Supporting Information

Mechanistic Models for LAH Reductions of Acetonitrile and Malononitrile. Aggregation Effects of Li^+ and AlH_3 on Imide-Enamide Equilibria

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Table S1. Results Computed at the MP2(full)/6-311+G* Level

Molecule	E_{tot}[a]	*VZPE*[b]	*TE*[b]	*S*[c]	*NI*	ν_1	ν_2	E_{SMD}[d]
$LiAlH_4$, **1a**, C_{2v}	-251.912005	18.31	20.89	61.94	0	194.5	487.5	
1b, C_{3v}	-251.911039	18.33	20.84	58.57	0	363.9	363.9	
1c, C_s	-251.908844	18.00	20.24	59.52	1	-257.8	483.3	
H_3CCN, **2**	-132.453794	28.48	30.81	60.56	0	335.8	335.8	
(*E*)-**3**	-384.419408	51.30	56.22	84.90	0	64.4	132.1	-384.436325
			53.83	74.31				
(*Z*)-**3**	-384.419016	51.36	56.25	85.13	0	54.7	93.4	
(*E*)-**4**	-384.412041	51.72	56.28	80.75	0	99.1	148.8	
(*Z*)-**4**	-384.422613	52.47	56.74	78.05	0	154.7	241.4	-384.436852
			54.49	68.08				
(*E*)-**5**	-384.401843	52.67	56.71	76.58	0	195.2	216.3	
(*Z*)-**5**	-384.410608	52.23	56.71	80.47	0	119.4	135.6	
$H_2C(CN)_2$, **6**	-224.524160	27.59	30.74	71.23	0	139.2	305.7	
(*E*)-**7**	-476.518241	50.23	55.93	92.07	0	54.8	98.0	-476.534563
(*E*)-**7b**	-476.501547	50.46	56.31	95.25	0	31.0	72.7	
(*Z*)-**7**	-476.502400	50.40	56.21	94.83	0	26.8	88.4	
(*E*,*Z*)-**8**	-476.513643	50.92	56.48	89.84	0	90.8	131.1	
(*E*,*E*)-**8**	-476.506211	51.10	56.81	93.04	0	54.4	88.3	
(*Z*,*Z*)-**8**	-476.526722	51.72	57.00	87.47	0	90.2	150.6	-476.540038
(*Z*,*E*)-**8**	-476.514693	51.58	56.98	88.68	0	99.4	120.5	
(*E*,*Z*)-**9**	-476.489222	50.99	56.58	90.60	0	87.1	102.6	
(*E*,*E*)-**9**	-476.491580	51.55	56.75	87.07	0	109.0	133.8	
(*Z*,*Z*)-**9**	-476.516202	51.57	56.77	86.07	0	132.0	182.6	
(*Z*,*E*)-**9**	-476.501523	51.55	56.82	88.27	0	74.9	129.8	
$AlH_3 \cdot Li^+$, **10**	-251.097234	13.50	16.13	61.34	0	291.7	318.7	
Li^+, **11**	-7.248435	0.00	0.89	31.80	0			
AlH_3, **12**	-243.815712	11.92	13.86	49.49	0	736.1	812.9	
$(AlH_3)_2$, **13**	-487.685242	28.36	31.45	68.07	0	221.4	383.4	
$(LiAlH_4)_2$, **14**	-503.892207	39.55	44.47	82.41	0	134.4	190.4	
LiH, **15**	-8.014789	2.04	3.52	40.82	0	1424.2		
$(LiH)_2$, **16**	-16.107787	7.60	9.69	54.47	0	523.5	600.9	
$(LiH)_2(AlH_3)$, **17**	-260.002796	23.53	27.07	70.03	0	193.1	312.4	
$(LiH)(AlH_3)_2$, **18**	-495.782895	33.77	37.96	77.71	0	84.7	221.1	

19	-140.508299	36.23	39.56	70.54	0	120.2	139.0	-140.528298
(*Z*)-**20**	-140.521776	37.17	39.88	64.99	0	346.1	389.0	-140.535491
(*E*)-**20a**	-140.502160	36.74	39.52	65.47	0	274.4	379.7	
(*E*)-**20b**	-140.504413	36.41	39.60	69.12	0	107.4	147.5	
(*Z*)-**21**	-232.613074	0.06	38.93	76.45	0	143.3	208.3	-232.630628
21b	-232.598489	35.38	39.61	81.47	0	40.6	122.6	
(*Z*,*Z*)-**22**	-232.651086	36.73	40.33	73.97	0	184.0	254.4	-232.663487
(*E*,*Z*)-**22a**	-232.613757	36.38	40.06	74.68	0	169.0	178.6	
(*E*,*Z*)-**22b**	-232.614414	36.15	40.21	79.20	0	86.9	103.0	
(*Z*,*E*)-**22**	-232.622830	36.50	40.24	75.40	0	146.5	176.6	
(*E*,*E*)-**22a**	-232.600753	35.99	39.83	76.24	0	143.8	176.5	
(*E*,*E*)-**22b**	-232.611438	36.08	40.20	79.07	0	106.0	110.3	
23	-132.984201	33.23	35.72	62.86	0	149.3	495.3	-133.066556
anti-**24a**	-132.993706	33.31	35.53	60.58	1	-137.4	500.2	
anti-**24b**	-132.993711	33.60	36.18	62.73	0	195.6	496.4	
syn-**24a**	-132.997282	33.43	35.62	60.51	1	-182.4	494.8	
syn-**24b**	-132.997298	33.81	36.31	62.21	0	252.6	495.3	-133.075139
25	-225.095663	32.10	35.74	76.36	0	35.1	142.4	-225.167121
(*anti*,*Z*)-**26**	-225.129019	33.86	37.14	72.01	0	159.8	192.8	
(*syn*,*Z*)-**26**	-225.136304	34.09	37.33	71.87	0	148.5	205.0	-225.204660
(*anti*,*E*)-**26**	-225.133587	33.99	37.25	71.54	0	132.9	186.4	
(*syn*,*E*)-**26**	-225.136001	34.05	37.30	71.58	0	133.5	186.4	

(a) Energies given in hartrees. 1 hartree = 627.51 kcal/mol.

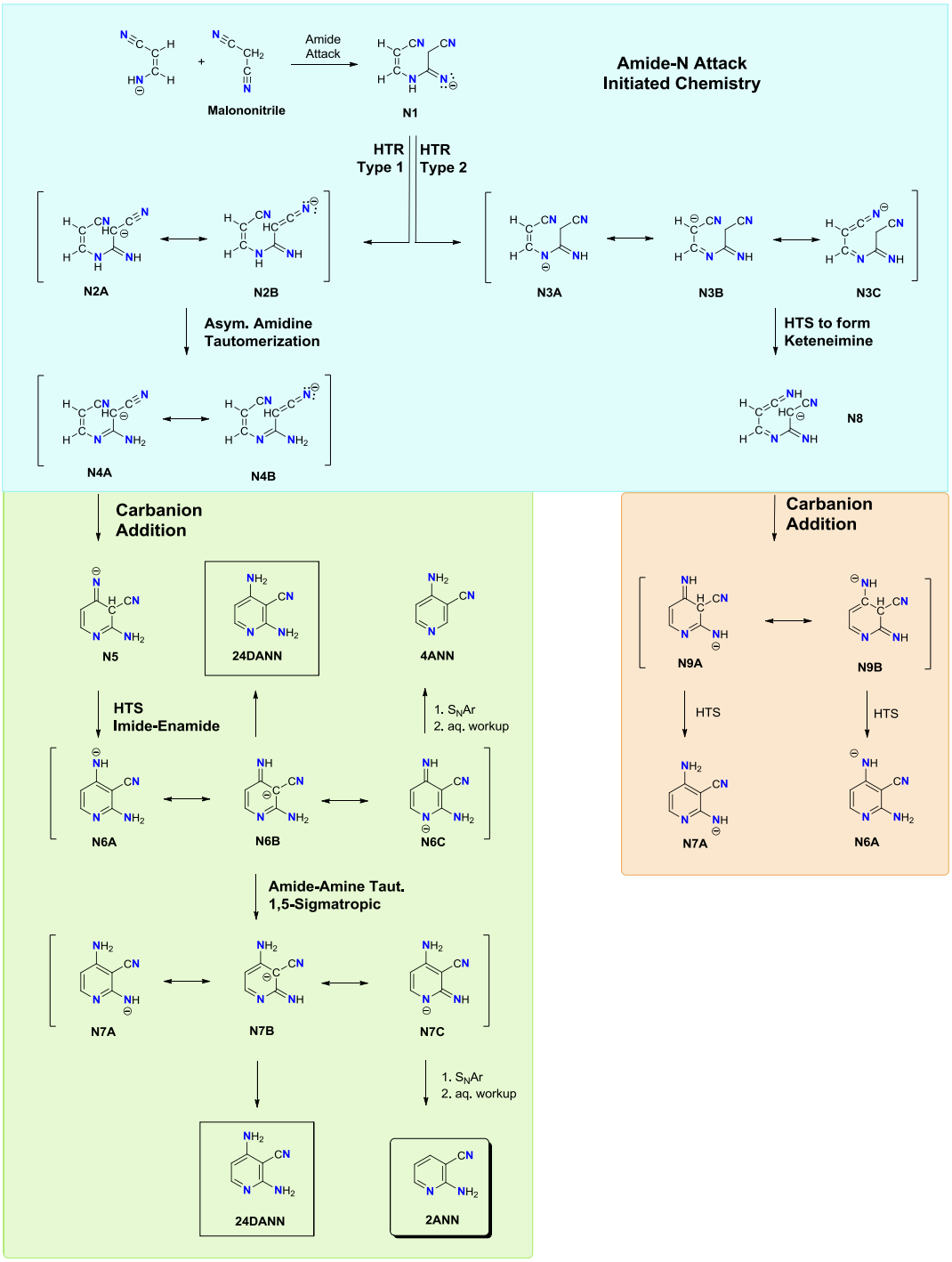
(b) Energies given in kcal/mol.

(c) Entropies given in cal/(mol K).

(d) Energies computed at the SMD(MP2(full)/6-311+G*) level and based on the MP2(full)/6-311+G* structures.

(e) The first stereochemical descriptor refers to the geometry about the CN bond.

(f) For **7**, the second stereochemical descriptor refers to the geometry about the CC bond.



Scheme S5B. Amide-N attack mechanism for the formation of 2,4-diaminonicotinonitrile (**24DANN**), 2-aminonicotinonitrile (**2ANN**), and 4-aminonicotinonitrrile (**4ANN**).

Possible mechanisms for the formation of 2-aminonicotinonitrile **2ANN** involving initial amide-N attack are outlined in Scheme S5B. The enamide attacks malononitrile to form the 1,5-dicyano-substituted imide **N1**. Imide **N1** can stabilize itself to a more conjugated imine and the hydrogen transfer reaction (HTR) may shift a hydrogen from the CH_2 (Type 1) or the NH group (Type 2), respectively. If the HTR Type 1 occurs, then it may be followed by HTR Type 2 to afford **N4**. If the HTR Type 2 occurs first, then the HTR Type 2 tautomerization could follow and also lead to **N4**. In addition, one might consider the tautomerization leading to **N8**.

The reaction of **N4** to **N5** involves an intramolecular carbanion addition and **N5** will then aromatize to **N6** ⇄ **N7** and react on as shown in Scheme 5. These same equilibrium **N6** ⇄ **N7** can be reached by the sequence **N1** → **N3** → **N8** → **N9**.

Cartesian Coordinates of Stationary Structures

$LiAlH_4$, **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-2.059348	0.000001	-0.000130
2	13	0	0.412646	0.000006	0.000054
3	1	0	1.192008	-1.389495	-0.000134
4	1	0	1.191592	1.389745	-0.000976
5	1	0	-0.784620	0.000321	1.207354
6	1	0	-0.785330	-0.000649	-1.206555

Acetonitrile, **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.185680	-0.000022	-0.000012
2	1	0	-1.559209	-0.754783	-0.692443
3	1	0	-1.559302	0.976957	-0.307520
4	1	0	-1.559552	-0.222272	0.999721
5	6	0	0.275967	0.000089	0.000085
6	7	0	1.448049	-0.000044	-0.000028

(*E*)-**3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.525570	0.011022	0.000003
2	1	0	-2.577396	1.100899	0.000043
3	1	0	-3.050458	-0.377322	0.878933
4	1	0	-3.050454	-0.377259	-0.878957
5	6	0	-1.095860	-0.455415	-0.000009
6	1	0	-0.986103	-1.555196	-0.000048
7	7	0	-0.078198	0.312134	0.000024
8	3	0	0.699484	2.040891	-0.000030
9	13	0	1.785671	-0.289135	0.000001
10	1	0	2.152708	-0.997115	1.385442
11	1	0	2.152637	-0.997279	-1.385373
12	1	0	2.322862	1.320774	-0.000095

(*Z*)-**3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.025974	-0.601385	-0.000111
2	1	0	2.677190	-0.637409	0.879322

3	1	0	2.677084	-0.637221	-0.879631
4	1	0	1.380278	-1.480377	-0.000180
5	6	0	1.234820	0.678919	0.000080
6	1	0	1.863973	1.586153	-0.000022
7	7	0	-0.035941	0.789551	0.000354
8	3	0	-1.549423	1.932043	-0.000476
9	13	0	-1.377171	-0.635522	0.000010
10	1	0	-1.368927	-1.438207	-1.383231
11	1	0	-1.370399	-1.437411	1.383719
12	1	0	-2.620887	0.518064	-0.000966

(*E*)-**4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.368810	0.080458	-0.034273
2	1	0	-2.646077	0.530921	0.917643
3	1	0	-3.161022	-0.096155	-0.751323
4	6	0	-1.126959	-0.439542	-0.242398
5	1	0	-0.914639	-0.913088	-1.203190
6	7	0	-0.026093	-0.307742	0.583063
7	13	0	1.762876	-0.023950	-0.099809
8	1	0	2.063749	-1.043752	-1.289402
9	1	0	1.368002	1.491497	-0.784353
10	1	0	2.742211	0.171967	1.143991
11	1	0	-0.262786	-0.194022	1.564933
12	3	0	-0.316519	1.557558	-0.240734

(*Z*)-**4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.781780	-0.751241	-0.190467
2	1	0	-1.100993	-1.588983	-0.320962
3	1	0	-2.842003	-0.953138	-0.268332
4	6	0	-1.337453	0.540583	-0.168306
5	1	0	-2.073044	1.346944	-0.177691
6	13	0	1.568842	-0.235643	-0.136107
7	1	0	1.159814	-1.160835	1.215746
8	1	0	1.521847	-1.168311	-1.429541
9	1	0	2.800040	0.735780	0.157032
10	3	0	-0.376984	-0.357113	1.562568
11	7	0	-0.019092	0.898044	0.009504
12	1	0	0.119388	1.900883	-0.008469

(*E*)-**5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.025358	1.272497	-0.127661
2	1	0	0.144137	1.536008	-1.182119
3	1	0	-0.207471	2.143086	0.486720
4	6	0	1.084506	0.440260	0.403673
5	1	0	1.204734	0.445373	1.491359
6	7	0	1.789397	-0.467325	-0.224077
7	1	0	1.648154	-0.362264	-1.233311
8	3	0	0.431629	-1.910701	0.211474
9	13	0	-1.428092	-0.214978	-0.025463
10	1	0	-0.941199	-1.149364	1.270425
11	1	0	-2.963691	0.181155	-0.082055
12	1	0	-0.799326	-1.272443	-1.141962

(*Z*)-**5**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021362	-0.955533	-0.516340
2	1	0	-0.126245	-0.708366	-1.577618
3	1	0	0.248133	-2.007037	-0.409443
4	6	0	-1.188599	-0.604198	0.258519
5	1	0	-1.452055	-1.258967	1.096780
6	7	0	-1.878582	0.488598	0.057375
7	1	0	-2.639059	0.579017	0.724312
8	3	0	-0.620872	1.745512	-0.677549
9	13	0	1.590238	0.185752	0.190278
10	1	0	1.605571	0.157469	1.792369
11	1	0	2.913517	-0.182217	-0.626201
12	1	0	1.049506	1.706983	-0.295861

Malononitrile, **6**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000055	0.847023	0.000018
2	1	0	0.000669	1.493556	0.882203
3	1	0	-0.000477	1.493731	-0.882038
4	6	0	1.216690	0.027368	-0.000650
5	7	0	2.207353	-0.599869	0.000272
6	6	0	-1.216700	0.027347	0.000557
7	7	0	-2.207419	-0.599805	-0.000232

(*E*)-**7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.835823	-1.039815	0.000003
2	1	0	2.299424	-1.491557	-0.883136

3	1	0	2.299401	-1.491546	0.883160
4	6	0	0.303527	-1.272050	-0.000011
5	1	0	0.032579	-2.340944	-0.000081
6	7	0	-0.508750	-0.310212	0.000060
7	3	0	-0.199689	1.645664	-0.000003
8	13	0	-2.396983	0.135882	-0.000009
9	1	0	-3.061088	-0.290641	-1.389397
10	1	0	-3.061102	-0.290422	1.389440
11	1	0	-2.020182	1.782884	-0.000127
12	6	0	2.038725	0.404145	-0.000003
13	7	0	1.966232	1.576655	-0.000012

(*E*)-**7b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.543967	0.714553	0.534499
2	1	0	-1.437698	1.665310	0.006931
3	1	0	-1.834917	0.927583	1.569933
4	6	0	-0.213093	-0.027491	0.521984
5	1	0	-0.244550	-0.996522	1.047949
6	7	0	0.835911	0.429467	-0.027236
7	3	0	1.731956	1.624319	-1.217950
8	13	0	2.585928	-0.482469	-0.002365
9	1	0	3.266692	-0.238812	1.420984
10	1	0	2.467020	-1.946189	-0.622586
11	1	0	3.190743	0.624437	-1.128639
12	6	0	-2.597678	-0.086614	-0.090565
13	7	0	-3.420454	-0.749373	-0.602120

(*Z*)-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.099001	-0.459759	0.283099
2	1	0	-1.014930	-0.851497	1.304058
3	1	0	-0.691817	-1.222724	-0.387812
4	6	0	-0.268789	0.819946	0.173504
5	1	0	-0.852300	1.751265	0.238880
6	7	0	0.994051	0.827835	0.038922
7	3	0	2.589452	1.849619	-0.184891
8	13	0	2.213967	-0.706409	-0.083262
9	1	0	2.283414	-1.442487	1.333490
10	1	0	1.905106	-1.542260	-1.409439
11	1	0	3.524693	0.333239	-0.294056
12	6	0	-2.508462	-0.231301	-0.029094
13	7	0	-3.629277	0.005824	-0.283649

(*E*,*Z*)-**8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.661115	1.091326	-0.146868
2	1	0	2.321268	1.847709	-0.546596
3	6	0	0.300290	1.259079	-0.002706
4	1	0	-0.168296	2.154245	-0.411380
5	7	0	-0.536954	0.340830	0.553132
6	13	0	-2.286688	-0.211571	-0.092572
7	1	0	-2.716692	0.878652	-1.175385
8	1	0	-1.686064	-1.597488	-0.863374
9	1	0	-3.220625	-0.654273	1.118058
10	1	0	-0.074829	-0.205351	1.279402
11	3	0	0.060282	-1.528306	-0.573312
12	6	0	2.066740	-0.253342	0.015590
13	7	0	2.097307	-1.436620	0.064945

(*E*,*E*)-**8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.484038	0.489967	-0.456681
2	6	0	0.306876	0.098778	0.093835
3	1	0	0.323244	-0.693369	0.843921
4	7	0	-0.953339	0.604897	-0.192448
5	13	0	-2.568644	-0.539022	-0.116392
6	1	0	-2.150262	-2.058396	0.093634
7	1	0	-3.064173	0.127128	1.361636
8	1	0	-3.528121	-0.033200	-1.283388
9	1	0	-0.911678	1.229647	-0.995610
10	3	0	-1.778188	1.305799	1.471818
11	1	0	1.522633	1.255204	-1.227617
12	6	0	2.714952	-0.094271	-0.043764
13	7	0	3.739068	-0.562607	0.298836

(*Z*,*Z*)-**8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.516286	0.938045	-0.437997
2	1	0	-2.253301	1.546909	-0.942128
3	6	0	-0.402365	1.450925	0.163919
4	1	0	-0.288347	2.535779	0.192725
5	13	0	1.907616	-0.356351	-0.389817
6	1	0	1.561677	-1.828562	0.298649
7	1	0	1.416467	-0.276480	-1.902833
8	1	0	3.333911	0.183802	0.078241
9	3	0	0.045350	-1.342651	1.103757
10	7	0	0.579992	0.668199	0.729181
11	1	0	1.141710	1.240758	1.354524
12	6	0	-1.709975	-0.449737	-0.247125
13	7	0	-1.733623	-1.579212	0.100019

(*Z*,*E*)-**8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.997288	-0.285514	-0.077802
2	1	0	-0.497755	-1.243064	-0.214006
3	6	0	-0.295588	0.897983	-0.144848
4	1	0	-0.858985	1.832618	-0.176219
5	13	0	2.366487	-0.508260	-0.154743
6	1	0	1.842944	-1.190777	1.292320
7	1	0	1.984836	-1.487683	-1.350831
8	1	0	3.786481	0.195252	-0.014388
9	3	0	0.540248	-0.076716	1.660361
10	7	0	1.060439	0.968548	-0.048674
11	1	0	1.408395	1.916179	-0.139548
12	6	0	-2.421564	-0.279935	-0.068299
13	7	0	-3.598204	-0.280006	-0.040048

(*E*,*Z*)-**9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.225649	-0.292636	0.851921
2	1	0	-0.099498	-0.707071	1.853359
3	6	0	-0.007499	1.132784	0.730249
4	1	0	0.773001	1.542295	1.378865
5	7	0	-0.494771	1.947810	-0.168572
6	1	0	-1.267011	1.486805	-0.663511
7	6	0	-1.366478	-0.780981	0.126260
8	7	0	-2.271421	-1.098027	-0.557548
9	3	0	1.043573	1.837883	-1.388826
10	13	0	1.588747	-0.886126	-0.173507
11	1	0	2.762081	-0.393204	0.799267
12	1	0	1.448396	-2.395814	-0.638842
13	1	0	1.559695	0.169494	-1.474810

(*E*,*E*)-**9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.442462	-0.270170	0.521228
2	1	0	-0.342801	-0.372481	1.605840
3	6	0	0.452934	-1.125977	-0.250204
4	1	0	0.168164	-1.307733	-1.290082
5	7	0	1.635581	-1.543726	0.104463
6	1	0	1.776684	-1.368536	1.103760
7	3	0	2.543970	0.082185	-0.728320
8	13	0	0.587293	1.519810	0.030372

9	1	0	1.181116	1.169035	-1.479517
10	1	0	-0.167800	2.886096	0.267842
11	1	0	2.009078	1.167044	0.801080
12	6	0	-1.817287	-0.255079	0.085169
13	7	0	-2.928477	-0.209152	-0.298172

(*Z*,*Z*)-**9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.038359	0.016367	-1.000588
2	1	0	-0.329822	-0.042951	-2.047188
3	6	0	0.493980	1.303224	-0.552064
4	1	0	0.212026	2.181930	-1.138415
5	7	0	1.179122	1.403721	0.545808
6	1	0	1.415979	2.370089	0.753466
7	6	0	0.759913	-1.067126	-0.515190
8	7	0	1.406864	-1.810218	0.137769
9	3	0	0.885229	-0.277859	1.618387
10	13	0	-1.795362	-0.141967	0.268260
11	1	0	-2.510567	1.286153	0.200117
12	1	0	-2.573402	-1.466111	-0.155722
13	1	0	-0.925308	-0.319275	1.667212

(*Z*,*E*)-**9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.388934	-0.162834	0.433975
2	1	0	-0.274250	-0.109819	1.525042
3	6	0	0.292616	-1.380154	-0.063314
4	1	0	-0.333923	-2.170892	-0.491860
5	7	0	1.578309	-1.523321	-0.018980
6	1	0	1.848808	-2.438939	-0.372186
7	3	0	2.638785	0.156525	-0.039639
8	13	0	0.645203	1.576903	-0.089213
9	1	0	1.563806	1.085667	-1.367724
10	1	0	-0.194899	2.914387	-0.133592
11	1	0	1.886209	1.473660	1.015920
12	6	0	-1.795382	-0.150814	0.094331
13	7	0	-2.928243	-0.128187	-0.222001

10, $LiAlH_4$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	2.170226	-0.000189	0.000001
2	13	0	-0.441852	0.000070	0.000000
3	1	0	-1.993510	-0.000962	0.000002

4	1	0	0.613723	-1.226232	-0.000001
5	1	0	0.613186	1.226844	-0.000001

12, AlH_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	0.000000	0.000000
2	1	0	0.000000	1.582520	0.000000
3	1	0	1.370502	-0.791260	0.000000
4	1	0	-1.370502	-0.791260	0.000000

13, $(AlH_3)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.305287	-0.000016	-0.000052
2	1	0	-1.993268	-1.416926	0.000177
3	1	0	-1.992658	1.417187	0.000355
4	1	0	-0.000139	-0.000920	-1.143378
5	1	0	0.000052	0.000385	1.143416
6	13	0	1.305368	-0.000006	0.000026
7	1	0	1.991903	1.417576	-0.000735
8	1	0	1.993049	-1.417021	0.000496

14, $(LiAlH_3)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.000605	-1.393778	0.000708
2	13	0	2.199705	-0.000007	-0.015307
3	1	0	1.711550	1.349349	-0.819458
4	1	0	3.640763	-0.002326	0.635195
5	1	0	1.710192	-1.348158	-0.820741
6	1	0	-1.711277	1.349691	0.818689
7	1	0	-0.887392	-0.001555	-1.041283
8	1	0	-1.711273	-1.347646	0.821700
9	1	0	-3.640143	-0.001221	-0.636762
10	13	0	-2.199707	0.000075	0.015019
11	3	0	0.000322	1.393831	0.000669
12	1	0	0.888446	0.000826	1.042275

15, LiH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000000	0.000000	0.401321

2	1	0	0.000000	0.000000	-1.203964

16, $(LiH)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-1.132031	0.000006	0.000000
2	1	0	-0.000014	-1.347402	0.000000
3	3	0	1.132031	-0.000006	0.000000
4	1	0	0.000014	1.347402	0.000000

17, $(LiH)_2(AlH_3)$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-1.536426	-1.267862	0.063915
2	1	0	0.133370	1.325742	-0.778388
3	1	0	-0.370527	-0.000008	1.230652
4	1	0	0.133373	-1.325735	-0.778400
5	1	0	2.285994	0.000002	0.348930
6	13	0	0.745990	0.000000	-0.014135
7	3	0	-1.536432	1.267860	0.063914
8	1	0	-2.661507	-0.000003	-0.222525

18, $(LiH)(AlH_3)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.522889	1.979330	0.000070
2	13	0	1.498279	-0.284094	-0.000029
3	1	0	2.598033	-1.411995	-0.000178
4	1	0	1.388535	0.810243	1.220933
5	1	0	-2.226522	-0.555680	-1.396716
6	1	0	-0.047602	-0.940336	-0.000988
7	1	0	-1.126509	1.440621	0.000042
8	1	0	-2.225163	-0.556294	1.397140
9	13	0	-1.599726	-0.141742	0.000005
10	1	0	1.389378	0.811316	-1.220136

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.423991	-0.326150	0.000080
2	1	0	-1.171994	-1.387992	-0.000034
3	1	0	-2.033978	-0.094667	-0.880742
4	1	0	-2.034127	-0.094859	0.880821

5	6	0	-0.156665	0.510214	0.000175
6	1	0	-0.373115	1.604160	0.000818
7	3	0	2.643428	-0.527442	0.000792
8	7	0	1.023837	0.064472	-0.000681

(*Z*)-**20**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.230718	0.037490	0.100230
2	1	0	-1.337906	0.770086	0.901671
3	1	0	-2.137119	-0.447798	-0.236473
4	1	0	1.971751	-0.518282	0.018981
5	6	0	0.009787	-0.560502	-0.104255
6	1	0	0.032310	-1.510642	-0.652475
7	3	0	0.217109	1.473341	-0.507023
8	7	0	1.163603	0.060669	0.216216

(*E*)-**20a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.216151	0.078290	0.155394
2	1	0	-1.274121	0.759785	1.008435
3	1	0	-2.152549	-0.358802	-0.172229
4	1	0	1.185618	0.481062	1.002257
5	6	0	-0.005285	-0.537601	-0.151356
6	1	0	-0.030657	-1.335539	-0.899628
7	3	0	0.300324	1.361653	-0.715952
8	7	0	1.242765	-0.125085	0.169256

(*E*)-**20b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.531313	0.078240	0.000214
2	1	0	-1.762160	1.140271	0.000266
3	1	0	-2.361344	-0.617369	-0.000060
4	1	0	0.705975	1.335784	0.000126
5	6	0	-0.250759	-0.373752	-0.000182
6	1	0	-0.111944	-1.460086	-0.000074
7	3	0	2.574182	-0.339187	0.000475
8	7	0	0.928480	0.341719	-0.000268

(*Z*)-**21**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.190396	-1.252472	0.000003
2	1	0	0.268299	-1.886439	0.888400
3	1	0	0.268303	-1.886463	-0.888375
4	6	0	1.370663	-0.139411	-0.000003
5	1	0	2.338851	-0.682721	-0.000004
6	7	0	1.204381	1.094134	-0.000002
7	3	0	-0.467926	1.915173	0.000010
8	6	0	-1.049007	-0.509000	-0.000003
9	7	0	-1.853522	0.350923	-0.000003

21b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.330108	0.802628	-0.203993
2	1	0	0.528095	1.786542	0.237659
3	1	0	0.032845	0.940485	-1.245792
4	6	0	-0.826578	0.113788	0.553607
5	1	0	-0.565797	-0.079403	1.615962
6	7	0	-1.929694	-0.181303	0.033459
7	3	0	-3.448796	-0.713616	-0.618291
8	6	0	1.552223	0.003508	-0.131426
9	7	0	2.503513	-0.679600	-0.042327

(*Z*,*Z*)-**22**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.104200	-1.203995	-0.000100
2	1	0	0.121555	-2.283293	0.000030
3	6	0	1.255094	-0.410854	0.000017
4	1	0	2.212941	-0.939063	0.000137
5	3	0	-0.478762	1.751965	-0.000150
6	7	0	1.236355	0.925223	-0.000012
7	1	0	2.181011	1.293605	0.000247
8	6	0	-1.080414	-0.465049	0.000033
9	7	0	-1.915283	0.382241	0.000060

(*E*,*Z*)-**22a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037087	1.109528	-0.003918
2	1	0	0.009142	2.176787	0.169350
3	6	0	1.246390	0.369924	-0.043129
4	1	0	2.148179	0.921097	0.233747
5	7	0	1.412835	-0.938037	-0.222648
6	1	0	0.576234	-1.341560	-0.667460

7	3	0	-0.023693	-0.772317	1.259150
8	6	0	-1.140414	0.350565	-0.152172
9	7	0	-1.915815	-0.550459	-0.108463

(*E*,*Z*)-**22b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454590	1.038422	0.000050
2	1	0	-0.775869	2.072020	-0.000127
3	6	0	0.881458	0.710012	-0.000172
4	1	0	1.581390	1.549191	-0.000319
5	7	0	1.446730	-0.520050	0.000160
6	1	0	0.708046	-1.224516	0.000610
7	6	0	-1.426223	0.006969	0.000357
8	7	0	-2.173002	-0.907167	-0.000295
9	3	0	3.188824	-0.979533	-0.000212

(*Z*,*E*)-**22**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.143691	0.378782	0.305649
2	1	0	0.054802	1.149524	1.051444
3	6	0	0.883797	-0.529790	-0.004302
4	1	0	0.597803	-1.507779	-0.407836
5	3	0	1.486092	1.407193	-0.665996
6	7	0	2.163545	-0.163737	0.078709
7	1	0	2.792356	-0.928215	-0.141480
8	6	0	-1.506142	0.065646	0.054491
9	7	0	-2.635977	-0.182396	-0.170019

(*E*,*E*)-**22a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.133906	0.357887	-0.350490
2	6	0	-0.892837	-0.507240	0.062680
3	1	0	-0.608484	-1.336442	0.717056
4	7	0	-2.211764	-0.317883	-0.065634
5	1	0	-2.381813	0.382269	-0.804357
6	3	0	-1.448200	1.242102	0.942086
7	1	0	-0.064903	1.084208	-1.141606
8	6	0	1.501750	0.063035	-0.087044
9	7	0	2.632176	-0.159037	0.158745

(*E*,*E*)-**22b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.374117	0.619238	-0.000051
2	1	0	0.296438	1.703103	0.000318
3	6	0	-0.743889	-0.174833	-0.000362
4	1	0	-0.567426	-1.254724	-0.000683
5	7	0	-2.050095	0.194348	-0.000115
6	1	0	-2.117476	1.210475	0.000578
7	3	0	-3.431806	-0.964023	0.000571
8	6	0	1.670532	0.044194	0.000039
9	7	0	2.747141	-0.436973	0.000161

23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160776	-0.149906	-0.000004
2	1	0	1.155901	-1.244161	-0.000207
3	1	0	1.695069	0.219910	0.887735
4	1	0	1.695212	0.220263	-0.887511
5	6	0	-0.300431	0.373134	0.000004
6	1	0	-0.248636	1.528128	-0.000006
7	7	0	-1.351373	-0.294787	-0.000002

anti-**24a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.235252	-0.155819	-0.000082
2	1	0	-1.415581	-1.228370	0.000127
3	1	0	-2.090513	0.512931	0.000217
4	1	0	1.977970	0.349135	-0.000048
5	6	0	0.056926	0.354196	0.000022
6	1	0	0.098124	1.462569	-0.000022
7	7	0	1.214280	-0.326647	0.000013

anti-**24b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.235655	-0.155889	-0.018719
2	1	0	-1.413586	-1.227834	0.030443
3	1	0	-2.088098	0.512776	0.055055
4	1	0	1.977875	0.349123	-0.004661
5	6	0	0.056868	0.354118	0.001723
6	1	0	0.097983	1.462507	-0.001951
7	7	0	1.214078	-0.326564	0.003299

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syn-**24a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.207814	-0.187937	-0.000083
2	1	0	-1.336682	-1.270242	0.000149
3	1	0	-2.104055	0.426110	0.000238
4	1	0	1.204616	-1.135434	0.000023
5	6	0	0.059678	0.399145	0.000003
6	1	0	0.054997	1.500295	0.000012
7	7	0	1.295706	-0.112567	0.000008

syn-**24b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208502	-0.188522	-0.025858
2	1	0	-1.332867	-1.268982	0.048826
3	1	0	-2.099385	0.426610	0.069704
4	1	0	1.204497	-1.134935	0.002376
5	6	0	0.059372	0.399089	0.003161
6	1	0	0.053836	1.500188	-0.000113
7	7	0	1.295528	-0.112326	0.002198

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.023947	0.741452	0.001105
2	1	0	0.147003	1.350961	0.890365
3	1	0	0.149148	1.351383	-0.887395
4	6	0	1.185102	-0.429116	0.001847
5	1	0	0.671933	-1.428480	0.006941
6	7	0	2.379897	-0.144062	-0.002386
7	6	0	-1.360429	0.184975	-0.000349
8	7	0	-2.347389	-0.464185	-0.001261

(*anti*,*Z*)-**26**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.067258	0.882816	-0.000046
2	1	0	-0.214583	1.957781	0.000104

3	1	0	2.639802	-0.923956	0.000024
4	6	0	1.245699	0.373697	0.000010
5	1	0	2.010659	1.171624	0.000039
6	7	0	1.620417	-0.893378	-0.000004
7	6	0	-1.219834	0.075946	0.000002
8	7	0	-2.218635	-0.563794	0.000009

(*syn*,*Z*)-**26**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018324	0.932380	-0.000034
2	1	0	-0.128919	2.011594	0.000072
3	1	0	0.843395	-1.501875	-0.000024
4	6	0	1.276390	0.352467	0.000008
5	1	0	2.094274	1.085087	0.000024
6	7	0	1.675188	-0.902043	0.000002
7	6	0	-1.178196	0.141723	0.000003
8	7	0	-2.144898	-0.548561	0.000006

(*anti*,*E*)-**26**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.060743	0.577475	-0.000006
2	1	0	0.106606	1.650729	0.000023
3	1	0	2.877878	-0.796413	0.000003
4	6	0	1.036445	-0.301470	0.000003
5	1	0	0.760503	-1.370540	0.000013
6	7	0	2.311485	0.051390	-0.000004
7	6	0	-1.380156	0.098758	0.000003
8	7	0	-2.499808	-0.298869	-0.000003

(*syn*,*E*)-**26**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040933	0.547163	-0.000006
2	1	0	0.143074	1.619674	0.000045
3	1	0	2.497907	0.864436	-0.000037
4	6	0	1.040723	-0.363489	0.000008
5	1	0	0.757216	-1.423771	0.000014
6	7	0	2.342412	-0.149577	-0.000003
7	6	0	-1.375347	0.110383	0.000004
8	7	0	-2.505962	-0.253949	-0.000006

Higher Level Energies, Selected Species

Up to QCISD(full,T)/6-311++G(2df,2pd)//MP2(full)/6-311+G* Level

(*E*)-3: MP2=-384.6218719, MP3=-384.6622892, MP4D=-384.681563, MP4DQ=-384.6638015, MP4SDQ=-384.6706826, QCISD=-384.6720306, QCISD(T)=-384.702477.

(*Z*)-4: MP2=-384.6275931, MP3=-384.6674404, MP4D=-384.6856071, MP4DQ=-384.6672959, MP4SDQ=-384.6739671, QCISD=-384.6752874, QCISD(T)=-384.7066911.

(*E*)-7: MP2=-476.7733304, MP3=-476.8030028, MP4D=-476.8330592, MP4DQ=-476.8038651, MP4SDQ=-476.8167855, QCISD=-476.817404, QCISD(T)=-476.8682527.

(*Z*,*Z*)-8: MP2=-476.7851281, MP3=-476.81324, MP4D=-476.8419963, MP4DQ=-476.811871, MP4SDQ=-476.8248385, QCISD=-476.8258814, QCISD(T)=-476.878103.

19: MP2=-140.6529916, MP3=-140.6742703, MP4D=-140.6885785, MP4DQ=-140.6729008, MP4SDQ=-140.679095, QCISD=-140.6796007, QCISD(T)=-140.7066005.

(*Z*)-20: MP2=-140.6697602, MP3=-140.6905456, MP4D=-140.7034612, MP4DQ=-140.6872736, MP4SDQ=-140.693394, QCISD=-140.6939439, QCISD(T)=-140.7217357.

(*Z*)-21: MP2=-232.8093449, MP3=-232.8200257, MP4D=-232.8449518, MP4DQ=-232.8176636, MP4SDQ=-232.8304799, QCISD= -232.8304134, QCISD(T)=-232.8782405.

(*Z*,*Z*)-22: MP2=-232.8528453, MP3=-232.8627551, MP4D=-232.8858243, MP4DQ=-232.8579598, MP4SDQ=-232.870196, QCISD=-232.8703315, QCISD(T)=-232.9185059.

23: MP2=-133.1276695, MP3=-133.1438337, MP4D=-133.1588292, MP4DQ=-133.1425315, MP4SDQ=-133.1504631, QCISD=-133.1522052, QCISD(T)=-133.1805224.

***syn*-24b**: MP2=-133.1475079, MP3=-133.1640616, MP4D=-133.1771809, MP4DQ=-133.1608653, MP4SDQ=-133.1675663, QCISD=-133.1679735, QCISD(T)=-133.1961307.

25: MP2=-225.2906236, MP3=-225.2956169,MP4D=-225.321414, MP4DQ=-225.2934915, MP4SDQ=-225.3076129, QCISD=-225.3076579, QCISD(T)=-225.3567182.

(*syn*,*Z*)-26: MP2=-225.3387979, MP3=-225.345017, MP4D=-225.3685871, MP4DQ=-225.3405924, MP4SDQ=-225.353401, QCISD=-225.3532091, QCISD(T)= -225.4015689.