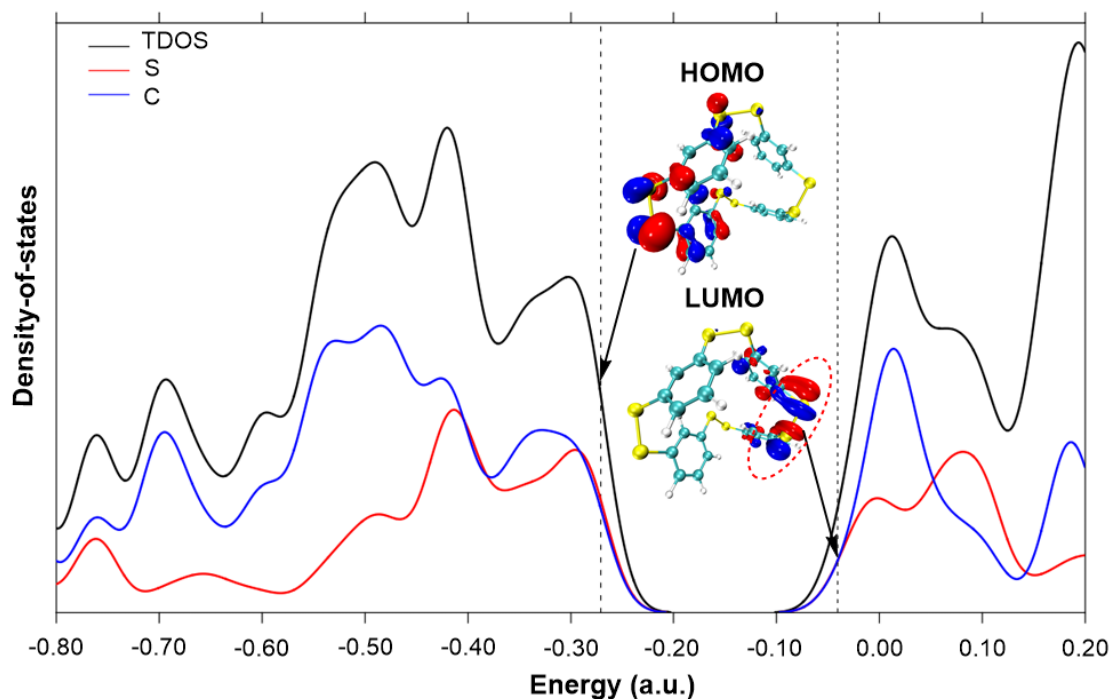
**Fig. S3** Total and partial (S and C atoms) density-of-states map of OPS (I).



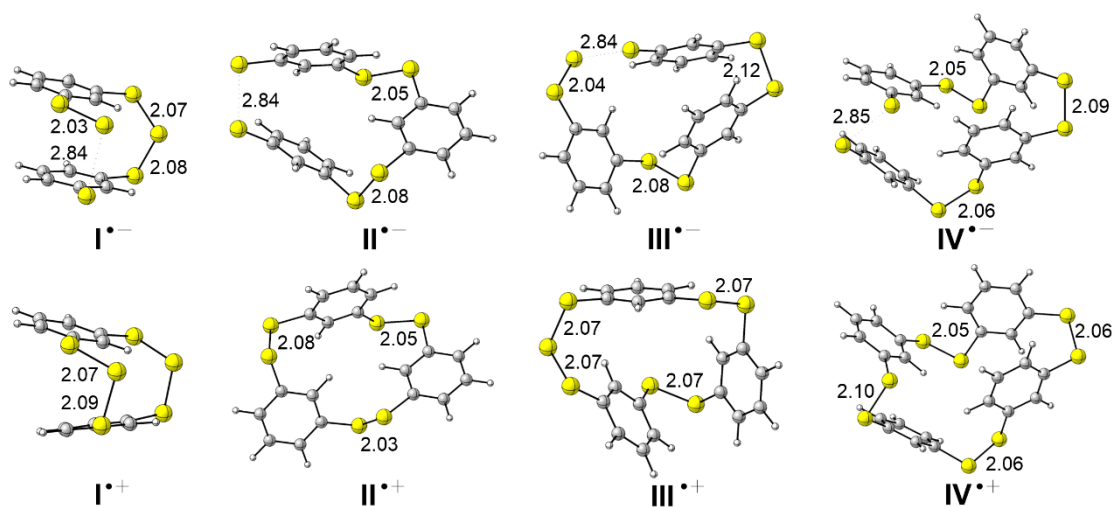
**Fig. S4** Total and partial (S and C atoms) density-of-states map of OPS (II).



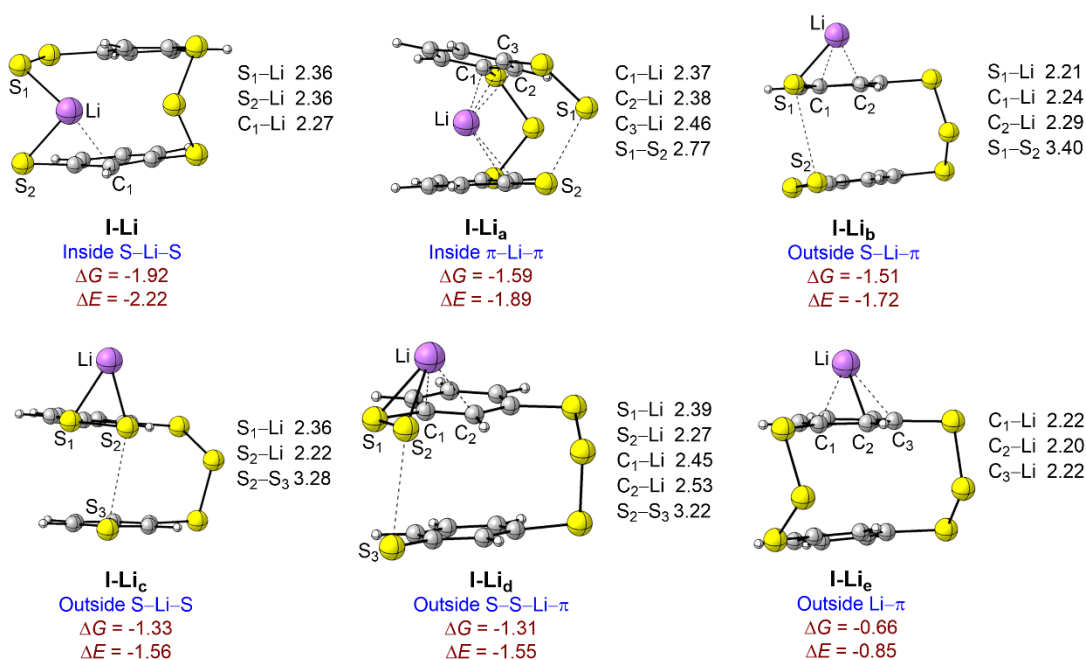
**Fig. S5** Total and partial (S and C atoms) density-of-states map of OPS (III).



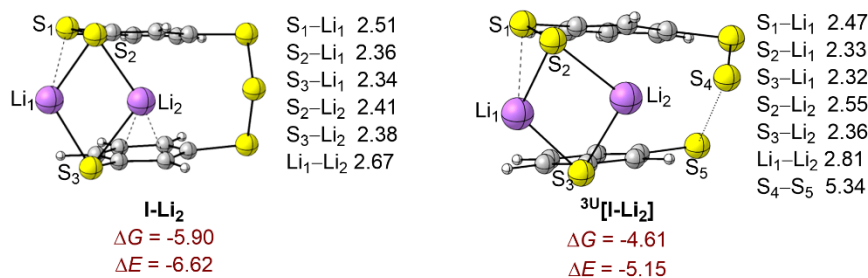
**Fig. S6** Total and partial (S and C atoms) density-of-states map of OPS (IV).



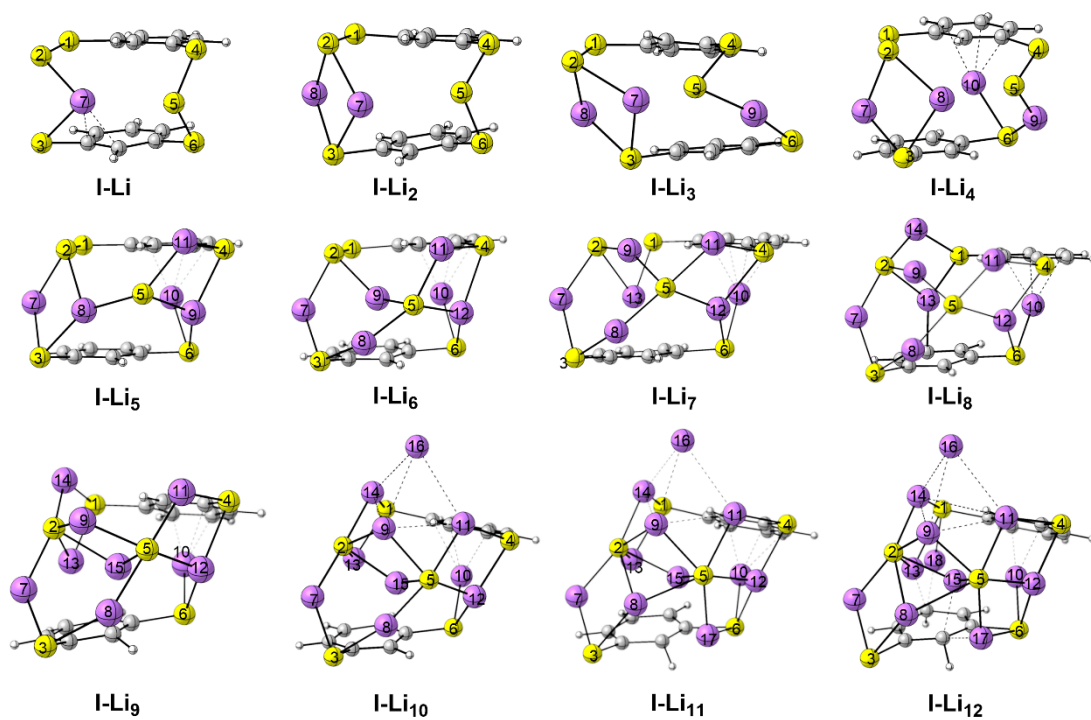
**Fig. S7** Optimized structures of cyclic OPSs (I-IV) and their key charged states. The key inter-atomic and bond lengths (in Å, black) are given.



**Fig. S8** Lithiation free energies ( $\Delta G$ , in eV) and electronic energies ( $\Delta E$ , in eV) of **I-Li** species in different configurations were compared at the UM06-2X-D3/cc-pVTZ level. The key bond lengths (in Å, black) are given.

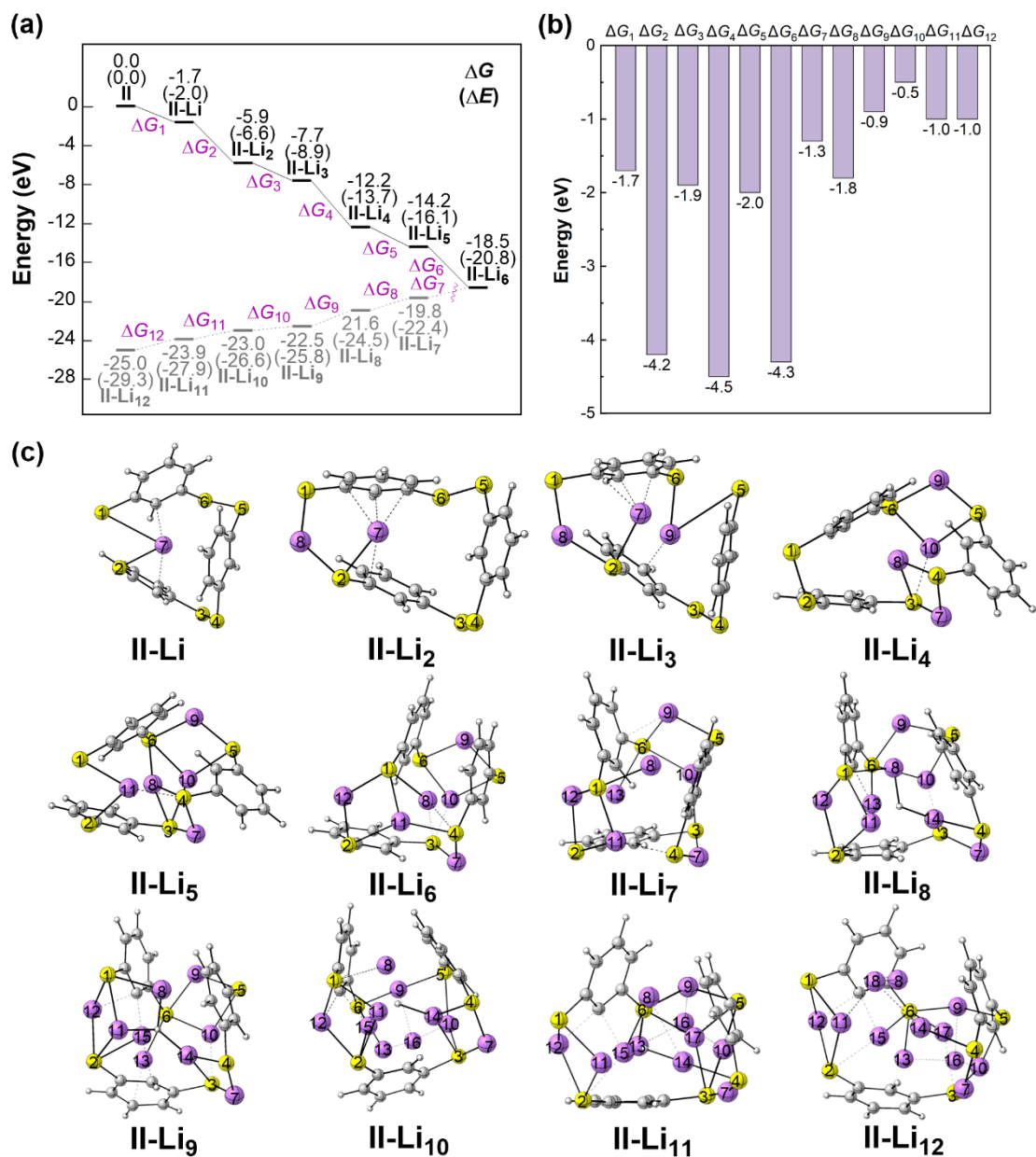


**Fig. S9** Optimized structures, lithiation free energies ( $\Delta G$ , in eV) and electronic energies ( $\Delta E$ , in eV) of closed-shell singlet states (**I-Li<sub>2</sub>**) and triplet states (**<sup>3</sup>U[I-Li<sub>2</sub>]**) of the LiPSs (**I-Li<sub>2</sub>**) at the (U)M06-2X-D3/cc-pVTZ level. The key bond lengths (in Å, black) are given.

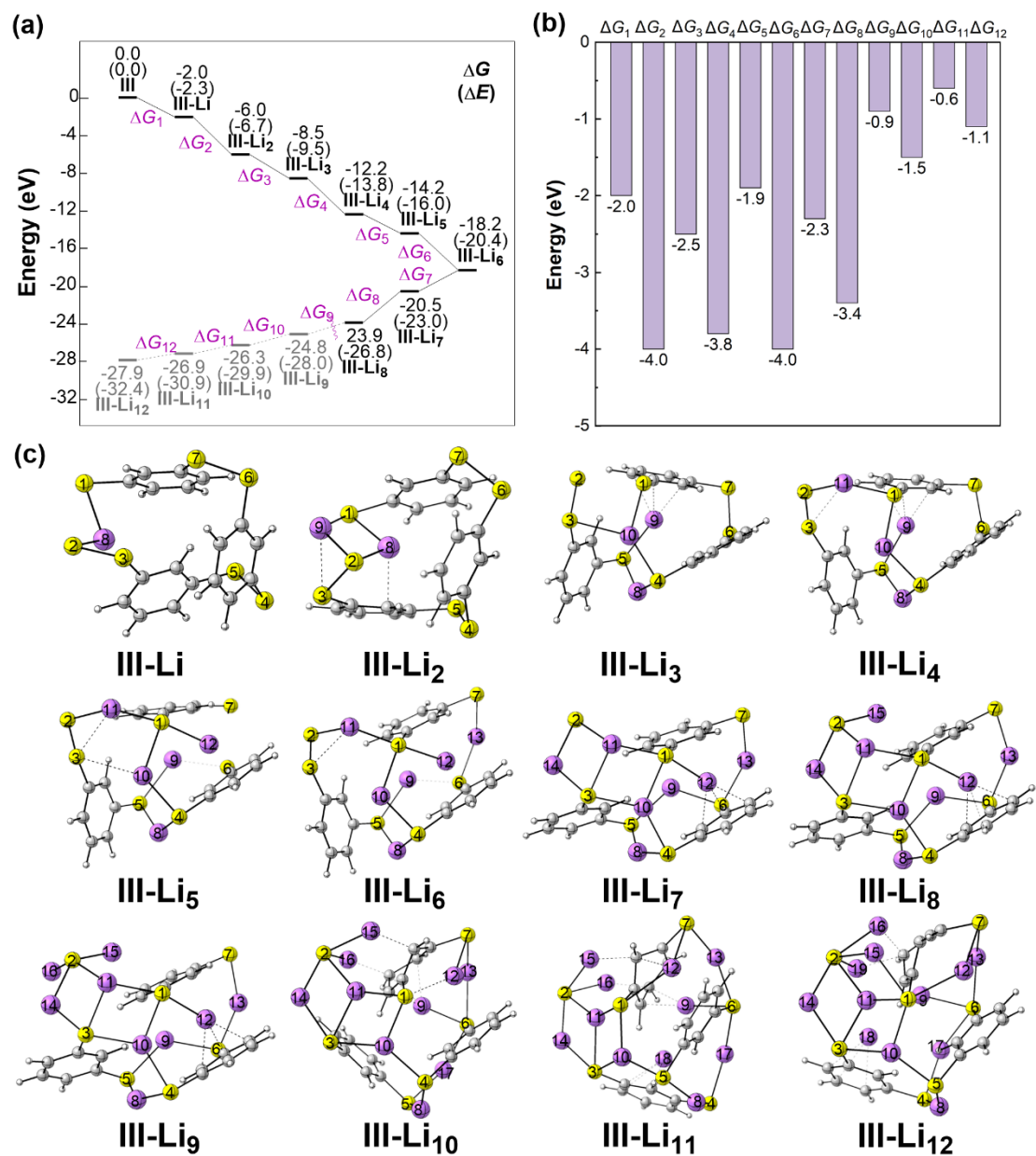


**Fig. S10** Geometric structures for LiPSs (I-Li~I-Li<sub>12</sub>).

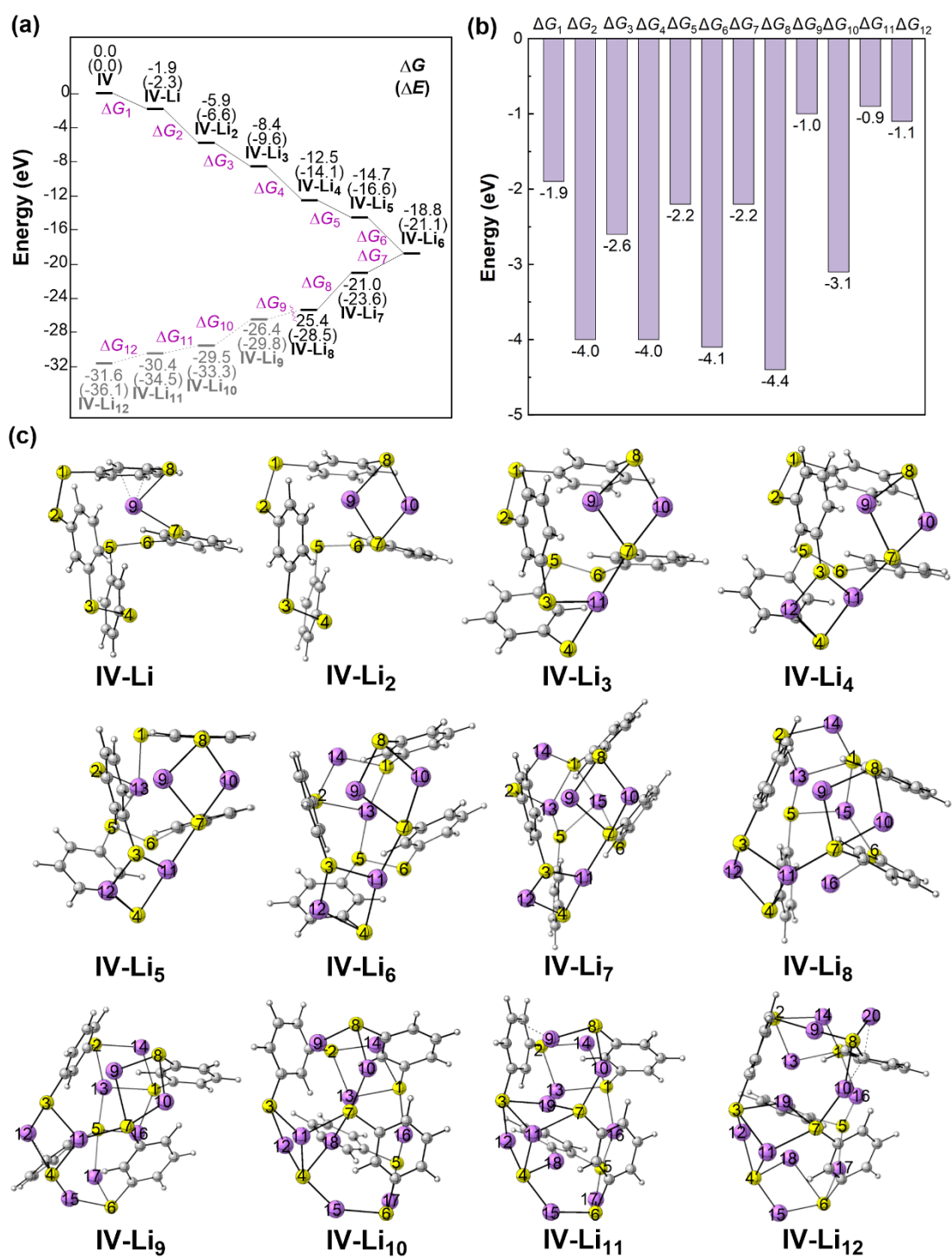




**Fig. S11** Relative Gibbs free energies ( $\Delta G$ , in eV) and the geometric structures involving the lithiation of the selected cyclic OPS **II** at the (U)M06-2X-D3/cc-pVTZ level.



**Fig. S12** Relative Gibbs free energies ( $\Delta G$ , in eV) and the geometric structures involving the lithiation of the selected cyclic OPS **III** at the (U)M06-2X-D3/cc-pVTZ level.



**Fig. S13** Relative Gibbs free energies ( $\Delta G$ , in eV) and the geometric structures involving the lithiation of the selected cyclic OPS **IV** at the (U)M06-2X-D3/cc-pVTZ level.

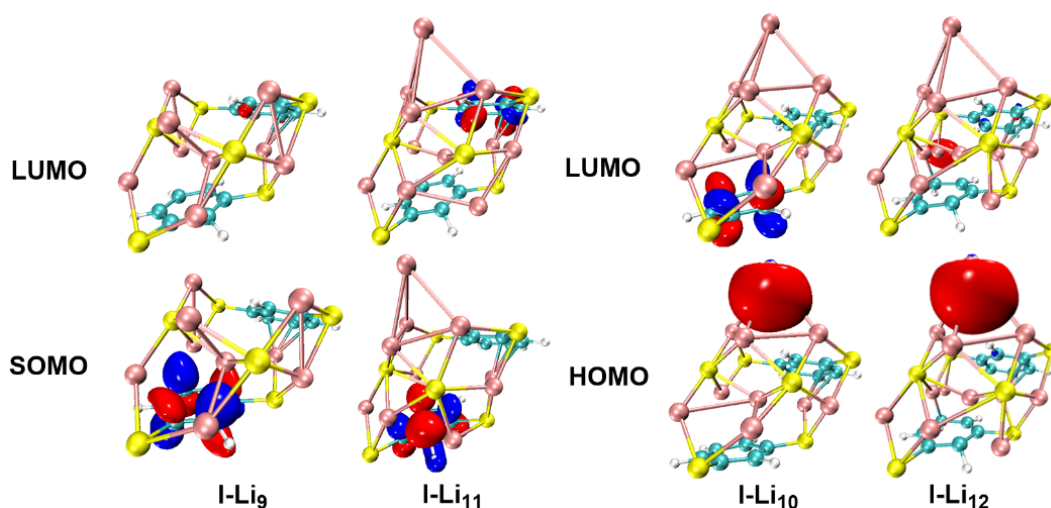


Fig. S14 Key molecular orbitals of the selected LiPSs (I-Li<sub>9</sub>~I-Li<sub>12</sub>).

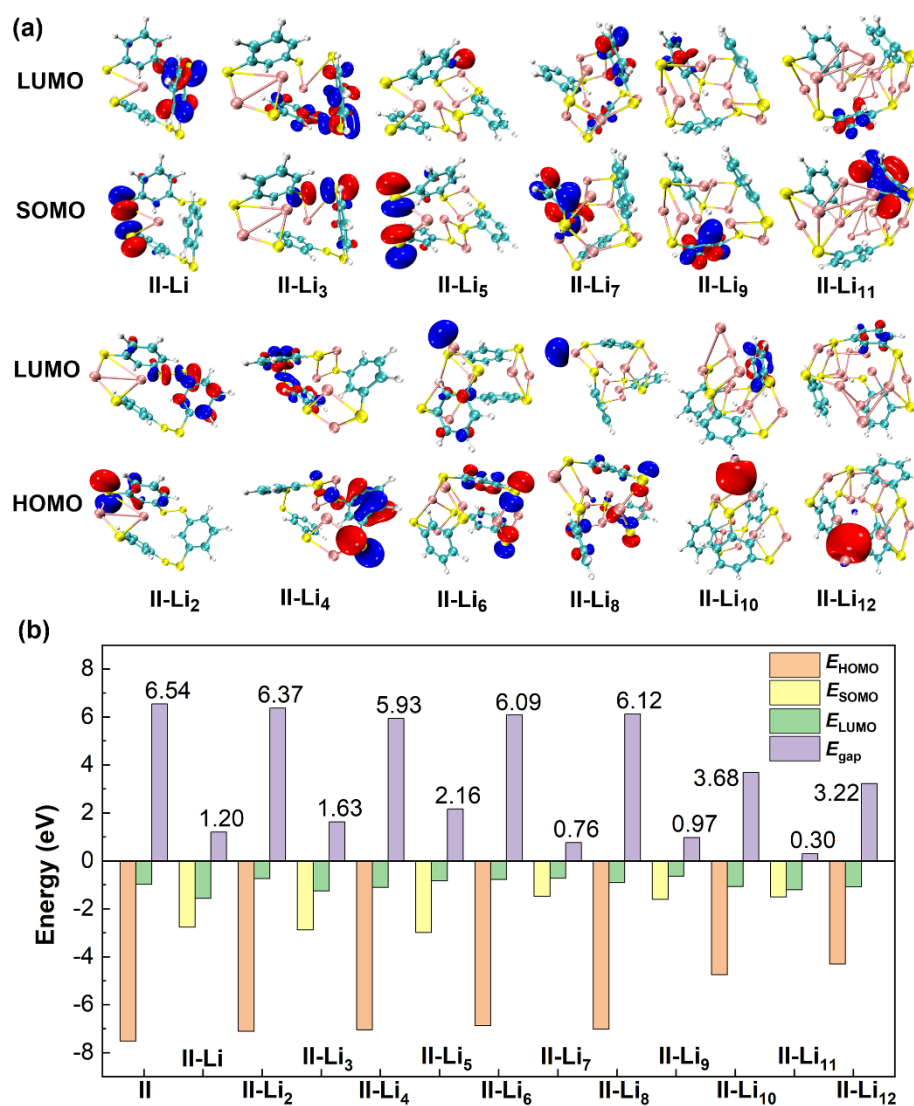


Fig. S15 Key molecular orbitals and their energy levels (in eV) of the LiPSs (II-Li<sub>n</sub>).

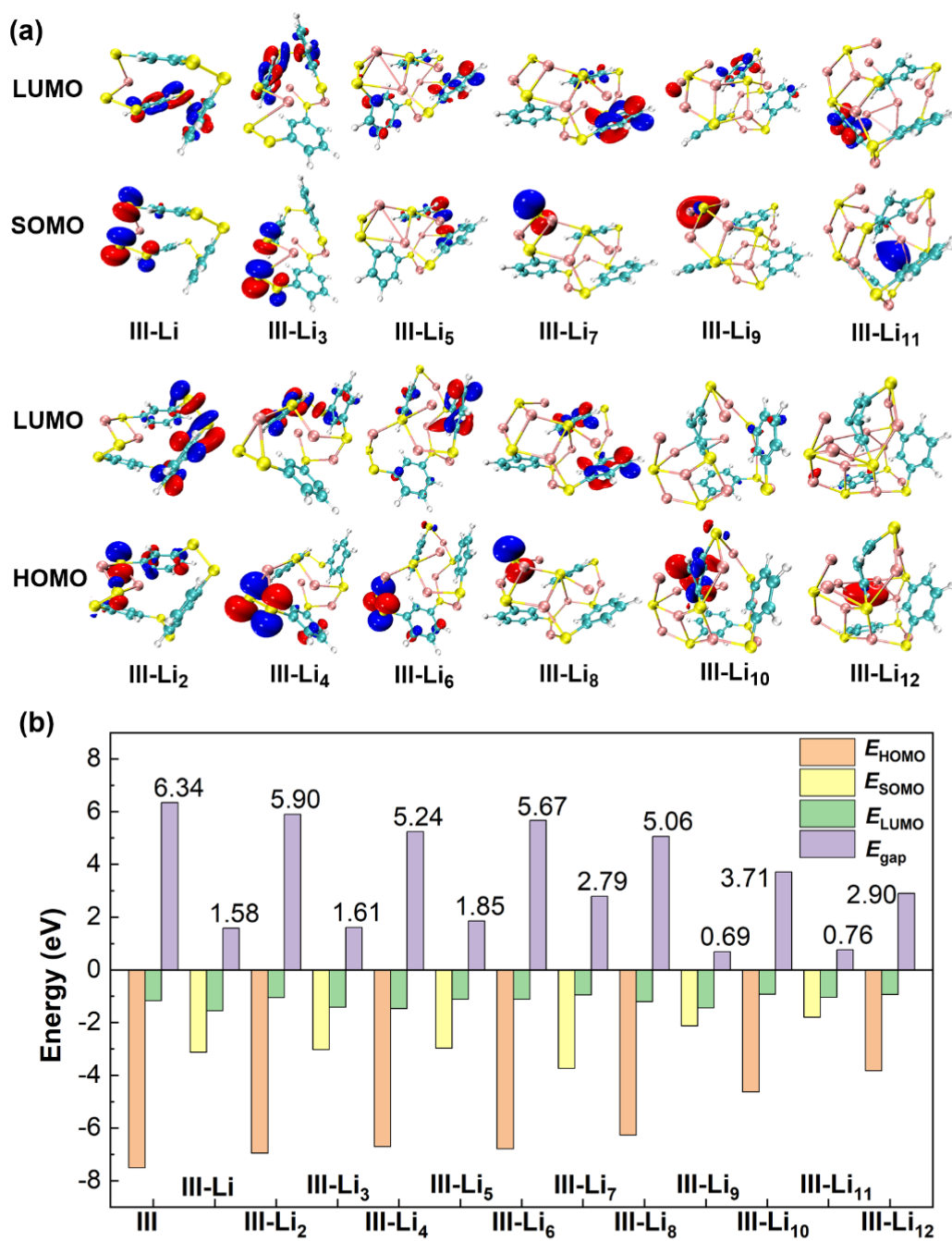


Fig. S16 Key molecular orbitals and their energy levels (in eV) of the LiPSs (III-Li<sub>n</sub>).

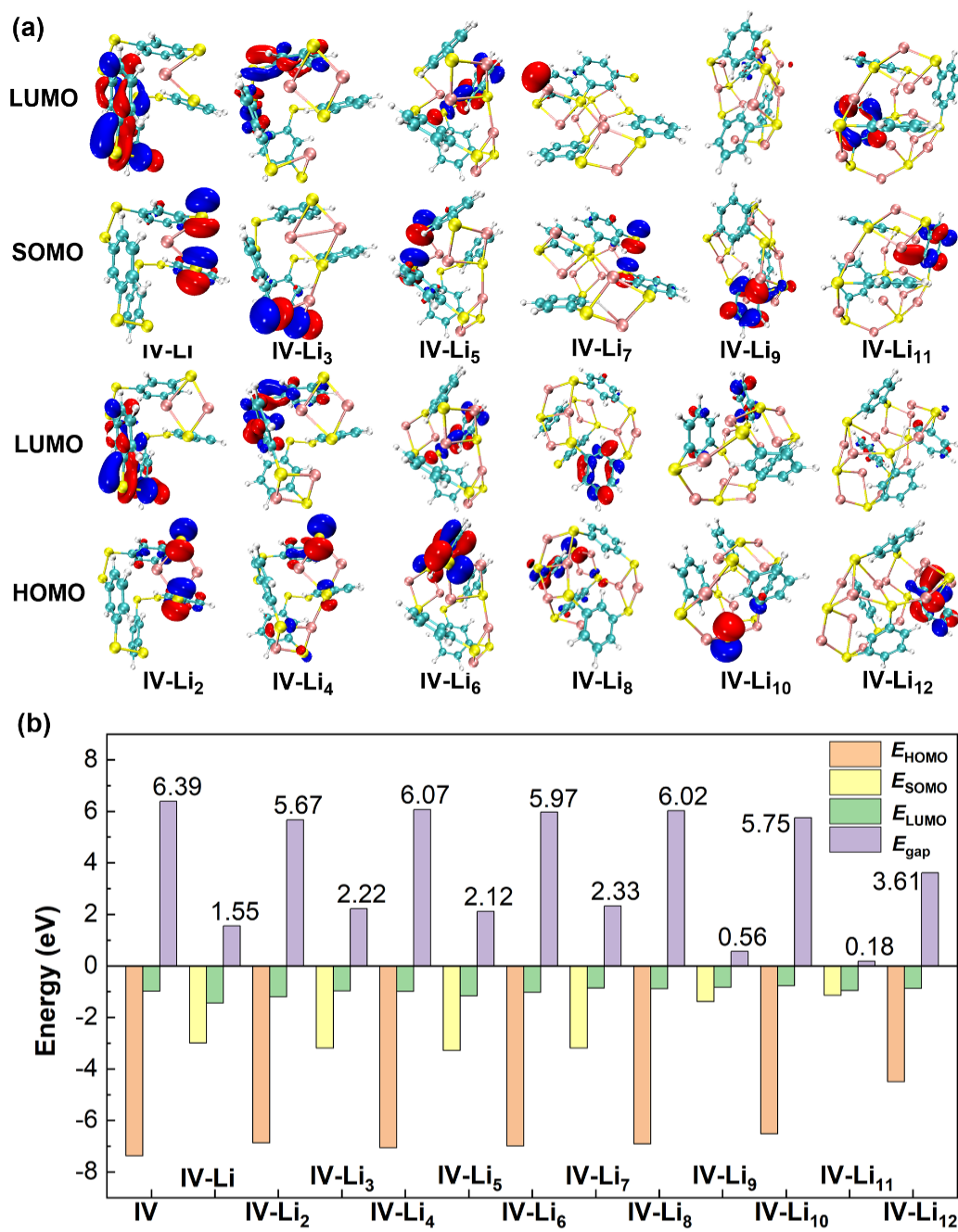
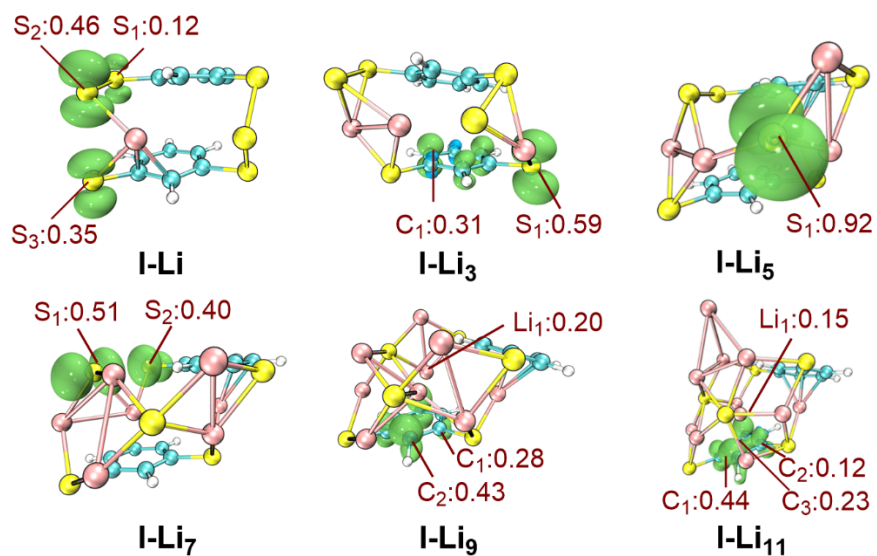
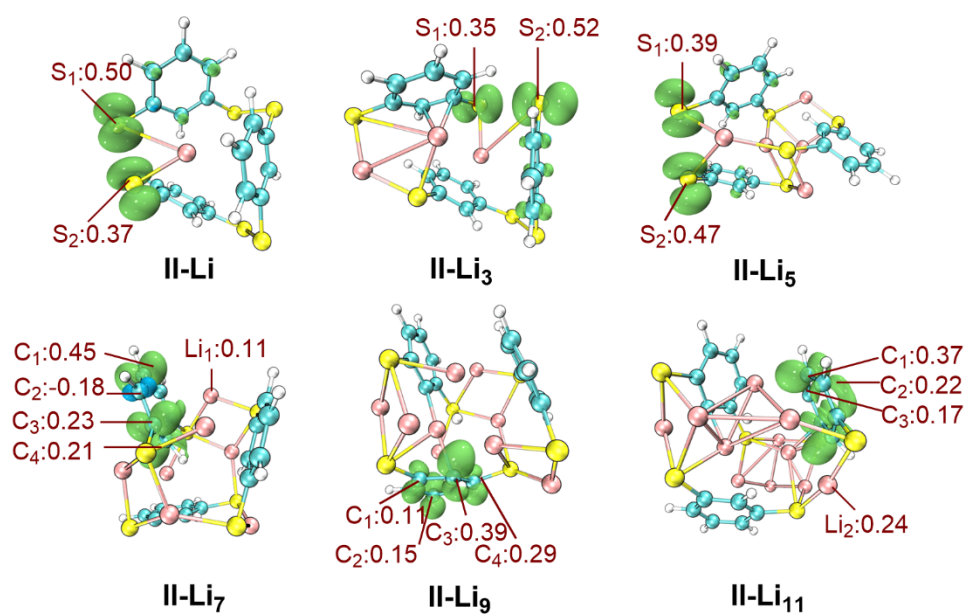


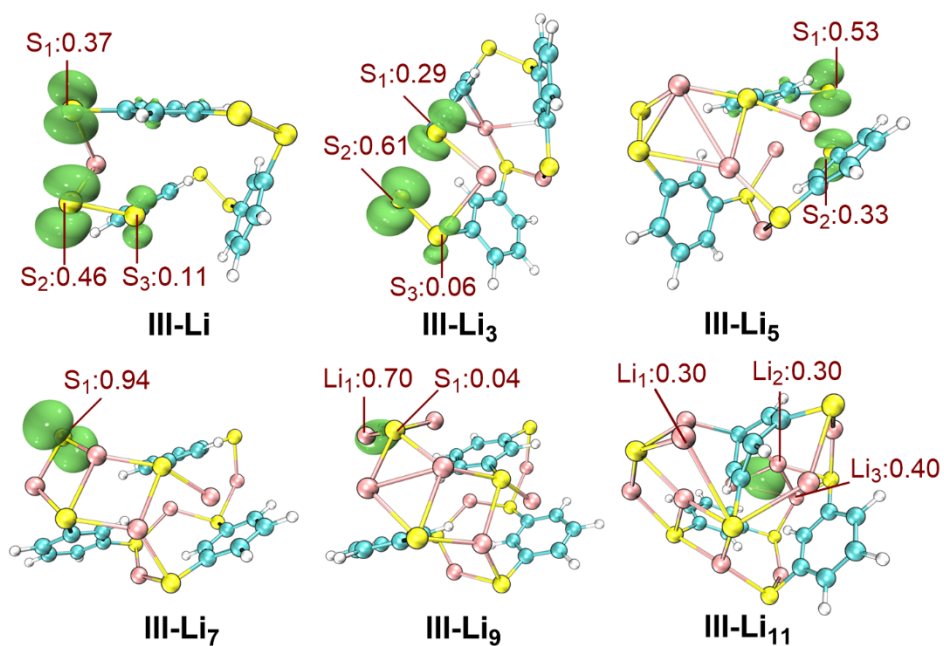
Fig. S17 Key molecular orbitals and their energy levels (in eV) of the LiPSs (IV-Li<sub>n</sub>).



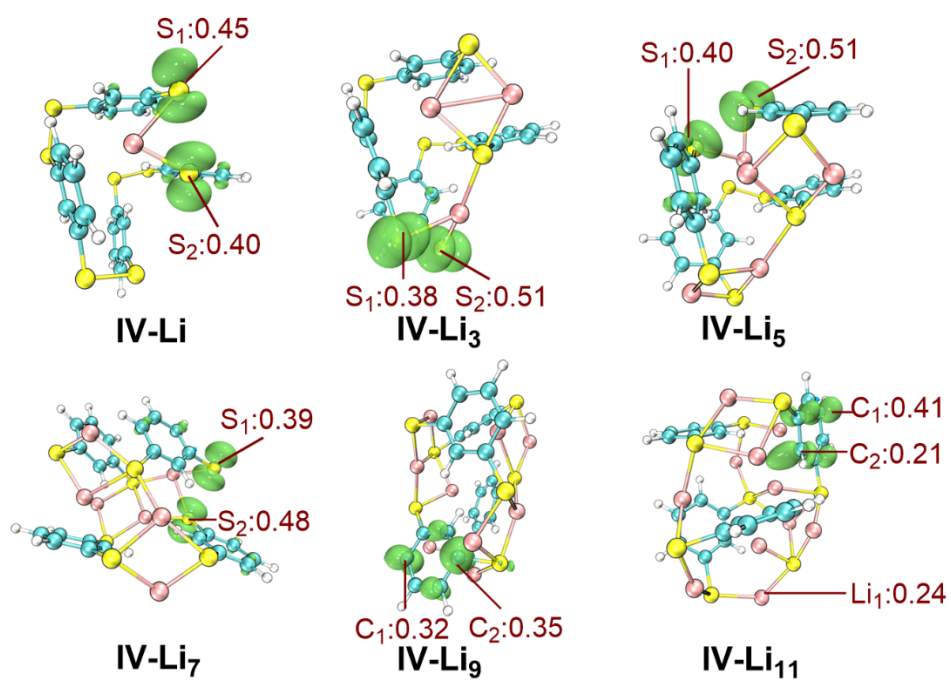
**Fig. S18** The spin densities of LiPSs (**I-Li<sub>n</sub>**) at the UM06-2X-D3/cc-pVTZ level.



**Fig. S19** The spin densities of LiPSs (**II-Li<sub>n</sub>**) at the UM06-2X-D3/cc-pVTZ level.



**Fig. S20** The spin densities of LiPSs (III-Li<sub>n</sub>) at the UM06-2X-D3/cc-pVTZ level.



**Fig. S21** The spin densities of LiPSs (IV-Li<sub>n</sub>) at the UM06-2X-D3/cc-pVTZ level.



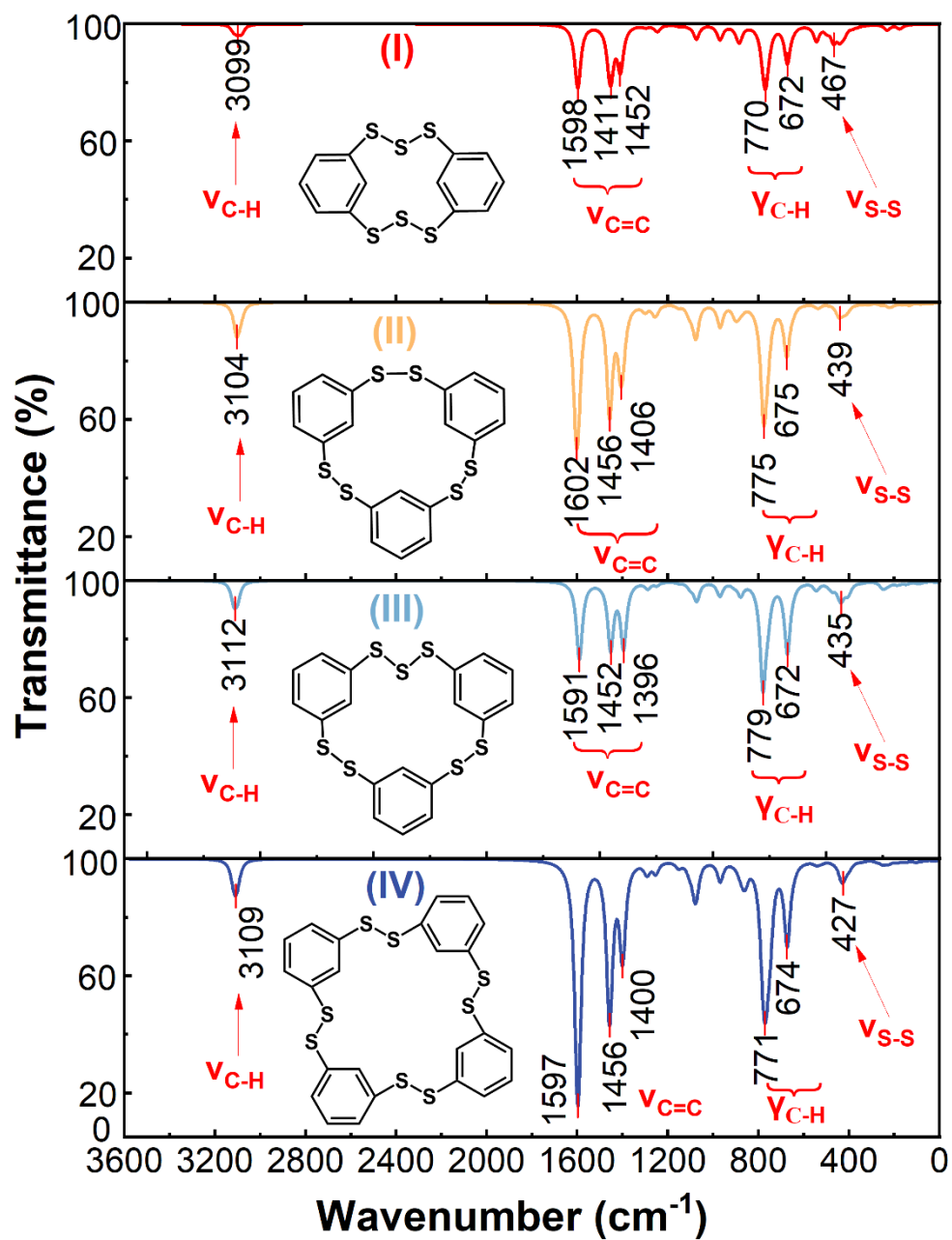


Fig. S22 Simulated infrared spectra for the cyclic OPSs (I~IV).

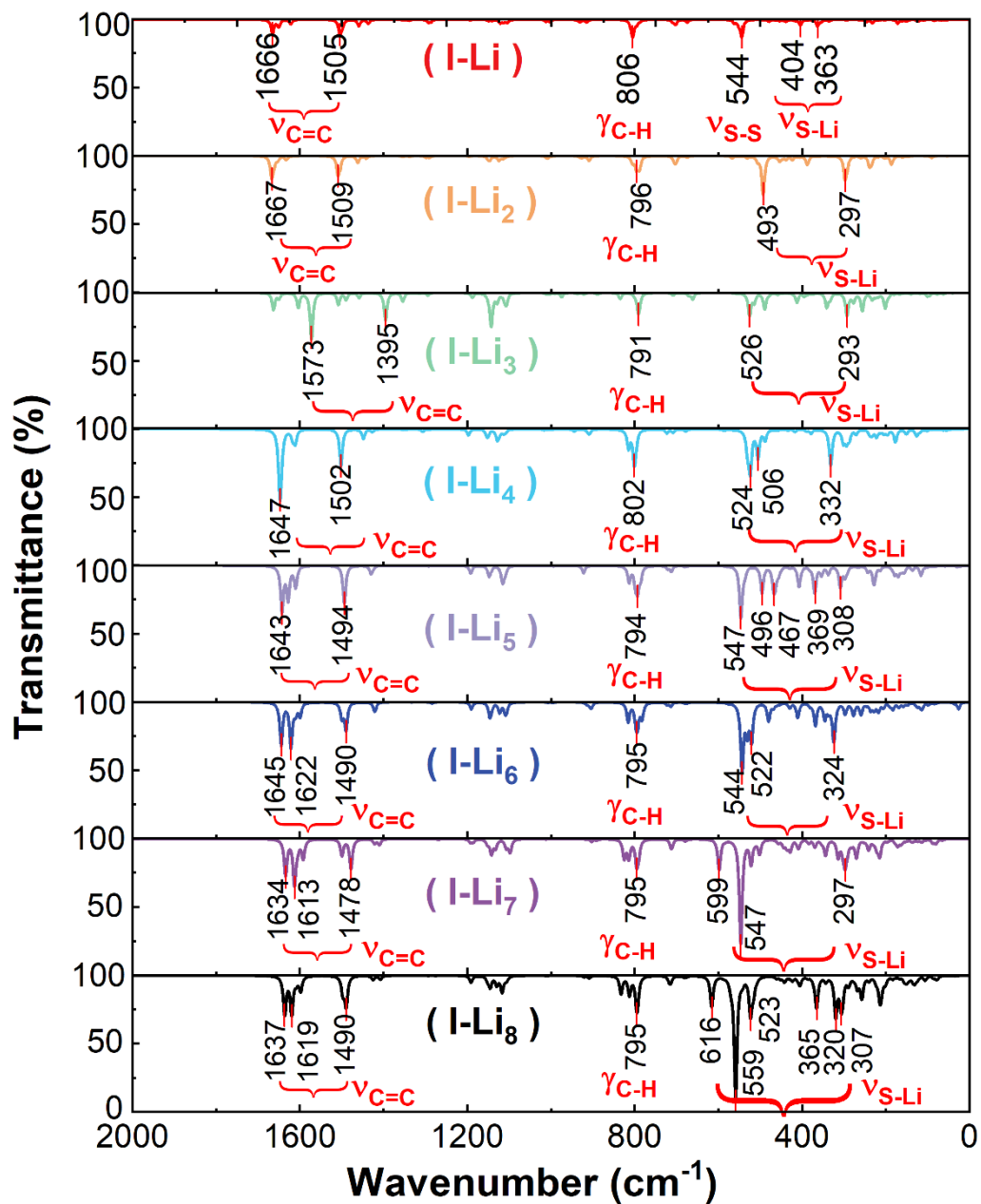


Fig. S23 Simulated infrared spectra for the LiPSs (I-Li<sub>n</sub>).

**Table S1** Key NPA atomic charges of LiPSs (**I-Li~I-Li<sub>12</sub>**) at the (U)M06-2X-D3/cc-pVTZ level. The atomic sequence numbers correspond to Fig. S10.

<b>I-Li</b>			<b>I-Li<sub>2</sub></b>			<b>I-Li<sub>3</sub></b>			<b>I-Li<sub>4</sub></b>		
<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>
<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>	
1	S	0.17629	1	S	0.06987	1	S	0.03166	1	S	0.17694
2	S	0.05367	2	S	-0.72419	2	S	-0.35379	2	S	-0.72219
3	S	0.06456	3	S	-0.56049	3	S	-0.27047	3	S	-0.52382
4	S	0.07577	4	S	0.15074	4	S	0.04315	4	S	0.10198
5	S	-0.02262	5	S	-0.03410	5	S	-0.35258	5	S	-0.71526
6	S	0.07786	6	S	0.14140	6	S	0.29218	6	S	-0.55413
7	Li	0.42192	7	Li	0.84917	7	Li	0.42097	7	Li	0.85424
			8	Li	0.84520	8	Li	0.39975	8	Li	0.81472
						9	Li	0.41378	9	Li	0.84586
									10	Li	0.87810
<b>I-Li<sub>5</sub></b>			<b>I-Li<sub>6</sub></b>			<b>I-Li<sub>7</sub></b>			<b>I-Li<sub>8</sub></b>		
<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>
<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>	
1	S	0.07314	1	S	0.16734	1	S	0.14384	1	S	-0.55173
2	S	-0.34443	2	S	-0.71925	2	S	-0.31218	2	S	-1.67804
3	S	-0.26530	3	S	-0.56799	3	S	-0.28363	3	S	-0.56775
4	S	-0.27394	4	S	-0.51298	4	S	-0.27010	4	S	-0.54393
5	S	0.06517	5	S	-1.68274	5	S	-0.84008	5	S	-1.68194
6	S	-0.27205	6	S	-0.52384	6	S	-0.25851	6	S	-0.53313
7	Li	0.43047	7	Li	0.85946	7	Li	0.43098	7	Li	0.85593
8	Li	0.39736	8	Li	0.87746	8	Li	0.42667	8	Li	0.84518
9	Li	0.39573	9	Li	0.76070	9	Li	0.40815	9	Li	0.81140
10	Li	0.43342	10	Li	0.86326	10	Li	0.42955	10	Li	0.85722
11	Li	0.43625	11	Li	0.86768	11	Li	0.43317	11	Li	0.86281
			12	Li	0.80873	12	Li	0.39349	12	Li	0.79213
						13	Li	0.39469	13	Li	0.80070
									14	Li	0.87678
<b>I-Li<sub>9</sub></b>			<b>I-Li<sub>10</sub></b>			<b>I-Li<sub>11</sub></b>			<b>I-Li<sub>12</sub></b>		
<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>	<b>N</b>	<b>Ato</b>	<b>Charge</b>
<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>		<b>o</b>	<b>m</b>	
1	S	-0.27469	1	S	-0.55947	1	S	-0.27003	1	S	-0.56740
2	S	-0.84369	2	S	-1.70147	2	S	-0.84370	2	S	-1.65434
3	S	-0.28181	3	S	-0.55169	3	S	-0.25428	3	S	-0.56705
4	S	-0.27709	4	S	-0.53530	4	S	-0.26742	4	S	-0.51510
5	S	-0.82829	5	S	-1.69809	5	S	-0.82172	5	S	-1.65150
6	S	-0.28966	6	S	-0.51246	6	S	-0.29211	6	S	-0.60968
7	Li	0.43060	7	Li	0.86947	7	Li	0.43637	7	Li	0.86805
8	Li	0.42237	8	Li	0.86259	8	Li	0.40796	8	Li	0.80950

9	Li	0.43630	9	Li	0.61045	9	Li	0.28057	9	Li	0.63144
10	Li	0.43332	10	Li	0.85968	10	Li	0.43432	10	Li	0.85239
11	Li	0.42852	11	Li	0.67400	11	Li	0.33030	11	Li	0.67116
12	Li	0.40865	12	Li	0.81758	12	Li	0.39889	12	Li	0.80013
13	Li	0.41509	13	Li	0.83782	13	Li	0.41421	13	Li	0.76667
14	Li	0.43713	14	Li	0.67763	14	Li	0.35497	14	Li	0.67344
15	Li	0.39391	15	Li	0.78064	15	Li	0.39611	15	Li	0.76201
			16	Li	-0.21757	16	Li	-0.08379	16	Li	-0.20804
						17	Li	0.43165	17	Li	0.85638
									18	Li	0.86327

**Table S2** Key NPA atomic charges of LiPSs (**II-Li-III-Li<sub>12</sub>**) at the (U)M06-2X-D3/cc-pVTZ level. The atomic sequence numbers correspond to Fig. S11.

II-Li			II-Li <sub>2</sub>			II-Li <sub>3</sub>			II-Li <sub>4</sub>		
N	Atom	Charge	N	Atom	Charge	N	Atom	Charge	N	Atom	Charge
1	S	0.22830	1	S	-0.49345	1	S	-0.26345	1	S	0.12686
2	S	0.07078	2	S	-0.58202	2	S	-0.27862	2	S	0.13498
3	S	0.08268	3	S	0.15928	3	S	0.08667	3	S	-0.58721
4	S	0.07865	4	S	0.16099	4	S	0.07945	4	S	-0.54149
5	S	0.06597	5	S	0.15461	5	S	0.24229	5	S	-0.57190
6	S	0.07892	6	S	0.17560	6	S	0.05423	6	S	-0.59224
7	Li	0.43911	7	Li	0.88636	7	Li	0.43760	7	Li	0.86110
			8	Li	0.83625	8	Li	0.42175	8	Li	0.80511
						9	Li	0.43711	9	Li	0.85297
									10	Li	0.81718
II-Li <sub>5</sub>			II-Li <sub>6</sub>			II-Li <sub>7</sub>			II-Li <sub>8</sub>		
N	Atom	Charge	N	Atom	Charge	N	Atom	Charge	N	Atom	Charge
	H	0.10833		H	0.19751	1	S	-0.30232	1	S	-0.58675
1	S	0.11577	1	S	-0.62401	2	S	-0.26241	2	S	-0.54951
2	S	0.14959	2	S	-0.53741	3	S	-0.28553	3	S	-0.63003
3	S	-0.29827	3	S	-0.60222	4	S	-0.28480	4	S	-0.54902
4	S	-0.30242	4	S	-0.61394	5	S	-0.27849	5	S	-0.54578
5	S	-0.28605	5	S	-0.56831	6	S	-0.30567	6	S	-0.60261
6	S	-0.29470	6	S	-0.54049	7	Li	0.42876	7	Li	0.87769
7	Li	0.43594	7	Li	0.86850	8	Li	0.45477	8	Li	0.83253
8	Li	0.43343	8	Li	0.80603	9	Li	0.43808	9	Li	0.84078
9	Li	0.42572	9	Li	0.84503	10	Li	0.40044	10	Li	0.81788
10	Li	0.40715	10	Li	0.80331	11	Li	0.40247	11	Li	0.82400
11	Li	0.39633	11	Li	0.82589	12	Li	0.44226	12	Li	0.85331
			12	Li	0.87100	13	Li	0.44136	13	Li	0.78858

II-Li <sub>9</sub>			II-Li <sub>10</sub>			II-Li <sub>11</sub>			II-Li <sub>12</sub>		
N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge
1	S	-0.30005	1	S	-0.56962	1	S	-0.28057	1	S	-0.58001
2	S	-0.29488	2	S	-0.51844	2	S	-0.26872	2	S	-0.52794
3	S	-0.32273	3	S	-0.61298	3	S	-0.29347	3	S	-0.62322
4	S	-0.27311	4	S	-0.55818	4	S	-0.28008	4	S	-0.55715
5	S	-0.28237	5	S	-0.60280	5	S	-0.32815	5	S	-0.61454
6	S	-0.31650	6	S	-0.68706	6	S	-0.38064	6	S	-0.75063
7	Li	0.43497	7	Li	0.87343	7	Li	0.42289	7	Li	0.85936
8	Li	0.42019	8	Li	0.85560	8	Li	0.43838	8	Li	0.61563
9	Li	0.42825	9	Li	0.72147	9	Li	0.35798	9	Li	0.73016
10	Li	0.40981	10	Li	0.62225	10	Li	0.33446	10	Li	0.62527
11	Li	0.42827	11	Li	0.83413	11	Li	0.40610	11	Li	0.63644
12	Li	0.43463	12	Li	0.84691	12	Li	0.42373	12	Li	0.84169
13	Li	0.43682	13	Li	0.52312	13	Li	0.31180	13	Li	0.61577
14	Li	0.39127	14	Li	0.75273	14	Li	0.42049	14	Li	0.43624
15	Li	0.36616	15	Li	0.76537	15	Li	0.38779	15	Li	0.76021
			16	Li	-0.10408	16	Li	-0.08373	16	Li	-0.16160
						17	Li	0.39762	17	Li	0.78024
									18	Li	0.05151

**Table S3** Key NPA atomic charges of LiPSs (**III-Li~III-Li<sub>12</sub>**) at the (U)M06-2X-D3/cc-pVTZ level. The atomic sequence numbers correspond to Fig. S12.

III-Li <sub>1</sub>			III-Li <sub>2</sub>			III-Li <sub>3</sub>			III-Li <sub>4</sub>		
N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge
1	S	0.06584	1	S	-0.55450	1	S	0.01512	1	S	-0.54482
2	S	0.05875	2	S	-0.73369	2	S	0.20428	2	S	-0.68850
3	S	0.15520	3	S	0.07579	3	S	0.10730	3	S	0.06801
4	S	0.07261	4	S	0.15083	4	S	-0.29036	4	S	-0.58243
5	S	0.06167	5	S	0.15296	5	S	-0.27711	5	S	-0.55868
6	S	0.06871	6	S	0.12920	6	S	0.06834	6	S	0.13688
7	S	0.07979	7	S	0.14007	7	S	0.06950	7	S	0.13751
8	Li	0.42990	8	Li	0.83480	8	Li	0.42482	8	Li	0.83783
						9	Li	0.42381	9	Li	0.85514
						10	Li	0.41045	10	Li	0.83211
									11	Li	0.83811
III-Li <sub>5</sub>			III-Li <sub>6</sub>			III-Li <sub>7</sub>			III-Li <sub>8</sub>		
N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge	N o	Ato m	Charge

1	S	-0.31121	1	S	-0.63107	1	S	-0.30369	1	S	-0.58699
2	S	-0.34235	2	S	-0.68580	2	S	0.10339	2	S	-1.68780
3	S	0.02560	3	S	0.07413	3	S	-0.28254	3	S	-0.55277
4	S	-0.27707	4	S	-0.55231	4	S	-0.26842	4	S	-0.52895
5	S	-0.26341	5	S	-0.53068	5	S	-0.26980	5	S	-0.56329
6	S	0.06999	6	S	-0.54582	6	S	-0.26993	6	S	-0.54263
7	S	0.25261	7	S	-0.48050	7	S	-0.25155	7	S	-0.48900
8	Li	0.42669	8	Li	0.84563	8	Li	0.42900	8	Li	0.86129
9	Li	0.42287	9	Li	0.84011	9	Li	0.41525	9	Li	0.83088
10	Li	0.41191	10	Li	0.83609	10	Li	0.40037	10	Li	0.79690
11	Li	0.43005	11	Li	0.86321	11	Li	0.39198	11	Li	0.79240
12	Li	0.43443	12	Li	0.87872	12	Li	0.43629	12	Li	0.87548
			13	Li	0.83994	13	Li	0.41733	13	Li	0.83744
						14	Li	0.42215	14	Li	0.87577
									15	Li	0.91194
III-Li <sub>9</sub>			III-Li <sub>10</sub>			III-Li <sub>11</sub>			III-Li <sub>12</sub>		
No	Atom	Charge	No	Atom	Charge	No	Atom	Charge	No	Atom	Charge
1	S	-0.29800	1	S	-0.57158	1	S	-0.28923	1	S	-0.59827
2	S	-0.82734	2	S	-1.63030	2	S	-0.81474	2	S	-1.65100
3	S	-0.28598	3	S	-0.56510	3	S	-0.27176	3	S	-0.57714
4	S	-0.26819	4	S	-0.57448	4	S	-0.29676	4	S	-0.59199
5	S	-0.28103	5	S	-0.61495	5	S	-0.28634	5	S	-0.59878
6	S	-0.27255	6	S	-0.63016	6	S	-0.30201	6	S	-0.61445
7	S	-0.24600	7	S	-0.56626	7	S	-0.28189	7	S	-0.56885
8	Li	0.43065	8	Li	0.84242	8	Li	0.42919	8	Li	0.85881
9	Li	0.41937	9	Li	0.82726	9	Li	0.42085	9	Li	0.35105
10	Li	0.40204	10	Li	0.80344	10	Li	0.40988	10	Li	0.81947
11	Li	0.40780	11	Li	0.74096	11	Li	0.36459	11	Li	0.71603
12	Li	0.44098	12	Li	0.86622	12	Li	0.43478	12	Li	0.87236
13	Li	0.42194	13	Li	0.83949	13	Li	0.41972	13	Li	0.83448
14	Li	0.43455	14	Li	0.87567	14	Li	0.43984	14	Li	0.89346
15	Li	0.45465	15	Li	0.84248	15	Li	0.42558	15	Li	0.85775
16	Li	0.44784	16	Li	0.80867	16	Li	0.40209	16	Li	0.83270
			17	Li	0.85908	17	Li	0.43714	17	Li	0.80789
						18	Li	0.46027	18	Li	-0.04556
									19	Li	0.70765

**Table S4** Key NPA atomic charges of LiPSs (IV-Li~IV-Li<sub>12</sub>) at the (U)M06-2X-D3/cc-pVTZ level. The atomic sequence numbers correspond to Fig. S13.

IV-Li			IV-Li <sub>2</sub>			IV-Li <sub>3</sub>			IV-Li <sub>4</sub>		
No	Atom	Charge	No	Atom	Charge	No	Atom	Charge	No	Atom	Charge

1	S	0.06877	1	S	0.13471	1	S	0.06548	1	S	0.12987
2	S	0.08595	2	S	0.16929	2	S	0.08018	2	S	0.14856
3	S	0.06316	3	S	0.12289	3	S	0.08471	3	S	-0.55218
4	S	0.07400	4	S	0.14550	4	S	0.19550	4	S	-0.53294
5	S	0.06239	5	S	0.12963	5	S	0.07924	5	S	0.16830
6	S	0.07167	6	S	0.14859	6	S	0.08323	6	S	0.16756
7	S	0.13970	7	S	-0.57161	7	S	-0.30540	7	S	-0.60548
8	S	0.10984	8	S	-0.55443	8	S	-0.28475	8	S	-0.58153
9	Li	0.41191	9	Li	0.83372	9	Li	0.42379	9	Li	0.85457
			10	Li	0.86469	10	Li	0.43202	10	Li	0.86123
						11	Li	0.40321	11	Li	0.80850
									12	Li	0.83897
IV-Li <sub>5</sub>			IV-Li <sub>6</sub>			IV-Li <sub>7</sub>			IV-Li <sub>8</sub>		
No	Atom	Charge	No	Atom	Charge	No	Atom	Charge	No	Atom	Charge
1	S	0.18939	1	S	-0.58464	1	S	-0.30867	1	S	-0.61441
2	S	0.09604	2	S	-0.58854	2	S	-0.28503	2	S	-0.57922
3	S	-0.28354	3	S	-0.56353	3	S	-0.28284	3	S	-0.58516
4	S	-0.26507	4	S	-0.53207	4	S	-0.31337	4	S	-0.54601
5	S	0.06587	5	S	0.12999	5	S	0.04594	5	S	-0.51945
6	S	0.08861	6	S	0.17564	6	S	0.17476	6	S	-0.56353
7	S	-0.29719	7	S	-0.59448	7	S	-0.31510	7	S	-0.61606
8	S	-0.27012	8	S	-0.55456	8	S	-0.28862	8	S	-0.54109
9	Li	0.41579	9	Li	0.82000	9	Li	0.40311	9	Li	0.82128
10	Li	0.43063	10	Li	0.86780	10	Li	0.43154	10	Li	0.87039
11	Li	0.40515	11	Li	0.81220	11	Li	0.39803	11	Li	0.79179
12	Li	0.41642	12	Li	0.83113	12	Li	0.42953	12	Li	0.86349
13	Li	0.39949	13	Li	0.78621	13	Li	0.39473	13	Li	0.76129
			14	Li	0.86430	14	Li	0.43952	14	Li	0.87522
						15	Li	0.41925	15	Li	0.79096
									16	Li	0.88688
IV-Li <sub>9</sub>			IV-Li <sub>10</sub>			IV-Li <sub>11</sub>			IV-Li <sub>12</sub>		
No	Atom	Charge	No	Atom	Charge	No	Atom	Charge	No	Atom	Charge
1	S	-0.28868	1	S	-0.57704	1	S	-0.30174	1	S	-0.62203
2	S	-0.28761	2	S	-0.56042	2	S	-0.30560	2	S	-0.54123
3	S	-0.28201	3	S	-0.52597	3	S	-0.30423	3	S	-0.55726
4	S	-0.31390	4	S	-1.66507	4	S	-0.81586	4	S	-1.64368
5	S	-0.31667	5	S	-0.59464	5	S	-0.29035	5	S	-0.55572
6	S	-0.26794	6	S	-0.57685	6	S	-0.28980	6	S	-0.58435
7	S	-0.30941	7	S	-0.60481	7	S	-0.29497	7	S	-0.58967
8	S	-0.27385	8	S	-0.55123	8	S	-0.26825	8	S	-0.65600
9	Li	0.41430	9	Li	0.84670	9	Li	0.42355	9	Li	0.78266
10	Li	0.44081	10	Li	0.87613	10	Li	0.43473	10	Li	0.86932
11	Li	0.39958	11	Li	0.84495	11	Li	0.42220	11	Li	0.84022
12	Li	0.44536	12	Li	0.84139	12	Li	0.42199	12	Li	0.83299

13	Li	0.40138	13	Li	0.80871	13	Li	0.41869	13	Li	0.82526
14	Li	0.43786	14	Li	0.88502	14	Li	0.44380	14	Li	0.73559
15	Li	0.42641	15	Li	0.85733	15	Li	0.44011	15	Li	0.88850
16	Li	0.41672	16	Li	0.83958	16	Li	0.42453	16	Li	0.85296
17	Li	0.43188	17	Li	0.84381	17	Li	0.42845	17	Li	0.85239
			18	Li	0.77214	18	Li	0.38914	18	Li	0.79399
						19	Li	0.39694	19	Li	0.77512
									20	Li	0.70694

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**Table S5** The calculated absolute electronic energies ( $E$ , in a.u.), thermal free energies $(G$ , in a.u.) calculated at the M06-2X-D3/cc-pVTZ level.

Species	Correction	$E$	$G$
<b>I</b>	0.126395	-2851.264050	-2851.137655
<b>II</b>	0.198701	-3082.287540	-3082.088839
<b>III</b>	0.197912	-3480.489872	-3480.291960
<b>IV</b>	0.271499	-4109.719512	-4109.448013

**Table S6** The calculated absolute electronic energies ( $E$ , in a.u.) of cyclic OPSs (**I-IV**)

and their key charged states at the (U)M06-2X-D3/cc-pVTZ level.

	0	-1	1	-2	2
	<b>Vertical</b>				
<b>I</b>	-2851.264050	-2851.285614	-2850.961329	-2851.315535	-2850.503570
<b>II</b>	-3082.287540	-3082.301476	-3081.988522	-3082.177894	-3081.554788
<b>III</b>	-3480.489888	-3480.510135	-3480.190686	-3480.407121	-3479.760906
<b>IV</b>	-4109.719512	-4109.739078	-4109.424230	-4109.633044	-4109.005949
	<b>Adiabatic</b>				
<b>I</b>	-2851.264050	-2851.317476	-2850.968780	-2851.221675	-2850.530189
<b>II</b>	-3082.287540	-3082.336205	-3081.998207	-3082.350439	-3081.572171
<b>III</b>	-3480.489888	-3480.541272	-3480.198834	-3480.562522	-3479.774452
<b>IV</b>	-4109.719512	-4109.773022	-4109.432844	-4109.788813	-4109.024060

**Table S7** The calculated absolute electronic energies ( $E$ , in a.u.), thermal free energies $(G$ , in a.u.), and the lithiation free energies ( $\Delta G$ , in eV) and the lithiation electronic energies ( $\Delta E$ , in eV) calculated at the (U)M06-2X-D3/ cc-pVTZ level.

Species	Correction	$E$ (a.u.)	$G$ (a.u.)	$\Delta E$ (eV)	$\Delta G$ (eV)
<b>I-Li</b>	0.123725	-2858.826179	-2858.702454	-2.22	-1.92
<b>I-Li<sub>a</sub></b>	0.124006	-2858.814248	-2858.690242	-1.89	-1.59
<b>I-Li<sub>b</sub></b>	0.120790	-2858.807864	-2858.687074	-1.72	-1.51
<b>I-Li<sub>c</sub></b>	0.121688	-2858.802189	-2858.680501	-1.56	-1.33
<b>I-Li<sub>d</sub></b>	0.121866	-2858.801648	-2858.679782	-1.55	-1.31
<b>I-Li<sub>f</sub></b>	0.119766	-2858.775851	-2858.656085	-0.85	-0.66
<b>I-Li<sub>2</sub></b>	0.125903	-2866.468580	-2866.342677	-6.62	-5.90
<sup>3U</sup> <b>[I-Li<sub>2</sub>]</b>	0.119635	-2866.414695	-2866.295060	-5.15	-4.61



**Table S8** The calculated absolute electronic energies ( $E$ , in a.u.), thermal free energies ( $G$ , in a.u.), the lithiation free energies ( $\Delta G$ , in eV) and the lithiation electronic energies ( $\Delta E$ , in eV) calculated at the M06-2X-D3/cc-pVTZ level.

Species	Correction (a.u.)	$E$ (a.u.)	$G$ (a.u.)	$\Delta E$ (eV)	$\Delta G$ (eV)
I-Li	0.123725	-2858.826179	-2858.702454	-2.2	-1.9
I-Li <sub>2</sub>	0.125903	-2866.468580	-2866.342677	-6.6	-5.9
I-Li <sub>3</sub>	0.123122	-2874.047835	-2873.924713	-9.3	-8.3
I-Li <sub>4</sub>	0.126477	-2881.682443	-2881.555966	-13.5	-12.0
I-Li <sub>5</sub>	0.123251	-2889.254758	-2889.131507	-16.0	-14.2
I-Li <sub>6</sub>	0.127047	-2896.899624	-2896.772577	-20.4	-18.2
I-Li <sub>7</sub>	0.126315	-2904.465607	-2904.339292	-22.8	-20.2
I-Li <sub>8</sub>	0.127514	-2912.116508	-2911.988994	-27.4	-24.5
I-Li <sub>9</sub>	0.128610	-2919.648669	-2919.520059	-28.8	-25.5
I-Li <sub>10</sub>	0.128760	-2927.182449	-2927.053689	-30.2	-26.5
I-Li <sub>11</sub>	0.129855	-2934.703091	-2934.573236	-31.3	-27.2
I-Li <sub>12</sub>	0.131113	-2942.234540	-2942.103427	-32.7	-28.2
II-Li	0.198998	-3089.843533	-3089.644535	-2.0	-1.7
II-Li <sub>2</sub>	0.199611	-3097.493038	-3097.293427	-6.6	-5.9
II-Li <sub>3</sub>	0.200501	-3105.056030	-3104.855529	-8.9	-7.7
II-Li <sub>4</sub>	0.200193	-3112.714228	-3112.514035	-13.7	-12.2
II-Li <sub>5</sub>	0.199261	-3120.280896	-3120.081635	-16.1	-14.2
II-Li <sub>6</sub>	0.202978	-3127.936261	-3127.733283	-20.8	-18.5
II-Li <sub>7</sub>	0.201117	-3135.475706	-3135.274589	-22.4	-19.8
II-Li <sub>8</sub>	0.199936	-3143.033743	-3142.833807	-24.5	-21.6
II-Li <sub>9</sub>	0.198250	-3150.560221	-3150.361971	-25.8	-22.5
II-Li <sub>10</sub>	0.199215	-3158.072339	-3157.873124	-26.6	-23.0
II-Li <sub>11</sub>	0.196233	-3165.598937	-3165.402704	-27.9	-23.9

<b>II-Li<sub>12</sub></b>	0.196228	-3173.131503	-3172.935275	-29.3	-25.0
<b>III-Li</b>	0.198303	-3488.056754	-3487.858451	-2.3	-2.0
<b>III-Li<sub>2</sub></b>	0.200073	-3495.698492	-3495.498419	-6.7	-6.0
<b>III-Li<sub>3</sub></b>	0.199619	-3503.282763	-3503.083144	-9.5	-8.5
<b>III-Li<sub>4</sub></b>	0.202079	-3510.918193	-3510.716114	-13.8	-12.2
<b>III-Li<sub>5</sub></b>	0.199855	-3518.481457	-3518.281602	-16.0	-14.2
<b>III-Li<sub>6</sub></b>	0.199807	-3526.123701	-3525.923894	-20.4	-18.2
<b>III-Li<sub>7</sub></b>	0.199392	-3533.700992	-3533.501600	-23.0	-20.5
<b>III-Li<sub>8</sub></b>	0.200212	-3541.319573	-3541.119361	-26.8	-23.9
<b>III-Li<sub>9</sub></b>	0.198612	-3548.845136	-3548.646524	-28.0	-24.8
<b>III-Li<sub>10</sub></b>	0.200381	-3556.395880	-3556.195499	-29.9	-26.3
<b>III-Li<sub>11</sub></b>	0.199943	-3563.911448	-3563.711505	-30.9	-26.9
<b>III-Li<sub>12</sub></b>	0.202334	-3571.448074	-3571.245740	-32.4	-27.9
<b>IV-Li</b>	0.273229	-4117.285482	-4117.012253	-2.3	-1.9
<b>IV-Li<sub>2</sub></b>	0.272531	-4124.924668	-4124.652137	-6.6	-5.9
<b>IV-Li<sub>3</sub></b>	0.273708	-4132.514020	-4132.240312	-9.6	-8.4
<b>IV-Li<sub>4</sub></b>	0.276921	-4140.159878	-4139.882957	-14.1	-12.5
<b>IV-Li<sub>5</sub></b>	0.275151	-4147.734627	-4147.459476	-16.6	-14.7
<b>IV-Li<sub>6</sub></b>	0.277084	-4155.380300	-4155.103216	-21.1	-18.8
<b>IV-Li<sub>7</sub></b>	0.273325	-4162.951029	-4162.677704	-23.6	-21.0
<b>IV-Li<sub>8</sub></b>	0.275740	-4170.610705	-4170.334965	-28.5	-25.4
<b>IV-Li<sub>9</sub></b>	0.276802	-4178.140886	-4177.864084	-29.8	-26.4
<b>IV-Li<sub>10</sub></b>	0.277099	-4185.749975	-4185.472876	-33.3	-29.5
<b>IV-Li<sub>11</sub></b>	0.275674	-4193.276390	-4193.000716	-34.5	-30.4
<b>IV-Li<sub>12</sub></b>	0.277743	-4200.814695	-4200.536952	-36.1	-31.6

**Table S9** Cartesian coordinates of all the studied molecules.

<b>I</b>			
C	-3.135642000	-1.314296000	0.000000000
C	-2.661946000	-0.812200000	-1.207216000

C	-1.723408000	0.221281000	-1.200590000
C	-1.260666000	0.754740000	0.000000000
C	-1.723408000	0.221281000	1.200590000
C	-2.661946000	-0.812200000	1.207216000
H	-3.860634000	-2.121868000	0.000000000
H	-3.007257000	-1.225689000	-2.149814000
H	-0.531123000	1.559753000	0.000000000
H	-3.007257000	-1.225689000	2.149814000
C	1.979231000	-0.319900000	0.000000000
C	1.573310000	-0.895090000	-1.201572000
C	0.816804000	-2.068400000	-1.205815000
C	0.454260000	-2.661167000	0.000000000
C	0.816804000	-2.068400000	1.205815000
C	1.573310000	-0.895090000	1.201572000
H	2.556917000	0.599833000	0.000000000
H	0.492513000	-2.490034000	-2.151828000
H	-0.148509000	-3.563091000	0.000000000
H	0.492513000	-2.490034000	2.151828000
S	-1.254327000	0.860218000	-2.812455000
S	0.665955000	1.565816000	-2.562503000
S	1.923766000	-0.086863000	-2.755720000
S	1.923766000	-0.086863000	2.755720000
S	0.665955000	1.565816000	2.562503000
S	-1.254327000	0.860218000	2.812455000

## II

C	2.388556000	-1.946076000	0.523847000
C	1.535646000	-1.695998000	-0.550685000
C	0.246951000	-2.230170000	-0.545544000
C	-0.186784000	-3.008665000	0.523674000
C	0.676364000	-3.254049000	1.589283000
C	1.962343000	-2.726893000	1.599008000
H	1.872804000	-1.072882000	-1.375294000
H	-1.192191000	-3.416245000	0.527715000
H	0.335302000	-3.860008000	2.422364000
H	2.633277000	-2.902874000	2.432982000
S	-0.747703000	-1.832997000	-1.984391000
S	-2.665149000	-2.239892000	-1.394525000
C	0.595484000	2.483838000	-0.661012000
C	1.087317000	2.579881000	-1.963359000

C	2.360953000	2.101096000	-2.260182000
C	3.147479000	1.527019000	-1.269426000
C	2.635516000	1.404631000	0.023920000
C	1.359965000	1.874640000	0.334255000
H	0.475910000	3.026764000	-2.741868000
H	2.741980000	2.184113000	-3.272822000
H	4.141294000	1.152606000	-1.492897000
H	0.968022000	1.759874000	1.340095000
S	4.016508000	-1.212206000	0.516685000
S	3.596071000	0.662211000	1.336048000
S	-0.996033000	3.256505000	-0.382119000
S	-1.674481000	2.510715000	1.412821000
C	-3.966894000	1.041169000	1.516244000
C	-4.785566000	-0.043268000	1.208355000
C	-4.358504000	-1.014916000	0.314694000
C	-3.092467000	-0.910880000	-0.271298000
C	-2.251237000	0.148593000	0.048418000
C	-2.705207000	1.127927000	0.933554000
H	-4.307569000	1.819522000	2.190651000
H	-5.770939000	-0.120812000	1.656163000
H	-5.004351000	-1.852910000	0.067978000
H	-1.260437000	0.226194000	-0.389848000

### III

C	0.620196000	-2.636912000	0.269763000
C	-0.702131000	-2.671509000	-0.182568000
C	-1.736389000	-2.310858000	0.679298000
C	-1.460588000	-1.868937000	1.975716000
C	-0.138485000	-1.795260000	2.398116000
C	0.902228000	-2.192538000	1.559003000
H	-0.930591000	-2.975476000	-1.199710000
H	-2.273943000	-1.577696000	2.632375000
H	0.089291000	-1.440886000	3.397931000
H	1.929157000	-2.162247000	1.907871000
C	2.668199000	1.656273000	0.000528000
C	2.550382000	2.065964000	-1.325199000
C	2.787159000	1.154701000	-2.355930000
C	3.115446000	-0.162048000	-2.064690000
C	3.210962000	-0.572936000	-0.730967000
C	2.999367000	0.333427000	0.301974000

H	2.266021000	3.089784000	-1.545032000
H	2.701240000	1.474817000	-3.388807000
H	3.283832000	-0.881954000	-2.859018000
H	3.072341000	0.015686000	1.337257000
C	-0.714040000	3.731541000	0.193465000
C	-1.613038000	3.981846000	-0.833019000
C	-2.401827000	2.951628000	-1.344211000
C	-2.252735000	1.655508000	-0.854549000
C	-1.313576000	1.381564000	0.144119000
C	-0.571107000	2.429483000	0.682614000
H	-0.119628000	4.533035000	0.620154000
H	-1.731862000	4.990468000	-1.214744000
H	-3.141258000	3.153278000	-2.112184000
H	-1.168297000	0.367172000	0.505571000
S	-3.404691000	-2.472244000	0.073444000
S	-3.268419000	0.390795000	-1.605319000
S	1.849431000	-3.221320000	-0.888347000
S	3.593720000	-2.265943000	-0.306337000
S	2.340663000	2.819931000	1.313033000
S	0.537240000	2.068986000	2.036679000
S	-4.127722000	-0.530929000	0.054194000

#### IV

C	-2.183832000	2.650887000	1.264046000
C	-2.705818000	1.724933000	2.163539000
C	-3.552735000	0.707984000	1.738656000
C	-3.859663000	0.606101000	0.383410000
C	-3.326356000	1.508858000	-0.534339000
C	-2.502126000	2.543393000	-0.086421000
H	-1.530692000	3.445255000	1.608068000
H	-2.453309000	1.805002000	3.215794000
H	-3.956690000	-0.009721000	2.444206000
H	-3.537296000	1.396582000	-1.595041000
C	1.322610000	2.774958000	-1.863982000
C	2.379381000	1.875700000	-1.927605000
C	3.121011000	1.579582000	-0.784476000
C	2.773351000	2.159666000	0.436721000
C	1.696772000	3.047743000	0.512204000
C	0.987261000	3.365334000	-0.643012000
H	0.752448000	3.022576000	-2.753737000

H	2.641008000	1.414864000	-2.874482000
H	3.964425000	0.897778000	-0.832889000
H	1.421864000	3.485823000	1.466606000
C	-2.117593000	-2.152125000	-0.534065000
C	-0.810626000	-2.588199000	-0.766258000
C	-0.271686000	-3.646741000	-0.044242000
C	-1.061549000	-4.280192000	0.913753000
C	-2.358441000	-3.856829000	1.164658000
C	-2.884470000	-2.785894000	0.435227000
H	-2.525891000	-1.325058000	-1.106322000
H	0.744791000	-3.978950000	-0.221915000
H	-0.650140000	-5.109814000	1.479187000
H	-2.958843000	-4.347930000	1.924419000
C	4.189537000	-2.663599000	-0.954767000
C	2.874198000	-2.197969000	-0.904873000
C	2.446294000	-1.423422000	0.171568000
C	3.348196000	-1.109698000	1.189916000
C	4.661413000	-1.579483000	1.151601000
C	5.074883000	-2.356097000	0.074572000
H	4.522986000	-3.260798000	-1.798796000
H	1.434464000	-1.032899000	0.213974000
H	5.348166000	-1.320698000	1.950321000
H	6.095247000	-2.722100000	0.029905000
S	-4.944100000	-0.654324000	-0.289238000
S	-4.547592000	-2.297772000	0.879099000
S	0.086657000	-1.634884000	-1.991365000
S	-1.935141000	3.676147000	-1.350223000
S	-0.294391000	4.609128000	-0.522119000
S	3.709838000	1.759721000	1.901275000
S	1.828612000	-2.665950000	-2.282557000
S	2.799080000	-0.028894000	2.499858000
<b>I-Li</b>			
C	-1.038733000	2.686484000	1.619412000
C	-2.024835000	2.131722000	0.801346000
C	-1.649567000	1.520998000	-0.390607000
C	-0.306424000	1.462846000	-0.774951000
C	0.674778000	1.947186000	0.081337000
C	0.300033000	2.575083000	1.279394000
H	-1.319110000	3.175702000	2.546694000



H	-3.070502000	2.159402000	1.087990000
H	-0.040805000	1.069349000	-1.753801000
H	1.067649000	2.965573000	1.941818000
C	0.256727000	-2.092418000	0.393642000
C	-0.814915000	-1.553264000	1.106269000
C	-0.582130000	-0.740893000	2.210555000
C	0.738795000	-0.461271000	2.575287000
C	1.806643000	-0.914944000	1.814206000
C	1.586215000	-1.728909000	0.682585000
H	0.061963000	-2.801436000	-0.411685000
H	-1.414098000	-0.307678000	2.755530000
H	0.928166000	0.169947000	3.438412000
H	2.824995000	-0.637677000	2.064548000
S	-2.929643000	0.799692000	-1.405755000
S	-2.349386000	-1.203557000	-1.418789000
S	-2.483999000	-1.879410000	0.544410000
S	2.873032000	-2.153438000	-0.436378000
S	2.719099000	0.600504000	-1.788789000
S	2.427046000	1.857733000	-0.225984000
Li	1.061273000	-1.044435000	-1.453269000

**I-Li<sub>a</sub>**

C	-0.149918000	2.255287000	2.363444000
C	-1.333885000	2.045946000	1.648256000
C	-1.264510000	1.780417000	0.274562000
C	-0.028462000	1.700708000	-0.374467000
C	1.159486000	1.872882000	0.351654000
C	1.086869000	2.164233000	1.728020000
H	-0.193714000	2.452950000	3.429525000
H	-2.296128000	2.067315000	2.148524000
H	0.030189000	1.447546000	-1.430229000
H	2.006135000	2.279983000	2.294131000
C	0.066645000	-1.836815000	-0.341796000
C	-1.145398000	-1.825691000	0.348960000
C	-1.181309000	-1.913707000	1.751097000
C	0.034699000	-2.020321000	2.443267000
C	1.250490000	-2.004336000	1.761829000
C	1.308806000	-1.932916000	0.340694000
H	0.080253000	-1.757797000	-1.424749000
H	-2.128237000	-1.890206000	2.278544000

H	0.028479000	-2.084236000	3.527114000
H	2.185554000	-2.057080000	2.309604000
S	-2.815084000	1.573319000	-0.598865000
S	-2.458291000	-0.105916000	-1.759415000
S	-2.719232000	-1.735477000	-0.509263000
S	2.816243000	-1.954205000	-0.499667000
S	2.485375000	0.397720000	-1.921423000
S	2.767114000	1.694869000	-0.377255000
Li	0.082798000	-0.032514000	1.249541000

**I-Li<sub>b</sub>**

C	0.636553000	0.426380000	2.525091000
C	-0.569872000	0.956033000	2.049181000
C	-0.561963000	1.670417000	0.859569000
C	0.633250000	1.852840000	0.147391000
C	1.861586000	1.348366000	0.628049000
C	1.824691000	0.623063000	1.842258000
H	0.636637000	-0.151604000	3.444401000
H	-1.501803000	0.791233000	2.578665000
H	0.591476000	2.306393000	-0.845473000
H	2.756331000	0.218342000	2.223724000
C	-0.562934000	-1.352464000	-0.643420000
C	-1.863221000	-1.377536000	-0.139527000
C	-2.167588000	-2.087288000	1.020867000
C	-1.157538000	-2.781540000	1.684823000
C	0.145548000	-2.747872000	1.208389000
C	0.436428000	-2.027323000	0.044648000
H	-0.321559000	-0.795972000	-1.544952000
H	-3.181389000	-2.082388000	1.407904000
H	-1.388553000	-3.336221000	2.588344000
H	0.938426000	-3.272324000	1.734204000
S	-2.098106000	2.352400000	0.242278000
S	-2.359551000	1.265745000	-1.509804000
S	-3.217359000	-0.530829000	-0.950505000
S	2.145415000	-2.070748000	-0.485856000
S	2.329838000	-0.922465000	-2.078570000
S	3.383049000	1.701915000	-0.195369000
Li	2.202737000	3.522596000	0.231484000

**I-Li<sub>c</sub>**

C	-0.703100000	3.016294000	1.642859000
C	-1.802383000	2.425278000	1.021202000
C	-1.599109000	1.569623000	-0.058989000
C	-0.310769000	1.296143000	-0.523543000
C	0.775343000	1.879052000	0.120047000
C	0.584501000	2.743204000	1.205396000
H	-0.856677000	3.680843000	2.487260000
H	-2.807788000	2.613376000	1.384834000
H	-0.144383000	0.601925000	-1.343281000
H	1.442116000	3.184562000	1.705307000
C	0.355117000	-2.158958000	0.228809000
C	-0.856928000	-1.773799000	0.789514000
C	-0.886810000	-0.976210000	1.938675000
C	0.307995000	-0.547009000	2.512571000
C	1.523387000	-0.905970000	1.942953000
C	1.566612000	-1.725975000	0.798435000
H	0.378907000	-2.777137000	-0.662851000
H	-1.843148000	-0.677653000	2.357044000
H	0.286238000	0.087571000	3.392483000
H	2.460360000	-0.558356000	2.365749000
S	-3.079961000	0.887913000	-0.807075000
S	-2.474600000	-0.929545000	-1.576260000
S	-2.401767000	-2.255059000	0.027354000
S	3.083043000	-2.189936000	0.091874000
S	2.418437000	0.258773000	-1.981736000
S	2.478969000	1.578232000	-0.360066000
Li	2.325094000	2.396266000	-2.566533000

**I-Li<sub>d</sub>**

C	-0.642714000	3.176366000	1.494577000
C	-1.751102000	2.546700000	0.922115000
C	-1.556429000	1.581605000	-0.059489000
C	-0.262763000	1.233789000	-0.474028000
C	0.837180000	1.869106000	0.109148000
C	0.641970000	2.850692000	1.096791000
H	-0.792859000	3.926421000	2.264611000
H	-2.755050000	2.795863000	1.250845000
H	-0.104186000	0.415971000	-1.176120000
H	1.501037000	3.339818000	1.546182000

C	0.342429000	-2.185986000	0.246980000
C	-0.861862000	-1.804347000	0.827205000
C	-0.878422000	-0.999757000	1.971434000
C	0.324823000	-0.561101000	2.520345000
C	1.532250000	-0.911382000	1.927089000
C	1.560350000	-1.734903000	0.785057000
H	0.353960000	-2.808623000	-0.641940000
H	-1.829001000	-0.704726000	2.405211000
H	0.316031000	0.074417000	3.399915000
H	2.473859000	-0.551986000	2.329202000
S	-3.051320000	0.872227000	-0.748028000
S	-2.473864000	-0.949036000	-1.526275000
S	-2.412213000	-2.278913000	0.075387000
S	3.063947000	-2.169985000	0.028963000
S	2.426334000	0.253129000	-1.996259000
S	2.536340000	1.564542000	-0.377724000
Li	1.231452000	2.158908000	-2.292759000

**I-Li<sub>e</sub>**

C	-2.839834000	1.753275000	0.000000000
C	-2.476986000	1.163648000	1.206043000
C	-1.760753000	-0.034765000	1.200731000
C	-1.402543000	-0.647863000	0.000000000
C	-1.760753000	-0.034765000	-1.200731000
C	-2.476986000	1.163648000	-1.206043000
H	-3.393497000	2.686663000	0.000000000
H	-2.734772000	1.633375000	2.150250000
H	-0.842562000	-1.578163000	0.000000000
H	-2.734772000	1.633375000	-2.150250000
C	1.858276000	-0.030782000	0.000000000
C	1.584186000	0.642980000	1.236761000
C	1.064865000	1.936048000	1.225626000
C	0.844261000	2.614859000	0.000000000
C	1.064865000	1.936048000	-1.225626000
C	1.584186000	0.642980000	-1.236761000
H	2.264440000	-1.034200000	0.000000000
H	0.835045000	2.419802000	2.169841000
H	0.460611000	3.627131000	0.000000000
H	0.835045000	2.419802000	-2.169841000
S	-1.437131000	-0.751573000	2.809053000

S	0.362942000	-1.714966000	2.603906000
S	1.847928000	-0.160604000	2.777851000
S	1.847928000	-0.160604000	-2.777851000
S	0.362942000	-1.714966000	-2.603906000
S	-1.437131000	-0.751573000	-2.809053000
Li	2.951385000	1.876304000	0.000000000

**I-Li<sub>2</sub>**

C	-0.660930000	2.567276000	2.041033000
C	-1.732505000	2.189794000	1.230111000
C	-1.476904000	1.687141000	-0.041751000
C	-0.167631000	1.566983000	-0.514952000
C	0.892497000	1.906211000	0.317296000
C	0.644779000	2.413429000	1.600452000
H	-0.849305000	2.964577000	3.033412000
H	-2.754339000	2.272529000	1.585500000
H	0.017860000	1.244409000	-1.535908000
H	1.477228000	2.691220000	2.240628000
C	0.000318000	-2.242633000	0.166346000
C	-1.161853000	-1.730588000	0.752979000
C	-1.098567000	-1.035240000	1.952589000
C	0.149088000	-0.836913000	2.551004000
C	1.310072000	-1.294990000	1.947635000
C	1.263558000	-2.004260000	0.731369000
H	-0.081847000	-2.856427000	-0.731250000
H	-2.002039000	-0.629104000	2.393975000
H	0.211631000	-0.288578000	3.485934000
H	2.275374000	-1.115469000	2.411960000
S	-2.880318000	1.262227000	-1.066989000
S	-2.422846000	-0.655463000	-1.710338000
S	-2.729726000	-1.920761000	-0.087693000
S	2.724607000	-2.536067000	-0.130307000
S	2.631207000	0.848844000	-2.047688000
S	2.600103000	1.826859000	-0.194929000
Li	3.698955000	-0.427731000	-0.372859000
Li	1.356198000	-1.109148000	-1.454416000

**<sup>3</sup>U[I-Li<sub>2</sub>]**

C	0.999450000	0.129339000	2.397482000
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C	1.140669000	-1.139191000	1.830203000
C	0.074650000	-1.659104000	1.105772000
C	-1.138348000	-0.976378000	1.010250000
C	-1.246023000	0.308926000	1.524092000
C	-0.163888000	0.865978000	2.220981000
H	1.835275000	0.567725000	2.932607000
H	2.081592000	-1.675733000	1.900294000
H	-2.008606000	-1.454647000	0.566540000
H	-0.236282000	1.875036000	2.615233000
C	1.602147000	0.551796000	-1.167362000
C	2.771936000	0.700244000	-0.390464000
C	3.006545000	1.923620000	0.277501000
C	2.084374000	2.951606000	0.166406000
C	0.932627000	2.786394000	-0.604433000
C	0.671624000	1.583141000	-1.286959000
H	1.443515000	-0.386362000	-1.693318000
H	3.910525000	2.035084000	0.866353000
H	2.258148000	3.896317000	0.671943000
H	0.228789000	3.608415000	-0.703424000
S	0.308718000	-3.194229000	0.232382000
S	-0.732143000	-3.017151000	-1.444114000
S	3.877301000	-0.610197000	-0.227211000
S	-0.760316000	1.399594000	-2.320765000
S	-3.794904000	0.315417000	-0.220452000
S	-2.729993000	1.274530000	1.319179000
Li	-2.522618000	2.109436000	-0.992306000
Li	-1.686095000	-0.546606000	-1.368147000

**I-Li<sub>3</sub>**

C	-0.531834000	1.967898000	1.742505000
C	-1.466473000	1.632581000	0.762426000
C	-1.055612000	1.572987000	-0.566954000
C	0.263048000	1.868047000	-0.913143000
C	1.204273000	2.120559000	0.077670000
C	0.801755000	2.184762000	1.416393000
H	-0.841009000	2.007586000	2.782469000
H	-2.492080000	1.396458000	1.030232000
H	0.552449000	1.915159000	-1.961061000
H	1.531974000	2.387666000	2.194471000
C	-0.480492000	-1.821129000	0.463426000

C	-1.547895000	-1.682093000	1.379737000
C	-1.256261000	-1.334487000	2.727883000
C	0.052823000	-1.090725000	3.096638000
C	1.085198000	-1.178781000	2.157003000
C	0.837413000	-1.552694000	0.816461000
H	-0.672461000	-2.165596000	-0.549432000
H	-2.071683000	-1.250078000	3.437992000
H	0.286154000	-0.817801000	4.120833000
H	2.108928000	-0.979222000	2.460777000
S	-2.199930000	1.123536000	-1.864351000
S	-1.137492000	-0.347670000	-2.955378000
S	-3.178206000	-1.851893000	0.877401000
S	2.119790000	-1.745984000	-0.375911000
S	3.188789000	1.448860000	-2.197759000
S	2.929285000	2.366462000	-0.318693000
Li	3.594055000	0.050319000	-0.397963000
Li	1.198169000	-0.203242000	-2.020802000
Li	-2.584696000	-1.211287000	-1.383120000

#### **I-Li<sub>4</sub>**

C	2.823982000	-1.735417000	1.563840000
C	3.266420000	-0.735467000	0.688773000
C	2.482641000	-0.421971000	-0.431000000
C	1.305006000	-1.129683000	-0.673207000
C	0.832479000	-2.093104000	0.223330000
C	1.606010000	-2.390231000	1.364309000
H	3.414438000	-1.970494000	2.443516000
H	4.173413000	-0.179236000	0.899901000
H	0.756077000	-0.939096000	-1.585675000
H	1.256969000	-3.127830000	2.080005000
C	-1.306528000	1.746653000	0.560234000
C	-0.548955000	1.494598000	1.713677000
C	-1.046716000	0.561474000	2.645642000
C	-2.279818000	-0.053069000	2.429933000
C	-3.021423000	0.217048000	1.285218000
C	-2.528304000	1.103727000	0.301914000
H	-0.955687000	2.482518000	-0.158815000
H	-0.492450000	0.374753000	3.562487000
H	-2.672808000	-0.738810000	3.174463000
H	-4.019396000	-0.209785000	1.178936000

S	2.955119000	0.917920000	-1.505608000
S	1.155045000	1.670210000	-2.310286000
S	1.050652000	2.235499000	1.964581000
S	-3.322615000	1.309995000	-1.268865000
S	-1.512566000	-2.066793000	-1.733979000
S	-0.712437000	-2.910684000	0.001524000
Li	-3.324919000	-0.959482000	-0.838506000
Li	-1.063602000	0.477068000	-1.754930000
Li	1.636108000	2.665551000	-0.270809000
Li	1.158921000	-0.042381000	1.534688000

**I-Li<sub>5</sub>**

C	-2.846339000	2.463517000	-0.371964000
C	-3.455179000	1.262916000	0.007201000
C	-2.862238000	0.027776000	-0.319232000
C	-1.646639000	0.048517000	-1.036172000
C	-1.030582000	1.248316000	-1.408747000
C	-1.633042000	2.473620000	-1.062142000
H	-3.313414000	3.405907000	-0.102903000
H	-4.378500000	1.269017000	0.574807000
H	-1.152209000	-0.878074000	-1.313906000
H	-1.158511000	3.410669000	-1.335478000
C	1.676930000	-0.324545000	1.580012000
C	0.748736000	0.620669000	2.041007000
C	1.014616000	1.984163000	1.802894000
C	2.169033000	2.369080000	1.124831000
C	3.072352000	1.418554000	0.660761000
C	2.835023000	0.043441000	0.873556000
H	1.507237000	-1.373158000	1.814992000
H	0.343743000	2.738582000	2.210644000
H	2.374170000	3.424550000	0.971669000
H	3.999107000	1.732140000	0.182605000
S	-3.605642000	-1.469454000	0.258996000
S	-0.254760000	-3.143875000	-0.004139000
S	-0.754397000	0.138338000	2.863967000
S	3.903165000	-1.188839000	0.163462000
S	1.142335000	-0.636468000	-2.575345000
S	0.490778000	1.326463000	-2.305766000
Li	3.076668000	0.179382000	-1.523487000
Li	1.747339000	-1.942334000	-0.491658000



Li	-1.503659000	-1.710194000	1.583168000
Li	-1.293792000	1.332001000	0.975372000
Li	-2.433662000	-3.180332000	-0.801152000

**I-Li<sub>6</sub>**

C	-3.197622000	2.421082000	-0.259982000
C	-3.693879000	1.144354000	0.022675000
C	-2.981519000	-0.006373000	-0.378229000
C	-1.773118000	0.191692000	-1.085655000
C	-1.254028000	1.467086000	-1.344037000
C	-1.974077000	2.599486000	-0.910158000
H	-3.758361000	3.293158000	0.062329000
H	-4.623138000	1.022534000	0.567589000
H	-1.238813000	-0.673084000	-1.466866000
H	-1.585316000	3.595764000	-1.094858000
C	1.552693000	-0.447822000	1.738738000
C	0.636057000	0.564119000	2.071222000
C	0.956114000	1.888858000	1.712413000
C	2.139770000	2.168869000	1.037699000
C	3.015103000	1.147935000	0.672580000
C	2.714750000	-0.192491000	0.994697000
H	1.328726000	-1.461095000	2.053829000
H	0.296112000	2.701152000	2.010403000
H	2.385011000	3.197091000	0.789784000
H	3.965663000	1.390779000	0.196834000
S	-3.558818000	-1.603228000	0.081462000
S	-0.073049000	-3.189812000	0.290905000
S	-0.900110000	0.164928000	2.864347000
S	3.706162000	-1.516917000	0.333341000
S	1.091773000	-0.126734000	-2.531246000
S	0.289893000	1.766036000	-2.157644000
Li	3.130515000	-0.036757000	-1.399401000
Li	2.159836000	-3.369109000	0.444062000
Li	0.711837000	-1.156969000	-0.396327000
Li	-1.620747000	1.328045000	1.040027000
Li	-1.996323000	-3.123706000	-0.832907000
Li	-1.518560000	-1.870914000	1.631782000

**I-Li<sub>7</sub>**

C	4.072537000	-1.635979000	0.239050000
C	4.143498000	-0.243634000	0.335905000
C	3.115418000	0.561808000	-0.201527000
C	2.038755000	-0.089903000	-0.839688000
C	1.936608000	-1.493270000	-0.924027000
C	2.978576000	-2.265816000	-0.360217000
H	4.868899000	-2.241342000	0.661851000
H	4.977249000	0.235673000	0.836194000
H	1.229717000	0.511012000	-1.244700000
H	2.923225000	-3.347620000	-0.410194000
C	-1.894298000	0.334981000	1.475494000
C	-0.864308000	-0.485469000	1.966939000
C	-1.049018000	-1.881086000	1.899210000
C	-2.218661000	-2.408054000	1.349032000
C	-3.211164000	-1.572739000	0.826597000
C	-3.056587000	-0.172087000	0.875639000
H	-1.754047000	1.408307000	1.552479000
H	-0.277971000	-2.545133000	2.276831000
H	-2.345340000	-3.484786000	1.296193000
H	-4.111305000	-2.000283000	0.394329000
S	3.168403000	2.303809000	0.086140000
S	-0.532539000	3.081714000	-0.672823000
S	0.604262000	0.249350000	2.628665000
S	-4.246303000	0.911988000	0.115166000
S	-1.477304000	-0.616513000	-2.690079000
S	0.559799000	-2.327699000	-1.646722000
Li	-3.543945000	-0.283573000	-1.770529000
Li	-2.700565000	2.701214000	-0.186402000
Li	-0.787678000	1.476565000	-2.238128000
Li	2.172235000	-0.888932000	1.366733000
Li	1.604441000	3.457187000	-1.214002000
Li	0.846193000	2.070854000	1.016953000
Li	-1.150562000	-1.223551000	-0.422282000
<b>I-Li<sub>8</sub></b>			
C	4.182811000	-1.656803000	0.398930000
C	4.174282000	-0.262603000	0.326199000
C	3.106233000	0.415467000	-0.303398000
C	2.068875000	-0.365819000	-0.855883000
C	2.051089000	-1.775650000	-0.774664000

C	3.130701000	-2.412919000	-0.124326000
H	5.007371000	-2.160332000	0.894623000
H	4.974913000	0.319847000	0.768021000
H	1.223324000	0.141777000	-1.318909000
H	3.129306000	-3.494019000	-0.043237000
C	-1.936842000	0.383199000	1.591393000
C	-0.856247000	-0.438734000	1.951510000
C	-1.008492000	-1.828062000	1.793677000
C	-2.202370000	-2.349433000	1.287539000
C	-3.242897000	-1.508323000	0.886490000
C	-3.115994000	-0.111354000	1.021780000
H	-1.825627000	1.449778000	1.766781000
H	-0.201629000	-2.498605000	2.073475000
H	-2.309172000	-3.424788000	1.178735000
H	-4.159826000	-1.929990000	0.484352000
S	3.077686000	2.178608000	-0.221405000
S	-0.657847000	2.995260000	-0.755520000
S	0.625099000	0.302196000	2.584154000
S	-4.372885000	0.999285000	0.419939000
S	-2.101848000	-0.561257000	-2.738376000
S	0.708882000	-2.768014000	-1.353660000
Li	-3.977689000	-0.083745000	-1.618178000
Li	-2.743846000	2.681280000	0.041940000
Li	-1.270090000	1.456718000	-2.276371000
Li	2.212087000	-0.892877000	1.416697000
Li	1.427010000	3.193180000	-1.510320000
Li	0.807698000	2.020216000	0.869670000
Li	-1.228784000	-1.346612000	-0.654900000
Li	-0.328859000	-1.818314000	-3.211494000

**I-Li<sub>9</sub>**

C	4.118316000	-1.644771000	0.540887000
C	4.078127000	-0.255557000	0.409444000
C	3.090082000	0.357821000	-0.389663000
C	2.162755000	-0.479118000	-1.045462000
C	2.182010000	-1.886324000	-0.918777000
C	3.178031000	-2.457658000	-0.098215000
H	4.879142000	-2.099944000	1.167827000
H	4.792590000	0.370568000	0.931742000
H	1.381633000	-0.017748000	-1.649137000

H	3.205992000	-3.535177000	0.018362000
C	-2.117869000	0.474620000	1.549769000
C	-0.984072000	-0.366115000	1.787869000
C	-1.080152000	-1.739803000	1.571410000
C	-2.310244000	-2.341792000	1.158790000
C	-3.439269000	-1.486515000	0.917229000
C	-3.362420000	-0.117157000	1.090987000
H	-2.152001000	1.408729000	2.118322000
H	-0.226374000	-2.375959000	1.806856000
H	-2.440393000	-3.416678000	1.230922000
H	-4.387483000	-1.930126000	0.610155000
S	3.035065000	2.125168000	-0.438759000
S	-0.739750000	2.936847000	-0.766696000
S	0.523390000	0.418959000	2.343182000
S	-4.626767000	1.008081000	0.514691000
S	-1.804353000	-0.457551000	-2.286656000
S	1.009812000	-2.967876000	-1.691234000
Li	-3.794006000	-0.407444000	-1.120818000
Li	-2.712618000	2.410168000	0.408458000
Li	-1.777285000	1.801092000	-2.454903000
Li	2.003422000	-0.938652000	1.258139000
Li	1.287039000	2.916174000	-1.727067000
Li	0.918658000	2.306391000	0.911248000
Li	-1.093763000	-2.139891000	-0.681318000
Li	-0.149069000	-1.647087000	-3.217532000
Li	-0.866837000	0.571716000	-0.273517000

**I-Li<sub>10</sub>**

C	4.215008000	-1.621082000	0.482664000
C	4.144884000	-0.225024000	0.438165000
C	3.113094000	0.415338000	-0.283103000
C	2.179688000	-0.408268000	-0.948198000
C	2.236658000	-1.816749000	-0.925150000
C	3.268864000	-2.417908000	-0.171801000
H	5.009293000	-2.096717000	1.050233000
H	4.870841000	0.382422000	0.967061000
H	1.382017000	0.074645000	-1.509822000
H	3.330241000	-3.499632000	-0.129677000
C	-2.128361000	0.385559000	1.720570000
C	-1.024178000	-0.457614000	1.910294000

C	-1.208720000	-1.844645000	1.700304000
C	-2.469178000	-2.333150000	1.354780000
C	-3.538594000	-1.468106000	1.107924000
C	-3.364810000	-0.079097000	1.234870000
H	-1.999284000	1.444571000	1.926113000
H	-0.386277000	-2.530369000	1.890503000
H	-2.622716000	-3.407537000	1.275349000
H	-4.508144000	-1.865004000	0.816966000
S	2.976067000	2.172933000	-0.255842000
S	-0.797698000	2.730091000	-0.734779000
S	0.528341000	0.247209000	2.374674000
S	-4.593860000	1.068931000	0.656467000
S	-1.973369000	-0.638398000	-2.169050000
S	1.081183000	-2.826670000	-1.809169000
Li	-3.962437000	-0.237950000	-1.197828000
Li	-2.958849000	2.697185000	-0.032089000
Li	-1.172426000	1.519095000	-2.799221000
Li	2.150350000	-0.987365000	1.278402000
Li	1.269969000	2.628066000	-1.892553000
Li	0.854796000	2.231335000	0.903552000
Li	-1.050528000	-2.318446000	-0.921156000
Li	0.067333000	-1.104465000	-3.245607000
Li	-1.035738000	0.482194000	-0.350905000
Li	1.208700000	1.430157000	-4.835544000

### I-Li<sub>11</sub>

C	3.867177000	-1.770971000	0.628134000
C	4.028207000	-0.389780000	0.473825000
C	3.164698000	0.332902000	-0.378499000
C	2.155294000	-0.389095000	-1.049574000
C	1.994143000	-1.786442000	-0.932166000
C	2.855995000	-2.467371000	-0.044142000
H	4.532454000	-2.312905000	1.293877000
H	4.809605000	0.140193000	1.006947000
H	1.511143000	0.155985000	-1.739519000
H	2.745233000	-3.539066000	0.080080000
C	-2.186537000	0.470011000	1.601970000
C	-0.962587000	-0.271040000	1.847053000
C	-0.907236000	-1.635367000	1.601207000
C	-2.071441000	-2.364414000	1.219782000

C	-3.296105000	-1.648859000	1.023319000
C	-3.370491000	-0.274998000	1.168519000
H	-2.439603000	1.246231000	2.345022000
H	0.014278000	-2.188613000	1.789012000
H	-2.061472000	-3.449223000	1.252656000
H	-4.201170000	-2.206551000	0.776647000
S	3.329609000	2.086840000	-0.540828000
S	-0.529238000	2.857239000	-0.635473000
S	0.463357000	0.681806000	2.402007000
S	-4.774379000	0.686495000	0.658887000
S	-2.075249000	-0.194167000	-2.045663000
S	0.797703000	-2.677668000	-1.875573000
Li	-4.083482000	-0.707957000	-1.041368000
Li	-2.858270000	1.647165000	-0.501455000
Li	-1.046608000	1.804322000	-2.768011000
Li	1.920202000	-0.763907000	1.267091000
Li	1.474330000	2.680052000	-2.009690000
Li	1.361927000	2.304328000	0.685951000
Li	-1.265810000	-2.079445000	-0.837248000
Li	-0.166710000	-0.899825000	-3.239460000
Li	-0.701283000	0.517404000	-0.239036000
Li	1.139811000	1.560874000	-4.921809000
Li	-1.124556000	2.412128000	1.546734000

### I-Li<sub>12</sub>

C	3.678681000	-1.811893000	0.781334000
C	3.896569000	-0.448152000	0.593375000
C	3.137409000	0.274375000	-0.355741000
C	2.155782000	-0.437501000	-1.078273000
C	1.935155000	-1.818340000	-0.913229000
C	2.709219000	-2.502304000	0.040966000
H	4.267715000	-2.349495000	1.518203000
H	4.642496000	0.078290000	1.178346000
H	1.577495000	0.102472000	-1.827651000
H	2.582875000	-3.572897000	0.176515000
C	-2.051802000	0.462303000	1.391939000
C	-0.780452000	-0.212716000	1.809718000
C	-0.595342000	-1.560833000	1.720746000
C	-1.596087000	-2.537094000	1.184775000
C	-2.927174000	-1.855402000	0.947741000

C	-3.145791000	-0.514530000	1.067711000
H	-2.414528000	1.060113000	2.252318000
H	0.313388000	-1.988347000	2.167322000
H	-1.726414000	-3.359852000	1.904702000
H	-3.783778000	-2.501839000	0.743246000
S	3.389350000	2.004945000	-0.562908000
S	-0.386965000	2.994873000	-0.710974000
S	0.499462000	0.898158000	2.456426000
S	-4.716797000	0.261181000	0.696672000
S	-2.124769000	-0.033190000	-2.178901000
S	0.692512000	-2.666138000	-1.862409000
Li	-4.033776000	-0.885138000	-1.128034000
Li	-2.997042000	1.493470000	-0.423178000
Li	-1.048705000	1.985199000	-2.782793000
Li	1.626190000	-0.682232000	1.204890000
Li	1.564712000	2.659921000	-2.035271000
Li	1.422629000	2.420838000	0.696432000
Li	-1.473217000	-1.743309000	-0.751329000
Li	-0.237739000	-0.792238000	-3.297981000
Li	-0.736907000	0.720350000	-0.330460000
Li	1.185140000	1.524512000	-4.968940000
Li	-1.161276000	2.432495000	1.427017000
Li	-0.247297000	-3.705785000	0.035275000

## II-Li

C	3.005080000	-1.027829000	-0.077734000
C	2.160411000	-0.311984000	0.803693000
C	2.303529000	1.070321000	0.967007000
C	3.295272000	1.768596000	0.277277000
C	4.105163000	1.077066000	-0.621422000
C	3.953543000	-0.291526000	-0.814800000
H	1.422136000	-0.854365000	1.394348000
H	3.411306000	2.837138000	0.426749000
H	4.870458000	1.614522000	-1.173304000
H	4.586222000	-0.824319000	-1.516831000
S	1.177923000	1.894090000	2.085981000
S	0.501075000	3.453040000	0.867858000
C	-2.448297000	-1.277802000	0.923344000
C	-2.093321000	-1.734972000	2.191639000
C	-1.018505000	-2.614040000	2.313298000

C	-0.265090000	-2.995621000	1.208318000
C	-0.596572000	-2.511400000	-0.067015000
C	-1.722330000	-1.680147000	-0.196646000
H	-2.643183000	-1.412348000	3.070467000
H	-0.749754000	-2.988658000	3.296155000
H	0.602520000	-3.635954000	1.320519000
H	-2.034555000	-1.380820000	-1.190572000
S	2.889530000	-2.765856000	-0.254604000
S	0.394184000	-2.820066000	-1.509653000
S	-3.801527000	-0.105883000	0.851348000
S	-3.797151000	0.538829000	-1.112263000
C	-1.434804000	0.936091000	-2.422947000
C	-0.136799000	1.424407000	-2.585278000
C	0.447526000	2.202810000	-1.584599000
C	-0.281128000	2.500078000	-0.424846000
C	-1.585263000	2.031303000	-0.268604000
C	-2.160490000	1.246803000	-1.267607000
H	-1.875536000	0.295050000	-3.181201000
H	0.420193000	1.186312000	-3.486356000
H	1.460639000	2.575566000	-1.691679000
H	-2.133953000	2.248184000	0.643292000
Li	0.557144000	-0.546557000	-0.962907000

## II-Li<sub>2</sub>

C	-3.507866000	-1.034245000	-0.183467000
C	-2.513145000	-1.066345000	0.818613000
C	-1.288507000	-1.718859000	0.623541000
C	-1.008524000	-2.356286000	-0.591324000
C	-1.997914000	-2.357870000	-1.584685000
C	-3.216031000	-1.711959000	-1.393369000
H	-2.709776000	-0.552402000	1.755239000
H	-0.059391000	-2.851020000	-0.757322000
H	-1.796944000	-2.853472000	-2.529342000
H	-3.961603000	-1.707868000	-2.181585000
S	-0.122056000	-1.574765000	1.972842000
S	1.402065000	-2.863843000	1.481287000
C	0.900725000	2.405930000	0.773410000
C	0.233028000	2.432979000	1.998060000
C	-1.155938000	2.353445000	2.008302000
C	-1.873344000	2.236589000	0.822118000



C	-1.207697000	2.201513000	-0.414674000
C	0.195378000	2.287041000	-0.420546000
H	0.789803000	2.499852000	2.927752000
H	-1.687337000	2.369876000	2.954951000
H	-2.956860000	2.151049000	0.863075000
H	0.722056000	2.276443000	-1.370580000
S	-5.013335000	-0.167380000	0.058490000
S	-2.056823000	2.000492000	-1.973918000
S	2.687965000	2.548317000	0.863537000
S	3.356893000	1.805669000	-0.925595000
C	3.800996000	-0.728580000	-1.774050000
C	3.676046000	-2.111392000	-1.760588000
C	2.925516000	-2.746084000	-0.772753000
C	2.315257000	-1.976507000	0.215800000
C	2.438758000	-0.588312000	0.223577000
C	3.178612000	0.031879000	-0.778556000
H	4.380708000	-0.238310000	-2.550474000
H	4.159730000	-2.701511000	-2.532031000
H	2.809416000	-3.825602000	-0.774943000
H	1.959984000	-0.008660000	1.005685000
Li	-1.470877000	-0.091139000	-1.123826000
Li	-4.228202000	1.473857000	-1.307230000

### II-Li<sub>3</sub>

C	-3.831459000	0.147310000	-0.061205000
C	-2.873329000	-0.071187000	0.950310000
C	-2.076512000	-1.229426000	1.014313000
C	-2.280978000	-2.240888000	0.052238000
C	-3.253133000	-2.059839000	-0.939296000
C	-4.003235000	-0.881653000	-1.017739000
H	-2.744433000	0.689910000	1.711951000
H	-1.688763000	-3.148112000	0.106102000
H	-3.412430000	-2.842670000	-1.675449000
H	-4.735555000	-0.745019000	-1.806137000
S	-0.848596000	-1.367472000	2.287302000
S	0.868043000	-3.319674000	1.249661000
C	2.044861000	1.948724000	0.771762000
C	1.401853000	2.261810000	1.981703000
C	0.028425000	2.511028000	1.974221000
C	-0.717880000	2.395519000	0.800642000

C	-0.091591000	2.054777000	-0.412045000
C	1.305079000	1.875889000	-0.411381000
H	1.962951000	2.292972000	2.910447000
H	-0.475093000	2.747829000	2.905885000
H	-1.795357000	2.537794000	0.832535000
H	1.792793000	1.645575000	-1.350099000
S	-4.737545000	1.657006000	-0.137472000
S	-0.972148000	1.779964000	-1.929202000
S	3.769390000	1.497696000	0.893279000
S	4.173974000	0.594855000	-0.927045000
C	2.328155000	-0.831517000	-2.301603000
C	1.313279000	-1.774203000	-2.467505000
C	0.853835000	-2.514684000	-1.386313000
C	1.419860000	-2.353153000	-0.102273000
C	2.457502000	-1.411181000	0.051044000
C	2.900942000	-0.663361000	-1.040897000
H	2.654642000	-0.219952000	-3.137005000
H	0.872547000	-1.916134000	-3.449696000
H	0.075263000	-3.258488000	-1.520458000
H	2.933852000	-1.303507000	1.023822000
Li	-1.768024000	-0.334086000	-1.168024000
Li	-3.158505000	2.542974000	-1.484946000
Li	0.578412000	0.143785000	1.228925000

#### **II-Li<sub>4</sub>**

C	-2.793075000	1.698787000	-0.132547000
C	-1.923423000	1.129103000	-1.069405000
C	-0.647927000	1.677364000	-1.292257000
C	-0.295125000	2.835935000	-0.580109000
C	-1.171721000	3.409965000	0.336290000
C	-2.418150000	2.840649000	0.577565000
H	-2.230222000	0.253159000	-1.635464000
H	0.681379000	3.286187000	-0.736680000
H	-0.867386000	4.296395000	0.882614000
H	-3.098173000	3.269613000	1.305174000
S	0.457444000	0.845847000	-2.414591000
S	4.239797000	0.350246000	-2.009012000
C	-0.692122000	-2.296968000	-0.210467000
C	-1.201906000	-2.862889000	-1.387177000
C	-2.565039000	-2.822921000	-1.661455000

C	-3.452666000	-2.193378000	-0.791646000
C	-2.955449000	-1.601934000	0.366618000
C	-1.593390000	-1.679207000	0.670954000
H	-0.516650000	-3.335392000	-2.083378000
H	-2.939094000	-3.276644000	-2.573809000
H	-4.510706000	-2.126953000	-1.022043000
H	-1.243923000	-1.229269000	1.601046000
S	-4.408001000	0.972492000	0.103238000
S	-3.992207000	-0.604197000	1.422202000
S	1.061295000	-2.294467000	0.105191000
S	0.994134000	0.850271000	2.405294000
C	3.525003000	-0.301272000	2.477492000
C	4.668756000	-0.812295000	1.847606000
C	4.903991000	-0.590944000	0.501193000
C	4.019202000	0.211357000	-0.248372000
C	2.918474000	0.771691000	0.411696000
C	2.607151000	0.477575000	1.753457000
H	3.353318000	-0.479987000	3.537949000
H	5.369788000	-1.409708000	2.423308000
H	5.762375000	-1.031897000	0.006694000
H	2.233537000	1.422355000	-0.128909000
Li	1.490633000	-1.424678000	2.247042000
Li	0.084801000	0.139693000	0.279494000
Li	2.555210000	1.813161000	-2.608067000
Li	2.126302000	-0.829713000	-1.515230000

## **II-Li<sub>5</sub>**

C	-2.458880000	1.871448000	0.028712000
C	-1.767185000	1.140710000	-0.962087000
C	-0.518009000	1.563144000	-1.446719000
C	0.022228000	2.761240000	-0.949261000
C	-0.650690000	3.491836000	0.022342000
C	-1.869127000	3.049156000	0.525354000
H	-2.226156000	0.244305000	-1.375903000
H	0.977068000	3.129058000	-1.318475000
H	-0.215383000	4.412231000	0.398616000
H	-2.393450000	3.619980000	1.285774000
S	0.354954000	0.533296000	-2.616376000
S	4.214915000	0.494809000	-1.899386000
C	-0.521341000	-2.601402000	-0.494025000

C	-1.165837000	-2.753995000	-1.730447000
C	-2.541308000	-2.549336000	-1.828020000
C	-3.293454000	-2.128627000	-0.732946000
C	-2.664128000	-1.933974000	0.502596000
C	-1.298687000	-2.237109000	0.614752000
H	-0.584938000	-3.020611000	-2.606936000
H	-3.027473000	-2.682906000	-2.789450000
H	-4.350233000	-1.906062000	-0.833669000
H	-0.843322000	-2.139981000	1.594760000
S	-4.009924000	1.328041000	0.677132000
S	-3.501144000	-1.225472000	1.884905000
S	1.258095000	-2.719556000	-0.335657000
S	0.506802000	0.297241000	2.153344000
C	3.211138000	-0.113989000	2.536961000
C	4.507559000	-0.338550000	2.053666000
C	4.826977000	-0.116654000	0.722999000
C	3.858623000	0.400406000	-0.158733000
C	2.591377000	0.703439000	0.356563000
C	2.224479000	0.393534000	1.676891000
H	2.962325000	-0.318285000	3.575407000
H	5.265510000	-0.721229000	2.730727000
H	5.814921000	-0.350895000	0.342408000
H	1.840889000	1.146768000	-0.290016000
Li	1.629478000	-1.776811000	1.796441000
Li	-2.072891000	0.711228000	2.039940000
Li	2.418846000	1.608612000	-2.832771000
Li	2.257861000	-0.985619000	-1.696379000
Li	-0.049233000	-0.391473000	-0.191100000

## **II-Li<sub>6</sub>**

C	-0.695757000	1.656787000	0.374017000
C	-0.500479000	1.032952000	-0.864699000
C	0.213430000	1.654901000	-1.911286000
C	0.689229000	2.957710000	-1.685236000
C	0.487685000	3.589549000	-0.453715000
C	-0.179797000	2.948712000	0.576294000
H	-0.980446000	0.076070000	-1.076607000
H	1.153143000	3.505681000	-2.505490000
H	0.857572000	4.600350000	-0.307343000
H	-0.325862000	3.431475000	1.536161000

S	0.541719000	0.814833000	-3.441383000
S	3.750299000	-0.093622000	-1.432118000
C	-1.225716000	-2.561758000	-0.924758000
C	-2.029326000	-2.090103000	-1.975576000
C	-3.359952000	-1.780836000	-1.725402000
C	-3.904087000	-1.884333000	-0.438540000
C	-3.113059000	-2.338412000	0.634404000
C	-1.797384000	-2.727711000	0.338392000
H	-1.598932000	-1.944274000	-2.960893000
H	-3.987094000	-1.431876000	-2.540359000
H	-4.952526000	-1.645285000	-0.265456000
H	-1.202428000	-3.126811000	1.155267000
S	-1.562603000	0.843037000	1.697969000
S	-3.633444000	-2.194969000	2.325679000
S	0.525562000	-2.809860000	-1.122738000
S	0.962136000	-2.073866000	2.848154000
C	1.839744000	0.571598000	2.700355000
C	2.451721000	1.631929000	2.037837000
C	3.053873000	1.461937000	0.792370000
C	3.102452000	0.195439000	0.198261000
C	2.574394000	-0.882636000	0.927800000
C	1.886910000	-0.711559000	2.138559000
H	1.310725000	0.730594000	3.633710000
H	2.422850000	2.621928000	2.483406000
H	3.485533000	2.314494000	0.275647000
H	2.694573000	-1.869392000	0.491056000
Li	1.181277000	-3.516338000	1.018361000
Li	0.185418000	-0.727412000	0.613192000
Li	2.521929000	1.581379000	-2.456126000
Li	1.645679000	-1.027460000	-2.330525000
Li	-1.390268000	-1.334201000	2.881261000
Li	-3.566744000	-0.170953000	1.128363000

## **II-Li<sub>7</sub>**

C	-0.616413000	2.098474000	0.753815000
C	-0.713494000	1.108145000	-0.330380000
C	-0.362350000	1.575362000	-1.656656000
C	-0.204341000	2.924463000	-1.914824000
C	-0.320406000	3.894981000	-0.871260000
C	-0.485431000	3.455835000	0.439596000

H	-0.422523000	0.079581000	-0.074172000
H	-0.071189000	3.248406000	-2.946137000
H	-0.216073000	4.949886000	-1.093078000
H	-0.523659000	4.174629000	1.254258000
S	-0.162850000	0.386105000	-2.991325000
S	3.336153000	0.186224000	-1.320772000
C	-1.061948000	-2.941133000	-1.310095000
C	-1.908378000	-3.025555000	-2.430888000
C	-3.224017000	-2.560554000	-2.341065000
C	-3.724854000	-1.993156000	-1.163385000
C	-2.903321000	-1.897967000	-0.021291000
C	-1.589968000	-2.387057000	-0.134070000
H	-1.526230000	-3.429938000	-3.361543000
H	-3.865059000	-2.614862000	-3.215766000
H	-4.742118000	-1.619488000	-1.118966000
H	-0.943251000	-2.279302000	0.731289000
S	-0.930009000	1.608648000	2.468722000
S	-3.443286000	-1.121304000	1.469368000
S	0.645226000	-3.433648000	-1.385429000
S	0.734244000	-2.161435000	2.911190000
C	2.503161000	-0.024032000	3.203537000
C	3.347324000	0.965174000	2.689006000
C	3.592353000	1.081163000	1.314498000
C	2.994663000	0.175412000	0.416447000
C	2.124487000	-0.786786000	0.956110000
C	1.868085000	-0.923773000	2.328848000
H	2.311089000	-0.088228000	4.268615000
H	3.815532000	1.668452000	3.371081000
H	4.259642000	1.847545000	0.935500000
H	1.620837000	-1.454606000	0.264398000
Li	0.961802000	-3.539856000	0.979654000
Li	1.239706000	1.342107000	1.698076000
Li	1.760962000	1.649485000	-2.204453000
Li	1.465417000	-1.236868000	-2.089378000
Li	-1.287672000	-0.792897000	2.635298000
Li	-2.618912000	1.036854000	0.873596000
Li	-1.835527000	-0.704974000	-1.777869000

**II-Li<sub>8</sub>**

C	-1.009187000	2.622150000	0.702268000
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C	-1.146234000	1.616552000	-0.279719000
C	-0.518969000	1.866901000	-1.526641000
C	0.071610000	3.107597000	-1.817958000
C	0.126730000	4.101813000	-0.826591000
C	-0.375127000	3.859361000	0.440391000
H	-0.312541000	-0.626528000	1.276218000
H	0.431996000	3.327988000	-2.825321000
H	0.578184000	5.062602000	-1.056848000
H	-0.296035000	4.606620000	1.223852000
S	-0.398984000	0.497559000	-2.702022000
S	3.339233000	0.073750000	-1.628288000
C	-1.144483000	-3.011920000	-1.075659000
C	-1.753889000	-2.908487000	-2.329790000
C	-3.018932000	-2.332296000	-2.431019000
C	-3.650530000	-1.785559000	-1.316917000
C	-3.068201000	-1.892780000	-0.041193000
C	-1.861636000	-2.609874000	0.061218000
H	-1.216667000	-3.225090000	-3.217819000
H	-3.484559000	-2.239357000	-3.406992000
H	-4.590345000	-1.253534000	-1.422660000
H	-1.441488000	-2.759202000	1.051798000
S	-1.556018000	2.232905000	2.378354000
S	-3.730015000	-1.016426000	1.358424000
S	0.614748000	-3.348853000	-0.968458000
S	2.157971000	-3.051671000	2.716317000
C	2.397666000	-0.295052000	2.859155000
C	2.525055000	0.967542000	2.283294000
C	2.774232000	1.119222000	0.910857000
C	2.994596000	-0.015624000	0.109087000
C	2.946859000	-1.278453000	0.728840000
C	2.588332000	-1.451206000	2.074208000
H	2.135763000	-0.401626000	3.906670000
H	2.397341000	1.852997000	2.902800000
H	2.853263000	2.112316000	0.474689000
H	3.176048000	-2.150566000	0.121978000
Li	1.636409000	-4.422162000	0.892650000
Li	0.334922000	1.003974000	1.355701000
Li	1.660735000	1.540400000	-2.249152000
Li	1.331103000	-1.217546000	-2.032390000
Li	-1.717511000	-0.245944000	2.397393000
Li	-3.013394000	1.224525000	0.706467000

Li	-1.280200000	-0.434292000	-0.587813000
Li	0.683007000	-1.982087000	1.105028000

**II-Li<sub>9</sub>**

C	-0.850332000	2.713706000	0.725507000
C	-0.885275000	1.637799000	-0.196291000
C	-0.449583000	1.936415000	-1.513562000
C	-0.030227000	3.224884000	-1.880157000
C	0.015744000	4.247924000	-0.917918000
C	-0.378819000	4.002529000	0.383424000
H	-0.330844000	-0.551031000	1.872933000
H	0.211747000	3.449408000	-2.919349000
H	0.348522000	5.240156000	-1.208391000
H	-0.348777000	4.786411000	1.133641000
S	-0.323175000	0.640728000	-2.770810000
S	3.330436000	0.255745000	-1.465513000
C	-1.091751000	-2.995452000	-1.238493000
C	-1.861235000	-3.197108000	-2.368942000
C	-3.205524000	-2.722381000	-2.428476000
C	-3.715530000	-1.948132000	-1.348973000
C	-2.968521000	-1.747445000	-0.193569000
C	-1.654381000	-2.357970000	-0.059955000
H	-1.414064000	-3.668882000	-3.239830000
H	-3.826134000	-2.939351000	-3.289017000
H	-4.696445000	-1.487325000	-1.427483000
H	-1.422282000	-2.776679000	0.934918000
S	-1.432071000	2.432269000	2.416715000
S	-3.567950000	-0.696647000	1.140648000
S	0.672174000	-3.304365000	-1.224457000
S	2.018856000	-3.147796000	2.619319000
C	2.433630000	-0.430946000	2.991656000
C	2.644540000	0.865553000	2.526940000
C	2.873779000	1.124963000	1.165812000
C	2.987835000	0.053130000	0.264294000
C	2.847223000	-1.251748000	0.768863000
C	2.508019000	-1.522499000	2.101598000
H	2.193005000	-0.613654000	4.033577000
H	2.606528000	1.697261000	3.227275000
H	3.022620000	2.143070000	0.815923000
H	2.997631000	-2.076796000	0.079290000



Li	1.627986000	-4.351527000	0.649863000
Li	0.449238000	1.042045000	1.670577000
Li	1.715904000	1.735609000	-2.154831000
Li	1.353252000	-1.079235000	-1.934713000
Li	-1.825535000	-0.049949000	2.709700000
Li	-2.877788000	1.557941000	0.692391000
Li	-1.968918000	-0.977115000	-2.308130000
Li	0.414840000	-2.009590000	1.160344000
Li	-1.282560000	-0.318452000	0.323642000

### **II-Li<sub>10</sub>**

C	-1.403674000	2.758747000	1.270777000
C	-1.665997000	2.053891000	0.060364000
C	-0.744995000	2.246202000	-0.985783000
C	0.319749000	3.169305000	-0.902285000
C	0.488691000	3.904356000	0.271402000
C	-0.348668000	3.687505000	1.370192000
H	-0.360264000	-0.167463000	0.979186000
H	1.011548000	3.294393000	-1.730633000
H	1.307648000	4.614527000	0.347506000
H	-0.177755000	4.209759000	2.306678000
S	-0.788395000	1.154963000	-2.425554000
S	3.291409000	-0.349191000	-1.829925000
C	-1.006656000	-3.194518000	-0.999251000
C	-1.621273000	-3.263778000	-2.261818000
C	-2.868706000	-2.658138000	-2.453333000
C	-3.497387000	-1.949227000	-1.427963000
C	-2.928614000	-1.914861000	-0.140405000
C	-1.710757000	-2.597287000	0.050581000
H	-1.120794000	-3.781186000	-3.073840000
H	-3.348605000	-2.727425000	-3.427366000
H	-4.438841000	-1.440140000	-1.605178000
H	-1.311575000	-2.626868000	1.064074000
S	-2.363106000	2.333906000	2.721808000
S	-3.622770000	-0.982502000	1.187565000
S	0.686976000	-3.707779000	-0.781910000
S	1.576384000	-2.385691000	2.941743000
C	2.298807000	0.266020000	2.617250000
C	2.662355000	1.355624000	1.827974000
C	2.960118000	1.204779000	0.466303000

C	2.995168000	-0.077946000	-0.104726000
C	2.765998000	-1.175176000	0.744922000
C	2.324372000	-1.031619000	2.069365000
H	1.984061000	0.405419000	3.646189000
H	2.670462000	2.351287000	2.266299000
H	3.189154000	2.069983000	-0.148154000
H	2.880042000	-2.171191000	0.327313000
Li	1.326928000	-4.147728000	1.458162000
Li	0.502611000	1.499643000	0.794624000
Li	1.411653000	0.535447000	-2.967041000
Li	1.887738000	-2.233572000	-2.378847000
Li	-1.704970000	0.069330000	2.335682000
Li	-3.531778000	1.455896000	0.845759000
Li	-1.051743000	-1.100608000	-3.132363000
Li	0.553596000	-1.630762000	0.808898000
Li	-1.662491000	0.040387000	-0.368379000
Li	0.981614000	-1.629504000	-5.315877000

## II-Li<sub>11</sub>

C	-1.726565000	2.844674000	1.161757000
C	-1.637699000	1.882437000	0.116281000
C	-0.532221000	1.995597000	-0.741850000
C	0.402891000	3.043585000	-0.662225000
C	0.257328000	3.989199000	0.354240000
C	-0.782523000	3.882545000	1.283666000
H	-0.564463000	0.009784000	1.939295000
H	1.246167000	3.093063000	-1.343487000
H	0.982507000	4.792452000	0.446298000
H	-0.863060000	4.592493000	2.100983000
S	-0.175744000	0.611573000	-1.857782000
S	3.387534000	-0.821027000	-1.965040000
C	-1.084330000	-3.058937000	-1.245818000
C	-1.758031000	-3.130542000	-2.476592000
C	-3.029363000	-2.557215000	-2.609424000
C	-3.637180000	-1.895812000	-1.545685000
C	-3.014480000	-1.866800000	-0.282074000
C	-1.755825000	-2.485014000	-0.151713000
H	-1.287228000	-3.638437000	-3.312926000
H	-3.549135000	-2.630983000	-3.562431000
H	-4.612585000	-1.436372000	-1.664794000

H	-1.282585000	-2.497035000	0.829386000
S	-3.020905000	2.641673000	2.380418000
S	-3.765481000	-0.999987000	1.071949000
S	0.593324000	-3.613513000	-1.108630000
S	2.236204000	-2.455677000	3.186329000
C	2.593349000	0.219909000	2.483170000
C	2.713425000	1.279614000	1.515734000
C	3.022658000	0.953074000	0.167360000
C	3.132465000	-0.360935000	-0.248866000
C	2.843446000	-1.423859000	0.695607000
C	2.667924000	-1.107443000	2.093248000
H	2.480879000	0.459223000	3.540875000
H	2.845848000	2.303757000	1.858688000
H	3.191288000	1.750811000	-0.551804000
H	3.285721000	-2.397804000	0.451513000
Li	1.543677000	-3.256484000	1.086992000
Li	0.447136000	1.684686000	1.321059000
Li	1.774494000	0.364941000	-3.192155000
Li	1.946631000	-2.585673000	-2.844798000
Li	-2.292506000	0.400666000	2.509277000
Li	-3.675978000	1.372237000	0.470063000
Li	-1.157114000	-0.999098000	-3.267840000
Li	0.604465000	-0.902310000	2.862717000
Li	-1.526401000	-0.176564000	0.143712000
Li	0.840418000	-1.498650000	-5.617376000
Li	1.222329000	-1.090904000	-0.758266000

### **II-Li<sub>12</sub>**

C	-1.995817000	2.786027000	1.132129000
C	-1.779532000	1.854194000	0.073925000
C	-0.571922000	1.985872000	-0.636190000
C	0.394247000	2.962409000	-0.338205000
C	0.142769000	3.856513000	0.707297000
C	-1.041115000	3.775398000	1.442861000
H	-0.002783000	-0.425512000	1.066456000
H	1.326118000	3.012461000	-0.892519000
H	0.884853000	4.608745000	0.959924000
H	-1.219810000	4.451718000	2.273147000
S	-0.138518000	0.728156000	-1.865678000
S	3.555177000	-0.823573000	-2.114693000

C	-1.092369000	-2.997526000	-1.240905000
C	-1.699150000	-3.107827000	-2.500890000
C	-2.995533000	-2.604947000	-2.686290000
C	-3.681112000	-1.976035000	-1.651835000
C	-3.116217000	-1.911220000	-0.360181000
C	-1.844462000	-2.481919000	-0.176093000
H	-1.162089000	-3.575634000	-3.320132000
H	-3.466783000	-2.700777000	-3.661861000
H	-4.668404000	-1.557421000	-1.816617000
H	-1.405975000	-2.445157000	0.818534000
S	-3.471760000	2.626186000	2.129603000
S	-3.923809000	-1.044475000	0.951245000
S	0.632200000	-3.364844000	-1.014661000
S	2.180132000	-2.500755000	2.968552000
C	2.831242000	0.109935000	2.331117000
C	3.098148000	1.137360000	1.424556000
C	3.314786000	0.868710000	0.075838000
C	3.343901000	-0.460467000	-0.385630000
C	3.124814000	-1.487572000	0.547594000
C	2.788304000	-1.224698000	1.889849000
H	2.642394000	0.334857000	3.377008000
H	3.123931000	2.166313000	1.776857000
H	3.494106000	1.676368000	-0.627007000
H	3.197137000	-2.517212000	0.204581000
Li	1.161570000	-3.649320000	1.256151000
Li	0.032459000	1.539502000	1.591427000
Li	1.837892000	0.442755000	-3.137570000
Li	1.915820000	-2.418683000	-2.822923000
Li	-2.687649000	0.412359000	2.652278000
Li	-3.814257000	1.273449000	0.251302000
Li	-1.104282000	-0.938924000	-3.203455000
Li	0.376113000	-0.887546000	2.834730000
Li	-1.560495000	-0.204086000	0.061030000
Li	0.857331000	-1.390437000	-5.585921000
Li	1.047713000	-0.863917000	-0.363834000
Li	-0.671725000	1.176313000	4.743002000
<b>III-Li</b>			
C	0.546104000	2.285957000	0.889996000
C	1.870201000	1.968193000	0.589439000

C	2.564488000	1.004887000	1.339764000
C	1.874420000	0.341467000	2.374710000
C	0.551673000	0.663253000	2.661810000
C	-0.122774000	1.637970000	1.930132000
H	2.382267000	2.457453000	-0.234544000
H	2.402522000	-0.394373000	2.976728000
H	0.036659000	0.155782000	3.471801000
H	-1.150866000	1.892579000	2.165409000
S	4.244511000	0.610736000	0.959390000
S	1.597329000	-0.311931000	-1.957378000
C	-3.087855000	-0.615080000	-0.582999000
C	-2.669250000	-0.835819000	-1.892691000
C	-2.131754000	0.217910000	-2.635121000
C	-1.986522000	1.474910000	-2.063211000
C	-2.411270000	1.691256000	-0.747463000
C	-2.979406000	0.656524000	-0.012660000
H	-2.728697000	-1.834596000	-2.312874000
H	-1.795481000	0.045481000	-3.652239000
H	-1.525740000	2.286173000	-2.617624000
H	-3.279313000	0.816348000	1.018888000
S	-0.177215000	3.566471000	-0.131017000
S	-2.217400000	3.279148000	0.053633000
S	-3.570621000	-2.010351000	0.419069000
S	-2.002990000	-1.976707000	1.811959000
C	-0.036600000	-3.620890000	0.772009000
C	1.058877000	-3.893525000	-0.044616000
C	1.566666000	-2.912443000	-0.896382000
C	0.998574000	-1.630150000	-0.898915000
C	-0.072933000	-1.340272000	-0.050414000
C	-0.607210000	-2.346786000	0.760559000
H	-0.454502000	-4.388184000	1.414955000
H	1.501445000	-4.884494000	-0.044477000
H	2.395957000	-3.132471000	-1.563738000
H	-0.468580000	-0.328333000	-0.012569000
S	3.630963000	-0.498406000	-1.821931000
Li	3.019508000	-1.239630000	0.362329000
<b>III-Li<sub>2</sub></b>			
C	2.288469000	1.974386000	-0.445729000
C	1.120512000	2.358589000	0.222082000

C	-0.068474000	2.609932000	-0.491607000
C	-0.044223000	2.426594000	-1.888312000
C	1.123230000	2.048193000	-2.540146000
C	2.301367000	1.826902000	-1.830124000
H	1.135223000	2.473185000	1.303744000
H	-0.961691000	2.586837000	-2.445606000
H	1.116224000	1.922401000	-3.618456000
H	3.211956000	1.526425000	-2.337540000
S	-1.600462000	2.994124000	0.306309000
S	-3.117539000	-0.016314000	2.383309000
C	0.930760000	-2.475901000	-0.074351000
C	0.768310000	-2.778544000	1.275982000
C	1.673045000	-2.281451000	2.215323000
C	2.736684000	-1.489385000	1.809016000
C	2.896004000	-1.184127000	0.452285000
C	1.993621000	-1.668462000	-0.493850000
H	-0.074730000	-3.383498000	1.596576000
H	1.528196000	-2.504482000	3.266793000
H	3.446528000	-1.097206000	2.530007000
H	2.123939000	-1.427418000	-1.545146000
S	3.745340000	1.682365000	0.546661000
S	4.289065000	-0.219546000	-0.110682000
S	-0.200265000	-3.242641000	-1.236586000
S	-0.865057000	-1.682346000	-2.411707000
C	-3.188092000	-0.270091000	-2.189710000
C	-4.195582000	0.397136000	-1.496686000
C	-4.202484000	0.441834000	-0.107294000
C	-3.196860000	-0.212791000	0.604631000
C	-2.222865000	-0.947254000	-0.076763000
C	-2.199170000	-0.944337000	-1.473244000
H	-3.174431000	-0.273478000	-3.274890000
H	-4.968769000	0.918948000	-2.051004000
H	-4.953735000	1.019896000	0.420785000
H	-1.479931000	-1.502879000	0.490296000
S	-1.037870000	-0.007522000	2.774101000
Li	-0.686280000	0.715085000	0.467673000
Li	-1.795614000	2.159580000	2.469972000

### III-Li<sub>3</sub>

C	-2.682651000	1.773572000	0.542226000
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C	-1.852010000	1.518613000	-0.556275000
C	-0.506995000	1.953018000	-0.575639000
C	-0.046005000	2.689717000	0.536990000
C	-0.879363000	2.946865000	1.629141000
C	-2.196727000	2.482868000	1.652188000
H	-2.238031000	0.965181000	-1.407638000
H	0.979004000	3.047432000	0.542586000
H	-0.485566000	3.490955000	2.481411000
H	-2.841257000	2.660321000	2.505968000
S	0.507565000	1.592352000	-1.968112000
S	4.049271000	0.722764000	-1.348577000
C	-1.008700000	-2.156671000	-1.209865000
C	-1.559943000	-2.120700000	-2.497138000
C	-2.890618000	-1.759391000	-2.697503000
C	-3.709570000	-1.411168000	-1.627444000
C	-3.165434000	-1.417693000	-0.344035000
C	-1.840152000	-1.799630000	-0.136969000
H	-0.933521000	-2.382050000	-3.343893000
H	-3.292365000	-1.747108000	-3.705803000
H	-4.739698000	-1.108567000	-1.783033000
H	-1.458649000	-1.813471000	0.882689000
S	-4.368126000	1.177333000	0.517567000
S	-4.084806000	-0.825179000	1.069138000
S	0.693683000	-2.619037000	-0.968249000
S	0.608385000	-0.653330000	2.802603000
C	3.019960000	-1.855887000	2.271749000
C	4.155202000	-2.114187000	1.497285000
C	4.476814000	-1.304191000	0.419822000
C	3.670365000	-0.189996000	0.145790000
C	2.549531000	0.087084000	0.924408000
C	2.179488000	-0.767978000	1.979292000
H	2.781042000	-2.492767000	3.120713000
H	4.787516000	-2.961748000	1.742521000
H	5.345158000	-1.514931000	-0.196108000
H	1.949912000	0.965821000	0.700678000
S	3.144630000	2.530019000	-1.178876000
Li	0.897986000	-2.507505000	1.341617000
Li	-0.792469000	0.571891000	1.390257000
Li	1.580369000	-0.475483000	-1.422586000

**III-Li<sub>4</sub>**

C	2.487830000	2.073399000	-0.300294000
C	1.743655000	1.519515000	0.749607000
C	0.354191000	1.741577000	0.858675000
C	-0.249786000	2.583581000	-0.098775000
C	0.497074000	3.144106000	-1.139295000
C	1.863875000	2.882503000	-1.262615000
H	2.234684000	0.897281000	1.492258000
H	-1.317089000	2.785319000	-0.036616000
H	-0.002179000	3.768451000	-1.873148000
H	2.443868000	3.295119000	-2.080869000
S	-0.531655000	0.952024000	2.172278000
S	-4.471716000	0.608826000	1.096538000
C	1.516952000	-2.270011000	0.926314000
C	2.123660000	-2.339033000	2.186353000
C	3.398421000	-1.817456000	2.398154000
C	4.101903000	-1.199386000	1.368343000
C	3.497068000	-1.100329000	0.115945000
C	2.230969000	-1.641366000	-0.105098000
H	1.584109000	-2.808716000	3.002154000
H	3.847310000	-1.893614000	3.383510000
H	5.085525000	-0.773152000	1.535083000
H	1.801154000	-1.559800000	-1.102005000
S	4.243134000	1.746592000	-0.399157000
S	4.244074000	-0.180929000	-1.220979000
S	-0.107774000	-2.948303000	0.666080000
S	-0.578053000	-0.585658000	-2.752613000
C	-2.636483000	-2.240268000	-1.970687000
C	-3.667327000	-2.649450000	-1.121135000
C	-4.174341000	-1.790885000	-0.157944000
C	-3.675331000	-0.478685000	-0.074696000
C	-2.611083000	-0.082112000	-0.889739000
C	-2.049626000	-0.970054000	-1.829613000
H	-2.304548000	-2.898608000	-2.773855000
H	-4.090326000	-3.642907000	-1.232402000
H	-4.993206000	-2.099615000	0.483778000
H	-2.258022000	0.943874000	-0.831833000
S	-4.019353000	2.561411000	0.515010000
Li	-0.382208000	-2.620351000	-1.596577000
Li	0.719228000	0.767196000	-1.335235000
Li	-1.354051000	-0.979221000	1.041769000



Li	-2.649468000	1.942071000	2.182853000
<b>III-Li<sub>5</sub></b>			
C	2.607503000	2.480384000	-0.238956000
C	1.883077000	1.949179000	0.842612000
C	0.483645000	1.891043000	0.856157000
C	-0.220845000	2.511724000	-0.186758000
C	0.482920000	3.108172000	-1.237182000
C	1.876972000	3.068739000	-1.291146000
H	2.469257000	1.596713000	1.692665000
H	-1.306443000	2.546400000	-0.170677000
H	-0.073346000	3.585724000	-2.038217000
H	2.416234000	3.493525000	-2.131762000
S	-0.302584000	0.947493000	2.163363000
S	-4.225301000	0.378837000	1.245362000
C	1.276299000	-2.430788000	1.075837000
C	2.023175000	-2.510420000	2.268315000
C	3.282051000	-1.892637000	2.341158000
C	3.825623000	-1.183895000	1.263559000
C	3.118553000	-1.118976000	0.042415000
C	1.859497000	-1.748037000	-0.003336000
H	1.609817000	-3.028074000	3.126814000
H	3.839037000	-1.943722000	3.272065000
H	4.782627000	-0.681345000	1.353005000
H	1.316736000	-1.670803000	-0.938583000
S	4.337629000	2.249744000	-0.313144000
S	3.685393000	-0.273654000	-1.386001000
S	-0.373516000	-3.076400000	0.938442000
S	-0.422078000	-0.753679000	-2.709357000
C	-2.648555000	-2.251251000	-2.145917000
C	-3.729094000	-2.649871000	-1.356030000
C	-4.182459000	-1.849998000	-0.317416000
C	-3.575721000	-0.601923000	-0.104704000
C	-2.483988000	-0.203600000	-0.882806000
C	-1.963485000	-1.045993000	-1.886659000
H	-2.332973000	-2.865516000	-2.988125000
H	-4.227336000	-3.591031000	-1.567350000
H	-5.027864000	-2.151339000	0.291764000
H	-2.040141000	0.773771000	-0.723124000
S	-3.915890000	2.380595000	0.734560000

Li	-0.538594000	-2.777876000	-1.405336000
Li	1.352784000	0.672064000	-1.695517000
Li	-1.480732000	-0.960514000	1.104142000
Li	-2.452084000	1.885237000	2.344782000
Li	1.678941000	-0.317084000	1.842887000

### III-Li<sub>6</sub>

C	2.839127000	2.767156000	0.441429000
C	1.936608000	2.039476000	1.251834000
C	0.634220000	1.733409000	0.847484000
C	0.176782000	2.203084000	-0.400357000
C	1.032792000	2.983364000	-1.184884000
C	2.338616000	3.255820000	-0.784029000
H	2.281508000	1.755519000	2.247998000
H	-0.861239000	2.071506000	-0.686299000
H	0.657637000	3.401535000	-2.116197000
H	2.982036000	3.874470000	-1.403415000
S	-0.376667000	0.737626000	1.952062000
S	-4.363276000	0.773659000	0.907682000
C	1.311987000	-2.511009000	0.959095000
C	2.115161000	-2.522795000	2.117551000
C	3.349370000	-1.858676000	2.110896000
C	3.804722000	-1.148133000	0.991995000
C	3.030290000	-1.133726000	-0.186166000
C	1.816704000	-1.840488000	-0.164119000
H	1.763423000	-3.028209000	3.010034000
H	3.955339000	-1.861734000	3.011858000
H	4.740301000	-0.600185000	1.042255000
H	1.232782000	-1.829533000	-1.077399000
S	4.509088000	2.983891000	0.933602000
S	3.427033000	-0.247430000	-1.662669000
S	-0.311273000	-3.226277000	0.908046000
S	-0.646209000	-1.113891000	-2.812066000
C	-2.819583000	-2.519536000	-1.862997000
C	-3.864869000	-2.754744000	-0.965591000
C	-4.291188000	-1.764295000	-0.092828000
C	-3.700859000	-0.488993000	-0.163579000
C	-2.635636000	-0.261065000	-1.039039000
C	-2.139080000	-1.285356000	-1.871004000
H	-2.549231000	-3.285222000	-2.590841000

H	-4.358450000	-3.721722000	-0.962051000
H	-5.110637000	-1.945389000	0.595307000
H	-2.219028000	0.737331000	-1.102929000
S	-3.645936000	2.597436000	0.191008000
Li	-0.619109000	-3.055470000	-1.429203000
Li	1.064170000	0.430093000	-1.872781000
Li	-1.468520000	-1.120173000	0.835521000
Li	-2.368353000	1.988408000	1.924166000
Li	1.724718000	-0.293744000	1.651219000
Li	4.611232000	1.585316000	-0.832815000

### III-Li<sub>7</sub>

C	2.571700000	2.738441000	-0.097661000
C	1.854645000	2.152874000	0.966424000
C	0.532166000	1.700373000	0.837490000
C	-0.120951000	1.857483000	-0.398420000
C	0.555872000	2.485205000	-1.451041000
C	1.880060000	2.900787000	-1.317890000
H	2.346724000	2.108502000	1.939114000
H	-1.153952000	1.551364000	-0.530105000
H	0.030363000	2.649538000	-2.388848000
H	2.386858000	3.387511000	-2.145446000
S	-0.234490000	0.947750000	2.275209000
S	-3.670056000	-0.766394000	1.823533000
C	1.503670000	-2.429516000	1.421535000
C	2.280208000	-2.203369000	2.576484000
C	3.481647000	-1.492172000	2.478675000
C	3.928658000	-0.964662000	1.259474000
C	3.186938000	-1.195495000	0.083850000
C	2.003773000	-1.947488000	0.202572000
H	1.930837000	-2.566893000	3.536644000
H	4.064087000	-1.310203000	3.376817000
H	4.840301000	-0.376973000	1.226149000
H	1.457766000	-2.139499000	-0.714162000
S	4.238934000	3.248699000	0.117728000
S	3.601670000	-0.572813000	-1.517993000
S	-0.079804000	-3.226270000	1.495098000
S	-0.378153000	-1.315443000	-2.599696000
C	-3.144828000	-1.485583000	-2.699303000
C	-4.396913000	-1.557555000	-2.110684000

C	-4.564969000	-1.365058000	-0.732417000
C	-3.461048000	-1.046947000	0.072466000
C	-2.205041000	-0.919852000	-0.552065000
C	-2.009744000	-1.182627000	-1.918291000
H	-3.016557000	-1.674547000	-3.759414000
H	-5.261337000	-1.803668000	-2.719972000
H	-5.536665000	-1.527435000	-0.269653000
H	-1.340887000	-0.603598000	0.031752000
S	-3.660370000	2.853763000	0.345564000
Li	-0.729663000	-2.818474000	-0.774519000
Li	1.295938000	0.239978000	-1.742161000
Li	-1.314267000	-1.302944000	2.171864000
Li	-2.534537000	1.490333000	1.898056000
Li	1.804103000	-0.097798000	1.731597000
Li	4.737196000	1.406347000	-1.062275000
Li	-4.748542000	0.829816000	0.318621000

### III-Li<sub>8</sub>

C	2.452796000	2.912576000	-0.228850000
C	1.827017000	2.273613000	0.864461000
C	0.565612000	1.665232000	0.777032000
C	-0.115762000	1.705983000	-0.460184000
C	0.464090000	2.393163000	-1.543397000
C	1.723234000	2.981917000	-1.438488000
H	2.347805000	2.290736000	1.821070000
H	-1.102741000	1.266080000	-0.564220000
H	-0.083970000	2.444240000	-2.483325000
H	2.163573000	3.497941000	-2.285699000
S	-0.105105000	0.888213000	2.244572000
S	-3.628030000	-0.743041000	1.815027000
C	1.544190000	-2.486880000	1.471099000
C	2.344629000	-2.350601000	2.625515000
C	3.557647000	-1.656767000	2.555328000
C	3.992468000	-1.053348000	1.366696000
C	3.223992000	-1.187499000	0.192264000
C	2.029716000	-1.925609000	0.280229000
H	2.005417000	-2.774846000	3.564160000
H	4.161391000	-1.553695000	3.451979000
H	4.923047000	-0.495382000	1.350367000
H	1.454015000	-2.046391000	-0.630651000

S	4.067462000	3.581372000	-0.079956000
S	3.637253000	-0.462283000	-1.366109000
S	-0.043624000	-3.269012000	1.524633000
S	-0.339855000	-1.442787000	-2.587853000
C	-3.116277000	-1.391549000	-2.721410000
C	-4.377740000	-1.350125000	-2.146198000
C	-4.546840000	-1.168403000	-0.767926000
C	-3.431092000	-0.986189000	0.061465000
C	-2.161624000	-0.982785000	-0.548002000
C	-1.972883000	-1.216478000	-1.918913000
H	-2.993547000	-1.565678000	-3.784657000
H	-5.254300000	-1.490533000	-2.771861000
H	-5.538637000	-1.221361000	-0.324619000
H	-1.279458000	-0.762976000	0.052396000
S	-3.363720000	3.041525000	0.711059000
Li	-0.742856000	-2.911954000	-0.751577000
Li	1.302273000	0.126619000	-1.773211000
Li	-1.319915000	-1.334425000	2.157548000
Li	-2.504552000	1.518982000	2.124838000
Li	1.906515000	-0.197315000	1.917841000
Li	4.687454000	1.558195000	-0.859344000
Li	-4.440623000	1.153607000	0.321402000
Li	-1.387679000	3.602800000	0.036480000

### III-Li<sub>9</sub>

C	2.503742000	2.820212000	-0.175557000
C	1.816914000	2.236246000	0.914471000
C	0.557970000	1.627569000	0.782826000
C	-0.064142000	1.629485000	-0.483151000
C	0.561636000	2.291399000	-1.558295000
C	1.828164000	2.859989000	-1.416627000
H	2.285905000	2.294968000	1.896157000
H	-1.044855000	1.183626000	-0.627761000
H	0.041056000	2.334540000	-2.515299000
H	2.306772000	3.350423000	-2.258383000
S	-0.172966000	0.889565000	2.244657000
S	-3.631784000	-0.807109000	1.801906000
C	1.573344000	-2.455126000	1.493933000
C	2.348007000	-2.235415000	2.652199000
C	3.546854000	-1.519661000	2.563414000

C	3.991282000	-0.976017000	1.349750000
C	3.247512000	-1.192476000	0.172369000
C	2.068123000	-1.952172000	0.280912000
H	2.000383000	-2.612746000	3.607635000
H	4.130487000	-1.349164000	3.463020000
H	4.907526000	-0.395372000	1.319404000
H	1.514861000	-2.139777000	-0.632585000
S	4.124935000	3.452969000	0.025209000
S	3.667940000	-0.540614000	-1.416809000
S	0.003080000	-3.274070000	1.562081000
S	-0.330360000	-1.540528000	-2.586917000
C	-3.104267000	-1.480912000	-2.729752000
C	-4.366820000	-1.446411000	-2.159011000
C	-4.539263000	-1.268377000	-0.779299000
C	-3.425563000	-1.075592000	0.048984000
C	-2.155050000	-1.061166000	-0.555430000
C	-1.962059000	-1.301171000	-1.924679000
H	-2.977918000	-1.650763000	-3.793109000
H	-5.241222000	-1.589866000	-2.786668000
H	-5.531471000	-1.337389000	-0.337572000
H	-1.276018000	-0.831727000	0.045882000
S	-3.446906000	2.921385000	0.517506000
Li	-0.694952000	-2.975193000	-0.722630000
Li	1.330532000	0.033315000	-1.826601000
Li	-1.295837000	-1.364483000	2.176006000
Li	-2.521220000	1.431947000	1.988540000
Li	1.882347000	-0.117987000	1.811176000
Li	4.695752000	1.502679000	-0.953694000
Li	-4.558316000	0.953861000	0.342796000
Li	-1.366180000	3.522280000	-0.133175000
Li	-3.662840000	3.139273000	-1.733358000

### III-Li<sub>10</sub>

C	1.679754000	2.854125000	-0.294031000
C	0.876804000	2.807318000	0.962511000
C	0.083057000	1.564775000	0.978198000
C	-0.582939000	1.216790000	-0.179423000
C	-0.375076000	2.050632000	-1.400992000
C	1.027719000	2.549208000	-1.468226000
H	1.462051000	2.980910000	1.872075000

H	-1.189515000	0.314106000	-0.219487000
H	-0.771451000	1.624839000	-2.329741000
H	1.489457000	2.754119000	-2.438924000
S	0.002824000	0.683843000	2.533792000
S	-3.625596000	-0.597156000	1.352206000
C	1.517361000	-2.304176000	1.708394000
C	2.613603000	-1.983065000	2.522058000
C	3.692097000	-1.276913000	1.997820000
C	3.738777000	-0.911027000	0.646288000
C	2.662275000	-1.242459000	-0.187830000
C	1.552313000	-1.888367000	0.369626000
H	2.601423000	-2.275085000	3.566491000
H	4.531731000	-1.026974000	2.640089000
H	4.614449000	-0.415009000	0.238356000
H	0.669087000	-2.063494000	-0.242995000
S	3.450859000	3.056616000	-0.108360000
S	2.699659000	-0.882580000	-1.952500000
S	0.121956000	-3.203383000	2.349824000
S	-0.659634000	-3.885281000	-1.936495000
C	-1.901686000	-1.549314000	-2.792027000
C	-2.756457000	-0.458693000	-2.631639000
C	-3.355043000	-0.186656000	-1.405821000
C	-3.102909000	-1.012797000	-0.300571000
C	-2.307874000	-2.151133000	-0.496669000
C	-1.682517000	-2.429395000	-1.721403000
H	-1.455773000	-1.755865000	-3.761045000
H	-2.951422000	0.193921000	-3.478163000
H	-3.993815000	0.686952000	-1.298617000
H	-2.180653000	-2.830923000	0.341852000
S	-3.149623000	3.398838000	1.190491000
Li	-0.240288000	-4.313726000	0.345942000
Li	0.810115000	0.366459000	-1.373257000
Li	-1.321281000	-1.275217000	2.227249000
Li	-2.071418000	1.403479000	1.668263000
Li	2.380277000	1.237234000	1.354103000
Li	3.202913000	1.503658000	-1.699438000
Li	-4.570041000	1.661455000	1.214490000
Li	-0.891485000	3.940586000	1.497931000
Li	-2.108245000	3.075653000	-0.797792000
Li	1.246293000	-2.676945000	-2.511967000

**III-Li<sub>11</sub>**

C	2.034477000	3.009028000	-0.014741000
C	1.191770000	2.851847000	1.204151000
C	0.314883000	1.680364000	1.069683000
C	-0.304523000	1.488160000	-0.150077000
C	-0.026067000	2.459802000	-1.252527000
C	1.413130000	2.861231000	-1.231863000
H	1.746463000	2.903674000	2.147326000
H	-0.984703000	0.642383000	-0.287591000
H	-0.400409000	2.159175000	-2.240212000
H	1.924269000	3.131065000	-2.161090000
S	0.029648000	0.739898000	2.567479000
S	-3.454537000	-0.336553000	0.921997000
C	1.506607000	-2.275832000	1.614218000
C	2.514244000	-2.004402000	2.550021000
C	3.646479000	-1.292177000	2.165259000
C	3.823905000	-0.858799000	0.843838000
C	2.834365000	-1.136138000	-0.111807000
C	1.680451000	-1.812506000	0.304241000
H	2.395017000	-2.341731000	3.573643000
H	4.423281000	-1.087367000	2.896759000
H	4.738894000	-0.352374000	0.548862000
H	0.879561000	-1.967998000	-0.415455000
S	3.803069000	3.109077000	0.245473000
S	3.019503000	-0.671447000	-1.830373000
S	0.035774000	-3.179377000	2.067306000
S	-0.479172000	-3.683790000	-2.301879000
C	-2.714337000	-2.295067000	-3.181971000
C	-3.731028000	-1.346843000	-3.030062000
C	-3.947766000	-0.696017000	-1.809445000
C	-3.161752000	-1.020679000	-0.686248000
C	-2.121722000	-1.951102000	-0.872387000
C	-1.872207000	-2.599409000	-2.094405000
H	-2.544342000	-2.774925000	-4.139257000
H	-4.355454000	-1.096680000	-3.882099000
H	-4.746830000	0.032097000	-1.717726000
H	-1.477816000	-2.180100000	-0.028829000
S	-2.838866000	3.628385000	1.317878000
Li	-0.027657000	-4.197610000	-0.027224000
Li	1.061125000	0.695090000	-1.564176000



Li	-1.283948000	-1.168246000	2.123586000
Li	-1.883402000	1.542987000	1.482319000
Li	2.617183000	1.198994000	1.429613000
Li	3.568301000	1.667275000	-1.458713000
Li	-4.305012000	2.006048000	0.856212000
Li	-0.577788000	3.856869000	1.971563000
Li	-1.582952000	3.698812000	-0.579860000
Li	1.118118000	-1.901773000	-2.829600000
Li	-1.667345000	-0.322769000	-2.587595000

### III-Li<sub>12</sub>

C	2.203856000	3.263126000	0.284959000
C	1.143897000	3.027238000	1.338158000
C	0.438522000	1.770466000	1.025848000
C	0.093862000	1.573179000	-0.289161000
C	0.387882000	2.703086000	-1.241157000
C	1.775743000	3.196819000	-1.007719000
H	1.528948000	3.098885000	2.360983000
H	-0.408592000	0.642040000	-0.598287000
H	0.137308000	2.564006000	-2.304299000
H	2.448717000	3.400994000	-1.846727000
S	-0.079194000	0.794320000	2.448113000
S	-3.521010000	-0.445278000	0.900187000
C	1.424719000	-2.173864000	1.579239000
C	2.488470000	-1.922776000	2.459649000
C	3.598130000	-1.208360000	2.018878000
C	3.689407000	-0.749922000	0.696565000
C	2.633411000	-0.983750000	-0.198260000
C	1.506525000	-1.666558000	0.277342000
H	2.435290000	-2.292803000	3.477682000
H	4.428701000	-1.032349000	2.697699000
H	4.599758000	-0.262321000	0.357302000
H	0.659389000	-1.790525000	-0.394327000
S	3.923072000	3.114277000	0.776084000
S	2.726762000	-0.458309000	-1.901430000
S	0.001892000	-3.115959000	2.103438000
S	-0.517799000	-3.783019000	-2.280185000
C	-2.951623000	-2.687869000	-3.078884000
C	-4.076138000	-1.880683000	-2.886271000
C	-4.277100000	-1.179802000	-1.692583000

C	-3.343674000	-1.298602000	-0.651796000
C	-2.219434000	-2.104506000	-0.864870000
C	-1.992929000	-2.808472000	-2.056425000
H	-2.803760000	-3.215066000	-4.015069000
H	-4.805241000	-1.785373000	-3.685185000
H	-5.158246000	-0.559617000	-1.566397000
H	-1.480384000	-2.174234000	-0.074323000
S	-2.616871000	3.442920000	0.720788000
Li	-0.045496000	-4.152612000	0.004703000
Li	0.650214000	0.762441000	-2.283233000
Li	-1.423237000	-1.211360000	2.111929000
Li	-1.787567000	1.247252000	0.851603000
Li	2.593208000	1.288540000	1.750551000
Li	3.462862000	1.704986000	-0.996223000
Li	-4.244943000	1.883227000	0.575998000
Li	-0.913044000	3.128690000	2.374894000
Li	-0.363336000	4.231436000	0.115376000
Li	0.839329000	-1.880408000	-2.891157000
Li	-2.130537000	-0.382747000	-2.899186000
Li	-1.777842000	2.725359000	-1.430186000

#### IV-Li

C	0.807523000	3.394284000	0.302532000
C	0.316180000	3.546920000	1.603944000
C	-0.992664000	3.179494000	1.918312000
C	-1.825524000	2.691241000	0.907981000
C	-1.330503000	2.508998000	-0.384799000
C	-0.004320000	2.834932000	-0.689628000
H	1.805501000	3.736511000	0.048450000
H	0.954478000	3.985340000	2.366728000
H	-1.376992000	3.294119000	2.925817000
H	-1.987090000	2.112654000	-1.154879000
C	2.980823000	-0.192981000	-2.012170000
C	3.270366000	-1.307627000	-1.223550000
C	3.465067000	-1.186977000	0.149161000
C	3.417119000	0.072872000	0.775435000
C	3.211655000	1.196360000	-0.047329000
C	2.949667000	1.064961000	-1.411942000
H	2.779204000	-0.295883000	-3.073440000
H	3.305048000	-2.290501000	-1.682872000

H	3.633401000	-2.068483000	0.759948000
H	3.289227000	2.186546000	0.393899000
C	-2.180534000	-0.572143000	-0.442453000
C	-2.019202000	-1.172885000	-1.691237000
C	-3.134244000	-1.649338000	-2.383295000
C	-4.403931000	-1.511408000	-1.829087000
C	-4.572037000	-0.890366000	-0.592758000
C	-3.456832000	-0.419446000	0.100003000
H	-1.324529000	-0.216935000	0.119652000
H	-2.999684000	-2.123774000	-3.350006000
H	-5.270029000	-1.880289000	-2.368499000
H	-5.560907000	-0.767760000	-0.163261000
C	0.409154000	-4.370138000	0.553662000
C	0.414107000	-3.146138000	-0.117038000
C	0.551960000	-1.961318000	0.595353000
C	0.631402000	-1.970431000	1.994745000
C	0.650627000	-3.205384000	2.661291000
C	0.551729000	-4.388215000	1.939889000
H	0.283031000	-5.296644000	0.001650000
H	0.588597000	-1.017270000	0.060937000
H	0.727397000	-3.219288000	3.742915000
H	0.558563000	-5.339270000	2.462731000
S	-3.558253000	2.377918000	1.225092000
S	-3.608720000	0.346288000	1.704936000
S	-0.374131000	-1.270936000	-2.388745000
S	0.502701000	2.526484000	-2.373712000
S	2.578583000	2.554472000	-2.330025000
S	3.470615000	0.279648000	2.521874000
S	0.214332000	-3.199899000	-1.896196000
S	0.649099000	-0.477893000	2.915394000
Li	1.453882000	1.250664000	1.596738000

#### IV-Li<sub>2</sub>

C	-0.843210000	-3.246462000	0.396475000
C	-0.357014000	-3.366936000	1.701621000
C	0.969773000	-3.059767000	2.001151000
C	1.823847000	-2.657354000	0.973247000
C	1.339727000	-2.514224000	-0.328169000
C	0.001826000	-2.790164000	-0.619792000
H	-1.857807000	-3.547672000	0.154471000

H	-1.014496000	-3.738098000	2.484387000
H	1.348446000	-3.148016000	3.013382000
H	2.017098000	-2.194276000	-1.115852000
C	-2.819080000	0.149176000	-2.178548000
C	-3.157889000	1.308102000	-1.478972000
C	-3.573006000	1.251380000	-0.152760000
C	-3.690160000	0.022129000	0.518294000
C	-3.399636000	-1.141714000	-0.214611000
C	-2.940360000	-1.077986000	-1.532685000
H	-2.464350000	0.195423000	-3.203023000
H	-3.073666000	2.271969000	-1.970893000
H	-3.805929000	2.168583000	0.381296000
H	-3.565063000	-2.111413000	0.250281000
C	2.318489000	0.536369000	-0.439085000
C	2.160544000	1.155670000	-1.679734000
C	3.275977000	1.647627000	-2.360784000
C	4.543737000	1.506089000	-1.804095000
C	4.709376000	0.865475000	-0.577178000
C	3.594187000	0.380474000	0.105637000
H	1.465261000	0.166580000	0.117757000
H	3.143040000	2.134442000	-3.321543000
H	5.410468000	1.885906000	-2.334913000
H	5.697455000	0.738966000	-0.146943000
C	-0.449054000	4.296852000	0.557069000
C	-0.365713000	3.078150000	-0.127000000
C	-0.431525000	1.879150000	0.566714000
C	-0.455270000	1.854668000	1.970261000
C	-0.547360000	3.081680000	2.649813000
C	-0.569795000	4.284702000	1.939913000
H	-0.397102000	5.235869000	0.014925000
H	-0.428443000	0.941333000	0.019996000
H	-0.526217000	3.090854000	3.737320000
H	-0.630766000	5.224183000	2.480433000
S	3.574352000	-2.418532000	1.261638000
S	3.746451000	-0.387027000	1.710859000
S	0.522592000	1.246882000	-2.398417000
S	-0.465288000	-2.576359000	-2.330841000
S	-2.534723000	-2.624087000	-2.338183000
S	-4.100848000	-0.132971000	2.238722000
S	-0.106290000	3.161319000	-1.896146000
S	-0.335092000	0.317372000	2.858090000

Li	-1.878726000	-1.053719000	1.711847000
Li	-2.443555000	1.267478000	3.097053000

#### IV-Li<sub>3</sub>

C	-0.598223000	-3.199340000	-0.052168000
C	-0.382471000	-3.563476000	1.282195000
C	0.737985000	-3.108695000	1.974506000
C	1.704635000	-2.314677000	1.326459000
C	1.464566000	-1.921309000	0.000005000
C	0.316642000	-2.348588000	-0.678552000
H	-1.446096000	-3.590728000	-0.603531000
H	-1.089490000	-4.226192000	1.774997000
H	0.895553000	-3.391651000	3.010307000
H	2.189478000	-1.293268000	-0.511511000
C	-2.634010000	0.660449000	-2.117610000
C	-3.127315000	1.587286000	-1.199533000
C	-3.504163000	1.198580000	0.083200000
C	-3.435195000	-0.147505000	0.477253000
C	-3.001654000	-1.078246000	-0.478026000
C	-2.558552000	-0.678740000	-1.739678000
H	-2.307691000	0.967725000	-3.105105000
H	-3.192703000	2.634611000	-1.480176000
H	-3.858921000	1.945102000	0.790122000
H	-3.028464000	-2.133709000	-0.229017000
C	2.619689000	1.436031000	-0.580821000
C	2.159170000	1.228708000	-1.878482000
C	2.876713000	0.415832000	-2.759266000
C	4.047861000	-0.199972000	-2.319537000
C	4.487357000	-0.037771000	-1.011098000
C	3.761328000	0.768144000	-0.121893000
H	2.087982000	2.093104000	0.097947000
H	2.517671000	0.261572000	-3.771941000
H	4.610015000	-0.827890000	-3.003154000
H	5.369739000	-0.556386000	-0.652249000
C	-1.041033000	4.273471000	0.759772000
C	-0.448183000	3.198057000	0.084226000
C	-0.288842000	1.972289000	0.721033000
C	-0.587117000	1.843682000	2.084085000
C	-1.151284000	2.931855000	2.765793000
C	-1.404106000	4.128163000	2.090097000

H	-1.195130000	5.219212000	0.249268000
H	0.100563000	1.114172000	0.176540000
H	-1.318146000	2.870225000	3.840486000
H	-1.850276000	4.963121000	2.620876000
S	3.176193000	-1.862912000	2.199751000
S	4.200620000	0.823164000	1.583142000
S	0.544437000	1.756966000	-2.437134000
S	0.156897000	-1.789877000	-2.371695000
S	-1.873459000	-1.940957000	-2.806230000
S	-3.796788000	-0.737446000	2.117142000
S	0.182135000	3.571006000	-1.545441000
S	-0.225380000	0.321521000	2.953537000
Li	-1.441008000	-1.351965000	1.591653000
Li	-2.507662000	0.820869000	3.179822000
Li	2.137859000	0.213940000	2.634346000

#### IV-Li<sub>4</sub>

C	0.826782000	-3.615337000	0.088909000
C	0.673610000	-3.958109000	-1.253282000
C	-0.375334000	-3.432670000	-2.011979000
C	-1.309216000	-2.550444000	-1.435724000
C	-1.092890000	-2.141792000	-0.104958000
C	-0.047404000	-2.681564000	0.653302000
H	1.622508000	-4.046567000	0.687098000
H	1.366720000	-4.658849000	-1.709276000
H	-0.508179000	-3.731853000	-3.046578000
H	-1.756376000	-1.405882000	0.349273000
C	2.892722000	0.437877000	2.089518000
C	3.357180000	1.367347000	1.160173000
C	3.601437000	1.003064000	-0.162065000
C	3.421896000	-0.321748000	-0.587469000
C	3.033970000	-1.262662000	0.375353000
C	2.724025000	-0.884930000	1.681678000
H	2.663201000	0.729017000	3.109266000
H	3.500830000	2.400498000	1.463073000
H	3.933304000	1.755605000	-0.873924000
H	2.983310000	-2.307284000	0.092185000
C	-2.507772000	1.404098000	0.770490000
C	-1.988102000	0.921454000	1.966709000
C	-2.695015000	-0.021959000	2.725975000

C	-3.927522000	-0.464217000	2.266462000
C	-4.440834000	-0.005101000	1.051236000
C	-3.723865000	0.914722000	0.259583000
H	-1.982445000	2.164268000	0.203222000
H	-2.288912000	-0.386212000	3.663552000
H	-4.504038000	-1.164364000	2.862863000
H	-5.441825000	-0.309096000	0.742187000
C	1.301450000	4.076107000	-0.386881000
C	0.642735000	2.979670000	0.185481000
C	0.364565000	1.852712000	-0.576461000
C	0.611914000	1.851000000	-1.955485000
C	1.244060000	2.962722000	-2.532230000
C	1.612051000	4.052452000	-1.738336000
H	1.548850000	4.942265000	0.219075000
H	-0.083087000	0.974875000	-0.117419000
H	1.375506000	3.010971000	-3.612730000
H	2.108217000	4.904632000	-2.191750000
S	-2.678986000	-2.003543000	-2.404605000
S	-4.265975000	1.347345000	-1.374162000
S	-0.335837000	1.297465000	2.542265000
S	0.065967000	-2.147898000	2.355648000
S	2.111513000	-2.156985000	2.777290000
S	3.611115000	-0.874442000	-2.270098000
S	0.088123000	3.192491000	1.870106000
S	0.093777000	0.465708000	-2.956637000
Li	1.243315000	-1.452940000	-1.801348000
Li	2.389485000	0.822521000	-3.198778000
Li	-2.279001000	0.368568000	-2.460608000
Li	-4.278925000	-0.968297000	-1.091598000

#### IV-Li<sub>5</sub>

C	-0.901070000	-2.875455000	-2.297220000
C	-0.965377000	-4.047296000	-1.548219000
C	-0.161177000	-4.220067000	-0.420943000
C	0.741544000	-3.215735000	-0.021678000
C	0.788267000	-2.028426000	-0.778700000
C	-0.025934000	-1.841291000	-1.913630000
H	-1.534507000	-2.735787000	-3.166968000
H	-1.669974000	-4.824412000	-1.826107000
H	-0.227892000	-5.127061000	0.169902000

H	1.469549000	-1.228729000	-0.487927000
C	-3.725299000	1.906705000	-0.388883000
C	-4.454354000	1.449847000	0.697607000
C	-4.515277000	0.087233000	1.004449000
C	-3.844830000	-0.855965000	0.202789000
C	-3.157763000	-0.382062000	-0.930037000
C	-3.082813000	0.981180000	-1.231409000
H	-3.662636000	2.967219000	-0.609558000
H	-4.982532000	2.162323000	1.325508000
H	-5.144221000	-0.258851000	1.824971000
H	-2.710371000	-1.093954000	-1.617854000
C	3.198976000	1.065611000	0.320986000
C	2.976227000	1.341085000	-1.020375000
C	3.538464000	0.549024000	-2.028068000
C	4.361696000	-0.504342000	-1.656745000
C	4.580178000	-0.798377000	-0.309192000
C	3.955798000	-0.054933000	0.710417000
H	2.785988000	1.700646000	1.098082000
H	3.343938000	0.760911000	-3.074170000
H	4.844075000	-1.102861000	-2.422792000
H	5.298111000	-1.578536000	-0.049400000
C	-0.769547000	3.878947000	1.494947000
C	0.165696000	3.053457000	0.870939000
C	0.100514000	1.665841000	1.040633000
C	-0.846686000	1.084887000	1.895124000
C	-1.756481000	1.928784000	2.542497000
C	-1.726595000	3.301607000	2.325788000
H	-0.737571000	4.952778000	1.344409000
H	0.844398000	1.014406000	0.586764000
H	-2.483387000	1.507183000	3.230313000
H	-2.453099000	3.937085000	2.822723000
S	1.685723000	-3.461903000	1.455136000
S	4.013959000	-0.547493000	2.414053000
S	1.877808000	2.644218000	-1.598805000
S	0.043608000	-0.348075000	-2.850478000
S	-2.216397000	1.540480000	-2.673199000
S	-3.759493000	-2.572097000	0.668004000
S	1.522085000	3.863165000	0.027731000
S	-0.763499000	-0.656096000	2.237548000
Li	-1.431944000	-2.192520000	0.208427000
Li	-3.028118000	-1.223438000	2.367254000



Li	1.606725000	-1.261116000	2.462559000
Li	3.740248000	-2.485607000	1.167186000
Li	-0.315418000	1.406317000	-1.336830000

**IV-Li<sub>6</sub>**

C	-0.839042000	-2.897854000	-2.262269000
C	-0.928578000	-4.054317000	-1.488975000
C	-0.094285000	-4.246097000	-0.388769000
C	0.871641000	-3.277280000	-0.049849000
C	0.960593000	-2.120365000	-0.847172000
C	0.112023000	-1.909911000	-1.952277000
H	-1.511812000	-2.750528000	-3.100555000
H	-1.688221000	-4.794060000	-1.720561000
H	-0.184277000	-5.134710000	0.226121000
H	1.697401000	-1.353276000	-0.607194000
C	-4.129614000	2.173143000	-0.185494000
C	-4.901476000	1.492213000	0.741792000
C	-4.777638000	0.108512000	0.907881000
C	-3.868031000	-0.619984000	0.121801000
C	-3.084291000	0.094101000	-0.804549000
C	-3.200206000	1.479702000	-0.982374000
H	-4.231639000	3.245572000	-0.314028000
H	-5.625161000	2.037685000	1.341282000
H	-5.436540000	-0.425373000	1.590110000
H	-2.368813000	-0.475985000	-1.401093000
C	3.334670000	1.016751000	0.335030000
C	3.137258000	1.285439000	-1.011636000
C	3.736333000	0.499444000	-2.003115000
C	4.569117000	-0.538002000	-1.610077000
C	4.759066000	-0.827214000	-0.256937000
C	4.095650000	-0.093289000	0.745197000
H	2.896802000	1.648540000	1.100822000
H	3.558593000	0.702132000	-3.053700000
H	5.079652000	-1.129641000	-2.363126000
H	5.482197000	-1.595433000	0.023762000
C	-0.775284000	3.783585000	1.294232000
C	0.238699000	2.971394000	0.787731000
C	0.208656000	1.590541000	1.004609000
C	-0.786837000	1.006826000	1.799820000
C	-1.780011000	1.836666000	2.330552000

C	-1.782052000	3.200685000	2.058230000
H	-0.775340000	4.848675000	1.090370000
H	0.996919000	0.949169000	0.619691000
H	-2.552776000	1.418561000	2.969521000
H	-2.579257000	3.822055000	2.454034000
S	1.839316000	-3.525488000	1.410191000
S	4.106366000	-0.592441000	2.448247000
S	2.033240000	2.569609000	-1.618451000
S	0.259880000	-0.429972000	-2.915608000
S	-2.228507000	2.375609000	-2.177756000
S	-3.660247000	-2.374875000	0.359378000
S	1.620054000	3.789561000	-0.004922000
S	-0.692886000	-0.724822000	2.190532000
Li	-1.274855000	-2.221446000	0.141339000
Li	-2.998852000	-1.156111000	2.180023000
Li	1.696772000	-1.326485000	2.422864000
Li	3.877592000	-2.509186000	1.159228000
Li	-0.214202000	1.383348000	-1.398001000
Li	-1.822998000	0.489817000	-3.471229000

#### IV-Li<sub>7</sub>

C	-2.431837000	2.659733000	2.204421000
C	-2.838525000	3.682309000	1.348448000
C	-1.957960000	4.232438000	0.416401000
C	-0.625716000	3.776523000	0.338303000
C	-0.234147000	2.738562000	1.206871000
C	-1.114417000	2.168639000	2.147151000
H	-3.133314000	2.231472000	2.912451000
H	-3.866919000	4.027268000	1.382823000
H	-2.282995000	5.019136000	-0.255441000
H	0.778068000	2.341935000	1.147761000
C	-3.383731000	-3.359501000	0.718842000
C	-4.502004000	-3.048437000	-0.046904000
C	-4.746007000	-1.745194000	-0.473925000
C	-3.856607000	-0.713822000	-0.152764000
C	-2.715587000	-1.042597000	0.604189000
C	-2.467624000	-2.353109000	1.046929000
H	-3.209680000	-4.371919000	1.067323000
H	-5.205703000	-3.834307000	-0.305862000
H	-5.632943000	-1.512464000	-1.053986000

H	-1.961741000	-0.275377000	0.793419000
C	3.254420000	0.279153000	0.279059000
C	3.694691000	-0.875560000	0.937978000
C	5.062766000	-1.164294000	0.979936000
C	5.962164000	-0.311702000	0.350804000
C	5.516974000	0.812563000	-0.336524000
C	4.151132000	1.120122000	-0.386753000
H	2.189488000	0.508013000	0.250134000
H	5.401883000	-2.059001000	1.490161000
H	7.023824000	-0.536919000	0.378543000
H	6.219512000	1.456427000	-0.854884000
C	-0.187883000	-3.620586000	-1.749613000
C	0.919733000	-2.796484000	-1.478310000
C	0.780689000	-1.402255000	-1.613588000
C	-0.434320000	-0.828902000	-1.994415000
C	-1.509193000	-1.679108000	-2.299642000
C	-1.387510000	-3.055989000	-2.175566000
H	-0.087361000	-4.698529000	-1.652777000
H	1.644768000	-0.774356000	-1.418381000
H	-2.475269000	-1.283528000	-2.607618000
H	-2.239753000	-3.691031000	-2.395894000
S	0.457141000	4.473764000	-0.872983000
S	3.607305000	2.516050000	-1.346745000
S	2.563502000	-2.010041000	1.681673000
S	-0.575136000	0.882266000	3.238579000
S	-1.069943000	-2.730953000	2.104453000
S	-4.190662000	0.951493000	-0.691665000
S	2.423957000	-3.504167000	-0.866962000
S	-0.616907000	0.946152000	-2.077429000
Li	-2.044273000	1.895221000	-0.102319000
Li	-2.892844000	0.916689000	-2.589941000
Li	1.291493000	2.373857000	-1.857282000
Li	2.588734000	4.060482000	-0.000626000
Li	0.531370000	-0.823458000	1.999742000
Li	-2.157266000	-0.824908000	2.980045000
Li	0.689130000	-3.453193000	0.699806000
<b>IV-Li<sub>8</sub></b>			
C	-3.715312000	2.232878000	0.979901000
C	-3.888703000	2.844711000	-0.264260000

C	-2.811662000	3.422949000	-0.937515000
C	-1.527547000	3.424116000	-0.354390000
C	-1.368852000	2.806060000	0.895146000
C	-2.446543000	2.214166000	1.584012000
H	-4.559437000	1.778935000	1.487235000
H	-4.872336000	2.845249000	-0.724005000
H	-2.952920000	3.894813000	-1.903780000
H	-0.391533000	2.823357000	1.373229000
C	-1.165907000	-3.684848000	0.824126000
C	-1.754030000	-4.035996000	-0.383214000
C	-2.677184000	-3.194834000	-1.006628000
C	-3.001539000	-1.947550000	-0.446816000
C	-2.355151000	-1.586765000	0.751034000
C	-1.470069000	-2.448887000	1.410444000
H	-0.466441000	-4.352385000	1.315916000
H	-1.508953000	-4.990430000	-0.839039000
H	-3.185658000	-3.520535000	-1.912278000
H	-2.553209000	-0.586761000	1.145009000
C	2.782067000	1.271817000	0.520960000
C	3.227226000	0.585776000	1.668942000
C	4.558745000	0.118262000	1.679800000
C	5.387172000	0.322723000	0.576172000
C	4.932238000	1.009745000	-0.553282000
C	3.623099000	1.532688000	-0.583645000
H	1.740028000	1.592801000	0.484708000
H	4.916229000	-0.426212000	2.546334000
H	6.399703000	-0.068999000	0.589991000
H	5.585149000	1.177899000	-1.402053000
C	1.396012000	-3.453780000	-2.094733000
C	1.459982000	-2.541250000	-1.025023000
C	0.760567000	-1.331197000	-1.137429000
C	0.073978000	-0.990061000	-2.312528000
C	0.046686000	-1.905611000	-3.374076000
C	0.693646000	-3.138303000	-3.246907000
H	1.919340000	-4.399707000	-2.006421000
H	0.749764000	-0.631236000	-0.302071000
H	-0.426495000	-1.626123000	-4.313483000
H	0.668152000	-3.843157000	-4.072541000
S	-0.201366000	4.213409000	-1.219042000
S	3.113946000	2.520216000	-1.958474000
S	2.183091000	0.241345000	3.040960000

S	-2.210377000	1.539527000	3.208693000
S	-0.782472000	-2.022512000	3.005923000
S	-4.123004000	-0.833383000	-1.260233000
S	2.479529000	-2.920812000	0.382468000
S	-0.796573000	0.563389000	-2.475148000
Li	-2.588661000	0.988873000	-0.829712000
Li	-2.299965000	-1.250409000	-2.613775000
Li	0.739404000	2.294474000	-2.315522000
Li	1.981324000	3.953771000	-0.479905000
Li	-0.165846000	0.400183000	2.830481000
Li	-2.747905000	-0.742688000	3.231626000
Li	1.501362000	-1.947256000	2.305892000
Li	3.507193000	-0.912686000	-0.158968000

**IV-Li<sub>9</sub>**

C	-2.436187000	2.840528000	2.415714000
C	-2.598330000	3.890353000	1.513444000
C	-1.583913000	4.230448000	0.618047000
C	-0.365000000	3.520714000	0.619315000
C	-0.217420000	2.457180000	1.532157000
C	-1.234129000	2.110702000	2.445340000
H	-3.237275000	2.575969000	3.097046000
H	-3.540016000	4.429393000	1.486647000
H	-1.715599000	5.044494000	-0.086185000
H	0.718165000	1.902182000	1.544585000
C	-3.689147000	-3.121589000	0.561423000
C	-4.773711000	-2.719619000	-0.206858000
C	-4.986572000	-1.373206000	-0.514565000
C	-4.105983000	-0.386306000	-0.045774000
C	-2.988475000	-0.815998000	0.702392000
C	-2.763460000	-2.166124000	1.014746000
H	-3.530881000	-4.167222000	0.803077000
H	-5.476317000	-3.463674000	-0.570494000
H	-5.856811000	-1.072046000	-1.089987000
H	-2.231345000	-0.087672000	0.999623000
C	2.835399000	0.220564000	0.115928000
C	3.264895000	-0.757093000	0.993032000
C	4.665735000	-1.002021000	1.188825000
C	5.586218000	-0.180446000	0.482681000
C	5.171695000	0.808365000	-0.379806000

C	3.756327000	1.087565000	-0.587074000
H	1.765476000	0.326149000	-0.070873000
H	4.993092000	-1.648053000	1.996442000
H	6.651516000	-0.326639000	0.644267000
H	5.902655000	1.421974000	-0.900473000
C	0.828643000	-3.643994000	-1.870403000
C	1.673582000	-2.534662000	-2.080738000
C	1.079981000	-1.265280000	-2.140491000
C	-0.295224000	-1.060434000	-1.960932000
C	-1.119698000	-2.184119000	-1.777033000
C	-0.550999000	-3.461882000	-1.746259000
H	1.258410000	-4.639247000	-1.822801000
H	1.707035000	-0.401815000	-2.337236000
H	-2.191729000	-2.075997000	-1.635303000
H	-1.194671000	-4.322791000	-1.590432000
S	0.877165000	3.977767000	-0.550078000
S	3.314869000	1.751276000	-2.249212000
S	2.141241000	-1.952045000	1.716412000
S	-1.005721000	0.828820000	3.652299000
S	-1.338393000	-2.672846000	1.956250000
S	-4.363660000	1.329043000	-0.440294000
S	3.428446000	-2.737232000	-2.253836000
S	-0.930610000	0.605306000	-1.987947000
Li	-2.111017000	1.995098000	0.077431000
Li	-3.233831000	0.369869000	-2.183571000
Li	0.958585000	2.130962000	-2.040033000
Li	3.030990000	3.076076000	-0.326022000
Li	0.310594000	-0.828616000	2.606716000
Li	-2.485867000	-0.884429000	3.051382000
Li	4.188593000	-0.451313000	-2.114073000
Li	0.346464000	-2.412687000	0.173127000
Li	3.731742000	-2.710147000	0.064056000

#### IV-Li<sub>10</sub>

C	-1.844121000	3.395343000	2.588709000
C	-2.089926000	4.450887000	1.703378000
C	-1.347487000	4.609732000	0.526948000
C	-0.312764000	3.700291000	0.211719000
C	-0.113004000	2.620672000	1.098710000
C	-0.826554000	2.462767000	2.300250000

H	-2.424722000	3.290279000	3.498333000
H	-2.885005000	5.155536000	1.927882000
H	-1.542047000	5.441962000	-0.140617000
H	0.668315000	1.914212000	0.844901000
C	-2.994904000	-2.995898000	1.067541000
C	-4.274164000	-2.714612000	0.602705000
C	-4.647453000	-1.415552000	0.256831000
C	-3.731470000	-0.359334000	0.368071000
C	-2.421046000	-0.663848000	0.793801000
C	-2.040483000	-1.968453000	1.153396000
H	-2.714695000	-4.003773000	1.355807000
H	-5.001807000	-3.516445000	0.520366000
H	-5.658498000	-1.203267000	-0.075893000
H	-1.662934000	0.119848000	0.797478000
C	2.762413000	-0.712339000	0.118181000
C	3.099497000	-1.703820000	1.063336000
C	3.370599000	-1.275229000	2.373698000
C	3.316710000	0.088154000	2.683376000
C	2.923591000	1.025604000	1.718112000
C	2.620461000	0.669589000	0.381507000
H	2.618079000	-1.085968000	-0.908985000
H	3.628964000	-2.007660000	3.131754000
H	3.536972000	0.411652000	3.697405000
H	2.815389000	2.060939000	2.043267000
C	0.880963000	-3.735282000	-2.502130000
C	1.566653000	-2.641707000	-3.062667000
C	0.900460000	-1.411072000	-3.117029000
C	-0.337165000	-1.194363000	-2.498863000
C	-1.011455000	-2.297833000	-1.950503000
C	-0.411564000	-3.559469000	-1.991750000
H	1.346828000	-4.716575000	-2.490374000
H	1.372778000	-0.561589000	-3.601082000
H	-1.985399000	-2.181591000	-1.483560000
H	-0.951140000	-4.416379000	-1.594119000
S	0.729905000	3.927180000	-1.187162000
S	2.817673000	1.563475000	-3.118912000
S	3.114648000	-3.438416000	0.649215000
S	-0.398952000	1.173303000	3.441736000
S	-0.406592000	-2.325826000	1.777144000
S	-4.228777000	1.294270000	-0.077301000
S	3.247108000	-2.766531000	-3.638671000

S	-0.910616000	0.485091000	-2.329946000
Li	-2.348824000	2.544125000	0.494114000
Li	-3.156238000	0.380460000	-1.877754000
Li	0.667828000	2.357227000	-3.066924000
Li	2.770633000	2.491879000	-0.987725000
Li	1.067667000	-0.291378000	2.076524000
Li	-1.659424000	-0.708546000	3.043480000
Li	3.701767000	-0.374582000	-3.737278000
Li	0.916114000	-2.983810000	-0.098106000
Li	3.960996000	-3.290186000	-1.494284000
Li	1.525254000	0.536876000	-1.448759000

#### IV-Li<sub>11</sub>

C	-2.029627000	3.507629000	2.631091000
C	-2.256151000	4.481129000	1.616659000
C	-1.400154000	4.530879000	0.480165000
C	-0.359417000	3.626135000	0.333730000
C	-0.197210000	2.560874000	1.308206000
C	-1.013572000	2.572241000	2.505933000
H	-2.658258000	3.492555000	3.515778000
H	-3.050105000	5.208216000	1.730200000
H	-1.546064000	5.296364000	-0.275057000
H	0.820588000	2.199076000	1.437256000
C	-2.871109000	-3.033858000	0.983797000
C	-4.037018000	-2.819634000	0.258353000
C	-4.470897000	-1.527721000	-0.046686000
C	-3.735323000	-0.411992000	0.380644000
C	-2.532172000	-0.644219000	1.079620000
C	-2.090054000	-1.939535000	1.390087000
H	-2.555303000	-4.039136000	1.245251000
H	-4.630567000	-3.670425000	-0.062800000
H	-5.404150000	-1.373060000	-0.579985000
H	-1.901645000	0.212022000	1.326472000
C	2.262171000	-1.122053000	0.135015000
C	2.989333000	-1.964047000	1.000697000
C	3.625303000	-1.363405000	2.100540000
C	3.554498000	0.015753000	2.264915000
C	2.857164000	0.818823000	1.347184000
C	2.154649000	0.289989000	0.235572000
H	1.723546000	-1.630361000	-0.677028000



H	4.170752000	-1.982477000	2.804934000
H	4.050319000	0.479130000	3.113775000
H	2.857863000	1.893977000	1.542985000
C	0.938657000	-3.496767000	-2.393824000
C	1.568681000	-2.446727000	-3.083889000
C	0.864925000	-1.241998000	-3.228467000
C	-0.327178000	-0.985536000	-2.540594000
C	-0.914804000	-2.028078000	-1.806843000
C	-0.300589000	-3.281647000	-1.783912000
H	1.417064000	-4.470196000	-2.328381000
H	1.287217000	-0.444550000	-3.833772000
H	-1.846204000	-1.873186000	-1.269828000
H	-0.802520000	-4.105820000	-1.276834000
S	0.806567000	3.719155000	-1.018414000
S	3.073204000	1.617630000	-3.155420000
S	3.033521000	-3.731621000	0.752334000
S	-0.586853000	1.398033000	3.777178000
S	-0.586424000	-2.204799000	2.323917000
S	-4.293496000	1.236135000	0.008423000
S	3.265975000	-2.561748000	-3.617383000
S	-0.972194000	0.670872000	-2.545729000
Li	-2.460908000	2.547073000	0.687125000
Li	-3.168689000	0.524160000	-1.833800000
Li	0.850621000	2.343088000	-3.055766000
Li	2.750500000	2.321005000	-0.955683000
Li	0.692195000	0.017690000	2.265757000
Li	-1.881571000	-0.468404000	3.408264000
Li	3.858941000	-0.230518000	-4.147552000
Li	0.767886000	-3.107037000	0.617756000
Li	3.703170000	-3.330515000	-1.438329000
Li	2.346961000	-0.063338000	-1.853341000
Li	0.290091000	1.353851000	-0.481433000

#### IV-Li<sub>12</sub>

C	-1.959236000	3.555404000	2.453522000
C	-2.277501000	4.256185000	1.277806000
C	-1.392429000	4.325916000	0.207447000
C	-0.116794000	3.739920000	0.322646000
C	0.179317000	3.032799000	1.496276000
C	-0.731619000	2.875562000	2.555613000

H	-2.653228000	3.536174000	3.291787000
H	-3.241910000	4.751526000	1.203904000
H	-1.656133000	4.862988000	-0.696908000
H	1.173800000	2.622230000	1.620625000
C	-2.359605000	-2.931215000	1.249501000
C	-3.536602000	-2.938088000	0.409842000
C	-4.063923000	-1.731043000	-0.004572000
C	-3.483674000	-0.482162000	0.326968000
C	-2.417309000	-0.437795000	1.406781000
C	-1.801333000	-1.766664000	1.702196000
H	-2.002221000	-3.878946000	1.657080000
H	-3.962197000	-3.876775000	0.076895000
H	-4.957275000	-1.721446000	-0.627893000
H	-1.603061000	0.303247000	1.177950000
C	1.861349000	-1.067024000	0.229205000
C	2.588139000	-2.033365000	0.962753000
C	3.482334000	-1.568701000	1.940695000
C	3.636868000	-0.200980000	2.145647000
C	2.904676000	0.722616000	1.383235000
C	1.974562000	0.340104000	0.383537000
H	1.130293000	-1.454999000	-0.492148000
H	4.036903000	-2.285914000	2.536809000
H	4.328490000	0.152282000	2.906291000
H	3.070496000	1.779791000	1.614838000
C	0.693743000	-3.333905000	-2.640038000
C	1.429620000	-2.255755000	-3.155205000
C	0.813949000	-0.996626000	-3.195391000
C	-0.399200000	-0.743772000	-2.550363000
C	-1.091196000	-1.821691000	-1.975252000
C	-0.560461000	-3.106033000	-2.070541000
H	1.093607000	-4.345731000	-2.686041000
H	1.330490000	-0.170439000	-3.673462000
H	-2.028286000	-1.674948000	-1.446232000
H	-1.130374000	-3.939519000	-1.665529000
S	1.107507000	3.859130000	-0.954203000
S	3.259532000	1.588609000	-2.941145000
S	2.314387000	-3.776645000	0.735494000
S	-0.301682000	1.843364000	3.927239000
S	-0.505782000	-1.843591000	2.946630000
S	-4.526215000	1.014869000	0.244941000
S	3.170505000	-2.419441000	-3.528574000

S	-0.938699000	0.950971000	-2.410103000
Li	-2.875536000	1.741241000	1.644308000
Li	-3.035430000	0.689160000	-1.435412000
Li	1.058336000	2.406712000	-2.945608000
Li	2.868300000	2.231650000	-0.778697000
Li	0.888780000	0.121702000	2.649358000
Li	-1.801125000	0.026302000	3.599615000
Li	3.950240000	-0.179238000	-4.115456000
Li	0.073312000	-2.979988000	0.973525000
Li	2.937794000	-3.541313000	-1.473585000
Li	2.580721000	-0.271210000	-1.790974000
Li	0.335352000	1.518553000	-0.410249000
Li	-4.471832000	-0.477915000	2.075574000

END-----

## Notes and references

- 1 G. Kresse and J. Hafner, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1993, **47**, 558-561.
- 2 G. Kresse and D. Joubert, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1999, **59**, 1758-1775.
- 3 P. E. Blöchl, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1994, **50**, 17953-17979.
- 4 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
- 5 S. Nosé, *J. Chem. Phys.*, 1984, **81**, 511-519.