Chemistry of Heterocyclic Compounds **2023**, *59*(3), 145–154

Unveiling the exclusive stereo and site selectivity in [3+2] cycloaddition reactions of a tricyclic strained alkene with nitrile oxides from the molecular electron density theory perspective

Asmita Mondal[1], Nivedita Acharjee[1]*

[1] *Department of Chemistry, Durgapur Government College, Durgapur, West Bengal 713214, India; e-mail: nivchem@gmail.com*

SUPPLEMENTARY INFORMATION

Index

Table S1. MPWB1K/6-311G(d,p) calculated C-C and C-O bond distances along with the GEDT in average number of electrons and the bond development indices $l_{C\text{-}C}$ and $l_{O\text{-}C}$ of the optimized TSs in gas phase.

TS	C-C	C-O	GEDT	$l_{C\text{-}C}$	$l_{O\text{-}C}$	Δa
TS1	2.224	2.402	0.02	0.50	0.32	0.17
TS2	2.072	2.505	0.04	0.60	0.24	0.36
TS3	2.133	2.364	0.01	0.57	0.35	0.22
TS4	2.098	2.419	0.04	0.59	0.31	0.28
TS5	2.215	2.404	0.02	0.52	0.32	0.20
TS6	2.122	2.407	0.05	0.58	0.31	0.27
TS7	2.208	2.202	0.02	0.53	0.46	0.07
TS8	2.187	2.243	0.05	0.55	0.43	0.12

Table S2. MPWB1K/6-311G(d,p) calculated total electronic energies, in a.u, of the reactants involved in the *zw-type* 32CA reactions of BNO **2** and CNO **10** with SA **8**

Reactants	Gas phase	DCM
2	-399.530839	-399.541277
8	-577.837187	-577.855948
10	-168.532260	-168.540606

Table S3. MPWB1K /6-311G(d,p) total enthalpies (H, in a.u.), entropies (S, in cal·mol^{-1}K^{-1}) and Gibbs free energies (G, in a.u.), computed at 25 ºC in DCM, of the reactants involved in the *zw-type* 32CA reactions of BNO **2** and CNO **10** with SA **8**

Reactants	H	S	G
2	-399.427887	84.600	-399.468083
8	-577.609134	98.169	-577.655777
10	-168.515371	54.084	-168.541068

Table S4. MPWB1K/6-311G(d,p) calculated total electronic energies, in a.u, of the stationary points involved in the *zw-type* 32CA reactions of BNO **2** and CNO **10** with SA **8**

TSs	Gas phase	DCM	Products	Gas phase	DCM
TS1	-746.349775	-746.374147	**14**	-746.467246	-746.493175
TS2	-746.335940	-746.354615	**15**	-746.455902	-746.476513
TS3	-746.341000	-746.363669	**16**	-746.451053	-746.476896
TS4	-746.346683	-746.365111	**17**	-746.447351	-746.466663
TS5	-977.350826	-977.376030	**9**	-977.467906	-977.495306
TS6	-977.331045	-977.351403	**11**	-977.450075	-977.472215
TS7	-977.339046	-977.362413	**12**	-977.444786	-977.472921
TS8	-977.344233	-977.360605	**13**	-977.445301	-977.465074

Table S5. MPWB1K /6-311G(d,p) total enthalpies (H, in a.u.), entropies (S, in cal·mol^{-1}K^{-1}) and Gibbs free energies (G, in a.u.), computed at 25 ºC in DCM, of the stationary points involved in the *zw-type* 32CA reactions of BNO **2** and CNO **10** with SA **8**

TSs	H	S	G	Products	H	S	G
TS1	-746.101675	113.005	-746.155368	**14**	-746.215229	106.472	-746.265817
TS2	-746.081247	109.600	-746.133321	**15**	-746.196668	102.948	-746.245582
TS3	-746.091504	118.002	-746.147571	**16**	-746.19841	108.740	-746.250076
TS4	-746.091119	109.215	-746.143011	**17**	-746.187935	106.922	-746.238736
TS5	-977.014371	134.713	-977.078377	**9**	-977.130003	124.032	-977.188935
TS6	-976.989196	129.979	-977.050953	**11**	-977.105401	129.484	-977.166924
TS7	-977.002357	133.142	-977.065617	**12**	-977.106926	131.011	-977.169174
TS8	-976.997519	131.303	-977.059906	**13**	-977.097787	127.552	-977.158391

MPWB1K/6-311G(d,p) gas phase computed Cartesian coordinates of the stationary points involved in the 32CA reaction of BNO **2** and CNO **10** with SA **8** in gas phase

2 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.462793	-0.000037	0.000000
2	7	0	2.612560	-0.000011	0.000002
3	8	0	3.802579	0.000019	0.000002
4	6	0	0.042928	-0.000043	-0.000004
5	6	0	-0.654700	1.202704	-0.000012
6	6	0	-0.654745	-1.202722	0.000004
7	6	0	-2.032268	1.196226	0.000011
8	1	0	-0.110282	2.131543	-0.000019
9	6	0	-2.032345	-1.196178	-0.000008
10	1	0	-0.110420	-2.131615	0.000002
11	6	0	-2.723293	0.000027	0.000002
12	1	0	-2.568666	2.130481	0.000018
13	1	0	-2.568742	-2.130433	0.000005
14	1	0	-3.800659	0.000080	0.000005

8 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.450744	-1.097945	-0.502844
2	6	0	0.658293	-1.880346	0.481894
3	6	0	-0.658158	-1.880390	0.481886
4	6	0	-1.450654	-1.098038	-0.502854
5	6	0	-0.773875	0.204296	-0.935367
6	1	0	1.227630	-2.475734	1.178271
7	1	0	1.581107	-1.724467	-1.391686
8	1	0	-1.580980	-1.724577	-1.391689
9	1	0	-1.227466	-2.475817	1.178253
10	8	0	2.713823	-0.859356	0.076149
11	1	0	3.263272	-0.430493	-0.571396
12	8	0	-2.713754	-0.859531	0.076133
13	1	0	-3.263252	-0.430770	-0.571438
14	6	0	-1.110407	1.424200	-0.035113
15	1	0	-2.130897	1.771606	-0.137093
16	6	0	-0.000056	2.373806	-0.463741
17	1	0	-0.000090	3.298609	0.104120
18	1	0	-0.000029	2.585726	-1.531888
19	6	0	-0.662523	1.093441	1.359321
20	6	0	0.773894	0.204350	-0.935345
21	6	0	1.110312	1.424246	-0.035047
22	1	0	2.130795	1.771692	-0.136959
23	6	0	0.662352	1.093409	1.359345
24	1	0	-1.125103	0.439874	-1.939082
25	1	0	1.125144	0.439986	-1.939041
26	1	0	1.316497	0.769611	2.149309
27	1	0	-1.316712	0.769673	2.149260

10 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.163931
2	1	0	0.000000	0.000000	-2.218928
3	7	0	0.000000	0.000000	-0.017427
4	8	0	0.000000	0.000000	1.165563

14 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.842408	1.421600	0.039362
2	6	0	-1.936209	0.647555	-1.227426
3	6	0	-1.920075	-0.671088	-1.232845
4	6	0	-1.807478	-1.450345	0.028179
5	6	0	-0.894593	-0.782658	1.057858
6	1	0	-2.058240	1.223232	-2.131722
7	1	0	-2.847943	1.471834	0.470170
8	1	0	-2.810476	-1.523294	0.462613
9	1	0	-2.027301	-1.242433	-2.141508
10	8	0	-1.415990	2.722478	-0.290406
11	1	0	-1.441343	3.257620	0.495842
12	8	0	-1.354952	-2.737424	-0.312212
13	1	0	-1.319178	-3.267370	0.477220
14	6	0	0.597234	-1.104077	0.917024
15	1	0	0.860949	-2.117280	1.193928
16	6	0	1.211980	0.018297	1.742355
17	1	0	2.296733	0.023757	1.699997
18	1	0	0.890095	0.009847	2.780510
19	6	0	1.083609	-0.742605	-0.473026
20	6	0	-0.917484	0.769912	1.068267
21	6	0	0.566397	1.131863	0.927510
22	1	0	0.794398	2.149005	1.225000
23	6	0	1.046128	0.787047	-0.484880
24	8	0	2.468262	-1.084684	-0.607069
25	6	0	2.488989	1.063468	-0.718991
26	1	0	2.939018	2.034107	-0.838489
27	7	0	3.222455	0.039995	-0.778603
28	1	0	-1.198806	-1.140151	2.040393
29	1	0	-1.235515	1.108601	2.053261
30	1	0	0.424106	1.234018	-1.251392
31	1	0	0.541221	-1.238241	-1.268435

15 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.604525	-1.187445	-0.681104
2	6	0	0.796260	-2.020801	0.244145
3	6	0	-0.515832	-2.119657	0.178590
4	6	0	-1.369665	-1.384177	-0.794238
5	6	0	-0.705707	-0.122477	-1.362398
6	1	0	1.361400	-2.586346	0.968806
7	1	0	1.923575	-1.842152	-1.497626
8	1	0	-1.566417	-2.054359	-1.630591
9	1	0	-1.047467	-2.770557	0.856399
10	8	0	2.758337	-0.758350	0.015231
11	1	0	3.379850	-0.418222	-0.619481
12	8	0	-2.637579	-1.108745	-0.262112
13	1	0	-2.486132	-0.694150	0.588633
14	6	0	-1.170302	1.222717	-0.793753
15	1	0	-2.191138	1.452886	-1.070552
16	6	0	-0.078659	2.134644	-1.362190
17	1	0	-0.158354	3.166128	-1.027409
18	1	0	-0.036629	2.114390	-2.447883
19	6	0	-0.889189	1.437383	0.688215
20	6	0	0.843528	-0.014476	-1.300910
21	6	0	1.072392	1.375060	-0.694676
22	1	0	2.068565	1.759818	-0.880393
23	6	0	0.633805	1.551368	0.763423
24	8	0	-1.227746	0.382138	1.583402
25	6	0	0.907409	0.568613	1.840290
26	1	0	1.866185	0.340287	2.268165
27	7	0	-0.112650	-0.014090	2.293902
28	1	0	0.955714	2.538929	1.087162
29	1	0	-1.404919	2.328032	1.037286
30	1	0	-0.994740	-0.077352	-2.409565
31	1	0	1.203570	0.076435	-2.324789

16 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.213570	-0.743445	0.420676
2	6	0	1.201299	0.778906	0.424994
3	6	0	0.426702	-1.362593	-0.715730
4	1	0	1.018185	-1.195201	-1.614150
5	6	0	0.401045	1.415372	-0.704908
6	1	0	0.960802	1.271263	-1.627440
7	8	0	0.344612	-2.753939	-0.588047
8	1	0	-0.053939	-2.951820	0.254407
9	8	0	0.334712	2.806380	-0.541015
10	1	0	-0.201233	2.986427	0.226173
11	6	0	-0.967463	0.796013	-0.908688
12	1	0	-1.332040	1.176905	-1.859611
13	6	0	-0.946733	-0.746737	-0.934550
14	1	0	-1.279050	-1.104183	-1.905724
15	6	0	-2.062690	-1.122361	0.077220
16	1	0	-2.416992	-2.140460	-0.027645
17	6	0	-2.074439	1.107082	0.136545
18	1	0	-2.447181	2.123962	0.089352
19	6	0	-1.634084	-0.705863	1.456708
20	1	0	-1.325428	-1.370575	2.246285
21	6	0	-1.638946	0.620362	1.491757
22	1	0	-1.335504	1.244718	2.315585
23	6	0	-3.057958	-0.004542	-0.229441
24	1	0	-3.367926	0.021879	-1.271703
25	1	0	-3.925266	-0.025704	0.422058
26	8	0	2.588807	-1.113509	0.288369
27	7	0	3.373120	0.000699	0.223177
28	6	0	2.662065	1.037113	0.304487
29	1	0	3.126008	2.006637	0.260291
30	1	0	0.867698	-1.140639	1.372349
31	1	0	0.820773	1.164599	1.368656

17 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.877224	-0.832540	0.841032
2	6	0	1.775182	1.307231	0.810505
3	1	0	1.842971	2.301449	1.216637
4	7	0	2.015602	0.322075	1.556940
5	6	0	1.694898	-0.534043	-0.549788
6	1	0	2.624782	-0.819110	-1.035152
7	6	0	1.472405	0.968556	-0.610197
8	1	0	2.235845	1.442116	-1.223022
9	6	0	0.591631	-1.403131	-1.114619
10	1	0	0.756352	-1.411798	-2.191911
11	6	0	0.127306	1.463566	-1.173804
12	1	0	0.284632	1.552499	-2.245448
13	8	0	0.774278	-2.724599	-0.691509
14	1	0	0.928225	-2.692443	0.250776
15	8	0	-0.114552	2.780398	-0.750263
16	1	0	-0.406396	2.744508	0.156609
17	6	0	-1.103695	0.575705	-0.995639
18	1	0	-1.734780	0.775625	-1.858244
19	6	0	-0.843657	-0.945145	-0.900989
20	1	0	-1.413707	-1.442999	-1.682306
21	6	0	-1.547836	-1.333383	0.423725
22	1	0	-1.700337	-2.400139	0.524386
23	6	0	-1.982624	0.844786	0.255726
24	1	0	-2.542398	1.770861	0.197688
25	6	0	-0.859877	-0.646628	1.568441
26	1	0	-0.202074	-1.116744	2.276214
27	6	0	-1.127541	0.649304	1.475498
28	1	0	-0.741064	1.428597	2.110980
29	6	0	-2.787117	-0.451525	0.290424
30	1	0	-3.352209	-0.635666	-0.621149
31	1	0	-3.439092	-0.509111	1.155571

9 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.724976	2.190477	0.166347
2	6	0	-2.119083	1.775099	-1.206436
3	6	0	-2.992548	0.808327	-1.412470
4	6	0	-3.633778	0.083111	-0.284277
5	6	0	-2.690665	-0.121293	0.901693
6	1	0	-1.682628	2.334315	-2.019459
7	1	0	-2.472734	2.906006	0.522392
8	1	0	-4.481224	0.687409	0.057140
9	1	0	-3.312842	0.529079	-2.403987
10	8	0	-0.477661	2.843832	0.071824
11	1	0	-0.260764	3.206253	0.924696
12	8	0	-4.110701	-1.139623	-0.789177
13	1	0	-4.571187	-1.598250	-0.094286
14	6	0	-1.801618	-1.369414	0.826611
15	1	0	-2.334440	-2.301975	0.965373
16	6	0	-0.734343	-1.023471	1.856191
17	1	0	0.066182	-1.755703	1.893745
18	1	0	-1.135921	-0.874226	2.855056
19	6	0	-0.983707	-1.354592	-0.450275
20	6	0	-1.670294	1.021820	1.150925
21	6	0	-0.331414	0.278724	1.176993
22	1	0	0.471409	0.840084	1.640943
23	6	0	0.004346	-0.212044	-0.234756
24	8	0	-0.175237	-2.534366	-0.523245
25	6	0	1.293349	-0.960861	-0.313688
26	7	0	1.145190	-2.210476	-0.469202
27	1	0	-3.308082	-0.233159	1.791452
28	1	0	-1.833484	1.425684	2.148906
29	1	0	-0.040184	0.577186	-0.976386
30	1	0	-1.580813	-1.305159	-1.352707
31	6	0	2.613916	-0.348828	-0.223213
32	6	0	2.737573	1.032821	-0.192642
33	6	0	3.759792	-1.134706	-0.173165
34	6	0	3.987259	1.617858	-0.116290
35	1	0	1.855047	1.653411	-0.238236
36	6	0	5.000942	-0.546510	-0.095733
37	1	0	3.655201	-2.206294	-0.198476
38	6	0	5.119917	0.832257	-0.066522
39	1	0	4.073696	2.692061	-0.098912
40	1	0	5.883282	-1.164410	-0.057732
41	1	0	6.093935	1.289650	-0.006079

11 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534160	0.100457	2.076659
2	6	0	0.517590	-1.299820	1.584247
3	6	0	1.553833	-1.850336	0.984519
4	6	0	2.825757	-1.127317	0.705309
5	6	0	2.639832	0.386011	0.545501
6	1	0	-0.386795	-1.855977	1.777841
7	1	0	0.941441	0.079989	3.092889
8	1	0	3.490596	-1.284064	1.554976
9	1	0	1.523541	-2.882355	0.669007
10	8	0	-0.794586	0.562353	2.128219
11	1	0	-0.817164	1.365391	2.637504
12	8	0	3.511795	-1.680008	-0.384864
13	1	0	2.868183	-1.767489	-1.086193
14	6	0	2.549164	0.937331	-0.882492
15	1	0	3.495510	0.879762	-1.405121
16	6	0	2.010172	2.340688	-0.585185
17	1	0	1.794981	2.919516	-1.480373
18	1	0	2.667605	2.915778	0.061312
19	6	0	1.378081	0.424571	-1.709006
20	6	0	1.414718	1.028386	1.246811
21	6	0	0.748967	1.835722	0.125308
22	1	0	0.076103	2.598614	0.500648
23	6	0	0.150806	1.049170	-1.051587
24	8	0	1.129867	-0.976686	-1.700963
25	6	0	-0.732073	-0.150367	-0.949524
26	7	0	-0.176528	-1.215925	-1.357317
27	1	0	-0.328220	1.774413	-1.706581
28	1	0	1.503557	0.718660	-2.748509
29	1	0	3.539358	0.843714	0.950383
30	1	0	1.787558	1.789453	1.932346
31	6	0	-2.139738	-0.141614	-0.565199
32	6	0	-2.768526	1.055689	-0.264474
33	6	0	-2.869880	-1.321313	-0.507538
34	6	0	-4.104059	1.079527	0.079493
35	1	0	-2.206265	1.975184	-0.289979
36	6	0	-4.201750	-1.296188	-0.159394
37	1	0	-2.377093	-2.249926	-0.741973
38	6	0	-4.824548	-0.096360	0.133876
39	1	0	-4.581953	2.017651	0.310372
40	1	0	-4.759546	-2.217428	-0.116206
41	1	0	-5.867344	-0.080117	0.405797

12 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.823216	1.396137	0.495155
2	6	0	-0.079172	0.179046	0.309633
3	6	0	1.923962	1.545308	-0.534359
4	1	0	1.430542	1.880876	-1.444572
5	6	0	0.272781	-0.659288	-0.919118
6	1	0	-0.033992	-0.095485	-1.798429
7	8	0	2.802017	2.581720	-0.195240
8	1	0	3.183268	2.381141	0.654569
9	8	0	-0.471958	-1.844476	-0.972856
10	1	0	-0.134839	-2.434015	-0.304437
11	6	0	1.757127	-0.954591	-1.056810
12	1	0	1.885297	-1.350392	-2.061323
13	6	0	2.671639	0.266143	-0.852427
14	1	0	3.231955	0.466058	-1.762073
15	6	0	3.701713	-0.238904	0.193688
16	1	0	4.600939	0.362966	0.242162
17	6	0	2.374826	-2.007714	-0.093064
18	1	0	2.072677	-3.027820	-0.303009
19	6	0	2.996887	-0.489618	1.497923
20	1	0	3.081057	0.116835	2.384293
21	6	0	2.207957	-1.542951	1.328282
22	1	0	1.526737	-1.961069	2.050579
23	6	0	3.853531	-1.677329	-0.296861
24	1	0	4.169902	-1.746855	-1.335179
25	1	0	4.503854	-2.270906	0.336972
26	8	0	-0.036208	2.529743	0.374884
27	7	0	-1.326412	2.129566	0.251482
28	6	0	-1.412718	0.865346	0.219990
29	1	0	1.245483	1.418792	1.498233
30	1	0	-0.041440	-0.464861	1.184880
31	6	0	-2.729738	0.235038	0.129621
32	6	0	-2.955501	-1.033445	0.638650
33	6	0	-3.793067	0.936593	-0.425116
34	6	0	-4.217577	-1.589516	0.601082
35	1	0	-2.140402	-1.589239	1.068541
36	6	0	-5.050607	0.377399	-0.467896
37	1	0	-3.613644	1.923879	-0.815878
38	6	0	-5.267866	-0.887883	0.045292
39	1	0	-4.379763	-2.575628	1.004437
40	1	0	-5.865833	0.929740	-0.905867
41	1	0	-6.252083	-1.325495	0.009436

13 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.854747	-2.019501	-0.727293
2	6	0	-0.896830	-0.976109	-0.019378
3	7	0	-0.420701	-1.631627	-0.994303
4	6	0	1.173633	-1.756222	0.641449
5	1	0	1.193614	-2.724661	1.135492
6	6	0	0.037125	-0.883789	1.157226
7	1	0	-0.459356	-1.370565	1.994529
8	6	0	2.569481	-1.170353	0.713021
9	1	0	2.892856	-1.310680	1.744582
10	6	0	0.479333	0.492806	1.697759
11	1	0	0.837935	0.271206	2.701266
12	8	0	3.436247	-1.946944	-0.064456
13	1	0	3.019338	-2.052587	-0.917240
14	8	0	-0.610339	1.346802	1.904108
15	1	0	-0.964064	1.594894	1.052997
16	6	0	1.629038	1.219019	1.007364
17	1	0	2.064343	1.850882	1.778305
18	6	0	2.721820	0.310942	0.411569
19	1	0	3.680886	0.582894	0.846891
20	6	0	2.799628	0.785101	-1.061142
21	1	0	3.690870	0.441385	-1.570783
22	6	0	1.280521	2.157839	-0.178227
23	1	0	0.788132	3.073422	0.126931
24	6	0	1.492652	0.519868	-1.750779
25	1	0	1.316118	-0.256264	-2.472398
26	6	0	0.590506	1.343991	-1.234472
27	1	0	-0.461287	1.378972	-1.465710
28	6	0	2.663697	2.288171	-0.813609
29	1	0	3.418331	2.684705	-0.137017
30	1	0	2.642101	2.863988	-1.732707
31	6	0	-2.269687	-0.472010	-0.099323
32	6	0	-3.012146	-0.206948	1.042417
33	6	0	-2.860197	-0.291843	-1.345926
34	6	0	-4.320510	0.222802	0.938091
35	1	0	-2.562032	-0.318698	2.013810
36	6	0	-4.163304	0.140551	-1.444827
37	1	0	-2.279311	-0.502852	-2.228281
38	6	0	-4.899013	0.397838	-0.302096
39	1	0	-4.887109	0.423522	1.832369
40	1	0	-4.607727	0.280532	-2.416527
41	1	0	-5.918433	0.738525	-0.379959

TS1 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.955211	1.437839	0.058830
2	6	0	-2.150997	0.657976	-1.191350
3	6	0	-2.142857	-0.658913	-1.205055
4	6	0	-1.935321	-1.463642	0.027646
5	6	0	-1.009338	-0.791212	1.044291
6	1	0	-2.334836	1.235285	-2.083991
7	1	0	-2.936250	1.551244	0.531913
8	1	0	-2.914019	-1.603945	0.498789
9	1	0	-2.318664	-1.219770	-2.109597
10	8	0	-1.479772	2.712295	-0.314053
11	1	0	-1.446896	3.258397	0.464246
12	8	0	-1.438249	-2.717394	-0.379086
13	1	0	-1.348638	-3.271147	0.389375
14	6	0	0.495143	-1.119192	0.843720
15	1	0	0.763524	-2.137771	1.090319
16	6	0	1.116042	-0.010530	1.679546
17	1	0	2.199729	-0.014452	1.632306
18	1	0	0.787406	-0.024476	2.716611
19	6	0	0.852132	-0.669636	-0.535946
20	6	0	-1.018666	0.757999	1.060234
21	6	0	0.478531	1.105985	0.866393
22	1	0	0.727601	2.123524	1.142849
23	6	0	0.868309	0.689017	-0.530470
24	8	0	3.213319	-1.110515	-0.503703
25	6	0	3.040624	1.152739	-0.639051
26	1	0	3.340765	2.171740	-0.720496
27	7	0	3.486518	0.055462	-0.592257
28	1	0	-1.284889	-1.154369	2.033573
29	1	0	-1.301275	1.096187	2.056405
30	1	0	0.681323	1.301889	-1.395888
31	1	0	0.786762	-1.306240	-1.398613

Rotational constants (GHZ): 0.8296672 0.5025959 0.3978660

TS2 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354120	-1.084988	-1.161785
2	6	0	0.016446	-1.723080	-1.222684
3	6	0	-1.109563	-1.068766	-1.428239
4	6	0	-1.227555	0.405330	-1.589708
5	6	0	0.015243	1.186922	-1.138543
6	1	0	0.019822	-2.800010	-1.143009
7	1	0	1.806317	-1.214835	-2.149152
8	1	0	-1.369334	0.600215	-2.652497
9	1	0	-2.041503	-1.608330	-1.508955
10	8	0	2.139794	-1.807618	-0.228712
11	1	0	3.050305	-1.563501	-0.356595
12	8	0	-2.399405	0.885443	-0.986518
13	1	0	-2.470220	0.448896	-0.136952
14	6	0	-0.178624	2.002558	0.156499
15	1	0	-0.860051	2.831726	0.026397
16	6	0	1.289811	2.317817	0.478825
17	1	0	1.409833	2.854378	1.414545
18	1	0	1.807858	2.846326	-0.321350
19	6	0	-0.480372	1.142871	1.353351
20	6	0	1.329413	0.409936	-0.851703
21	6	0	1.669821	0.835852	0.590222
22	1	0	2.692059	0.614891	0.873305
23	6	0	0.638435	0.401717	1.617108
24	8	0	-2.080847	-0.783862	1.351993
25	6	0	0.021041	-1.575977	1.668209
26	1	0	0.820970	-2.274718	1.762184
27	7	0	-1.164479	-1.548351	1.571410
28	1	0	0.944800	0.150447	2.620663
29	1	0	-1.300881	1.317571	2.021282
30	1	0	0.225362	1.920783	-1.912017
31	1	0	2.110383	0.861763	-1.461129

TS3 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.997431	-0.693656	0.619894
2	6	0	1.071591	0.660081	0.617655
3	6	0	0.343508	-1.404399	-0.521090
4	1	0	1.026882	-1.391333	-1.367556
5	6	0	0.415092	1.413023	-0.509615
6	1	0	1.043953	1.341594	-1.395495
7	8	0	0.126730	-2.762423	-0.253452
8	1	0	-0.406932	-2.823295	0.533133
9	8	0	0.340120	2.789223	-0.241327
10	1	0	-0.227538	2.907648	0.514651
11	6	0	-0.937775	0.824448	-0.890322
12	1	0	-1.187119	1.238643	-1.864157
13	6	0	-0.959507	-0.715411	-0.958038
14	1	0	-1.157467	-1.039999	-1.976001
15	6	0	-2.216013	-1.074869	-0.116460
16	1	0	-2.591344	-2.072377	-0.308425
17	6	0	-2.143360	1.146209	0.035044
18	1	0	-2.463091	2.181035	-0.012913
19	6	0	-1.931917	-0.730930	1.319814
20	1	0	-1.699592	-1.433905	2.103401
21	6	0	-1.879187	0.590214	1.407360
22	1	0	-1.594838	1.164548	2.273454
23	6	0	-3.120794	0.095972	-0.487349
24	1	0	-3.304664	0.176702	-1.556356
25	1	0	-4.058286	0.088059	0.059183
26	8	0	3.233607	-1.187600	0.031629
27	7	0	3.535322	-0.024353	-0.031136
28	6	0	3.104959	1.072472	0.124456
29	1	0	3.369216	2.100650	0.022629
30	1	0	1.226961	-1.270188	1.500296
31	1	0	1.208774	1.190167	1.549220

TS4 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.204195	-1.124798	1.030440
2	6	0	2.177417	1.128611	0.826336
3	1	0	2.391806	2.153064	1.031889
4	7	0	2.363943	0.045823	1.285935
5	6	0	1.397559	-0.565397	-1.180898
6	1	0	2.328992	-1.056791	-1.411860
7	6	0	1.359895	0.787624	-1.075705
8	1	0	2.224586	1.337754	-1.424743
9	6	0	0.196299	-1.434848	-1.286584
10	1	0	0.154772	-1.721042	-2.340059
11	6	0	0.075946	1.567964	-1.159473
12	1	0	0.022615	1.913610	-2.189906
13	8	0	0.378148	-2.643103	-0.598330
14	1	0	0.864656	-2.428768	0.195737
15	8	0	0.143480	2.764271	-0.415845
16	1	0	0.019799	2.535052	0.500767
17	6	0	-1.205955	0.779628	-0.872805
18	1	0	-1.944342	1.126827	-1.590903
19	6	0	-1.143115	-0.768655	-0.949979
20	1	0	-1.852754	-1.094014	-1.706339
21	6	0	-1.738527	-1.201035	0.411153
22	1	0	-2.034979	-2.240315	0.432119
23	6	0	-1.833042	1.018584	0.528479
24	1	0	-2.232242	2.017780	0.654315
25	6	0	-0.785472	-0.769775	1.488604
26	1	0	-0.137306	-1.420879	2.046485
27	6	0	-0.847844	0.553354	1.567353
28	1	0	-0.266886	1.184475	2.219571
29	6	0	-2.822201	-0.140123	0.567933
30	1	0	-3.536336	-0.125605	-0.253036
31	1	0	-3.342319	-0.208474	1.517806

TS5 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.863790	2.196236	0.203882
2	6	0	-2.413152	1.848550	-1.132873
3	6	0	-3.291085	0.880897	-1.301334
4	6	0	-3.804574	0.062090	-0.171352
5	6	0	-2.781480	-0.143814	0.946263
6	1	0	-2.075318	2.458858	-1.955914
7	1	0	-2.534912	2.934117	0.654020
8	1	0	-4.667522	0.588772	0.250025
9	1	0	-3.709671	0.657743	-2.270218
10	8	0	-0.603840	2.805125	-0.004267
11	1	0	-0.293834	3.138617	0.831380
12	8	0	-4.237319	-1.162636	-0.716492
13	1	0	-4.615066	-1.687431	-0.018559
14	6	0	-1.872111	-1.392724	0.758083
15	1	0	-2.384042	-2.336140	0.894616
16	6	0	-0.759092	-1.052076	1.736530
17	1	0	0.043621	-1.781216	1.718684
18	1	0	-1.113918	-0.911465	2.755335
19	6	0	-1.164372	-1.215556	-0.545815
20	6	0	-1.755785	0.998525	1.150914
21	6	0	-0.404888	0.255372	1.045141
22	1	0	0.433242	0.810324	1.449639
23	6	0	-0.261179	-0.216424	-0.382452
24	8	0	0.368251	-3.067787	-0.502271
25	6	0	1.710479	-1.225762	-0.352164
26	7	0	1.333958	-2.350335	-0.432990
27	1	0	-3.330938	-0.290799	1.875122
28	1	0	-1.845953	1.372861	2.169757
29	1	0	0.076665	0.414973	-1.186843
30	1	0	-1.539455	-1.589685	-1.479954
31	6	0	2.867741	-0.389117	-0.232974
32	6	0	2.752228	0.994643	-0.259220
33	6	0	4.125191	-0.969925	-0.088630
34	6	0	3.881136	1.779834	-0.143617
35	1	0	1.784193	1.455176	-0.368926
36	6	0	5.243248	-0.175371	0.024131
37	1	0	4.208999	-2.043381	-0.070126
38	6	0	5.126496	1.202037	-0.001928
39	1	0	3.783389	2.852671	-0.168207
40	1	0	6.212007	-0.634608	0.132915
41	1	0	6.004002	1.820851	0.086909

TS6 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.797881	-0.894813	1.869652
2	6	0	-0.796073	0.584414	1.964327
3	6	0	-1.778682	1.342700	1.519511
4	6	0	-2.992493	0.833725	0.825783
5	6	0	-2.825573	-0.570554	0.232259
6	1	0	0.044802	1.011063	2.489581
7	1	0	-1.206937	-1.272938	2.811655
8	1	0	-3.792761	0.787055	1.564253
9	1	0	-1.753797	2.411318	1.668624
10	8	0	0.543404	-1.322465	1.766426
11	1	0	0.580738	-2.246764	1.988590
12	8	0	-3.451462	1.750433	-0.133171
13	1	0	-2.678489	2.056319	-0.605764
14	6	0	-2.638491	-0.606663	-1.298420
15	1	0	-3.531855	-0.313125	-1.832043
16	6	0	-2.146541	-2.054594	-1.456741
17	1	0	-1.888454	-2.302484	-2.481403
18	1	0	-2.840152	-2.795505	-1.058715
19	6	0	-1.389625	0.093351	-1.762118
20	6	0	-1.649977	-1.447407	0.733382
21	6	0	-0.915667	-1.817831	-0.572019
22	1	0	-0.233735	-2.652269	-0.452440
23	6	0	-0.318770	-0.634321	-1.319358
24	8	0	-0.723081	2.227282	-0.870306
25	6	0	0.988088	0.788507	-0.441727
26	7	0	0.367385	1.809206	-0.544732
27	1	0	0.570271	-0.770000	-1.915949
28	1	0	-1.379601	0.808193	-2.561839
29	1	0	-3.753063	-1.105590	0.419255
30	1	0	-2.068059	-2.388616	1.087856
31	6	0	2.361473	0.395020	-0.258618
32	6	0	2.731852	-0.940057	-0.237985
33	6	0	3.340018	1.378296	-0.146989
34	6	0	4.061421	-1.285954	-0.120625
35	1	0	1.970526	-1.697830	-0.289456
36	6	0	4.663887	1.023392	-0.019013
37	1	0	3.047489	2.414576	-0.165863
38	6	0	5.030857	-0.309202	-0.010750
39	1	0	4.341184	-2.326550	-0.109256
40	1	0	5.413803	1.792464	0.066752
41	1	0	6.068565	-0.583811	0.082397

TS7 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.960227	1.247871	0.716873
2	6	0	0.153964	0.151024	0.779940
3	6	0	1.760861	1.528180	-0.513789
4	1	0	1.075844	1.893769	-1.274567
5	6	0	0.267642	-0.943399	-0.258244
6	1	0	-0.457925	-0.794078	-1.053695
7	8	0	2.677911	2.571769	-0.330675
8	1	0	3.242840	2.342584	0.400837
9	8	0	-0.090696	-2.186383	0.306106
10	1	0	0.515198	-2.359683	1.021204
11	6	0	1.659001	-1.040151	-0.897291
12	1	0	1.521304	-1.500656	-1.871974
13	6	0	2.446746	0.276127	-1.060639
14	1	0	2.644975	0.457842	-2.113471
15	6	0	3.812248	-0.053508	-0.397045
16	1	0	4.602112	0.630735	-0.680112
17	6	0	2.669331	-1.943418	-0.133318
18	1	0	2.418193	-2.996110	-0.171568
19	6	0	3.576371	-0.232160	1.077617
20	1	0	3.827764	0.477511	1.849249
21	6	0	2.890238	-1.355464	1.234114
22	1	0	2.479036	-1.728753	2.158384
23	6	0	3.959613	-1.510423	-0.818578
24	1	0	3.938660	-1.649502	-1.897184
25	1	0	4.838543	-1.983786	-0.392872
26	8	0	-0.465503	2.894172	0.390178
27	7	0	-1.455739	2.208542	0.274240
28	6	0	-1.803498	1.063288	0.320507
29	1	0	1.190227	1.819820	1.599523
30	1	0	-0.201216	-0.174378	1.747876
31	6	0	-2.993940	0.285153	0.109509
32	6	0	-3.043389	-1.059892	0.441237
33	6	0	-4.117614	0.902410	-0.437302
34	6	0	-4.205226	-1.775252	0.230621
35	1	0	-2.169840	-1.547949	0.836209
36	6	0	-5.270599	0.180095	-0.636473
37	1	0	-4.071306	1.947102	-0.694699
38	6	0	-5.319290	-1.162023	-0.303469
39	1	0	-4.234199	-2.821531	0.486268
40	1	0	-6.136334	0.665779	-1.055827
41	1	0	-6.223508	-1.725716	-0.463754

TS8 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.643609	2.405900	-0.785136
2	6	0	1.110524	1.141070	-0.107987
3	7	0	0.462367	1.905371	-0.763700
4	6	0	-1.332675	1.547445	1.169627
5	1	0	-1.278548	2.592430	1.426181
6	6	0	-0.304780	0.716694	1.504701
7	1	0	0.459216	1.120914	2.155743
8	6	0	-2.702619	1.072304	0.821067
9	1	0	-3.282860	1.225697	1.733902
10	6	0	-0.530177	-0.761887	1.686463
11	1	0	-0.752209	-0.873597	2.747070
12	8	0	-3.315067	1.900573	-0.128870
13	1	0	-2.649464	2.098076	-0.784661
14	8	0	0.643729	-1.517696	1.524570
15	1	0	0.922360	-1.442782	0.615566
16	6	0	-1.705533	-1.368026	0.919324
17	1	0	-2.137333	-2.121540	1.573346
18	6	0	-2.830578	-0.408554	0.458014
19	1	0	-3.767942	-0.750079	0.890017
20	6	0	-2.934540	-0.710897	-1.058310
21	1	0	-3.847706	-0.337699	-1.501209
22	6	0	-1.334698	-2.107688	-0.393747
23	1	0	-0.785560	-3.025527	-0.225825
24	6	0	-1.656913	-0.276918	-1.718526
25	1	0	-1.542721	0.593972	-2.338561
26	6	0	-0.703743	-1.113708	-1.328422
27	1	0	0.343231	-1.068018	-1.582161
28	6	0	-2.718893	-2.219675	-1.023639
29	1	0	-3.437194	-2.744632	-0.396852
30	1	0	-2.689690	-2.662689	-2.013926
31	6	0	2.422403	0.546867	-0.129273
32	6	0	3.077732	0.204494	1.044661
33	6	0	3.043053	0.322851	-1.355514
34	6	0	4.342081	-0.341688	0.991130
35	1	0	2.584740	0.341994	1.990267
36	6	0	4.306787	-0.222317	-1.397577
37	1	0	2.527528	0.591204	-2.262553
38	6	0	4.959628	-0.554689	-0.225367
39	1	0	4.844623	-0.606608	1.906225
40	1	0	4.783042	-0.389004	-2.349514
41	1	0	5.947142	-0.983987	-0.261427

MPWB1K/6-311G(d,p) gas phase computed Cartesian coordinates of the stationary points involved in the 32CA reaction of BNO **2** and CNO **10** with SA **8** in DCM

2 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.459789	-0.000021	-0.000001
2	7	0	2.606098	-0.000004	-0.000003
3	8	0	3.807641	0.000010	-0.000005
4	6	0	0.039145	-0.000015	0.000001
5	6	0	-0.652951	1.205993	0.000001
6	6	0	-0.652974	-1.206004	0.000001
7	6	0	-2.031534	1.198446	-0.000001
8	1	0	-0.106793	2.137338	0.000002
9	6	0	-2.031561	-1.198427	0.000005
10	1	0	-0.106841	-2.137364	0.000001
11	6	0	-2.721485	0.000015	0.000004
12	1	0	-2.569559	2.134708	-0.000001
13	1	0	-2.569601	-2.134681	0.000003
14	1	0	-3.801602	0.000028	0.000005

8 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.453125	-1.097418	-0.498823
2	6	0	0.660710	-1.882149	0.485391
3	6	0	-0.656985	-1.883038	0.485664
4	6	0	-1.450531	-1.099990	-0.498734
5	6	0	-0.773642	0.201844	-0.930764
6	1	0	1.228567	-2.484612	1.181272
7	1	0	1.579735	-1.721131	-1.391236
8	1	0	-1.575947	-1.724303	-1.390879
9	1	0	-1.223925	-2.486189	1.181691
10	8	0	2.721310	-0.861351	0.071679
11	1	0	3.273921	-0.430296	-0.588176
12	8	0	-2.719292	-0.865633	0.071384
13	1	0	-3.272606	-0.436487	-0.589118
14	6	0	-1.113364	1.424530	-0.036905
15	1	0	-2.135649	1.768634	-0.144115
16	6	0	-0.002160	2.372249	-0.470239
17	1	0	-0.003433	3.302878	0.090280
18	1	0	-0.001700	2.575664	-1.540006
19	6	0	-0.664965	1.102246	1.359810
20	6	0	0.774225	0.203631	-0.930319
21	6	0	1.110509	1.427097	-0.035332
22	1	0	2.132193	1.773566	-0.141013
23	6	0	0.660851	1.104194	1.361022
24	1	0	-1.125739	0.434667	-1.935027
25	1	0	1.126367	0.437842	-1.934236
26	1	0	1.314492	0.785130	2.156946
27	1	0	-1.319064	0.781332	2.154494

10 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.165395
2	1	0	0.000000	0.000000	-2.231282
3	7	0	0.000000	0.000000	-0.022228
4	8	0	0.000000	0.000000	1.172406

14 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.812217	1.449102	0.032958
2	6	0	-1.911216	0.677420	-1.235992
3	6	0	-1.922770	-0.642856	-1.241591
4	6	0	-1.835762	-1.421531	0.022889
5	6	0	-0.908551	-0.773174	1.050554
6	1	0	-2.016275	1.253214	-2.145650
7	1	0	-2.819290	1.511476	0.460936
8	1	0	-2.841509	-1.461130	0.457445
9	1	0	-2.038039	-1.209657	-2.155403
10	8	0	-1.365945	2.747028	-0.286141
11	1	0	-1.401313	3.284399	0.511698
12	8	0	-1.418920	-2.726298	-0.303138
13	1	0	-1.429522	-3.259136	0.498778
14	6	0	0.576432	-1.120083	0.906490
15	1	0	0.816708	-2.143405	1.173936
16	6	0	1.207129	-0.016093	1.746109
17	1	0	2.293325	-0.025463	1.713834
18	1	0	0.877003	-0.031608	2.781548
19	6	0	1.068872	-0.751049	-0.478593
20	6	0	-0.906249	0.779323	1.067488
21	6	0	0.583631	1.118491	0.942264
22	1	0	0.826726	2.129480	1.252371
23	6	0	1.064801	0.778772	-0.471513
24	8	0	2.452078	-1.118503	-0.626336
25	6	0	2.510173	1.036621	-0.698200
26	1	0	2.975332	2.006259	-0.797953
27	7	0	3.228405	0.003215	-0.777874
28	1	0	-1.214339	-1.131477	2.032647
29	1	0	-1.228658	1.121222	2.050117
30	1	0	0.459676	1.249372	-1.238262
31	1	0	0.517997	-1.223514	-1.283169

15 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622124	-1.182671	-0.658938
2	6	0	0.814007	-2.016613	0.267258
3	6	0	-0.497236	-2.129642	0.193489
4	6	0	-1.347797	-1.406890	-0.791698
5	6	0	-0.695463	-0.142834	-1.365167
6	1	0	1.378099	-2.579947	0.998604
7	1	0	1.947001	-1.841694	-1.471267
8	1	0	-1.536522	-2.084754	-1.625487
9	1	0	-1.028306	-2.788462	0.868399
10	8	0	2.769134	-0.743104	0.038115
11	1	0	3.375124	-0.351078	-0.598692
12	8	0	-2.627385	-1.143216	-0.261660
13	1	0	-2.480994	-0.687834	0.570254
14	6	0	-1.175198	1.206162	-0.816126
15	1	0	-2.194787	1.434257	-1.106765
16	6	0	-0.083232	2.118216	-1.384986
17	1	0	-0.174121	3.152578	-1.061222
18	1	0	-0.031789	2.083596	-2.470183
19	6	0	-0.908124	1.445085	0.664023
20	6	0	0.853376	-0.022311	-1.292909
21	6	0	1.067623	1.374170	-0.700025
22	1	0	2.063665	1.763705	-0.881763
23	6	0	0.612975	1.565302	0.751189
24	8	0	-1.250755	0.397495	1.575605
25	6	0	0.886482	0.599798	1.840997
26	1	0	1.845648	0.390668	2.285520
27	7	0	-0.132940	0.018174	2.299812
28	1	0	0.928502	2.558458	1.069577
29	1	0	-1.430958	2.339071	0.997435
30	1	0	-0.974275	-0.112627	-2.416632
31	1	0	1.219128	0.060816	-2.315588

16 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.202996	-0.739521	0.435187
2	6	0	1.189884	0.782562	0.429873
3	6	0	0.432658	-1.357676	-0.711376
4	1	0	1.018735	-1.152776	-1.608768
5	6	0	0.390665	1.404793	-0.711240
6	1	0	0.950608	1.241004	-1.633119
7	8	0	0.395176	-2.756414	-0.614151
8	1	0	-0.060452	-3.009405	0.193528
9	8	0	0.334947	2.799875	-0.574841
10	1	0	-0.142966	3.026522	0.226890
11	6	0	-0.977191	0.781140	-0.913258
12	1	0	-1.333165	1.145807	-1.875507
13	6	0	-0.949370	-0.763528	-0.920452
14	1	0	-1.288380	-1.131617	-1.887290
15	6	0	-2.055576	-1.131393	0.104141
16	1	0	-2.399460	-2.157366	0.022553
17	6	0	-2.090539	1.099599	0.120632
18	1	0	-2.469336	2.114544	0.054055
19	6	0	-1.625307	-0.683456	1.473261
20	1	0	-1.298301	-1.334111	2.270213
21	6	0	-1.644954	0.644155	1.483190
22	1	0	-1.335590	1.291974	2.289484
23	6	0	-3.061257	-0.029500	-0.225315
24	1	0	-3.370106	-0.026444	-1.268908
25	1	0	-3.930204	-0.047712	0.425686
26	8	0	2.588416	-1.106188	0.308259
27	7	0	3.368256	0.019161	0.231564
28	6	0	2.646777	1.049826	0.302524
29	1	0	3.106359	2.025470	0.254247
30	1	0	0.858912	-1.139200	1.386413
31	1	0	0.814530	1.178989	1.372437

17 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.839646	-0.928954	0.910268
2	6	0	1.807812	1.221964	0.843897
3	1	0	1.884532	2.223234	1.237261
4	7	0	2.024125	0.240031	1.602070
5	6	0	1.654291	-0.646383	-0.481575
6	1	0	2.568345	-0.982639	-0.972902
7	6	0	1.518061	0.869009	-0.572711
8	1	0	2.327966	1.284533	-1.174656
9	6	0	0.500608	-1.416380	-1.094644
10	6	0	0.220764	1.413718	-1.190774
11	6	0	-1.065903	0.633259	-0.972387
12	1	0	-1.692350	0.867645	-1.831791
13	6	0	-0.905397	-0.898997	-0.874962
14	1	0	-1.495662	-1.362335	-1.664612
15	6	0	-1.639092	-1.239789	0.445932
16	1	0	-1.865352	-2.294723	0.545907
17	6	0	-1.913089	0.967850	0.280586
18	1	0	-2.393686	1.936901	0.224473
19	6	0	-0.907385	-0.604794	1.592011
20	1	0	-0.276426	-1.132141	2.285693
21	6	0	-1.077279	0.708386	1.497543
22	1	0	-0.624807	1.470337	2.109904
23	6	0	-2.810790	-0.268416	0.306750
24	1	0	-3.382332	-0.409737	-0.609338
25	1	0	-3.472277	-0.283050	1.167966
26	1	0	0.395570	1.397534	-2.269757
27	1	0	0.679984	-1.325249	-2.173870
28	8	0	-0.004072	2.738226	-0.776271
29	1	0	0.694772	3.296544	-1.134143
30	8	0	0.517046	-2.765993	-0.717967
31	1	0	1.366277	-3.149874	-0.960856

9 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.701827	2.193707	0.160100
2	6	0	-2.101735	1.777345	-1.211561
3	6	0	-2.983843	0.816626	-1.416790
4	6	0	-3.631664	0.094766	-0.289193
5	6	0	-2.692365	-0.108931	0.900120
6	1	0	-1.663563	2.330812	-2.031322
7	1	0	-2.442593	2.917772	0.516107
8	1	0	-4.477789	0.702166	0.051888
9	1	0	-3.304748	0.544064	-2.413105
10	8	0	-0.446390	2.832233	0.067105
11	1	0	-0.231558	3.208504	0.927303
12	8	0	-4.113758	-1.130259	-0.789480
13	1	0	-4.598987	-1.577137	-0.088280
14	6	0	-1.812767	-1.364031	0.830219
15	1	0	-2.359031	-2.290570	0.969694
16	6	0	-0.745524	-1.023101	1.862368
17	1	0	0.051364	-1.760678	1.908783
18	1	0	-1.152414	-0.867612	2.858035
19	6	0	-0.993950	-1.351735	-0.444850
20	6	0	-1.664323	1.027431	1.148870
21	6	0	-0.330988	0.275770	1.183830
22	1	0	0.470896	0.836673	1.651415
23	6	0	0.003882	-0.218983	-0.227525
24	8	0	-0.187954	-2.540358	-0.526449
25	6	0	1.289197	-0.970963	-0.310249
26	7	0	1.139764	-2.220176	-0.473514
27	1	0	-3.313367	-0.217000	1.788088
28	1	0	-1.826160	1.437398	2.144752
29	1	0	-0.035052	0.569810	-0.970377
30	1	0	-1.585071	-1.296421	-1.351348
31	6	0	2.610842	-0.358866	-0.220747
32	6	0	2.727362	1.024157	-0.183186
33	6	0	3.761050	-1.140072	-0.178181
34	6	0	3.975085	1.615545	-0.109570
35	1	0	1.840233	1.639557	-0.215440
36	6	0	5.001074	-0.546288	-0.103297
37	1	0	3.669562	-2.214999	-0.204058
38	6	0	5.112743	0.834019	-0.069025
39	1	0	4.056249	2.692216	-0.084663
40	1	0	5.888211	-1.161491	-0.070257
41	1	0	6.086791	1.296865	-0.010019

11 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622125	-1.182670	-0.658938
2	6	0	0.814008	-2.016612	0.267259
3	6	0	-0.497235	-2.129642	0.193490
4	6	0	-1.347796	-1.406891	-0.791697
5	6	0	-0.695463	-0.142835	-1.365167
6	1	0	1.378101	-2.579946	0.998605
7	1	0	1.947002	-1.841693	-1.471267
8	1	0	-1.536521	-2.084755	-1.625486
9	1	0	-1.028304	-2.788462	0.868400
10	8	0	2.769134	-0.743102	0.038115
11	1	0	3.375124	-0.351076	-0.598692
12	8	0	-2.627384	-1.143218	-0.261659
13	1	0	-2.480994	-0.687835	0.570254
14	6	0	-1.175199	1.206161	-0.816126
15	1	0	-2.194788	1.434255	-1.106765
16	6	0	-0.083233	2.118216	-1.384987
17	1	0	-0.174123	3.152578	-1.061223
18	1	0	-0.031791	2.083595	-2.470184
19	6	0	-0.908125	1.445085	0.664023
20	6	0	0.853376	-0.022311	-1.292909
21	6	0	1.067622	1.374170	-0.700025
22	1	0	2.063664	1.763706	-0.881764
23	6	0	0.612974	1.565303	0.751189
24	8	0	-1.250755	0.397495	1.575605
25	6	0	0.886482	0.599799	1.840997
26	1	0	1.845648	0.390670	2.285520
27	7	0	-0.132940	0.018175	2.299812
28	1	0	0.928500	2.558459	1.069576
29	1	0	-1.430959	2.339070	0.997434
30	1	0	-0.974275	-0.112628	-2.416632
31	1	0	1.219128	0.060816	-2.315588

12 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.202996	-0.739521	0.435187
2	6	0	1.189884	0.782562	0.429873
3	6	0	0.432658	-1.357676	-0.711376
4	1	0	1.018735	-1.152776	-1.608768
5	6	0	0.390665	1.404793	-0.711240
6	1	0	0.950608	1.241004	-1.633119
7	8	0	0.395175	-2.756414	-0.614151
8	1	0	-0.060453	-3.009405	0.193528
9	8	0	0.334948	2.799875	-0.574841
10	1	0	-0.142965	3.026522	0.226890
11	6	0	-0.977191	0.781140	-0.913258
12	1	0	-1.333165	1.145807	-1.875507
13	6	0	-0.949370	-0.763528	-0.920452
14	1	0	-1.288380	-1.131617	-1.887290
15	6	0	-2.055576	-1.131393	0.104141
16	1	0	-2.399460	-2.157365	0.022553
17	6	0	-2.090539	1.099599	0.120632
18	1	0	-2.469336	2.114545	0.054055
19	6	0	-1.625307	-0.683455	1.473261
20	1	0	-1.298301	-1.334110	2.270213
21	6	0	-1.644954	0.644156	1.483190
22	1	0	-1.335590	1.291975	2.289484
23	6	0	-3.061257	-0.029499	-0.225315
24	1	0	-3.370106	-0.026443	-1.268908
25	1	0	-3.930204	-0.047711	0.425686
26	8	0	2.588416	-1.106188	0.308259
27	7	0	3.368256	0.019160	0.231564
28	6	0	2.646777	1.049826	0.302524
29	1	0	3.106359	2.025469	0.254247
30	1	0	0.858912	-1.139200	1.386413
31	1	0	0.814530	1.178989	1.372437

13 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.839646	-0.928954	0.910268
2	6	0	1.807812	1.221964	0.843897
3	1	0	1.884532	2.223234	1.237261
4	7	0	2.024125	0.240031	1.602070
5	6	0	1.654291	-0.646383	-0.481575
6	1	0	2.568345	-0.982639	-0.972902
7	6	0	1.518061	0.869009	-0.572711
8	1	0	2.327966	1.284533	-1.174656
9	6	0	0.500608	-1.416380	-1.094644
10	6	0	0.220764	1.413718	-1.190774
11	6	0	-1.065903	0.633259	-0.972387
12	1	0	-1.692350	0.867645	-1.831791
13	6	0	-0.905397	-0.898997	-0.874962
14	1	0	-1.495662	-1.362335	-1.664612
15	6	0	-1.639092	-1.239789	0.445932
16	1	0	-1.865352	-2.294723	0.545907
17	6	0	-1.913089	0.967850	0.280586
18	1	0	-2.393686	1.936901	0.224473
19	6	0	-0.907385	-0.604794	1.592011
20	1	0	-0.276426	-1.132141	2.285693
21	6	0	-1.077279	0.708386	1.497543
22	1	0	-0.624807	1.470337	2.109904
23	6	0	-2.810790	-0.268416	0.306750
24	1	0	-3.382332	-0.409737	-0.609338
25	1	0	-3.472277	-0.283050	1.167966
26	1	0	0.395570	1.397534	-2.269757
27	1	0	0.679984	-1.325249	-2.173870
28	8	0	-0.004072	2.738226	-0.776271
29	1	0	0.694772	3.296544	-1.134143
30	8	0	0.517046	-2.765993	-0.717967
31	1	0	1.366277	-3.149874	-0.960856

TS1 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.950885	1.446424	0.059413
2	6	0	-2.160116	0.664886	-1.188414
3	6	0	-2.161354	-0.653188	-1.202012
4	6	0	-1.948298	-1.462423	0.027780
5	6	0	-1.017921	-0.791419	1.041193
6	1	0	-2.350961	1.239525	-2.084665
7	1	0	-2.928719	1.567284	0.539144
8	1	0	-2.924043	-1.603473	0.506326
9	1	0	-2.353224	-1.208971	-2.109783
10	8	0	-1.467816	2.718216	-0.314139
11	1	0	-1.435562	3.271503	0.472442
12	8	0	-1.454422	-2.717845	-0.382994
13	1	0	-1.377256	-3.282718	0.392167
14	6	0	0.485074	-1.129558	0.839743
15	1	0	0.738990	-2.153074	1.087472
16	6	0	1.111293	-0.024363	1.677461
17	1	0	2.195863	-0.033195	1.631090
18	1	0	0.780243	-0.038824	2.713729
19	6	0	0.842734	-0.678117	-0.538407
20	6	0	-1.018110	0.757740	1.058445
21	6	0	0.480498	1.098124	0.866453
22	1	0	0.734167	2.115275	1.143485
23	6	0	0.868884	0.679505	-0.530800
24	8	0	3.288420	-1.111240	-0.515960
25	6	0	3.014877	1.150452	-0.621842
26	1	0	3.238081	2.197575	-0.681863
27	7	0	3.511299	0.077398	-0.588219
28	1	0	-1.291136	-1.155758	2.030926
29	1	0	-1.297676	1.098263	2.054803
30	1	0	0.695488	1.294725	-1.400037
31	1	0	0.787146	-1.311350	-1.407044

TS2 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.140061	1.394484	-1.076216
2	6	0	0.302065	1.713850	-1.219408
3	6	0	1.236798	0.826942	-1.501377
4	6	0	1.012595	-0.636139	-1.655971
5	6	0	-0.355866	-1.124957	-1.156606
6	1	0	0.550907	2.764007	-1.137825
7	1	0	-1.608052	1.643556	-2.034172
8	1	0	1.076606	-0.868158	-2.719861
9	1	0	2.260719	1.146494	-1.645814
10	8	0	-1.682462	2.251766	-0.090464
11	1	0	-2.641998	2.219389	-0.160500
12	8	0	2.081109	-1.350708	-1.074859
13	1	0	2.241493	-0.934842	-0.224333
14	6	0	-0.300259	-2.009020	0.110760
15	1	0	0.150598	-2.977024	-0.070195
16	6	0	-1.782001	-1.969920	0.515424
17	1	0	-1.976242	-2.488559	1.449684
18	1	0	-2.453470	-2.335669	-0.260823
19	6	0	0.261454	-1.283126	1.298585
20	6	0	-1.435557	-0.073883	-0.786059
21	6	0	-1.788361	-0.442980	0.668383
22	1	0	-2.709267	0.012886	1.013714
23	6	0	-0.625485	-0.299675	1.635688
24	8	0	2.352971	0.287934	1.259931
25	6	0	0.439877	1.450002	1.687719
26	1	0	-0.209869	2.283850	1.862026
27	7	0	1.596297	1.210798	1.539063
28	1	0	-0.799005	-0.000386	2.661405
29	1	0	1.078523	-1.641825	1.898412
30	1	0	-0.767109	-1.763600	-1.934988
31	1	0	-2.332052	-0.321104	-1.352561

TS3 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.984642	-0.660124	0.636877
2	6	0	1.028841	0.693304	0.617854
3	6	0	0.383544	-1.371296	-0.527603
4	1	0	1.053066	-1.241683	-1.379601
5	6	0	0.362855	1.405370	-0.531054
6	1	0	0.991278	1.303244	-1.417058
7	8	0	0.288628	-2.758446	-0.344514
8	1	0	-0.165822	-2.940837	0.480945
9	8	0	0.276231	2.790190	-0.315500
10	1	0	-0.202715	2.955322	0.501105
11	6	0	-0.982581	0.784659	-0.901805
12	1	0	-1.229758	1.164762	-1.891511
13	6	0	-0.963603	-0.757124	-0.927358
14	1	0	-1.176401	-1.113534	-1.933491
15	6	0	-2.189192	-1.129314	-0.049068
16	1	0	-2.529993	-2.149231	-0.192201
17	6	0	-2.200676	1.099042	0.006302
18	1	0	-2.555412	2.120788	-0.082465
19	6	0	-1.908928	-0.711852	1.368452
20	1	0	-1.633294	-1.377420	2.173024
21	6	0	-1.910028	0.614018	1.399793
22	1	0	-1.634441	1.241162	2.234262
23	6	0	-3.138532	-0.009121	-0.466767
24	1	0	-3.327711	0.017239	-1.538172
25	1	0	-4.075182	-0.027090	0.082874
26	8	0	3.294596	-1.142825	0.092454
27	7	0	3.542893	0.041503	-0.002231
28	6	0	3.063243	1.119665	0.115034
29	1	0	3.270539	2.166621	0.003399
30	1	0	1.211990	-1.225792	1.527252
31	1	0	1.150456	1.241215	1.543794

TS4 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.357474	-1.016900	0.979835
2	6	0	1.997649	1.221711	0.900734
3	1	0	1.942233	2.254197	1.181987
4	7	0	2.341076	0.159877	1.306735
5	6	0	1.440742	-0.430937	-1.200962
6	1	0	2.407154	-0.838330	-1.457993
7	6	0	1.293960	0.908851	-1.038477
8	1	0	2.123811	1.536155	-1.350377
9	6	0	0.307959	-1.387570	-1.311240
10	6	0	-0.049109	1.582058	-1.127612
11	6	0	-1.262725	0.698494	-0.857817
12	1	0	-2.021113	0.992903	-1.580609
13	6	0	-1.078179	-0.838145	-0.953929
14	1	0	-1.763124	-1.207801	-1.714511
15	6	0	-1.636301	-1.329630	0.404204
16	1	0	-1.852145	-2.390981	0.416272
17	6	0	-1.911117	0.874547	0.540113
18	1	0	-2.380100	1.841510	0.672434
19	6	0	-0.722387	-0.827736	1.487596
20	1	0	-0.007192	-1.426619	2.026901
21	6	0	-0.892264	0.486806	1.569918
22	1	0	-0.351957	1.182034	2.189610
23	6	0	-2.803614	-0.361584	0.562567
24	1	0	-3.511500	-0.399406	-0.263978
25	1	0	-3.323541	-0.483389	1.508422
26	1	0	-0.122917	1.918491	-2.165490
27	1	0	0.279671	-1.666756	-2.368369
28	8	0	-0.128103	2.718169	-0.292050
29	1	0	0.399457	3.419053	-0.688353
30	8	0	0.600405	-2.588660	-0.634777
31	1	0	1.047845	-2.332266	0.172275

TS5 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.862024	2.194456	0.186750
2	6	0	-2.424913	1.835824	-1.142446
3	6	0	-3.308928	0.869598	-1.295753
4	6	0	-3.812869	0.060433	-0.153734
5	6	0	-2.775236	-0.140335	0.950328
6	1	0	-2.096300	2.439276	-1.977746
7	1	0	-2.531825	2.933431	0.639324
8	1	0	-4.666297	0.594629	0.279349
9	1	0	-3.738582	0.646290	-2.262833
10	8	0	-0.604654	2.802664	-0.032881
11	1	0	-0.304988	3.182862	0.798810
12	8	0	-4.262455	-1.168635	-0.679407
13	1	0	-4.661635	-1.675967	0.034401
14	6	0	-1.866973	-1.388844	0.756374
15	1	0	-2.385245	-2.329960	0.895334
16	6	0	-0.750181	-1.045935	1.731330
17	1	0	0.054466	-1.774625	1.711995
18	1	0	-1.103701	-0.904300	2.750382
19	6	0	-1.162675	-1.209100	-0.548623
20	6	0	-1.749586	1.003459	1.142538
21	6	0	-0.397525	0.261688	1.038441
22	1	0	0.436809	0.822213	1.443033
23	6	0	-0.254560	-0.214374	-0.388601
24	8	0	0.397988	-3.099229	-0.516418
25	6	0	1.716415	-1.234236	-0.351939
26	7	0	1.359267	-2.362901	-0.439404
27	1	0	-3.313975	-0.291163	1.885152
28	1	0	-1.833719	1.386840	2.158640
29	1	0	0.090264	0.407437	-1.199315
30	1	0	-1.530723	-1.586959	-1.486756
31	6	0	2.865485	-0.384047	-0.227675
32	6	0	2.742011	0.999181	-0.246536
33	6	0	4.125273	-0.963093	-0.088270
34	6	0	3.868421	1.789463	-0.129843
35	1	0	1.771445	1.456418	-0.346961
36	6	0	5.240864	-0.163466	0.025267
37	1	0	4.216914	-2.038600	-0.074059
38	6	0	5.117198	1.214612	0.005312
39	1	0	3.765956	2.864358	-0.146331
40	1	0	6.213878	-0.620173	0.130211
41	1	0	5.994177	1.838202	0.095310

TS6 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777495	-0.834983	1.896632
2	6	0	-0.801406	0.646420	1.955053
3	6	0	-1.793553	1.379782	1.489250
4	6	0	-2.995720	0.834277	0.802588
5	6	0	-2.815274	-0.586147	0.254081
6	1	0	0.031220	1.104107	2.472174
7	1	0	-1.184606	-1.197746	2.847079
8	1	0	-3.806592	0.806876	1.532054
9	1	0	-1.784840	2.454081	1.613262
10	8	0	0.569120	-1.238380	1.804664
11	1	0	0.608981	-2.188727	1.950936
12	8	0	-3.450565	1.727055	-0.191280
13	1	0	-2.677105	1.979874	-0.696581
14	6	0	-2.637321	-0.673133	-1.276784
15	1	0	-3.538720	-0.419066	-1.820957
16	6	0	-2.119196	-2.116372	-1.387577
17	1	0	-1.864476	-2.394899	-2.405896
18	1	0	-2.796978	-2.853606	-0.957173
19	6	0	-1.404233	0.034707	-1.767432
20	6	0	-1.622648	-1.428266	0.775963
21	6	0	-0.886564	-1.828211	-0.519734
22	1	0	-0.189711	-2.647461	-0.376250
23	6	0	-0.319292	-0.659419	-1.309441
24	8	0	-0.724743	2.251318	-0.917390
25	6	0	0.974526	0.791904	-0.472717
26	7	0	0.365070	1.817293	-0.586851
27	1	0	0.571120	-0.787877	-1.909805
28	1	0	-1.407455	0.743281	-2.576175
29	1	0	-3.733732	-1.128290	0.468493
30	1	0	-2.025518	-2.365409	1.158245
31	6	0	2.345863	0.390334	-0.277639
32	6	0	2.714256	-0.945991	-0.261128
33	6	0	3.323639	1.373362	-0.148677
34	6	0	4.042963	-1.294150	-0.130997
35	1	0	1.956915	-1.707040	-0.328481
36	6	0	4.647015	1.016102	-0.007534
37	1	0	3.035303	2.413545	-0.163826
38	6	0	5.012751	-0.317933	-0.003372
39	1	0	4.321248	-2.337522	-0.122918
40	1	0	5.397766	1.786059	0.092133
41	1	0	6.051330	-0.594867	0.100479

TS7 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029089	1.232544	-0.757147
2	6	0	-0.165655	0.192394	-0.889216
3	6	0	-1.713351	1.454386	0.550643
4	1	0	-0.954209	1.786039	1.259455
5	6	0	-0.133477	-0.890205	0.164243
6	1	0	0.575020	-0.635755	0.950804
7	8	0	-2.649924	2.498270	0.511527
8	1	0	-3.278252	2.335713	-0.196225
9	8	0	0.356922	-2.095334	-0.371237
10	1	0	-0.136524	-2.306400	-1.168357
11	6	0	-1.494035	-1.103829	0.834481
12	1	0	-1.292476	-1.611381	1.776110
13	6	0	-2.322754	0.167013	1.108789
14	1	0	-2.440642	0.309395	2.181125
15	6	0	-3.719044	-0.198250	0.532509
16	1	0	-4.520380	0.424862	0.914254
17	6	0	-2.501191	-2.004411	0.070761
18	1	0	-2.194742	-3.043342	0.017029
19	6	0	-3.585871	-0.276153	-0.962659
20	1	0	-3.921924	0.474948	-1.662783
21	6	0	-2.846706	-1.343476	-1.235963
22	1	0	-2.463590	-1.632343	-2.203328
23	6	0	-3.760078	-1.684129	0.872167
24	1	0	-3.652557	-1.886464	1.935997
25	1	0	-4.644533	-2.178006	0.480294
26	8	0	0.382380	3.021186	-0.540144
27	7	0	1.390732	2.341723	-0.444561
28	6	0	1.744778	1.201073	-0.483686
29	1	0	-1.358871	1.805741	-1.608967
30	1	0	0.146683	-0.105611	-1.882772
31	6	0	2.873408	0.370077	-0.171891
32	6	0	3.161967	-0.762786	-0.918946
33	6	0	3.683528	0.717812	0.905827
34	6	0	4.264164	-1.529183	-0.599112
35	1	0	2.516634	-1.040231	-1.736211
36	6	0	4.782663	-0.051979	1.215139
37	1	0	3.446183	1.595847	1.487340
38	6	0	5.075123	-1.176191	0.463129
39	1	0	4.489449	-2.408853	-1.183283
40	1	0	5.412460	0.223522	2.047908
41	1	0	5.935845	-1.780960	0.707957

TS8 (DCM)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.668456	2.379899	-0.920124
2	6	0	1.101435	1.163506	-0.184523
3	7	0	0.449370	1.891205	-0.875161
4	6	0	-1.317259	1.592782	1.106251
5	1	0	-1.261357	2.650836	1.312700
6	6	0	-0.278622	0.784102	1.457932
7	1	0	0.494905	1.221764	2.078225
8	6	0	-2.687873	1.094764	0.802228
9	1	0	-3.254780	1.280297	1.719005
10	6	0	-0.498626	-0.685158	1.708734
11	1	0	-0.708915	-0.746217	2.777218
12	8	0	-3.322808	1.890228	-0.169398
13	1	0	-2.690587	2.010629	-0.877475
14	8	0	0.677196	-1.449169	1.567699
15	1	0	0.957623	-1.405365	0.656656
16	6	0	-1.680362	-1.331453	0.985289
17	1	0	-2.103558	-2.054594	1.679738
18	6	0	-2.814583	-0.397365	0.494938
19	1	0	-3.746261	-0.726746	0.950599
20	6	0	-2.930590	-0.763548	-1.006552
21	1	0	-3.850716	-0.414196	-1.459254
22	6	0	-1.322459	-2.129118	-0.297834
23	1	0	-0.769859	-3.040256	-0.097474
24	6	0	-1.660021	-0.358323	-1.699678
25	1	0	-1.553636	0.483644	-2.362856
26	6	0	-0.702452	-1.177626	-1.281934
27	1	0	0.341122	-1.147368	-1.551904
28	6	0	-2.713910	-2.269491	-0.905985
29	1	0	-3.424952	-2.764701	-0.247174
30	1	0	-2.696287	-2.757437	-1.876097
31	6	0	2.408211	0.558601	-0.165728
32	6	0	3.092758	0.357504	1.025218
33	6	0	2.988315	0.178445	-1.373525
34	6	0	4.350280	-0.207831	1.003239
35	1	0	2.636360	0.632838	1.962222
36	6	0	4.246547	-0.383439	-1.383433
37	1	0	2.449638	0.337639	-2.295963
38	6	0	4.929040	-0.578260	-0.196302
39	1	0	4.880912	-0.361328	1.930921
40	1	0	4.694847	-0.671950	-2.322454
41	1	0	5.913498	-1.022140	-0.205937