

## The mechanism of replacement of aluminum atom in 1-ethyl-3-alkylaluminumolanes by boron atom with boron halides

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**Table S1.** Calculated (PBE/3 $\zeta$ ) thermodynamic parameters for all optimized compounds and intermediates at T = 298.15 K ([S] = cal/(mol\*K); [H] = [G] = kcal/mol).

Compound	H <sup>0</sup>	G <sup>0</sup>	S <sup>0</sup>
<b>3</b>	-349412.4	-349445.6	111.2
<b>4</b>	-203540.8	-203560.1	64.6
<b>4'</b>	-881674.7	-881696.5	73.0
<b>5a</b>	-552953.5	-552996.9	145.7
<b>5a'</b>	-1231086.9	-1231134.9	160.9
<b>5b</b>	-552953.2	-552997.3	147.7
<b>5b'</b>	-1231087.0	-1231133.5	156.0
<b>6a</b>	-552973.2	-553015.2	140.6
<b>6a + THF</b>	-1231118.6	-1231162.1	145.8
<b>6a + 2THF</b>	-1522454.1	-1522517.4	212.3
<b>6a'</b>	-1231118.6	-1231162.1	145.8
<b>6a'_1</b>	-1231116.0	-1231161.3	152.0
<b>6a'_2</b>	-1231116.7	-1231159.2	142.5
<b>6a'_3</b>	-1231116.9	-1231161.3	148.8
<b>6a'_4</b>	-1231119.3	-1231162.4	144.5
<b>6a'_5</b>	-1231119.6	-1231162.8	145.0
<b>6a'_6</b>	-1231117.2	-1231161.6	148.8
<b>6a'_7</b>	-1231117.8	-1231162.5	150.0
<b>6a'_8</b>	-1231116.6	-1231162.8	155.1
<b>6a'_9</b>	-1231118.2	-1231163.5	151.9
<b>6a'_10</b>	-1231112.9	-1231157.9	151.0
<b>6b</b>	-552973.3	-553015.2	140.4
<b>6b + THF</b>	-1231117.5	-1231160.8	145.1
<b>6b + 2THF</b>	-1522450.7	-1522512.9	208.6
<b>6b'</b>	-1231117.5	-1231160.8	145.1
<b>7a</b>	-552988.7	-553031.4	143.5
<b>7a + THF</b>	-1231141.8	-1231186.6	150.2
<b>7a + 2THF</b>	-1522479.1	-1522549.1	234.7
<b>7a'</b>	-1231141.8	-1231186.6	150.2
<b>7b</b>	-552988.7	-553030.9	141.9
<b>7b + THF</b>	-1231141.0	-1231185.6	149.5
<b>7b + 2THF</b>	-1522456.5	-1522531.1	250.3

<b>7b'</b>	-1231141.0	-1231185.6	149.5
<b>8</b>	-327001.6	-327026.6	84.1
<b>8'</b>	-779109.5	-779136.5	90.5
<b>9</b>	-225978.1	-226005.4	91.5
<b>9'</b>	-452025.5	-452053.6	94.1
<b>10a</b>	-756513.9	-756569.0	184.6
<b>10a'</b>	-2112792.4	-2112851.9	199.5
<b>10b</b>	-756514.1	-756568.0	181.0
<b>10b'</b>	-2112792.1	-2112851.6	199.8
<b>11a</b>	-756535.4	-756585.7	168.9
<b>11a'</b>	-2112818.2	-2112874.8	189.7
<b>11b</b>	-756536.4	-756587.0	169.7
<b>11b'</b>	-2112820.2	-2112877.6	192.5
<b>12</b>	-429525.9	-429562.5	122.6
<b>12'</b>	-1333703.2	-1333742.9	133.0
<b>13a</b>	-429520.4	-429559.1	129.7
<b>13a'</b>	-1333700.1	-1333745.2	151.3
<b>13b</b>	-429520.4	-429559.2	130.1
<b>13b'</b>	-1333700.1	-1333744.4	148.5
<b>14</b>	-4860932.9	-4860957.2	81.3
<b>15</b>	-5210344.5	-5210396.3	173.6
<b>16</b>	-5210345.3	-5210390.2	150.9
<b>17</b>	-5210378.0	-5210426.1	161.6
<b>18</b>	-5210404.4	-5210451.4	157.7
<b>19</b>	-3431953.1	-3431981.9	96.3
<b>20</b>	-1778445.2	-1778474.1	96.9
<b>21</b>	-5210344.4	-5210397.1	176.8
<b>22</b>	-5210377.3	-5210425.3	161.2
<b>23</b>	-5210404.4	-5210451.4	157.6
<b>24</b>	-10071310.9	-10071378.0	224.9
<b>25</b>	-10071340.0	-10071403.1	211.8
<b>26</b>	-6639380.1	-6639423.3	144.6
<b>27</b>	-10071309.9	-10071376.0	221.7
<b>28</b>	-10071297.0	-10071357.0	201.5
<b>29</b>	-10071341.0	-10071402.9	207.6
<b>30a</b>	-6639377.9	-6639425.3	159.1

<b>30b</b>	-6639377.7	-6639425.2	159.5
<b>33</b>	-698839.8	-698891.7	174.2
<b>34a</b>	-1580540.6	-1580604.5	214.3
<b>34b</b>	-1580545.5	-1580612.2	223.8
<b>TS(5a-6a)</b>	-552953.8	-552994.0	134.7
<b>TS(5a'-6a')</b>	-1231084.0	-1231126.0	141.2
<b>TS(5b-6b)</b>	-552952.8	-552993.3	135.9
<b>TS(5b'-6b')</b>	-1231083.8	-1231126.3	142.5
<b>TS(6a-7a)</b>	-552976.6	-553016.0	132.1
<b>TS(6a-7a) + THF</b>	-1231116.7	-1231157.5	136.6
<b>TS(6a-7a) + 2THF</b>	-1522434.9	-1522500.0	218.2
<b>TS(6a'-7a')</b>	-1231116.7	-1231157.5	136.6
<b>TS(6b-7b)</b>	-552969.4	-553009.0	132.9
<b>TS(6b-7b) + THF</b>	-1231111.9	-1231153.1	137.9
<b>TS(6b-7b) + 2THF</b>	-1522435.7	-1522500.1	215.9
<b>TS(6b'-7b')</b>	-1231111.9	-1231153.1	137.9
<b>TS(10a-11a)</b>	-756509.9	-756558.5	163.2
<b>TS(10a'-11a')</b>	-2112782.7	-2112836.1	179.1
<b>TS(10b-11b)</b>	-756511.4	-756559.5	161.2
<b>TS(10b'-11b')</b>	-2112777.9	-2112832.3	182.3
<b>TS(12-13a)</b>	-429499.9	-429532.5	109.4
<b>TS(12'-13a')</b>	-1333669.0	-1333704.4	118.9
<b>TS(12-13b)</b>	-429501.2	-429533.8	109.5
<b>TS(12'-13b')</b>	-1333668.2	-1333703.5	118.3
<b>TS(15-16)</b>	-5210336.0	-5210382.5	155.8
<b>TS(16-17)</b>	-5210344.0	-5210387.2	145.1
<b>TS(17-18)</b>	-5210378.8	-5210422.7	147.0
<b>TS(21-22)</b>	-5210330.8	-5210376.4	152.8
<b>TS(22-23)</b>	-5210379.3	-5210423.1	147.1
<b>TS(24-25)</b>	-10071296.6	-10071356.9	202.3
<b>TS(26-30a)</b>	-6639353.0	-6639392.8	133.6
<b>TS(26-30b)</b>	-6639353.0	-6639392.8	133.5
<b>TS(27-28)</b>	-10071294.8	-10071353.9	198.3
<b>TS(28-29)</b>	-10071298.4	-10071358.6	201.8
<b>TS(33-34a)</b>	-1580497.5	-1580557.1	199.9
<b>TS(33-34b)</b>	-1580492.8	-1580555.0	208.6

**Table S2.** Calculated (PBE/3 $\zeta$ ) relative thermodynamic parameters for intermediate **6a'** and its ten possible\* conformers at T = 298.15 K ( $[\Delta S] = \text{cal}/(\text{mol}\cdot\text{K})$ ;  $[\Delta H] = [\Delta G] = \text{kcal/mol}$ ).

Conformer	$\Delta H^0$	$\Delta G^0$	$\Delta S^0$
<b>6a'</b>	0.9	1.4	3.3
<b>6a'_1</b>	3.6	2.2	9.5
<b>6a'_2</b>	2.9	4.3	0.0
<b>6a'_3</b>	2.7	2.2	6.4
<b>6a'_4</b>	0.2	1.1	2.0
<b>6a'_5</b>	0.0	0.7	2.6
<b>6a'_6</b>	2.4	1.9	6.4
<b>6a'_7</b>	1.8	1.0	7.5
<b>6a'_8</b>	3.0	0.7	12.7
<b>6a'_9</b>	1.4	0.0	9.4
<b>6a'_{10}</b>	6.7	5.5	8.6

\* 80 possible conformers of intermediate **6a** were found in the Avogadro 1.93.0 program, and then the 10 most energetically favorable ones were optimized in the PRIRODA-06 (PBE/3 $\zeta$ ) program

**Table S3.** Thermodynamic and activation parameters of reaction **6**  $\rightarrow$  **7** calculated by M06-2X/cc-pVDZ method at T = 298 K ( $\Delta H$ ,  $\Delta G$  [kcal/mol]) in gas phase, THF, toluene, and dichloromethane (CPCM).

Solvent	Reaction	$\Delta H^0$	$\Delta G^0$	$\Delta H^\ddagger$	$\Delta G^\ddagger$
Gas phase	<b>6a</b> $\rightarrow$ <b>7a</b>	-13.9	-14.0	2.1	6.0
	<b>6b</b> $\rightarrow$ <b>7b</b>	-20.3	-22.2	8.2	9.7
THF	<b>6a</b> $\rightarrow$ <b>7a</b>	-13.7	-13.8	2.5	6.4
	<b>6b</b> $\rightarrow$ <b>7b</b>	-21.0	-22.9	8.5	9.9
Toluene	<b>6a</b> $\rightarrow$ <b>7a</b>	-13.7	-13.8	2.5	6.4
	<b>6b</b> $\rightarrow$ <b>7b</b>	-20.7	-22.6	8.4	9.9
CH <sub>2</sub> Cl <sub>2</sub>	<b>6a</b> $\rightarrow$ <b>7a</b>	-13.7	-13.8	2.5	6.4
	<b>6b</b> $\rightarrow$ <b>7b</b>	-21.1	-23.0	8.5	9.9

### Cartesian coordinates (PBE/3c)

**3**

6	0.95389614	2.49109994	1.01381071
13	0.51431413	1.13768685	-0.36859271
6	-1.40241127	1.61882103	-0.53922865
6	-1.60287201	2.51187684	0.71563145
6	-0.32758036	3.36135883	0.96953288
6	1.61085304	-0.23980905	-1.28338207
6	3.04765167	-0.43154480	-0.76022781
1	-0.24090922	4.09299054	0.14533849
1	1.05351470	2.00801217	2.00284859
1	-1.71406378	1.83801571	1.58904756
1	1.86912089	3.08333581	0.87234114
1	-1.56177808	2.22474761	-1.45255951
1	-0.46016441	3.95120949	1.89230278
1	1.05652642	-1.19417281	-1.24025524
1	1.63050818	0.01902970	-2.35799206
1	3.59853436	-1.19671261	-1.32943494
1	3.62890512	0.50033158	-0.82046047
1	3.05695047	-0.74305012	0.29471627
1	-2.12373856	0.79134459	-0.59091455
6	-2.85556421	3.40258478	0.65972374
1	-2.86350089	4.06055803	1.54617176
1	-2.77053212	4.06886098	-0.21690200
6	-4.17844738	2.63446205	0.59254099
1	-4.29085214	1.96482073	1.45913507
1	-4.24170138	2.01869548	-0.31558968
1	-5.03698043	3.32112270	0.58953551

**4**

9	1.35215225	0.40759772	0.14462021
9	0.20173101	0.31767145	-1.84165172
5	0.20410054	0.33539530	-0.51551482
9	-0.94135121	0.27582001	0.15045958

**4'**

17	1.68926350	-0.87473353	0.12119101
17	2.40524060	-0.93489764	3.07241857
5	2.89828057	-0.94354770	1.38953185
17	4.60001152	-1.03198961	0.97509688

**5a**

6	0.08346562	1.89116266	1.37323019
13	-0.10520810	0.90386637	-0.34896176
6	-1.68437265	1.92513196	-0.97424778
6	-1.65744613	3.15626039	-0.02735129
6	-1.23365093	2.71017912	1.39738313
6	1.07927278	-0.38501266	-1.27873466
6	2.21392227	-1.02298860	-0.45506850

1	-1.15139876	3.58479893	2.06157746
1	0.26549505	1.36944417	2.32634263
1	0.94696376	2.57552096	1.26946662
1	-0.86981976	3.84463109	-0.39524968
1	-2.04864167	2.08631220	1.80781137
1	0.43944477	-1.16884449	-1.72107203
1	1.50120278	0.15032314	-2.14941196
1	2.83874799	-1.69655506	-1.06235077
1	2.88024784	-0.26128681	-0.02398858
1	1.82370830	-1.61577231	0.38516877
1	-2.60949041	1.34584417	-0.79227168
1	-1.71153728	2.22375373	-2.03231610
6	-2.98660829	3.93321151	-0.03925791
1	-3.26111847	4.12704084	-1.08903165
1	-3.77667937	3.27562496	0.36440574
6	-2.97780103	5.26149526	0.72699671
1	-2.18237601	5.92613992	0.35609095
1	-2.81593226	5.11610761	1.80394945
1	-3.93401320	5.79068815	0.60662725
9	0.10546433	-1.49888214	2.83756906
5	-1.02151742	-0.97804974	2.38188981
9	-1.30205044	-1.05594430	1.07242341
9	-1.90321965	-0.43592524	3.20390738

### 5a'

6	1.21962000	3.31451169	-0.16915734
13	0.87253372	1.37335310	-0.41024259
6	-1.05879552	1.44262587	0.04539698
6	-1.18025603	2.86396791	0.65698591
6	-0.23583928	3.84366129	-0.09165244
6	1.99175713	-0.09148718	-1.14917626
6	3.51548133	0.13221794	-1.14668909
1	-0.62997927	3.97422152	-1.11636050
1	1.74932924	3.51654648	0.77787013
1	-0.81758580	2.81003291	1.70260714
1	1.80052980	3.81423042	-0.95780971
1	-1.65666169	1.38850981	-0.88573360
1	-0.28928472	4.83702924	0.38562567
1	1.73822442	-1.03008322	-0.62760081
1	1.63944425	-0.24754529	-2.18642378
1	4.05889075	-0.69597884	-1.62825000
1	3.79146775	1.05583800	-1.67651781
1	3.91182050	0.22222663	-0.12400867
1	-1.45457364	0.66024039	0.70768581
6	-2.61804346	3.40958389	0.69669762
1	-2.59284179	4.45341034	1.05565949
1	-3.00496355	3.44999263	-0.33687664
6	-3.57909768	2.60082898	1.57230727
1	-3.21984479	2.55278984	2.61180498
1	-3.68509123	1.56949710	1.20758599

1	-4.58087869	3.05351369	1.58709865
17	1.60266600	0.28765498	2.60354108
17	4.48950542	0.08902227	3.52480126
5	3.03718582	1.03931397	3.30710676
17	2.99028218	2.71944827	3.78796896

**5b**

6	0.68610035	2.44027514	1.16181877
13	0.25449592	1.13823949	-0.27106064
6	-1.60237010	1.79463028	-0.58390131
6	-1.55806696	3.16723145	0.14520848
6	-0.71509821	3.04239162	1.44271932
6	1.35836438	-0.15258774	-1.29319592
6	2.68560743	-0.58506667	-0.64063868
1	-0.64152026	4.02146851	1.94181376
1	1.15778524	2.04350969	2.07217223
1	1.36741669	3.22291951	0.78277221
1	-1.01942812	3.87439715	-0.51752590
1	-1.26447955	2.38266480	2.13946957
1	0.73586896	-1.03548142	-1.51958080
1	1.55673358	0.30805173	-2.27876622
1	3.25645466	-1.27780742	-1.27875559
1	3.33523435	0.27814045	-0.43349685
1	2.51785689	-1.09328547	0.32048281
1	-2.38907583	1.17106455	-0.11343465
1	-1.91360825	1.90072769	-1.63413828
6	-2.96326214	3.74574905	0.39071076
1	-3.52349040	3.70379331	-0.55774104
1	-3.49740393	3.07655360	1.08835656
6	-2.99683855	5.18239108	0.92566556
1	-2.45086970	5.86528153	0.25674773
1	-2.54510858	5.26171524	1.92399454
1	-4.03054133	5.54895974	1.00171000
9	-0.70694463	-0.77829150	1.35630182
5	-2.02691747	-1.00846423	1.30246998
9	-2.51632315	-1.75712857	0.32924356
9	-2.81017826	-0.52345448	2.25053016

**5b'**

6	0.51418518	2.97463524	-0.51706195
13	0.03951053	1.08130820	-0.90068479
6	-1.73335504	1.13308227	0.00117730
6	-1.62743568	2.45833041	0.80459235
6	-0.84887475	3.51713090	-0.02224896
6	1.15921984	-0.44649324	-1.50651020
6	1.96225979	-1.07041453	-0.34241175
1	-1.47257398	3.78914466	-0.89367200
1	1.25509536	3.00602352	0.30273640
1	-1.01937118	2.25297357	1.70863082
1	0.93855319	3.58235862	-1.32889706



1	-2.55492735	1.21536463	-0.73496005
1	-0.73856322	4.43813172	0.57554582
1	0.51917202	-1.21732719	-1.96615765
1	1.85284643	-0.10859024	-2.29404998
1	2.58021668	-1.91990431	-0.67362277
1	2.64333148	-0.34045826	0.12146572
1	1.30160679	-1.44608794	0.45422010
1	-1.97842581	0.27359110	0.64140884
6	-2.98134158	3.01461031	1.27806829
1	-2.81653482	3.99738558	1.75331083
1	-3.60847968	3.20368465	0.38882286
6	-3.73533298	2.10533615	2.25230624
1	-3.13323396	1.90544220	3.15205319
1	-3.97974809	1.13754792	1.79242830
1	-4.67801381	2.56708980	2.57923355
17	-0.78290782	1.81905614	-3.72525303
17	-2.45377685	0.99510687	-6.11396291
5	-1.88960619	0.67113089	-4.49171258
17	-2.40058908	-0.75650108	-3.62676323

**6a**

6	-0.35121151	1.75269031	2.03022411
13	-0.47157607	0.26123627	-0.50106715
6	-1.69904750	1.76188494	-0.88005515
6	-1.69925120	2.91572057	0.15506256
6	-1.70689080	2.35583847	1.59337249
6	1.21616046	-0.21070195	-1.40340609
6	2.02883263	-1.35868308	-0.77443573
1	-1.98080652	3.14677780	2.30531078
1	0.20733441	2.48444810	2.64197536
1	0.34771201	1.62879319	1.17006616
1	-0.76658385	3.49718044	0.02524422
1	-2.50089380	1.59514995	1.66280261
1	0.95709214	-0.45775754	-2.44963001
1	1.83152371	0.70287816	-1.48140289
1	2.93306245	-1.58665635	-1.35937249
1	2.35093580	-1.11505832	0.24773388
1	1.43667238	-2.28180011	-0.70625725
1	-2.71729378	1.33096804	-0.91528208
1	-1.50146665	2.16497391	-1.88722584
6	-2.87770548	3.87823394	-0.09644644
1	-2.92877942	4.08275796	-1.17800212
1	-3.81753178	3.35841942	0.15882462
6	-2.79729314	5.21047976	0.65674745
1	-1.87263980	5.75143967	0.40457270
1	-2.81830898	5.07454343	1.74732578
1	-3.64364090	5.86066042	0.39428451
9	0.72550000	-0.31654557	3.02870305
5	-0.38843782	0.40683435	2.85108621
9	-1.02478049	-0.83987568	0.68146791

9 -1.47437860 0.02264542 3.52665278

**6a + THF**

6 1.61368795 3.72521340 0.98318122  
13 0.67122226 0.58420515 -0.39726111  
6 -0.73545844 1.99548322 -0.28918706  
6 -0.85569189 2.86545452 0.98752279  
6 0.11466106 4.06279830 0.97130706  
6 2.27734459 0.69396030 -1.57286115  
6 2.98896477 -0.63738075 -1.88271735  
1 -0.10561219 4.67076746 0.07643347  
1 2.18976218 4.65351748 0.78220662  
1 -0.61242584 2.24345532 1.86829535  
1 1.89444491 3.07565691 0.13725493  
1 -0.68963243 2.66200230 -1.17153523  
1 -0.10634568 4.70357675 1.83967133  
1 2.01473406 1.20949168 -2.51489851  
1 2.99788272 1.36941876 -1.07850347  
1 3.90483810 -0.49678566 -2.47876346  
1 3.27979979 -1.15907679 -0.95883054  
1 2.34537378 -1.32672168 -2.45400551  
1 -1.67652586 1.42561478 -0.40484935  
6 -2.29045530 3.39841803 1.20035050  
1 -2.27233957 4.13042945 2.02576279  
1 -2.60123883 3.95712185 0.29981521  
6 -3.33255838 2.32551019 1.52980090  
1 -3.04770592 1.76656874 2.43367161  
1 -3.44969657 1.59813704 0.71325401  
1 -4.31850216 2.77731205 1.70947700  
17 1.06893018 -0.38926735 1.52309353  
17 3.90019803 2.49411805 2.25207184  
5 2.26854169 3.18529982 2.29739604  
17 1.51384325 3.35822407 3.88866821  
6 -0.61815147 -3.07314358 -2.20390611  
6 -1.55607461 -2.08934061 -2.92087730  
6 -0.28133625 -2.34353195 -0.90846028  
6 -0.91244621 -0.74721347 -2.60604200  
1 0.28948779 -3.24142899 -2.80064284  
1 -1.00935269 -2.53189956 -0.10868280  
1 -2.56919182 -2.13797807 -2.49690638  
1 -1.60830943 0.10031019 -2.58659286  
1 -1.62223408 -2.26853148 -4.00112227  
1 -0.07129496 -0.52141660 -3.27956292  
1 0.72928868 -2.52587807 -0.52877026  
1 -1.08770587 -4.04510024 -2.00879955  
8 -0.38596387 -0.90550397 -1.24431579

**6a + 2THF**

6 1.88890042 3.77410829 1.04780135  
13 0.56863671 0.06977622 0.47342924

6	-0.52876867	1.73249408	0.54178364
6	-0.42649812	2.71969955	1.73964308
6	0.39424868	3.97509614	1.38347144
6	2.30595972	-0.13816270	-0.50539388
6	3.32145762	-1.13944669	0.07641214
1	-0.09943365	4.46030433	0.52190833
1	2.24579245	4.72035990	0.59857001
1	0.06414721	2.22151818	2.59274328
1	1.98410232	3.01197791	0.25453799
1	-0.40671562	2.30297341	-0.39934702
1	2.08531250	-0.40790047	-1.55602679
1	2.77132414	0.86084426	-0.56923945
1	4.25362033	-1.18869641	-0.51168182
1	3.59061559	-0.87582252	1.10906485
1	2.91094195	-2.15936673	0.11975460
1	-1.56207892	1.33901260	0.50173531
17	0.31389530	-1.28455954	2.17087352
17	2.80763949	1.62809337	2.81944349
5	2.84966948	3.40666508	2.27505655
17	2.72397258	4.56131455	3.72969120
6	-0.85146144	-2.72512729	-2.39940776
6	-1.76249496	-1.55363891	-2.79762974
6	-0.55622146	-2.44052810	-0.92955518
6	-1.12549004	-0.39063312	-2.05156296
1	0.07494333	-2.70593515	-2.99097236
1	-1.29845860	-2.87648441	-0.24867495
1	-2.78908705	-1.72040456	-2.44129199
1	-1.81247913	0.42486823	-1.79797877
1	-1.79333822	-1.38048089	-3.88062098
1	-0.25483114	0.01595092	-2.59105048
1	0.44704240	-2.73893856	-0.60415967
1	-1.32737866	-3.70407579	-2.53537905
8	-0.66464966	-0.97426217	-0.78889677
6	6.30752202	3.37634425	0.41515951
6	5.90660446	4.85959628	0.40894797
6	5.00422709	2.69365793	0.78425432
6	4.96474165	4.97708413	1.60333313
1	7.07346168	3.17873708	1.17829103
1	4.30584005	2.63722533	-0.06247859
1	5.37899596	5.10576251	-0.52338528
1	4.11592591	5.65032955	1.44911446
1	6.76387564	5.53688940	0.50795103
1	5.47242634	5.23639014	2.53856223
1	5.09588736	1.71406279	1.25966802
1	6.68406006	3.03010016	-0.55542108
8	4.42834081	3.60077314	1.80360248
1	0.32629170	4.68929344	2.21956787
6	-1.82037313	3.16400248	2.23476248
1	-1.69039899	3.98727857	2.95762474
1	-2.38377885	3.58453058	1.38237358

6	-2.63648782	2.05355301	2.90341383
1	-2.10802182	1.65687495	3.78258293
1	-2.81762224	1.20715979	2.22500644
1	-3.61555907	2.42728154	3.23682642

**6a'**

6	1.46782119	3.84857366	0.42727675
13	0.88051981	0.37600815	0.12501442
6	-0.64616777	1.64072186	-0.03949026
6	-0.87051699	2.77932362	0.98416538
6	-0.06614299	4.04207367	0.62288267
6	2.26037923	0.09924983	-1.26830171
6	3.41534814	-0.85920795	-0.92740195
1	-0.46662054	4.45634142	-0.31757930
1	1.90026336	4.82105598	0.14591788
1	-0.54481657	2.43883609	1.98627132
1	1.64084652	3.15665241	-0.41081839
1	-0.64498407	2.07020297	-1.05843374
1	-0.23122674	4.80879830	1.39626913
1	1.71443904	-0.27489325	-2.15460286
1	2.65813645	1.08163654	-1.57851912
1	4.09827452	-1.00142168	-1.77940609
1	4.01917468	-0.48379709	-0.08779297
1	3.04155004	-1.84950018	-0.63203941
1	-1.51337391	0.95751445	-0.00884820
6	-2.35910923	3.16886282	1.11992350
1	-2.42767993	4.10017630	1.70848304
1	-2.75343145	3.40711379	0.11691526
6	-3.23548497	2.10408529	1.78520168
1	-2.87461714	1.87335896	2.79854430
1	-3.24797476	1.16367242	1.21655218
1	-4.27485465	2.45045622	1.87019250
17	0.48719829	-1.31426683	1.41775870
17	2.41459828	1.57729526	2.00259974
5	2.16516965	3.33775804	1.71771900
17	2.71976081	4.39474918	3.00633345

**6a'\_1**

6	-0.44635160	4.59358816	-0.77223570
13	1.13985658	1.01403426	-0.39007037
6	-0.74271885	1.52970464	-0.07853614
6	-0.95815625	2.67366557	0.93739905
6	-0.12796166	3.92995021	0.58840808
6	1.98560242	0.70234684	-2.14504949
6	3.43998392	0.19950056	-2.15397087
1	-0.24493628	4.67557704	1.39020312
1	-0.42833164	3.85623743	-1.58812226
1	-0.56558612	2.32643722	1.91025404
1	0.37800884	5.29918520	-0.99960929
1	-1.21361995	1.77014342	-1.04770707

1	0.94218522	3.65025413	0.60024495
1	1.32987900	0.00038301	-2.69180994
1	1.90393094	1.64974603	-2.70887738
1	3.81628900	0.05810760	-3.17870631
1	4.11412774	0.90509865	-1.64878129
1	3.53821798	-0.76173674	-1.63038501
1	-1.25794139	0.61954783	0.27620229
6	-2.44549779	3.01775953	1.15286095
1	-2.50879427	3.87708918	1.84044054
1	-2.88851691	3.34995680	0.19661691
6	-3.28988196	1.87084665	1.71645554
1	-2.86595164	1.49830791	2.66149180
1	-3.35209285	1.02479316	1.01817323
1	-4.31673100	2.20485630	1.91957742
17	2.34020827	0.69889483	1.36055594
17	-2.11785580	6.70016766	0.34481794
5	-1.72912269	5.48188971	-0.88194349
17	-2.78321125	5.41414721	-2.30542718

**6a'\_2**

6	-0.20514290	4.92603754	-0.53582525
13	-1.06608176	1.92609516	-2.07933516
6	-0.46974900	1.87197248	-0.17368365
6	-0.90714411	2.84808797	0.94134788
6	-0.19423178	4.21296671	0.85024270
6	-2.60722907	0.88764782	-2.76221929
6	-2.92355714	0.99559951	-4.26435396
1	-0.61915708	4.88988800	1.60829796
1	0.36415270	4.32237728	-1.25887796
1	-0.56337748	2.42351643	1.90503005
1	0.34249973	5.87547350	-0.40995169
1	-0.75374686	0.84725180	0.13013571
1	0.86483672	4.07248929	1.11637100
1	-2.38779603	-0.16563816	-2.50482710
1	-3.49663928	1.14678946	-2.16182028
1	-3.75979000	0.34179870	-4.55707245
1	-3.20064759	2.02103395	-4.55159501
1	-2.05473146	0.71900841	-4.87774218
1	0.63369675	1.85591477	-0.22080986
6	-2.43354174	2.99523185	1.08066100
1	-2.63986270	3.72173722	1.88393875
1	-2.86394213	3.42700092	0.15975123
6	-3.16488754	1.68598776	1.39484166
1	-2.75787821	1.22113667	2.30579177
1	-3.07306761	0.95791372	0.57711261
1	-4.23680169	1.86287739	1.55927261
17	0.55026324	2.27328907	-3.48053534
17	-2.58001313	6.63075832	-0.56058979
5	-1.60220088	5.27778243	-1.11322792
17	-2.30081197	4.31822405	-2.47640801

**6a'\_3**

6	-0.63595166	4.82327267	-0.71602780
13	-1.47386031	-0.20187462	-0.51844894
6	-0.82074835	1.64602275	-0.77480796
6	-0.83055447	2.51407861	0.50391367
6	-0.06170582	3.84713143	0.33526805
6	-0.74558462	-1.54187965	0.73641581
6	-1.74311478	-2.58335640	1.27889655
1	-0.00656212	4.35560154	1.31150992
1	-0.82161162	4.31040409	-1.67078404
1	-0.27856123	1.96524843	1.29112786
1	0.15146058	5.57091889	-0.94272099
1	0.21174381	1.58548190	-1.16472852
1	0.97441673	3.60094000	0.05510972
1	0.06703078	-2.05832087	0.19252871
1	-0.24383160	-1.01573611	1.56638915
1	-1.24848201	-3.32642428	1.92300967
1	-2.53835692	-2.11307719	1.87641971
1	-2.23692129	-3.12842687	0.46242060
1	-1.42114630	2.11520643	-1.57203412
6	-2.25534083	2.73417622	1.04481304
1	-2.19764865	3.35254711	1.95416398
1	-2.84943914	3.30834655	0.31273906
6	-3.00939589	1.44284319	1.37616010
1	-2.40949777	0.77379776	2.01384946
1	-3.33297349	0.89742503	0.46687664
1	-3.94441842	1.64736501	1.91640903
17	-2.93134530	-0.92467620	-1.92751625
17	-1.97398644	6.50849257	1.25191562
5	-1.86527759	5.70569665	-0.32696680
17	-3.15801530	6.05496534	-1.48781095

**6a'\_4**

6	1.45931779	4.19623127	1.04066569
13	1.29868541	1.05608096	-0.52766828
6	-0.32206869	2.21356833	-0.42908336
6	-0.75703509	2.85857824	0.90334293
6	-0.08813598	4.22462774	1.13217426
6	1.71270988	-0.01601250	-2.13686112
6	3.07445926	-0.73234771	-2.17043866
1	-0.48676500	4.95306542	0.40616409
1	1.86017543	3.37239614	1.64939621
1	-0.44498360	2.19714841	1.73229253
1	1.84275352	5.13514998	1.48391775
1	-0.37385559	2.95197606	-1.24956571
1	-0.37185460	4.59333262	2.12970611
1	0.89971755	-0.76204257	-2.20934474
1	1.59211945	0.62842545	-3.02431911
1	3.18541548	-1.36041339	-3.06785769

1	3.91107310	-0.01770607	-2.17240077
1	3.21039149	-1.38064946	-1.29333447
1	-1.07297148	1.45121070	-0.72091405
6	-2.28879781	3.03169127	1.01068385
1	-2.50999930	3.65574574	1.89351719
1	-2.64400401	3.60157303	0.13480928
6	-3.07197514	1.72136927	1.13109368
1	-2.73919571	1.14139045	2.00482478
1	-2.95180006	1.08374221	0.24334687
1	-4.14714583	1.91645589	1.24786673
17	1.97404052	0.26937930	1.36950333
17	1.68304237	5.40246708	-1.60518001
5	2.02955170	4.16322347	-0.40316173
17	3.20534497	2.88471266	-0.92869558

**6a'\_5**

6	1.42213822	3.31734724	0.33567472
13	-1.61809191	1.98225928	-1.88242543
6	-1.18664489	1.68953619	0.03870262
6	-1.02799577	2.86527461	1.02282799
6	0.00679103	3.89602244	0.53455672
6	-1.69628446	0.45887600	-3.14022891
6	-1.74642298	0.79090123	-4.64230609
1	-0.34829180	4.35696134	-0.40173234
1	1.76223915	2.79556993	1.24441559
1	-0.65368937	2.46386283	1.98650224
1	2.13169486	4.16361362	0.21487715
1	-1.94730933	0.98401361	0.41790672
1	0.06692444	4.70921319	1.27495990
1	-0.84833662	-0.21233392	-2.91991394
1	-2.59734031	-0.11683279	-2.85736495
1	-1.85560739	-0.11443953	-5.25939565
1	-2.58768267	1.45743764	-4.87874505
1	-0.83083680	1.30121067	-4.97571952
1	-0.26436348	1.07355494	0.03700019
6	-2.36171649	3.57614483	1.32804024
1	-2.14458357	4.44863715	1.96712196
1	-2.78121864	3.97510169	0.39042283
6	-3.40383018	2.70128758	2.03125314
1	-3.00331457	2.27577457	2.96431598
1	-3.73793543	1.86674361	1.39873053
1	-4.29609161	3.28908817	2.28880973
17	-2.62015822	3.78456628	-2.52648840
17	0.95751745	2.76509827	-2.51225516
5	1.72096440	2.43272786	-0.90623873
17	2.93318693	1.15527148	-0.89815408

**6a'\_6**

6	0.01966346	4.87957498	1.46408199
13	0.92869853	0.94572496	-0.14034397

6	-0.96701398	1.54199797	-0.11905422
6	-1.26108543	2.73752103	0.81023121
6	-0.52078972	4.00853918	0.32235410
6	2.28491504	1.32454334	-1.52957491
6	2.23924399	0.30115210	-2.68630515
1	0.31530486	3.72965854	-0.33923426
1	-0.78213613	5.14942490	2.17459849
1	-0.87812904	2.48646279	1.81796578
1	0.36589974	5.86013503	1.08107393
1	-1.26648878	1.80396538	-1.15097666
1	-1.20466976	4.60308190	-0.30478564
1	2.13699944	2.34349657	-1.92465913
1	3.28426848	1.31305000	-1.06575665
1	3.00406601	0.51290874	-3.44965889
1	2.41527987	-0.72317198	-2.32612458
1	1.26502262	0.30268996	-3.19915656
1	-1.57394230	0.66819165	0.16941569
6	-2.76792551	3.03271807	0.97528608
1	-2.88558812	3.98875139	1.51568643
1	-3.20110983	3.19263795	-0.02721143
6	-3.55547856	1.94961377	1.71623343
1	-3.14288156	1.77775829	2.72184767
1	-3.53561436	0.99078513	1.17989103
1	-4.60906872	2.23958262	1.83275061
17	1.37957428	-0.70954559	1.16624907
17	2.12811876	2.84645165	1.79177356
5	1.21873427	4.31040063	2.28322385
17	1.81109747	5.11604604	3.73418340

### 6a'\_7

6	0.12540639	4.78697308	1.51180141
13	0.79819200	0.84287497	-0.29220248
6	-1.04190792	1.58775874	-0.24452770
6	-1.24952458	2.73411653	0.76813086
6	-0.45987933	3.99437202	0.33502366
6	2.14222786	1.14226366	-1.71021583
6	3.55681783	0.58168461	-1.48272735
1	0.36063790	3.71140823	-0.34399363
1	-0.65536099	5.04100389	2.25074215
1	-0.85347427	2.40255852	1.74709625
1	0.49432210	5.77582877	1.17424309
1	-1.31711261	1.94116514	-1.25510454
1	-1.12320181	4.64473368	-0.25785493
1	1.70298664	0.69417034	-2.62185588
1	2.18244173	2.22447134	-1.92485040
1	4.20850013	0.74703257	-2.35464701
1	4.04582470	1.05186485	-0.61727013
1	3.53382953	-0.49915831	-1.28596941
1	-1.71278241	0.74278273	-0.01613627
6	-2.73518045	3.09001455	0.99483005



1	-2.79176682	4.02067465	1.58679190
1	-3.18910131	3.32197222	0.01589813
6	-3.55098777	2.00690549	1.70450064
1	-3.12426699	1.77281673	2.69141253
1	-3.58155357	1.07312968	1.12587546
1	-4.58922696	2.33276729	1.85788196
17	1.14973937	-0.80647434	1.04836098
17	2.18138329	2.68595313	1.67903742
5	1.32199812	4.13844250	2.27489362
17	1.95572057	4.84088456	3.76240113

**6a'\_8**

6	-0.33486399	5.19576485	1.63976869
13	-0.84794460	1.76969757	-1.88769985
6	-0.41953289	1.60990389	0.04270246
6	-0.91138890	2.75752852	0.95500455
6	-0.18178588	4.06968926	0.60136936
6	-2.41193828	0.97387916	-2.79292341
6	-2.57965698	1.24734229	-4.29771095
1	0.88828290	3.85439192	0.46377624
1	-1.38803791	5.47709643	1.78897193
1	-0.64526468	2.50100269	1.99934748
1	0.13630840	6.11482083	1.23454238
1	-0.83139130	0.64730309	0.38930518
1	-0.54487445	4.43085975	-0.37781855
1	-2.35677435	-0.11456483	-2.60479687
1	-3.30943186	1.30194828	-2.23803660
1	-3.46497359	0.73864945	-4.70915242
1	-2.69171873	2.32139050	-4.50216359
1	-1.70556866	0.90619659	-4.86953916
1	0.67621696	1.52239555	0.13189269
6	-2.44161307	2.92949475	0.90801184
1	-2.73064033	3.78889529	1.53311704
1	-2.73815617	3.19917324	-0.12507328
6	-3.24157555	1.70618276	1.36644058
1	-2.94863656	1.40676959	2.38396322
1	-3.08971281	0.84074505	0.70681513
1	-4.31859080	1.92368360	1.38049003
17	0.57188027	2.78908768	-3.13369190
17	1.83937090	4.05447970	3.22519839
5	0.35409935	4.99832424	3.03020492
17	-0.28208643	5.79748832	4.47771445

**6a'\_9**

6	-0.27681730	4.95387050	1.93483434
13	-1.33225358	0.05843036	-0.51753848
6	-0.72696875	1.93949489	-0.57130929
6	-0.95542469	2.74284688	0.72782653
6	-0.28150272	4.12863745	0.63178219
6	-0.71488322	-1.33257881	0.74104328

6	-1.69220252	-2.48852551	1.02639608
1	0.75778799	3.98561576	0.29978238
1	-1.29587014	5.18925869	2.27456452
1	-0.47278950	2.19800969	1.56272270
1	0.17616394	5.94260148	1.71470243
1	0.35267377	1.93624741	-0.80574884
1	-0.78249853	4.70705093	-0.16257329
1	0.22116765	-1.73580395	0.31201339
1	-0.40810922	-0.84315989	1.68113874
1	-1.24462639	-3.25007671	1.68322024
1	-2.60927340	-2.13265519	1.51908976
1	-2.00217673	-2.99052331	0.09933412
1	-1.21902012	2.44810635	-1.41874941
6	-2.45414514	2.86220653	1.06789659
1	-2.57268504	3.42141994	2.00839148
1	-2.95305851	3.46068425	0.28651044
6	-3.17852915	1.52118498	1.21896632
1	-2.63834354	0.83945764	1.89538886
1	-3.34886305	1.01980500	0.24500516
1	-4.18743593	1.64987334	1.63585493
17	-2.55873120	-0.61869054	-2.15293839
17	2.09984673	3.55343561	2.88878186
5	0.56825963	4.41023389	3.13284005
17	0.07329866	4.70075234	4.80862132

### 6a'\_10

6	-0.43525371	4.74784530	-0.86222957
13	1.19429554	1.08636164	-0.40927965
6	-0.68146265	1.64132784	-0.12793716
6	-0.89045957	2.79489185	0.87726860
6	-0.10648054	4.07231781	0.48703776
6	2.02849374	0.66016980	-2.14533981
6	3.44827620	0.06740978	-2.12990153
1	-0.21337153	4.81134595	1.29599857
1	-0.59977884	4.01091619	-1.66340226
1	-0.41655577	2.47957256	1.82326660
1	0.46491369	5.30472286	-1.19928945
1	-1.13063048	1.86970284	-1.10878537
1	0.96561076	3.80026951	0.48457315
1	1.33134041	-0.01478751	-2.67431713
1	2.00877730	1.59292101	-2.73887991
1	3.82314566	-0.12117966	-3.14750510
1	4.16120910	0.74075493	-1.63418742
1	3.48183199	-0.88575606	-1.58377826
1	-1.22197184	0.74526452	0.23244377
6	-2.38155465	3.02487889	1.23744237
1	-2.69781693	2.17927805	1.87068728
1	-2.45159030	3.91933189	1.87811315
6	-3.38352159	3.14174724	0.08344392
1	-3.40854724	2.22822389	-0.52690982

1	-3.16951835	3.98006705	-0.59483249
1	-4.39698486	3.30268949	0.47706386
17	2.40138967	0.87658490	1.35227635
17	-1.99411223	6.84486543	0.45824745
5	-1.54154184	5.84992574	-0.93370240
17	-2.29985114	6.25372626	-2.48559549

**6b**

6	0.17035345	1.72819660	1.75777240
13	0.38872803	0.38156285	0.33882478
6	-1.65253098	2.49464474	-0.68609052
6	-1.63378567	3.23933242	0.66844082
6	-1.24485597	2.33859369	1.85750593
6	2.00214104	-0.14736189	-0.66089120
6	3.30961986	0.56676377	-0.26976012
1	-1.31319542	2.94005841	2.77771966
1	0.42222832	1.23763068	2.71570459
1	0.92458033	2.52638541	1.64028212
1	-0.85643378	4.02323433	0.58834261
1	-1.99474211	1.53708377	1.95823772
1	2.10883742	-1.24043079	-0.54760215
1	1.79131901	-0.00366676	-1.73497969
1	4.16379258	0.21527215	-0.86835475
1	3.24017759	1.65495929	-0.41447135
1	3.56554642	0.40117927	0.78718280
1	-1.89530031	3.22042690	-1.48582853
1	-0.63037841	2.17896842	-0.98784015
6	-2.97554803	3.96713883	0.90391500
1	-3.26348173	4.47421191	-0.03238345
1	-3.76401191	3.22516533	1.10581602
6	-2.94538939	5.00822810	2.02829710
1	-2.15376569	5.75363192	1.85730816
1	-2.76966076	4.55188517	3.01195256
1	-3.90227655	5.54567906	2.08479026
9	-1.02774163	-0.49874811	-0.01075053
5	-2.64394970	1.28364642	-0.91944968
9	-2.65587182	0.66877883	-2.10995699
9	-3.60652740	0.93637080	-0.05799500

**6b + THF**

6	1.44174461	3.86578376	0.56593504
13	0.53060350	0.20722456	-0.08087065
6	-0.82065981	1.67044551	0.05243940
6	-0.79970281	2.69133993	1.21650469
6	-0.07455397	4.01608806	0.91142147
6	2.32706591	0.35593518	-0.93488611
6	2.98503748	-0.97131734	-1.35990783
1	-0.54570309	4.42120966	-0.00428673
1	1.77409986	4.76759019	0.03228369
1	-0.38480189	2.23556342	2.12960932

1	1.54311748	3.02954363	-0.14900361
1	-0.89470748	2.22195367	-0.90449853
1	2.27452261	1.04095971	-1.80103277
1	2.99042388	0.86223776	-0.21249511
1	3.99950119	-0.82753521	-1.76503952
1	3.06896133	-1.66507190	-0.51025336
1	2.40455403	-1.48758237	-2.14223035
1	-1.76430812	1.09682671	0.12222237
1	-1.83624330	2.96947122	1.47375590
17	0.48016448	-1.16797839	1.62019209
17	2.39746569	2.10937558	2.70627209
5	2.42723953	3.60037991	1.75266166
17	3.68570311	4.77827359	2.18677557
6	-0.68409467	-2.88388440	-2.79246691
6	-1.40421460	-1.68904540	-3.43649823
6	-0.53563154	-2.44820503	-1.33941265
6	-0.72997206	-0.50584797	-2.75727302
1	0.30216297	-3.03161740	-3.25498257
1	-1.41274287	-2.69652919	-0.72728131
1	-2.47730586	-1.70762736	-3.19836376
1	-1.35685664	0.39005387	-2.67424354
1	-1.29058442	-1.65460032	-4.52708936
1	0.22893897	-0.24572084	-3.23164791
1	0.36772387	-2.81368275	-0.84045604
1	-1.24902518	-3.82025804	-2.87764533
8	-0.45772326	-0.97216084	-1.39214753
6	-0.31386325	5.04563530	2.03263446
1	-1.39084864	5.04832935	2.26810191
1	0.19226538	4.70762360	2.95430502
6	0.12249858	6.47542634	1.69640117
1	-0.38295695	6.83548596	0.78715319
1	1.20586545	6.55138149	1.53018007
1	-0.13228118	7.16482823	2.51353132

**6b + 2THF**

6	1.76320392	3.84258993	0.51737955
13	0.56597264	0.06042629	-0.09373087
6	-0.62493498	1.65532794	0.04123239
6	-0.51315359	2.73085356	1.15153954
6	0.23521418	4.02038321	0.75201452
6	2.22427547	-0.07883956	-1.21382410
6	3.31701315	-1.05086649	-0.73048770
1	-0.17762296	4.31953018	-0.23219861
1	2.14166821	4.80638854	0.12913100
1	-0.06817872	2.31086828	2.06624072
1	1.87483499	3.13269759	-0.32228337
1	-0.65872666	2.16461691	-0.94202401
1	1.92906207	-0.34669068	-2.24627770
1	2.64901419	0.93587969	-1.30485321
1	4.20456836	-1.05362928	-1.38598775

1	3.65176130	-0.79980142	0.28643428
1	2.94852753	-2.08624183	-0.67921096
1	-1.61667940	1.17396563	0.14092695
1	-1.53149717	3.04603217	1.43582831
17	0.45473613	-1.37199516	1.55881907
17	2.63290782	1.53145297	2.08881272
5	2.74268694	3.34588505	1.68498125
17	2.82493756	4.35692873	3.24493998
6	-0.95184273	-2.74928054	-2.93010058
6	-1.93231451	-1.60848102	-3.24186251
6	-0.55495610	-2.47096990	-1.48267354
6	-1.28428269	-0.43283572	-2.52606862
1	-0.07499807	-2.68952411	-3.59052916
1	-1.21928232	-2.95093509	-0.75288073
1	-2.92300296	-1.81757365	-2.81339637
1	-1.97903342	0.35573494	-2.21530633
1	-2.05017459	-1.42242469	-4.31683524
1	-0.46693067	0.00892625	-3.11907501
1	0.48362418	-2.72648087	-1.24287150
1	-1.40067879	-3.74386022	-3.04307054
8	-0.71969013	-1.01368004	-1.30594413
6	6.15720253	3.24248966	-0.29687915
6	5.87106233	4.74828215	-0.18368519
6	4.80483082	2.63563654	0.02346129
6	4.92516037	4.84441601	1.01118694
1	6.90371230	2.92610539	0.44514329
1	4.10320353	2.71153199	-0.81930737
1	5.37739126	5.10978971	-1.09665583
1	4.11773281	5.57372211	0.88983080
1	6.77717089	5.34554423	-0.02393027
1	5.43573958	5.01940274	1.96374850
1	4.81930856	1.61356986	0.40969094
1	6.50853666	2.94765219	-1.29351460
8	4.31162557	3.49144176	1.12373098
6	-0.13003573	5.16379651	1.72244805
1	-1.23091720	5.22362416	1.74839822
1	0.18880069	4.90725616	2.74299427
6	0.42391677	6.54074132	1.34447494
1	0.16700709	6.80391204	0.30589860
1	1.51730672	6.58379080	1.44648599
1	0.00852185	7.32127626	1.99799469

**6b'**

6	0.58412546	2.58829768	-0.49080920
13	1.08010557	1.32958627	-1.94625109
6	-1.97233886	0.91312692	0.02484383
6	-1.85627446	2.42962790	0.40210172
6	-0.83160816	3.20607464	-0.44556129
6	1.88307684	-0.46884604	-1.74305563
6	1.40887316	-1.33927984	-0.56587054

1	-1.22842565	3.35186971	-1.46551669
1	0.83543848	2.15679079	0.49442442
1	-1.47874010	2.43314518	1.44110534
1	1.31426110	3.40472354	-0.63889694
1	-2.63798276	0.42688657	0.75292483
1	-0.78009817	4.21775221	-0.00908408
1	1.74992813	-1.00628280	-2.69669681
1	2.97292577	-0.29961389	-1.66686578
1	1.95583068	-2.29353387	-0.51036060
1	1.54731041	-0.83306190	0.40160403
1	0.34067258	-1.59263777	-0.64928257
1	-0.97454425	0.46341984	0.15233926
6	-3.21621273	3.15089850	0.40516918
1	-3.02472859	4.21326611	0.62821744
1	-3.64826421	3.13194672	-0.60993020
6	-4.23751599	2.61078416	1.41107005
1	-3.82444640	2.61022648	2.43116491
1	-4.55256539	1.58480189	1.17502094
1	-5.14268117	3.23345674	1.41944892
17	1.55530636	2.31471644	-3.81295874
17	-1.36379260	0.60106768	-2.82137305
5	-2.48393193	0.60034255	-1.40868048
17	-4.15196884	0.20523740	-1.80308913

7a

6	2.12218478	1.85643323	-4.09416615
13	3.65364154	1.28903086	-0.34547256
6	1.63281154	3.67553644	-2.33388464
6	0.37770320	3.37868486	-3.20077809
6	0.93970728	2.76868684	-4.51305934
6	5.15101966	0.03120120	-0.30300991
6	6.53598964	0.65774097	-0.04536627
1	0.17349487	2.23447234	-5.09013523
1	2.87322423	1.67604587	-4.87591087
1	1.75042433	0.85932485	-3.78806881
1	-0.19538008	2.58721463	-2.68444855
1	1.31690304	3.58592631	-5.15177337
1	4.92839085	-0.71871437	0.47557913
1	5.15315040	-0.53237827	-1.25095095
1	7.32823948	-0.10556496	-0.00793703
1	6.81252090	1.37337209	-0.83362188
1	6.56050092	1.20579063	0.90701435
1	2.07628019	4.64357265	-2.64990112
1	1.44702125	3.76072045	-1.25477989
6	-0.54196294	4.58817889	-3.39914007
1	-0.80772843	4.99452681	-2.40965524
1	0.02615394	5.38272855	-3.91451696
6	-1.82437318	4.28096066	-4.17951560
1	-2.40466955	3.48598532	-3.68745263
1	-1.60815972	3.95106895	-5.20547125

1	-2.46812104	5.16898134	-4.24724761
9	3.62979304	2.64574664	0.65548107
5	2.60918612	2.55799395	-2.79300506
9	2.10233868	0.77709916	-0.83117613
9	3.82882337	2.26172066	-2.15574846

**7a + THF**

6	-1.94677701	2.22242922	2.36900709
13	2.34590561	-0.20339887	-1.05457113
6	-1.93049235	2.85993735	-0.11556179
6	-1.73816531	4.11213697	0.78375712
6	-1.19335577	3.55075179	2.12014552
6	1.69765643	0.49685891	-2.77818248
6	2.10100000	-0.33038836	-4.01414519
1	-0.11762023	3.33981847	2.00499218
1	-2.92513853	2.41754701	2.85167415
1	-2.74108598	4.53644927	0.98132817
1	-1.42596464	1.51056691	3.02423294
1	-0.95886847	2.59249599	-0.58133786
1	-1.29746972	4.27344137	2.94248903
1	0.60104205	0.61433266	-2.73642130
1	2.09177021	1.52321854	-2.87213383
1	1.73925554	0.12133305	-4.95108703
1	3.19363138	-0.42326234	-4.09450877
1	1.69799563	-1.35426301	-3.97161654
1	-2.64203085	2.98154316	-0.94363156
6	-0.86201000	5.21863523	0.18713911
1	-0.70123315	5.99571315	0.95372076
1	0.13275831	4.79539211	-0.03469499
6	-1.44138062	5.86624845	-1.07429028
1	-2.43240496	6.30236893	-0.87640857
1	-1.55497554	5.13458572	-1.88699330
1	-0.79044560	6.67161721	-1.44238147
17	4.43178209	-0.73331997	-0.89131198
17	1.60051592	0.78371014	0.73823240
5	-2.24771223	1.72485390	0.91432468
17	-2.89032610	0.11161615	0.49990170
6	0.86997631	-3.88555976	0.38493286
6	-0.35298980	-2.96573890	0.24666852
6	2.02863692	-2.92610795	0.16971846
6	0.03768515	-2.05926983	-0.91081717
1	0.86281229	-4.66549208	-0.39002284
1	2.27831963	-2.35780003	1.07646283
1	-0.49785383	-2.37342603	1.16025533
1	-0.37074859	-1.04481323	-0.83552556
1	-1.27988792	-3.51269316	0.03549512
1	-0.19647392	-2.49162401	-1.89276395
1	2.93449127	-3.36887985	-0.25562887
1	0.92830034	-4.37155115	1.36670701
8	1.51930236	-1.96207773	-0.83898239

**7a + 2THF**

6	3.23957099	3.82932294	-1.54504894
13	0.94971001	0.52472371	-4.70522058
6	1.07330088	4.72328875	-0.49686725
6	1.79976558	5.83166535	-1.30608714
6	2.69124454	5.05892323	-2.30923066
6	-0.10056976	-0.34662449	-6.12565240
6	0.54031058	-1.61145462	-6.72846665
1	2.06916866	4.71299337	-3.15110217
1	4.13592039	4.11023966	-0.95942684
1	2.47114349	6.36706864	-0.60959445
1	3.53624619	2.98972963	-2.18898119
1	0.19396427	4.36736530	-1.07347958
1	-1.11102360	-0.57155914	-5.74274575
1	-0.25789130	0.40614426	-6.91691653
1	-0.07803366	-2.04956403	-7.52769907
1	1.52767602	-1.39295865	-7.16033380
1	0.69254748	-2.39517925	-5.96987168
1	0.68917157	5.02959226	0.48569125
17	3.03160020	0.94907618	-5.09640331
17	-0.03723569	2.12864704	-3.61633831
5	2.10394894	3.54576462	-0.50608382
17	1.95804684	2.05640626	0.48500015
6	1.68586234	-1.60480929	-1.12204895
6	0.17496187	-1.32791949	-1.16042125
6	2.20532569	-0.76081376	-2.27391246
6	-0.12400070	-1.31932606	-2.65191859
1	1.89397300	-2.67095764	-1.29245937
1	2.34847435	0.28921499	-1.98865248
1	-0.04410768	-0.34500252	-0.72166874
1	-0.94215162	-0.64739539	-2.93866590
1	-0.41454148	-2.08876580	-0.63403332
1	-0.29623543	-2.32475689	-3.05979176
1	3.10481719	-1.14317824	-2.76626910
1	2.14609287	-1.30436081	-0.17282439
8	1.11667443	-0.81219368	-3.28707769
6	2.65561815	5.05252482	3.75119741
6	3.60981605	3.82836123	3.78435679
6	3.24568535	5.92690338	2.63509906
6	4.53376422	4.05271530	2.56639157
1	2.61211214	5.58402081	4.71095096
1	2.50179127	6.50560756	2.07252501
1	3.04739600	2.89170588	3.68785410
1	4.70840607	3.15011340	1.96744392
1	4.18891387	3.77993742	4.71582774
1	5.51021584	4.46443803	2.88500451
1	4.00673501	6.62313387	3.03915186
1	1.63642347	4.73976043	3.48954029
8	3.86473140	5.00689604	1.72452987



1	3.48213967	5.69723373	-2.72944334
6	0.88247165	6.86018290	-1.97579463
1	1.49442291	7.51862470	-2.61563088
1	0.19304690	6.32799855	-2.65352692
6	0.07929594	7.71777427	-0.99280747
1	0.74656055	8.26783622	-0.31147016
1	-0.59272495	7.10197723	-0.37771825
1	-0.53949136	8.45699844	-1.52095296

**7a'**

6	0.28173044	3.94877694	0.37122397
13	0.64846194	-0.55838101	-2.18762371
6	-1.38774109	2.06541944	-0.15277189
6	-1.94825861	3.02999183	0.93133938
6	-1.17326793	4.35342327	0.71821163
6	2.33055876	-1.02367878	-3.09209351
6	2.67063938	-0.21666862	-4.35780184
1	-1.61392483	4.89181381	-0.13767206
1	0.84896411	3.73432962	1.29921296
1	-1.65408479	2.62484346	1.91751325
1	0.86525212	4.70720637	-0.16843114
1	-1.90733322	2.24390494	-1.11839496
1	-1.24121727	5.01898806	1.59010687
1	3.14629245	-0.95759727	-2.35287301
1	2.24946816	-2.09724716	-3.33724672
1	3.59831512	-0.57475832	-4.82993675
1	1.87008574	-0.28591489	-5.10765226
1	2.81117287	0.85196763	-4.13787890
1	-1.51316597	0.99376534	0.05000272
6	-3.47031401	3.20332136	0.92004917
1	-3.74240332	3.98774604	1.64639468
1	-3.77298779	3.58352734	-0.07122160
6	-4.24737872	1.92298999	1.24036718
1	-3.97016144	1.52862585	2.22944226
1	-4.05118554	1.13530748	0.49946982
1	-5.33012526	2.10937421	1.24751149
17	0.14579840	-1.52960212	-0.34185872
17	1.38936486	1.75069968	-1.26620450
5	0.06534958	2.57794428	-0.34191028
17	-1.04811323	0.06093940	-3.34625990

**7b**

6	0.58201815	2.71895463	2.51289431
13	0.64337510	0.93388872	-1.17942648
6	-1.14554321	3.52057474	0.77504672
6	-0.55411461	4.71538189	1.57315432
6	-0.03529063	4.08948244	2.89575405
6	1.50263979	-0.82334739	-1.19135820
6	0.54474988	-2.02390024	-1.32534078
1	0.67298537	4.74396346	3.42066905

1	0.62238561	1.98062839	3.32597602
1	1.62456731	2.84947299	2.16325561
1	0.32443113	5.08052869	1.01074647
1	-0.89174576	3.92836259	3.57296645
1	2.23095066	-0.83059825	-2.02055549
1	2.11043004	-0.91599270	-0.27583213
1	1.08963996	-2.97997442	-1.35350652
1	-0.16100582	-2.07838893	-0.48323482
1	-0.05763092	-1.96091443	-2.24279984
1	-2.17713687	3.31455208	1.13122883
1	-1.22133256	3.67437329	-0.30983733
6	-1.52807294	5.88408008	1.75669945
1	-1.90357410	6.18825565	0.76606689
1	-2.40724138	5.52535363	2.32070699
6	-0.92339195	7.10202319	2.46293752
1	-0.04146578	7.47514294	1.92087093
1	-0.60953105	6.86441529	3.48922306
1	-1.64978288	7.92447379	2.52224264
9	-0.71759896	1.24080669	-2.12661375
5	-0.25533658	2.34197472	1.25625468
9	1.52644717	2.33816090	-0.79141809
9	-0.25727067	1.06121683	0.67415036

**7b + THF**

6	-1.49280784	2.93829960	2.09859353
13	2.59733715	-0.23453662	-1.01639825
6	-0.89750569	3.83587399	-0.22898012
6	-0.56142853	4.85652453	0.88516564
6	-0.39456513	4.03263804	2.18561567
6	2.39709905	0.62143341	-2.77953831
6	2.75269467	-0.27195427	-3.98380486
1	0.58432936	3.52280657	2.13265556
1	-2.45717487	3.35085854	2.46404383
1	-1.40720467	5.55475774	1.00960156
1	-1.30426324	2.03797825	2.69913943
1	0.03385069	3.36967391	-0.60734774
1	1.36996580	1.01210663	-2.88189147
1	3.04373283	1.51562507	-2.77491566
1	2.64997314	0.26321203	-4.94082235
1	3.78818800	-0.63607118	-3.92042066
1	2.10645802	-1.16180556	-4.03942545
1	-1.40841372	4.25360209	-1.10742900
1	0.32918530	5.46337883	0.66687603
17	4.42783777	-1.30077403	-0.60309860
17	1.89657385	0.90265471	0.70451582
5	-1.65731947	2.71540655	0.55739304
17	-2.59974920	1.39590219	-0.18930803
6	0.01844339	-3.39529933	0.06477374
6	-0.89112605	-2.18846443	-0.21243801
6	1.40342473	-2.77036291	0.05514479

6	-0.11199576	-1.41386004	-1.26505170
1	-0.07370713	-4.14709193	-0.73221417
1	1.65049045	-2.28151314	1.00789053
1	-1.01405108	-1.57948551	0.69342957
1	-0.24754950	-0.32786172	-1.20421995
1	-1.88555337	-2.47432036	-0.57608885
1	-0.30529258	-1.76437792	-2.28757804
1	2.21852888	-3.43562281	-0.24582809
1	-0.19714539	-3.87854491	1.02574233
8	1.31714138	-1.71315539	-0.98399891
6	-0.42072752	4.88744810	3.45675378
1	0.32011529	5.69852335	3.35417033
1	-1.40641414	5.37985834	3.53210888
6	-0.13561036	4.10485229	4.74247215
1	0.84702827	3.61233215	4.69414457
1	-0.89126651	3.32514245	4.91540212
1	-0.13525452	4.76703021	5.61971250

**7b + 2THF**

6	4.85666975	2.26141842	0.15295046
13	1.61167786	-0.64587288	-2.63979876
6	3.02327235	0.76649223	-0.83826846
6	3.23135106	2.05594939	-1.66815368
6	4.67060667	2.53513591	-1.36191628
6	0.18247256	0.65009966	-3.01396044
6	-1.00161396	0.01981483	-3.77673866
1	5.36729746	1.87512212	-1.91212206
1	4.38339762	3.08248002	0.73203543
1	2.51584871	2.81607938	-1.31667103
1	5.89767471	2.19556689	0.49641822
1	3.49219880	-0.12246503	-1.32203879
1	-0.16153678	1.07966951	-2.06002375
1	0.60906523	1.48173039	-3.59594696
1	-1.79949782	0.75620603	-3.95919684
1	-0.69274642	-0.37242127	-4.75688371
1	-1.44854725	-0.81632024	-3.21923043
1	1.98800890	0.53912378	-0.52054350
1	3.07683009	1.92187564	-2.74866469
17	1.20502719	-2.38723738	-1.46242568
17	3.20838114	-0.91707742	-4.04442566
5	3.96814764	1.00577432	0.41629411
17	3.99783693	-0.00994248	1.86083789
6	-2.19211729	-0.54548048	1.74847468
6	-1.09690331	-1.56937358	2.08229141
6	-1.52593827	0.24141713	0.62262166
6	0.18333704	-0.74475255	1.91492617
1	-2.38796251	0.10936388	2.61068196
1	-1.64151932	-0.28446780	-0.34279820
1	-1.11705272	-2.39523043	1.35694189
1	1.02190906	-1.33483795	1.51980561

1	-1.19058290	-1.99304087	3.09029021
1	0.49594731	-0.27608528	2.86297062
1	-1.90359921	1.26837533	0.51203262
1	-3.13844232	-1.00794445	1.43889042
8	-0.12581034	0.31805504	0.97003178
6	0.26686599	5.88606913	1.17033794
6	-0.35846611	4.53497017	1.61407705
6	1.78235851	5.59470632	1.15704912
6	0.86584298	3.65450820	1.91204630
1	0.02450054	6.70505618	1.86009657
1	2.31536681	6.03272665	0.30326537
1	-0.95262510	4.09868965	0.80044785
1	0.72508739	2.59265168	1.67281217
1	-1.01125729	4.63921282	2.49069924
1	1.16993689	3.75300351	2.97241018
1	2.25730006	5.94932879	2.09198840
1	-0.08864926	6.17298364	0.17264102
8	1.90979246	4.16709247	1.06405205
6	4.92948439	3.97828690	-1.80665618
1	4.64721805	4.07902485	-2.86830890
1	4.25451860	4.64307888	-1.24100310
6	6.37995256	4.43578468	-1.62534853
1	7.07130252	3.78862725	-2.18579023
1	6.68162696	4.41120879	-0.56849282
1	6.52006096	5.46414876	-1.98670823

**7b'**

6	0.81117661	2.47142919	1.20679749
13	1.56106756	0.31228504	-1.96842210
6	-1.68275698	2.49362743	0.58652842
6	-1.33162017	3.67454642	1.53610868
6	0.19248659	3.88355488	1.35159417
6	1.06368549	-1.19090881	-3.13148138
6	1.94507437	-1.29893049	-4.39307368
1	0.36866917	4.44843177	0.42152906
1	0.95173406	2.01019956	2.20659473
1	-1.49926960	3.32527029	2.57227002
1	1.79282727	2.43016019	0.71780093
1	-1.82819416	2.87833605	-0.44587118
1	0.63071456	4.46550677	2.17445523
1	1.12996154	-2.12045053	-2.54266701
1	0.00538782	-1.07362598	-3.41558255
1	1.64270356	-2.14874314	-5.02408684
1	1.87969253	-0.39323671	-5.01359600
1	3.00475250	-1.44377235	-4.13703502
1	-2.59877117	1.93980343	0.83236563
6	-2.15427578	4.94891047	1.32146222
1	-1.74086869	5.74691111	1.96085904
1	-2.01357675	5.28639737	0.28012215
6	-3.64853927	4.78770431	1.61628688

1	-3.81416394	4.46518081	2.65533592
1	-4.11291255	4.04110414	0.95616426
1	-4.18564189	5.73528354	1.47210673
17	3.36418621	0.23260821	-0.81570413
17	0.99892789	2.32037868	-2.52285045
5	-0.35362923	1.68789304	0.53993612
17	-0.22813441	-0.00392030	-0.14979589

## 8

13	-0.66519635	-2.33822170	-9.14458315
6	0.66602313	-1.72134803	-10.43497164
6	2.12187281	-2.13505826	-10.15163745
1	0.34236295	-2.06400984	-11.43156465
1	0.57857818	-0.62160684	-10.47547277
1	2.81054407	-1.70366696	-10.89319368
1	2.45478821	-1.79973101	-9.15972080
1	2.24822775	-3.22616067	-10.17885183
9	-2.30781903	-2.21313285	-9.44454561
9	-0.22798766	-2.99879588	-7.66884407

## 8'

17	-2.27670519	1.98949658	-2.92903211
13	-3.77475515	0.72077397	-2.13617554
6	-5.42307206	1.44656492	-1.36518875
1	-5.12584844	2.27745542	-0.70350203
1	-5.96971631	1.92720813	-2.19517942
6	-6.32778260	0.44613688	-0.62458136
1	-5.82416585	0.01513918	0.25171408
1	-6.62285575	-0.39267614	-1.26982594
1	-7.24970028	0.93072501	-0.27007669
17	-3.40023488	-1.36090449	-2.23953026

## 9

6	-2.02551104	1.48007183	-3.00372665
6	-0.68825031	3.59179897	-2.38879379
6	-2.08740631	3.59850077	-1.71974731
6	-2.94879986	2.65443407	-2.59904090
1	-3.86581406	2.32811393	-2.08957035
1	-2.32842499	0.94881653	-3.91697260
1	-2.00606100	0.71738536	-2.20083771
1	-1.98412682	3.12116111	-0.72660615
1	-3.26303043	3.20231218	-3.50341841
1	-0.67433864	4.32795934	-3.21868422
1	0.13793025	3.87494463	-1.72077081
6	-2.67783526	4.99801815	-1.51409405
1	-1.95149577	5.60899139	-0.95296953
1	-2.78522542	5.48142146	-2.50121842
6	-4.02407821	5.01697051	-0.78211647
1	-3.94453438	4.53498353	0.20415183
1	-4.80323467	4.48880929	-1.34960934

1	-4.37286875	6.04680367	-0.62159031
5	-0.60489985	2.15935556	-3.03480976
9	0.50895990	1.59825387	-3.53631223

**9'**

6	-2.01231022	1.33257681	-3.09983950
6	-0.53535359	3.33611765	-2.50846598
6	-1.92222043	3.44603905	-1.82185383
6	-2.85360297	2.56647617	-2.69328986
1	-3.78759452	2.30109084	-2.17903771
1	-2.36185967	0.80578004	-3.99844527
1	-2.02683307	0.57954316	-2.28673290
1	-1.84231306	2.96276453	-0.82957228
1	-3.13183422	3.13404178	-3.59847982
1	-0.48769811	4.05723092	-3.35155382
1	0.32006728	3.57779760	-1.86211430
6	-2.40401636	4.88587347	-1.61218328
1	-1.62594512	5.44259113	-1.06415924
1	-2.49092031	5.37381129	-2.59902026
6	-3.73333777	5.00490116	-0.85908204
1	-3.67279965	4.52230699	0.12818223
1	-4.55745770	4.53211380	-1.41171990
1	-4.00425951	6.05782895	-0.69831371
5	-0.55216286	1.90595656	-3.15055841
17	0.85351916	1.06643124	-3.83074097

**10a**

6	0.15110514	2.75486546	1.25959060
13	-0.33296766	0.20030120	-0.11096245
6	-2.13207365	1.02088828	-0.17227671
6	-2.21378648	2.51168988	0.24520162
6	-1.37392038	2.76086056	1.51594095
6	0.84729427	-0.29449178	-1.60853487
6	2.28432458	-0.70610442	-1.23527930
1	-1.64631467	3.72504381	1.96680278
1	0.52181026	3.79190031	1.16231059
1	0.40501791	2.35099938	0.25149442
1	-1.78151564	3.12216509	-0.57012977
1	-1.63664964	1.99195029	2.25999905
1	0.34408823	-1.11778953	-2.14841033
1	0.85662704	0.54175832	-2.32951306
1	2.86437691	-1.00846882	-2.12051308
1	2.82888885	0.11627901	-0.75036051
1	2.29174534	-1.54842090	-0.52977478
1	-2.75659277	0.43396924	0.52814069
1	-2.56197729	0.89190937	-1.18023637
6	-3.67990254	2.95535912	0.42267323
1	-4.25679118	2.58920462	-0.44211562
1	-4.09878056	2.44579736	1.30758264
6	-3.88835439	4.46872737	0.54466506

1	-3.48858806	4.99438633	-0.33561336
1	-3.39897295	4.88652972	1.43575633
1	-4.95780420	4.71060723	0.61787142
9	2.34194899	1.75892010	2.06235712
5	1.06143691	2.04461193	2.33367390
9	0.19856557	-0.23695947	1.45059928
9	0.64857836	1.84743761	3.58795751
9	-5.20336752	-0.13412011	-2.12096860
9	-5.75638445	-0.40687064	0.09369228
5	-5.04809551	-0.77022614	-0.96649824
9	-4.19610087	-1.78510474	-0.88039101

**10a'**

6	1.09373789	3.71309224	1.30049958
13	-0.35193257	0.16012728	-1.21138226
6	-1.54567112	1.64935632	-0.67466302
6	-1.04439486	2.47306966	0.53418567
6	0.17569590	3.33160503	0.12938182
6	0.92221206	0.12533093	-2.72038711
6	1.57198107	-1.22538104	-3.06824486
1	0.77323517	2.79674605	-0.62717564
1	0.52638523	4.18165813	2.12239201
1	-0.72089739	1.77089767	1.32610819
1	1.79945640	4.50857864	0.98693636
1	-1.70728873	2.32657781	-1.53257066
1	-0.18918714	4.24348720	-0.37209860
1	0.39351716	0.53903417	-3.59742971
1	1.70358471	0.87217524	-2.48971558
1	2.26688969	-1.13566680	-3.91760181
1	2.13534962	-1.63216666	-2.21714302
1	0.81901637	-1.98013254	-3.33723006
1	-2.52549991	1.19643460	-0.44738018
6	-2.15005973	3.36239744	1.14406087
1	-1.69382342	4.07015568	1.85723570
1	-2.58288307	3.97756753	0.33625182
6	-3.25972057	2.59417729	1.86665313
1	-2.85078953	1.99328788	2.69257878
1	-3.79237942	1.90984108	1.19130419
1	-4.00379408	3.28310124	2.29033760
17	-0.42479785	-1.57146980	0.07054816
17	2.31797152	1.06163163	1.05441954
5	2.00335404	2.59125824	1.89942981
17	2.83201291	2.83110021	3.44326345
17	-4.69481889	-1.23034371	-5.06948115
17	-2.88802972	1.16041728	-4.55565842
5	-3.40487089	-0.46709994	-4.16939612
17	-2.61903128	-1.35604618	-2.86439418

**10b**

6	0.23752996	1.26414736	1.60638338
---	------------	------------	------------

13	0.19486457	-0.00865834	0.10127599
6	-1.71790828	2.27604216	-0.63000290
6	-1.51005120	2.96658868	0.73746227
6	-1.10099299	1.99154586	1.85925892
6	1.64723485	-0.56568468	-1.10648827
6	2.99829184	0.14762250	-0.90931317
1	-1.03720133	2.56122348	2.79941351
1	0.51867906	0.68518023	2.50540165
1	1.05107705	1.99303072	1.43941899
1	-0.67484504	3.68115859	0.60839296
1	-1.90635294	1.25307862	2.00285685
1	1.76544420	-1.65665600	-0.98271416
1	1.29056561	-0.44260801	-2.14332530
1	3.76406565	-0.22749102	-1.60515532
1	2.91609061	1.23191637	-1.07430128
1	3.39066286	0.00814538	0.10867779
1	-1.96873567	3.04950911	-1.38125169
1	-0.75859877	1.89100950	-1.04171330
6	-2.75302977	3.80075264	1.11738425
1	-3.08001654	4.36156508	0.22570889
1	-3.58279263	3.12415752	1.37562996
6	-2.52345650	4.79748903	2.25879283
1	-1.69226538	5.48060108	2.02766200
1	-2.29112115	4.29617615	3.20803250
1	-3.42135981	5.40898648	2.42440253
9	-1.30857980	-0.78229491	-0.10317732
5	-2.83263934	1.16584418	-0.80688691
9	-3.00479629	0.60004589	-2.00896639
9	-3.74451654	0.87709867	0.12736182
9	1.98390500	1.62226644	4.80386353
9	1.45517097	3.70469609	3.98646010
5	2.23228828	2.62922284	3.97612285
9	3.27551286	2.57292127	3.15693317

**10b'**

6	0.37398788	3.10035079	1.42424364
13	1.13905845	1.26688905	1.40909734
6	-2.44518726	2.33253307	-1.08249628
6	-1.91877164	2.68349750	0.31925473
6	-0.55767425	3.41473788	0.23612471
6	0.61496061	-0.32612769	2.45717835
6	-0.82240601	-0.36823653	3.00462031
1	-0.04773913	3.15231808	-0.70573062
1	-0.15617489	3.27348604	2.37678369
1	-1.75857467	1.73388627	0.86162207
1	1.23287632	3.79225287	1.41952507
1	-2.51553344	3.24054055	-1.70889761
1	-0.75245324	4.50037001	0.16946462
1	0.82299895	-1.21737807	1.84258240
1	1.33852938	-0.38705142	3.29020928



1	-0.99397624	-1.24918167	3.64241683
1	-1.05928051	0.52054441	3.60860712
1	-1.56353814	-0.41162111	2.19255490
1	-3.49044923	1.96715231	-1.03338762
6	-2.93379982	3.50367578	1.13940920
1	-2.42466321	3.88320379	2.04030235
1	-3.22206362	4.39436093	0.55512472
6	-4.18594313	2.73308830	1.56728707
1	-3.92058731	1.85051887	2.16842968
1	-4.77404440	2.38560420	0.70528997
1	-4.84807133	3.36409617	2.17629538
17	2.94780903	1.05880121	0.25220529
17	-2.04511303	0.93220729	-3.58778593
5	-1.67888033	1.23756158	-1.88770323
17	-0.44163943	0.18031402	-1.15406010
17	0.94783075	2.44405611	5.66219172
17	3.61821722	3.55349912	6.59690574
5	2.63956908	2.79515551	5.35985614
17	3.35632200	2.38216146	3.80850571

### 11a

6	-1.32321432	-5.81981621	-5.91953641
13	-0.56615728	-2.17875818	-8.89718240
6	-2.14581241	-2.47275801	-5.65357070
6	-1.12118314	-3.40661247	-4.94647229
6	-1.67471247	-4.84332208	-4.77983580
6	0.92211070	-1.45267168	-9.93237013
6	2.32626222	-1.89981297	-9.47939573
1	-1.27355787	-5.26217630	-3.84450914
1	-1.53342167	-6.85231154	-5.57852849
1	-0.23732604	-5.81489976	-6.10885549
1	-0.21877387	-3.46941223	-5.57827612
1	-2.76711932	-4.79583768	-4.64312039
1	0.75723560	-1.74031993	-10.98491825
1	0.84238986	-0.35307889	-9.92050754
1	3.11314557	-1.47585573	-10.12137702
1	2.54338680	-1.58188614	-8.44906235
1	2.43191678	-2.99340429	-9.50840694
1	-2.57518839	-2.98896483	-6.52920196
1	-2.98539694	-2.25594686	-4.97535945
6	-0.70536545	-2.78873082	-3.59458596
1	-0.52636520	-1.70684959	-3.72918777
1	-1.55330536	-2.86371179	-2.89210549
6	0.54728903	-3.41192889	-2.97220084
1	1.41432064	-3.30340437	-3.64038533
1	0.41662484	-4.48400049	-2.76813818
1	0.79551844	-2.92551276	-2.01885667
9	-1.66855122	-6.47179418	-8.33607038
5	-2.05601830	-5.71431225	-7.30260450
9	-0.47376230	-3.74318269	-8.24163164

9 -3.18205216 -5.00381988 -7.48718721  
9 -2.15796618 -1.63850723 -9.07673539  
9 -1.88910536 0.08464378 -5.86578906  
5 -1.53023416 -1.14992169 -6.17067413  
9 -0.43338995 -1.18959113 -7.04403267

**11a'**

6 -0.26156827 4.98036355 0.73073767  
13 0.31006132 -1.22330289 -1.03645137  
6 -2.15364856 2.08288040 -1.17014002  
6 -1.47971561 2.77931784 0.04763415  
6 -1.04224488 4.20543654 -0.34759474  
6 1.66846038 -2.09314675 -2.15784824  
6 1.21339448 -2.53897753 -3.55833151  
1 -0.41798671 4.15425189 -1.25542456  
1 -0.85830601 5.11782044 1.64351058  
1 -0.58172466 2.19636112 0.31513291  
1 -0.09110136 6.01048943 0.35599584  
1 -3.09256100 2.60335723 -1.41713087  
1 -1.93858149 4.78440447 -0.62788606  
1 2.53960441 -1.42056094 -2.22064744  
1 2.01768266 -2.96241142 -1.57286464  
1 2.02297218 -3.05051722 -4.10067997  
1 0.36202595 -3.23165741 -3.50463926  
1 0.89575531 -1.68653658 -4.17592661  
1 -2.42504781 1.05179570 -0.87741160  
6 -2.42567918 2.77974153 1.26384187  
1 -1.92233829 3.29510726 2.09633113  
1 -3.31514758 3.38733619 1.01988555  
6 -2.86012202 1.39412319 1.75124191  
1 -1.99171811 0.75344242 1.96092786  
1 -3.49001765 0.87327257 1.01685368  
1 -3.44617602 1.48064099 2.67667479  
17 0.83897148 -0.47906923 0.89706264  
17 2.24597957 3.72103184 -0.07869259  
5 1.17281600 4.47760858 1.10713041  
17 1.82543116 4.73787089 2.73049482  
17 -1.68736129 2.65794344 -4.00515502  
17 0.29663512 1.05589193 -2.43378253  
5 -1.28167800 1.96220413 -2.44542318  
17 -1.76253596 -1.73171377 -1.25379123

**11b**

6 -0.35091687 4.32571688 -0.02900762  
13 0.65125399 0.41847506 -0.52249916  
6 -2.73645434 2.28311487 0.22927555  
6 -2.41315297 3.40014686 1.25777093  
6 -0.92683343 3.80311968 1.29644850  
6 1.43231134 -1.34631886 -0.22784075  
6 2.45819729 -1.43239288 0.91982523

1	-0.80293082	4.58685575	2.05812801
1	-0.85386747	5.26599407	-0.32260834
1	-0.53787149	3.63181041	-0.86428090
1	-2.98593633	4.28855172	0.93391420
1	-0.32084179	2.95470336	1.64999466
1	0.60810848	-2.06053003	-0.06533793
1	1.89988439	-1.65908613	-1.17719037
1	2.87982282	-2.44478848	1.01004351
1	3.29639458	-0.73823845	0.76718430
1	2.00659317	-1.18082302	1.89044975
1	-3.82834818	2.17738054	0.13178557
1	-2.38674848	2.57933929	-0.77700561
6	-2.94309416	2.99523580	2.64900527
1	-3.97167592	2.61521760	2.53248791
1	-2.34368269	2.14768110	3.02909278
6	-2.95002890	4.11756924	3.69161619
1	-3.51737070	4.98774634	3.32850075
1	-1.93646757	4.45724806	3.94242940
1	-3.42237910	3.77872200	4.62389935
9	-0.58257521	0.67361549	-1.66811443
5	-2.15618361	0.85901039	0.45148905
9	-2.82205175	-0.27023640	0.27030126
9	-0.85288880	0.63782170	0.92993003
9	1.51005579	1.82632780	-0.14902189
9	1.90259127	4.65613167	1.12313207
5	1.19622529	4.59028531	-0.01302659
9	1.86729996	4.84967912	-1.14270500

**11b'**

6	-0.69546612	2.79960966	1.69665494
13	-0.05160112	0.00575361	4.27724571
6	-1.96410904	3.79318663	-1.86453510
6	-1.76557441	2.85620327	-0.65513171
6	-1.20001334	3.66394720	0.53167833
6	0.73881546	-0.42339170	6.02299638
6	2.27605603	-0.42542575	6.09381860
1	-0.36965392	4.29237228	0.17286961
1	-1.50246706	2.16989863	2.11696156
1	-1.01620925	2.09297872	-0.92922393
1	0.03663230	2.04940236	1.33744229
1	-2.64789970	4.61759160	-1.59976153
1	-1.97342280	4.36295074	0.89197404
1	0.30815866	0.26003863	6.77337493
1	0.34491880	-1.42170290	6.28409561
1	2.63369940	-0.72211140	7.09139660
1	2.71373080	-1.12119423	5.36447290
1	2.69851464	0.56775535	5.88130621
1	-2.49301822	3.24862693	-2.67274896
6	-3.07113227	2.12602970	-0.28402104
1	-2.92677820	1.58765289	0.66536693

1	-3.85739486	2.87745524	-0.09517007
6	-3.55659834	1.11796394	-1.33037925
1	-2.78770881	0.35765781	-1.53171188
1	-3.81369022	1.59804947	-2.28562394
1	-4.45701068	0.59555413	-0.97917360
17	-2.18103040	0.18000514	4.08499779
17	-0.80659446	5.88762096	-3.49698337
5	-0.70136651	4.37898254	-2.57511153
17	0.86146937	3.54521108	-2.58241630
17	0.56106596	2.57915579	4.32676560
17	0.22153434	5.25434068	3.03004436
5	-0.03602990	3.52702066	2.89124937
17	0.95285731	-0.55541197	2.46992089

## 12

6	-0.40240343	4.08985067	0.04779360
6	-3.03132240	2.38325499	0.23253461
6	-2.58307864	3.42666038	1.27982322
6	-1.05160697	3.58796136	1.35393601
1	-0.81846861	4.30428771	2.15470142
1	0.61577535	4.46180010	0.27662088
1	-0.93390068	4.97132733	-0.34672738
1	-2.99336550	4.40127988	0.95368156
1	-0.59593756	2.63123859	1.65454482
1	-4.13726772	2.35772411	0.20236992
1	-2.76832590	2.70455587	-0.79150036
6	-3.20166723	3.12407752	2.66146514
1	-4.26997254	2.89278515	2.51456636
1	-2.74503253	2.21150218	3.07626605
6	-3.08769692	4.26599566	3.67717033
1	-3.52652089	5.19443629	3.28120196
1	-2.04489868	4.47734844	3.95100273
1	-3.62152292	4.01492926	4.60424748
5	-2.57592968	0.88629969	0.38265218
9	-2.87145216	-0.00114280	-0.57632895
9	-1.92766806	0.39781941	1.44781415
9	-0.03802220	1.73560413	-0.85964454
5	-0.18721932	3.04952378	-1.09991313
9	-0.08665160	3.41774764	-2.38339347

## 12'

6	-0.52648403	3.26850852	1.71504624
6	-1.40966110	3.47440339	-1.29091749
6	-2.06334748	2.52152172	-0.26356026
6	-1.95628200	3.04914216	1.18208460
1	-2.53268425	3.98504460	1.26644008
1	-0.53761595	3.11830160	2.81598312
1	-1.53917106	1.55067477	-0.30728275
1	0.16046966	2.48421069	1.35952856
1	-1.65103477	4.52386125	-1.06001853

1	-2.46473288	2.31789494	1.82943787
1	-1.88414924	3.30161910	-2.28112827
6	-3.54692296	2.26149706	-0.59976612
1	-4.00949371	1.74087020	0.25476168
1	-4.06947465	3.22948391	-0.68689149
6	-3.77891162	1.42867881	-1.86357342
1	-3.29191278	0.44562901	-1.78354675
1	-3.38886751	1.92072549	-2.76682505
1	-4.85173936	1.25849346	-2.02901634
17	1.00244948	4.71939892	-2.29808628
5	0.10096490	3.33546194	-1.66071775
17	0.95781008	1.78424244	-1.59904799
17	1.91639181	4.81477846	1.78070967
17	-0.75757737	6.17612567	1.45665130
5	0.16054067	4.66889484	1.60875025

### 13a

6	-0.23073695	3.93229100	0.53540652
6	-2.33665273	2.48055966	0.83118222
6	-2.48151887	3.83819715	1.56845335
6	-1.02424011	4.31232172	1.80953667
1	-0.96535061	5.38206916	2.05187779
1	0.85300126	3.82209286	0.68201103
1	-0.35353542	4.71380727	-0.23954998
1	-2.94864300	4.55155214	0.86314952
1	-0.61289598	3.76194740	2.67360055
1	-2.17333925	1.67384618	1.57543459
1	-3.21875323	2.17853501	0.24899993
6	-3.35276304	3.77665929	2.82791085
1	-4.33091404	3.34466078	2.55959992
1	-2.89111335	3.06905166	3.53905486
6	-3.56992259	5.12969098	3.51370047
1	-4.02570163	5.85456623	2.82223627
1	-2.62481240	5.56043975	3.87329698
1	-4.23887236	5.03119588	4.38004987
5	-1.66515088	-0.32803283	-1.84409450
9	-0.69207288	-0.50014648	-2.72895735
9	-2.76333984	0.34019212	-2.18391894
9	-1.58791056	-0.90365743	-0.64837912
5	-0.99468710	2.65348174	0.03727180
9	-0.55045063	1.82390779	-0.93686792

### 13a'

6	-0.79982222	3.13798722	1.79148234
6	-1.17382172	2.21536547	-0.57083304
6	-2.46477886	2.10224591	0.28426251
6	-2.29278845	3.17396766	1.38814742
1	-2.53190916	4.16334048	0.96201878
1	-0.42094119	4.05652155	2.26050793
1	-2.45111040	1.11166473	0.77736728

1	-0.62216161	2.33004981	2.52884926
1	-1.29291874	3.03650890	-1.30877735
1	-2.98020003	3.01202662	2.23112679
1	-0.91920879	1.32223064	-1.15745456
6	-3.78040593	2.22956896	-0.49067139
1	-4.61629055	2.25671593	0.22888618
1	-3.78871181	3.20469600	-1.00834552
6	-4.02258800	1.10671960	-1.50398871
1	-4.02937981	0.12322059	-1.01017096
1	-3.24158652	1.08646888	-2.27737305
1	-4.98929247	1.23100224	-2.01168730
17	0.85672719	5.36784829	-3.20478433
5	1.22740953	6.25683245	-1.73968858
17	2.86336367	6.79899310	-1.42825650
17	1.65581646	2.73918267	0.16856644
17	-0.05140562	6.61919733	-0.59064258
5	-0.09543110	2.69710789	0.46047380

**13b**

6	-0.26253395	3.93716779	0.52823296
6	-2.35382926	2.46236968	0.81480511
6	-2.50174470	3.82780296	1.53011031
6	-1.06084870	4.33600776	1.79730336
1	0.82425121	3.86129126	0.67540394
1	-0.40999190	4.70850084	-0.25579603
1	-3.00632470	4.54002632	0.85405511
1	-0.65529922	3.74972906	2.64371074
1	-2.20773279	1.65421130	1.55773256
1	-3.22209697	2.16368605	0.21105978
5	-1.62890263	-0.34707384	-1.84765828
9	-0.61668455	-0.54515891	-2.68181419
9	-2.69607587	0.33789524	-2.24710098
9	-1.62193472	-0.91401226	-0.64530156
5	-0.99771923	2.63873852	0.04239612
9	-0.52684449	1.79707677	-0.90855616
6	-0.96224488	5.82206334	2.15888124
1	0.10243656	6.09867714	2.23340091
1	-1.37326372	6.41472004	1.32245948
6	-1.67485960	6.20530026	3.46026804
1	-1.28529973	5.62482573	4.31028562
1	-2.75733651	6.02454715	3.40021966
1	-1.53010766	7.27002293	3.69101967
1	-3.10500857	3.77255893	2.44643765

**13b'**

6	-2.02785418	3.77255885	1.93409099
6	-1.74099979	3.74393848	-0.61267017
6	-2.50102174	2.48264379	-0.12137912
6	-3.10238767	2.90078443	1.24225665
1	-4.00533514	3.50893231	1.06115618

1	-2.40745604	4.45488180	2.70706214
1	-1.74702201	1.69702581	0.07495380
1	-1.28325163	3.12811096	2.44212416
1	-2.45751314	4.43699596	-1.10239363
1	-3.41512964	2.03168589	1.83930020
1	-0.95283172	3.55814422	-1.35482410
6	-3.53538551	1.91529301	-1.09860379
1	-4.09349581	1.10650965	-0.59695950
1	-4.27515213	2.70346900	-1.32415483
6	-2.93774606	1.38161231	-2.40421926
1	-2.20827157	0.58186162	-2.20655425
1	-2.42140680	2.17399234	-2.96448986
1	-3.71813739	0.96718200	-3.05768085
17	-0.12670756	5.77409976	0.83594169
5	-1.29101704	4.43833395	0.71909076
17	2.13153709	2.15301918	0.60733608
17	4.03439401	4.51584922	0.44836490
17	2.49142958	3.63743649	-2.01738236
5	2.88242238	3.44324753	-0.31888070

**14**

35	-4.18674732	0.37705476	-4.06565210
5	-4.47005361	2.02873680	-3.13503194
35	-3.81403459	3.67059811	-3.87518442
35	-5.42194082	2.03994229	-1.47109165

**15**

6	0.69577302	2.19581431	1.19556601
13	0.69331173	0.91099188	-0.31397758
6	-0.98685427	1.56797454	-1.14127471
6	-1.19614585	2.88506601	-0.34949337
6	-0.75548583	2.74595732	1.13307537
6	1.95247510	-0.53832383	-0.81329940
6	1.63458702	-1.31611991	-2.10458734
1	0.95275215	1.81886194	2.19621608
1	1.40649513	3.01893217	0.98590202
1	-0.58436966	3.68461580	-0.80688103
1	-1.42052068	1.98797183	1.59375605
1	2.96133884	-0.09158608	-0.87403647
1	2.01121957	-1.23127716	0.04566129
1	2.37737248	-2.10299232	-2.30944898
1	0.65019038	-1.80389365	-2.05161116
1	1.61288424	-0.65296957	-2.98183493
1	-1.81347965	0.86289973	-0.93890655
1	-0.97971684	1.72910127	-2.22885008
35	-4.18717473	0.37655561	-4.06593449
5	-4.46872240	2.02863907	-3.13467847
35	-3.81453755	3.67096209	-3.87511265
35	-5.42234166	2.04017519	-1.47123450
6	-0.92381899	4.05128098	1.93162814

1	-0.49522698	3.89853410	2.93567284
1	-0.30661387	4.83325986	1.45474108
6	-2.36720051	4.54886923	2.07654799
1	-3.00541258	3.77829366	2.53564907
1	-2.81100460	4.81579699	1.10768800
1	-2.41249658	5.44122335	2.71723280
1	-2.24121241	3.22833127	-0.40272597

## 16

6	0.44892239	2.27135091	0.81606087
13	0.22378677	0.76722991	-0.41356162
6	-1.69306425	1.64190590	-1.14057231
6	-1.72453955	2.94029923	-0.32115939
6	-0.96754108	2.86039560	1.02348196
6	1.00341320	-0.88385389	-1.12237829
6	1.58289981	-0.74920617	-2.54859110
1	0.92982621	2.00201923	1.76777799
1	1.10514280	3.01980145	0.33311199
1	-1.31108573	3.74867032	-0.94438117
1	-1.53221676	2.15744943	1.66663300
1	1.78127004	-1.20929105	-0.41161206
1	0.21421394	-1.65233181	-1.10922049
1	2.02037570	-1.70279176	-2.87720288
1	0.80144525	-0.48226828	-3.27315803
1	2.37647397	0.00989704	-2.60696351
1	-1.79229991	0.71505142	-0.49975420
1	-0.82466852	1.57485587	-1.86296116
35	-2.44295951	-0.48667316	-3.07773826
5	-2.89775183	1.33929519	-2.23069912
35	-2.88317068	2.81391223	-3.62997714
35	-4.66336543	1.24318850	-1.22503511
6	-0.92080098	4.21682591	1.74950617
1	-0.31982215	4.09578594	2.66545837
1	-0.37107876	4.93353221	1.11511195
6	-2.29163783	4.79388518	2.11857841
1	-2.87085672	4.08343985	2.72696407
1	-2.88924175	5.03915398	1.23062932
1	-2.17722707	5.71661480	2.70377382
1	-2.78147180	3.18246829	-0.14823437

## 17

6	0.41252664	2.83377084	-0.43777284
13	0.52562323	1.21582719	-1.56792008
6	-2.38809346	1.91065825	-1.31117970
6	-2.13142857	3.05390063	-0.31749584
6	-0.82317431	2.91561038	0.48594428
6	0.52736130	-0.66393154	-0.95467935
6	1.78477898	-1.46802585	-1.34722770
1	1.32504708	2.84435067	0.18656568
1	0.47083982	3.73470412	-1.07198541



1	-2.12230870	4.01297414	-0.86068896
1	-0.89299597	1.97479446	1.06723784
1	0.38813825	-0.67964595	0.13943297
1	-0.36599826	-1.15276576	-1.38041223
1	1.71009591	-2.51877456	-1.02823990
1	1.94053983	-1.46451497	-2.43534201
1	2.69502494	-1.05438501	-0.88803681
1	-2.19042350	0.92572764	-0.84801646
1	-1.69769725	1.98634162	-2.18613025
35	0.91238385	1.53221049	-3.82936030
5	-3.78837569	1.82125284	-2.01376202
35	-5.00565125	3.31467963	-2.07912875
35	-4.31830321	0.18750823	-2.89749775
6	-0.67199053	4.06510997	1.50626249
1	0.30980367	3.95590713	1.99438207
1	-0.63256804	5.02044325	0.95509299
6	-1.75663497	4.13287891	2.58743777
1	-1.83922026	3.17677360	3.12675451
1	-2.74561604	4.37106314	2.17264168
1	-1.51882007	4.91003613	3.32721361
1	-2.97989363	3.10613260	0.37979820

**18**

6	-1.21975820	2.04716290	-0.11020322
13	0.14014852	-0.59136516	-2.80789761
6	-3.07467304	3.40660774	-1.24808146
6	-2.75136667	3.94677817	0.16867520
6	-2.11565598	2.76309895	0.93992762
6	1.78713819	0.34914608	-2.27414887
6	3.00265793	-0.59306461	-2.16199699
1	-0.97260341	1.00184846	0.12190477
1	-0.24728889	2.58031832	-0.18177289
1	-2.01129266	4.76129627	0.08807318
1	-2.92950633	2.06453647	1.20924353
1	1.98372247	1.13962987	-3.01675971
1	1.60828937	0.85502069	-1.31146787
1	3.91241813	-0.04690212	-1.86856069
1	2.83792444	-1.38072812	-1.41209939
1	3.21600582	-1.09252181	-3.11821845
1	-3.17786205	4.17063046	-2.03045560
1	-4.03964180	2.86053857	-1.23435463
35	-0.04866030	-1.38011358	-4.96873034
5	-1.96662307	2.32558245	-1.44439739
35	-1.61427714	1.47246646	-3.18673916
35	-0.98987861	-1.84741893	-1.22699387
6	-1.37240948	3.15077299	2.22285178
1	-0.88231718	2.25171502	2.63045005
1	-0.56008471	3.85136687	1.96126153
6	-2.26388908	3.77397815	3.30177527
1	-3.08331893	3.09390030	3.57877205

1 -2.71237927 4.71918573 2.96462409  
1 -1.68825025 3.98856908 4.21270850  
1 -3.63359808 4.35857652 0.67649834

**19**

13 1.72957834 0.62258349 -3.41501987  
6 1.66035727 -0.34600227 -1.70936384  
6 1.16597051 -1.80087892 -1.76241610  
1 2.67539005 -0.28732176 -1.28032773  
1 1.03234061 0.26219755 -1.03587745  
1 1.15648273 -2.25384130 -0.75967521  
1 0.14643438 -1.87010721 -2.16585485  
1 1.80683938 -2.42488602 -2.40031624  
35 2.42508920 2.78996233 -3.49764967  
35 1.12944250 -0.34100595 -5.38967498

**20**

6 -1.49764691 1.59649107 -0.13069800  
6 -2.96175452 3.42974181 -1.14983928  
6 -2.62083606 3.74999493 0.33030102  
6 -2.28406601 2.37282897 0.95429882  
1 -1.50892436 0.50348010 -0.02151404  
1 -0.42879706 1.88862617 -0.10623715  
1 -1.69352782 4.35375079 0.33509355  
1 -3.22674781 1.84166997 1.17324117  
1 -2.88232587 4.28208679 -1.83854957  
1 -4.01761879 3.09055433 -1.21270949  
5 -2.08299219 2.17301610 -1.46653398  
35 -1.76399110 1.44225015 -3.23269110  
6 -3.70902177 4.54262389 1.06311102  
1 -3.93268001 5.45398304 0.48435412  
1 -4.63774076 3.94519964 1.06376967  
6 -3.34655464 4.93405257 2.49973308  
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1 -4.14098952 5.54051013 2.95689737  
1 -1.73519564 2.45994811 1.90214689

**21**

6 0.69576071 2.10812950 1.36083800  
13 0.59757467 0.99270980 -0.27657642  
6 -1.06992531 1.80438662 -0.97829390  
6 -1.18597733 3.07985182 -0.09907705  
6 -0.71137232 2.76122880 1.34492983  
6 1.76269843 -0.44381893 -0.99369973  
6 2.99289204 -0.82395655 -0.14781743  
1 0.90825717 1.59881146 2.31162614  
1 1.47568709 2.88329654 1.25028349  
1 -0.48084410 3.83143304 -0.50772449  
1 -1.44240635 2.06095769 1.79006281

1	1.12524669	-1.33073743	-1.16124514
1	2.07612188	-0.13543215	-2.00751949
1	3.58757719	-1.62459103	-0.61498710
1	3.66374677	0.03500767	0.00063843
1	2.70297194	-1.17594241	0.85315339
1	-1.92836953	1.13668047	-0.76924192
1	-1.11417060	2.03650923	-2.05250460
35	-3.44171008	-0.53607966	-4.02827705
5	-4.31696197	1.13495184	-3.68506775
35	-3.86791808	2.68156096	-4.72529490
35	-5.64713449	1.25616986	-2.31126891
6	-2.59507135	3.69782891	-0.14384548
1	-2.89169522	3.80400080	-1.20004777
1	-3.30520673	2.97750247	0.29940654
6	-2.73730899	5.05769260	0.55034405
1	-2.02286785	5.78714213	0.13878843
1	-2.55877669	4.99007983	1.63230219
1	-3.74746340	5.46776329	0.40821574
1	-0.74020901	3.67191782	1.96346961

22

6	0.51627654	2.59970322	-0.32880560
13	0.54720630	0.96890517	-1.44784141
6	-2.30690868	2.03080021	-1.37584443
6	-2.04185121	3.07960130	-0.26659923
6	-0.75860186	2.75762246	0.52515722
6	0.24613493	-0.87998049	-0.81781554
6	-0.38387523	-1.85587836	-1.82960454
1	1.39345186	2.55227628	0.34069480
1	0.66846604	3.48807869	-0.96300821
1	-1.90248412	4.05647254	-0.76224855
1	-0.93723564	1.84029840	1.11576126
1	1.23710091	-1.25856089	-0.50572190
1	-0.35111679	-0.84048403	0.10897030
1	-0.45336424	-2.87612651	-1.42230799
1	-1.40198912	-1.54888523	-2.11106306
1	0.20304659	-1.90755539	-2.75696634
1	-2.34101447	1.01603218	-0.94523661
1	-1.47174671	2.06785437	-2.11456512
35	1.17411887	1.21077436	-3.66189085
5	-3.56795386	2.25980416	-2.28038789
35	-3.87630106	3.96221160	-3.14109045
35	-4.82592464	0.83794734	-2.63067798
6	-3.26993824	3.18609006	0.66124552
1	-4.16803132	3.34242374	0.04022543
1	-3.41710388	2.21692401	1.16896367
6	-3.20020522	4.30918425	1.70083427
1	-3.01464453	5.28093046	1.21928490
1	-2.40652225	4.14251242	2.44117139
1	-4.14942114	4.38586117	2.24895667

1 -0.60621380 3.56212637 1.26205298

**23**

6 -1.49353351 1.58870352 -0.12334660  
13 -0.63009948 -0.99749813 -3.06248779  
6 -2.95655165 3.42951282 -1.14963057  
6 -2.61576509 3.75051915 0.33297370  
6 -2.27996621 2.37334499 0.95845107  
6 1.15362434 -0.56659638 -2.34521758  
6 2.08158124 -1.79623298 -2.27550534  
1 -1.50702381 0.49560204 -0.01401916  
1 -0.42413995 1.88204496 -0.10384858  
1 -1.68939658 4.35497444 0.33637023  
1 -3.22101040 1.84103832 1.17836278  
1 1.59798328 0.21218094 -2.98612816  
1 1.03414914 -0.12352962 -1.34316865  
1 3.07414629 -1.53188975 -1.87920724  
1 1.66794347 -2.57991370 -1.62406995  
1 2.23478820 -2.24384556 -3.26817850  
1 -2.87891709 4.27955454 -1.84115365  
1 -4.01150211 3.08633148 -1.21266684  
35 -0.84424001 -1.47375500 -5.31071071  
5 -2.08318095 2.17283146 -1.44041702  
35 -1.79735936 1.46960382 -3.26001331  
35 -2.14872762 -2.08923246 -1.70032444  
6 -3.70849453 4.54261244 1.05936736  
1 -3.93040180 5.45288110 0.47860728  
1 -4.63609879 3.94384575 1.05692174  
6 -3.35069503 4.93440418 2.49665726  
1 -2.42367930 5.52658970 2.52683090  
1 -3.20494742 4.05136892 3.13444936  
1 -4.14743488 5.54062955 2.94932208  
1 -1.72769634 2.46088332 1.90342303

**24**

6 -1.31340192 6.27173436 -3.80425421  
13 -0.66971405 5.82572427 -5.61907491  
6 -3.35435897 7.12327044 -5.94039911  
6 -3.60852675 7.21048012 -4.42758848  
6 -2.83998137 6.16757343 -3.59213626  
6 -0.92737520 4.10451841 -6.55438252  
6 -0.94057523 4.14157736 -8.09398930  
1 -0.80887158 5.57354155 -3.11137241  
1 -0.96304867 7.28153933 -3.53054377  
1 -3.34744596 8.22081188 -4.07254825  
1 -3.17534792 5.16605485 -3.92690776  
1 -0.10517004 3.45201619 -6.20570525  
1 -1.84728216 3.63319572 -6.16779864  
1 -1.01914806 3.13166865 -8.52459896  
1 -1.78758196 4.72783542 -8.47943233

1	-0.02571592	4.60222073	-8.49157213
1	-3.38916218	6.07520265	-6.29284348
1	-2.33362545	7.50113447	-6.19190527
35	0.72214778	7.36194937	-6.65581992
5	-4.25563448	7.96718007	-6.90882840
35	-5.33075019	9.44395136	-6.29325089
35	-4.27050942	7.56846062	-8.79906579
6	-3.19406298	6.28407371	-2.09340047
1	-2.56527305	5.56681144	-1.54196130
1	-2.89532037	7.28582059	-1.73947628
6	-4.66343632	6.02522124	-1.74152876
1	-4.99475555	5.04530803	-2.11804642
1	-5.33360278	6.78946488	-2.15835044
1	-4.80683975	6.02645098	-0.65197466
1	-4.68691083	7.09341262	-4.24821376
35	0.80070649	8.55605112	-0.01223858
5	1.63257849	7.06961619	-0.89201042
35	1.50080186	5.31323719	-0.12774633
35	2.58497777	7.33215920	-2.53159970

25

6	0.29915052	4.22435776	1.59414002
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6	-1.24032175	2.08208086	-0.16462983
6	-1.62732033	3.55059570	0.06394867
6	-1.23348124	4.10018184	1.44925262
6	2.35734614	-1.06360684	-3.13120807
6	2.00373564	-2.52542972	-3.45043668
1	0.78664381	3.27617455	1.28626107
1	0.68459055	4.97739303	0.88734055
1	-1.16647150	4.17706888	-0.71748671
1	-1.59642235	3.39214402	2.21531796
1	3.29416107	-0.77654793	-3.64116554
1	2.55198186	-0.92635738	-2.05538008
1	2.81633675	-3.20894672	-3.16068641
1	1.10002248	-2.85519032	-2.91647916
1	1.81521643	-2.67109109	-4.52327143
1	-1.68950008	1.44348900	0.62429896
1	-0.15415917	1.92339461	-0.04498154
35	1.32529079	2.47885102	-2.95367947
5	-1.64179932	1.43160061	-1.51633160
35	-2.84019946	2.15789016	-2.80825759
35	-0.97600253	-0.42159025	-1.88190197
6	-1.89372909	5.46760129	1.72319668
1	-1.45420222	5.88807097	2.64291757
1	-1.62080357	6.16401667	0.91154395
6	-3.41573830	5.42883838	1.88840102
1	-3.70630307	4.74285902	2.69789618
1	-3.92817163	5.10501037	0.97197092
1	-3.80346652	6.42521558	2.14151470

1	-2.71435702	3.64989806	-0.06829460
35	0.11186127	3.70717605	4.61144349
5	0.88596177	4.49166492	3.01802866
35	-0.08769037	0.10167538	-5.66986146
35	2.48765662	5.54850288	3.24861390

## 26

6	0.33538250	4.30907516	0.54071612
6	-1.41586092	2.43556137	-1.27704990
6	-1.94910169	3.39643854	-0.19410824
6	-0.99673700	3.66271991	0.98905478
1	0.16472305	5.06848079	-0.23889118
1	0.73589269	4.89887962	1.39552333
1	-2.22954258	4.35847357	-0.65420982
1	-0.76796932	2.69260918	1.46424140
1	-2.28045765	1.89806382	-1.72390453
1	-0.81868108	1.62369932	-0.83200242
5	-0.70835776	2.97140750	-2.56274995
35	-1.00124938	4.75517640	-3.25711246
35	0.39047374	1.78563834	-3.62516670
6	-1.67767155	4.54943442	2.05497054
1	-0.93817998	4.75183846	2.84709102
1	-1.91891460	5.52813456	1.60519053
6	-2.93258722	3.95345658	2.70088922
1	-2.72755857	2.95518964	3.11645752
1	-3.76414075	3.85755972	1.98981573
1	-3.28204421	4.59062024	3.52519968
1	-2.87557642	2.96899060	0.21454438
35	1.88503037	1.68137351	0.93130459
5	1.58366079	3.44294444	0.18218238
35	2.99284412	4.17758534	-0.92098185

## 27

6	4.94473309	3.35126025	-2.07238329
13	6.10170620	2.74752656	-3.55895692
6	3.95598299	0.63424416	-3.08528940
6	3.43640729	1.25321968	-1.76391585
6	4.46722881	2.21668032	-1.14320062
6	7.74191176	1.66124629	-3.37560613
6	8.06587202	0.69778404	-4.53313816
1	5.53415191	4.07595320	-1.48251748
1	4.08571585	3.91285794	-2.47436249
1	2.52797018	1.83261257	-2.00529275
1	5.33138717	1.62248797	-0.79326221
1	8.56984146	2.38377674	-3.25230031
1	7.69187179	1.11560713	-2.41792359
1	9.02730114	0.18457146	-4.37904036
1	7.29587708	-0.08012345	-4.64264149
1	8.12318323	1.22897890	-5.49331154
1	4.92717665	0.13732318	-2.92184988

1	4.10573486	1.44967165	-3.83224748
35	5.61879229	3.53514858	-5.68016178
5	2.98890346	-0.33946287	-3.84457947
35	1.16014280	0.16448760	-4.21477189
35	3.59813270	-2.04713840	-4.50741852
6	3.04064084	0.13362506	-0.77891696
1	2.36001063	-0.56451720	-1.29471046
1	3.94119621	-0.45201837	-0.52449799
6	2.35617094	0.61342405	0.50500818
1	1.47155384	1.22570273	0.27505222
1	3.02638320	1.21387414	1.13422362
1	2.02150988	-0.24343700	1.10594617
1	4.01851219	2.65119734	-0.23601317
35	3.40989549	7.52714133	-1.02448970
5	2.93061667	6.12957918	0.19355471
35	1.31675609	5.12991830	-0.07682290
35	4.06215146	5.73045953	1.69088590

28

6	4.57601810	3.63249863	-1.70149699
13	5.70137857	2.95174105	-3.42787398
6	3.88134418	0.87659964	-3.04830566
6	3.34827801	1.33410899	-1.66859557
6	4.33913639	2.28814455	-0.97817735
6	7.41669043	2.07209623	-3.06821466
6	7.87750624	1.07448193	-4.14651253
1	5.62961650	4.00601281	-1.69656387
1	4.01600728	3.80235998	-2.65292126
1	2.40188252	1.87651592	-1.82832426
1	5.29236387	1.75739520	-0.81424008
1	8.13899678	2.90400894	-2.98481842
1	7.38832795	1.60104746	-2.07370720
1	8.88169590	0.68941462	-3.91767176
1	7.20464980	0.20801479	-4.21991704
1	7.92038749	1.54090964	-5.14009740
1	4.88514738	0.42772980	-2.95293200
1	3.91951114	1.74637249	-3.75843235
35	5.09370010	3.75377933	-5.46564240
5	2.95900288	-0.10765077	-3.87552142
35	1.11931725	0.33293566	-4.20742945
35	3.67432357	-1.73101596	-4.62150703
6	3.05857374	0.10306889	-0.78500707
1	2.41964575	-0.59154189	-1.35608443
1	4.00333085	-0.43717905	-0.59841195
6	2.36509748	0.41955122	0.54353610
1	1.44220778	0.99347751	0.37996356
1	3.00458434	1.00116059	1.22022030
1	2.09790731	-0.51007526	1.06387225
1	3.96498753	2.54195350	0.02271819
35	4.52188569	6.57115771	-2.15925150

5 3.96225179 5.02111564 -0.95070860  
35 1.94313789 4.83987670 -0.82139001  
35 4.81791843 5.16775645 0.88784516

**29**

6 4.91911936 2.56987500 -1.65663736  
13 5.76259158 4.64914231 -4.94466315  
6 3.38589786 -0.04813673 -2.61995749  
6 3.24137716 0.64061623 -1.24615507  
6 4.55455666 1.32898148 -0.82181416  
6 5.52563853 6.35467954 -5.89914567  
6 6.21403881 7.58809542 -5.29062940  
1 5.96879377 2.86719679 -1.44484317  
1 4.94596521 2.34322275 -2.73586870  
1 2.45509812 1.41153027 -1.32682835  
1 5.37618809 0.59773404 -0.89604961  
1 5.91180172 6.16450262 -6.91627863  
1 4.44386063 6.52442077 -6.02776652  
1 6.08242666 8.47685955 -5.92627057  
1 5.80791251 7.83750502 -4.29924470  
1 7.29370779 7.42769487 -5.16409779  
1 4.08080378 -0.90099369 -2.54328548  
1 3.87047089 0.63471987 -3.34903206  
35 7.75717831 4.18655564 -3.87944285  
5 2.08984006 -0.49918517 -3.36694482  
35 0.42031530 0.47193652 -3.21765636  
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6 2.77710661 -0.38963264 -0.19588739  
1 1.94836389 -0.97534788 -0.62669669  
1 3.59538470 -1.10922681 -0.01832924  
6 2.30753533 0.20613482 1.13465913  
1 1.47857453 0.91171291 0.97797106  
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1 1.94905589 -0.58491848 1.80779356  
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35 4.63008762 2.78256756 -5.70481768  
5 4.12322509 3.87745762 -1.42428120  
35 4.18340864 5.33666725 -2.76497204  
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**30a**

6 -0.90891408 5.14427091 -0.06460370  
6 -1.80204770 3.09073675 -1.30176918  
6 -2.72653563 3.46837865 -0.11342708  
6 -1.81329897 4.27510920 0.84332424  
1 -1.43941291 6.07299767 -0.35477197  
1 0.03256564 5.47443747 0.39548110  
1 -3.49893552 4.16076766 -0.49871059  
1 -1.18666118 3.56836641 1.41452395  
1 -2.32557840 2.83400515 -2.23300840



1	-1.21172672	2.18993946	-1.03060557
5	-0.78138018	4.27571230	-1.36358387
35	0.45004533	4.62341160	-2.82184730
35	1.94503739	0.30580038	-1.82769270
35	2.33295101	2.30010188	0.79822250
5	2.93851507	1.66270357	-0.90902780
35	4.54105664	2.37149548	-1.67920321
6	-3.43663462	2.27107306	0.52829611
1	-3.97716859	1.71818962	-0.25762726
1	-2.67050377	1.57803752	0.91799516
6	-4.41508260	2.64179606	1.64781459
1	-5.18757099	3.33612317	1.28394087
1	-3.90276151	3.12501464	2.49170701
1	-4.92636737	1.75050873	2.03781443
1	-2.38323182	4.86520860	1.57422993

**30b**

6	-0.61677755	4.70789093	-0.36706503
6	-2.14532655	3.09711749	-1.63513332
6	-2.65920174	3.36736322	-0.19937293
6	-1.42102273	3.81656388	0.61607002
1	-1.05363840	5.72931636	-0.37012375
1	0.44314292	4.84449723	-0.11129651
1	-3.38997945	4.19446589	-0.22165592
1	-0.81538029	2.91406599	0.82186418
1	-2.91173989	3.14424564	-2.42082400
1	-1.71566819	2.07757104	-1.69869053
5	-0.94316861	4.09501326	-1.77049792
35	-0.01077789	4.50590692	-3.41916128
35	1.96496027	0.82467689	-0.93126378
6	-1.73691821	4.49150197	1.95524484
1	-0.79499437	4.85652621	2.39706556
1	-2.35073134	5.38886670	1.76152497
6	-2.44969226	3.58610299	2.96537541
1	-1.85686065	2.68218519	3.17170924
1	-3.43394287	3.26299764	2.59804824
1	-2.60758895	4.10619225	3.92062459
1	-3.16616898	2.50008097	0.24571633
35	2.59418992	2.45007908	1.89485857
5	2.86326832	2.23582600	0.00657042
35	4.01739405	3.43429728	-0.93858320

**33**

6	-2.67556496	0.14075338	0.79855271
13	-0.71682319	0.35768878	1.09807977
6	-0.49657770	1.86658425	-0.47739930
6	-1.93799190	2.37643150	-0.12758871
6	-3.04351537	1.29507050	-0.17856238
6	3.00800544	-0.95988862	0.01091323
6	2.57954732	0.37564525	-0.64404255

13	0.65933610	0.11236932	-1.07241470
6	0.52516449	-1.32896699	0.57865740
6	1.98642314	-1.36418893	1.09547691
6	0.04423254	1.05898723	2.80358065
6	-0.75741631	2.16515969	3.51645704
6	0.05213030	-0.64341835	-2.82150750
6	-0.61839653	-2.03085646	-2.83007212
1	2.98039096	-1.74659084	-0.77034569
6	5.00047060	-2.24581104	1.07291826
1	-3.97341573	1.78968503	0.15702817
6	-4.58841444	0.01491584	-1.78778170
1	-2.98358259	-0.83797068	0.40232381
1	3.21676022	0.59986594	-1.51350154
1	2.72543936	1.19780324	0.07896428
1	0.40161929	-2.05996163	-0.24644502
1	-2.19864749	3.22304957	-0.78457373
1	2.09103122	-0.67338065	1.94871801
1	2.22133670	-2.36967531	1.47856357
1	-0.61080345	0.08491453	-3.31932315
1	0.95783566	-0.67921128	-3.45324691
1	-0.90268154	-2.34872459	-3.84575544
1	0.05066953	-2.80896647	-2.43110591
1	-1.53272212	-2.05110910	-2.21766553
1	4.94235271	-3.02607268	0.29840056
1	6.05606652	-2.14729022	1.36398228
1	4.45033206	-2.60686989	1.95306212
1	-3.21172017	0.26067169	1.75389855
6	4.44903791	-0.91230885	0.55441858
1	-0.41590106	1.95207721	-1.58115570
1	0.24444768	2.58382336	-0.09098170
1	-0.13967103	-1.78886768	1.33916518
1	-1.91911020	2.78696753	0.89652934
6	-3.28936608	0.80737465	-1.61572310
1	0.13620553	0.18989525	3.48140725
1	1.07965471	1.40264066	2.64109897
1	-0.32712138	2.42268246	4.49739908
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1	-1.80249651	1.86703290	3.69082369
1	-5.46162001	0.62952419	-1.52192109
1	-4.71631925	-0.31748851	-2.82767122
1	-4.60578559	-0.87955610	-1.14880058
1	-2.43795140	0.18715104	-1.94021962
1	-3.31016836	1.67970976	-2.29232875
1	4.49448147	-0.15274070	1.35426857
1	5.10305928	-0.54334033	-0.25222671

**34a**

6	-5.15220273	-0.68836183	0.31666387
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6 -2.76679958 -0.40376921 1.25116167  
6 -3.93173139 0.26446041 0.48069378  
6 2.47546914 -1.94851456 -0.02727067  
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6 -0.31372307 -0.81053249 3.51616487  
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1 0.69417697 -4.42102756 -2.62782207  
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1 -5.48151117 -0.99434202 1.32101735  
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1 -2.17886538 0.13660980 4.20568213  
1 -1.67068170 -1.24167617 5.18809608  
1 -4.91123295 2.59168880 -0.75660642  
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1 3.80844230 -0.72938923 -1.19689351  
17 -2.17749572 -3.77904515 3.10586282

5 -5.09131052 -1.96787195 -0.58682668  
17 -4.73681180 -1.90841421 -2.32896316  
17 -5.54660295 -3.55578279 0.05485223

**34b**

6 -4.14355343 -0.13495180 0.19360937  
13 -2.59025299 -0.83756864 1.20649566  
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1 -0.34925927 0.64780260 0.87519581  
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1 -3.16472062 -1.38116091 5.07991085  
1 -4.36516506 -1.10696946 3.80727637  
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1	-5.28937617	-0.16259046	-2.49733614
1	-2.77029297	-0.24871383	-2.18414740
1	-2.67324893	1.47631396	-2.55656710
1	3.65472057	-2.54208176	-0.51912669
1	2.16949122	-2.96967131	-1.35911296
17	-2.01126301	-3.03224405	0.60514125
5	3.27623390	-3.55979500	4.53196339
17	3.93869416	-2.11015504	5.30817931
17	3.88594797	-5.12296326	5.10077451

### TS(5a-6a)

$v = 81.20i \text{ cm}^{-1}$

6	-0.05127758	1.75052493	1.47926007
13	-0.24812462	0.74412537	-0.25077369
6	-1.79107161	1.81175319	-0.88051776
6	-1.68928453	3.07854329	0.01187019
6	-1.29723023	2.67241553	1.45567594
6	1.08189955	-0.33448685	-1.24484483
6	2.20767832	-1.01084469	-0.43964607
1	-1.13664014	3.57041593	2.07285656
1	0.14695558	1.36608773	2.49067496
1	0.85789270	2.35012535	1.26268868
1	-0.86179509	3.70239251	-0.38326718
1	-2.15471984	2.13813406	1.90214304
1	0.52906305	-1.08846062	-1.83261225
1	1.51847993	0.34186691	-2.00291298
1	2.91992711	-1.54135367	-1.09087775
1	2.78465116	-0.28036906	0.14645323
1	1.81154086	-1.74910900	0.27249917
1	-2.73812193	1.28536492	-0.65837416
1	-1.82051047	2.07010932	-1.94894336
6	-2.96815728	3.93472588	-0.03910949
1	-3.22545570	4.10279860	-1.09756779
1	-3.79869761	3.34394875	0.38570729
6	-2.87898135	5.28941340	0.67387462
1	-2.04018728	5.88663408	0.28429473
1	-2.73401916	5.17694766	1.75719542
1	-3.79850604	5.87315710	0.52402457
9	0.27218520	-1.25625924	2.66693432
5	-0.87598161	-0.78704126	2.20498419
9	-1.22020243	-1.05891026	0.91317597
9	-1.80500106	-0.30517393	3.01400831

### TS(5a'-6a')

$v = 160.99i \text{ cm}^{-1}$

6	1.47146505	3.06726566	0.53726126
13	1.02219686	1.11725948	0.11960705
6	-0.93445938	1.29018470	0.40607966

6	-1.06396502	2.74464039	0.92498660
6	0.03709765	3.60914369	0.26206145
6	1.95605884	0.08528389	-1.29528179
6	3.49480276	0.07466472	-1.31475755
1	-0.14975457	3.61471645	-0.82814166
1	1.85633414	3.53493960	1.44740739
1	-0.85831133	2.73740521	2.01181245
1	2.19251364	3.34179978	-0.25164629
1	-1.45248260	1.19306420	-0.56651582
1	-0.04819108	4.65699538	0.59373853
1	1.57024903	-0.94878578	-1.25898415
1	1.57528580	0.49308320	-2.25058686
1	3.89284355	-0.49956844	-2.16618255
1	3.90788672	1.09144560	-1.38714459
1	3.90979406	-0.37464290	-0.40084016
1	-1.39827592	0.55681187	1.08007837
6	-2.45564019	3.36641281	0.71924590
1	-2.42782488	4.42285765	1.03814174
1	-2.67940864	3.37727595	-0.36222006
6	-3.57958370	2.64509382	1.46781476
1	-3.38373767	2.62745399	2.55080112
1	-3.68384024	1.60439363	1.13038094
1	-4.54619461	3.14476172	1.31191937
17	1.91033897	-0.06761399	2.19721598
17	4.20891574	1.96140401	2.05930688
5	2.55580174	1.60884675	2.54745560
17	1.80339013	2.46310167	3.89437242

### TS(5b-6b)

$\nu = 118.15i \text{ cm}^{-1}$

6	0.63308415	2.36319548	1.30673952
13	0.18241887	0.95952651	-0.01700882
6	-1.72836550	1.56149811	-0.30895008
6	-1.59899102	3.01530682	0.25014869
6	-0.75532541	3.00614676	1.55027801
6	1.29382456	-0.08749514	-1.27675974
6	2.64860501	-0.57037086	-0.72047078
1	-0.66373925	4.02810861	1.95019160
1	1.10059636	2.02014086	2.24100093
1	1.32555382	3.10364850	0.87050239
1	-1.02446604	3.60298816	-0.49445991
1	-1.30646202	2.42409438	2.31038967
1	0.70336518	-0.94579843	-1.63997496
1	1.46246990	0.54188548	-2.16935158
1	3.23426261	-1.12012583	-1.47374393
1	3.26853029	0.27086674	-0.37633535
1	2.51811324	-1.24316198	0.14046328
1	-2.64530026	1.12791306	0.12781951
1	-1.93816384	1.56002328	-1.39187902
6	-2.97144496	3.69297805	0.41062102

1	-3.53768495	3.55311336	-0.52477085
1	-3.53583124	3.15380029	1.19164873
6	-2.92463555	5.18824886	0.74543137
1	-2.35056247	5.74462164	-0.01124448
1	-2.46060398	5.37796195	1.72288168
1	-3.93728572	5.61513897	0.77288054
9	-0.50460413	-0.72768989	1.27311270
5	-1.86521939	-0.69857168	1.06103793
9	-2.35345730	-1.42478974	0.06610060
9	-2.62736696	-0.28233480	2.06335878

**TS(5b'-6b')**

$\nu = 147.01i \text{ cm}^{-1}$

6	0.60242801	2.99317088	-0.87489096
13	0.13638765	1.12248140	-1.35470924
6	-1.79928264	1.21541722	-0.70062247
6	-1.56582333	2.38405408	0.31096360
6	-0.75959842	3.51904372	-0.36537917
6	1.20034866	-0.54409014	-1.18424397
6	1.49554039	-0.92956663	0.28067335
1	-1.35225762	3.90356932	-1.21306075
1	1.34635706	2.99611307	-0.06008561
1	-0.93382042	1.99489818	1.13584658
1	1.01842592	3.61509477	-1.67963672
1	-2.72054062	1.43266255	-1.25243555
1	-0.64423942	4.35857851	0.34088879
1	0.67074377	-1.36837676	-1.68959919
1	2.14881573	-0.41372689	-1.73273833
1	2.09571275	-1.85021468	0.35380135
1	2.05373470	-0.14015314	0.80686206
1	0.57068028	-1.10491771	0.85163598
1	-1.97351542	0.24464862	-0.20814101
6	-2.87446650	2.89781091	0.93697478
1	-2.63629122	3.76404945	1.57741058
1	-3.51918315	3.28050414	0.12701041
6	-3.63999977	1.85817916	1.75984560
1	-3.01630976	1.46355306	2.57645538
1	-3.95953423	1.00743705	1.14196534
1	-4.54033609	2.29755168	2.21184816
17	-0.17319124	1.14093274	-3.87838220
17	-2.45311322	-0.80772777	-3.22093002
5	-1.91119171	0.86012792	-3.37475602
17	-3.04474590	2.15368518	-3.76741865

**TS(6a-7a)**

$\nu = 124.17i \text{ cm}^{-1}$

6	-2.72739051	1.96108872	-0.01726373
13	0.38174703	0.59943404	-0.33404869
6	-0.71141636	1.24015715	-1.92017788
6	-1.29784842	2.66556829	-1.98343247

6	-2.71567127	2.66478421	-1.38944768
6	1.51431168	-1.00074865	-0.47321365
6	2.88434263	-0.76247454	-1.14288440
1	-3.09989686	3.68958303	-1.28981278
1	-3.75369133	1.92691054	0.38570167
1	-2.10957453	2.52231212	0.70020607
1	-0.67002459	3.31959075	-1.35052006
1	-3.39492279	2.13540056	-2.08055806
1	1.66449602	-1.39471469	0.54640568
1	0.96070882	-1.78519056	-1.01631712
1	3.49127425	-1.68040883	-1.17441955
1	2.77842225	-0.41420963	-2.18185983
1	3.47066646	-0.00252670	-0.60612279
1	-1.33009310	0.53076458	-2.49353342
1	0.23898783	1.24458431	-2.50639429
6	-1.26624015	3.23140784	-3.41671772
1	-0.23342531	3.15716264	-3.79522813
1	-1.87746495	2.58191752	-4.06737490
6	-1.73675987	4.68443915	-3.54650681
1	-1.16338897	5.34678517	-2.88034076
1	-2.80088216	4.79748817	-3.29721416
1	-1.60079528	5.04876335	-4.57438176
9	-1.20159150	-0.00435823	0.74010732
5	-2.19387788	0.50368181	-0.16845679
9	0.91746889	1.92516563	0.57540821
9	-2.84994763	-0.48625986	-0.78186408

**TS(6a-7a) + THF**

$\nu = 207.78i \text{ cm}^{-1}$

6	1.31392999	3.71914804	1.87147082
13	1.30211989	0.53322275	-0.55948770
6	0.14772590	2.19871786	-0.01324523
6	-0.87352629	2.71150211	1.02551758
6	-0.22284448	3.79848422	1.92331131
6	2.06804568	0.99872014	-2.33337130
6	3.20208153	0.10221214	-2.86168860
1	-0.55320896	4.79451186	1.58823374
1	1.76163544	4.08143387	2.81193524
1	-1.16551208	1.86189640	1.66580749
1	1.71372308	4.36123393	1.07336360
1	0.64985380	3.04370388	-0.50963481
1	-0.58241357	3.68420080	2.95568770
1	1.24531712	1.04467440	-3.07024814
1	2.43190146	2.03686947	-2.25291604
1	3.59770160	0.46011575	-3.82556853
1	4.04188596	0.06146630	-2.15374959
1	2.87249716	-0.93698817	-3.01065032
1	-0.46148550	1.74594617	-0.82690474
6	-2.15952000	3.27405259	0.38430486
1	-2.73359272	3.78567938	1.17542942



1	-1.87680719	4.05770088	-0.33977322
6	-3.07188093	2.24856431	-0.29290135
1	-3.41236033	1.48879327	0.42731688
1	-2.56857566	1.72924373	-1.12278490
1	-3.96651614	2.73242301	-0.70964730
17	2.14318827	-1.25050434	0.39865963
17	3.38114987	1.93975613	0.80911904
5	1.77809151	2.23543286	1.64617165
17	1.32666139	1.02478604	2.91315395
6	-1.35944067	-2.60594225	-0.34654982
6	-1.32497990	-2.57770683	-1.88216415
6	-1.19900446	-1.13593797	0.01495088
6	-0.24145152	-1.54631222	-2.15657267
1	-0.51337748	-3.18594548	0.04553752
1	-2.15561356	-0.59665182	0.02428897
1	-2.29117367	-2.24699074	-2.29001586
1	-0.34712236	-1.00975166	-3.10640321
1	-1.07578595	-3.55151680	-2.32185492
1	0.76550511	-1.97992942	-2.07374097
1	-0.65701790	-0.96998145	0.95399099
1	-2.29208203	-3.02246509	0.05398586
8	-0.39096593	-0.54600105	-1.08122351

**TS(6a-7a) + 2THF**

$\nu = 211.67i \text{ cm}^{-1}$

6	1.66419053	4.00697245	-1.52820474
13	1.28271069	0.10884603	-0.67998894
6	0.19575048	1.76152709	-1.37578096
6	-0.60370801	3.00181537	-0.92021438
6	0.17270020	4.29785376	-1.28034449
6	1.61038983	-1.00590672	-2.29266733
6	2.64691764	-2.13598524	-2.16225064
1	-0.27058013	4.75050956	-2.18149261
1	2.29077868	4.88098030	-1.27900049
1	-0.71170208	2.95430967	0.17679996
1	1.84790196	3.78707171	-2.59009981
1	0.53713105	1.88433767	-2.41534014
1	0.64358154	-1.41468829	-2.63920028
1	1.92515867	-0.31299304	-3.09110098
1	2.79887282	-2.67055492	-3.11353542
1	3.62370290	-1.74682290	-1.84183973
1	2.35085036	-2.88413736	-1.41166652
1	-0.55074755	0.93911567	-1.44443992
17	2.39519915	-0.47527246	1.11920418
17	3.53056712	1.76514446	-1.23965508
5	2.13316975	2.79873245	-0.64632974
17	2.02910988	2.99030541	1.15453290
6	-1.11887947	-1.44551758	2.29661594
6	-1.42093290	-2.56933858	1.29359535
6	-0.94859651	-0.23186475	1.39320333

6	-0.47126272	-2.23946736	0.15242385
1	-0.18278541	-1.65170039	2.83259955
1	-1.90233643	0.26284938	1.16596085
1	-2.46674913	-2.52385504	0.95682701
1	-0.80430206	-2.57773734	-0.83546286
1	-1.22921360	-3.56936368	1.70224515
1	0.54877944	-2.59723040	0.35381378
1	-0.21977466	0.49695714	1.76825240
1	-1.92225590	-1.29659281	3.02882672
8	-0.43172426	-0.76498168	0.10859594
6	6.19466856	6.60550290	0.70621966
6	5.16385406	7.36961698	1.58236873
6	5.31026881	5.73558545	-0.20388413
6	3.80235964	6.90890836	1.02116548
1	6.88737681	5.99681511	1.30211871
1	5.70451824	5.59919690	-1.21858278
1	5.28852051	8.45450008	1.47317430
1	3.05313915	7.70765228	0.95032866
1	5.25965336	7.12618847	2.64873780
1	3.38780640	6.08180479	1.62790178
1	5.13817512	4.74179436	0.25137281
1	6.78994434	7.30763291	0.10826383
8	4.06557603	6.44423102	-0.31233391
1	0.04952025	5.03359782	-0.47288931
6	-2.02260678	3.06211570	-1.52375760
1	-2.43902359	4.05980631	-1.30381218
1	-1.93935129	3.00432218	-2.62285959
6	-3.00743391	2.00256772	-1.02309916
1	-3.14900698	2.08064327	0.06588919
1	-2.66768922	0.98017535	-1.24915118
1	-3.99304900	2.12707737	-1.49359406

**TS(6a'-7a')**

$\nu = 188.65i \text{ cm}^{-1}$

6	1.41121941	3.50085951	1.41474234
13	0.69618449	0.18571648	-0.07432506
6	-0.30521335	1.31486787	1.31274193
6	-0.91780239	2.68567058	0.95558886
6	0.20055042	3.63073305	0.48100667
6	0.15975426	0.20509107	-1.97651015
6	1.04761077	-0.65614422	-2.89534639
1	0.49322890	3.35794725	-0.54798750
1	1.14105445	3.82810895	2.43144868
1	-1.33840432	3.11974649	1.88211294
1	2.23184513	4.15923918	1.07998006
1	-1.08484291	0.51910831	1.25368069
1	-0.15937975	4.67032946	0.44297016
1	-0.88256495	-0.15707692	-2.02199970
1	0.13195874	1.24540609	-2.34063924
1	0.68409686	-0.64951771	-3.93443871

1	2.08655650	-0.29415851	-2.91407103
1	1.07720136	-1.70286823	-2.56151044
1	-0.03273090	1.24935197	2.37365323
6	-2.06355398	2.61734678	-0.06988609
1	-2.29464295	3.64618071	-0.39243524
1	-1.71494982	2.08887402	-0.97276672
6	-3.34659193	1.96460317	0.45306151
1	-3.73256479	2.50252173	1.33182029
1	-3.18828220	0.91708613	0.74924051
1	-4.13307805	1.96965228	-0.31422640
17	1.15794209	-1.72982283	0.78722236
17	2.80579958	1.38569769	-0.09202635
5	1.96917764	2.03760003	1.47954508
17	2.62391416	1.28825635	2.94822920

### TS(6b-7b)

$\nu = 157.44i \text{ cm}^{-1}$

6	0.48190032	2.19499953	1.37766596
13	0.27594751	0.88615627	-0.15728216
6	-0.01578556	4.49200888	-0.20914075
6	0.09561649	4.72777993	1.33017745
6	-0.16512304	3.40435418	2.08295876
6	1.94600328	0.18351700	-0.92318268
6	1.75880557	-0.82826463	-2.07202403
1	0.22960379	3.48562184	3.10694338
1	0.40273853	1.34018255	2.08637271
1	1.56719239	2.39165091	1.28055571
1	1.13519704	5.03161784	1.54352015
1	-1.25043879	3.24158876	2.18242219
1	2.56304674	1.03357227	-1.26194755
1	2.52343453	-0.28488517	-0.10680603
1	2.72231893	-1.20718679	-2.44652055
1	1.16494551	-1.69573339	-1.75109998
1	1.23148711	-0.37978383	-2.92698745
1	-0.53611798	5.33892357	-0.68719416
1	0.97828277	4.43283038	-0.67326808
6	-0.82847202	5.86274133	1.80281752
1	-0.59766814	6.76651308	1.21525301
1	-1.87161427	5.59560811	1.56146299
6	-0.71386943	6.19331622	3.29435151
1	0.32372081	6.43950261	3.56705716
1	-1.03664610	5.35499497	3.92687974
1	-1.34010556	7.05891761	3.55134168
9	-1.06019853	-0.14231968	-0.03753541
5	-0.80425151	3.17688952	-0.47818877
9	-0.39050161	2.24424228	-1.48996796
9	-2.08274783	2.98651330	-0.14040250

### TS(6b-7b) + THF

$\nu = 218.47i \text{ cm}^{-1}$

6	1.43284438	3.52964630	2.04904074
13	1.37399328	0.47176702	-0.60070265
6	0.22630467	2.06742248	0.11585722
6	-0.71624720	2.47713678	1.26159206
6	-0.11870423	3.65641612	2.05726441
6	2.05021114	1.04187283	-2.37908339
6	3.15205753	0.17295492	-3.01170957
1	-0.37692529	4.58157399	1.51272220
1	1.85063629	3.76830487	3.04123195
1	-0.88648936	1.62413113	1.93787989
1	1.87802165	4.25361418	1.35211832
1	0.67244363	2.95820356	-0.35288191
1	1.18875616	1.12435502	-3.06693538
1	2.42026179	2.07427774	-2.26339564
1	3.49530491	0.57769799	-3.97714141
1	4.02929170	0.09874348	-2.35357433
1	2.81258005	-0.85801037	-3.19235426
1	-0.42730404	1.66172612	-0.68775420
1	-1.70437914	2.76673788	0.86811693
17	2.24539305	-1.35722667	0.22809814
17	3.47763312	1.87365068	0.74153079
5	1.91162482	2.07387586	1.67884495
17	1.57855324	0.76085716	2.88386596
6	-1.42755717	-2.57713545	-0.40157259
6	-1.39056190	-2.53805115	-1.93720311
6	-1.16379100	-1.12535151	-0.02278941
6	-0.24336272	-1.57554769	-2.20213429
1	-0.62404370	-3.21893344	-0.01604162
1	-2.08171637	-0.52237084	0.01664613
1	-2.33316440	-2.14255870	-2.34263277
1	-0.31008581	-1.02978818	-3.15029408
1	-1.20456333	-3.52249826	-2.38437275
1	0.73536173	-2.06900028	-2.11371303
1	-0.59478157	-1.01197030	0.90848342
1	-2.38597494	-2.93292057	-0.00369625
8	-0.34210189	-0.57212935	-1.12610276
6	-0.73908600	3.76179588	3.45923518
1	-1.83336487	3.65298534	3.36467057
1	-0.39596159	2.90765765	4.06551461
6	-0.43074085	5.07534107	4.18324618
1	-0.81044118	5.93821383	3.61535237
1	0.65069476	5.21921672	4.32176024
1	-0.89590958	5.09896486	5.17872867

**TS(6b-7b) + 2THF**

$\nu = 220.64i \text{ cm}^{-1}$

6	1.91152651	3.96293556	-1.44218726
13	1.40509182	-0.01715191	-0.98028462
6	0.53757377	1.67142959	-1.85933681
6	-0.36234851	2.88341944	-1.55738277

6	0.41055425	4.20209486	-1.77541129
6	2.24640149	-1.03423363	-2.46486491
6	3.19694673	-2.17817593	-2.06876419
1	0.34624530	4.44515364	-2.85056105
1	2.34246864	4.82087623	-0.89816796
1	-0.72605957	2.83619327	-0.51828346
1	2.49997193	3.86552061	-2.36583106
1	1.15954847	1.86530865	-2.74677348
1	1.44364199	-1.41697490	-3.12144910
1	2.79298723	-0.30222272	-3.08260365
1	3.64724485	-2.66590369	-2.94806763
1	4.01845376	-1.81358102	-1.43592979
1	2.68356043	-2.95999923	-1.48912483
1	-0.14497940	0.86184107	-2.20097763
1	-1.25664126	2.87191351	-2.20183593
17	1.89163146	-0.69384236	1.04602345
17	3.66809951	1.70904028	-0.75712428
5	2.12297439	2.68651274	-0.54940798
17	1.49900207	2.74254264	1.15675174
6	-1.81258163	-2.74148552	-0.12106826
6	-1.91770194	-1.61496784	0.91862984
6	-0.49736247	-2.41412863	-0.81100227
6	-1.40512733	-0.40247776	0.15188130
1	-2.64869659	-2.69669429	-0.83396133
1	0.36888823	-2.76391331	-0.23093037
1	-1.26283960	-1.82323915	1.77535153
1	-0.86317759	0.31591563	0.77974320
1	-2.94055694	-1.46169107	1.28433385
1	-2.19631500	0.10899691	-0.41392343
1	-0.42421626	-2.75843981	-1.84902102
1	-1.79456792	-3.74023427	0.33269720
8	-0.45159987	-0.94106482	-0.84724643
6	4.50258061	5.36056645	2.51032031
6	5.60531165	5.33415706	1.41731801
6	3.43733879	6.31669031	1.93193817
6	5.12461907	6.38513596	0.40493721
1	4.88152430	5.72714400	3.47346202
1	2.40635786	5.96323740	2.05911905
1	5.65757174	4.34423531	0.94639387
1	5.37209431	6.15238547	-0.63864424
1	6.60102855	5.57317072	1.81375344
1	5.52876709	7.38655726	0.65310306
1	3.52802279	7.32455908	2.38076137
1	4.08860943	4.35782359	2.67136806
8	3.69436568	6.39694804	0.51993522
6	-0.23437317	5.36617576	-1.00688206
1	-1.32290468	5.34107990	-1.18997944
1	-0.09999683	5.19628230	0.07405726
6	0.30871634	6.74649123	-1.38769299
1	0.16487669	6.94510321	-2.46091566

1	1.38242497	6.83363453	-1.16856550
1	-0.20705738	7.54098381	-0.82973494

**TS(6b'-7b')**

$\nu = 159.73i \text{ cm}^{-1}$

6	0.11179076	2.09654572	-0.83790251
13	0.58959324	0.77044462	-2.30296336
6	-2.37574089	0.98574782	-0.08748394
6	-2.04813672	2.39866864	0.48920524
6	-0.95949502	3.08137742	-0.36260198
6	2.06863825	-0.43927864	-1.79747801
6	1.99174083	-1.12945165	-0.42498834
1	-1.41635586	3.58614577	-1.22739187
1	0.50918754	1.53770917	0.02897723
1	-1.62658641	2.23948229	1.49706079
1	0.96284283	2.70357544	-1.22487693
1	-3.45170880	0.76745689	0.02870156
1	-0.49146360	3.87528158	0.24273652
1	2.14595111	-1.19162820	-2.60034620
1	2.99589167	0.15573791	-1.87296157
1	2.85032866	-1.79717775	-0.25384060
1	1.98416937	-0.40130565	0.40013918
1	1.08285433	-1.74135993	-0.32459619
1	-1.84790788	0.20624639	0.47950431
6	-3.27979297	3.30604495	0.64448646
1	-2.92771405	4.32717696	0.86759060
1	-3.80541992	3.36959091	-0.32222032
6	-4.25233286	2.86560923	1.74219710
1	-3.75694856	2.84580410	2.72450236
1	-4.65736083	1.86025263	1.55453871
1	-5.10631724	3.55344061	1.81233961
17	0.65346395	1.56324509	-4.29754336
17	-1.34554140	-0.76276675	-2.25358010
5	-2.01922395	0.85932689	-1.59923346
17	-2.75667129	1.85284739	-2.86681882

**TS(10a-11a)**

$\nu = 109.80i \text{ cm}^{-1}$

6	-1.28777300	-5.81764799	-6.18341372
13	-0.81072965	-2.45981794	-7.84559126
6	-1.77512157	-2.46663391	-6.09702964
6	-0.68313614	-3.39148166	-5.41497607
6	-1.24354609	-4.78258017	-5.04094283
6	0.88535939	-1.56226030	-8.27472576
6	2.09670058	-2.48869917	-8.50756622
1	-0.61211238	-5.19728190	-4.24015398
1	-1.43597969	-6.81967521	-5.73604956
1	-0.30414482	-5.88863596	-6.67645133
1	0.17771385	-3.59559929	-6.10163853
1	-2.24607049	-4.64898294	-4.60464130

1	0.70443758	-0.96015980	-9.18228888
1	1.11182937	-0.82893396	-7.48254821
1	2.99061221	-1.92174255	-8.80914964
1	2.36287177	-3.05062493	-7.59978790
1	1.89478710	-3.22813378	-9.29536124
1	-2.72548768	-3.01021697	-6.15103830
1	-1.92145345	-1.60163374	-5.43845201
6	-0.05893314	-2.65456137	-4.21175608
1	0.15431438	-1.61758114	-4.51709360
1	-0.82327069	-2.58777008	-3.41880018
6	1.22532304	-3.27948181	-3.65974467
1	2.00635064	-3.32723243	-4.43346139
1	1.06578809	-4.29880706	-3.28177580
1	1.61971779	-2.68093027	-2.82716508
9	-2.33990935	-6.55869988	-8.35531895
5	-2.39209907	-5.73729931	-7.30020840
9	-1.20018650	-3.90308537	-8.66003514
9	-3.52226436	-5.02265056	-7.16246064
9	-2.23674433	-1.13631524	-8.72065875
9	-4.04643293	-1.11503287	-7.26120767
5	-2.81452371	-0.71317733	-7.52298798
9	-2.30366563	0.38489712	-6.97619112

### TS(10a'-11a')

$\nu = 167.34i \text{ cm}^{-1}$

6	0.69836978	4.00620212	0.44759579
13	-0.90985552	-0.06453880	-1.40264985
6	-2.06675996	1.58733424	-1.08387655
6	-1.18893316	2.20308661	0.06811364
6	-0.28481806	3.30073333	-0.52924305
6	1.02738135	-0.04218872	-1.77345614
6	1.58886820	-1.39660114	-2.24880495
1	0.28873578	2.87981175	-1.36924344
1	0.13672974	4.47152398	1.26969997
1	-0.53844896	1.43431950	0.53871923
1	1.17791770	4.82177657	-0.11737879
1	-2.37204295	2.43817831	-1.70043312
1	-0.93888901	4.07375207	-0.96576825
1	1.25517409	0.74421909	-2.51084953
1	1.53918764	0.25662000	-0.84376310
1	2.68029363	-1.35330635	-2.38309488
1	1.37683827	-2.19876481	-1.52749866
1	1.15703911	-1.70233114	-3.21323777
1	-2.98901390	1.14385993	-0.68228906
6	-2.10727659	2.73295642	1.19187568
1	-1.49965229	3.33610561	1.88435420
1	-2.84239197	3.42109472	0.74082040
6	-2.82125003	1.64994818	2.00526994
1	-2.09714174	0.97626719	2.48512428
1	-3.48849998	1.03131600	1.39003452

1	-3.43130216	2.10636830	2.79678232
17	-1.65182650	-1.60923340	-0.10138243
17	3.26823325	2.71576867	0.05565610
5	1.83103603	3.08920027	1.01890359
17	1.73778065	2.37420681	2.63534790
17	-4.12297799	1.25967850	-3.40808003
17	-1.31414807	2.17988909	-4.26806847
5	-2.37312680	1.01674432	-3.44788808
17	-1.84070003	-0.75919748	-3.57765708

**TS(10b-11b)**

$\nu = 184.48i \text{ cm}^{-1}$

6	0.65806262	2.18840595	1.70670419
13	0.94046765	0.43232762	0.75274475
6	-1.62805297	2.33759523	-0.47781257
6	-1.53817494	3.22936949	0.78087376
6	-0.83464069	2.53823155	1.96696534
6	2.43945440	0.07124064	-0.46149589
6	3.78901258	0.69742591	-0.05667320
1	-0.89201274	3.20838310	2.83627986
1	1.27282460	2.57845443	2.53412776
1	1.05933742	2.81740190	0.88204491
1	-0.92207625	4.10825800	0.50955027
1	-1.40778209	1.63873986	2.24016032
1	2.53819563	-1.02370580	-0.55285028
1	2.15162702	0.41432057	-1.47020395
1	4.58094522	0.46808361	-0.78571015
1	3.72781327	1.79358243	0.01708956
1	4.13517528	0.32847488	0.92008234
1	-2.08843125	2.92653210	-1.29372890
1	-0.62333966	2.11233252	-0.88177743
6	-2.92932523	3.76972376	1.17768808
1	-3.44703355	4.09360619	0.25945932
1	-3.53428304	2.95116783	1.59746095
6	-2.89737642	4.94673291	2.15859672
1	-2.29531845	5.77825832	1.76168235
1	-2.47768090	4.66423268	3.13409999
1	-3.91184676	5.32789023	2.34066187
9	-0.53755462	-0.37162367	0.50805191
5	-2.43969858	0.98371731	-0.42821020
9	-2.49079331	0.20922102	-1.52168867
9	-3.24457001	0.63366716	0.58419379
9	1.50683961	-0.49509224	2.52081168
9	0.46449815	0.74675437	4.18480456
5	1.50261003	0.61938120	3.37354607
9	2.69772964	1.12146308	3.66860083

**TS(10b'-11b')**

$\nu = 354.03i \text{ cm}^{-1}$

6	0.57146578	2.60050671	1.69954241
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13	1.29471197	0.67959299	1.97978146
6	-2.22311978	3.05553043	-0.96799378
6	-1.64142046	2.59225593	0.38216752
6	-0.26090457	3.24904423	0.60283053
6	0.23528023	-0.79055016	2.74645113
6	-0.77404473	-0.41259855	3.84522968
1	0.32036837	3.19790612	-0.33029977
1	0.05893169	2.48007370	2.66483294
1	-1.49288536	1.49874770	0.33461921
1	1.64113719	2.84743353	1.62704543
1	-2.28504838	4.15675484	-0.99891780
1	-0.41160224	4.32312504	0.81187067
1	-0.28310476	-1.27717970	1.90145805
1	0.94678570	-1.54671598	3.11759020
1	-1.33531139	-1.29020966	4.20013461
1	-0.27787925	0.03008362	4.72070682
1	-1.51697105	0.31747501	3.48960889
1	-3.27710878	2.72272702	-1.05438497
6	-2.60139381	2.89412181	1.54909597
1	-2.08367620	2.72179686	2.50708405
1	-2.84693580	3.96953363	1.53566084
6	-3.88919132	2.06508156	1.54600532
1	-3.66791790	0.98753840	1.56929216
1	-4.50646285	2.26010808	0.65750306
1	-4.50496310	2.29798136	2.42534081
17	2.96920996	0.24108823	0.72333118
17	-1.80079364	3.41004515	-3.80832002
5	-1.55990424	2.53887620	-2.28791634
17	-0.61674919	1.04243195	-2.35654034
17	0.10369556	4.27480954	4.37898564
17	2.56894740	4.88608853	2.69988117
5	1.39074799	3.65982094	3.27951259
17	2.22879042	2.04045266	3.93145115

### TS(12-13a)

$\nu = 231.39i \text{ cm}^{-1}$

6	-0.35411775	3.94333273	0.09146280
6	-2.64935113	2.71119992	0.05803605
6	-2.47470758	3.65450934	1.29348430
6	-0.95622425	3.83192307	1.50170667
1	-0.72860010	4.70003308	2.13484354
1	0.73239439	3.77917193	0.05936947
1	-0.53611182	4.94839454	-0.32672797
1	-2.87981332	4.63768604	0.99257678
1	-0.55385848	2.94204015	2.01392573
1	-3.36622657	1.91070049	0.31861578
1	-3.21868856	3.17511154	-0.76763459
6	-3.25254847	3.19417266	2.53548372
1	-4.30904468	3.04320293	2.25676778
1	-2.87153050	2.21208200	2.85733120

6	-3.18328010	4.18348840	3.70303016
1	-3.54695444	5.17829021	3.40393255
1	-2.15666763	4.29996046	4.07691465
1	-3.80294637	3.84052500	4.54293079
5	-1.76960693	0.94497858	-0.01514126
9	-2.42943451	0.23301910	-0.95300805
9	-1.77306431	0.50417442	1.26368454
9	-0.43510416	1.32706932	-0.44205634
5	-1.15863098	2.89695437	-0.77773996
9	-1.21003850	2.89484706	-2.12690374

**TS(12'-13a')**

$\nu = 208.09i \text{ cm}^{-1}$

6	-1.01725013	3.84546365	1.84420229
6	-1.29833944	3.56370268	-0.71090136
6	-2.04612406	2.41101603	0.06089491
6	-2.16762128	2.85761460	1.53989900
1	-3.14469846	3.33685338	1.70288212
1	-1.36902153	4.88587671	1.80116314
1	-1.43977559	1.49741854	-0.00323420
1	-0.58052977	3.69463174	2.84173608
1	-1.88577199	4.47742012	-0.55600357
1	-2.12838791	1.97809461	2.19644842
1	-1.43199388	3.25963740	-1.76908230
6	-3.41330954	2.12291846	-0.57807528
1	-3.95184911	1.45390475	0.11377457
1	-4.00045188	3.05614660	-0.61742825
6	-3.36186732	1.47126046	-1.96186871
1	-2.78459031	0.53569003	-1.93876761
1	-2.90370282	2.12855322	-2.71613583
1	-4.37315568	1.23322088	-2.31880558
17	-0.32295907	5.73560746	-2.28511675
5	0.16433488	4.23095573	-1.38322209
17	1.21019524	3.09966362	-2.31059431
17	0.97196816	1.99310244	0.85753450
17	1.25657359	4.96302360	0.24478013
5	0.05689176	3.54768621	0.72493551

**TS(12-13b)**

$\nu = 237.79i \text{ cm}^{-1}$

6	-0.36956958	3.95535067	0.07297891
6	-2.64182698	2.75198353	-0.01044304
6	-2.46757842	3.56047224	1.29844435
6	-0.95870491	3.85745320	1.49377087
1	0.72391158	3.84215824	0.04971068
1	-0.59487271	4.94485104	-0.36667432
1	-3.02662977	4.50702499	1.21905831
1	-0.50907670	2.97426608	1.98143165
1	-3.46653874	2.02233834	0.05941400
1	-3.04968769	3.37224991	-0.83351396

5	-1.81606784	0.95576433	0.02781088
9	-2.40211345	0.22034628	-0.94044475
9	-1.99589532	0.59548292	1.31807979
9	-0.43934450	1.28012685	-0.26584841
5	-1.12460953	2.86681837	-0.78192827
9	-1.07695663	2.74873211	-2.12317304
6	-0.67593816	5.07794951	2.37656944
1	0.41142472	5.25815008	2.38976015
1	-1.12835663	5.96774952	1.90430177
6	-1.18351215	4.94174771	3.81602975
1	-0.74479795	4.06041768	4.30728172
1	-2.27705342	4.83491514	3.85409321
1	-0.91742239	5.82419482	4.41429417
1	-2.88561751	3.01316344	2.15225784

### TS(12'-13b')

$\nu = 196.83i \text{ cm}^{-1}$

6	-0.35081436	3.17912691	1.11612567
6	-1.22557836	2.94105865	-1.32672704
6	-2.20560128	2.25932093	-0.32662135
6	-1.88111311	2.85002905	1.06430319
1	-2.48064858	3.74533978	1.27058060
1	-0.16926373	3.36852937	2.19228171
1	-1.97245456	1.18172456	-0.29548870
1	0.17509258	2.25528358	0.84746741
1	-1.73347061	3.28815715	-2.23852974
1	-2.08315011	2.12701399	1.86810002
1	-0.44004651	2.24319982	-1.64833938
6	-3.69331694	2.40614234	-0.67627232
1	-4.29115451	2.06726071	0.18693884
1	-3.92464214	3.47531064	-0.81018661
6	-4.11568183	1.61714560	-1.91834307
1	-3.93512094	0.54010509	-1.78378154
1	-3.55987993	1.93866643	-2.81109478
1	-5.18533441	1.75304668	-2.12896750
17	-1.68206358	5.63741168	-0.36092903
5	-0.62253040	4.18298182	-0.55410155
17	1.14656556	4.74907997	-1.06006788
17	2.48598478	3.38122892	1.34512187
17	0.80572486	5.86770960	1.86767977
5	0.97706200	4.32458969	0.95986627

### TS(15-16)

$\nu = 279.49i \text{ cm}^{-1}$

6	0.54071922	2.25227326	1.06216274
13	0.45693960	0.94371350	-0.40725033
6	-1.30174365	1.65677417	-1.18477702
6	-1.43571369	2.95303777	-0.37086297
6	-0.90531423	2.80907948	1.08006368
6	1.56126607	-0.55629863	-1.05527446

6	1.17956116	-1.19324768	-2.40466162
1	0.85965039	1.87497761	2.04424611
1	1.24791081	3.05923564	0.79162060
1	-0.86283015	3.74641651	-0.87994724
1	-1.54954708	2.06035042	1.58172866
1	2.60491905	-0.19470222	-1.07715477
1	1.54994013	-1.31807188	-0.25411597
1	1.84654456	-2.03087621	-2.65824658
1	0.15162655	-1.58122018	-2.39718177
1	1.23943715	-0.46822297	-3.22860936
1	-1.91493852	0.79023668	-0.89984994
1	-0.98377082	1.68410166	-2.23302294
35	-2.77192456	-0.07834927	-3.51092520
5	-3.06661115	1.61555989	-2.52130864
35	-2.87345982	3.27476691	-3.58034133
35	-4.58860373	1.60095235	-1.25525135
6	-1.01664723	4.12166319	1.87654952
1	-0.53211999	3.96968124	2.85464075
1	-0.42127045	4.89457517	1.35939350
6	-2.44591501	4.62919455	2.09978011
1	-3.06292828	3.86624143	2.59771700
1	-2.94278723	4.89696534	1.15770658
1	-2.44537114	5.52407261	2.73777426
1	-2.48291101	3.28611508	-0.35114973

### TS(16-17)

$v = 56.88i \text{ cm}^{-1}$

6	0.44213685	2.51501656	0.27389331
13	0.11385170	0.91491287	-0.83404813
6	-1.90395751	1.89945718	-1.24494399
6	-2.03522611	3.01202923	-0.21487234
6	-0.93232373	2.91853939	0.87592081
6	0.83116398	-0.90747114	-0.99789441
6	1.77352558	-1.14998419	-2.19445318
1	1.17798810	2.33422313	1.07164875
1	0.84058311	3.33958901	-0.34445589
1	-1.96885246	3.97492877	-0.74548861
1	-1.24201767	2.11081289	1.56932182
1	1.35585953	-1.10564160	-0.04671066
1	-0.02697581	-1.59516458	-1.04484616
1	2.13741900	-2.18754799	-2.19591639
1	1.25777689	-0.97945649	-3.14898028
1	2.65581442	-0.49439214	-2.16656355
1	-1.84637861	0.89366630	-0.72123403
1	-1.00991262	2.11654040	-1.89112082
35	-1.75009229	0.07426675	-3.46374922
5	-2.94186406	1.51759484	-2.44241290
35	-3.28099708	3.10702776	-3.63407273
35	-4.62453205	0.67030930	-1.72522499
6	-0.83248826	4.21382217	1.70276662

1	-0.01912231	4.09610992	2.43664445
1	-0.52389535	5.03176147	1.02934910
6	-2.12150578	4.60133803	2.43527170
1	-2.46157472	3.79061666	3.09713781
1	-2.93875619	4.83124576	1.73844835
1	-1.95998179	5.49188661	3.05804042
1	-3.03269495	2.96457541	0.24243287

**TS(17-18)**

$\nu = 129.96i \text{ cm}^{-1}$

6	-0.39636286	2.92078102	-0.92330113
13	0.30743135	1.28393280	-1.90490445
6	-3.01721807	1.71884045	-0.84098029
6	-2.65378204	2.81099195	0.17960527
6	-1.13724044	2.84177142	0.41781529
6	0.80596921	-0.27718721	-0.79903269
6	1.35603568	-1.49164602	-1.56750699
1	0.68624553	3.10458223	-0.71288764
1	-0.68855614	3.80363783	-1.50528796
1	-2.98253032	3.79430807	-0.19680241
1	-0.85609890	1.89769035	0.92228382
1	1.56078519	0.08111824	-0.07606367
1	-0.06728727	-0.57278369	-0.19297009
1	1.64838560	-2.30728745	-0.88831103
1	0.60989404	-1.90243650	-2.26423687
1	2.23992606	-1.22407876	-2.16353259
1	-4.11257721	1.68627009	-0.98302247
1	-2.72479563	0.73099828	-0.45104253
35	1.75460329	1.95911011	-3.58363899
5	-2.37642983	1.96685308	-2.24421210
35	-2.81125392	3.49322210	-3.35909692
35	-1.71599686	0.35665201	-3.29556939
6	-0.71987354	3.99995735	1.35095152
1	0.37862934	3.99523263	1.43925441
1	-0.98358963	4.95499158	0.86550816
6	-1.32984030	3.94486400	2.75587108
1	-1.11024420	2.98433625	3.24636187
1	-2.42099121	4.07160732	2.73808896
1	-0.91789135	4.74250638	3.38956175
1	-3.19237579	2.63177626	1.12098578

**TS(21-22)**

$\nu = 348.30i \text{ cm}^{-1}$

6	0.65349391	2.44895227	0.91149612
13	0.42975019	1.02223064	-0.42168567
6	-1.41862649	1.69158689	-1.03720700
6	-1.69053913	2.90066253	-0.11741493
6	-0.82105912	2.83244571	1.17538935
6	1.41282520	-0.54875863	-1.08962682
6	2.72081374	-0.89861759	-0.35441181

1	-0.89086349	3.79457732	1.70384448
1	1.18699922	2.18740047	1.83522160
1	1.19926281	3.29587468	0.45873161
1	-1.36629410	3.79256289	-0.68398014
1	-1.27622924	2.08071359	1.84644409
1	0.71733503	-1.40550738	-1.08105576
1	1.60665644	-0.36385041	-2.16109054
1	3.21481980	-1.77335601	-0.80343405
1	3.44064903	-0.06787843	-0.38347001
1	2.54390100	-1.13390897	0.70506078
1	-1.97125785	0.75232076	-0.91136949
1	-0.95756234	1.86440243	-2.02201757
6	-3.17870701	3.08416933	0.23304705
1	-3.75653357	3.13583329	-0.69835843
1	-3.53524502	2.18391502	0.76309985
6	-3.48443576	4.33109076	1.07051528
1	-3.09347139	5.23807073	0.58459036
1	-3.05596663	4.27860854	2.08058590
1	-4.57032047	4.45807679	1.18113486
35	-1.55340588	0.27710094	-3.91848167
5	-2.65782646	1.55988735	-2.84337857
35	-2.70776332	3.41351518	-3.54213298
35	-4.40536815	0.80534147	-2.29219255

### TS(22-23)

$\nu = 123.41 \text{ i cm}^{-1}$

6	-0.28412774	2.63884426	-1.17832460
13	-0.07013134	0.85133141	-2.12385667
6	-3.14750676	2.22657748	-1.06866785
6	-2.50548241	3.20123223	-0.05798131
6	-1.04036322	2.78949962	0.14319481
6	-0.01041819	-0.75920977	-0.97838321
6	0.16321247	-2.09960454	-1.71403676
1	0.80324067	2.52061572	-0.95146834
1	-0.31560198	3.55053148	-1.78610858
1	-2.51824367	4.21205431	-0.50428065
1	-1.00934833	1.84336041	0.71243886
1	0.82738796	-0.60790399	-0.27403167
1	-0.92052330	-0.78157114	-0.35495955
1	0.22829031	-2.94583115	-1.01280245
1	-0.68101980	-2.30349564	-2.38978850
1	1.07537230	-2.10679671	-2.32728958
1	-4.20791642	2.50137622	-1.21826668
1	-3.14602614	1.20757646	-0.64776298
35	1.48768736	1.06242919	-3.82529917
5	-2.47239881	2.24428079	-2.47572242
35	-2.46309633	3.79829321	-3.63605927
35	-2.28903382	0.48407456	-3.47679818
6	-3.30773506	3.25057741	1.25367738
1	-4.35978380	3.46902128	1.00793021

1	-3.30236660	2.24647127	1.71217924
6	-2.80932019	4.28486177	2.26861715
1	-2.78039079	5.29180653	1.82582917
1	-1.80052954	4.05058238	2.63517733
1	-3.47436270	4.32492077	3.14243689
1	-0.53611013	3.54105802	0.77205009

**TS(24-25)**

$\nu = 394.73i \text{ cm}^{-1}$

6	0.41058594	3.09194143	-0.17792333
13	0.96500279	1.69934280	-1.63517895
6	-2.42339405	1.68454065	-0.78568689
6	-2.11519195	3.12297588	-0.35341868
6	-0.90178838	3.27111803	0.59560421
6	1.29594540	-0.19551599	-1.20283594
6	2.18001811	-0.95353442	-2.21135728
1	1.20670896	2.59072952	0.40034266
1	0.63708881	3.87095336	-0.91969889
1	-1.95840409	3.75592266	-1.24117406
1	-0.95094220	2.45382953	1.33735838
1	1.73955128	-0.23910919	-0.19333163
1	0.31404436	-0.69291873	-1.11934773
1	2.29822588	-2.01081568	-1.92991604
1	1.75104438	-0.92720375	-3.22295618
1	3.18828451	-0.51859885	-2.27451482
1	-2.53278465	1.03130133	0.10015316
1	-1.57632588	1.22960540	-1.33857160
35	0.28010873	2.27358228	-3.76554381
5	-3.67095040	1.42981315	-1.69825182
35	-4.81928515	2.84446410	-2.32746907
35	-4.10363876	-0.37979447	-2.22657395
6	-0.97157156	4.60303207	1.37672981
1	-0.01077948	4.76981535	1.88442235
1	-1.08902632	5.43508648	0.66311626
6	-2.08652880	4.65071880	2.42636815
1	-1.97058841	3.83914200	3.16033075
1	-3.08847935	4.56351661	1.98379541
1	-2.05562987	5.60160700	2.97560799
1	-3.00365954	3.52806328	0.15063849
35	2.83840391	3.57233738	2.12137476
5	2.21027022	4.07114550	0.31537992
35	3.22264647	3.00629570	-1.20623520
35	2.13974989	5.99494757	-0.06736304

**TS(26-30a)**

$\nu = 210.74i \text{ cm}^{-1}$

6	-0.06800831	4.08598688	-0.07702656
6	-1.73913248	2.62170722	-1.40892398
6	-2.40174669	3.27511611	-0.17701508
6	-1.22044779	3.52349275	0.77954879

1	-0.16421979	5.15896548	-0.31330432
1	0.81654824	4.16456890	0.59435122
1	-2.81170091	4.25665017	-0.47823802
1	-0.90581153	2.56718385	1.22966915
1	-2.38553713	2.62404363	-2.29650375
1	-1.51768028	1.56991519	-1.16362681
5	-0.39667080	3.45922802	-1.61452760
35	-0.30845827	4.79405085	-3.09066828
35	1.27374721	1.96116861	-2.08133616
35	2.07428613	1.98963342	1.13618075
5	1.72287502	3.12031050	-0.44904681
35	3.00499941	4.54726045	-0.85706517
6	-3.54138395	2.44427171	0.42600027
1	-4.27346077	2.22918136	-0.36906872
1	-3.13554803	1.46794171	0.74271660
6	-4.25673469	3.11629000	1.60281474
1	-4.66340033	4.09629665	1.31127405
1	-3.58129220	3.27376335	2.45569553
1	-5.09529992	2.50096733	1.95732330
1	-1.45915304	4.21002411	1.60398331

### TS(26-30b)

$\nu = 204.62i \text{ cm}^{-1}$

6	-0.08727060	4.08036716	-0.08013367
6	-1.75111110	2.62574430	-1.42984649
6	-2.40648878	3.30172023	-0.21091070
6	-1.25549176	3.54139262	0.78347973
1	-0.17487376	5.15567076	-0.31624212
1	0.78656982	4.15782263	0.60697798
1	-2.84981571	4.26949258	-0.50011061
1	-0.94340123	2.56099603	1.18584038
1	-2.38230369	2.63868860	-2.32751572
1	-1.54594948	1.57243920	-1.18476037
5	-0.39486137	3.45000325	-1.61470094
35	-0.27658515	4.77588043	-3.09777291
35	1.27267578	1.94141372	-2.04017326
6	-1.57923496	4.46834344	1.96297109
1	-0.66436763	4.62290280	2.55872846
1	-1.86389449	5.45959016	1.57012623
6	-2.68861922	3.93748686	2.87692466
1	-2.43178922	2.94444559	3.27465348
1	-3.64616559	3.84989213	2.34542450
1	-2.84495201	4.60935742	3.73194436
1	-3.20881766	2.69101145	0.22568090
35	2.04210748	2.00058304	1.18541974
5	1.70335615	3.11939809	-0.41378076
35	2.99466078	4.53870856	-0.82121978

### TS(27-28)

$\nu = 354.92i \text{ cm}^{-1}$



6	4.62948759	3.55331218	-1.80701293
13	5.76549382	2.93348326	-3.41222791
6	3.89785134	0.81786170	-3.04150654
6	3.33609118	1.31155167	-1.68538810
6	4.30159822	2.29331607	-0.99525309
6	7.47852027	2.00706488	-3.13681863
6	7.90624040	1.04187980	-4.25826545
1	5.50308050	4.16034631	-1.52670034
1	3.89650775	3.98455390	-2.49949031
1	2.38968399	1.84220738	-1.88400446
1	5.23499295	1.75852948	-0.74744258
1	8.22610124	2.81418494	-3.03053970
1	7.45920724	1.49464264	-2.16145270
1	8.90543803	0.62516495	-4.06380968
1	7.21288463	0.19380063	-4.35561022
1	7.94123941	1.54599336	-5.23369727
1	4.90811708	0.39237975	-2.91288342
1	3.94561756	1.67276178	-3.76377301
35	5.18118111	3.72895714	-5.47792691
5	3.00952085	-0.20475610	-3.84893084
35	1.16138916	0.18598221	-4.22080070
35	3.75998283	-1.83581512	-4.54672363
6	3.02917760	0.10642125	-0.77207042
1	2.39998302	-0.60367991	-1.33446318
1	3.97074994	-0.42761568	-0.55489185
6	2.31361107	0.45504183	0.53685599
1	1.39587056	1.02882386	0.34438509
1	2.94376740	1.04797250	1.21253850
1	2.03154689	-0.46150916	1.07264294
1	3.86673444	2.59353032	-0.03164197
35	4.44470013	6.68415438	-1.98577764
5	3.90646255	5.16248555	-0.80694928
35	1.93897641	4.86044447	-0.67711995
35	4.82865579	5.13670462	0.96646227

### TS(28-29)

$\nu = 236.45i \text{ cm}^{-1}$

6	4.75864277	2.81142301	-1.80520970
13	5.92335767	2.98144890	-3.50908041
6	3.59255261	-0.01684202	-2.69490686
6	3.13087141	0.82631966	-1.48941294
6	4.28670759	1.66781796	-0.91280735
6	7.87279216	2.71335665	-3.42713305
6	8.67731601	3.22288575	-4.63723916
1	5.56004429	3.40132309	-1.32559437
1	3.94653945	3.33497634	-2.33481104
1	2.34039659	1.51701498	-1.83130346
1	5.14024302	1.00491243	-0.69247855
1	8.23845894	3.17942711	-2.49605025
1	8.03582105	1.62828595	-3.29783797

1	9.74973768	2.99868761	-4.53382377
1	8.33152067	2.76265354	-5.57338754
1	8.58164456	4.31176988	-4.75793595
1	4.35446757	-0.74906545	-2.37988888
1	4.10650785	0.63298759	-3.43591253
35	4.81771450	2.63488881	-5.50646691
5	2.50806215	-0.73070555	-3.56641443
35	0.75281077	0.02805205	-3.85586234
35	2.92174988	-2.37890582	-4.48908614
6	2.51917371	-0.08675783	-0.40674185
1	1.82752808	-0.78985249	-0.89850322
1	3.32043208	-0.70718782	0.03150216
6	1.75813962	0.64513195	0.70303652
1	0.95160277	1.26381658	0.28338737
1	2.40924041	1.30114972	1.29730067
1	1.30132858	-0.07378634	1.39703417
1	3.97224403	2.08613288	0.05719537
35	5.40256889	5.54352407	-2.86400823
5	4.39009986	4.81844567	-1.18096071
35	2.46481646	5.19596312	-1.18509239
35	5.32167722	5.17853097	0.51689309

### TS(33-34a)

$\nu = 231.33i \text{ cm}^{-1}$

6	-3.43519756	-0.87066883	1.46240784
13	-1.36102195	-1.09161715	1.51161964
6	-1.08537786	0.36528028	-0.10650867
6	-2.40726555	1.09483572	0.26442387
6	-3.64027283	0.17871271	0.31211780
6	2.35544566	-2.40062099	0.29352863
6	1.86039401	-1.17162281	-0.50253933
13	-0.08606001	-1.47246572	-0.74189629
6	-0.08647655	-2.75319262	1.01551329
6	1.39593381	-2.67297128	1.47002450
6	-0.55812976	-0.26569428	3.13996173
6	-1.46587542	0.55591307	4.07234094
6	-0.87540523	-2.27659786	-2.38041229
6	0.03640791	-3.33877697	-3.03045786
1	2.30512349	-3.28335169	-0.37487517
6	4.42953208	-3.50596936	1.39685900
1	-4.49637862	0.81351224	0.60445313
6	-5.37996172	-1.02006824	-1.16434793
1	-4.43155928	-1.36282751	1.47092509
1	2.42146501	-1.06561934	-1.44399259
1	2.05508282	-0.25679156	0.08531457
1	-0.19648980	-3.52395381	0.22418428
1	-2.59631855	1.92020846	-0.44110981
1	1.51880872	-1.87090680	2.21660715
1	1.66895531	-3.61321413	1.97274935
1	-1.86283355	-2.71844749	-2.17475432

1	-1.06230429	-1.46553193	-3.10710482
1	-0.38915048	-3.72862814	-3.96825569
1	1.03171639	-2.93426299	-3.26855894
1	0.19208537	-4.20436697	-2.36816902
1	4.35149338	-4.37680404	0.72815386
1	5.49533920	-3.35281758	1.61813739
1	3.93295889	-3.76496407	2.34235241
1	-3.48842030	-0.35876153	2.44122416
6	3.82029003	-2.25737391	0.74847901
1	-1.04714676	0.38824341	-1.21705247
1	-0.23294351	0.98298298	0.21491680
1	-0.68453186	-3.23626536	1.80997211
1	-2.28388884	1.56531924	1.25376841
6	-3.97271322	-0.42469395	-1.06070721
1	-0.10588572	-1.08785873	3.71982226
1	0.29317816	0.35630190	2.81122423
1	-0.91455745	0.94165530	4.94397791
1	-1.90662483	1.42798868	3.56511688
1	-2.29831942	-0.04823755	4.46278983
1	-6.14522623	-0.26608697	-0.92611839
1	-5.57391087	-1.38258631	-2.18315479
1	-5.52414097	-1.87272938	-0.48688162
1	-3.22773620	-1.18986362	-1.32483663
1	-3.87090549	0.37898687	-1.81009924
1	3.88723723	-1.40372188	1.44541377
1	4.42250197	-1.97884717	-0.13144756
17	-2.70800959	-3.11146998	3.35682059
5	-3.73441818	-2.89725471	1.84583918
17	-3.21132266	-3.82079738	0.37200857
17	-5.51741014	-3.16403914	2.23498096

### TS(33-34b)

$\nu = 348.53i \text{ cm}^{-1}$

6	-3.39000314	-1.11861776	0.60241430
13	-1.63541034	-0.91427107	1.49215158
6	-0.88343718	0.43212220	-0.02103513
6	-2.27973954	1.11824203	0.14857284
6	-3.49963894	0.21637902	-0.18962900
6	2.68074572	-2.38112767	0.13611166
6	2.14380092	-1.04668576	-0.42533169
13	0.20395958	-1.41873738	-0.48869039
6	0.37440877	-2.72164795	1.31237437
6	1.91165893	-2.74087421	1.42539711
6	-1.19731705	-0.21706740	3.30081022
6	-2.43445474	-0.08081020	4.21110918
6	-0.60093808	-2.42876431	-2.00253805
6	-0.41371361	-1.77230797	-3.38556081
1	2.47573672	-3.17948884	-0.60531687
6	4.82374591	-3.70787987	0.76469987
1	-4.38637486	0.77015988	0.16456111

6	-4.99678610	-0.61722746	-2.09816979
1	-3.43914228	-1.99719090	-0.05483532
1	2.59725387	-0.81839443	-1.40220546
1	2.40994851	-0.22202470	0.25820911
1	-0.15197432	-3.48979765	0.73495154
1	-2.30087825	2.04353515	-0.44933623
1	2.19173618	-2.01534859	2.20683602
1	2.23063746	-3.72793806	1.79181646
1	-0.10315759	-3.41552031	-2.00530749
1	-1.66646675	-2.65017844	-1.82969341
1	-0.80257842	-2.40204315	-4.20107920
1	-0.93408524	-0.80397354	-3.45885339
1	0.64777712	-1.58016942	-3.60339204
1	4.58758542	-4.48552789	0.02264205
1	5.91846080	-3.63092201	0.82666136
1	4.46419867	-4.05845591	1.74175555
1	-4.19903322	-1.23298925	1.33764409
6	4.20424997	-2.36243140	0.36904666
1	-0.68600882	0.44784605	-1.11316191
1	-0.10518565	1.06483928	0.43010624
1	-0.12248874	-2.29660028	2.19192150
1	-2.38190905	1.45454912	1.19876935
6	-3.66213076	0.02227905	-1.70630428
1	-0.44325166	-0.84460163	3.80198708
1	-0.71226161	0.76597765	3.16645039
1	-2.17275452	0.34814410	5.19035873
1	-3.20481751	0.56878359	3.76791458
1	-2.90388904	-1.05701469	4.39823486
1	-5.84268492	0.00605878	-1.77165593
1	-5.07184087	-0.74138993	-3.18727194
1	-5.11786102	-1.60915103	-1.64050413
1	-2.83541560	-0.59802891	-2.08792190
1	-3.57186586	1.00359340	-2.20369145
1	4.42810635	-1.60483153	1.14039771
1	4.68214203	-2.00391566	-0.55678721
17	-2.13742363	-3.82372135	2.52845615
5	-0.34051956	-4.23857062	2.60636797
17	0.43800460	-3.91199971	4.20838000
17	0.11850570	-5.81307264	1.84363391

### The 3 $\zeta$ basis set

	basis	basis2
H	{5s2p}/[3s1p]	{5s2p}
B	{11s6p2d}/[6s3p2d]	{10s3p3d1f}
C	{11s6p2d}/[6s3p2d]	{10s3p3d1f}
F	{11s6p2d}/[6s3p2d]	{10s3p3d1f}
Al	{15s11p2d}/[10s6p2d]	{14s3p3d1f1g}
Cl	{15s11p2d}/[10s6p2d]	{14s3p3d1f1g}
Br	{18s14p9d}/[13s10p5d]	{18s3p3d1f1g}

\$BASIS

default=3z

set=3z

	1	4		
0	3	2.951830e+1	2.663542e-2	
		4.459397e+0	1.992677e-1	
		1.020214e+0	8.443136e-1	
0	1	2.789184e-1	1.0	
0	1	8.185002e-2	1.0	
1	1	1.020214e+0	1.0	

	5	11		
0	6	1.358868e+4	4.892238e-4	
		2.036685e+3	3.795693e-3	
		4.634536e+2	1.979014e-2	
		1.310157e+2	8.118179e-2	
		4.229295e+1	2.713876e-1	
		1.468394e+1	7.086939e-1	
0	1	5.272553e+0	1.0	
0	1	1.917192e+0	1.0	
0	1	6.072388e-1	1.0	
0	1	2.069688e-1	1.0	
0	1	6.607158e-2	1.0	
1	4	1.468394e+1	2.156235e-2	
		5.272553e+0	5.694623e-2	
		1.917192e+0	2.686221e-1	
		6.072388e-1	7.674997e-1	
1	1	2.069688e-1	1.0	
1	1	6.607158e-2	1.0	
2	1	6.072388e-1	1.0	
2	1	2.069688e-1	1.0	

	6	11		
0	6	2.192464e+4	4.524117e-4	

		3.285791e+3	3.511161e-3
		7.474901e+2	1.834054e-2
		2.109105e+2	7.595411e-2
		6.756323e+1	2.620972e-1
		2.308674e+1	7.228794e-1
0	1	8.151221e+0	1.0
0	1	2.947252e+0	1.0
0	1	9.660187e-1	1.0
0	1	3.231446e-1	1.0
0	1	1.010825e-1	1.0
1	4	2.308674e+1	2.068355e-2
		8.151221e+0	6.066722e-2
		2.947252e+0	2.747077e-1
		9.660187e-1	7.569660e-1
1	1	3.231446e-1	1.0
1	1	1.010825e-1	1.0
2	1	9.660187e-1	1.0
2	1	3.231446e-1	1.0

9 11

0	6	5.708712e+4	3.900913e-4
		8.554214e+3	3.028942e-3
		1.944314e+3	1.588079e-2
		5.453350e+2	6.713141e-2
		1.708447e+2	2.467701e-1
		5.590937e+1	7.474134e-1
0	1	1.888258e+1	1.0
0	1	6.650594e+0	1.0
0	1	2.215890e+0	1.0
0	1	7.191028e-1	1.0
0	1	2.115702e-1	1.0
1	4	5.590937e+1	1.993210e-2
		1.888258e+1	7.061877e-2
		6.650594e+0	3.007673e-1
		2.215890e+0	7.277287e-1
1	1	7.191028e-1	1.0
1	1	2.115702e-1	1.0
2	1	2.215890e+0	1.0
2	1	7.191028e-1	1.0

13 18

0	6	2.382966e+5	3.811725e-4
		3.569645e+4	2.962297e-3
		8.116019e+3	1.557456e-2
		2.284096e+3	6.609540e-2
		7.300537e+2	2.418684e-1
		2.546557e+2	7.476854e-1
0	1	9.502825e+1	1.0
0	1	3.741167e+1	1.0

0	1	1.536696e+1	1.0
0	1	6.290235e+0	1.0
0	1	2.543955e+0	1.0
0	1	1.012528e+0	1.0
0	1	3.453793e-1	1.0
0	1	1.253362e-1	1.0
0	1	4.096564e-2	1.0
1	6	7.300537e+2	1.232426e-3
		2.546557e+2	5.132843e-3
		9.502825e+1	2.674667e-2
		3.741167e+1	9.921941e-2
		1.536696e+1	3.081204e-1
		6.290235e+0	6.701420e-1
1	1	2.543955e+0	1.0
1	1	1.012528e+0	1.0
1	1	3.453793e-1	1.0
1	1	1.253362e-1	1.0
1	1	4.096564e-2	1.0
2	1	3.453793e-1	1.0
2	1	1.253362e-1	1.0

17 18

0	6	4.886680e+5	3.683119e-4
		7.319565e+4	2.862919e-3
		1.663917e+4	1.506844e-2
		4.678381e+3	6.424228e-2
		1.491358e+3	2.379472e-1
		5.186839e+2	7.529444e-1
0	1	1.935542e+2	1.0
0	1	7.648497e+1	1.0
0	1	3.167528e+1	1.0
0	1	1.322806e+1	1.0
0	1	5.558031e+0	1.0
0	1	2.335902e+0	1.0
0	1	8.433804e-1	1.0
0	1	3.183365e-1	1.0
0	1	1.082213e-1	1.0
1	6	1.491358e+3	1.074090e-3
		5.186839e+2	4.581779e-3
		1.935542e+2	2.412967e-2
		7.648497e+1	9.277696e-2
		3.167528e+1	2.982536e-1
		1.322806e+1	6.822171e-1
1	1	5.558031e+0	1.0
1	1	2.335902e+0	1.0
1	1	8.433804e-1	1.0
1	1	3.183365e-1	1.0
1	1	1.082213e-1	1.0
2	1	8.433804e-1	1.0
2	1	3.183365e-1	1.0

35 28

0	6	4.183132e+6	3.518723e-4
		6.264457e+5	2.736140e-3
		1.424236e+5	1.441783e-2
		4.008375e+4	6.165851e-2
		1.281741e+4	2.308731e-1
		4.483365e+3	7.608863e-1
0	1	1.686773e+3	1.0
0	1	6.705166e+2	1.0
0	1	2.774937e+2	1.0
0	1	1.186309e+2	1.0
0	1	5.205105e+1	1.0
0	1	2.339561e+1	1.0
0	1	1.059655e+1	1.0
0	1	4.688213e+0	1.0
0	1	2.015214e+0	1.0
0	1	7.912240e-1	1.0
0	1	3.004622e-1	1.0
0	1	1.010219e-1	1.0
1	5	1.281741e+4	2.089890e-3
		4.483365e+3	9.199630e-3
		1.686773e+3	4.878943e-2
		6.705166e+2	2.120892e-1
		2.774937e+2	7.960288e-1
1	1	1.186309e+2	1.0
1	1	5.205105e+1	1.0
1	1	2.339561e+1	1.0
1	1	1.059655e+1	1.0
1	1	4.688213e+0	1.0
1	1	2.015214e+0	1.0
1	1	7.912240e-1	1.0
1	1	3.004622e-1	1.0
1	1	1.010219e-1	1.0
2	5	2.774937e+2	5.848704e-3
		1.186309e+2	2.303397e-2
		5.205105e+1	1.032942e-1
		2.339561e+1	3.140592e-1
		1.059655e+1	6.729262e-1
2	1	4.688213e+0	1.0
2	1	2.015214e+0	1.0
2	1	7.912240e-1	1.0
2	1	3.004622e-1	1.0

\$END

\$Basis2



default=3z

set=3z

1 7

0	1	2.04937577e-01	1.0
0	1	5.52861763e-01	1.0
1	1	5.52861763e-01	1.0
0	1	1.49145966e+00	1.0
1	1	1.49145966e+00	1.0
0	1	4.02352281e+00	1.0
0	1	1.08542901e+01	1.0

5 17

0	1	1.28115547e-01	1.0
0	1	3.23423392e-01	1.0
1	1	3.23423392e-01	1.0
2	1	3.23423392e-01	1.0
0	1	8.16471480e-01	1.0
1	1	8.16471480e-01	1.0
2	1	8.16471480e-01	1.0
3	1	8.16471480e-01	1.0
0	1	2.06115480e+00	1.0
1	1	2.06115480e+00	1.0
2	1	2.06115480e+00	1.0
0	1	5.20331602e+00	1.0
0	1	1.31355964e+01	1.0
0	1	3.31603715e+01	1.0
0	1	8.37122431e+01	1.0
0	1	2.11328744e+02	1.0
0	1	5.33492309e+02	1.0

6 17

0	1	1.75774940e-01	1.0
0	1	4.40360864e-01	1.0
1	1	4.40360864e-01	1.0
2	1	4.40360864e-01	1.0
0	1	1.10321580e+00	1.0
1	1	1.10321580e+00	1.0
2	1	1.10321580e+00	1.0
3	1	1.10321580e+00	1.0
0	1	2.76383573e+00	1.0
1	1	2.76383573e+00	1.0
2	1	2.76383573e+00	1.0
0	1	6.92411041e+00	1.0
0	1	1.73466550e+01	1.0
0	1	4.34577760e+01	1.0
0	1	1.08872765e+02	1.0

0	1	2.72753926e+02	1.0
0	1	6.83317851e+02	1.0

9 17

0	1	3.44930222e-01	1.0
0	1	8.78520791e-01	1.0
1	1	8.78520791e-01	1.0
2	1	8.78520791e-01	1.0
0	1	2.23755047e+00	1.0
1	1	2.23755047e+00	1.0
2	1	2.23755047e+00	1.0
3	1	2.23755047e+00	1.0
0	1	5.69893411e+00	1.0
1	1	5.69893411e+00	1.0
2	1	5.69893411e+00	1.0
0	1	1.45149128e+01	1.0
0	1	3.69687893e+01	1.0
0	1	9.41577396e+01	1.0
0	1	2.39815263e+02	1.0
0	1	6.10798014e+02	1.0
0	1	1.55567335e+03	1.0

13 22

0	1	6.36338538e-02	1.0
0	1	1.46064791e-01	1.0
1	1	1.46064791e-01	1.0
2	1	1.46064791e-01	1.0
0	1	3.35276303e-01	1.0
1	1	3.35276303e-01	1.0
2	1	3.35276303e-01	1.0
3	1	3.35276303e-01	1.0
4	1	3.35276303e-01	1.0
0	1	7.69591345e-01	1.0
1	1	7.69591345e-01	1.0
2	1	7.69591345e-01	1.0
0	1	1.76651566e+00	1.0
0	1	4.05485013e+00	1.0
0	1	9.30748025e+00	1.0
0	1	2.13643380e+01	1.0
0	1	4.90395816e+01	1.0
0	1	1.12565181e+02	1.0
0	1	2.58381484e+02	1.0
0	1	5.93087410e+02	1.0
0	1	1.36136951e+03	1.0
0	1	3.12487995e+03	1.0

17 22

0	1	2.01070734e-01	1.0
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0	1	4.40284706e-01	1.0
1	1	4.40284706e-01	1.0
2	1	4.40284706e-01	1.0
0	1	9.64091681e-01	1.0
1	1	9.64091681e-01	1.0
2	1	9.64091681e-01	1.0
3	1	9.64091681e-01	1.0
4	1	9.64091681e-01	1.0
0	1	2.11107213e+00	1.0
1	1	2.11107213e+00	1.0
2	1	2.11107213e+00	1.0
0	1	4.62261589e+00	1.0
0	1	1.01221448e+01	1.0
0	1	2.21644664e+01	1.0
0	1	4.85335452e+01	1.0
0	1	1.06273933e+02	1.0
0	1	2.32708094e+02	1.0
0	1	5.09561051e+02	1.0
0	1	1.11578613e+03	1.0
0	1	2.44323756e+03	1.0
0	1	5.34995874e+03	1.0

35 26

0	1	1.57524529e-01	1.0
0	1	3.17148739e-01	1.0
1	1	3.17148739e-01	1.0
2	1	3.17148739e-01	1.0
0	1	6.38524826e-01	1.0
1	1	6.38524826e-01	1.0
2	1	6.38524826e-01	1.0
3	1	6.38524826e-01	1.0
4	1	6.38524826e-01	1.0
0	1	1.28556070e+00	1.0
1	1	1.28556070e+00	1.0
2	1	1.28556070e+00	1.0
0	1	2.58825692e+00	1.0
0	1	5.21101332e+00	1.0
0	1	1.04914854e+01	1.0
0	1	2.11228143e+01	1.0
0	1	4.25271794e+01	1.0
0	1	8.56212133e+01	1.0
0	1	1.72383691e+02	1.0
0	1	3.47065125e+02	1.0
0	1	6.98756360e+02	1.0
0	1	1.40682660e+03	1.0
0	1	2.83240512e+03	1.0
0	1	5.70256402e+03	1.0
0	1	1.14811388e+04	1.0
0	1	2.31153124e+04	1.0

**Table S4.** Energy effects and activation barriers of reactions calculated by PBE/3 $\zeta$ , PBE/6-31G(d,p), PBE(GD3)/6-31G(d,p), PBE0/6-31G(d,p), PBE0(GD3)/6-31G(d,p) methods.

Reaction	$\Delta E_r$ , kcal/mol					$\Delta E^\ddagger$ , kcal/mol				
	PBE/3 $\zeta$	PBE/6-31G(d,p)	PBE(GD3)/6-31G(d,p)	PBE0/6-31G(d,p)	PBE0(GD3)/6-31G(d,p)	PBE/3 $\zeta$	PBE/6-31G(d,p)	PBE(GD3)/6-31G(d,p)	PBE0/6-31G(d,p)	PBE0(GD3)/6-31G(d,p)
<b>3+4→5a</b>	-1.4	-6.2	-8.7	-5.3	-7.8					
<b>5a→6a</b>	-20.3	-20.5	-21.0	-20.4	-21.0	0.3	-1.4	-1.9	-1.0	-1.5
<b>6a→7a</b>	-15.2	-16.5	-15.9	-17.9	-17.1	-2.8	-6.8	-7.3	-6.5	-7.0
<b>7a→8+9</b>	10.0	16.8	19.1	17.3	19.7					
<b>3+4→5b</b>	-1.1	-5.2	-7.5	-4.5	-6.7					
<b>5b→6b</b>	-20.7	-21.8	-22.8	-21.7	-22.8	1.0	-1.6	-2.2	-1.0	-1.7
<b>6b→7b</b>	-15.1	-16.0	-15.2	-17.4	-16.4	4.5	1.0	0.9	1.7	1.6
<b>7b→8+9</b>	10.0	16.7	19.0	17.3	19.6					
<b>6a+4→10a</b>	-1.1	-2.6	-4.3	-2.3	-3.9					
<b>10a→11a</b>	-22.0	-26.5	-27.6	-26.9	-28.1	4.6	-2.1	-3.9	-0.9	-2.8
<b>11a→8+12</b>	9.0	16.6	19.5	16.8	19.7					
<b>12→13a</b>	6.1	8.0	9.7	7.2	9.1	27.7	24.0	23.6	25.6	25.1
<b>13a→4+9</b>	2.7	4.8	6.0	4.6	5.9					
<b>6b+4→10b</b>	-1.1	-2.7	-4.6	-2.4	-4.2					
<b>10b→11b</b>	-22.9	-27.6	-28.4	-28.2	-29.0	3.5	-3.2	-4.5	-2.4	-3.8
<b>11b→8+12</b>	10.1	18.3	21.2	18.6	21.5					
<b>12→13b</b>	6.1	8.0	9.7	7.2	9.1	26.4	23.2	23.0	24.6	24.3
<b>13b→4+9</b>	2.7	4.8	6.0	4.6	5.9					
<b>3+4'→5a'</b>	-0.9	-1.6	-4.7	-1.4	-4.4					
<b>5a'→6a'</b>	-33.1	-33.8	-36.2	-35.9	-38.6	3.4	3.0	0.7	4.1	1.7
<b>6a'→7a'</b>	-23.2	-22.8	-21.8	-24.5	-23.3	2.7	1.7	0.5	2.3	0.9
<b>7a'→8'+9'</b>	7.9	9.6	13.0	9.8	13.3					
<b>3+4'→5b'</b>	-1.2	-1.8	-4.8	-1.6	-4.6					
<b>5b'→6b'</b>	-31.8	-32.8	-35.8	-34.8	-38.0	3.8	3.3	1.2	4.5	2.2
<b>6b'→7b'</b>	-23.4	-22.5	-21.1	-24.4	-22.8	6.4	6.2	6.0	7.2	6.9
<b>7b'→8'+9'</b>	7.1	8.6	12.1	8.8	12.5					

<b>6a'+4'&gt;10a'</b>	-0.1	-0.7	-3.1	-0.5	-2.9					
<b>10a'→11a'</b>	-26.6	-27.0	-29.2	-28.8	-31.0	10.0	8.9	5.3	10.1	6.4
<b>11a'→8'+12'</b>	6.9	8.2	12.4	8.3	12.6					
<b>12'→13a'</b>	3.6	5.2	7.7	5.1	8.0	35.2	35.7	35.3	37.3	36.5
<b>13a'→4'+9'</b>	1.0	1.2	3.4	1.1	3.2					
<b>6b'+4'→10b'</b>	-0.7	-1.3	-3.6	-1.1	-3.4					
<b>10b'→11b'</b>	-28.8	-28.9	-28.8	-30.8	-30.8	15.2	15.7	14.1	17.1	15.4
<b>11b'→8'+12'</b>	8.6	9.9	12.3	10.0	12.6					
<b>12'→13b'</b>	3.6	5.1	7.7	5.1	8.0	35.9	36.4	36.2	38.0	37.4
<b>13b'→4'+9'</b>	1.0	1.2	3.4	1.2	3.3					
<b>3+14→15</b>	-0.4	-1.9	-4.3	-1.7	-4.1					
<b>15→16</b>	-1.3	-4.7	-8.1	-6.1	-10.0	9.2	5.9	2.9	6.6	3.2
<b>16→17</b>	-33.3	-36.6	-35.7	-37.4	-36.3	1.6	0.8	1.3	1.4	1.9
<b>17→18</b>	-26.8	-37.8	-37.6	-40.2	-40.0	-0.3	-10.4	-12.5	-10.0	-12.2
<b>18→19+20</b>	7.3	18.9	22.3	18.9	22.6					
<b>3+14→21</b>	-0.2	-1.7	-3.9	-1.5	-3.7					
<b>21→22</b>	-34.1	-40.7	-44.3	-43.0	-46.7	14.3	9.2	5.5	10.1	5.9
<b>22→23</b>	-27.5	-38.5	-37.5	-40.9	-39.8	-1.4	-11.4	-12.6	-11.0	-12.4
<b>23→19+20</b>	7.3	18.8	22.2	18.9	22.5					
<b>17+14→24</b>	-1.2	-4.2	-7.1	-4.0	-6.9					
<b>24→25</b>	-29.7	-43.3	-45.0	-46.0	-48.1	15.5	4.8	1.2	6.0	1.9
<b>25→26+19</b>	7.8	19.1	21.9	19.4	22.6					
<b>22+14→27</b>	-0.9	-2.7	-5.6	-2.5	-5.3					
<b>27→28</b>	12.9	8.1	4.1	7.6	3.0	16.1	11.0	7.5	11.6	7.4
<b>28→29</b>	-44.7	-55.7	-53.8	-57.8	-55.7	-0.3	-4.4	-2.7	-2.8	-0.9
<b>29→26+19</b>	8.9	21.2	25.2	21.4	25.7					
<b>26→30a</b>	2.7	6.1	8.9	6.2	9.3	28.6	25.1	24.8	26.8	26.2
<b>30a→14+20</b>	0.9	3.3	5.9	3.2	5.7					
<b>26→30b</b>	2.9	6.7	9.1	6.8	9.6	28.6	25.1	24.5	26.8	25.8
<b>30b→14+20</b>	0.7	2.8	5.7	2.5	5.4					
<b>33+4'→34a</b>	-28.4	-30.0	-35.1	-31.7	-36.9	16.7	15.2	7.7	16.0	8.1
<b>33+4'→34b</b>	-33.2	-33.0	-35.6	-34.6	-37.2	21.3	20.3	14.8	22.9	17.2
<b>6a+THF→ 7a+THF</b>	-27.1	-25.3	-23.2	-27.2	-24.9	16.8	16.7	14.6	17.8	15.5
<b>6a+2THF→ 7a+2THF</b>	-24.8	-22.2	-18.6	-22.4	-17.9	20.0	21.4	22.7	24.3	25.8

<b>6b+THF</b> → <b>7b+THF</b>	-29.7	-28.1	-25.5	-30.0	-27.2	14.0	14.2	13.2	15.1	13.9
<b>6b+2THF</b> → <b>7b+2THF</b>	-5.2	-1.7	2.3	0.8	5.7	15.7	17.6	19.3	20.2	22.1

It follows from Table S4 the results are not very sensitive to the functional and basis set.

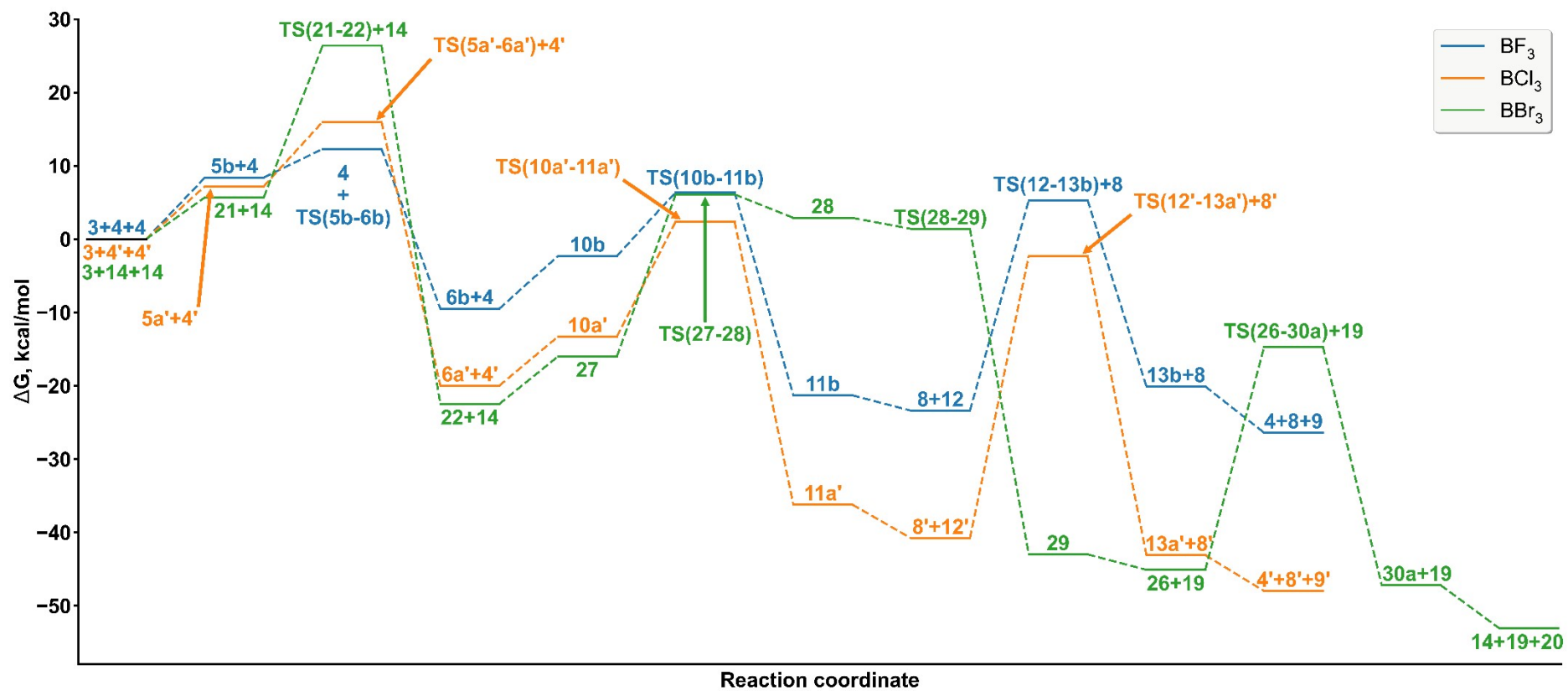


Figure S1. Energy diagram of route 2 of the reaction between 1,3-diethylalumolane and BHal<sub>3</sub>.