Supporting Information

Solvent Effects on the Reduction and Amination Reactions of Electrophiles by Lithium Dialkylaminoborohydrides

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General Methods. All reactions were performed in oven-dried, nitrogen cooled glassware. All air- and moisture-sensitive compounds were introduced via syringes or cannula through a rubber septum. THF was distilled from sodium-benzophenone. Compounds were not isolated. All reactions were analyzed by ^{11}B-NMR. ^{11}B-NMR spectra were recorded neat. Chemical shifts are reported relative to external standard BF_3*Et_2O (δ = 0 ppm).

General Procedure for the Preparation of LAB reagent 1 M solution in THF/Hexanes. Diisopropylamine (5.06 g, 7 mL, 50 mmol, 1 eq.) was mixed with anhydrous THF (18 mL) in a serum vial. The solution was cooled to 0^{o}C (ice bath) and borane dimethylsulfide (5 mL, 10 M, 50 mmol, 1eq) was added dropwise via syringe, stirred for 1 hour at 0^{o}C and analyzed by ^{11}B-NMR. The analysis showed the solution to be diisopropylamine-borane =-21.08 (q, *J* = 95.3 Hz). Then, *n*-butyllithium in hexanes (20 mL, 2.5 M, 50 mmol, 1eq) was measured in oven dried graduated cylinder and added dropwise via cannula needle to the solution of amine borane at 0 ^{o}C. After stirring at 0 ^{o}C for 1 h, an aliquot was taken and analyzed by ^{11}B-NMR (80.25 MHz, THF) which showed the solution to be lithium diisopropylaminoborohydride = -23.64 (q, *J* = 83.4 Hz). LAB reagent was transferred to an oven-dried, nitrogen cooled ampoule via a cannula needle.

Note that, although the chemical shift of the corresponding amine-borane complex is virtually identical to that of the LAB, the *J*-values of the amine-borane complex is different and range from 95-98 Hz.

General Procedure for the reaction of LAB reagent with alkyl halides. The following procedure for reaction of *i*Pr-LAB reagent with methyl iodide (Table 1, entry

1), is representative. A 50 mL, round bottom flask equipped with magnetic stirring bar and fitted with rubber septa was charged lithium diisopropylaminoborohydride (1M in THF, 5 mL, 5 mmol, 1 eq), 5 mL of anhydrous THF. The reaction was cooled to 0°C (ice bath) and methyl iodide (0.31 mL, 5 mmol, 1 eq) was added slowly drop-wise (caution: v. exothermic rxn). After all methyl iodide was added, the ice bath was removed and reaction was stirred at room temperature for one hour. After 1 hour, the ^{11}B-NMR (80.25 MHz, THF) showed formation of diisopropyl aminoborane complex (δ= 35.33 ppm, t, J = 125.11 Hz) and *N,N,N*-diisopropylmethyl amine borane (δ = -15.61 ppm (q, J = 98.31 Hz)

Diisopropyl aminoborane complex and *N,N,N*-diisopropylmethyl amine borane (Table 1, entries 1,2,3). ^{11}B-NMR (80.25 MHz, THF): 35.11 ppm (t, J = 128.08 Hz); -15.71 ppm (q, J = 98.31 Hz)

Diisopropyl aminoborane complex and *N,N,N*-diisopropylmethyl amine borane (Table 1, entry 4). ^{11}B-NMR (80.25 MHz, THF): 35.07 ppm (t, J = 125.11 Hz); -15.71 ppm (q, J = 95.34 Hz).

Diisopropyl aminoborane complex and *N,N,N*-diisopropylmethyl amine borane (Table 1, entry 5). ^{11}B-NMR (80.25 MHz, THF): 35.15 ppm (t, J = 125.03 Hz); -15.61 ppm (q, J = 95.01 Hz).

***N,N,N*-Diisopropylmethyl amine-borane (**Table 1, entries 6, 7). ^{11}B-NMR (80.25 MHz, THF): -15.61 ppm (q, J = 98.31 Hz).

Diisopropyl aminoborane (Table 1, entries 8, 9). ^{11}B-NMR (80.25 MHz, THF): 35.33 ppm (t, J = 128.08 Hz)

Diisopropyl aminoborane (Table 1, entries 10, 11). ^{11}B-NMR (80.25 MHz, THF): 35.33 ppm (t, J = 128.08 Hz)

***N,N,N*-Diisopropylmethyl amine-borane (**Table 2 entries 1, 2, 3). ^{11}B-NMR (80.25 MHz): -15.54 ppm (q, J = 97 Hz).

***N,N*-Dimethyloctylamine-borane (Scheme 6).** ^{11}B-NMR (80.25 MHz, THF): -6.78 ppm (q, J=96 Hz)

***N,N*-Dimethylcyclohexylamine-borane (Scheme 6).** ^{11}B-NMR (80.25 MHz, THF): -11.35 ppm (q, J=96 Hz)

Table S1 Dimethyl LAB monomer.2THF

SCF Done: E(RHF) = -629.586454852 A.U. after 9 cycles

Convg = 0.6036D-08 -V/T = 2.0018

S**2 = 0.0000

E2 = -0.1970993173D+01 EUMP2 = -0.63155744802514D+03

Framework group C1[X(C10H25BLiNO2)]

Deg. of freedom 114

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.202749	0.582927	-0.078053
2	7	0	-1.188067	2.276143	-0.067562
3	5	0	-1.388909	1.721177	1.395856
4	1	0	-0.296744	1.224038	1.741872
5	1	0	-2.228321	0.824798	1.349216
6	1	0	-1.696844	2.592912	2.195594
7	8	0	1.702114	0.237473	-0.178661
8	6	0	2.642980	0.506921	0.899166
9	6	0	3.981447	-0.016798	0.396690
10	6	0	3.550047	-1.196475	-0.476868
11	6	0	2.317595	-0.630514	-1.166259
12	1	0	2.297894	-0.026889	1.791961
13	1	0	2.622771	1.580728	1.098412
14	1	0	4.486786	0.741522	-0.212145
15	1	0	4.648867	-0.300705	1.215871
16	1	0	4.317276	-1.516301	-1.188612
17	1	0	3.278696	-2.055469	0.147990
18	1	0	2.587019	-0.024086	-2.040189
19	1	0	1.570823	-1.373392	-1.457389

20	8	0	-0.854442	-1.212659	-0.496846
21	6	0	-0.686312	-2.076989	0.664900
22	6	0	-1.896702	-2.998710	0.655249
23	6	0	-2.982054	-2.075227	0.097975
24	6	0	-2.224581	-1.323154	-0.985693
25	1	0	-0.664702	-1.448246	1.562651
26	1	0	0.272222	-2.592825	0.552312
27	1	0	-1.729090	-3.848521	-0.016960
28	1	0	-2.127720	-3.385430	1.652396
29	1	0	-3.847639	-2.614555	-0.299349
30	1	0	-3.321551	-1.377345	0.869552
31	1	0	-2.197369	-1.879306	-1.930761
32	1	0	-2.591599	-0.310455	-1.165763
33	6	0	-2.447387	2.708508	-0.663796
34	1	0	-2.298780	3.029625	-1.704724
35	1	0	-3.168111	1.885655	-0.647078
36	1	0	-2.891544	3.552308	-0.104996
37	6	0	-0.247429	3.395862	-0.089219
38	1	0	-0.058539	3.729601	-1.119535
39	1	0	-0.625804	4.256899	0.490728
40	1	0	0.704258	3.088716	0.357937

Table S2 Dimethyl LAB monomer.dioxane

SCF Done: E(RHF) = -473.425824017 A.U. after 7 cycles

Convg = 0.8804D-08 -V/T = 2.0022

S**2 = 0.0000

E2 = -0.1437718474D+01 EUMP2 = -0.47486354249088D+03

Framework group C1[X(C6H17BLiNO2)]

Deg. of freedom 78

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.324167	0.221560	0.022423
2	7	0	-2.240270	-0.051849	0.060720
3	5	0	-1.939795	1.340169	-0.620859
4	1	0	-1.157955	1.104338	-1.559556
5	1	0	-1.316545	2.006265	0.218539
6	1	0	-2.926807	1.930234	-1.017123
7	6	0	-3.065026	0.098574	1.257901
8	1	0	-3.198829	-0.868494	1.762621
9	1	0	-2.584604	0.794884	1.951842
10	1	0	-4.065142	0.498364	1.013429
11	6	0	-2.890096	-0.981335	-0.861625
12	1	0	-3.023203	-1.966277	-0.392460
13	1	0	-3.883456	-0.613780	-1.174801
14	1	0	-2.275759	-1.099524	-1.759530
15	6	0	2.122954	-0.530475	1.284705
16	6	0	1.762545	-1.514135	0.150593
17	8	0	1.208721	-0.764655	-0.945749
18	6	0	2.078200	0.337274	-1.265555
19	6	0	1.998093	1.357145	-0.106581
20	8	0	1.419515	0.698124	1.040803
21	1	0	2.636364	-2.083839	-0.193863
22	1	0	0.976251	-2.213472	0.444992
23	1	0	3.200585	-0.324117	1.330491
24	1	0	3.096720	-0.043754	-1.418914
25	1	0	1.708410	0.756097	-2.202879
26	1	0	1.322008	2.184772	-0.331222

27	1	0	2.985669	1.755485	0.161671
28	1	0	1.793753	-0.889804	2.261685

Table S3 Diisopropyl LAB monomer.2THF

SCF Done: E(RHF) = -785.712945520 A.U. after 8 cycles

Convg = .2618D-08 -V/T = 2.0016

S**2 = .0000

E2 = -.2521884825D+01 EUMP2 = -.78823483034554D+03

Framework group C1[X(C14H33BLiNO2)]

Deg. of freedom 150

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-.182671	-.277697	-.064157
2	7	0	1.812887	-.418234	-.212812
3	5	0	1.166656	-1.329901	-1.328353
4	1	0	.322643	-.604973	-1.898439
5	1	0	.540436	-2.227423	-.759272
6	1	0	1.919880	-1.789437	-2.167896
7	8	0	-.952302	1.516521	.021503
8	6	0	-.921007	2.578807	-.967850
9	6	0	-1.225759	3.853413	-.192658
10	6	0	-2.163862	3.339131	.901641
11	6	0	-1.512059	2.012795	1.264693
12	1	0	-1.689292	2.364399	-1.721828
13	1	0	.062246	2.564521	-1.443569
14	1	0	-.308935	4.257831	.251103

15	1	0	-1.673760	4.626974	-.823811
16	1	0	-2.243597	4.013492	1.759721
17	1	0	-3.169563	3.173998	.497373
18	1	0	-.693867	2.147924	1.984468
19	1	0	-2.199513	1.250350	1.641190
20	8	0	-1.927024	-1.127162	.426548
21	6	0	-2.829682	-.801079	-.674204
22	6	0	-3.657814	-2.056846	-.916069
23	6	0	-2.681317	-3.160775	-.507686
24	6	0	-2.035831	-2.548999	.722937
25	1	0	-2.219556	-.546684	-1.548440
26	1	0	-3.417686	.072478	-.377206
27	1	0	-4.542311	-2.069534	-.268330
28	1	0	-3.991197	-2.132765	-1.955521
29	1	0	-3.170244	-4.116363	-.293418
30	1	0	-1.924623	-3.314677	-1.284255
31	1	0	-2.663168	-2.665557	1.616182
32	1	0	-1.029911	-2.918164	.927401
33	6	0	2.525517	1.925265	.244014
34	6	0	2.492006	.769911	-.763210
35	1	0	1.515019	2.139823	.606847
36	1	0	3.155572	1.687438	1.108829
37	1	0	2.935773	2.831761	-.220033
38	6	0	3.892240	.512708	-1.335473
39	1	0	1.861425	1.082307	-1.607773
40	1	0	3.864187	-.303615	-2.062541
41	1	0	4.264325	1.413405	-1.840006
42	1	0	4.608778	.257521	-.546066
43	6	0	1.659823	-1.443204	2.018839
44	6	0	2.584034	-1.103838	.847141
45	1	0	1.197718	-.532104	2.418832

46	1	0	.868040	-2.123808	1.686818
47	1	0	2.205478	-1.938342	2.832421
48	6	0	3.335464	-2.357489	.386524
49	1	0	3.331859	-.396440	1.231881
50	1	0	3.990386	-2.142069	-.461173
51	1	0	3.949060	-2.749483	1.208321
52	1	0	2.633021	-3.136230	.075868

Table S4 Diisopropyl LAB monomer.dioxane

SCF Done: E(RHF) = -629.556303344 A.U. after 7 cycles

Convg = 0.9660D-08 -V/T = 2.0018

S**2 = 0.0000

E2 = -0.1985564834D+01 EUMP2 = -0.63154186817803D+03

Framework group C1[X(C10H25BLiNO2)]

Deg. of freedom 114

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.563303	0.125386	0.446381
2	7	0	-1.369753	-0.016756	0.286488
3	5	0	-0.985079	0.355990	1.775308
4	1	0	-0.365644	1.426645	1.732632
5	1	0	-0.154751	-0.512415	2.118614
6	1	0	-1.884292	0.403481	2.589364
7	6	0	-1.973255	-1.357928	0.158949
8	1	0	-1.448609	-1.970491	0.904576
9	6	0	-2.045945	1.034091	-0.506734
10	1	0	-2.638792	0.538099	-1.287729

11	6	0	2.439563	-0.716273	-1.303764
12	6	0	2.872894	0.748931	-1.079212
13	8	0	2.318981	1.184643	0.172451
14	6	0	2.995175	0.510700	1.254694
15	6	0	2.987252	-1.008074	0.965005
16	8	0	1.994654	-1.260570	-0.047064
17	1	0	3.965216	0.860059	-1.047581
18	1	0	2.473967	1.417744	-1.844471
19	1	0	3.257313	-1.331579	-1.703409
20	1	0	4.015110	0.906390	1.352117
21	1	0	2.421411	0.762992	2.149141
22	1	0	2.686632	-1.588301	1.839179
23	1	0	3.960835	-1.371814	0.609870
24	1	0	1.577198	-0.793953	-1.970301
25	6	0	-1.692171	-1.973539	-1.215238
26	1	0	-2.129106	-1.374890	-2.022845
27	1	0	-0.611522	-2.046107	-1.382472
28	1	0	-2.117284	-2.982555	-1.283337
29	6	0	-3.467896	-1.424383	0.493932
30	1	0	-4.072905	-0.889839	-0.247590
31	1	0	-3.804115	-2.468502	0.503836
32	1	0	-3.658436	-0.992337	1.480431
33	6	0	-0.995676	1.888318	-1.224383
34	1	0	-0.403167	1.265130	-1.907504
35	1	0	-1.461563	2.687715	-1.814515
36	1	0	-0.324067	2.360196	-0.496342
37	6	0	-2.996800	1.929240	0.294186
38	1	0	-2.444085	2.521709	1.028810
39	1	0	-3.522010	2.616289	-0.381975
40	1	0	-3.741500	1.338423	0.832691

Table S5 Dimethyl LAB monomer.2THF red anti CH3Cl

LABme_m_2THF_MeCl_red_TS_anti_6-31+Gd_MP2.arc

SCF Done: E(RHF) = -1128.62350829 A.U. after 8 cycles
Convg = 0.8737D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2243185563D+01 EUMP2 = -0.11308666938537D+04

Framework group C1[X(C11H28BClLiNO2)]
Deg. of freedom 129
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.239067	2.908113	2.013221
2	7	0	0.504728	1.834105	1.338513
3	3	0	0.917298	-0.053548	0.757883
4	6	0	-0.776084	1.630353	2.028273
5	1	0	2.212492	3.048037	1.538022
6	1	0	1.395447	2.654605	3.069390
7	1	0	0.695252	3.866366	1.967044
8	1	0	-1.317777	0.787574	1.588999
9	1	0	-1.422426	2.521884	1.962773
10	1	0	-0.603960	1.414368	3.090776
11	5	0	0.399790	2.009278	-0.187177
12	1	0	-0.750269	2.556887	-0.503391
13	1	0	0.364733	0.923148	-0.763640
14	1	0	1.249869	2.732155	-0.656119
15	6	0	-2.003302	1.987067	-1.093820

16	1	0	-1.528824	1.733799	-2.026122
17	1	0	-2.105050	1.251007	-0.321690
18	1	0	-2.519535	2.931012	-0.997062
19	17	0	-3.951634	0.977761	-1.940618
20	8	0	2.619842	-0.703425	0.177111
21	6	0	2.539291	-1.546173	-1.013355
22	6	0	3.767097	-1.194241	-1.842842
23	6	0	3.982056	0.277154	-1.481969
24	6	0	3.695043	0.267864	0.009196
25	1	0	1.610459	-1.299938	-1.540646
26	1	0	2.502734	-2.586421	-0.679516
27	1	0	4.629174	-1.794507	-1.530477
28	1	0	3.601640	-1.359748	-2.911433
29	1	0	4.989901	0.636618	-1.710799
30	1	0	3.256073	0.913491	-1.999443
31	1	0	4.558274	-0.075557	0.592122
32	1	0	3.339367	1.220800	0.406525
33	8	0	-0.413591	-1.456267	0.689212
34	6	0	-0.908028	-2.164010	1.867038
35	6	0	-2.206711	-2.845371	1.435265
36	6	0	-2.657051	-1.991126	0.247974
37	6	0	-1.333184	-1.694402	-0.423903
38	1	0	-1.074898	-1.418155	2.651857
39	1	0	-0.132464	-2.862968	2.195453
40	1	0	-2.011651	-3.873635	1.110619
41	1	0	-2.937964	-2.880016	2.248130
42	1	0	-3.355793	-2.500169	-0.421299
43	1	0	-3.132738	-1.060647	0.574634
44	1	0	-0.966213	-2.554998	-0.998624
45	1	0	-1.331180	-0.805237	-1.053990

Table S6 Dimethyl LAB monomer.2THF red gauche CH3Cl

SCF Done: E(RHF) = -1128.62923420 A.U. after 7 cycles

Convg = 0.5274D-08 -V/T = 2.0012

S**2 = 0.0000

E2 = -0.2246697453D+01 EUMP2 = -0.11308759316514D+04

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Framework group C1[X(C11H28BClLiNO2)]

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.934566	3.264619	1.358311
2	7	0	-0.105703	2.591034	0.578981
3	3	0	-0.450971	0.708603	0.089828
4	6	0	-1.420242	3.097633	1.000030
5	1	0	1.919746	2.870773	1.093571
6	1	0	0.774179	3.098843	2.431239
7	1	0	0.938553	4.352318	1.172412
8	1	0	-2.211207	2.607170	0.422424
9	1	0	-1.507303	4.185404	0.839269
10	1	0	-1.586110	2.891586	2.065982
11	5	0	0.059743	2.787057	-0.948477
12	1	0	1.286958	2.508151	-1.234742
13	1	0	-0.103779	3.920991	-1.357594
14	1	0	-0.616850	1.952027	-1.551177
15	6	0	2.246426	1.345156	-1.281269
16	1	0	1.847426	0.991801	-2.217811
17	1	0	3.069139	2.043954	-1.285809

18	1	0	1.884237	0.946193	-0.351399
19	17	0	3.744092	-0.414137	-1.278660
20	8	0	0.592897	-0.820997	0.548286
21	6	0	0.672958	-1.975146	-0.338762
22	6	0	1.184853	-3.091532	0.552928
23	6	0	2.206255	-2.346804	1.417765
24	6	0	1.537199	-0.994327	1.649703
25	1	0	1.381203	-1.749146	-1.141632
26	1	0	-0.333114	-2.130456	-0.740733
27	1	0	0.370904	-3.501555	1.164023
28	1	0	1.634456	-3.905633	-0.023692
29	1	0	2.426068	-2.858741	2.359799
30	1	0	3.134719	-2.206482	0.858912
31	1	0	0.953795	-0.961468	2.577056
32	1	0	2.246324	-0.161921	1.633166
33	8	0	-2.174402	-0.102908	-0.188969
34	6	0	-2.722382	-1.068306	0.749246
35	6	0	-3.734019	-1.866074	-0.058387
36	6	0	-4.284399	-0.796290	-1.003864
37	6	0	-3.026659	-0.019811	-1.368358
38	1	0	-3.200876	-0.519912	1.570478
39	1	0	-1.885203	-1.651083	1.142248
40	1	0	-3.231626	-2.657873	-0.626105
41	1	0	-4.500812	-2.326790	0.571602
42	1	0	-4.784893	-1.208551	-1.884918
43	1	0	-4.994813	-0.150750	-0.475165
44	1	0	-2.488849	-0.478042	-2.206524
45	1	0	-3.193014	1.037724	-1.586221

Table S7 Dimethyl LAB monomer.2THF SN2 backside CH3Cl

SCF Done: E(RHF) = -1128.64366453 A.U. after 10 cycles

Convg = 0.3615D-08 -V/T = 2.0012

S**2 = 0.0000

E2 = -0.2248732494D+01 EUMP2 = -0.11308923970198D+04

Framework group C1[X(C11H28BClLiNO2)]

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.477983	-3.328383	-1.000968
2	7	0	-1.972688	-2.542119	0.119347
3	3	0	0.535021	-0.409791	-0.045629
4	6	0	-2.517312	-3.041001	1.377197
5	1	0	-2.098612	-2.909519	-1.938588
6	1	0	-3.576447	-3.303071	-1.023224
7	1	0	-2.155880	-4.381117	-0.939455
8	1	0	-2.175868	-2.403320	2.199114
9	1	0	-2.189357	-4.073279	1.584081
10	1	0	-3.615913	-3.025763	1.353008
11	5	0	-0.427457	-2.459277	0.130990
12	1	0	0.118461	-3.548862	0.240357
13	1	0	-0.087759	-1.744260	1.090260
14	1	0	-0.064926	-1.936833	-0.936364
15	6	0	-2.685730	-0.559617	-0.138047
16	17	0	-3.337592	1.457896	-0.393515
17	1	0	-2.149495	-0.356018	0.773817
18	1	0	-3.684040	-0.964901	-0.080553

19	1	0	-2.158958	-0.593580	-1.077682
20	8	0	2.421613	-0.496531	-0.326848
21	6	0	3.366039	0.479986	0.191107
22	6	0	4.734890	-0.164295	0.023601
23	6	0	4.409528	-1.645885	0.224347
24	6	0	3.093185	-1.779194	-0.524340
25	1	0	3.129837	0.664012	1.246241
26	1	0	3.230924	1.406374	-0.373172
27	1	0	5.118326	0.008420	-0.988398
28	1	0	5.465575	0.224018	0.739473
29	1	0	5.179731	-2.316804	-0.167619
30	1	0	4.268381	-1.866724	1.288419
31	1	0	3.247234	-1.914905	-1.601038
32	1	0	2.425253	-2.558231	-0.151999
33	8	0	0.149109	1.432713	0.120355
34	6	0	-0.315448	2.165693	1.295185
35	6	0	-0.612595	3.583939	0.812264
36	6	0	0.225950	3.699721	-0.464238
37	6	0	0.089295	2.303861	-1.044065
38	1	0	0.496341	2.130644	2.030721
39	1	0	-1.199762	1.660913	1.690418
40	1	0	-1.674935	3.676334	0.573062
41	1	0	-0.351732	4.333681	1.565503
42	1	0	-0.145277	4.470325	-1.146663
43	1	0	1.275411	3.915418	-0.230034
44	1	0	-0.877380	2.163459	-1.537262
45	1	0	0.906292	2.001539	-1.706471

Table S8 Dimethyl LAB monomer.2THF SN2 frontside CH3Cl

LABme_m_2thf_MeCl_SN2_TS2_6-31+Gd_MP2.arc.txt

SCF Done: E(RHF) = -1128.58539687 A.U. after 11 cycles
Convg = 0.3565D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2268713770D+01 EUMP2 = -0.11308541106419D+04

Framework group C1[X(C11H28BClLiNO2)]
Deg. of freedom 129
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.055172	-0.275730	-0.216347
2	7	0	-1.427504	2.507265	-0.391216
3	6	0	-2.504323	2.559726	0.590874
4	5	0	-1.399406	1.187511	-1.236290
5	6	0	-1.465185	3.678272	-1.250837
6	1	0	-1.742458	0.256956	-0.521329
7	1	0	-0.250700	1.021774	-1.666149
8	1	0	-2.170062	1.263969	-2.181879
9	17	0	0.260073	1.034779	1.641977
10	6	0	0.463725	3.084431	0.637334
11	1	0	1.330540	3.033433	1.290592
12	1	0	-0.207663	3.874200	0.963852
13	1	0	0.761230	3.113295	-0.406915
14	1	0	-3.487956	2.476214	0.099805
15	1	0	-2.475909	3.511154	1.141528

16	1	0	-2.386568	1.737588	1.298136
17	1	0	-0.697285	3.588962	-2.025783
18	1	0	-1.289256	4.600461	-0.674633
19	1	0	-2.440945	3.770190	-1.749507
20	8	0	-0.667570	-2.077399	0.108824
21	6	0	-1.204853	-2.605472	-1.138926
22	6	0	-2.691774	-2.806862	-0.885262
23	6	0	-2.710352	-3.161329	0.603104
24	6	0	-1.669357	-2.200752	1.158308
25	1	0	-0.689357	-3.549518	-1.353357
26	1	0	-0.986360	-1.885144	-1.932895
27	1	0	-3.231622	-1.870889	-1.062665
28	1	0	-3.119717	-3.585880	-1.524054
29	1	0	-3.690786	-3.024030	1.069377
30	1	0	-2.396769	-4.200757	0.755669
31	1	0	-2.091231	-1.208021	1.351364
32	1	0	-1.156660	-2.556794	2.055899
33	8	0	1.857894	-0.831395	-0.735157
34	6	0	2.517521	-1.604587	0.308882
35	6	0	3.742571	-0.790148	0.693770
36	6	0	4.125983	-0.157685	-0.645293
37	6	0	2.760872	0.205125	-1.212512
38	1	0	2.788102	-2.580412	-0.113557
39	1	0	1.799259	-1.749272	1.118622
40	1	0	3.464403	-0.016725	1.417714
41	1	0	4.534943	-1.409155	1.126423
42	1	0	4.778420	0.715212	-0.544880
43	1	0	4.627499	-0.891524	-1.287056
44	1	0	2.409281	1.170082	-0.830556
45	1	0	2.708870	0.208205	-2.304369

Table S9 Dimethyl LAB monomer.dioxane red anti CH3Cl

SCF Done: E(RHF) = -972.460230469 A.U. after 8 cycles

Convg = 0.8047D-08 -V/T = 2.0013

S**2 = 0.0000

E2 = -0.1704720760D+01 EUMP2 = -0.97416495122897D+03

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.307871	3.329564	-0.524135
2	7	0	-0.189186	1.950126	-0.044063
3	3	0	1.202050	0.573184	-0.213138
4	6	0	-0.594994	1.869608	1.367065
5	1	0	0.014869	3.383134	-1.566107
6	1	0	0.319823	3.997219	0.078665
7	1	0	-1.347506	3.689006	-0.462070
8	1	0	-0.497269	0.839633	1.728452
9	1	0	-1.643830	2.177900	1.503870
10	1	0	0.033794	2.521386	1.986522
11	5	0	-0.877801	0.907613	-0.924505
12	1	0	-2.158428	0.893446	-0.675329
13	1	0	-0.501453	-0.221085	-0.596187
14	1	0	-0.765131	1.118410	-2.109725
15	6	0	-3.214139	-0.010446	-0.373799
16	1	0	-2.873608	-0.257737	0.617089
17	1	0	-3.961718	0.757311	-0.502775
18	1	0	-3.017279	-0.692534	-1.184370
19	17	0	-5.041787	-1.467955	0.159243
20	6	0	3.865845	-0.264057	-0.292954

21	6	0	3.335204	-0.307876	1.159877
22	8	0	1.963000	-0.746787	1.128188
23	6	0	1.875598	-1.991580	0.400804
24	6	0	2.183333	-1.696235	-1.087409
25	8	0	2.734762	-0.361444	-1.179339
26	1	0	3.922135	-0.982540	1.796030
27	1	0	3.312640	0.681022	1.624970
28	1	0	4.557613	-1.087696	-0.509021
29	1	0	2.580926	-2.707201	0.841435
30	1	0	0.858330	-2.358987	0.545432
31	1	0	1.282154	-1.681655	-1.702681
32	1	0	2.899119	-2.410395	-1.513109
33	1	0	4.362408	0.680070	-0.525327

Table S10 Dimethyl LAB monomer.dioxane red gauche CH3Cl

LABme_m_dioxane_MeCl_red_TS_gauche_6-31+Gd_MP2.arc.txt

SCF Done: E(RHF) = -972.461085360 A.U. after 7 cycles
Convg = 0.9299D-08 -V/T = 2.0013
S**2 = 0.0000
E2 = -0.1715393197D+01 EUMP2 = -0.97417647855723D+03

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.374210	-0.279858	-0.482637
2	7	0	-2.147383	-0.930493	-0.003822
3	3	0	-0.508625	0.005040	-0.523365

4	6	0	-2.407774	-1.573346	1.286007
5	1	0	-3.191779	0.192128	-1.454108
6	1	0	-3.702783	0.489018	0.230380
7	1	0	-4.198009	-1.001809	-0.607315
8	1	0	-1.494387	-2.041669	1.663726
9	1	0	-3.184219	-2.351506	1.200659
10	1	0	-2.742653	-0.831790	2.023005
11	5	0	-1.622265	-1.912394	-1.076137
12	1	0	-0.546564	-2.445823	-0.557281
13	1	0	-1.229988	-1.270797	-2.048025
14	1	0	-2.328585	-2.858865	-1.351520
15	6	0	0.901876	-2.149614	-0.294079
16	1	0	1.065710	-1.754579	-1.282529
17	1	0	0.671847	-1.526147	0.557481
18	1	0	1.084037	-3.201076	-0.126710
19	17	0	3.120540	-1.654914	0.121531
20	6	0	1.663548	1.472042	0.594808
21	6	0	1.487623	1.731981	-0.912810
22	8	0	0.066739	1.801019	-1.210349
23	6	0	-0.563113	2.697365	-0.272862
24	6	0	-0.561732	2.006900	1.111280
25	8	0	0.407534	0.942209	1.080724
26	1	0	1.967059	2.663655	-1.238905
27	1	0	1.876096	0.904806	-1.512309
28	1	0	1.902226	2.384064	1.156785
29	1	0	-0.013996	3.647300	-0.268153
30	1	0	-1.574103	2.878651	-0.644320
31	1	0	-1.516553	1.524462	1.332630
32	1	0	-0.314146	2.708662	1.918731
33	1	0	2.419011	0.706525	0.778038

Table S11 Dimethyl LAB monomer.dioxane SN2 backside CH3Cl

SCF Done: E(RHF) = -972.473445415 A.U. after 8 cycles

Convg = 0.3376D-08 -V/T = 2.0012

S**2 = 0.0000

E2 = -0.1722956847D+01 EUMP2 = -0.97419640226241D+03

Framework group C1[X(C7H20BClLiNO2)]

Deg. of freedom 93

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.655509	-0.621235	1.200167
2	7	0	2.837935	-0.485066	0.000000
3	3	0	-0.281393	0.038698	-0.000089
4	6	0	3.655637	-0.621088	-1.200096
5	1	0	3.035413	-0.443785	2.085825
6	1	0	4.477414	0.107359	1.192714
7	1	0	4.088001	-1.632528	1.289563
8	1	0	3.035634	-0.443537	-2.085799
9	1	0	4.088145	-1.632368	-1.289566
10	1	0	4.477537	0.107510	-1.192470
11	5	0	1.605947	-1.444268	-0.000126
12	1	0	1.909079	-2.626328	-0.000212
13	1	0	0.926853	-1.198540	-1.009061
14	1	0	0.926768	-1.198713	1.008791
15	6	0	1.635290	1.374860	0.000033
16	17	0	-0.080812	2.571189	-0.000023
17	1	0	1.418848	0.911572	-0.947044
18	1	0	2.431193	2.110030	0.000130

19	1	0	1.418721	0.911468	0.947030
20	6	0	-2.098670	-1.773801	-0.775741
21	6	0	-2.098733	-1.773709	0.775853
22	8	0	-1.852255	-0.428073	1.228639
23	6	0	-2.914653	0.431232	0.774826
24	6	0	-2.914818	0.431064	-0.774820
25	8	0	-1.852391	-0.428176	-1.228676
26	1	0	-3.053455	-2.120765	1.192398
27	1	0	-1.285183	-2.375639	1.183466
28	1	0	-3.053293	-2.121088	-1.192320
29	1	0	-3.865097	0.071404	1.190829
30	1	0	-2.691697	1.417665	1.183085
31	1	0	-2.692108	1.417448	-1.183338
32	1	0	-3.865295	0.071002	-1.190544
33	1	0	-1.284971	-2.375622	-1.183219

Table S12 Dimethyl LAB monomer.dioxane SN2 frontside CH3Cl

SCF Done: E(RHF) = -972.428603915 A.U. after 9 cycles
Convg = 0.7107D-08 -V/T = 2.0013
S**2 = 0.0000
E2 = -0.1732977622D+01 EUMP2 = -0.97416158153683D+03

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.277957	-0.062533	-0.426631
2	7	0	2.434631	-0.580296	-0.115559
3	6	0	3.291934	0.080768	-1.096752

4	5	0	1.339505	-1.505686	-0.761964
5	6	0	3.239356	-1.337952	0.830209
6	1	0	0.807461	-0.911346	-1.693471
7	1	0	0.511495	-1.767027	0.121577
8	1	0	1.825073	-2.544499	-1.172404
9	17	0	0.696210	1.941711	-0.369190
10	6	0	1.765387	0.925256	1.434729
11	1	0	1.264338	1.785533	1.864800
12	1	0	2.843132	1.045787	1.455836
13	1	0	1.372732	-0.006465	1.831056
14	1	0	3.864961	-0.664015	-1.672336
15	1	0	4.001549	0.752171	-0.593529
16	1	0	2.676251	0.663649	-1.781100
17	1	0	2.588745	-1.819909	1.567502
18	1	0	3.957833	-0.689692	1.353278
19	1	0	3.805078	-2.126734	0.313984
20	6	0	-2.494445	0.920407	0.871684
21	6	0	-2.908934	0.823586	-0.617216
22	8	0	-2.143190	-0.225214	-1.235303
23	6	0	-2.512097	-1.495604	-0.666952
24	6	0	-2.332871	-1.418536	0.869083
25	8	0	-1.640382	-0.196781	1.179285
26	1	0	-3.977922	0.602047	-0.739275
27	1	0	-2.666497	1.735024	-1.166370
28	1	0	-3.364131	0.906904	1.543001
29	1	0	-3.545682	-1.734868	-0.951601
30	1	0	-1.834573	-2.220893	-1.121495
31	1	0	-1.705217	-2.228326	1.244094
32	1	0	-3.293564	-1.428778	1.401770
33	1	0	-1.894105	1.808861	1.068977

Table S13 Diisopropyl LAB monomer.2THF red anti CH3Cl

SCF Done: E(RHF) = -1284.75350161 A.U. after 9 cycles
Convg = 0.7777D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2791271372D+01 EUMP2 = -0.12875447729804D+04

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.328345	-1.315180	2.451190
2	7	0	-0.923713	-0.973816	1.065760
3	3	0	0.894659	-0.161389	0.528456
4	6	0	-1.165686	-2.056712	0.079438
5	1	0	-1.360843	-2.410018	2.521027
6	1	0	-0.957538	-1.595216	-0.896900
7	5	0	-1.272894	0.417357	0.547753
8	1	0	-2.488108	0.487571	0.086698
9	1	0	-0.585679	0.668204	-0.444819
10	1	0	-1.198092	1.290876	1.386045
11	6	0	-3.278943	0.976112	-1.025542
12	1	0	-2.811587	1.946890	-1.047913
13	1	0	-2.943566	0.211731	-1.706437
14	1	0	-4.190882	0.835839	-0.465317
15	17	0	-4.628248	1.720530	-2.806501
16	8	0	1.975504	1.424440	0.916667
17	6	0	2.184472	2.176913	-0.320878
18	6	0	2.203783	3.645570	0.084604
19	6	0	1.298716	3.649404	1.317445

20	6	0	1.721699	2.363831	2.003609
21	1	0	1.350033	1.953897	-0.994410
22	1	0	3.119052	1.829610	-0.770645
23	1	0	3.218293	3.960608	0.354486
24	1	0	1.844551	4.294573	-0.719319
25	1	0	1.438523	4.528671	1.953697
26	1	0	0.245181	3.588655	1.025253
27	1	0	2.651676	2.488796	2.572373
28	1	0	0.956565	1.923098	2.643446
29	8	0	2.084340	-0.948568	-0.765080
30	6	0	3.495147	-1.173850	-0.496674
31	6	0	4.155626	-1.145502	-1.864862
32	6	0	3.087443	-1.813636	-2.733038
33	6	0	1.798337	-1.229808	-2.167749
34	1	0	3.607524	-2.153776	-0.014546
35	1	0	3.821933	-0.390206	0.191871
36	1	0	4.323308	-0.111490	-2.187482
37	1	0	5.115125	-1.671174	-1.877105
38	1	0	3.199429	-1.604583	-3.800803
39	1	0	3.110185	-2.900046	-2.592015
40	1	0	1.522784	-0.283885	-2.647782
41	1	0	0.948342	-1.915255	-2.209304
42	6	0	-2.610034	-2.569280	0.024565
43	1	0	-3.322278	-1.751788	-0.110260
44	1	0	-2.723955	-3.257691	-0.821013
45	1	0	-2.875492	-3.118537	0.934497
46	6	0	-0.197205	-3.228670	0.267189
47	1	0	-0.352912	-3.979253	-0.517439
48	1	0	0.842910	-2.890369	0.222367
49	1	0	-0.356508	-3.727499	1.229485
50	6	0	-2.706525	-0.780336	2.852774

51	1	0	-2.980817	-1.161408	3.844257
52	1	0	-2.699139	0.312555	2.897982
53	1	0	-3.480683	-1.086561	2.145462
54	6	0	-0.265342	-0.835434	3.437868
55	1	0	0.713630	-1.265978	3.194265
56	1	0	-0.190935	0.256570	3.409968
57	1	0	-0.520930	-1.125836	4.464063

Table S14 Diisopropyl LAB monomer.2THF red gauche CH3Cl

LABipr_m_2thf_MeCl_red_TS_gauche_MP2.arc.txt

SCF Done: E(RHF) = -1284.75175523 A.U. after 8 cycles
Convg = 0.4378D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2801949669D+01 EUMP2 = -0.12875537048954D+04

Framework group C1[X(C15H36BClLiNO2)]
Deg. of freedom 165
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.812161	-1.435673	0.002124
2	7	0	-2.304738	-0.071319	0.285654
3	3	0	-0.372765	0.140007	-0.272354
4	6	0	-3.227027	1.014409	-0.145453
5	1	0	-2.099969	-2.105856	0.504117
6	1	0	-3.880786	0.592108	-0.919561
7	5	0	-1.718902	0.083748	1.703440

8	1	0	-0.560410	-0.577942	1.675193
9	1	0	-2.284727	-0.479009	2.619177
10	1	0	-1.387686	1.227859	1.939759
11	6	0	0.927447	-0.715016	2.014270
12	1	0	0.883947	0.116093	2.698687
13	1	0	0.752716	-1.713841	2.385935
14	1	0	1.194882	-0.573173	0.984836
15	17	0	3.189887	-0.896709	2.316569
16	8	0	0.739766	-1.234635	-1.155523
17	6	0	2.112628	-0.952014	-1.588102
18	6	0	2.823574	-2.298795	-1.637649
19	6	0	2.062132	-3.106525	-0.585640
20	6	0	0.634779	-2.656293	-0.837022
21	1	0	2.564069	-0.281069	-0.851623
22	1	0	2.055972	-0.453087	-2.560157
23	1	0	2.721607	-2.757822	-2.627961
24	1	0	3.887602	-2.198441	-1.405338
25	1	0	2.180325	-4.188188	-0.705204
26	1	0	2.393032	-2.819370	0.417585
27	1	0	0.185802	-3.170781	-1.695965
28	1	0	-0.030652	-2.747588	0.024640
29	8	0	0.825859	1.662390	-0.366178
30	6	0	1.082119	2.421119	-1.574699
31	6	0	2.388656	3.142859	-1.299747
32	6	0	2.206816	3.527655	0.170055
33	6	0	1.541574	2.286614	0.754600
34	1	0	0.258909	3.129409	-1.735294
35	1	0	1.113113	1.712237	-2.406599
36	1	0	3.235784	2.457472	-1.417489
37	1	0	2.539960	4.003184	-1.959014
38	1	0	3.147723	3.757533	0.678132

39	1	0	1.549004	4.400360	0.252097
40	1	0	2.272611	1.561519	1.124621
41	1	0	0.807964	2.504248	1.535627
42	6	0	-2.774662	-1.746335	-1.497406
43	1	0	-3.029304	-2.797898	-1.677181
44	1	0	-3.499139	-1.137361	-2.049778
45	1	0	-1.780697	-1.555247	-1.915388
46	6	0	-4.193964	-1.753128	0.582792
47	1	0	-4.423260	-2.814524	0.429873
48	1	0	-4.222050	-1.548817	1.656503
49	1	0	-4.981145	-1.172120	0.089835
50	6	0	-2.434207	2.145733	-0.798287
51	1	0	-1.903619	1.781243	-1.687009
52	1	0	-3.098951	2.959711	-1.113115
53	1	0	-1.701683	2.554421	-0.093590
54	6	0	-4.123266	1.569605	0.967311
55	1	0	-4.869381	2.249983	0.537680
56	1	0	-4.651652	0.773221	1.495958
57	1	0	-3.533644	2.128745	1.699352

Table S15 Diisopropyl LAB monomer.2THF SN2 CH3Cl

SCF Done: E(RHF) = -1284.75886778 A.U. after 8 cycles
Convg = 0.5650D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2803356167D+01 EUMP2 = -0.12875622239470D+04

Framework group C1[X(C15H36BClLiNO2)]
Deg. of freedom 165
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.356726	0.249848	-1.059973
2	7	0	2.369165	0.091182	0.045219
3	3	0	-0.936682	0.430900	-0.412392
4	6	0	2.990688	0.000941	1.398357
5	1	0	2.733194	0.380604	-1.956047
6	1	0	3.999585	-0.410855	1.266311
7	5	0	1.207117	1.131077	-0.066328
8	1	0	1.524673	2.305302	-0.001118
9	1	0	0.382822	0.901845	0.833072
10	1	0	0.672040	0.946598	-1.171037
11	6	0	1.252772	-1.652696	-0.496880
12	17	0	-0.039204	-3.294019	-1.113322
13	1	0	0.555499	-1.320351	0.248697
14	1	0	2.053867	-2.306728	-0.202884
15	1	0	1.253050	-1.216031	-1.480557
16	8	0	-2.076159	1.946125	-0.753005
17	6	0	-2.806975	2.306044	0.458442
18	6	0	-2.882662	3.827476	0.451442
19	6	0	-1.593609	4.206328	-0.280477
20	6	0	-1.547464	3.155923	-1.375988
21	1	0	-2.240904	1.932881	1.320463
22	1	0	-3.778395	1.805531	0.422719
23	1	0	-3.757296	4.167055	-0.115105
24	1	0	-2.947249	4.239561	1.462914
25	1	0	-1.605736	5.225409	-0.679139
26	1	0	-0.724905	4.096284	0.377748
27	1	0	-2.198886	3.414426	-2.219714
28	1	0	-0.544013	2.923394	-1.736132

29	8	0	-2.145408	-0.893957	0.173559
30	6	0	-2.096111	-1.781658	1.331321
31	6	0	-3.065832	-2.917918	1.023356
32	6	0	-4.041197	-2.272381	0.035803
33	6	0	-3.104804	-1.412527	-0.793577
34	1	0	-2.404026	-1.189119	2.200832
35	1	0	-1.068292	-2.126546	1.461785
36	1	0	-2.529046	-3.739313	0.540808
37	1	0	-3.553863	-3.294448	1.927689
38	1	0	-4.578575	-3.005383	-0.573650
39	1	0	-4.774809	-1.646872	0.558512
40	1	0	-2.560808	-2.006323	-1.535099
41	1	0	-3.575262	-0.544907	-1.265415
42	6	0	4.228275	-0.991925	-1.283611
43	1	0	3.643837	-1.863775	-1.584619
44	1	0	4.947730	-0.785789	-2.084124
45	1	0	4.805012	-1.253871	-0.390275
46	6	0	4.257795	1.487097	-0.955473
47	1	0	4.998089	1.375252	-0.155409
48	1	0	4.807610	1.610517	-1.896384
49	1	0	3.675810	2.394051	-0.777360
50	6	0	2.228277	-0.962040	2.314378
51	1	0	1.182548	-0.650620	2.412111
52	1	0	2.257636	-1.994373	1.957977
53	1	0	2.675763	-0.941982	3.314931
54	6	0	3.127482	1.346841	2.126083
55	1	0	3.724782	1.201355	3.035134
56	1	0	3.613168	2.109530	1.516605
57	1	0	2.144499	1.726197	2.420849

Table S16 Diisopropyl LAB monomer.dioxane red anti CH3Cl

SCF Done: E(RHF) = -1128.59261410 A.U. after 9 cycles
Convg = 0.5601D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2253825313D+01 EUMP2 = -0.11308464394094D+04

Framework group C1[X(C11H28BClLiNO2)]
Deg. of freedom 129
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.648346	1.250702	1.398617
2	7	0	0.213937	1.168787	-0.018558
3	3	0	-1.278960	-0.131462	-0.099279
4	6	0	0.125845	2.467340	-0.728711
5	1	0	0.807484	0.207078	1.706313
6	1	0	0.053226	3.252933	0.034376
7	5	0	0.781825	-0.023678	-0.779289
8	1	0	2.079487	-0.086421	-0.711778
9	1	0	0.511332	-0.031375	-1.959945
10	1	0	0.415232	-1.064883	-0.221834
11	6	0	3.190280	-0.934134	-0.463327
12	1	0	3.879645	-0.205754	-0.863434
13	1	0	3.039561	-0.997262	0.601755
14	1	0	2.855897	-1.744048	-1.091071
15	17	0	5.114057	-2.279629	-0.043499
16	6	0	-3.692710	-0.641031	0.954363
17	6	0	-3.970280	-0.674920	-0.568075

18	8	0	-2.734227	-0.983749	-1.237282
19	6	0	-2.369334	-2.351792	-0.945189
20	6	0	-2.325040	-2.523535	0.593556
21	8	0	-2.389319	-1.209926	1.192344
22	1	0	-4.720158	-1.429407	-0.837630
23	1	0	-4.294624	0.294527	-0.951710
24	1	0	-4.444484	-1.199522	1.526655
25	1	0	-3.094930	-3.026767	-1.416299
26	1	0	-1.391224	-2.495187	-1.407485
27	1	0	-1.385933	-2.965295	0.931066
28	1	0	-3.161038	-3.124235	0.973312
29	1	0	-3.640576	0.378481	1.344832
30	6	0	-0.453412	1.831624	2.288767
31	1	0	-1.354954	1.208504	2.252529
32	1	0	-0.121314	1.874705	3.332234
33	1	0	-0.721130	2.848990	1.982774
34	6	0	1.970765	1.992361	1.614944
35	1	0	1.872244	3.062244	1.401178
36	1	0	2.283833	1.890795	2.660191
37	1	0	2.764922	1.582172	0.985896
38	6	0	-1.164214	2.510339	-1.549268
39	1	0	-1.180034	1.695553	-2.282594
40	1	0	-2.039551	2.415703	-0.892535
41	1	0	-1.256299	3.456586	-2.095410
42	6	0	1.339013	2.780078	-1.608196
43	1	0	1.401547	2.081390	-2.447337
44	1	0	1.255169	3.795155	-2.015035
45	1	0	2.270709	2.717513	-1.040745

Table S17 Diisopropyl LAB monomer.dioxane red gauche CH3Cl

SCF Done: E(RHF) = -1128.59102832 A.U. after 9 cycles
Convg = 0.5594D-08 -V/T = 2.0012
S**2 = 0.0000
E2 = -0.2262281260D+01 EUMP2 = -0.11308533095759D+04

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.666392	0.656152	-0.801862
2	7	0	-1.716514	-0.327860	-0.211246
3	3	0	0.047502	0.551300	-0.316877
4	6	0	-2.272639	-1.088226	0.938425
5	1	0	-2.167557	1.024560	-1.710723
6	1	0	-3.126282	-0.517034	1.325648
7	5	0	-1.013373	-1.139312	-1.326312
8	1	0	-0.152546	-1.919678	-0.732332
9	1	0	-0.324446	-0.359600	-1.990502
10	1	0	-1.649016	-1.888387	-2.031722
11	6	0	1.307087	-2.130965	-0.560085
12	1	0	1.542617	-1.861600	-1.574791
13	1	0	1.365746	-1.417273	0.244459
14	1	0	1.141373	-3.170583	-0.315917
15	17	0	3.601264	-2.403456	-0.238958
16	6	0	2.752476	1.011727	0.213856
17	6	0	2.294206	1.618573	-1.125289
18	8	0	0.999067	2.249030	-0.929448

19	6	0	1.064439	3.083205	0.242958
20	6	0	1.129391	2.150750	1.472327
21	8	0	1.561555	0.850171	1.027033
22	1	0	3.002583	2.361534	-1.513150
23	1	0	2.129801	0.855067	-1.890259
24	1	0	3.455339	1.660347	0.751438
25	1	0	1.941943	3.737875	0.167936
26	1	0	0.166358	3.704480	0.239094
27	1	0	0.147541	1.996013	1.928376
28	1	0	1.820861	2.525594	2.238306
29	1	0	3.198687	0.020366	0.095137
30	6	0	-1.240028	-1.162179	2.062912
31	1	0	-1.648066	-1.692569	2.931697
32	1	0	-0.341722	-1.698475	1.740935
33	1	0	-0.944305	-0.158053	2.385911
34	6	0	-2.778698	-2.489656	0.586817
35	1	0	-3.504791	-2.468914	-0.228965
36	1	0	-1.952440	-3.141563	0.286679
37	1	0	-3.259745	-2.936911	1.465034
38	6	0	-2.871651	1.855141	0.127717
39	1	0	-3.318230	1.555388	1.081698
40	1	0	-1.918238	2.353408	0.339794
41	1	0	-3.538849	2.590948	-0.335816
42	6	0	-4.012427	0.070526	-1.239567
43	1	0	-4.608579	-0.255511	-0.380402
44	1	0	-4.591045	0.833310	-1.773546
45	1	0	-3.868075	-0.780194	-1.910759

Table S18 Diisopropyl LAB monomer.dioxane SN2 CH3Cl

SCF Done: E(RHF) = -1128.59767626 A.U. after 10 cycles

Convg = 0.3591D-08 -V/T = 2.0012

S**2 = 0.0000

E2 = -0.2272542089D+01 EUMP2 = -0.11308702183496D+04

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framework group C1[X(C11H28BClLiNO2)]

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.783867	0.245469	-1.275639
2	7	0	-1.993705	-0.096380	-0.067271
3	3	0	1.277947	0.242328	-0.152516
4	6	0	-2.824443	-0.519698	1.092837
5	1	0	-2.027000	0.480537	-2.038354
6	1	0	-3.827623	-0.098996	0.948284
7	5	0	-0.774068	-1.036832	-0.395509
8	1	0	-1.049016	-2.160430	-0.771863
9	1	0	-0.054821	-1.126010	0.609575
10	1	0	-0.123095	-0.493819	-1.299103
11	6	0	-0.604577	1.646366	0.271863
12	17	0	1.296802	2.628252	0.300702
13	1	0	-0.308937	0.913216	0.996822
14	1	0	-1.245023	2.441156	0.631678
15	1	0	-0.568898	1.478013	-0.788185
16	6	0	2.820224	-1.939431	0.470686
17	6	0	2.704291	-1.781850	-1.065527

18	8	0	2.772774	-0.376637	-1.385539
19	6	0	3.977430	0.186591	-0.834963
20	6	0	3.874736	0.142139	0.709708
21	8	0	2.712550	-0.631224	1.063767
22	1	0	3.503930	-2.312843	-1.598960
23	1	0	1.733309	-2.114882	-1.436411
24	1	0	3.775658	-2.387651	0.774620
25	1	0	4.838524	-0.380728	-1.212782
26	1	0	4.029955	1.210009	-1.210326
27	1	0	3.707766	1.130961	1.137971
28	1	0	4.763295	-0.310968	1.169638
29	1	0	1.998197	-2.528490	0.879498
30	6	0	-2.286540	0.057310	2.404029
31	1	0	-1.258855	-0.278743	2.583188
32	1	0	-2.309401	1.151025	2.403030
33	1	0	-2.899278	-0.291896	3.243451
34	6	0	-2.980090	-2.039109	1.244784
35	1	0	-3.709301	-2.247496	2.038063
36	1	0	-3.326409	-2.514452	0.325475
37	1	0	-2.028196	-2.499769	1.524075
38	6	0	-3.650185	1.494366	-1.088020
39	1	0	-3.055110	2.354781	-0.769844
40	1	0	-4.133716	1.751618	-2.037610
41	1	0	-4.445335	1.336626	-0.351970
42	6	0	-3.637473	-0.899965	-1.834781
43	1	0	-4.475292	-1.133034	-1.168122
44	1	0	-4.058789	-0.603739	-2.803243
45	1	0	-3.039376	-1.802672	-1.980216

Table S19 Diisopropyl LAB monomer.2THF red anti CH3Br

SCF Done: E(RHF) = -3395.18737484 A.U. after 8 cycles
Convg = 0.5304D-08 -V/T = 2.0039
S**2 = 0.0000
E2 = -0.2776995456D+01 EUMP2 = -0.33979643702987D+04

Framework group C1[X(C15H36BBrLiNO2)]
Deg. of freedom 165
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.105360	2.407102	1.871845
2	7	0	-0.319456	1.695191	0.588083
3	3	0	-1.493045	-0.002202	0.464822
4	6	0	-0.625257	2.581412	-0.559199
5	1	0	-0.552218	3.404420	1.773078
6	1	0	-0.647522	1.910443	-1.429523
7	5	0	0.628376	0.549574	0.258899
8	1	0	1.777033	0.939595	-0.194940
9	1	0	0.165812	-0.106210	-0.676945
10	1	0	0.863047	-0.148400	1.223214
11	6	0	3.053870	0.293938	-0.503643
12	1	0	2.652390	-0.703264	-0.567313
13	1	0	3.161881	0.881125	-1.402658
14	1	0	3.508477	0.629108	0.414611
15	35	0	5.244943	-0.717149	-1.047772
16	8	0	-1.616485	-1.829306	1.168392
17	6	0	-1.474868	-2.763264	0.051303

18	6	0	-0.745281	-3.976134	0.614480
19	6	0	0.102529	-3.351935	1.723916
20	6	0	-0.866139	-2.342080	2.311108
21	1	0	-0.888867	-2.267584	-0.730641
22	1	0	-2.476835	-2.984209	-0.328397
23	1	0	-1.456973	-4.695620	1.035466
24	1	0	-0.151356	-4.486056	-0.149580
25	1	0	0.447658	-4.079281	2.464938
26	1	0	0.974065	-2.838653	1.304493
27	1	0	-1.577865	-2.808934	3.003303
28	1	0	-0.386423	-1.490926	2.795994
29	8	0	-3.019085	-0.072004	-0.703370
30	6	0	-4.321902	-0.526994	-0.242423
31	6	0	-4.999272	-1.084733	-1.483701
32	6	0	-4.476455	-0.141324	-2.568885
33	6	0	-3.022637	0.046300	-2.155839
34	1	0	-4.866377	0.335703	0.162273
35	1	0	-4.147669	-1.254515	0.554663
36	1	0	-4.666267	-2.111554	-1.673936
37	1	0	-6.090068	-1.086253	-1.398716
38	1	0	-4.568718	-0.546515	-3.580757
39	1	0	-5.011327	0.814358	-2.531010
40	1	0	-2.372429	-0.738944	-2.559355
41	1	0	-2.609717	1.024223	-2.414811
42	6	0	0.446628	3.639131	-0.844679
43	1	0	1.432700	3.178554	-0.955188
44	1	0	0.211101	4.167764	-1.776052
45	1	0	0.497042	4.386653	-0.045345
46	6	0	-2.006835	3.228830	-0.429475
47	1	0	-2.247156	3.795558	-1.337476
48	1	0	-2.778391	2.466599	-0.278151

49	1	0	-2.046643	3.931211	0.410219
50	6	0	1.368348	2.592447	2.246242
51	1	0	1.450570	3.224294	3.139211
52	1	0	1.835418	1.628529	2.469635
53	1	0	1.933009	3.068622	1.440610
54	6	0	-0.854133	1.688296	2.993458
55	1	0	-1.925356	1.624849	2.765499
56	1	0	-0.457218	0.676110	3.125076
57	1	0	-0.739224	2.216348	3.947791

Table S20 Diisopropyl LAB monomer.2THF red gauche CH3Br

SCF Done: E(RHF) = -3395.18978112 A.U. after 8 cycles
Convg = 0.2129D-08 -V/T = 2.0040
S**2 = 0.0000
E2 = -0.2788533249D+01 EUMP2 = -0.33979783143735D+04

Framework group C1[X(C15H36BBrLiNO2)]
Deg. of freedom 165
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.012516	-1.643593	-0.174390
2	7	0	2.559254	-0.257607	-0.449364
3	3	0	0.761659	0.071309	0.428266
4	6	0	3.613873	0.770999	-0.240464
5	1	0	2.193334	-2.280017	-0.535251
6	1	0	4.354573	0.334819	0.442511
7	5	0	1.742574	-0.129057	-1.748989

8	1	0	0.518191	-0.584897	-1.457443
9	1	0	2.041314	-0.859324	-2.673101
10	1	0	1.539169	1.025141	-2.060744
11	6	0	-1.024279	-0.500201	-1.563124
12	1	0	-0.961295	0.177194	-2.400456
13	1	0	-1.064151	-1.563183	-1.747946
14	1	0	-1.101201	-0.129009	-0.560848
15	35	0	-3.429188	-0.353847	-1.528664
16	8	0	-0.325450	-1.251129	1.405972
17	6	0	-1.611335	-0.900546	2.020148
18	6	0	-2.423000	-2.191207	2.073710
19	6	0	-1.820797	-3.014508	0.933627
20	6	0	-0.348915	-2.665608	1.052414
21	1	0	-2.087700	-0.144594	1.389405
22	1	0	-1.400437	-0.482734	3.009535
23	1	0	-2.281365	-2.701561	3.033365
24	1	0	-3.489860	-1.995497	1.933566
25	1	0	-1.999233	-4.089269	1.040687
26	1	0	-2.227437	-2.683694	-0.026299
27	1	0	0.143795	-3.233246	1.852437
28	1	0	0.222265	-2.778106	0.128390
29	8	0	-0.274097	1.710330	0.668072
30	6	0	-0.339233	2.448843	1.918492
31	6	0	-1.354547	3.552304	1.672685
32	6	0	-1.074394	3.895441	0.209030
33	6	0	-0.877347	2.518475	-0.402963
34	1	0	0.654728	2.859999	2.134170
35	1	0	-0.618461	1.744572	2.706494
36	1	0	-2.374606	3.168047	1.785994
37	1	0	-1.221449	4.397705	2.354664
38	1	0	-1.891519	4.440110	-0.273148

39	1	0	-0.160439	4.495074	0.126213
40	1	0	-1.828891	2.051547	-0.677972
41	1	0	-0.191687	2.496478	-1.253422
42	6	0	3.175948	-1.890434	1.328323
43	1	0	3.422009	-2.941799	1.520767
44	1	0	3.987480	-1.283679	1.745797
45	1	0	2.255603	-1.648628	1.871096
46	6	0	4.267425	-2.082686	-0.935525
47	1	0	4.447946	-3.150323	-0.762318
48	1	0	4.143058	-1.927851	-2.010804
49	1	0	5.157113	-1.539655	-0.598542
50	6	0	3.026896	1.993085	0.463755
51	1	0	2.636439	1.716903	1.450740
52	1	0	3.791283	2.766912	0.607111
53	1	0	2.211440	2.422637	-0.128450
54	6	0	4.353057	1.197539	-1.514362
55	1	0	5.217961	1.819078	-1.249990
56	1	0	4.712628	0.335954	-2.081027
57	1	0	3.699520	1.783113	-2.166722

Table S21 Diisopropyl LAB monomer.2THF SN2 CH3Br

SCF Done: E(RHF) = -3395.19759273 A.U. after 8 cycles
Convg = 0.5097D-08 -V/T = 2.0040
S**2 = 0.0000
E2 = -0.2791310088D+01 EUMP2 = -0.33979889028140D+04

Framework group C1[X(C15H36BBrLiNO2)]
Deg. of freedom 165
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.275185	0.642690	0.511304
2	7	0	-2.446541	-0.305050	-0.278731
3	3	0	0.621169	0.561663	-1.283653
4	6	0	-3.158830	-1.553422	-0.664755
5	1	0	-2.603938	1.496408	0.688807
6	1	0	-3.925220	-1.741752	0.097987
7	5	0	-1.689251	0.413247	-1.447187
8	1	0	-2.379209	0.884736	-2.331234
9	1	0	-0.893316	-0.388087	-1.965889
10	1	0	-1.054343	1.339799	-0.927079
11	6	0	-0.684478	-0.668960	0.995384
12	35	0	1.243473	-0.956872	2.141077
13	1	0	-0.294167	-1.068211	0.078663
14	1	0	-1.265468	-1.316254	1.629022
15	1	0	-0.744789	0.396853	1.145824
16	8	0	1.532510	2.233566	-0.897642
17	6	0	0.994858	3.444128	-1.516815
18	6	0	0.843350	4.467241	-0.388958
19	6	0	0.773501	3.585654	0.860707
20	6	0	1.771758	2.496845	0.516725
21	1	0	0.033087	3.178291	-1.966026
22	1	0	1.690766	3.759764	-2.299929
23	1	0	1.720068	5.122625	-0.339329
24	1	0	-0.042377	5.094340	-0.526122
25	1	0	1.034309	4.117996	1.780652
26	1	0	-0.227306	3.154653	0.975474
27	1	0	2.806742	2.844423	0.638605
28	1	0	1.640798	1.556326	1.057032

29	8	0	2.021755	-0.728899	-1.296292
30	6	0	1.901377	-2.184425	-1.322088
31	6	0	3.238862	-2.714716	-0.821703
32	6	0	4.206310	-1.604339	-1.235292
33	6	0	3.385187	-0.363950	-0.932182
34	1	0	1.693697	-2.475784	-2.357867
35	1	0	1.064343	-2.472718	-0.683298
36	1	0	3.216961	-2.811657	0.268085
37	1	0	3.482253	-3.688388	-1.258138
38	1	0	5.147123	-1.623388	-0.676409
39	1	0	4.435055	-1.663368	-2.305891
40	1	0	3.404300	-0.121885	0.135710
41	1	0	3.648107	0.517226	-1.521450
42	6	0	-3.695832	0.101262	1.883173
43	1	0	-2.841491	-0.190891	2.498102
44	1	0	-4.240130	0.884054	2.424033
45	1	0	-4.370082	-0.757292	1.798641
46	6	0	-4.513223	1.194884	-0.208881
47	1	0	-5.291886	0.429697	-0.301757
48	1	0	-4.934179	2.021708	0.376660
49	1	0	-4.262778	1.568658	-1.204241
50	6	0	-2.224062	-2.767975	-0.665989
51	1	0	-1.382598	-2.601828	-1.346940
52	1	0	-1.836268	-3.000534	0.329176
53	1	0	-2.771332	-3.648300	-1.022984
54	6	0	-3.862202	-1.490465	-2.028929
55	1	0	-4.478599	-2.389458	-2.157004
56	1	0	-4.506283	-0.616266	-2.130291
57	1	0	-3.127345	-1.460886	-2.839004

Table S22 Diisopropyl LAB monomer.dioxane red anti CH3Br

SCF Done: E(RHF) = -3239.02490899 A.U. after 8 cycles
Convg = 0.3137D-08 -V/T = 2.0041
S**2 = 0.0000
E2 = -0.2240324991D+01 EUMP2 = -0.32412652339799D+04

Framework group C1[X(C11H28BBrLiNO2)]
Deg. of freedom 129
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.731360	1.992486	-1.337846
2	7	0	0.729587	1.323779	-0.015897
3	3	0	1.865599	-0.304882	0.101300
4	6	0	0.818017	2.232210	1.154235
5	1	0	0.532638	1.187858	-2.058458
6	1	0	1.195413	3.197406	0.793902
7	5	0	-0.210494	0.130802	0.095213
8	1	0	-1.454656	0.439708	-0.069643
9	1	0	-0.125917	-0.410099	1.183049
10	1	0	0.035365	-0.662732	-0.812776
11	6	0	-2.758194	-0.133584	-0.056958
12	1	0	-3.093119	0.500701	0.749196
13	1	0	-2.957057	0.149399	-1.079009
14	1	0	-2.454390	-1.144644	0.159106
15	35	0	-5.094773	-1.039046	-0.054558
16	6	0	4.379706	-1.019480	-0.459603
17	6	0	4.167197	-1.649925	0.936268

18	8	0	2.751158	-1.814641	1.133335
19	6	0	2.269777	-2.858918	0.255705
20	6	0	2.722507	-2.525685	-1.186175
21	8	0	3.153739	-1.147415	-1.208393
22	1	0	4.657266	-2.627212	1.031363
23	1	0	4.519298	-1.001709	1.741252
24	1	0	5.198349	-1.499090	-1.011628
25	1	0	2.656948	-3.826827	0.598158
26	1	0	1.183363	-2.847906	0.363788
27	1	0	1.901863	-2.600847	-1.901604
28	1	0	3.551391	-3.160679	-1.523711
29	1	0	4.574373	0.054902	-0.405219
30	6	0	2.106632	2.575619	-1.668033
31	1	0	2.868417	1.787343	-1.665840
32	1	0	2.099548	3.035348	-2.662969
33	1	0	2.401956	3.348179	-0.949411
34	6	0	-0.372515	3.039706	-1.508658
35	1	0	-0.211699	3.907680	-0.859812
36	1	0	-0.388109	3.399582	-2.543829
37	1	0	-1.354796	2.613416	-1.283899
38	6	0	1.847221	1.684847	2.146369
39	1	0	1.555754	0.687000	2.496901
40	1	0	2.839221	1.627526	1.677123
41	1	0	1.933786	2.330815	3.028018
42	6	0	-0.522384	2.483113	1.849616
43	1	0	-0.895699	1.567714	2.318541
44	1	0	-0.401540	3.240322	2.633765
45	1	0	-1.277467	2.841754	1.145441

Table S23 Diisopropyl LAB monomer.dioxane red gauche CH3Br

SCF Done: E(RHF) = -3239.02415672 A.U. after 8 cycles
Convg = 0.5618D-08 -V/T = 2.0041
S**2 = 0.0000
E2 = -0.2248338785D+01 EUMP2 = -0.32412724955041D+04

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.238632	0.002734	-0.813428
2	7	0	-2.042567	-0.653347	-0.215341
3	3	0	-0.592474	0.681995	-0.321398
4	6	0	-2.350359	-1.533826	0.941973
5	1	0	-2.869637	0.487459	-1.729485
6	1	0	-3.328373	-1.226209	1.334555
7	5	0	-1.131211	-1.235296	-1.323676
8	1	0	-0.085303	-1.723302	-0.720763
9	1	0	-0.693524	-0.294820	-1.993958
10	1	0	-1.521198	-2.141205	-2.024293
11	6	0	1.387328	-1.520990	-0.521183
12	1	0	1.556329	-1.215764	-1.539774
13	1	0	1.232354	-0.803425	0.267480
14	1	0	1.496460	-2.563372	-0.257581
15	35	0	3.781239	-1.166009	-0.122430
16	6	0	1.839910	1.939118	0.272185
17	6	0	1.272165	2.350158	-1.098516
18	8	0	-0.157223	2.573023	-0.958060

19	6	0	-0.383454	3.412050	0.190554
20	6	0	-0.092289	2.564383	1.448181
21	8	0	0.723719	1.443233	1.054160
22	1	0	1.743408	3.259948	-1.491565
23	1	0	1.367689	1.554322	-1.842118
24	1	0	2.295615	2.780533	0.809051
25	1	0	0.264328	4.295239	0.122433
26	1	0	-1.423846	3.740215	0.141875
27	1	0	-1.000526	2.132648	1.877730
28	1	0	0.427161	3.142017	2.223984
29	1	0	2.568400	1.127642	0.197854
30	6	0	-1.331818	-1.306297	2.059203
31	1	0	-1.572767	-1.921171	2.934684
32	1	0	-0.321406	-1.575772	1.736198
33	1	0	-1.324666	-0.256792	2.372847
34	6	0	-2.439459	-3.023652	0.600135
35	1	0	-3.148073	-3.216411	-0.208269
36	1	0	-1.464235	-3.414842	0.294124
37	1	0	-2.765230	-3.583734	1.485036
38	6	0	-3.782978	1.103163	0.101120
39	1	0	-4.115429	0.700750	1.063951
40	1	0	-3.017688	1.863637	0.295556
41	1	0	-4.640365	1.601889	-0.365410
42	6	0	-4.357655	-0.954145	-1.235991
43	1	0	-4.832890	-1.426617	-0.369505
44	1	0	-5.132936	-0.398999	-1.776866
45	1	0	-3.974095	-1.735842	-1.896981

Table S24 Diisopropyl LAB monomer.dioxane SN2 CH3Br

SCF Done: E(RHF) = -3239.03350169 A.U. after 9 cycles
Convg = 0.5783D-08 -V/T = 2.0041
S**2 = 0.0000
E2 = -0.2255511550D+01 EUMP2 = -0.32412890132375D+04

Deg. of freedom 129

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.893914	0.012296	-1.336462
2	7	0	-2.183133	-0.235879	-0.059214
3	3	0	1.059871	-0.310443	-0.078047
4	6	0	-3.086218	-0.362210	1.116088
5	1	0	-2.093741	0.054647	-2.090292
6	1	0	-4.021021	0.155691	0.867853
7	5	0	-1.085978	-1.354748	-0.184896
8	1	0	-1.485726	-2.487790	-0.374481
9	1	0	-0.393076	-1.354239	0.844958
10	1	0	-0.365192	-1.052152	-1.146997
11	6	0	-0.602584	1.389682	0.072939
12	35	0	1.436853	2.331561	0.091589
13	1	0	-0.414274	0.756877	0.919799
14	1	0	-1.214555	2.261609	0.260355
15	1	0	-0.534779	1.043326	-0.943403
16	6	0	2.445442	-2.522136	0.577721
17	6	0	2.388685	-2.426440	-0.969722
18	8	0	2.484662	-1.037477	-1.343280

19	6	0	3.723169	-0.491470	-0.852332
20	6	0	3.697322	-0.536967	0.696933
21	8	0	2.479171	-1.184346	1.112461
22	1	0	3.202700	-2.984928	-1.450479
23	1	0	1.430358	-2.768892	-1.363874
24	1	0	3.330942	-3.067736	0.929590
25	1	0	4.556879	-1.070146	-1.272044
26	1	0	3.767081	0.531293	-1.229031
27	1	0	3.663241	0.461162	1.134497
28	1	0	4.552530	-1.088190	1.110299
29	1	0	1.547329	-2.985331	0.989277
30	6	0	-2.506480	0.339351	2.346858
31	1	0	-1.534791	-0.089933	2.617133
32	1	0	-2.389086	1.414546	2.182521
33	1	0	-3.177262	0.201934	3.203157
34	6	0	-3.445383	-1.806564	1.491351
35	1	0	-4.215554	-1.793869	2.273136
36	1	0	-3.827823	-2.372904	0.640295
37	1	0	-2.570137	-2.334613	1.880817
38	6	0	-3.622348	1.359991	-1.365373
39	1	0	-2.952704	2.188846	-1.120666
40	1	0	-4.023678	1.536753	-2.370052
41	1	0	-4.468010	1.387129	-0.670457
42	6	0	-3.853979	-1.103361	-1.769178
43	1	0	-4.731843	-1.146278	-1.114772
44	1	0	-4.210759	-0.906924	-2.787775
45	1	0	-3.357625	-2.076747	-1.758231