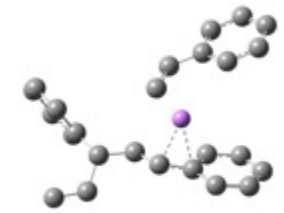
Supporting Information

Mechanism of formation anionic isotactic polystyrene initiated by Li carbanions in cyclohexane in the presence of Na-tosylate II. DFT calculations.

Tianwen Bai[a,]*, Jun Ling[b,c], Thieo E. Hogen-Esch[b,]*

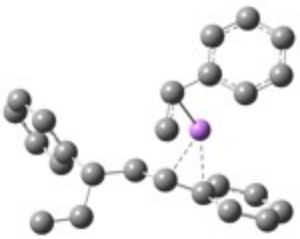
a. College of Biological, Chemical Sciences and Engineering, Jiaxing University, Zhejiang, 314001, China.
b. Department of Chemistry and Loker Hydrocarbon Research Institute, University of Southern California, Los Angeles, CA 90089-1661, USA.
c. MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Department of Polymer Science and Engineering, Zhejiang University, Hangzhou 310027, China.

3-Dimensional geometries of important intermediates

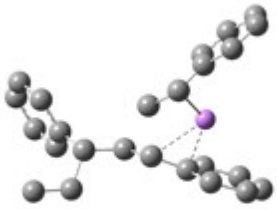


2-r-pro-m

2-r-pro-r



TS-3-r-pro-m



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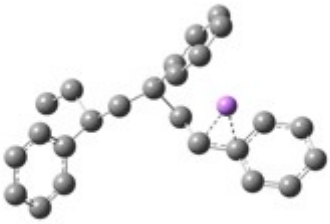

4-r-pro-m

4-r-pro-r

Figure S1. 3-Dimensional geometries of intermediates.

Tables of detailed parameters

Table S1. Calculated geometries of the LDPP *pro-m* and *pro-r* dimer anions **1**.

Isomers	Torsions		Li-carbon distances (nm) [c]						
	1-phenyl	3-phenyl	1-phenyl				3-phenyl		
	(a)	(b)	C_1	C_Q	C_Z	C_E	C_Q'	C_Z'	C_E'
1-*pro-m*	-28.0°	31.3°	0.22	0.21	0.23	0.30	0.25	0.23	0.30
1-*pro-r*	27.0°	17.2°	0.22	0.22	0.23	0.30	0.24	0.27	0.24

(a) CH_2-C_1-C_Q-C_Z dihedral angels. (b) H-C_3-C_Q-C_E dihedral angels. (c) C_Q (C_Q'), C_Z (C_Z') and C_E (C_E') are quaternary and aryl carbons (*Z*) and (*E*) with respect to the chain.

Table S2. Selected parameters and Li -aryl carbon distances in trimer anion **4**.

Isomers	(a)	(b)	(c)	C_Q	C_Z	C_E	C_Q'	C_Z'	C_E'
4-*m-pro-si*	-28.1°	33.9°	0.15^7	0.21	0.22	0.30	0.25	0.23	0.30
4-*m-pro-re*	26.6°	16.8°	0.15^6	0.21	0.23	0.30	0.24	0.28	0.23
4-*r-pro-si*	-26.7°	-15.8°	0.15^6	0.21	0.23	0.30	0.24	0.27	0.24
4-*r-pro-re*	28.9°	-33.3°	0.15^7	0.21	0.22	0.30	0.25	0.23	0.30

(a) CH_2 -C_1-C_Q-C_Z dihedral angles of the 1-phenyl group. (b) H-C_3-C_Q-C_E dihedral angles of 3-phenyl group.(c) Formed C_1-CH_2 bond lengths (nm). C_Q, C_Z and C_E are the quaternary, "cis- "and "trans" like carbons respectively of the 1- and 3- phenyl groups of interest. Distances from Li ion to C_Q, and C_Q' and to the other 4 carbons of the 1- and 3-phenyl groups.

Table S3. Calculated Li carbon distances of styrene-LDPP complexes **2**. [a]

Isomers [b]	(c)	Li- distances				Li- styrene distances			
		(d)	C_Q	C_Z	C_E	CH_2	C_Q'	C_Z'	C_E'
2-*pro-m-pro-si*	-20.8°	0.35	0.21	0.23	0.30	0.23	0.29	0.34	0.39
2-*pro-m-pro-re*	-14.1°	0.38	0.21	0.31	0.23	0.24	0.24	0.27	0.33
2-*pro-r-pro-si*	13.1°	0.38	0.21	0.31	0.23	0.24	0.24	0.27	0.33
2-*pro-r-pro-re*	17.1°	0.35	0.21	0.23	0.31	0.23	0.29	0.34	0.38

(a) All distances in nm. (b) Monomer presentation *si* or *re* (see Schemes 1-3). (c) 1-Phenyl rotation given as CH_2-C_1-C_Q-C_Z dihedral angle. (d) Distances between C-1 and vinyl methylene (nm).

Table S4. Li-Carbon distances (nm) and 1-phenyl torsion angles for transition states **3**.

Isomers	1-phenyl torsions [c]	Li-Carbanion				Li-styrene [a]		
		(b)	C_Q	C_Z	C_E	C_Q'	C_Z'	C_E'
3-*pro-m-pro-si*	-19.0°	0.21^9	0.22	0.23	0.32	0.23	0.25	0.34
3-*pro-m-pro-re*	-20.0°	0.22^3	0.21	0.27	0.23	0.22	0.24	0.33
3-*pro-r-pro-si*	18.8°	0.22^2	0.21	0.26	0.23	0.22	0.24	0.32
3-*pro-r-pro-re*	19.9°	0.21^6	0.22	0.23	0.32	0.23	0.25	0.33

(a) Li-vinyl distances are 0.21 and 0.22-0.23 nm for CH and CH_2 respectively. (b) Carbanion-vinyl methylene distances. (c) 1-phenyl torsions expressed as CH_2-C_1-C_Q-C_Z dihedral angle.

Table S5. Conformations of LDPP

Isomers	Conformers [a]	Dihedral angles of LDPP [b]			Phenyl torsions	
		C_1-C_2	C_2-C_3	C_3-C_4	1-phenyl	3-phenyl
1-*pro-m*	g, t [c]	130.1°	69.6°	174.4°	-28.0°	31.3°
1-*pro-r*	t, t	-127.7°	-176.1°	173.2°	27.0°	17.2°

(a) Trans-gauche nomenclature of C_Q-C_1-C_2-C_3 , C_1-C_2-C_3-C_4 and C_2-C_3-C_4-C_5 dihedral angles. (b) Chain carbons C_2-C_3 are flanked by C_1 and C_4. (c) C_3-C_4 conformation is "trans-like".

Table S6. Relative conformations of LDPP monomer complexes **2**.[a]

Isomers	1-phenyl torsion	LDPP-styrene dihedral intermolecular angles			Dihedral angles of LDPP [a]			
		C_1'-C_2'	C_2'-C_1	C_1-C_2 [b]	C_1-C_2[c]	C_2-C_3	C_3-C_4	(d)
2-*pro-m-pro-si*	-21°	94.0	81.6	78.6	-172.6	-173.5	172.6	19
2-*pro-m-pro-re*	-14°	-69.4	118.2	37.6	-172.4	-175.4	172.3	67
2-*pro-r-pro- si*	13°	68.7	-117.7	-41.5	-174.8	-71.1	172.6	66
2-*pro-r-pro- re*	17°	-98.3	-65.2	-84.9	168.0	-73.7	170.1	-6

(a) Styrene vinyl carbons indicated with primes. (b) C_2'-C_1-C_2-C_3 dihedral angle. (c) Phenyl carbon (C_Q) adjoins carbanion C_1. (d) Dihedral of CH'-CH_2'-C_1-C_2.

Table S7. Conformations of transition states **3**. [a][b][c]

Isomers	1-Phenyl torsions	LDPP-styrene dihedral intermolecular angles [d]			Dihedral angles of LDPP			
		C_1'-C_2'	C_2'-C_1	C_1-C_2	C_1-C_2	C_2-C_3	C_3-C_4	(e)
3-*pro-m-pro-si*	-19°	91.3°	50.0°	71.8°	-161.1°	-176.1°	172.7°	-5.8°
3-*pro-m-pro-re*	-20°	-89.0°	148.6°	66.6°	-161.6°	-177.8°	172.8°	-51.5°
3-*pro-r-pro-si*	19°	88.8°	-145.5°	-72.1°	156.7°	-71.7°	171.5°	54.1°
3-*pro-r- pro-re*	20°	-90.9°	-52.3°	-77.7°	154.6°	-72.0°	171.4°	3.8°

(a) Styrene vinyl carbons indicated with primes. (b) C_2'-C_1-C_2-C_3 dihedral angle. (c) Phenyl carbon (C_Q) adjoins C_1. (d) Dihedral angles between long axes of monomer and anion benzyl groups. (e) Dihedral of CH'-CH_2'-C_1-C_2.

Table 8. Conformations of LTPH **4**

Isomers	Conformer[b]	LTPH-Dihedral angles [a] [b] [c]						
		(d)	(e)	C_1-C_2	C_2-C_3	C_3-C_4	C_4-C_5	C_5-C_6
4-*m-pro-m*	*(g) g, g, t, t*	-28.1°	33.9°	129.4°	66.7°	69.8°	-176.2°	173.0°
4-*m-pro-r*	*(g) t, g, t, t*	26.6°	16.8°	-127.8°	-176.6°	72.9°	-174.3°	173.8°
4-*r-pro-r*	*(g) t, g$^-$, g$^-$, t*	-26.7°	15.7°	127.8°	177.5°	-69.8°	-67.8°	174.7°
4-*r-pro-m*	*(g) g$^-$, g$^-$, g$^-$,t*	28.9°	33.3°	-128.8°	-66.8°	-72.3°	-69.6°	174.0°

(a) Conventional numbering of the trimer anion.; Dihedrals (C_1-C_2), (C_2-C_3) and C_3-C_4) correspond to (C_1'-C_2'), (C_1'-C_2') and (C_1-C_2) of Table 7. (b) Dihedrals (C_4-C_5) and (C_5-C_6) correspond to (C_2-C_3) and (C_3-C_4) in Table 7. (c) Dihedral (C_1-C_2) of Table 7 is not included in conformers. (d) Torsion angles of the 1-phenyl group. (e) Torsion dihedral angles of 3-phenyl group.

Table S9. Selected Li aryl carbon LDPP (**5**) in the presence of SMBS.

LDPP	(a)	(b)	C_1	C_Q	C_Z	C_E	C_Q'	C_Z'	C_E'	SO_3	Na [(c)]
5-*pro-m*	-19.1°	25.4°	0.22	0.28	0.37	0.35	0.29	0.25	0.36	0.21/0.22	0.34
5-*pro-r*	20.3°	-0.2°	0.22	0.29	0.37	0.36	0.26	0.28	0.30	0.20/0.21	0.35

(a) Dihedral of 1-phenyl CH_2-C_1-C_Q-C_Z. (b) Dihedral angles of 3-phenyl: H-C_3-C_Q'-C_E'. (c) Na ion is coordinated to two sulfonate oxygens (0.24 nm) and the 1-phenyl group (0.27-0.28 nm).

Table S10. Conformations of LDPP-SMBS.

Isomers	Conformers[(a)]	Dihedral angles of LDPP			Phenyl torsions	
		C_1-C_2 [(b)]	C_2-C_3 [(c)]	C_3-C_4	1-phenyl	3-phenyl
5-*pro-m*	*(t) g t*	179.1°	64.5°	168.9°	-19.1°	25.4°
5-*pro-r*	*(t) t t*	178.2°	-174.2°	173.2°	20.3°	-0.2°

(a) Trans-gauche nomenclature of the C_1-C_2-C_3-C_4 and C_2-C_3-C_4-C_5-dihedral angles. (b) Phenyl carbon adjoins carbanion C_1. Distances of Na ion to 1-phenyl carbons are about 0.27 nm. (c) C_2-C_3 is flanked by C_1 and C_4.

Table S11. Selected distances parameters of SMBS/styrene-complexes **6**.

Isomers	Li-Carbanion Distances					Li-styrene distances					SO_3-distances	
	(a)	C_1	C_Q	C_Z	C_E	CH_2[(b)]	C_Q'	C_Z'	C_E'	CH_2[(c)]	Li	Na[(d)]
6-*pro-m* +S_{si}	-28.6°	0.21	0.24	0.27	0.34	0.25	0.34	0.36	0.46	0.32	0.18	0.19/0.21
6-*pro-m* +S_{re}	-28.6°	0.21	0.23	0.26	0.33	0.25	0.38	0.44	0.48	0.31	0.18	0.23/0.23
6-*pro-r* +S_{si}	23.5°	0.21	0.23	0.29	0.30	0.29	0.39	0.41	0.49	0.32	0.21	0.23/0.23
6-*pro-r* +S_{re}	26.9°	0.21	0.24	0.27	0.34	0.25	0.35	0.37	0.46	0.33	0.18	0.23/0.24

(a) Torsion of 1-phenyl group. (b) Li-CH_2 vinyl distances. (c) C_1(carbanion)-CH_2 distances. (d) Na distances to styrene phenyl carbons are 0.28-0.31 nm.

Table S12. Selected distances to Li in transition states **7**.[(a)]

Isomers	Li-Carbanion Distances					Li-monomer distances					SO_3-distances	
	(a)	C_1	C_Q	C_Z	C_E	CH_2	C_Q'	C_Z'	C_E'	CH_2[(b)]	Li	Na [(c)]
7-*pro-m* +S_{si}	-29.0°	0.22	0.25	0.27	0.36	0.23	0.29	0.33	0.40	0.32	0.19	0.23/0.24
7-*pro-m* +S_{re}	-26.0°	0.22	0.24	0.26	0.34	0.24	0.32	0.38	0.41	0.31	0.19	0.23/0.23
7-*pro-r* +S_{si}	21.5°	0.23	0.24	0.27	0.33	0.23	0.31	0.37	0.40	0.32	0.21[(d)]	0.23/0.23
7-*pro-r* +S_{re}	30.0°	0.22	0.25	0.27	0.36	0.23	0.29	0.33	0.40	0.33	0.19	0.24/0.24

(a) 1-Phenyl rotation degrees of benzyl anion (CH_2-C_1-C_Q-C_Z dihedral angle). (b) Carbanion to vinyl methylene distances (nm). (c) Na distances to styrene phenyl carbons are 0.27-29 nm. (d) Bis-coordinate Li- distances to SO_3 are 0.21 and 0.22 nm.

Table S13. Selected distances to Li ion for stereoisomers of LTPH, **9** in the presence of SMBS.

Isomers	1-phenyl		Li-carbanion distances				Li-3-Ph distances			SO_3 distances [c]	
	(a)	(b)	C_1	C_Q	C_Z	C_E	C_Q'	C_Z'	C_E'	Li	Na
8-*m-pro-m*	-20°	30°	0.22	0.28	0.37	0.35	0.28	0.25	0.35	0.21	0.24
8-*m-pro-r*	27°	45°	0.22	0.28	0.37	0.34	0.29	0.25	0.37	0.21	0.24
8-*r-pro-r*	-27°	-43°	0.22	0.29	0.37	0.33	0.29	0.25	0.38	0.21	0.24
8-*r-pro-m*	-19°	-27°	0.22	0.28	0.37	0.35	0.29	0.25	0.36	0.21	0.24

(a) CH_2-C_1-C_Q-C_Z dihedral angle. (b) H-C_3-C_Q'-C_E' dihedral angle. (c) Li and Na ion are bis-coordinated averages ±0.004 nm.

Table S14. Conformations of LDPP monomer complexes in the presence of SMBS.

Isomers	LDPP-styrene dihedral intermolecular angles.[a][b][c]			Dihedral angles of LDPP			Phenyl Torsions	
	C_1'-C_2'	C_2'-C_1	C_1-C_2	C_1-C_2[d]	C_2-C_3	C_3-C_4	1-Ph	(e)
6-*pro-m-pro-si*	81.9°	62.9°	52.4°	173.6°	-176.3°	172.7°	-28.6°	18.7°
6-*pro-m-pro-re*	-106.4°	57.7°	45.2°	172.0°	-179.1°	171.1°	-29.1°	6.7°
6- *pro-r-pro-si*	73.4°	-90.1°	-118.4°	88.5°	-62.6°	171.6°	23.5°	-9.1°
6- *pro-r-pro-re*	-80.9°	-58.5°	-67.0°	176.3°	-69.8°	172.2°	26.9°	17.1°

(a) Conformers using conventional carbon numbering with central bonds of dihedrals shown. (b) Styrene carbons indicated with primes. (c) Dihedral angle C_2'-C_1 is C_1'-C_2'-C_1-C_2. (d) Phenyl carbon adjoins carbanion C_1. (e) Monomer-phenyl dihedral angles: C_Z-C_Q-CH-CH_2.

Table S15. Conformations of transition states **(7**) SMBS.

Isomers	LDPP-styrene dihedral angles [a][b][c]			Dihedral angles of LDPP			Phenyl Torsions	
	C_1'-C_2'	C_2'-C_1	C_1-C_2	C_1-C_2 [d]	C_2-C_3	C_3-C_4	1-Ph	(e)
7-*pro-m-pro-si*	91.0°	65.6°	49.1°	-177.9°	-177.1°	172.2°	-28.8°	18.7°
7-*pro-m-pro-re*	-104.0°	65.2°	53.2°	-173.5°	-175.7°	173.5°	-26.3°	9.1°
7- *pro-r-pro-si*	91.2°	-73.3°	-76.3°	145.3°	-74.7°	169.3°	21.5°	-10.1°
7- *pro-r-pro-re*	-90.6°	66.5°	-43.9°	-177.5°	-62.4°	175.6°	30.2°	18.4°

(a) Conformers using conventional carbon numbering with central bonds of dihedrals shown. (b) Styrene carbons indicated with primes. (c) Dihedral angle C_2'-C_1 is C_1'-C_2'-C_1-C_2. (d) Phenyl carbon adjoins carbanion C_1. (e) Monomer-phenyl dihedral angles: C_Z-C_Q-CH-CH_2.

Table S16. Conformations of LTPH-SMBS **8**.

Isomers	Conformers	LTPH-Dihedral angles						
		1-Ph[a]	3-Ph[b]	C_1-C_2[c]	C_2-C_3[d]	C_3-C_4	C_4-C_5	C_5-C_6
8-*m-pro-m*	*t, g, g, t, t*	-19.9°	30.1°	178.4°	61.2°	62.4°	-175.9°	173.2°
8-*m-pro-r*	*g-, g, g, t, t*	26.8°	44.8°	-115.4°	75.2°	73.3°	-173.4°	174.1°
8-*r-pro-r*	*g, g-, g-, g-, t*	-26.7°	-43.4°	115.1°	75.7°	-77.1°	-76.3°	170.8°
8-*r-pro-m*	*t, g-, g-, g-, t*	19.1°	-26.7°	-179.8°	-60.5°	-69.8 °	-57.3°	176.1°

(a) Dihedral 1-phenyl torsions. (b) Dihedrals 3-phenyl torsions. (c) C_1 adjoins C_Q. (d) Central dihedral is indicated,

i.e. C_2-C_3 is flanked by C_1 and C_4.

Optimized geometries of critical TSs

3-m-pro-m

C	0.433391	-0.130546	0.428086
H	0.952481	-0.188604	1.394393
C	1.500227	-0.081280	-0.652023
C	2.858250	-0.040107	-0.316083
C	1.158726	-0.060451	-2.011771
C	3.847056	0.017811	-1.300143
H	3.146963	-0.050399	0.733060
C	2.140482	-0.002865	-2.999098
H	0.112686	-0.093698	-2.307963
C	3.491018	0.036007	-2.647376
H	4.894443	0.048333	-1.011404
H	1.850663	0.009063	-4.046588
H	4.256570	0.079697	-3.417106
C	-0.425504	1.149681	0.450578
H	-1.212832	1.020503	1.205566
H	-0.940431	1.252215	-0.514307
C	-0.467109	-1.375776	0.298665
H	-1.220394	-1.294496	1.116935
H	-1.055803	-1.287946	-0.628415
C	0.252381	-2.703398	0.357664
C	-0.437512	-3.875035	-0.166585
C	0.264158	-5.088873	-0.406780
C	-1.849385	-3.911872	-0.355417
C	-0.397010	-6.248208	-0.776735
H	1.347119	-5.093534	-0.304496
C	-2.505755	-5.091805	-0.720532
H	-2.433563	-2.995272	-0.274256
C	-1.793181	-6.269225	-0.924485
H	0.177277	-7.153751	-0.957336
H	-3.583903	-5.077195	-0.860657
H	-2.304174	-7.183403	-1.210369
H	1.302438	-2.666462	0.077843
Li	-1.204382	-3.370519	1.817347
C	-2.619404	-5.730171	5.196409
C	-2.630889	-4.414078	5.678867
C	-1.758401	-6.048858	4.148230
H	-3.266284	-6.485497	5.632093
C	-1.812521	-3.443538	5.122022
H	-3.290196	-4.145767	6.501016
C	-0.925067	-5.081486	3.585184
H	-1.725211	-7.063951	3.760246
C	-0.923248	-3.739795	4.055043
H	-1.835807	-2.428798	5.513401
H	-0.245078	-5.385367	2.789490
C	-0.102271	-2.696678	3.468798
H	-0.239198	-1.691316	3.859913
C	0.851256	-2.899868	2.454379
H	1.273184	-3.893771	2.303176
H	1.574830	-2.107498	2.298416
C	0.358315	2.424751	0.751057
H	1.123430	2.613949	-0.008462
H	-0.306594	3.294227	0.780668
H	0.862406	2.359548	1.722529

3-m-pro-r

C	0.814502	0.535068	-0.092434
H	1.160135	0.718079	0.933980
C	2.005749	0.008727	-0.874631
C	3.270623	-0.078934	-0.281351
C	1.880315	-0.389170	-2.213340
C	4.375741	-0.547995	-0.994197
H	3.393785	0.229126	0.755047
C	2.978920	-0.858563	-2.930968
H	0.910947	-0.336748	-2.703782
C	4.233554	-0.940655	-2.323855
H	5.346510	-0.605052	-0.508570
H	2.855117	-1.163584	-3.966892
H	5.090076	-1.307259	-2.882920
C	0.314070	1.883543	-0.648270
H	-0.580544	2.175269	-0.081589
H	-0.015553	1.741472	-1.686527
C	-0.347974	-0.478550	-0.034465
H	-1.164821	-0.009565	0.538110
H	-0.747301	-0.596532	-1.056291
C	0.008447	-1.831187	0.545838
C	-0.867648	-2.956150	0.278267
C	-0.431847	-4.282108	0.579537
C	-2.226290	-2.819101	-0.132605
C	-1.287867	-5.378913	0.461066
H	0.606211	-4.438293	0.866351
C	-3.063289	-3.921761	-0.253597
H	-2.613587	-1.832242	-0.369866
C	-2.609983	-5.213561	0.046751
H	-0.910073	-6.373045	0.687507
H	-4.087804	-3.774591	-0.587053

H	-3.273113	-6.067914	-0.045928
H	1.054208	-2.101345	0.408174
Li	-1.157183	-2.926963	2.332807
C	-1.155602	-3.247043	5.574297
C	-1.018243	-2.360658	4.472160
C	-2.353980	-3.377623	6.257041
H	-0.288578	-3.823425	5.889164
C	-2.180921	-1.629771	4.100260
C	0.227170	-2.271965	3.737496
C	-3.488203	-2.646595	5.872524
H	-2.412805	-4.059644	7.101884
C	-3.385830	-1.774609	4.792251
H	-2.130919	-0.900918	3.291272
H	1.020839	-2.955220	4.030272
C	0.462584	-1.370335	2.684298
H	-4.425755	-2.757781	6.408507
H	-4.248445	-1.190316	4.481036
H	-0.125477	-0.453985	2.630044
H	1.496455	-1.236525	2.388094
C	1.341752	3.010695	-0.586490
H	2.230097	2.777523	-1.182047
H	0.919359	3.946331	-0.967782
H	1.670319	3.191043	0.443941

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C	-0.240182	0.156294	-0.017187
H	-0.605193	0.712778	0.857059
C	1.264711	0.025063	0.139630
C	1.915715	0.548376	1.262823
C	2.042178	-0.633996	-0.823580
C	3.296000	0.419249	1.425288
H	1.332933	1.065972	2.021960
C	3.421050	-0.767334	-0.666707
H	1.567466	-1.049336	-1.709670
C	4.054734	-0.240972	0.460117
H	3.776633	0.835767	2.306649
H	4.002498	-1.282685	-1.426859
H	5.129434	-0.343752	0.582461
C	-0.625467	0.962628	-1.272711
H	-1.715563	0.932219	-1.390762
H	-0.213323	0.460730	-2.158373
C	-0.921414	-1.230770	-0.013314
H	-0.703054	-1.721595	-0.974572
H	-0.399689	-1.848491	0.750971
C	-2.410991	-1.199198	0.255824
C	-3.225318	-2.297123	-0.254903
C	-4.642321	-2.190599	-0.309065
C	-2.670993	-3.559879	-0.612249
C	-5.438177	-3.267396	-0.664120
H	-5.103182	-1.234052	-0.072234
C	-3.486137	-4.641719	-0.959390
H	-1.589503	-3.682714	-0.672339
C	-4.871453	-4.511980	-0.980446
H	-6.517773	-3.142534	-0.699353
H	-3.024093	-5.587833	-1.230499
H	-5.502188	-5.352388	-1.253144
H	-2.884905	-0.229868	0.116156
Li	-2.201830	-2.936825	1.575764
H	-4.306824	-2.969715	2.776368
C	-3.661308	-3.520696	3.460369
C	-2.393506	-2.992927	3.829774
C	-4.130199	-4.725677	3.986084
C	-1.637426	-3.759244	4.756988
C	-1.854073	-1.769843	3.267678
C	-3.367571	-5.454902	4.895700
H	-5.107092	-5.090724	3.678595
C	-2.115827	-4.951563	5.277399
H	-0.663810	-3.386621	5.067670
H	-0.840899	-1.502701	3.556967
C	-2.553350	-0.915220	2.390955
H	-3.734863	-6.392420	5.301861
H	-1.507022	-5.501984	5.990847
H	-3.643994	-0.927633	2.390940
H	-2.146126	0.083347	2.271474
C	-0.158223	2.415996	-1.242317
H	0.931735	2.485592	-1.165335
H	-0.464331	2.945088	-2.150801
H	-0.586193	2.951865	-0.386684

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C	0.155282	0.632718	-0.122651
H	0.265916	0.747099	0.964707
C	1.514656	0.921096	-0.735596
C	2.621437	1.200203	0.074858
C	1.707212	0.895924	-2.124507
C	3.879603	1.447452	-0.476941
H	2.495680	1.225210	1.155417
C	2.961212	1.141449	-2.681932
H	0.867933	0.681804	-2.782299
C	4.054496	1.418781	-1.859605

H	4.721716	1.663187	0.175533
H	3.085156	1.116784	-3.761593
H	5.031869	1.611225	-2.293564
C	-0.914756	1.639311	-0.587529
H	-1.891356	1.320940	-0.202284
H	-0.995852	1.592444	-1.681895
C	-0.275286	-0.825516	-0.405943
H	-0.568473	-0.888906	-1.467021
H	0.614390	-1.468047	-0.314326
C	-1.390613	-1.330371	0.487969
C	-2.219719	-2.430104	0.031319
C	-3.406483	-2.769711	0.748453
C	-1.839342	-3.323658	-1.012912
C	-4.158799	-3.901186	0.425809
H	-3.747927	-2.104575	1.538926
C	-2.603421	-4.441162	-1.327737
H	-0.938585	-3.121739	-1.585754
C	-3.768268	-4.748834	-0.611371
H	-5.063263	-4.114735	0.990259
H	-2.286144	-5.086221	-2.143552
H	-4.355146	-5.627357	-0.860300
H	-1.994133	-0.542176	0.935557
Li	-1.346078	-3.497547	1.585007
H	1.081005	-3.667021	1.557525
C	0.764482	-4.361620	2.335820
C	-0.114865	-3.922795	3.365015
C	1.294336	-5.654489	2.331708
C	-0.431007	-4.872876	4.373512
C	-0.721203	-2.607443	3.361860
C	0.971965	-6.560978	3.337633
H	1.971714	-5.946162	1.532755
C	0.104910	-6.150303	4.361674
H	-1.101259	-4.574932	5.176666
H	-1.467254	-2.407429	4.127153
C	-0.392589	-1.587298	2.449359
H	1.384293	-7.565259	3.332033
H	-0.154527	-6.842955	5.158734
H	-0.720575	-0.589200	2.717384
H	0.584665	-1.602993	1.966268
C	-0.642561	3.077616	-0.153396
H	0.310702	3.441996	-0.550061
H	-1.431372	3.750716	-0.505447
H	-0.599657	3.160148	0.939210

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C	0.102350	0.048010	0.024095
H	0.227995	0.070013	1.116858
C	1.493245	-0.016301	-0.582392
C	2.633412	0.127035	0.216872
C	1.677710	-0.194382	-1.960982
C	3.915864	0.090060	-0.333845
H	2.515080	0.273513	1.288776
C	2.954765	-0.232724	-2.517863
H	0.812900	-0.311312	-2.609992
C	4.081609	-0.091570	-1.705764
H	4.783608	0.202805	0.311030
H	3.070956	-0.375962	-3.589131
H	5.077431	-0.123301	-2.139370
C	-0.632689	1.344111	-0.376843
H	-1.649333	1.300150	0.035503
H	-0.744682	1.364933	-1.469522
C	-0.761290	-1.180856	-0.326183
H	-1.757112	-1.001136	0.109036
H	-0.950300	-1.180497	-1.415437
C	-0.168641	-2.520902	0.086007
C	-0.883617	-3.743677	-0.242953
C	-0.180829	-4.973650	-0.367414
C	-2.294871	-3.811104	-0.375497
C	-0.841584	-6.177160	-0.573023
H	0.906454	-4.960988	-0.322513
C	-2.951611	-5.024487	-0.573398
H	-2.889408	-2.901896	-0.327018
C	-2.238546	-6.219916	-0.667021
H	-0.262987	-7.092954	-0.673284
H	-4.035402	-5.030286	-0.658692
H	-2.753905	-7.161926	-0.831124
H	0.893481	-2.581778	-0.143854
Li	-1.491763	-2.405657	1.795765
C	-5.632447	-1.001166	2.746322
C	-5.813496	0.117404	3.556984
C	-6.513461	-1.279208	1.702269
S	-4.228554	-2.062024	3.021400
C	-6.890919	0.965637	3.311908
H	-5.128546	0.307715	4.377150
C	-7.585443	-0.421207	1.472806
H	-6.367786	-2.165999	1.093701
O	-3.931921	-2.047872	4.482810
O	-4.607280	-3.440043	2.580173
O	-3.110187	-1.500891	2.197595
C	-7.789213	0.715711	2.266769
H	-7.038438	1.835041	3.948061

H	-8.279079	-0.641386	0.664728
C	-8.935775	1.651306	1.990098
H	-9.188663	2.246930	2.871716
H	-8.682634	2.348910	1.182396
H	-9.831813	1.105273	1.679393
Na	-3.580356	-4.398655	4.418212
C	-1.807863	-6.254717	5.451001
C	-1.571061	-5.048732	6.134352
C	-1.483244	-6.319905	4.087373
H	-2.203060	-7.121972	5.971675
C	-1.039701	-3.946679	5.471690
H	-1.796448	-4.973038	7.195839
C	-0.945578	-5.221251	3.418522
H	-1.655212	-7.239220	3.532764
C	-0.685547	-3.994734	4.092958
H	-0.865436	-3.025595	6.021655
H	-0.727890	-5.309933	2.356719
C	-0.076550	-2.843864	3.469402
H	-0.113867	-1.920089	4.045844
C	0.664254	-2.849180	2.286956
H	0.990782	-3.794991	1.863785
H	1.324739	-2.010920	2.096880
C	0.047552	2.627362	0.093281
H	1.050685	2.731922	-0.332397
H	-0.534088	3.507575	-0.200645
H	0.145717	2.645444	1.185310

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C	0.112649	0.031399	-0.045563
H	0.084634	0.069973	1.053104
C	1.573488	-0.027598	-0.455959
C	2.595086	0.086847	0.494030
C	1.944662	-0.176494	-1.800141
C	3.940709	0.051791	0.123667
H	2.333921	0.208287	1.543462
C	3.285599	-0.212258	-2.178023
H	1.176049	-0.272080	-2.563471
C	4.291696	-0.098514	-1.216684
H	4.712606	0.141262	0.883804
H	3.546507	-0.332333	-3.226400
H	5.337302	-0.128293	-1.510810
C	-0.575906	1.311148	-0.562204
H	-1.630753	1.269632	-0.262840
H	-0.563331	1.304379	-1.660791
C	-0.679151	-1.216115	-0.483179
H	-1.729199	-1.042330	-0.202897
H	-0.697257	-1.250357	-1.588354
C	-0.142369	-2.529143	0.060807
C	-0.724505	-3.779904	-0.400537
C	0.013037	-4.992925	-0.315075
C	-2.055640	-3.888383	-0.880875
C	-0.543177	-6.215084	-0.664784
H	1.052318	-4.951569	0.005427
C	-2.607764	-5.121603	-1.228620
H	-2.664838	-2.995655	-0.996455
C	-1.864654	-6.296176	-1.121576
H	0.061659	-7.116267	-0.593429
H	-3.631376	-5.157320	-1.594065
H	-2.297035	-7.253422	-1.397851
H	0.945315	-2.555659	0.083970
Li	-1.816746	-2.676536	1.454376
C	-1.807848	-2.092647	5.535573
C	-0.989830	-1.836178	4.399553
C	-2.011741	-1.140265	6.529025
H	-2.266975	-3.072911	5.635130
C	-0.431207	-0.530080	4.314495
C	-0.722624	-2.888952	3.451042
C	-1.432739	0.137642	6.432317
H	-2.622160	-1.395062	7.392237
C	-0.639516	0.422680	5.310042
H	0.186789	-0.268686	3.461288
H	-1.228282	-3.835294	3.647811
C	0.232172	-2.861842	2.436158
H	-1.567594	0.872385	7.220476
H	-0.173094	1.400395	5.212486
H	0.953868	-2.053068	2.382838
H	0.576003	-3.811429	2.041381
Na	-3.243669	0.055318	4.384282
O	-3.604080	0.292620	2.103132
S	-4.364903	-0.995377	2.058855
C	-5.832615	-0.717565	1.087995
O	-3.604969	-2.077996	1.363159
O	-4.802112	-1.387946	3.430770
C	-5.837918	0.278160	0.114374
C	-6.949646	-1.528228	1.289681
C	-6.978682	0.459455	-0.665507
H	-4.965710	0.910575	-0.016080
C	-8.079435	-1.333583	0.501163
H	-6.934574	-2.288998	2.063694
C	-8.112443	-0.342919	-0.490731
H	-6.987377	1.241771	-1.420585

H	-8.953748	-1.960144	0.661164
C	-9.332514	-0.161350	-1.353867
H	-9.366107	-0.919775	-2.145461
H	-10.253231	-0.260122	-0.770321
H	-9.339426	0.819632	-1.836914
C	0.042826	2.610558	-0.052567
H	1.086833	2.711837	-0.366341
H	-0.506254	3.479613	-0.430653
H	0.018970	2.656104	1.042849

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C	0.044767	0.066043	-0.072867
H	0.018903	0.185953	1.020783
C	1.502685	0.124707	-0.489117
C	2.499328	0.482686	0.427469
C	1.896504	-0.165704	-1.803833
C	3.842376	0.549482	0.051381
H	2.217519	0.721932	1.451099
C	3.235824	-0.103317	-2.185685
H	1.146376	-0.445545	-2.539645
C	4.216790	0.254831	-1.258886
H	4.594054	0.836985	0.782380
H	3.514627	-0.332690	-3.211131
H	5.260392	0.307372	-1.557206
C	-0.766959	1.228588	-0.680878
H	-1.827831	1.060046	-0.458095
H	-0.674690	1.182105	-1.774574
C	-0.606587	-1.294327	-0.414597
H	-0.841002	-1.297349	-1.492668
H	0.149323	-2.082658	-0.290938
C	-1.866077	-1.568990	0.396362
C	-2.973658	-2.292478	-0.204021
C	-4.276540	-2.214755	0.364060
C	-2.831598	-3.144531	-1.331482
C	-5.347537	-2.922259	-0.159326
H	-4.434961	-1.560440	1.219327
C	-3.917263	-3.846989	-1.855192
H	-1.862204	-3.243270	-1.813821
C	-5.182408	-3.748256	-1.279552
H	-6.327992	-2.823505	0.301056
H	-3.765390	-4.477325	-2.727981
H	-6.024613	-4.296666	-1.691333
H	-2.208904	-0.704820	0.963050
Li	-1.452966	-3.749122	0.866425
H	1.379041	-2.000127	2.262956
C	1.609249	-2.925448	2.782363
C	0.547854	-3.759227	3.237112
C	2.945361	-3.273812	2.970672
C	0.933471	-4.969543	3.879806
C	-0.847229	-3.440738	3.073733
C	3.299431	-4.475582	3.604001
H	3.721035	-2.601181	2.611941
C	2.269271	-5.313584	4.063036
H	0.155583	-5.639963	4.236280
H	-1.548823	-4.216245	3.379368
C	-1.363099	-2.221512	2.644039
H	4.341681	-4.736514	3.760702
H	2.512928	-6.245263	4.567930
H	-2.414364	-2.024282	2.826407
H	-0.729418	-1.340651	2.627794
O	0.082068	-4.708873	-0.137417
S	-0.540188	-6.081291	0.065756
C	-0.944318	-6.745866	-1.537391
O	-1.806870	-5.923297	0.818941
O	0.480901	-6.982202	0.670642
C	-2.206190	-7.293449	-1.748631
C	0.019190	-6.757489	-2.547075
C	-2.500713	-7.861742	-2.987572
H	-2.943356	-7.264310	-0.953159
C	-0.293594	-7.322081	-3.778245
H	0.999798	-6.324701	-2.375268
C	-1.556357	-7.884636	-4.019453
H	-3.485392	-8.292322	-3.152356
H	0.455280	-7.328828	-4.566746
C	-1.887542	-8.474071	-5.364314
H	-2.114712	-7.684892	-6.091316
H	-1.048677	-9.052428	-5.764169
H	-2.758770	-9.132354	-5.308917
Na	1.884505	-5.252530	1.293070
C	-0.354081	2.612948	-0.187952
H	0.692873	2.829633	-0.424885
H	-0.968915	3.392742	-0.649813
H	-0.473547	2.698788	0.898873

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C	0.029940	0.016812	0.076242
H	-0.030194	0.038989	1.174718
C	1.505347	-0.027224	-0.284052
C	2.484636	-0.107698	0.712625
C	1.928443	-0.003956	-1.620889

C	3.841784	-0.162527	0.391640
H	2.178847	-0.132781	1.756428
C	3.282420	-0.059548	-1.948260
H	1.193094	0.058345	-2.419692
C	4.246490	-0.138582	-0.942101
H	4.581407	-0.225372	1.185674
H	3.585422	-0.040681	-2.992090
H	5.302096	-0.180727	-1.196640
C	-0.650861	1.296909	-0.443947
H	-1.715009	1.266017	-0.183646
H	-0.610279	1.304795	-1.541700
C	-0.673753	-1.273884	-0.407496
H	-0.638303	-1.293623	-1.511637
H	-0.032445	-2.117361	-0.109377
C	-2.114073	-1.451614	0.056314
C	-2.832213	-2.665855	-0.308589
C	-4.250547	-2.650881	-0.399573
C	-2.204205	-3.921829	-0.506981
C	-4.983269	-3.806707	-0.635310
H	-4.770677	-1.699766	-0.301922
C	-2.946421	-5.079659	-0.733630
H	-1.119947	-3.999853	-0.487788
C	-4.339723	-5.040112	-0.793261
H	-6.067031	-3.746392	-0.707275
H	-2.423085	-6.022760	-0.869393
H	-4.912581	-5.943877	-0.980209
H	-2.716805	-0.563141	-0.119678
Li	-1.268481	-2.616044	1.677253
H	-4.180696	-3.419273	2.278428
C	-3.959867	-3.621499	3.323847
C	-2.993106	-2.830830	4.007499
C	-4.631939	-4.662489	3.962967
C	-2.728517	-3.190215	5.360084
C	-2.310371	-1.703563	3.418953
C	-4.368255	-4.985807	5.302612
H	-5.369961	-5.232337	3.403465
C	-3.406913	-4.226687	5.993395
H	-1.989410	-2.618443	5.914899
H	-1.470225	-1.309554	3.989744
C	-2.718857	-1.000388	2.282264
H	-4.913962	-5.781357	5.801397
H	-3.192110	-4.442972	7.037580
H	-3.722583	-1.153697	1.894955
H	-2.322452	-0.000292	2.142587
C	2.229169	-6.366739	1.288807
C	3.512467	-6.828777	1.010623
C	2.024708	-5.562821	2.408985
H	1.390021	-6.637788	0.656055
C	4.598531	-6.496107	1.831482
H	3.672261	-7.461724	0.140961
C	3.083341	-5.222306	3.248242
S	0.399374	-4.916926	2.743423
C	4.360753	-5.693292	2.954271
C	5.987834	-6.972975	1.501848
H	2.901369	-4.610045	4.125734
O	0.288300	-3.642413	1.965297
O	-0.596975	-5.936520	2.290291
O	0.290004	-4.702940	4.215147
H	5.186903	-5.434273	3.612198
H	5.970527	-7.953268	1.016338
H	6.484521	-6.276554	0.815098
H	6.609498	-7.047887	2.398719
Na	-1.923504	-5.578001	4.151516
C	-0.043864	2.587457	0.103532
H	1.008179	2.690231	-0.180774
H	-0.581144	3.463896	-0.274110
H	-0.094270	2.614459	1.198677