Electronic Supplementary Information for the paper entitled:

A computational study of regioselectivity in aluminum hydride ring-opening of *cis*- and *trans*- 4-*t*-butyl and 3-methylcyclohexene oxides.

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TABLE S1. Single point free energies of activation at B3LYP/6-31+G*(PCM) geometries with ether for ring opening of *cis*- and *trans*- **1** and **2** with $LiAlH_4$ (Li^+-O bond in *exo* position).

		$\Delta G^{\ddagger a,b,c}$			
		MP2/ 6-31+G*(PCM)	**wb97xd/ 6-31+G*(PCM)**	**B3LYP/ 6-311+G(2d,p)(PCM)**	**mPW1PW91/ 6-311+G(2d,p)(PCM)**
***cis*-4-*t*-butyl**					
ψ_{ax}-*cis*-**1**-TS_1	chair	15.7 (7.9)	14.3 (6.9)	15.0 (7.5)	16.4 (7.6)
ψ_{ax}-*cis*-**1**-TS_2	twist-boat	15.9 (8.1)	14.6 (7.2)	15.3 (7.8)	16.6 (7.8)
ψ_{eq}-*cis*-**1**-TS_1	twist-boat	12.0 (4.2)	11.3 (3.9)	10.7 (3.2)	12.1 (3.3)
ψ_{eq}-*cis*-**1**-TS_2	chair	**7.8 (0.0)**	**7.4 (0.0)**	**7.5 (0.0)**	**8.8 (0.0)**
***trans*-4-*t*-butyl**					
ψ_{ax}-*trans*-**1**-TS_1	twist-boat	16.1 (7.4)	14.8 (6.7)	14.3 (6.3)	15.8 (6.4)
ψ_{ax}-*trans*-**1**-TS_2	chair	16.7 (8.0)	14.7 (6.6)	15.5 (7.5)	16.9 (7.5)
ψ_{eq}-*trans*-**1**-TS_1	chair	**8.7 (0.0)**	**8.1 (0.0)**	**8.0 (0.0)**	**9.4 (0.0)**
ψ_{eq}-*trans*-**1**-TS_2	twist-boat	11.4 (2.7)	10.6 (2.5)	10.3 (2.3)	11.7 (2.3)
***cis*-3-methyl**					
ψ_{ax}-*cis*-**2**-TS_1	twist-boat	13.1 (4.4)	11.8 (3.6)	11.5 (3.4)	12.8 (3.4)
ψ_{ax}-*cis*-**2**-TS_2	chair	11.1 (2.4)	10.1 (1.9)	10.5 (2.4)	11.7 (2.3)
ψ_{eq}-*cis*-**2**-TS_1	chair	**8.7 (0.0)**	**8.2 (0.0)**	**8.1 (0.0)**	**9.4 (0.0)**
ψ_{eq}-*cis*-**2**-TS_2	twist-boat	12.5 (3.8)	11.5 (3.3)	10.7 (2.6)	12.2 (2.8)
***trans*-3-methyl**					
ψ_{ax}-*trans*-**2**-TS_1	chair	9.2 (0.4)	8.2 (0.3)	9.0 (0.3)	10.1 (0.2)
ψ_{ax}-*trans*-**2**-TS_2	twist-boat	14.5 (5.6)	13.0 (5.1)	13.8 (5.1)	15.0 (5.2)
ψ_{eq}-*trans*-**2**-TS_1	twist-boat	12.4 (3.6)	11.2 (3.3)	10.9 (2.2)	12.3 (2.4)
ψ_{eq}-*trans*-**2**-TS_2	chair	**8.8 (0.0)**	**7.9 (0.0)**	**8.7 (0.0)**	**9.9 (0.0)**

[a]All energies relative to separated reactants (3-methyl- and 4-*t*-butyl-cyclohexene oxide-Li^+ + AlH_4^-) with lowest energy conformer. [b]All single point calculations performed on B3LYP/6-31+G*(PCM) optimized geometries, relative free energies of activation ($\Delta\Delta G^{\ddagger}$) relative to the lowest energy transition state in parenthesis. [c]Free energy corrections to electronic energies calculated at 298 K at B3LYP/6-31+G*(PCM) frequencies.

Table S2: Electronic Energies, ZPVE and G_{corr} at B3LYP/6-31+G*(PCM) at 298 K and 1 atm for all structures

	ε_0 (hartrees)	**ZPVE (hartrees)**	**G_{corr} (hartrees)**
AlH_4^-	-244.925612008	0.0240576	0.002182
11-Li^+ (*endo*)	-317.316106976	0.1543411	0.123423
11-Li^+ (*exo*)	-317.317962987	0.154727	0.124048
11-TS_1	-562.246961937	0.178632	0.140444
11-TS_2	-562.241694107	0.178658	0.140216
ψ_{ax}-*cis*-**1**-Li^+ (*endo*)	-474.559994669	0.268103	0.231405
ψ_{ax}-*cis*-**1**-Li^+ (*exo*)	-474.559943909	0.267071	0.229261
ψ_{ax}-*cis*-**1**-TS_1	-719.489222686	0.2918825	0.247848
ψ_{ax}-*cis*-**1**-TS_2	-719.488733055	0.2915745	0.247566
ψ_{eq}-***cis***-**1**-Li^+ (*endo*)	-474.569889205	0.266589	0.228873
ψ_{eq}-***cis***-**1**-Li^+ (*exo*)	-474.571013074	0.266990	0.229541
ψ_{eq}-***cis***-**1**-TS_1	-719.495498695	0.291587	0.246980
ψ_{eq}-***cis***-**1**-TS_2	-719.500293511	0.291386	0.246503
ψ_{ax}-*trans*-**1**-Li^+ (*endo*)	-474.563141417	0.268332	0.231740
ψ_{ax}-*trans*-**1**-Li^+ (*exo*)	-474.564811393	0.267200	0.230004
ψ_{ax}-*trans*-**1**-TS_1	-719.489222043	0.2915697	0.246980
ψ_{ax}-*trans*-**1**-TS_2	-719.488949890	0.292094	0.248497
ψ_{eq}-*trans*-**1**-Li^+ (*endo*)	-474.569743287	0.267522	0.230600
ψ_{eq}-*trans*-**1**-Li^+ (*exo*)	-474.570391447	0.266664	0.229103
ψ_{eq}-*trans*-**1**-TS_1	-719.499772790	0.291685	0.247159
ψ_{eq}-*trans*-**1**-TS_2	-719.495402545	0.291354	0.246435
ψ_{ax}-*cis*-**2**	-349.178635388	0.179931	0.148593
ψ_{ax}-*cis*-**2**-Li^+ (*endo*)	-356.629727294	0.183682	0.151688
ψ_{ax}-*cis*-**2**-Li^+ (*exo*)	-356.631254990	0.182192	0.149209
ψ_{ax}-*cis*-**2**-TS_1	-601.555272109	0.206402	0.165470
ψ_{ax}-*cis*-**2**-TS_2	-601.559689517	0.207262	0.167908
ψ_{eq}-*cis*-**2**	-349.180467720	0.179797	0.148428
ψ_{eq}-*cis*-**2**-Li^+ (*endo*)	-356.631082626	0.183359	0.151000
ψ_{eq}-*cis*-**2**-Li^+ (*exo*)	-356.632818981	0.181694	0.148482
ψ_{eq}-*cis*-**2**-TS_1	-601.562609975	0.206707	0.167076
ψ_{eq}-*cis*-**2**-TS_2	-601.557207695	0.206563	0.165994
ψ_{ax}-*trans*-**2**	-349.1783759	0.179742	0.148338
ψ_{ax}-*trans*-**2**-Li^+ (*endo*)	-356.629952823	0.183000	0.150522
ψ_{ax}-*trans*-**2**-Li^+ (*exo*)	-356.630909244	0.181878	0.148399
ψ_{ax}-*trans*-**2**-TS_1	-601.559724207	0.206635	0.166405
ψ_{ax}-*trans*-**2**-TS_2	-601.553597106	0.207180	0.167896
ψ_{eq}-*trans*-**2**	-349.1802208	0.179837	0.148414
ψ_{eq}-*trans*-**2**-Li^+ (*endo*)	-356.632193737	0.181958	0.149129

ψ_{eq}-*trans*-**2**-Li^+ (*exo*)	-356.632860083	0.1821389	0.149336
ψ_{eq}-*trans*-**2**-TS_1	-601.557045691	0.206718	0.166967
ψ_{eq}-*trans*-**2**-TS_2	-601.561145898	0.206800	0.167276
ψ_{ax}-*cis*-**12**-Li^+ (exo)	-356.62903791	0.182223	0.149619
ψ_{ax}-*cis*-**12**-TS_1	-601.5580824	0.206856	0.16737
ψ_{ax}-*cis*-**12**-TS_2	-601.5531024	0.206588	0.16630
ψ_{eq}-*cis*-**12**-Li^+ (exo)	-356.63367102	0.181452	0.147357
ψ_{eq}-*cis*-**12**-TS_1	-601.5579658	0.206650	0.16626
ψ_{eq}-*cis*-**12**-TS_2	-601.5631554	0.206724	0.16643
ψ_{ax}-*trans*-**12**-Li^+ (exo)	-356.63088165	0.182093	0.149187
ψ_{ax}-*trans*-**12**-TS_1	-601.5544783	0.207007	0.167293
ψ_{ax}-*trans*-**12**-TS_2	-601.5584793	0.206598	0.16685
ψ_{eq}-*trans*-**12**-Li^+ (exo)	-356.6334551	0.181770	0.148870
ψ_{eq}-*trans*-**12**-TS_1	-601.5630748	0.206285	0.16553
ψ_{eq}-*trans*-**12**-TS_2	-601.5578477	0.206731	0.16663

[a]Electronic energies.

Table S3: Electronic Energies, ZPVE and G_{corr} at B3LYP/6-31+G*(PCM) at 298 K and 1 atm for **11**.

Structure	**ε_0 (hartrees)**	**ZPVE (hartrees)**	**G_{corr} (hartrees)**
AlH_4^-	-244.925612008	0.0240576	0.002182
11	-309.864727428	0.1518034	0.122203
C1-opening	-554.752193054	0.1764827	0.140660
C2-opening	-554.758355838	0.1762748	0.140563

[a]Electronic energies.

Table S4: Electronic energies ε_0 (hartrees) for single point calculations at the B3LYP/6-31+G* (PCM) geometries for all structures.

Structure	**MP2/ 6-31+G*(PCM)**	**wb97xd/ 6-31+G*(PCM)**	**B3LYP/ 6-311+G(2d,p)(PCM)**	**mPW1PW91/ 6-311+G(2d,p)(PCM)**
AlH_4^-	-244.3569766	-244.892432023	-244.953407977	-244.924948846
11-Li^+ (*exo*)	-316.2385985	-317.230983767	-317.400735717	-317.318791631
11-TS_1	-560.5965772	-562.125769634	-562.356942308	-562.244409703
11-TS_2	-560.5900061	-562.119737360	-562.351886732	-562.239157716
ψ_{ax}-*cis*-**1**-Li^+ (*exo*)	-472.9037473	-474.437710641	-474.684573202	-474.565882169
ψ_{ax}-*cis*-**1**-TS_1	-717.2629075	-719.333305947	-719.640981263	-719.491839980
ψ_{ax}-*cis*-**1**-TS_2	-717.2623872	-719.332509280	-719.640213165	-719.491297092
ψ_{eq}-*cis*-**1**-Li^+ (*exo*)	-472.9148862	-474.447511695	-474.695297076	-474.576943750
ψ_{eq}-*cis*-**1**-TS_1	-717.2679531	-719.337144438	-719.646956529	-719.497832439
ψ_{eq}-*cis*-**1**-TS_2	-717.2741799	-719.342868862	-719.651557395	-719.502588836

ψ_{ax}-*trans*-**1**-Li^+ (*exo*)	-472.910125	-474.443633635	-474.689125399	-474.570925507
ψ_{ax}-*trans*-**1**-TS_1	-717.2614377	-719.331361370	-719.641044758	-719.491747140
ψ_{ax}-*trans*-**1**-TS_2	-717.2620299	-719.333083804	-719.640620198	-719.491472746
ψ_{eq}-*trans*-**1**-Li^+ (*exo*)	-472.9143987	-474.446883633	-474.694685227	-474.576310796
ψ_{eq}-*trans*-**1**-TS_1	-717. 2733677	-719.342310460	-719.651173231	-719.502226444
ψ_{eq}-*trans*-**1**-TS_2	-717.2684185	-719.337586907	-719.646819777	-719.497788614
ψ_{ax}-*cis*-**2**-Li^+ (*exo*)	-355.4074732	-356.534880311	-356.724601068	-356.633387831
ψ_{ax}-*cis*-**2**-TS_1	-599.7599351	-601.424417990	-601.675865895	-601.554050700
ψ_{ax}-*cis*-**2**-TS_2	-599.7655274	-601.429525459	-601.680038684	-601.558250601
ψ_{eq}-*cis*-**2**-Li^+ (*exo*)	-355.408960	-356.536011983	-356.726036938	-356.634724772
ψ_{eq}-*cis*-**2**-TS_1	-599.7684472	-601.431862105	-601.682906739	-601.561085851
ψ_{eq}-*cis*-**2**-TS_2	-599.7612811	-601.425513161	-601.677697157	-601.555580313
ψ_{ax}-*trans*-**2**-Li^+ (*exo*)	-355.4067884	-356.534449045	-356.724163848	-356.632903938
ψ_{ax}-*trans*-**2**-TS_1	-599.7656847	-601.430126645	-601.680077338	-601.558509546
ψ_{ax}-*trans*-**2**-TS_2	-599.7588404	-601.4239711	-601.673853484	-601.552116908
ψ_{eq}-*trans*-**2**-Li^+ (*exo*)	-355.4085185	-356.535817784	-356.726024588	-356.634747908
ψ_{eq}-*trans*-**2**-TS_1	-599.7611915	-601.425876227	-601.677502581	-601.555592829
ψ_{eq}-*trans*-**2**-TS_2	-599.7671568	-601.431399514	-601.681377863	-601.559717550

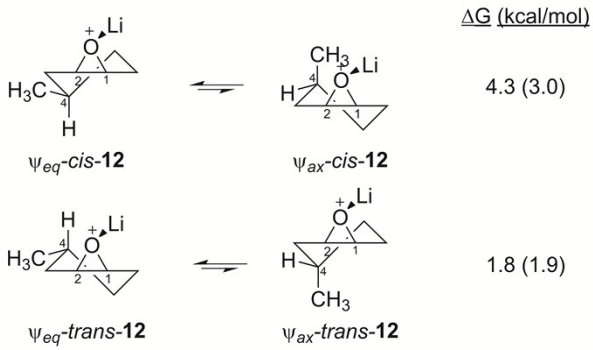
[a]Electronic energies.

TABLE S5: Relative free energies of activation at B3LYP/6-31+G*(PCM) with ether for ring opening of *cis*- and *trans*-**12** with $LiAlH_4$ (Li^+-O bond in *exo* position).

	T.S.	$\Delta G^{\ddagger a,b}$	$\Delta\Delta G^{\ddagger c}$	k_f/k_s
***cis*-4-methyl**				
ψ_{ax}-*cis*-**12**-TS_1	chair	10.4	3.8	0.3
ψ_{ax}-*cis*-**12**-TS_2	twist-boat	12.8	6.2	0.005
ψ_{eq}-*cis*-**12**-TS_1	twist-boat	9.7	3.1	1
ψ_{eq}-*cis*-**12**-TS_2	chair	6.6	**0.0**	188
***trans*-4-methyl**				
ψ_{ax}-*trans*-**12**-TS_1	twist-boat	12.1	6.5	.009
ψ_{ax}-*trans*-**12**-TS_2	chair	9.3	3.7	1
ψ_{eq}-*trans*-**12**-TS_1	chair	5.6	**0.0**	526
ψ_{eq}-*trans*-**12**-TS_2	twist-boat	9.5	4.0	0.89

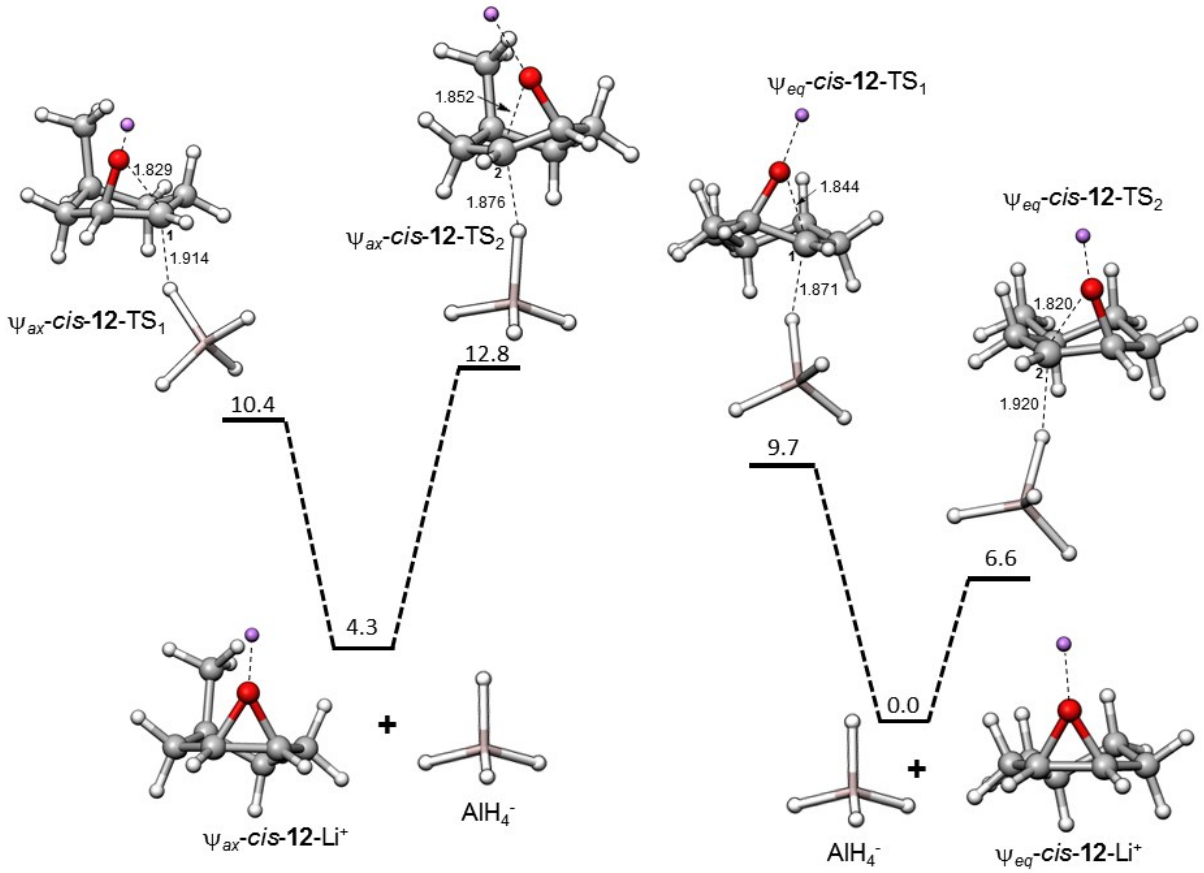
[a]All energies relative to separated reactants (*cis*- and *trans*- 4-methylcyclohexene oxide-Li^+ + AlH_4^-) with the lowest energy conformer. [b]Free energy corrections to electronic energies calculated at 298 K at B3LYP/6-31+G*(PCM) frequencies. [c]Relative free energies of activation ($\Delta\Delta G^{\ddagger}$) relative to the lowest energy transition state.

Scheme S1: Pseudoequatorial preference for lithiated (and neutral) *cis*- and *trans*-**12**



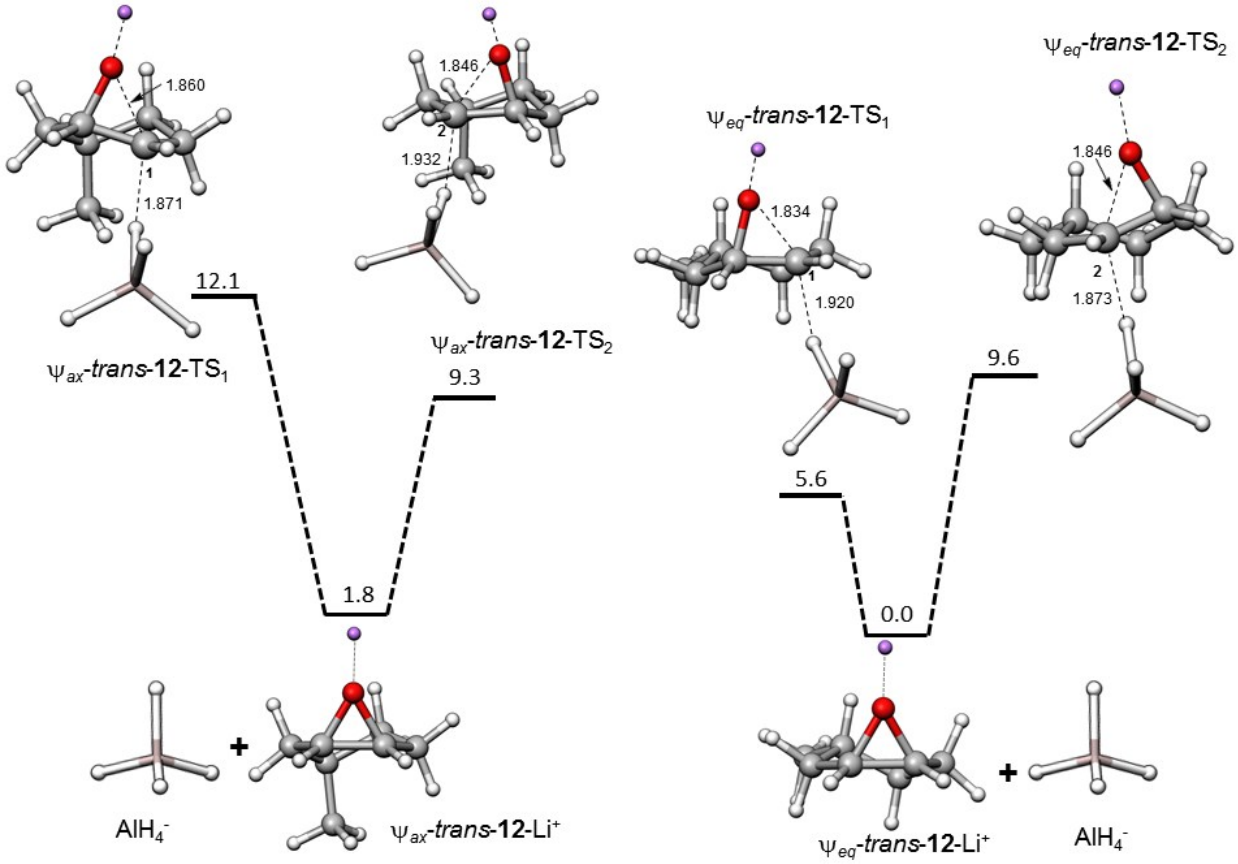
Geometry optimizations performed at B3LYP/6-31+G*(PCM). Free energy corrections to electronic energies calculated at 298 K. Depicted free energies are in kcal/mol and are relative to the pseudoequatorial conformer; the pseudoequatorial preference of the corresponding neutral compounds is shown in parenthesis.

FIGURE S1. Reaction coordinate for the ring opening of *cis*-**12**-Li^+ with AlH_4^-.



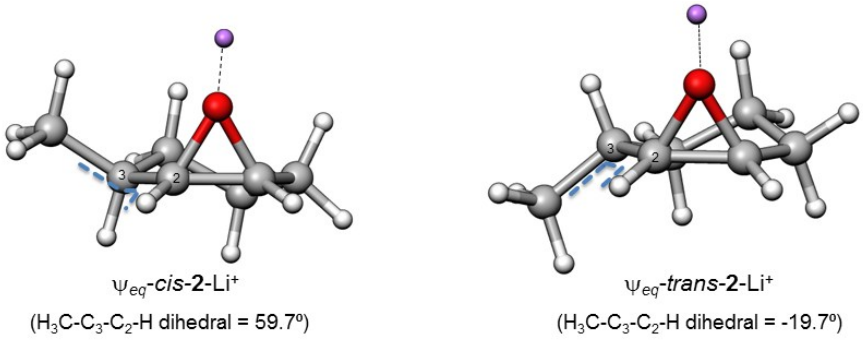
Structures optimized at B3LYP/6-31+G*(PCM). Free energies provided in kcal/mol and relative to separated ψ_{eq}-*cis*-**12**-Li^+ and AlH_4^-.

FIGURE S2. Reaction coordinate for the ring opening of *trans*-**12**-Li^+ with AlH_4^-.



Structures optimized at B3LYP/6-31+G*(PCM). Free energies provided in kcal/mol and relative to separated ψ*eq*-*trans*-**12**-Li^+ and AlH_4^-.

FIGURE S3: H_3C-C_3-C_2-H dihedral angles for ψ*eq*-*cis*-**2**-$Li^+$and ψ*eq*-*trans*-**2**-Li^+



Structures optimized at B3LYP/6-31+G*(PCM).

B3LYP/6-31+G*(PCM) Cartesian coordinates for **11**-Li^+, *cis*-**1**-Li^+, *trans*-**1**-Li^+, *cis*-**2**-Li^+, *trans*-**2**-Li^+, *cis*-**12**-Li^+, and *trans*-**12**-Li^+ systems.

11-Li^+ (NIMAG = 0)

1 1

C	-0.49553	1.52086	-0.02620
H	-0.71907	2.37954	-0.67016
C	-1.72681	0.60034	0.07687
H	-2.17339	0.48315	-0.92058
C	-1.36961	-0.78729	0.62670
H	-2.27439	-1.39646	0.73307
C	-0.38421	-1.51118	-0.30644
H	-0.01556	-2.44008	0.14805
H	-0.89493	-1.80084	-1.23608
C	0.78904	-0.64919	-0.70633
C	0.73273	0.81929	-0.57650
H	1.38994	1.40893	-1.21389
H	-0.23947	1.93141	0.95987
H	1.46942	-1.07242	-1.44475
H	-2.48597	1.07927	0.70569
H	-0.93293	-0.69163	1.62961
O	1.49384	0.01511	0.39015
Li	3.21734	0.01376	1.21980

11-TS_1 (NIMAG = 1)

0 1

C	-1.30271	-0.26885	1.43261
H	-0.56285	-0.79156	2.05463
C	-0.96205	-1.75625	-0.59275
H	-1.44063	-2.47574	-1.26848
H	-0.13976	-2.28436	-0.09147
C	-0.37508	-0.59815	-1.41705
H	-1.12799	-0.21342	-2.11761
H	0.46893	-0.93932	-2.02456
C	0.08642	0.54934	-0.55268
C	-0.58200	0.86378	0.71437
H	-2.04563	0.16508	2.11517
C	-1.96353	-1.26096	0.46180
H	-2.36460	-2.11141	1.02698
H	-0.01271	1.49797	1.40444
H	0.77207	1.28275	-0.95366
H	1.66121	-0.35798	0.06396
H	-2.81572	-0.77843	-0.03507
Al	3.30050	-0.06750	0.21655
H	3.44891	1.55421	0.06640
H	3.77169	-0.59055	1.68349
H	4.03989	-0.85490	-1.00307
O	-1.37449	1.59257	-0.21159
Li	-1.65656	3.28705	-0.77380

11-TS_2 (NIMAG = 1)

0 1

C	1.69119	-1.22336	-0.87301
H	2.59468	-0.60387	-0.92507
H	1.88004	-2.12145	-1.47354
C	1.40869	-1.60686	0.58625
H	2.21935	-2.23175	0.98067
H	0.49650	-2.21798	0.61965
C	1.22322	-0.36859	1.48676
H	2.19805	0.02151	1.80919
H	0.67723	-0.65000	2.39530
C	0.49035	0.78705	0.79635
H	-0.14758	1.34752	1.49003
C	0.49986	-0.45778	-1.47897
H	-0.29195	-1.16021	-1.76078
H	0.79031	0.05907	-2.40230
C	-0.10453	0.54230	-0.52292
H	-0.80079	1.27967	-0.89850
H	-1.63781	-0.41288	-0.02868
O	1.31335	1.62345	-0.00457
Li	1.42416	3.37069	-0.45664
Al	-3.29173	-0.17011	0.09738
H	-3.46623	1.45133	-0.01682
H	-3.77183	-0.74026	1.54241
H	-3.97950	-0.94550	-1.15776

ψ_{ax}-*cis*-**1**-Li^+ (NIMAG = 0)

1 1

C	-1.32017	1.54930	-0.64587
H	-1.85217	2.50124	-0.75899
C	-0.13165	1.75248	0.31272
H	-0.51879	2.26521	1.20487
C	0.58345	0.47286	0.81281
H	1.20003	0.81715	1.65420
C	-0.47069	-0.48139	1.45519
H	-0.11728	-1.51799	1.48917
H	-0.60284	-0.18609	2.50532
C	-1.86762	-0.47059	0.87553
C	-2.30061	0.51400	-0.13137
H	-3.36022	0.75738	-0.18860
H	-0.98968	1.26110	-1.64983
H	-2.63168	-0.90871	1.51759
H	0.58450	2.44497	-0.13825
C	1.64174	-0.20085	-0.14021
C	2.47163	-1.21120	0.68749
C	2.61882	0.87718	-0.66068
C	1.04965	-0.94721	-1.35187
O	-2.03451	-0.87271	-0.52302
Li	-2.84097	-2.39289	-1.34175

H	1.85895	-1.41026	-1.93077
H	0.50674	-0.27697	-2.02591
H	0.36146	-1.74112	-1.04449
H	3.26940	-1.64173	0.07026
H	1.86703	-2.04573	1.06102
H	2.94389	-0.72606	1.55114
H	3.45809	0.40436	-1.18500
H	3.03423	1.47252	0.16276
H	2.14005	1.56366	-1.36767

ψ_{ax}-*cis*-**1**-TS_1 (NIMAG = 1)

0 1

C	-0.07834	0.11939	1.37420
H	0.53209	-0.54040	2.00684
C	-0.13407	-1.38766	-0.66323
H	-0.76342	-1.95927	-1.35394
H	0.56827	-2.10674	-0.22225
C	0.70251	-0.37991	-1.47449
H	0.07182	0.21285	-2.14491
H	1.40973	-0.91785	-2.11420
C	1.47831	0.56793	-0.60193
C	0.91797	1.02910	0.66889
H	-0.67026	0.72681	2.06626
C	-0.98204	-0.79700	0.49495
H	-1.20507	-1.65023	1.15125
H	1.64282	1.43946	1.38301
C	-2.41963	-0.27921	0.09973
C	-3.29177	-1.51124	-0.24353
C	-3.08234	0.42837	1.30244
C	-2.45330	0.68067	-1.10670
H	2.34791	1.07933	-0.99004
H	2.73776	-0.76676	-0.02040
Al	4.37519	-0.78900	0.31876
H	4.81133	0.78855	0.31793
H	5.10625	-1.61178	-0.88149
H	4.58075	-1.47892	1.77761
O	0.39022	2.00149	-0.22154
Li	0.88784	3.69659	-0.67779
H	-2.14793	0.17744	-2.03238
H	-1.79379	1.53811	-0.94995
H	-3.47764	1.04561	-1.26201
H	-2.88441	-2.08416	-1.08437
H	-4.30500	-1.19630	-0.52364
H	-3.37829	-2.18992	0.61491
H	-4.14680	0.59952	1.09755
H	-2.62910	1.40458	1.50810
H	-3.01351	-0.17727	2.21588

ψ_{ax}-*cis*-**1**-TS_2 (NIMAG = 1)

0 1

C	-0.02970	0.09598	-1.04768
H	-0.06698	-0.61389	-1.87725
C	0.39057	0.11002	1.50073
H	1.25316	0.22742	2.16399
H	-0.26868	-0.61608	1.99042
C	-0.35549	1.45474	1.42037
H	0.29602	2.23252	1.00568
H	-0.64388	1.77930	2.42711
C	-1.59143	1.35420	0.51858
H	-2.53413	1.26872	1.07123
C	-1.42606	0.45071	-0.62454
H	0.42120	1.01582	-1.43921
C	0.83251	-0.47430	0.12206
H	0.60577	-1.54729	0.15240
C	2.37211	-0.38178	-0.16251
C	3.12976	-1.26105	0.85802
C	2.68055	-0.93905	-1.57047
C	2.90655	1.06262	-0.07021
H	-2.28190	0.23938	-1.24588
H	-1.84631	-1.32419	0.06861
Al	-3.27662	-2.19156	0.06440
H	-4.38292	-1.11485	-0.48509
H	-3.59292	-2.66660	1.58709
H	-3.09475	-3.43625	-0.96791
O	-1.62186	2.29904	-0.54388
Li	-3.07209	3.08164	-1.33699
H	2.27119	-0.30698	-2.36665
H	2.27089	-1.94984	-1.69673
H	3.76509	-0.99788	-1.72616
H	2.41423	1.73220	-0.78620
H	3.98107	1.08267	-0.29272
H	2.77224	1.48410	0.93288
H	2.78943	-2.30335	0.80825
H	2.99665	-0.91483	1.88894
H	4.20638	-1.24971	0.64586

ψ_{eq}-*cis*-**1**-Li^+ *exo* (NIMAG = 0)

1 1

C	0.38763	-1.13748	-0.42020
H	0.03404	-1.80045	-1.21643
C	-0.46161	0.15774	-0.38984
H	-0.52042	0.51489	-1.43106
C	0.27951	1.24798	0.41158
H	0.48398	0.89554	1.43004
H	-0.33464	2.14828	0.50739
C	1.60198	1.63905	-0.26785

H	2.17187	2.34089	0.35532
H	1.39903	2.15766	-1.21565
C	2.46197	0.44411	-0.59347
C	1.86746	-0.90209	-0.66096
H	2.38396	-1.65401	-1.25560
H	0.28233	-1.69870	0.51787
H	3.37564	0.63413	-1.15573
C	-1.94510	-0.08147	0.06065
C	-2.78545	1.17758	-0.24958
C	-2.55659	-1.25596	-0.73534
C	-2.05324	-0.39115	1.56879
O	2.66289	-0.50035	0.50657
Li	4.04298	-1.11033	1.66698
H	-1.46185	-1.26992	1.85412
H	-3.09626	-0.60212	1.83483
H	-1.72314	0.45356	2.18424
H	-2.44338	-1.10751	-1.81743
H	-3.62942	-1.33713	-0.52277
H	-2.10070	-2.21769	-0.47440
H	-2.74306	1.42835	-1.31736
H	-2.45244	2.05387	0.31709
H	-3.83702	1.00440	0.00934

ψ_{eq}-*cis*-**1**-TS_1 (NIMAG = 1)

0 1

C	0.27255	0.48332	-1.16763
H	0.17900	-0.22632	-1.99660
C	0.87138	-0.23802	0.06661
H	0.37133	-1.21715	0.12713
C	0.49850	0.52761	1.35312
H	0.85663	1.56089	1.29106
H	0.97144	0.07463	2.23052
C	-1.02401	0.53006	1.57974
H	-1.30149	1.25871	2.35206
H	-1.35013	-0.44695	1.95202
C	-1.80130	0.82315	0.32132
H	-2.84949	1.08024	0.38709
C	-1.09972	1.12242	-0.93052
H	-1.72522	1.09190	-1.83051
H	0.93475	1.28801	-1.51417
C	2.40147	-0.55363	-0.07562
C	2.83048	-1.54616	1.02833
C	2.67360	-1.22951	-1.43802
C	3.27267	0.71542	0.03525
H	-2.42292	-0.89788	-0.05870
Al	-3.71202	-1.95965	-0.17305
H	-5.02622	-1.07367	0.22148
H	-3.43137	-3.15572	0.89515
H	-3.77093	-2.48447	-1.71319
O	-1.07767	2.40017	-0.31338

Li	-1.84981	4.04676	-0.32573
H	2.50300	-0.54884	-2.27956
H	2.03241	-2.10936	-1.57936
H	3.71704	-1.56458	-1.49353
H	3.00546	1.46602	-0.71856
H	4.32951	0.46143	-0.11679
H	3.18608	1.18385	1.02260
H	3.88435	-1.82465	0.90127
H	2.23462	-2.46695	0.98532
H	2.72546	-1.12344	2.03364

ψ_{eq}-*cis*-**1**-TS_2 (NIMAG = 1)

0 1

C	-0.05051	-0.02051	-0.99481
H	-0.13424	-0.98259	-1.50615
C	0.86363	-0.12721	0.24722
H	0.46385	-0.95859	0.84835
C	0.72564	1.15486	1.09844
H	1.04207	2.02776	0.51411
H	1.37918	1.10711	1.97591
C	-0.71869	1.36945	1.57942
H	-0.80725	2.32354	2.11635
H	-1.00313	0.57715	2.28545
C	-1.72234	1.35609	0.43768
H	-2.76046	1.38553	0.78958
C	-1.45029	0.43583	-0.66809
H	0.36869	0.68382	-1.72503
C	2.34353	-0.51763	-0.09832
C	3.09189	-0.88990	1.20153
C	2.36399	-1.75964	-1.01753
C	3.10625	0.62758	-0.79794
H	-2.24380	0.25588	-1.37983
H	-1.97367	-1.24382	0.09476
Al	-3.30794	-2.25008	0.14501
H	-4.39343	-1.55063	-0.85865
H	-3.83962	-2.28074	1.68354
H	-2.83961	-3.71441	-0.38982
O	-1.44578	2.26755	-0.61540
Li	-2.31794	3.39174	-1.74400
H	1.97889	-1.54082	-2.01994
H	1.76639	-2.57847	-0.59662
H	3.39200	-2.12359	-1.13740
H	2.60965	0.94747	-1.72230
H	4.11676	0.29619	-1.06901
H	3.21190	1.50534	-0.15008
H	4.11080	-1.22601	0.97105
H	2.58304	-1.70607	1.73044
H	3.17657	-0.04210	1.88986

ψ_{ax}-*trans*-**1**-Li^+ (NIMAG = 0)

1 1

C	0.51950	-0.08851	-0.87902
C	-0.46705	-1.26166	-0.63223
C	-1.56227	-0.97126	0.38049
C	-1.89090	0.40220	0.80098
C	-1.12973	1.58160	0.24897
C	-0.28968	1.22671	-0.98943
H	-0.95788	-1.52536	-1.57800
H	0.06494	-2.16217	-0.31099
H	0.94292	-0.24936	-1.87968
H	-2.36595	0.54158	1.77172
H	-1.83674	2.38784	0.01163
H	-0.49564	1.96627	1.05670
H	-0.96453	1.12010	-1.84929
H	0.36818	2.06734	-1.22804
H	-1.82604	-1.78201	1.05811
C	1.76882	-0.09376	0.07996
C	2.69759	-1.25671	-0.34468
C	2.56815	1.21753	-0.07722
C	1.42208	-0.28599	1.57359
O	-2.75611	-0.29749	-0.15065
Li	-4.64332	-0.59490	-0.33931
H	3.51638	1.14961	0.46991
H	2.02622	2.08454	0.31736
H	2.80716	1.41737	-1.12976
H	2.34586	-0.32812	2.16366
H	0.88320	-1.22335	1.75616
H	0.82153	0.53501	1.97737
H	3.58672	-1.28936	0.29655
H	3.03730	-1.13232	-1.38057
H	2.20618	-2.23392	-0.26820

ψ_{ax}-*trans*-**1**-TS_1 (NIMAG = 1)

0 1

C	-0.68182	-0.85071	1.29753
C	-1.30379	-0.55493	-0.10595
H	-1.80706	-1.48249	-0.40971
C	-0.23160	-0.27668	-1.19646
H	-0.60486	-0.60888	-2.17186
H	-0.03120	0.79879	-1.29422
C	0.75727	-0.34771	1.52422
H	0.75769	0.74150	1.63811
H	1.15179	-0.75192	2.46399
C	1.68723	-0.67239	0.38514
C	1.11986	-0.93039	-0.93786
H	1.80655	-0.79599	-1.78208
H	-0.68600	-1.93290	1.45559
H	-1.30161	-0.42350	2.09220

C	-2.43762	0.53199	-0.08327
C	-3.62874	0.01515	0.75497
C	-1.95068	1.87073	0.50897
C	-2.96043	0.78108	-1.51590
H	2.71559	-0.95191	0.56136
H	2.43215	1.06806	0.10955
Al	3.97988	1.67772	-0.07945
H	4.85391	0.38256	-0.56360
H	4.46000	2.20735	1.38338
H	3.93373	2.85398	-1.20095
O	1.08337	-2.25304	-0.43096
Li	2.11350	-3.71830	-0.27606
H	-2.20795	1.25214	-2.15754
H	-3.83171	1.44764	-1.49022
H	-3.27340	-0.15693	-1.99385
H	-1.11005	2.29023	-0.05605
H	-1.63459	1.76467	1.55337
H	-2.76036	2.61115	0.48746
H	-4.02253	-0.92294	0.34163
H	-4.44473	0.74885	0.75257
H	-3.35943	-0.16741	1.80136

ψ_{ax}-*trans*-**1**-TS_2 (NIMAG = 1)

0 1

C	-1.20068	-0.73986	-0.51850
C	-0.82445	-1.75497	0.59676
H	-1.67245	-1.90258	1.27370
H	-0.64687	-2.72625	0.11875
C	0.05974	-0.36124	-1.36004
H	-0.05403	0.60892	-1.84830
H	0.15479	-1.08073	-2.18402
C	1.39346	-0.35712	-0.66305
C	1.63804	-1.12624	0.55847
H	2.51040	-0.81613	1.14691
H	-1.83711	-1.29653	-1.22053
C	-2.13350	0.44910	-0.06545
C	-2.34616	1.43909	-1.23352
C	-1.61474	1.23903	1.15380
C	-3.52217	-0.13527	0.28850
C	0.42404	-1.40999	1.42672
H	0.25628	-0.53634	2.06594
H	0.66154	-2.24961	2.09431
H	2.25488	-0.00162	-1.20926
H	1.39144	1.45980	-0.00291
Al	2.63301	2.55513	0.24782
H	2.37529	3.82853	-0.73147
H	3.97931	1.72542	-0.17976
H	2.64183	2.95357	1.82468
O	1.91747	-2.12468	-0.41163
Li	3.51651	-2.75201	-1.04314

H	-0.60280	1.62201	0.99070
H	-1.61099	0.62647	2.06266
H	-2.27169	2.09745	1.34621
H	-2.61181	0.91778	-2.16318
H	-1.46010	2.05368	-1.42577
H	-3.16599	2.12750	-0.99426
H	-3.97261	-0.64231	-0.57519
H	-4.20394	0.66734	0.59611
H	-3.47523	-0.85484	1.11343

ψ_{eq}-*trans*-**1**-Li^+ (NIMAG = 0)

1 1

C	1.63106	1.65884	0.18952
H	1.99193	2.59866	-0.24484
C	0.14201	1.46310	-0.15019
H	-0.00332	1.66826	-1.21954
C	-0.35225	0.03583	0.16553
C	0.40736	-0.95405	-0.74850
H	0.22235	-1.99327	-0.45348
H	0.05923	-0.85908	-1.78656
C	1.90181	-0.73485	-0.77589
C	2.50407	0.52982	-0.32032
H	3.48624	0.79684	-0.70737
H	1.77187	1.74400	1.27545
H	2.45810	-1.34101	-1.49049
H	-0.43857	2.21423	0.39354
H	-0.06198	-0.19343	1.20247
C	-1.91168	-0.13480	0.11509
C	-2.55212	0.68581	1.25713
C	-2.28920	-1.61588	0.34049
C	-2.51155	0.33193	-1.22817
O	2.55969	-0.66720	0.53061
Li	3.87488	-1.64281	1.52433
H	-2.08694	-0.21032	-2.08162
H	-2.35632	1.40365	-1.39645
H	-3.59385	0.15379	-1.23693
H	-1.99519	-2.25288	-0.50111
H	-3.37517	-1.71404	0.45694
H	-1.82062	-2.01463	1.25034
H	-2.37575	1.76151	1.14996
H	-2.16274	0.37429	2.23524
H	-3.63846	0.53509	1.26845

ψ_{eq}-*trans*-**1**-TS_1 (NIMAG = 1)

0 1

C	1.13072	0.25270	0.17337
C	0.28678	-0.49770	1.22758
H	-0.02798	-1.46840	0.82388

H	0.87094	-0.70041	2.13121
C	-0.97298	0.28470	1.63143
H	-0.69735	1.16829	2.22216
H	-1.62013	-0.32630	2.26864
C	0.27085	0.45955	-1.09373
H	0.08564	-0.50128	-1.59254
H	0.78516	1.10149	-1.81781
C	-1.08601	1.09494	-0.81320
H	-1.71859	1.11270	-1.70896
C	-1.76492	0.74274	0.43586
H	1.34858	1.25337	0.57710
C	2.52911	-0.40443	-0.10725
C	3.26206	0.36603	-1.22860
C	2.41179	-1.88674	-0.52104
C	3.40451	-0.31306	1.16315
H	-2.80519	1.01656	0.54238
H	-2.44678	-1.00832	0.03182
Al	-3.95545	-1.62244	-0.35038
H	-4.42150	-2.57317	0.88623
H	-3.82931	-2.42773	-1.75827
H	-4.90613	-0.29704	-0.48620
O	-1.04126	2.33608	-0.12328
Li	-2.05726	3.81939	0.06335
H	2.78908	0.22566	-2.20674
H	4.29752	0.01341	-1.31463
H	3.29319	1.44360	-1.01830
H	1.78883	-2.01634	-1.41391
H	1.98482	-2.50177	0.27928
H	3.40492	-2.29246	-0.75256
H	4.40799	-0.70903	0.96211
H	2.99049	-0.88877	1.99805
H	3.51696	0.72836	1.49281

ψ_{eq}-*trans*-**1**-TS_2 (NIMAG = 1)

0 1

C	1.06152	0.33459	0.03243
C	0.46383	0.29090	1.45360
H	0.05936	-0.71175	1.64179
H	1.23375	0.46647	2.21252
C	-0.66402	1.32318	1.64218
H	-0.24507	2.32704	1.79461
H	-1.23868	1.07618	2.54314
C	-0.03473	-0.09400	-0.97297
H	-0.12042	-1.18537	-1.00709
H	0.21929	0.22087	-1.99128
C	-1.40560	0.44627	-0.64635
H	-2.19094	0.35178	-1.38407
C	-1.61257	1.40623	0.44247
H	-2.65817	1.54655	0.74112
H	1.30774	1.38270	-0.19028

C	2.39891	-0.46801	-0.13305
C	2.82631	-0.48348	-1.61772
C	2.27547	-1.92290	0.36558
C	3.51793	0.23766	0.66524
H	-2.15789	-1.09451	0.11710
Al	-3.57785	-1.97714	0.00497
H	-3.25756	-3.25669	-0.94933
H	-4.63708	-0.94817	-0.69637
H	-4.02951	-2.40073	1.50824
O	-1.19993	2.29278	-0.58872
Li	-2.05773	3.42837	-1.72100
H	2.14663	-1.07762	-2.23894
H	3.82695	-0.92180	-1.71991
H	2.86494	0.53302	-2.03230
H	1.47750	-2.47076	-0.14969
H	2.07188	-1.96862	1.44139
H	3.21300	-2.46404	0.18476
H	4.47288	-0.28507	0.52766
H	3.31113	0.26027	1.74089
H	3.65260	1.27310	0.32568

ψ_{ax}-*cis*-**2**-Li^+ (NIMAG = 0)

1 1

C	1.45551	-1.23955	-0.05061
C	1.41445	0.14882	0.53912
C	0.13012	0.80987	0.83349
C	-1.21423	0.13982	0.57846
C	-1.05831	-1.35325	0.20012
C	0.13253	-1.62860	-0.72910
H	2.29396	0.46473	1.10009
H	2.29920	-1.31405	-0.74882
H	-1.98971	-1.70604	-0.25894
H	-0.92279	-1.93973	1.11946
H	0.02049	-1.07718	-1.67086
H	0.16250	-2.69243	-0.99062
H	0.12969	1.60173	1.58216
H	1.67113	-1.93169	0.77601
H	-1.74745	0.18886	1.53738
C	-2.04031	0.93668	-0.44659
H	-2.12610	1.99250	-0.15989
H	-3.05396	0.52712	-0.51346
H	-1.58959	0.88943	-1.44402
O	0.91116	1.19433	-0.35436
Li	1.54826	2.85310	-1.01429

ψ_{ax}-*cis*-**2**-TS_1 (NIMAG = 1)

0 1

C	0.49605	-0.04628	0.90473

C	-0.26788	-0.86816	-0.03950
H	0.28177	-1.72826	-0.44532
C	-1.08071	-0.16790	-1.14309
C	-0.00402	1.31617	1.32156
H	0.78222	2.04326	1.08956
H	-0.12522	1.33442	2.41176
C	-1.31121	1.71033	0.61086
C	-1.25249	1.35075	-0.88099
H	1.24290	-0.54369	1.50769
H	-2.15673	1.70867	-1.39039
H	-2.15739	1.20402	1.08882
H	-1.47105	2.78900	0.72993
H	-0.40847	1.88917	-1.33282
H	1.92725	0.46778	-0.16603
H	-0.49453	-0.28196	-2.06461
C	-2.42012	-0.89033	-1.35348
H	-3.07400	-0.77476	-0.48178
H	-2.27347	-1.96537	-1.52371
H	-2.94036	-0.48324	-2.22846
O	-0.96438	-1.17134	1.16303
Li	-0.96204	-2.79472	2.01541
Al	3.45487	-0.11205	-0.55037
H	3.43818	-0.52527	-2.12377
H	3.63458	-1.41411	0.42207
H	4.52440	1.06445	-0.20908

ψ_{ax}-*cis*-**2**-TS_2 (NIMAG = 1)

0 1

C	0.50368	-1.12056	-0.63894
H	-0.27354	-1.83755	-0.92715
C	1.05788	-1.53770	0.74172
H	0.21926	-1.87793	1.36440
C	1.78187	-0.39601	1.47223
H	2.65483	-0.06962	0.89333
H	2.15860	-0.75538	2.43794
C	0.83876	0.79531	1.69886
H	1.37875	1.64632	2.13508
H	0.04766	0.51850	2.40968
C	0.17069	1.25346	0.40956
H	-0.59250	2.02124	0.58983
C	-0.20079	0.21868	-0.56230
H	1.72794	-2.39756	0.61417
C	1.56889	-1.16242	-1.75390
H	1.93404	-2.18959	-1.87262
H	1.14722	-0.84340	-2.71482
H	2.41662	-0.51220	-1.52079
H	-0.83866	0.51722	-1.38335
H	-1.78726	-0.45023	0.24503
Al	-3.43294	-0.21313	0.04575
H	-3.97525	-1.44182	-0.87541

H	-3.54549	1.21774	-0.73942
H	-4.12124	-0.16611	1.51818
O	1.06804	1.56433	-0.64451
Li	1.06902	2.85723	-1.93871

ψ_{eq}-*cis*-**2**-Li^+ *exo* (NIMAG = 0)

0 1

C	-1.05904	-0.55349	0.42856
C	-0.32915	0.73930	0.72892
C	1.11810	0.88834	0.49414
C	1.95005	-0.24701	-0.07237
C	1.20949	-1.59729	-0.05962
C	-0.24828	-1.46009	-0.51732
H	-0.79432	1.38022	1.47879
H	-1.13853	-1.06434	1.40138
H	2.24240	0.02118	-1.09636
H	2.87784	-0.31716	0.50736
H	1.74502	-2.31198	-0.69489
H	1.22700	-2.00910	0.95927
H	-0.28434	-1.05393	-1.53756
H	-0.72705	-2.44591	-0.55322
C	-2.48101	-0.28442	-0.08616
H	-3.02344	-1.22649	-0.22353
H	-3.05392	0.33153	0.61798
H	-2.45733	0.23065	-1.05423
H	1.64932	1.64261	1.07316
O	0.15007	1.49553	-0.43393
Li	-0.14135	3.31550	-0.96786

ψ_{eq}-*cis*-**2**-TS_1 (NIMAG = 1)

0 1

C	-1.24263	-0.03839	-1.01958
C	-0.53836	2.04136	0.27753
H	-0.89066	2.98463	0.71285
H	0.19761	2.29821	-0.49582
C	0.16001	1.20814	1.36334
H	-0.47467	1.14255	2.25677
H	1.09616	1.67892	1.67939
C	0.45930	-0.19473	0.89802
H	1.20145	-0.78603	1.41624
C	-0.41728	-0.88686	-0.05091
C	-1.70542	1.27797	-0.36624
H	-2.18542	1.90519	-1.12870
H	0.02401	-1.75835	-0.55122
H	1.90921	0.33874	-0.23717
H	-2.47059	1.05920	0.39176
H	-0.56114	0.21370	-1.84646
C	-2.41597	-0.84529	-1.59057

H	-2.97503	-0.25188	-2.32406
H	-2.06773	-1.75642	-2.09380
H	-3.11234	-1.13956	-0.79560
O	-1.04741	-1.19730	1.18359
Li	-1.06117	-2.52167	2.43483
Al	3.42625	-0.22684	-0.65788
H	3.52515	-0.23125	-2.28186
H	3.48991	-1.73753	-0.03389
H	4.51785	0.75899	0.04129

ψ_{eq}-*cis*-**2**-TS_2 (NIMAG = 1)

0 1

C	0.55328	1.04726	-0.67102
C	1.14615	-1.29333	-1.46951
H	1.88547	-1.88720	-2.02092
H	0.22963	-1.29535	-2.07492
C	0.85656	-1.95722	-0.10829
H	1.77886	-2.36853	0.32367
H	0.16681	-2.79876	-0.24491
C	0.27473	-0.99202	0.92937
H	-0.43711	-1.48619	1.60181
C	-0.13373	0.34602	0.48334
C	1.63206	0.15486	-1.31914
H	1.88593	0.57343	-2.30122
H	2.54517	0.18401	-0.71072
H	-0.73185	0.93230	1.16859
H	-1.76133	-0.06055	-0.32905
Al	-3.42216	0.03972	-0.12283
H	-3.95134	1.19509	-1.14007
H	-3.61074	0.46769	1.44307
H	-4.04735	-1.42733	-0.44228
O	1.23690	-0.20377	1.61310
Li	1.54049	0.37836	3.29429
H	-0.23195	1.21450	-1.41829
C	1.09531	2.42769	-0.26669
H	0.30664	3.05778	0.16278
H	1.49583	2.94782	-1.14507
H	1.90258	2.33038	0.46829

ψ_{ax}-*trans*-**2**-Li^+ *exo* (NIMAG = 0)

1 1

C	-0.90448	-0.83416	0.36821
C	0.39784	-0.95435	-0.39887
C	1.19274	0.22888	-0.78196
C	0.75540	1.63452	-0.41431
C	-0.69665	1.70330	0.09588
C	-1.03154	0.54744	1.04935
H	0.51163	-1.85740	-0.99931
H	-0.89178	-1.60808	1.14976

H	1.44977	2.01847	0.34495
H	0.87690	2.27444	-1.29613
H	-0.86001	2.66399	0.59723
H	-1.38083	1.68309	-0.76206
H	-0.36366	0.58837	1.91982
H	-2.05263	0.65871	1.43334
H	1.86425	0.13262	-1.63365
C	-2.08012	-1.15250	-0.57557
H	-1.97748	-2.15286	-1.01283
H	-3.02486	-1.12553	-0.02218
H	-2.15326	-0.43466	-1.40052
O	1.61510	-0.61946	0.34096
Li	3.09400	-1.64142	0.96587

ψ_{ax}-*trans*-**2**-TS_1 (NIMAG = 1)

0 1

C	1.44591	-0.71671	-0.80993
C	0.92516	-0.74764	1.70452
H	1.37290	-0.86320	2.69924
H	0.19637	-1.55950	1.58971
C	0.18400	0.59707	1.63382
H	0.83361	1.40523	1.99468
H	-0.70025	0.59539	2.27818
C	-0.24453	0.93599	0.22751
C	0.55040	0.51871	-0.93479
C	2.01100	-0.85486	0.62209
H	2.53386	-1.81611	0.71001
H	0.02605	0.54805	-1.89785
H	2.76164	-0.07111	0.78908
H	2.29100	-0.54657	-1.49412
C	0.70716	-1.98024	-1.28542
H	0.35827	-1.86715	-2.31935
H	1.37609	-2.84854	-1.25112
H	-0.16902	-2.20014	-0.66689
H	-1.01301	1.67887	0.06625
H	-1.70241	-0.31249	0.22568
Al	-3.34133	-0.20189	-0.08659
H	-4.01102	-1.66826	0.12255
H	-3.45840	0.33627	-1.62355
H	-3.90768	0.90975	0.96642
O	1.17686	1.74451	-0.58980
Li	1.25331	3.47801	-1.09720

ψ_{ax}-*trans*-**2**-TS_2 (NIMAG = 1)

0 1

C	-0.74686	1.03589	-0.87645
C	-1.37231	0.63653	1.56781
H	-2.12951	0.83703	2.33579
H	-0.46748	1.17868	1.87274

C	-1.06669	-0.87267	1.51859
H	-1.99410	-1.45550	1.59940
H	-0.43769	-1.15254	2.37196
C	-0.37760	-1.30323	0.21924
H	0.37449	-2.08340	0.38710
C	0.02703	-0.25952	-0.72752
H	-1.23185	0.97307	-1.86052
C	-1.84543	1.16604	0.20736
H	-2.13693	2.22070	0.28917
H	-2.73728	0.61049	-0.10658
C	0.16778	2.27647	-0.93394
H	0.98833	2.13884	-1.64625
H	-0.42346	3.14331	-1.25287
H	0.61054	2.49387	0.04203
H	0.71484	-0.54229	-1.51366
H	1.60417	0.34743	0.16316
Al	3.19016	-0.17856	0.29889
H	4.16869	1.07041	-0.05820
H	3.30217	-1.38241	-0.80443
H	3.39274	-0.73006	1.81696
O	-1.25414	-1.59544	-0.86302
Li	-1.25072	-2.88662	-2.15588

ψ_{eq}-*trans*-**2**-Li^+ (NIMAG = 0)

1 1

C	-1.32362	1.26538	0.52673
C	-1.22642	-0.22063	0.76958
C	-0.03225	-0.98340	0.35974
C	1.15797	-0.32363	-0.32922
C	1.08074	1.21643	-0.25766
C	-0.32727	1.75945	-0.53421
H	-1.83202	-0.61732	1.58405
H	-2.35575	1.52398	0.25643
H	1.11203	-0.62467	-1.38608
H	1.80130	1.64199	-0.96612
H	1.39788	1.54159	0.74479
H	-0.65957	1.44853	-1.53324
H	-0.31628	2.85529	-0.53248
H	0.17443	-1.91638	0.88429
H	-1.12031	1.75723	1.48885
C	2.47480	-0.84949	0.26314
H	3.33088	-0.38204	-0.23553
H	2.56575	-1.93556	0.14187
H	2.54718	-0.62013	1.33377
O	-1.27091	-1.06513	-0.42648
Li	-2.43400	-2.44538	-1.05248

ψ_{eq}-*trans*-**2**-TS_1 (NIMAG = 1)

0 1

C	-0.19522	-1.04652	0.09917
C	0.47476	-0.07423	0.97130
H	-0.12490	0.25464	1.82987
C	1.24921	1.09411	0.33207
C	0.34757	-1.37008	-1.27098
H	-0.46965	-1.23308	-1.98730
H	0.61090	-2.43449	-1.30870
C	1.54585	-0.48551	-1.66142
C	1.32975	0.96321	-1.20407
H	-0.90854	-1.71730	0.55785
H	2.13610	1.60635	-1.57926
H	2.46292	-0.88286	-1.20964
H	1.67988	-0.52547	-2.74913
H	0.39587	1.34114	-1.64481
H	2.26941	1.01738	0.73752
C	0.66297	2.45130	0.74597
H	-0.37719	2.54970	0.41202
H	1.23686	3.27389	0.30197
H	0.68033	2.57997	1.83576
H	-1.70502	-0.06198	-0.41063
Al	-3.33830	0.10453	-0.07597
H	-3.52935	-0.60183	1.38568
H	-4.13930	-0.69666	-1.24572
H	-3.68289	1.69348	-0.04481
O	1.25098	-1.23363	1.24125
Li	1.45509	-2.28211	2.70156

ψ_{eq}-*trans*-**2**-TS_2 (NIMAG = 1)

0 1

C	0.57607	-1.30923	-0.06796
C	-0.01132	-0.21359	0.70736
C	0.52524	1.20111	0.62070
C	1.28046	-0.95588	-1.36992
H	0.51982	-0.94413	-2.16260
H	1.98784	-1.75881	-1.61705
C	1.99304	0.40430	-1.31058
C	1.05252	1.50450	-0.79521
H	-0.04936	-2.20451	-0.16766
H	1.56883	2.47301	-0.78197
H	2.87015	0.33364	-0.65360
H	2.36471	0.66570	-2.30912
H	0.19553	1.60549	-1.47573
H	1.38459	1.22574	1.30606
C	-0.47701	2.25243	1.12052
H	-1.33947	2.32667	0.45183
H	0.00970	3.23357	1.17189
H	-0.84634	2.00761	2.12422
H	-0.70609	-0.47402	1.49526
H	-1.61526	0.12471	-0.35505

Al	-3.16689	-0.48994	-0.43205
H	-3.23798	-1.48310	-1.72168
H	-4.20312	0.75960	-0.54719
H	-3.35220	-1.31586	0.96890
O	1.39668	-1.31159	1.09363
Li	1.60361	-2.33841	2.57054

ψ_{ax}-*cis*-**12**-Li^+ (NIMAG = 0)

1 1

C	-0.01343	1.62130	-0.43048
H	-0.13573	2.69674	-0.25763
C	1.32138	1.14898	0.17847
H	1.41051	1.56745	1.19081
C	1.45477	-0.38403	0.27013
H	2.39121	-0.59436	0.80369
C	0.31645	-0.95558	1.15085
H	0.25488	-2.04776	1.05177
H	0.54561	-0.75734	2.20774
C	-1.04766	-0.35347	0.91130
C	-1.21359	0.90345	0.15840
H	-2.09848	1.50514	0.36032
H	-0.02305	1.48155	-1.51865
H	-1.81285	-0.61422	1.64230
H	2.15243	1.56402	-0.40439
C	1.56464	-1.06420	-1.10552
H	1.71174	-2.14533	-0.99051
H	2.42489	-0.66926	-1.65967
H	0.66934	-0.91263	-1.71618
O	-1.55915	-0.38331	-0.46211
Li	-3.10421	-1.16872	-1.27053

ψ_{ax}-*cis*-**12**-TS_1 (NIMAG = 1)

0 1

C	-1.05922	-0.05752	1.43993
H	-0.37544	-0.55875	2.13904
C	-0.65283	-1.61258	-0.51939
H	-1.11302	-2.34476	-1.19524
H	0.15210	-2.13291	0.01535
C	-0.01838	-0.48308	-1.35011
H	-0.73670	-0.07995	-2.07464
H	0.82447	-0.86652	-1.93352
C	0.46992	0.65294	-0.48714
C	-0.24664	1.02287	0.73738
H	-1.83193	0.42873	2.05137
C	-1.69383	-1.11873	0.50857
H	-1.94503	-1.97944	1.14468
H	0.32385	1.62689	1.45386
C	-3.00733	-0.65648	-0.14642

H	-3.45371	-1.47311	-0.72878
H	-3.73624	-0.35692	0.61798
H	-2.85449	0.19897	-0.81034
H	1.21992	1.33391	-0.86434
H	1.95121	-0.32906	0.22308
Al	3.62250	-0.31254	0.18940
H	3.99828	0.80135	-0.94708
H	4.12595	-1.80387	-0.22299
H	4.13171	0.14371	1.66789
O	-0.93550	1.79550	-0.23591
Li	-1.01322	3.53543	-0.73607

ψ_{ax}-*cis*-**12**-TS_2 (NIMAG = 1)

0 1

C	0.20381	-0.34790	-1.27656
H	-0.72725	-0.78626	-1.64993
C	0.46618	-1.31271	1.04943
H	0.96225	-2.08564	1.65060
H	-0.60587	-1.54536	1.06247
C	0.67549	0.06610	1.70670
H	1.71639	0.19885	2.02846
H	0.05716	0.12700	2.60996
C	0.32974	1.23975	0.78134
H	-0.20173	2.04570	1.29916
C	-0.17875	0.92244	-0.55814
H	0.78430	-0.08667	-2.17082
C	0.95914	-1.39024	-0.40875
H	0.68007	-2.37994	-0.79392
C	2.48822	-1.28261	-0.52876
H	2.97859	-2.07047	0.05713
H	2.80518	-1.40270	-1.57340
H	2.85136	-0.31416	-0.17118
H	-0.63226	1.72671	-1.12182
H	-1.96850	0.50882	-0.12702
Al	-3.52749	-0.09830	-0.15214
H	-3.76363	-0.86781	1.26338
H	-3.55801	-1.12095	-1.42417
H	-4.53839	1.16376	-0.35150
O	1.39384	1.72475	-0.01695
Li	2.73468	2.33333	-1.02185

ψ_{eq}-*cis*-**12**-Li^+ (NIMAG = 0)

1 1

C	-0.47144	-1.23851	-0.31992
H	-0.82874	-1.94854	-1.07564
C	-1.41822	-0.01997	-0.25967
H	-1.59779	0.30895	-1.29518
C	-0.75755	1.15257	0.48398
H	-0.51645	0.84858	1.51212
H	-1.46233	1.98916	0.56110
C	0.51286	1.63538	-0.23545
H	1.05147	2.37891	0.36656
H	0.24224	2.13527	-1.17641
C	1.44869	0.50739	-0.59514
C	0.96900	-0.88612	-0.64071
H	1.51902	-1.59128	-1.26186
H	-0.48718	-1.77535	0.63949
H	2.31753	0.77079	-1.19770
C	-2.76844	-0.40629	0.35512
H	-3.46951	0.43612	0.32453
H	-3.22735	-1.24425	-0.18401
H	-2.65081	-0.70691	1.40472
O	1.77796	-0.41498	0.49162
Li	3.26560	-0.91608	1.57336

ψ_{eq}-*cis*-**12**-TS_1 (NIMAG = 1)

0 1

C	1.09793	-0.14784	-1.25194
H	0.72343	-0.71789	-2.11121
C	1.39186	-1.11581	-0.08442
H	0.55876	-1.83230	-0.03092
C	1.43214	-0.36337	1.25616
H	2.21236	0.40782	1.21841
H	1.70243	-1.05389	2.06522
C	0.07269	0.27992	1.58479
H	0.17445	1.03466	2.37494
H	-0.61585	-0.47680	1.97532
C	-0.58467	0.91153	0.38210
H	-1.44074	1.55710	0.52254
C	0.10284	0.96628	-0.91258
H	-0.53587	1.23032	-1.76329
H	2.02724	0.34198	-1.57727
C	2.68114	-1.90673	-0.33650
H	2.84775	-2.65518	0.44826
H	2.64348	-2.43292	-1.29882
H	3.55309	-1.23847	-0.35495
H	-1.85302	-0.41429	0.01733
Al	-3.45885	-0.85254	-0.15877
H	-3.83981	-1.75246	1.14412

H	-3.58960	-1.67541	-1.55708
H	-4.28182	0.55807	-0.19377
O	0.66703	2.09848	-0.26891
Li	0.72632	3.89036	-0.16306

ψ_{eq}-*cis*-**12**-TS_2 (NIMAG = 1)

0 1

C	0.45716	-0.53771	-1.11188
H	-0.17784	-1.24317	-1.65786
C	1.18667	-1.25022	0.04383
H	0.42309	-1.78829	0.62479
C	1.85264	-0.22747	0.98230
H	2.62485	0.32581	0.42935
H	2.36467	-0.75512	1.79749
C	0.83369	0.75766	1.57615
H	1.34092	1.53809	2.15912
H	0.16059	0.23047	2.26614
C	-0.02583	1.42407	0.51192
H	-0.82924	2.03328	0.94191
C	-0.39456	0.62083	-0.65709
H	1.19170	-0.15731	-1.83528
C	2.19182	-2.27467	-0.49557
H	2.66919	-2.82576	0.32388
H	1.70295	-3.00661	-1.15076
H	2.98506	-1.78254	-1.07499
H	-1.17232	1.00221	-1.30403
H	-1.77049	-0.49672	0.08166
Al	-3.42699	-0.70314	0.13331
H	-4.05251	0.76904	-0.20197
H	-3.82600	-1.21292	1.62674
H	-3.80021	-1.79072	-1.02232
O	0.69288	2.07478	-0.52421
Li	0.85467	3.54264	-1.54709

ψ_{ax}-*trans*-**12**-Li^+ (NIMAG = 0)

1 1

C	-1.41716	-0.33522	0.55726
C	-0.30760	-1.39401	0.35403
C	0.85236	-0.90702	-0.49696
C	1.05614	0.52748	-0.77646
C	0.10242	1.56743	-0.24096
C	-0.79303	1.03505	0.89153
H	0.09704	-1.71180	1.32393
H	-0.72841	-2.29129	-0.11555
H	-2.01241	-0.64890	1.42458

H	1.61480	0.80049	-1.67138
H	0.67216	2.44463	0.09256
H	-0.50917	1.90515	-1.08769
H	-0.20407	0.94674	1.81364
H	-1.58426	1.76673	1.09358
H	1.28681	-1.62322	-1.19255
C	-2.36394	-0.27286	-0.65391
H	-2.88890	-1.22690	-0.78266
H	-3.12049	0.51026	-0.52206
H	-1.83004	-0.06517	-1.58969
O	1.88843	-0.14888	0.21955
Li	3.77478	-0.31360	0.54988

ψ_{ax}-*trans*-**12**-TS_1 (NIMAG = 1)

0 1

C	1.81647	-0.48211	1.06265
C	1.70409	-1.14441	-0.32565
H	2.71842	-1.44091	-0.62586
C	1.17610	-0.13848	-1.38585
H	2.01452	0.37795	-1.87179
H	0.64667	-0.68551	-2.17615
C	0.47231	0.07051	1.57162
H	-0.16822	-0.74383	1.92598
H	0.62837	0.72718	2.43663
C	-0.29053	0.82375	0.51033
C	0.25517	0.95991	-0.84578
H	-0.46736	1.29316	-1.60055
H	2.54419	0.33564	1.01477
H	2.19743	-1.21124	1.78920
C	0.85204	-2.42609	-0.28392
H	1.22152	-3.11805	0.48404
H	-0.20083	-2.21040	-0.06981
H	0.89059	-2.94607	-1.24923
H	-1.07986	1.50280	0.79863
H	-1.69741	-0.37503	0.22191
Al	-3.35334	-0.33441	-0.04422
H	-3.70947	1.26122	-0.07192
H	-4.06102	-1.09763	1.20644
H	-3.63789	-1.05127	-1.47572
O	0.92926	2.03226	-0.20366
Li	0.80193	3.83089	-0.11759

ψ_{ax}-*trans*-**12**-TS_2 (NIMAG = 1)

0 1

C	1.42213	-1.29283	-0.57407
C	2.17680	-0.49460	0.51162
H	2.79203	-1.18064	1.10812
H	2.86519	0.20879	0.02664
C	0.51672	-0.35274	-1.40954
H	-0.20220	-0.92967	-2.00144
H	1.12999	0.20123	-2.13221
C	-0.24541	0.66744	-0.60209
C	0.27446	1.18363	0.66864
H	-0.46477	1.66334	1.32143
H	2.17314	-1.69903	-1.26590
C	0.65306	-2.49087	0.00769
H	0.18349	-3.07701	-0.79199
H	-0.14178	-2.18234	0.69322
H	1.33688	-3.15444	0.55239
C	1.23547	0.28997	1.44055
H	0.64084	-0.39301	2.06108
H	1.81672	0.91643	2.13029
H	-1.05877	1.20713	-1.06518
H	-1.67543	-0.48766	-0.00656
Al	-3.31938	-0.26877	0.21013
H	-4.07839	-1.06426	-0.99118
H	-3.52935	1.35020	0.08228
H	-3.71733	-0.81947	1.68811
O	0.89821	2.07199	-0.24702
Li	0.56554	3.76615	-0.80715

ψ_{eq}-*trans*-**12**-Li^+ (NIMAG = 0)

1 1

C	0.47499	1.68186	0.07977
H	0.65161	2.61491	-0.46801
C	-0.99749	1.25476	-0.06706
H	-1.30740	1.37320	-1.11605
C	-1.24137	-0.20419	0.35338
C	-0.42849	-1.14803	-0.55496
H	-0.46638	-2.17959	-0.17943
H	-0.87855	-1.16706	-1.55910
C	1.01179	-0.73404	-0.73236
C	1.45209	0.63922	-0.42881
H	2.34886	1.00731	-0.92481

H	0.71241	1.89036	1.13152
H	1.59339	-1.31183	-1.45031
H	-1.62935	1.92948	0.52298
H	-0.88363	-0.32879	1.38573
C	-2.73073	-0.56744	0.31744
H	-3.30572	0.06448	1.00447
H	-2.89275	-1.61304	0.60737
H	-3.14469	-0.43099	-0.69020
O	1.75527	-0.45988	0.50018
Li	3.30511	-1.23407	1.31001

ψ_{eq}-*trans*-**12**-TS_1 (NIMAG = 1)

0 1

C	1.98426	-0.44280	-0.02710
C	1.07942	-1.02588	1.07373
H	0.52912	-1.88533	0.66518
H	1.69033	-1.40271	1.90418
C	0.07055	0.00013	1.61408
H	0.58473	0.74599	2.23433
H	-0.66968	-0.48299	2.25946
C	1.12491	0.06407	-1.20054
H	0.66869	-0.79185	-1.71929
H	1.75154	0.58529	-1.93770
C	0.00232	0.99898	-0.77183
H	-0.66907	1.24624	-1.60315
C	-0.65354	0.72966	0.51140
H	2.52208	0.41852	0.39509
C	3.02068	-1.46702	-0.50589
H	3.66546	-1.04493	-1.28733
H	2.53077	-2.35758	-0.92191
H	3.66458	-1.79469	0.31997
H	-1.57739	1.24937	0.72373
H	-1.78477	-0.75787	0.06889
Al	-3.39869	-0.96312	-0.32113
H	-4.08626	-1.81650	0.88290
H	-3.47387	-1.72143	-1.75891
H	-3.99345	0.55957	-0.39926
O	0.41275	2.12688	-0.01082
Li	-0.08115	3.87118	0.09068

ψ_{eq}-*trans*-**12**-TS_2 (NIMAG = 1)

0 1

C	1.70062	-0.78264	-0.20136
C	1.25163	-0.69553	1.26696
H	0.44631	-1.42590	1.42836
H	2.07653	-0.98790	1.92957
C	0.75076	0.70978	1.65679
H	1.59663	1.36537	1.90424
H	0.12808	0.64191	2.55693
C	0.50097	-0.49389	-1.12969
H	-0.12186	-1.39203	-1.21440
H	0.84420	-0.26701	-2.14770
C	-0.38639	0.62682	-0.64649
H	-1.13119	1.03707	-1.31468
C	-0.04386	1.40599	0.54787
H	-0.85577	2.02839	0.94138
H	2.45832	-0.00600	-0.37305
C	2.32417	-2.14397	-0.53318
H	2.61203	-2.20436	-1.59081
H	1.61848	-2.96081	-0.33194
H	3.22368	-2.32133	0.06920
H	-1.80092	-0.39567	0.03240
Al	-3.43948	-0.73784	0.01065
H	-3.60761	-2.15345	-0.77727
H	-4.11994	0.50309	-0.80520
H	-3.94458	-0.80757	1.55607
O	0.74301	2.07074	-0.42855
Li	0.91978	3.53763	-1.44619