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endo-Mode Cyclizations of Vinylogous *N*-Acyliminium Ions as a Route to the Synthesis of Condensed Thiazolidines

Milovan Stojanović,[a,b] Rade Marković,[a,c] Erich Kleinpeter,[b] Marija Baranac-Stojanović[a,b,c*]

[a]*Center for Chemistry ICTM, P.O.Box 473, 11000 Belgrade, Serbia*

[b]*Chemisches Institut der Universität Potsdam, Karl-Liebknecht Str.24-25, D-14476 Potsdam (Golm), Germany*

[c]*Faculty of Chemistry, University of Belgrade, Studentski trg 16, P.O.Box 158, 11000 Belgrade, Serbia*

Supplementary Data

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X, Y, Z Coordinates for the Optimized Structures of Products 18

18b-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.524832	-1.733170	-0.032374
2	6	0	0.149304	-0.053415	-0.473893
3	6	0	-1.112674	0.474639	-0.426055
4	1	0	-1.286781	1.512369	-0.687088
5	6	0	-2.261122	-0.304463	-0.031955
6	8	0	-2.260772	-1.486299	0.317739
7	7	0	1.283294	0.613831	-0.884837
8	6	0	2.534987	-0.007059	-0.453684
9	1	0	3.326704	0.291477	-1.160017
10	6	0	1.364130	2.084485	-0.903347
11	1	0	0.405967	2.508596	-1.206996
12	8	0	-3.403912	0.434121	-0.078070
13	6	0	-4.618734	-0.242174	0.311805
14	1	0	-4.777715	-1.101402	-0.349273
15	1	0	-4.504030	-0.623833	1.332347
16	6	0	-5.753080	0.761038	0.211308
17	1	0	-5.855578	1.136094	-0.812508
18	1	0	-6.695976	0.283110	0.498820
19	1	0	-5.582498	1.613646	0.877158
20	6	0	2.309225	-1.516225	-0.492785
21	6	0	3.083813	1.840022	0.902823
22	1	0	3.929984	2.112252	0.250689
23	1	0	2.097768	2.354610	-1.673239
24	6	0	1.819637	2.591319	0.472442
25	1	0	2.021567	3.668924	0.434079
26	1	0	1.023461	2.422424	1.207415
27	1	0	3.357375	2.068838	1.936534
28	8	0	2.887156	0.418251	0.851997
29	1	0	2.405925	-1.833575	-1.538022
30	6	0	3.239787	-2.339006	0.391889
31	1	0	2.999400	-3.404523	0.315346
32	1	0	4.277153	-2.205152	0.064121
33	1	0	3.165483	-2.033504	1.437856

18b-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.385946	0.178239	0.267701
2	6	0	-2.116857	1.567055	-0.302213
3	16	0	-0.283024	1.773183	-0.148383
4	6	0	-0.030069	0.008794	-0.075201
5	7	0	-1.226220	-0.652883	-0.094348
6	6	0	-1.345792	-2.081182	0.216121
7	6	0	-2.705712	-2.596751	-0.272449
8	6	0	-3.831311	-1.669185	0.175712
9	8	0	-3.571895	-0.331762	-0.282814
10	1	0	-2.360695	1.537040	-1.371401
11	6	0	1.206064	-0.576704	-0.007973
12	1	0	1.299287	-1.653220	0.079769

13	1	0	-2.475568	0.207924	1.372291
14	6	0	-2.888595	2.685108	0.389720
15	1	0	-0.538636	-2.621779	-0.284314
16	1	0	-1.236503	-2.237419	1.301869
17	1	0	-2.703872	-2.651022	-1.367365
18	1	0	-2.870909	-3.608125	0.117370
19	1	0	-4.791630	-1.955688	-0.260901
20	1	0	-3.930715	-1.667889	1.273002
21	1	0	-2.665523	3.657218	-0.061568
22	1	0	-2.647292	2.735376	1.456897
23	1	0	-3.963699	2.501908	0.283046
24	6	0	2.425283	0.193185	-0.037289
25	8	0	2.515574	1.421129	-0.099272
26	8	0	3.523545	-0.608770	0.025195
27	6	0	4.804330	0.058223	0.017570
28	6	0	5.877255	-1.010078	0.121177
29	1	0	4.847585	0.759554	0.858154
30	1	0	4.899252	0.639551	-0.906402
31	1	0	5.821875	-1.705228	-0.723308
32	1	0	5.771910	-1.582687	1.048737
33	1	0	6.867355	-0.541270	0.116565

18d-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.391033	-0.169368	-0.597635
2	6	0	2.113475	-1.615456	-0.167744
3	16	0	0.274050	-1.770975	-0.465910
4	6	0	0.028314	-0.021320	-0.217244
5	7	0	1.221044	0.622034	-0.217588
6	6	0	-1.192495	0.581199	-0.051462
7	6	0	-2.423339	-0.166752	-0.076610
8	8	0	-2.540471	-1.377008	-0.283057
9	8	0	-3.502110	0.634593	0.146103
10	6	0	-5.844936	1.064563	0.333321
11	6	0	-4.794238	-0.008498	0.114017
12	6	0	1.436787	2.033296	0.092184
13	6	0	2.931527	2.306308	-0.137404
14	16	0	3.805476	0.716276	0.193596
15	1	0	2.600591	-2.303870	-0.866230
16	1	0	2.534251	-0.132247	-1.687781
17	6	0	2.463548	-1.976916	1.274722
18	1	0	-1.252633	1.657493	0.072205
19	1	0	-6.843134	0.613435	0.318555
20	1	0	-5.705096	1.558890	1.300539
21	1	0	-5.798921	1.824477	-0.453941
22	1	0	-4.831285	-0.776767	0.894518
23	1	0	-4.921607	-0.509291	-0.852051
24	1	0	0.830480	2.674215	-0.561031
25	1	0	1.145152	2.227664	1.132246
26	1	0	3.317087	3.071106	0.540733
27	1	0	3.122132	2.616192	-1.169079
28	1	0	2.117344	-2.990201	1.500749
29	1	0	1.999346	-1.285753	1.984820
30	1	0	3.549173	-1.947418	1.424644

18d-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.393639	0.100344	0.354181
2	6	0	-2.129085	1.445812	-0.318604
3	16	0	-0.314900	1.743250	0.009997
4	6	0	-0.003503	-0.008960	0.133226
5	7	0	-1.172253	-0.691586	0.235067
6	6	0	1.240808	-0.582824	0.125179
7	6	0	2.445480	0.202879	0.024162
8	8	0	2.515079	1.433352	-0.008570
9	8	0	3.555232	-0.584362	-0.020386
10	6	0	5.915354	-0.950885	-0.107368
11	6	0	4.823323	0.102728	-0.093341
12	6	0	-1.320892	-2.141232	0.119993
13	6	0	-2.826094	-2.439110	0.213925
14	16	0	-3.692366	-0.946702	-0.437631
15	6	0	-2.994262	2.592392	0.192096
16	1	0	-2.657222	0.241770	1.413933
17	1	0	-2.233299	1.339908	-1.405287
18	1	0	1.342327	-1.658292	0.227655
19	1	0	6.896066	-0.465886	-0.163090
20	1	0	5.884175	-1.560401	0.802008
21	1	0	5.810051	-1.614013	-0.972596
22	1	0	4.844059	0.719929	-0.998448
23	1	0	4.917113	0.772850	0.768449
24	1	0	-0.903253	-2.473005	-0.839368
25	1	0	-0.782963	-2.656939	0.925955
26	1	0	-3.132938	-2.610063	1.249894
27	1	0	-3.109080	-3.306027	-0.387573
28	1	0	-2.714097	3.537167	-0.284806
29	1	0	-4.047080	2.399952	-0.045830
30	1	0	-2.899242	2.710597	1.276743

18f-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.287509	-1.826833	0.049164
2	6	0	0.040796	-0.140354	0.503261
3	6	0	1.279598	0.436916	0.425642
4	1	0	1.420502	1.481665	0.677762
5	6	0	2.445510	-0.300498	0.001919
6	8	0	2.474734	-1.477177	-0.363474
7	7	0	-1.104581	0.474790	0.952808
8	6	0	-2.342039	-0.185990	0.582525
9	1	0	-3.115489	0.071592	1.316338
10	6	0	-1.192710	1.923157	1.178179
11	1	0	-0.241393	2.279517	1.578115
12	8	0	3.564366	0.473166	0.038042
13	6	0	4.793263	-0.158361	-0.382494
14	1	0	4.980077	-1.033348	0.249833
15	1	0	4.679361	-0.510529	-1.413791
16	6	0	5.901881	0.870608	-0.259066
17	1	0	6.003417	1.215179	0.775514
18	1	0	6.854207	0.426672	-0.569018

19	1	0	5.703803	1.739332	-0.895822
20	6	0	-2.050943	-1.688134	0.613392
21	6	0	-2.941003	2.219373	-0.646011
22	1	0	-3.742805	2.412634	0.077283
23	16	0	-2.960176	0.425345	-1.081291
24	1	0	-2.064711	-1.989198	1.668879
25	1	0	-1.947930	2.077277	1.959383
26	6	0	-1.589997	2.684978	-0.093721
27	1	0	-1.657041	3.754350	0.147444
28	1	0	-0.812066	2.565668	-0.856979
29	1	0	-3.191200	2.745180	-1.572482
30	6	0	-2.981596	-2.596036	-0.184190
31	1	0	-2.692501	-3.643975	-0.052624
32	1	0	-4.010556	-2.484722	0.175617
33	1	0	-2.960015	-2.368868	-1.254236

18f-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.289391	1.784835	-0.485291
2	6	0	0.017198	0.235924	0.342384
3	6	0	-1.212672	-0.353960	0.459872
4	1	0	-1.319138	-1.320298	0.939193
5	6	0	-2.411138	0.259864	-0.058425
6	8	0	-2.482171	1.332757	-0.660767
7	7	0	1.195441	-0.260025	0.847977
8	6	0	2.398019	0.317701	0.280625
9	1	0	3.210328	0.230681	1.012482
10	6	0	1.327067	-1.630693	1.358618
11	1	0	0.408377	-1.906637	1.879917
12	8	0	-3.508883	-0.506979	0.183892
13	6	0	-4.766699	0.001742	-0.311076
14	1	0	-4.961403	0.978755	0.145099
15	1	0	-4.691697	0.148759	-1.394169
16	6	0	-5.840981	-1.009053	0.045711
17	1	0	-5.905599	-1.146876	1.130240
18	1	0	-6.813764	-0.657593	-0.315190
19	1	0	-5.633439	-1.980563	-0.415263
20	6	0	2.090700	1.784190	-0.037124
21	6	0	2.975146	-2.288517	-0.470590
22	1	0	3.821382	-2.335774	0.225730
23	16	0	2.945955	-0.613999	-1.247345
24	1	0	2.129445	-1.615575	2.107116
25	6	0	1.664734	-2.633732	0.245477
26	1	0	1.761917	-3.631260	0.694507
27	1	0	0.841527	-2.674708	-0.477397
28	1	0	3.173455	-2.988294	-1.288088
29	1	0	2.641372	2.112659	-0.925577
30	6	0	2.383212	2.717480	1.140954
31	1	0	3.459507	2.729069	1.352449
32	1	0	2.070768	3.740271	0.908868
33	1	0	1.854277	2.392284	2.042843

18h-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.238169	-2.488529	0.350254
2	6	0	-3.927396	-1.182506	0.752124
3	16	0	-2.810150	0.210005	1.198928
4	6	0	-2.024456	0.453564	-0.482409
5	6	0	-0.956152	-1.858824	-0.757960
6	6	0	-2.363424	-2.448168	-0.917537
7	1	0	-4.035489	-3.227693	0.187519
8	1	0	-2.636577	-2.858715	1.190855
9	1	0	-4.597531	-0.834529	-0.043560
10	1	0	-4.538799	-1.342109	1.646941
11	1	0	-2.805092	0.196917	-1.204714
12	6	0	-1.547839	1.887252	-0.758956
13	6	0	-2.389265	3.031716	-0.207405
14	7	0	-0.860196	-0.389301	-0.690771
15	6	0	1.531452	-0.502508	-0.266158
16	1	0	-0.497664	-2.282730	0.147210
17	1	0	-2.897530	-1.969539	-1.749019
18	1	0	-2.198075	-3.485969	-1.233009
19	6	0	0.347182	0.180242	-0.376333
20	16	0	0.194166	1.932772	-0.130900
21	6	0	2.772285	0.159235	0.055642
22	1	0	-1.480684	1.982043	-1.850769
23	8	0	2.919336	1.353479	0.323301
24	8	0	3.819059	-0.711458	0.042665
25	1	0	-0.341536	-2.180262	-1.607929
26	1	0	-1.975519	3.991948	-0.533693
27	1	0	-2.428974	3.023716	0.884932
28	1	0	-3.413749	2.959591	-0.588992
29	6	0	5.113429	-0.161654	0.370112
30	1	0	7.125247	-0.908360	0.515225
31	6	0	6.126590	-1.287349	0.272002
32	1	0	5.076506	0.264037	1.379227
33	1	0	5.343430	0.652178	-0.326315
34	1	0	6.153571	-1.702920	-0.740913
35	1	0	5.885289	-2.094877	0.971349
36	1	0	1.567726	-1.573048	-0.425391

18h-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.300752	-2.419088	-0.149216
2	6	0	3.962565	-1.198897	-0.794145
3	16	0	2.816410	0.097040	-1.418021
4	6	0	2.060204	0.603426	0.216420
5	6	0	1.070037	-1.637485	0.970121
6	6	0	2.500072	-2.165007	1.142964
7	1	0	4.109318	-3.124892	0.088192
8	1	0	2.655801	-2.919156	-0.883667
9	1	0	4.663305	-0.723035	-0.096984
10	1	0	4.536453	-1.505471	-1.675472
11	1	0	2.863978	0.504133	0.950562
12	6	0	1.563680	2.057319	0.187657

13	1	0	2.092999	2.627643	-0.581466
14	7	0	0.928721	-0.214307	0.610000
15	6	0	-1.470413	-0.458172	0.297711
16	1	0	0.565977	-2.241915	0.202653
17	1	0	3.070398	-1.536898	1.840101
18	1	0	2.379827	-3.130674	1.649878
19	16	0	-0.206399	1.935687	-0.339966
20	6	0	-0.302370	0.258167	0.237432
21	6	0	-2.735709	0.103583	-0.107354
22	6	0	1.701478	2.748754	1.547458
23	8	0	-2.921781	1.227243	-0.579011
24	8	0	-3.756470	-0.777495	0.081098
25	1	0	0.521919	-1.789224	1.908431
26	1	0	1.269914	3.753785	1.513319
27	1	0	2.761136	2.840981	1.816101
28	1	0	1.191085	2.181374	2.332867
29	6	0	-5.070735	-0.326706	-0.312246
30	1	0	-7.055598	-1.154505	-0.328560
31	6	0	-6.043185	-1.460186	-0.042732
32	1	0	-5.052282	-0.051539	-1.372633
33	1	0	-5.326978	0.571751	0.260252
34	1	0	-6.051175	-1.726102	1.019643
35	1	0	-5.776617	-2.351270	-0.620933
36	1	0	-1.472937	-1.480694	0.654401

X, Y, Z Coordinates for the Calculated Ground State (GS) and Transition State (TS) Structures 21 and 22

21a (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.808162	-1.927102	-0.401240
2	6	0	1.621415	-1.540164	-1.810488
3	16	0	-0.064354	-0.797544	-1.926086
4	6	0	-0.306939	-1.002518	-0.186675
5	7	0	0.834407	-1.640461	0.411051
6	6	0	1.040419	-1.742899	1.870686
7	6	0	1.918469	-0.551487	2.321763
8	6	0	-1.400168	-0.637174	0.511003
9	6	0	-2.518008	-0.000970	-0.211108
10	8	0	-2.483519	0.211884	-1.414893
11	8	0	-3.530792	0.296162	0.600324
12	6	0	-4.700021	0.918667	-0.019032
13	6	0	-5.723557	1.149808	1.072792
14	1	0	2.696742	-2.409550	-0.012475
15	1	0	2.389754	-0.797347	-2.066999
16	1	0	1.736144	-2.398937	-2.482871
17	1	0	1.566098	-2.680829	2.059386
18	1	0	0.077907	-1.775985	2.377309
19	1	0	2.107508	-0.681328	3.394022
20	1	0	1.370382	0.389123	2.183788
21	1	0	3.175842	0.171943	0.978946
22	1	0	-1.504829	-0.801329	1.575486

23	1	0	-5.064392	0.247052	-0.801462
24	1	0	-4.374798	1.848715	-0.494076
25	1	0	-5.330664	1.814065	1.848568
26	1	0	-6.023905	0.206142	1.538067
27	1	0	-6.614069	1.617256	0.640361
28	8	0	3.276526	1.128395	-0.529725
29	1	0	4.229774	1.199723	-0.708425
30	6	0	2.707391	2.456933	-0.679751
31	6	0	3.331455	3.466725	0.269204
32	1	0	1.639847	2.326346	-0.483135
33	1	0	2.817214	2.770488	-1.724637
34	1	0	2.857360	4.445878	0.141822
35	1	0	3.209108	3.160555	1.313690
36	1	0	4.402560	3.592048	0.069661
37	8	0	3.131976	-0.578817	1.615552

21a (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.250372	1.634689	0.891098
2	6	0	-0.802840	2.630643	-0.106263
3	16	0	0.868130	2.085862	-0.672986
4	6	0	0.835053	0.715438	0.446136
5	7	0	-0.392131	0.692641	1.181774
6	6	0	-0.905042	-0.486284	1.895388
7	6	0	-1.905763	-1.176724	0.925000
8	6	0	1.822094	-0.184692	0.619499
9	6	0	3.050259	-0.057437	-0.181483
10	8	0	3.208051	0.822433	-1.016334
11	8	0	3.942829	-1.003111	0.119210
12	6	0	5.204243	-0.958825	-0.612314
13	6	0	6.058707	-2.106166	-0.114071
14	1	0	-2.169791	1.710510	1.452395
15	1	0	-1.510141	2.672666	-0.942938
16	1	0	-0.765293	3.632897	0.339638
17	1	0	-1.428604	-0.129348	2.784928
18	1	0	-0.087207	-1.134900	2.201931
19	1	0	-2.395519	-1.963941	1.525241
20	1	0	-1.324154	-1.681425	0.133410
21	1	0	-3.456568	-0.689861	-0.690797
22	1	0	1.757231	-0.992306	1.336978
23	1	0	5.666926	0.016046	-0.433116
24	1	0	4.980860	-1.035623	-1.680451
25	1	0	5.571524	-3.068994	-0.296358
26	1	0	6.257719	-2.012362	0.957880
27	1	0	7.017532	-2.101379	-0.642543
28	8	0	-4.151005	-1.106180	-1.528644
29	1	0	-4.372486	-0.387795	-2.150874
30	6	0	-5.392070	-1.651950	-0.914112
31	6	0	-6.142932	-0.593489	-0.134315
32	1	0	-5.021587	-2.459391	-0.282005
33	1	0	-5.962626	-2.080368	-1.740022
34	1	0	-7.011048	-1.052742	0.350315
35	1	0	-5.498412	-0.162427	0.637197
36	1	0	-6.514616	0.204988	-0.787034
37	8	0	-2.788241	-0.225359	0.442544

21b (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.422464	-1.699823	0.556315
2	6	0	1.083514	1.279890	1.273251
3	7	0	0.174145	0.361320	1.335703
4	6	0	0.432471	-0.948233	2.003135
5	6	0	0.991331	-1.983791	1.017951
6	6	0	0.770260	2.460646	0.449483
7	16	0	-0.922292	2.182984	-0.232676
8	6	0	-1.019023	0.616784	0.581248
9	6	0	-2.057120	-0.240470	0.532789
10	1	0	3.099308	-1.714519	1.427168
11	1	0	2.746160	-2.504911	-0.114528
12	1	0	2.011030	1.155431	1.817565
13	1	0	-0.505823	-1.269820	2.456041
14	1	0	1.139651	-0.748381	2.812506
15	1	0	0.328548	-2.063572	0.149582
16	1	0	0.971748	-2.952789	1.531366
17	1	0	0.822266	3.380701	1.045269
18	1	0	1.515570	2.543350	-0.352494
19	1	0	-2.061051	-1.189611	1.052536
20	6	0	-3.241697	0.130476	-0.262213
21	8	0	-3.313302	1.183822	-0.879428
22	8	0	-4.188002	-0.805773	-0.214229
23	6	0	-5.411689	-0.533457	-0.965013
24	1	0	-7.280102	-1.528842	-1.293215
25	6	0	-6.351088	-1.699885	-0.739865
26	1	0	-5.140915	-0.409510	-2.017561
27	1	0	-5.824559	0.413798	-0.606795
28	1	0	-6.598876	-1.807550	0.320507
29	1	0	-5.909251	-2.636505	-1.093397
30	6	0	5.921435	-0.205632	-1.542623
31	6	0	6.175400	-0.078000	-0.052224
32	1	0	5.932307	0.780594	-2.026379
33	1	0	6.693820	-0.825614	-2.014300
34	1	0	7.139415	0.408436	0.126433
35	1	0	5.393964	0.525265	0.423969
36	1	0	6.193819	-1.063885	0.423322
37	8	0	4.632581	-0.828935	-1.725900
38	1	0	4.475092	-0.950694	-2.675087
39	8	0	2.474740	-0.440109	-0.107184
40	1	0	3.249833	-0.461433	-0.719086

21b (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.364082	1.924280	0.082294
2	6	0	1.258959	-0.365913	-1.530410
3	7	0	0.210466	0.393908	-1.377152
4	6	0	0.350785	1.870515	-1.507779
5	6	0	0.957472	2.456671	-0.228814
6	6	0	1.076048	-1.794992	-1.201350
7	16	0	-0.618563	-1.946480	-0.485008
8	6	0	-0.922220	-0.227114	-0.766437

9	6	0	-2.058793	0.431152	-0.465081
10	1	0	3.044856	2.182944	-0.748917
11	1	0	2.747139	2.439890	0.972836
12	1	0	2.125742	0.019973	-2.049897
13	1	0	-0.628368	2.287925	-1.740733
14	1	0	0.997501	2.045417	-2.372875
15	1	0	0.294760	2.252601	0.619264
16	1	0	1.005058	3.545162	-0.354697
17	1	0	1.182913	-2.409037	-2.104765
18	1	0	1.839533	-2.113219	-0.485127
19	1	0	-2.192943	1.487578	-0.657249
20	6	0	-3.168112	-0.314910	0.150346
21	8	0	-3.100370	-1.509378	0.405619
22	8	0	-4.225506	0.464072	0.386096
23	6	0	-5.385211	-0.183759	0.989864
24	1	0	-7.340024	0.421935	1.626973
25	6	0	-6.452434	0.875438	1.174016
26	1	0	-5.070438	-0.630448	1.937459
27	1	0	-5.706972	-0.991247	0.325785
28	1	0	-6.743070	1.313112	0.214122
29	1	0	-6.102925	1.676661	1.832376
30	6	0	5.470392	-0.794217	1.469295
31	6	0	6.008481	-0.281252	0.149107
32	1	0	5.115658	-1.828698	1.389247
33	1	0	6.228787	-0.742618	2.256265
34	1	0	6.840021	-0.911866	-0.180356
35	1	0	5.233951	-0.305918	-0.625276
36	1	0	6.372258	0.745484	0.249505
37	8	0	4.360634	0.065335	1.869696
38	1	0	4.031372	-0.203925	2.744054
39	8	0	2.324634	0.516960	0.300231
40	1	0	3.277104	0.233302	0.968769

21c (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.018405	-0.575412	1.222011
2	6	0	0.814087	-1.971769	0.773280
3	16	0	-0.937186	-2.035994	0.160071
4	6	0	-1.191951	-0.341024	0.574343
5	7	0	0.007401	0.232599	1.119218
6	1	0	1.934166	-0.226141	1.677725
7	6	0	1.837541	-2.440245	-0.279345
8	1	0	0.899558	-2.616098	1.660822
9	1	0	2.859431	-2.351889	0.101337
10	1	0	1.749944	-1.841238	-1.187581
11	6	0	-2.341758	0.349152	0.440233
12	1	0	-2.436002	1.388860	0.724819
13	6	0	0.090507	1.669769	1.495756
14	6	0	0.168034	2.633967	0.293591
15	6	0	-3.524407	-0.335549	-0.112018
16	8	0	-3.502302	-1.501547	-0.478386
17	8	0	-4.588006	0.468411	-0.155977
18	6	0	-5.818381	-0.113666	-0.684413
19	6	0	-6.888750	0.956404	-0.626830
20	1	0	-6.067360	-0.988788	-0.077358
21	1	0	-5.620597	-0.454718	-1.704803

22	1	0	-6.612027	1.824655	-1.232752
23	1	0	-7.060048	1.287690	0.401934
24	1	0	-7.827963	0.551356	-1.017267
25	1	0	0.966636	1.771752	2.139247
26	1	0	-0.794023	1.873390	2.102885
27	1	0	-0.520039	2.300270	-0.491664
28	6	0	1.559716	2.908503	-0.303501
29	1	0	-0.232493	3.587074	0.659362
30	6	0	2.209014	1.788357	-1.109318
31	1	0	2.254304	3.217424	0.488555
32	1	0	1.451516	3.770655	-0.973492
33	1	0	1.646463	-3.488161	-0.525016
34	1	0	1.509962	1.414010	-1.874428
35	1	0	3.366150	0.233220	-0.668801
36	8	0	2.625221	0.729375	-0.244162
37	1	0	3.081835	2.195531	-1.636561
38	8	0	4.756263	-0.693650	-1.219477
39	1	0	4.799299	-0.957435	-2.152078
40	6	0	6.065513	-0.228973	-0.813027
41	1	0	6.337804	0.663869	-1.391428
42	1	0	6.805070	-1.011229	-1.022719
43	6	0	6.017694	0.082860	0.670934
44	1	0	5.792877	-0.819251	1.249609
45	1	0	5.252383	0.837117	0.883695
46	1	0	6.985340	0.470835	1.004154

21c (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.983779	0.427714	-1.104334
2	1	0	-2.768614	1.050033	-1.536308
3	6	0	-1.556839	-0.688879	-2.048493
4	16	0	0.134617	-1.172253	-1.464387
5	6	0	0.362904	0.448351	-0.770042
6	6	0	-0.905110	2.489191	-0.110487
7	7	0	-0.834534	1.169335	-0.762024
8	6	0	-2.310727	2.921377	0.320200
9	1	0	-0.473770	3.241814	-0.781259
10	6	0	-2.506134	-1.873926	-2.192379
11	1	0	-1.434265	-0.211278	-3.027566
12	1	0	-0.270186	2.453597	0.783187
13	6	0	-2.980432	1.993385	1.352278
14	6	0	1.551070	0.912696	-0.307967
15	1	0	1.670592	1.928583	0.045092
16	1	0	-2.966506	3.069742	-0.547329
17	1	0	-2.192941	3.913652	0.769497
18	6	0	2.721060	0.037793	-0.289873
19	8	0	2.686070	-1.161477	-0.547752
20	8	0	3.836220	0.694597	0.069102
21	6	0	5.056505	-0.091405	0.122579
22	6	0	6.178750	0.838096	0.540171
23	1	0	5.228283	-0.531794	-0.864120
24	1	0	4.911251	-0.911691	0.832752
25	1	0	5.984655	1.272192	1.526113
26	1	0	6.301767	1.653113	-0.179700
27	1	0	7.119036	0.279168	0.589998
28	1	0	-2.258308	1.728865	2.136465

29	6	0	-3.609198	0.726858	0.782392
30	1	0	-3.792081	2.538017	1.851234
31	8	0	-2.664981	-0.160037	0.117314
32	1	0	-4.389272	0.964750	0.050527
33	1	0	-4.064130	0.120947	1.571295
34	1	0	-2.148244	-1.105204	0.824845
35	1	0	-3.496874	-1.537494	-2.517379
36	1	0	-2.615967	-2.430745	-1.258508
37	1	0	-2.125822	-2.565286	-2.949853
38	8	0	-1.860702	-2.079600	1.386071
39	1	0	-2.634093	-2.668338	1.452013
40	6	0	-1.085857	-2.055447	2.662146
41	1	0	-0.969842	-3.106699	2.931763
42	1	0	-1.700527	-1.548252	3.411347
43	6	0	0.242447	-1.378016	2.426196
44	1	0	0.121890	-0.327396	2.146205
45	1	0	0.809780	-1.410725	3.362716
46	1	0	0.821249	-1.883486	1.649129

21d (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.683583	-1.194506	1.581502
2	6	0	-1.532340	0.062851	2.329206
3	16	0	0.166787	0.683002	1.961585
4	6	0	0.435520	-0.640317	0.822707
5	7	0	-0.693744	-1.530014	0.806991
6	6	0	-0.814647	-2.648977	-0.153059
7	6	0	-1.414037	-2.168198	-1.489627
8	16	0	-3.132699	-1.548481	-1.344806
9	6	0	1.535907	-0.833602	0.068498
10	6	0	2.645943	0.131073	0.181460
11	8	0	2.602056	1.093603	0.934590
12	8	0	3.662963	-0.183113	-0.617957
13	6	0	4.825347	0.703198	-0.570936
14	6	0	5.856397	0.152182	-1.533357
15	1	0	-2.561148	-1.830096	1.626740
16	1	0	-2.280497	0.775198	1.942750
17	1	0	-1.696144	-0.080383	3.403604
18	1	0	-1.458023	-3.399945	0.308105
19	1	0	0.173737	-3.088787	-0.290975
20	1	0	-1.454479	-3.034108	-2.156378
21	1	0	-0.773992	-1.419793	-1.962268
22	1	0	-2.853292	-0.248386	-1.070207
23	1	0	1.650044	-1.671686	-0.606656
24	1	0	5.185978	0.730964	0.461156
25	1	0	4.492713	1.709341	-0.841872
26	1	0	5.466905	0.122667	-2.555519
27	1	0	6.164658	-0.857569	-1.245938
28	1	0	6.741436	0.796491	-1.522616
29	8	0	-3.014517	1.610081	0.000537
30	1	0	-3.978514	1.734458	0.019757
31	6	0	-2.437806	2.847842	-0.484880
32	6	0	-2.958585	3.228494	-1.861857
33	1	0	-1.359855	2.666425	-0.502771
34	1	0	-2.628661	3.646848	0.243209
35	1	0	-2.480381	4.152378	-2.204813

36	1	0	-2.751521	2.442096	-2.595157
37	1	0	-4.040870	3.406835	-1.842854

21d (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.824299	-1.800396	0.930220
2	6	0	-1.597424	-1.072485	2.195106
3	16	0	0.111213	-0.379875	2.096835
4	6	0	0.318083	-1.033899	0.468451
5	7	0	-0.841584	-1.777210	0.070079
6	6	0	-1.067365	-2.218526	-1.316781
7	6	0	-1.720953	-1.072997	-2.126819
8	16	0	-3.324959	-0.533232	-1.430022
9	6	0	1.407097	-0.887583	-0.313177
10	6	0	2.551226	-0.115641	0.203893
11	8	0	2.544254	0.408604	1.309172
12	8	0	3.557078	-0.069329	-0.668193
13	6	0	4.752191	0.657921	-0.244982
14	6	0	5.753006	0.587390	-1.379321
15	1	0	-2.713531	-2.377663	0.712270
16	1	0	-2.328935	-0.258907	2.285105
17	1	0	-1.716015	-1.735967	3.060383
18	1	0	-1.727892	-3.086399	-1.279112
19	1	0	-0.118205	-2.532581	-1.750941
20	1	0	-1.919467	-1.460145	-3.130407
21	1	0	-1.031117	-0.232128	-2.226831
22	1	0	-2.848606	0.713224	-0.515237
23	1	0	1.487227	-1.327392	-1.298733
24	1	0	5.123573	0.191472	0.671968
25	1	0	4.457580	1.684301	-0.007836
26	1	0	5.355349	1.052115	-2.286723
27	1	0	6.021093	-0.449160	-1.604888
28	1	0	6.664079	1.121951	-1.091631
29	8	0	-2.649339	1.796559	0.620161
30	1	0	-3.539672	2.164708	0.763614
31	6	0	-1.736069	2.909524	0.376445
32	6	0	-2.192828	3.795984	-0.768773
33	1	0	-0.775086	2.432920	0.170447
34	1	0	-1.638577	3.470826	1.311916
35	1	0	-1.469038	4.603202	-0.924205
36	1	0	-2.282439	3.230781	-1.702067
37	1	0	-3.161241	4.262603	-0.551341

21e (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.130781	-1.943986	0.156467
2	16	0	2.273099	-0.491111	-0.990502
3	6	0	0.938671	1.145215	1.027869
4	7	0	-0.003866	0.253695	1.151976
5	6	0	0.266563	-1.080489	1.755223
6	6	0	0.713375	-2.121728	0.717796
7	6	0	0.562463	2.399246	0.342868

8	16	0	-1.175631	2.169693	-0.237898
9	6	0	-1.247466	0.572765	0.517141
10	6	0	-2.311943	-0.254498	0.520247
11	1	0	2.860015	-1.830204	0.965065
12	1	0	2.401739	-2.838279	-0.409272
13	1	0	1.888326	0.993446	1.524827
14	1	0	-0.643002	-1.392216	2.269413
15	1	0	1.036718	-0.926666	2.515920
16	1	0	-0.017857	-2.178995	-0.096332
17	1	0	0.680503	-3.090309	1.232040
18	1	0	0.641365	3.244500	1.040106
19	1	0	1.239013	2.596043	-0.495493
20	1	0	-2.300512	-1.227071	0.994658
21	6	0	-3.547654	0.183477	-0.152577
22	1	0	3.640133	-0.514714	-1.055828
23	8	0	-3.637204	1.261586	-0.722913
24	8	0	-4.517854	-0.724556	-0.055726
25	6	0	-5.790793	-0.384995	-0.687702
26	1	0	-7.713282	-1.307679	-0.891046
27	6	0	-6.746527	-1.530820	-0.428277
28	1	0	-5.606118	-0.225495	-1.753983
29	1	0	-6.140493	0.558446	-0.259008
30	1	0	-6.905877	-1.676169	0.644534
31	1	0	-6.369235	-2.464528	-0.856388
32	6	0	6.569269	-0.089748	-0.720417
33	6	0	6.265188	0.781506	0.484231
34	1	0	6.710620	0.526941	-1.618679
35	1	0	7.490825	-0.662454	-0.553819
36	1	0	7.091675	1.475912	0.665755
37	1	0	5.356395	1.371721	0.319282
38	1	0	6.128991	0.167051	1.380281
39	8	0	5.467357	-0.999919	-0.910798
40	1	0	5.687685	-1.585027	-1.653184

21e (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.953391	2.360850	-0.711893
2	16	0	-2.136114	0.517444	-0.578358
3	6	0	-1.317855	0.368159	1.212230
4	7	0	-0.045182	0.969582	1.182200
5	6	0	-0.000669	2.417151	0.941117
6	6	0	-0.500801	2.789258	-0.462509
7	6	0	-1.138610	-1.091029	1.581756
8	16	0	0.489966	-1.588516	0.866783
9	6	0	0.987813	0.114612	0.760254
10	6	0	2.209102	0.515598	0.336352
11	1	0	-2.631576	2.839693	0.003606
12	1	0	-2.274147	2.623633	-1.722925
13	1	0	-2.005994	0.917090	1.858927
14	1	0	1.019017	2.767344	1.103181
15	1	0	-0.624269	2.892772	1.708088
16	1	0	0.154112	2.348243	-1.221597
17	1	0	-0.449783	3.878595	-0.579374
18	1	0	-1.116293	-1.180338	2.672945
19	1	0	-1.929774	-1.737406	1.195823
20	1	0	2.479845	1.560833	0.261525

21	6	0	3.211387	-0.479868	-0.039218
22	1	0	-3.863247	0.243679	-0.312444
23	8	0	3.007972	-1.687881	-0.038162
24	8	0	4.374856	0.088643	-0.397006
25	6	0	5.436600	-0.819822	-0.792324
26	1	0	7.468679	-0.629442	-1.460069
27	6	0	6.643164	0.022764	-1.156414
28	1	0	5.082350	-1.422959	-1.633992
29	1	0	5.641038	-1.498077	0.041677
30	1	0	6.975314	0.622485	-0.303249
31	1	0	6.415072	0.697493	-1.987578
32	6	0	-5.536139	-0.994814	-1.139786
33	6	0	-4.903949	-2.341729	-0.880343
34	1	0	-5.326294	-0.604935	-2.139018
35	1	0	-6.611609	-0.995186	-0.956025
36	1	0	-5.344183	-3.067666	-1.572134
37	1	0	-3.824582	-2.327561	-1.061028
38	1	0	-5.101535	-2.680341	0.140423
39	8	0	-4.982209	-0.010891	-0.148010
40	1	0	-5.502357	0.816384	-0.156858

21f (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.397990	0.867798	-0.877057
2	1	0	3.598558	-0.120729	1.380283
3	6	0	-0.735209	0.033387	-0.618682
4	16	0	-0.266481	-1.671693	-0.568155
5	6	0	1.459148	-1.237419	-1.050808
6	6	0	1.540978	0.239212	-0.981594
7	16	0	2.576557	0.765045	1.501047
8	6	0	3.393462	2.269695	0.803529
9	6	0	2.375243	3.351489	0.412381
10	6	0	1.556011	3.175084	-0.888776
11	6	0	0.262375	2.348431	-0.837576
12	6	0	-3.073030	-0.425528	-0.144013
13	6	0	-1.979667	0.517694	-0.430743
14	1	0	-2.209414	1.574064	-0.476948
15	8	0	-2.896271	-1.631561	-0.042619
16	1	0	1.658719	-1.549657	-2.086811
17	1	0	2.209049	-1.717260	-0.411552
18	1	0	2.424756	0.785377	-1.276677
19	1	0	4.059327	2.667805	1.573022
20	1	0	4.013977	1.984470	-0.053607
21	1	0	2.954071	4.275005	0.292589
22	1	0	1.693902	3.538378	1.252696
23	1	0	1.207720	4.174692	-1.174069
24	1	0	2.197765	2.860621	-1.721988
25	1	0	-0.380459	2.613567	-1.682483
26	1	0	-0.286938	2.576195	0.081377
27	1	0	3.794625	-2.631447	1.646519
28	8	0	4.090610	-2.095080	0.892915
29	6	0	5.372842	-2.608602	0.466971
30	6	0	5.861590	-1.774960	-0.702229
31	1	0	5.267911	-3.660851	0.172389
32	1	0	6.085503	-2.557882	1.300340
33	1	0	6.834575	-2.141773	-1.043912

34	1	0	5.163900	-1.833819	-1.544929
35	1	0	5.979787	-0.724760	-0.412423
36	6	0	-5.395767	-0.648413	0.294704
37	6	0	-6.614194	0.251202	0.410826
38	1	0	-5.498979	-1.385371	-0.508126
39	1	0	-5.189543	-1.188909	1.224138
40	6	0	-7.877408	-0.554927	0.734794
41	1	0	-6.432485	0.999720	1.191756
42	1	0	-6.745480	0.798453	-0.530562
43	1	0	-8.745209	0.106522	0.815173
44	1	0	-8.093240	-1.293629	-0.045731
45	1	0	-7.778305	-1.090837	1.685887
46	8	0	-4.245525	0.196113	-0.006037

21f (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.327801	1.010464	0.898034
2	1	0	-3.552490	-1.157844	-0.631350
3	6	0	0.780464	0.177523	0.688976
4	16	0	0.369591	-1.533598	0.964436
5	6	0	-1.280610	-1.025053	1.608786
6	6	0	-1.550503	0.335758	0.996955
7	16	0	-2.386962	0.146797	-0.802750
8	6	0	-3.357760	1.716938	-0.748665
9	6	0	-2.474340	2.971575	-0.750500
10	6	0	-1.557232	3.211566	0.468411
11	6	0	-0.236110	2.429580	0.507620
12	6	0	3.089144	-0.361040	0.127004
13	6	0	2.010997	0.606767	0.323482
14	1	0	2.231291	1.655006	0.171552
15	8	0	2.940523	-1.574859	0.206481
16	1	0	-1.241207	-0.918274	2.698462
17	1	0	-2.039139	-1.769893	1.363677
18	1	0	-2.309417	0.908627	1.528787
19	1	0	-3.988416	1.709602	-1.642496
20	1	0	-4.012733	1.692608	0.129942
21	1	0	-3.165398	3.820986	-0.824511
22	1	0	-1.871585	2.985953	-1.666863
23	1	0	-1.258785	4.265518	0.434388
24	1	0	-2.111360	3.102443	1.409566
25	1	0	0.444141	2.915561	1.215373
26	1	0	0.237110	2.482497	-0.482133
27	1	0	-3.696072	-2.837774	-1.032923
28	8	0	-4.184638	-2.140896	-0.550488
29	6	0	-5.591271	-2.044044	-1.053789
30	6	0	-6.384722	-1.192107	-0.091308
31	1	0	-5.948502	-3.074546	-1.087617
32	1	0	-5.551208	-1.632039	-2.065653
33	1	0	-7.423536	-1.154056	-0.435420
34	1	0	-6.372275	-1.618993	0.915112
35	1	0	-6.009596	-0.164458	-0.053044
36	6	0	5.390779	-0.637791	-0.385183
37	6	0	6.596701	0.236626	-0.687926
38	1	0	5.541858	-1.249889	0.510208
39	1	0	5.153813	-1.313174	-1.214313
40	6	0	7.854828	-0.600780	-0.942648

41	1	0	6.373904	0.860570	-1.562301
42	1	0	6.761224	0.919653	0.154503
43	1	0	8.712946	0.044958	-1.153300
44	1	0	8.108746	-1.217717	-0.072667
45	1	0	7.724275	-1.270658	-1.800713
46	8	0	4.255712	0.237981	-0.161840

21g (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.798707	0.679133	-0.501040
2	6	0	2.437556	2.033010	-0.039434
3	16	0	0.608357	2.026133	0.215371
4	6	0	0.515483	0.335100	-0.294462
5	7	0	1.817984	-0.162923	-0.642288
6	6	0	2.097173	-1.590972	-0.892603
7	6	0	2.512170	-2.260357	0.440109
8	7	0	3.667395	-1.571020	1.000874
9	1	0	3.635143	-1.545151	2.015978
10	6	0	-0.605018	-0.409463	-0.365125
11	6	0	-1.888567	0.214270	0.009476
12	8	0	-1.964547	1.375414	0.385617
13	8	0	-2.909264	-0.629928	-0.116655
14	6	0	-4.233162	-0.106039	0.219684
15	6	0	-5.233616	-1.219540	-0.008241
16	1	0	3.805546	0.374090	-0.753579
17	1	0	2.970295	2.268146	0.891409
18	1	0	2.738517	2.784801	-0.781185
19	1	0	2.910134	-1.639194	-1.620582
20	1	0	1.219590	-2.059053	-1.334737
21	1	0	2.685904	-3.322519	0.222579
22	1	0	1.674326	-2.204304	1.141113
23	1	0	-0.611849	-1.440549	-0.693776
24	1	0	-4.421267	0.764660	-0.414753
25	1	0	-4.207543	0.230250	1.260120
26	1	0	-5.017300	-2.082056	0.629454
27	1	0	-5.230251	-1.545415	-1.052793
28	1	0	-6.237998	-0.857758	0.234307
29	1	0	4.541528	-2.021221	0.738530

21g (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.833016	0.347945	-0.616975
2	6	0	2.538214	1.765359	-0.277676
3	16	0	0.748393	1.819691	0.181047
4	6	0	0.516008	0.163068	-0.404158
5	7	0	1.756146	-0.413217	-0.827600
6	6	0	2.034685	-1.842015	-0.687713
7	6	0	2.570331	-1.995520	0.774182
8	7	0	3.427116	-0.837079	1.064797
9	1	0	3.202680	-0.385815	1.949227
10	6	0	-0.661402	-0.487916	-0.461146

11	6	0	-1.876541	0.200399	0.005001
12	8	0	-1.851591	1.325250	0.486092
13	8	0	-2.970316	-0.543536	-0.159273
14	6	0	-4.233008	0.057386	0.262591
15	6	0	-5.328985	-0.953180	-0.004815
16	1	0	3.761654	0.068549	-1.101232
17	1	0	3.168233	2.130109	0.538263
18	1	0	2.738417	2.396659	-1.153658
19	1	0	2.796808	-2.120977	-1.419916
20	1	0	1.147243	-2.445341	-0.866090
21	1	0	3.114528	-2.937850	0.872630
22	1	0	1.726369	-2.003819	1.466568
23	1	0	-0.753605	-1.490148	-0.861863
24	1	0	-4.371246	0.984371	-0.301209
25	1	0	-4.149071	0.314840	1.322383
26	1	0	-5.163473	-1.874383	0.562217
27	1	0	-5.384752	-1.202036	-1.068900
28	1	0	-6.292539	-0.531858	0.299608
29	1	0	4.422992	-1.052163	1.054555

21j (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.038487	0.012054	-0.289673
2	1	0	-5.659532	0.698957	-0.485848
3	1	0	-3.008480	0.744176	-0.343420
4	6	0	0.333111	0.430665	-0.131971
5	16	0	0.439843	2.184379	0.048188
6	6	0	-1.391677	2.326321	-0.102923
7	6	0	-1.924517	0.959453	-0.275031
8	7	0	-4.902555	0.392095	0.123202
9	6	0	-5.048508	-1.050297	0.437680
10	6	0	-3.670028	-1.677596	0.678043
11	6	0	-2.834624	-1.762130	-0.623661
12	6	0	-1.350445	-1.439847	-0.480802
13	6	0	2.731141	0.099446	0.037543
14	6	0	1.365949	-0.434148	-0.130464
15	8	0	3.649422	-0.864341	0.016939
16	1	0	1.239769	-1.502371	-0.247282
17	8	0	2.954434	1.293539	0.177108
18	1	0	-1.677221	2.948445	-0.962309
19	1	0	-1.834954	2.794733	0.785915
20	1	0	6.952503	-1.403104	0.241996
21	1	0	-5.695040	-1.219892	1.307805
22	1	0	-5.529326	-1.542635	-0.414642
23	1	0	-3.793595	-2.680259	1.101478
24	1	0	-3.146799	-1.092434	1.447717
25	1	0	-2.874703	-2.783179	-1.018767
26	1	0	-3.270484	-1.131919	-1.408378
27	1	0	-0.796642	-1.737794	-1.375665
28	1	0	-0.912194	-1.957645	0.377617
29	6	0	5.039879	-0.441370	0.175257
30	1	0	5.790055	-2.204954	-0.831213
31	6	0	5.901311	-1.685915	0.125632
32	1	0	5.124264	0.090411	1.127240
33	1	0	5.271700	0.262658	-0.628983
34	1	0	5.641487	-2.377862	0.932499

35	1	0	-5.011409	0.934463	0.980355

21j (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.072930	-0.019811	-0.394745
2	1	0	-5.400857	0.969569	0.014951
3	1	0	-3.058315	0.688858	-0.466348
4	6	0	0.287001	0.415442	-0.185851
5	16	0	0.359532	2.166666	0.026755
6	6	0	-1.465019	2.284400	-0.206837
7	6	0	-1.977447	0.911911	-0.408852
8	7	0	-4.583341	0.482856	0.384769
9	6	0	-4.899496	-0.956782	0.564764
10	6	0	-3.610825	-1.780559	0.648312
11	6	0	-2.832940	-1.841385	-0.693782
12	6	0	-1.354544	-1.471699	-0.615095
13	6	0	2.684911	0.117383	0.051938
14	6	0	1.333964	-0.432088	-0.169267
15	8	0	3.617901	-0.833198	0.033082
16	1	0	1.229900	-1.499188	-0.314209
17	8	0	2.887501	1.309956	0.229535
18	1	0	-1.716173	2.905110	-1.078044
19	1	0	-1.952479	2.748591	0.660259
20	1	0	6.919629	-1.333662	0.344910
21	1	0	-5.514020	-1.133533	1.456689
22	1	0	-5.488758	-1.281296	-0.299588
23	1	0	-3.865980	-2.796001	0.968518
24	1	0	-2.977217	-1.370512	1.447953
25	1	0	-2.847950	-2.865873	-1.080994
26	1	0	-3.327484	-1.238156	-1.464949
27	1	0	-0.833712	-1.734224	-1.540887
28	1	0	-0.867840	-2.002123	0.208117
29	6	0	4.996424	-0.395610	0.242807
30	1	0	5.800158	-2.126038	-0.779792
31	6	0	5.876224	-1.627289	0.191196
32	1	0	5.045519	0.115416	1.208553
33	1	0	5.242815	0.329562	-0.538024
34	1	0	5.602219	-2.340725	0.974351
35	1	0	-4.420795	0.899835	1.303365

22 (GS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.977980	0.436154	-1.061044
2	6	0	1.897427	-1.034223	-1.098491
3	16	0	0.154930	-1.480673	-0.685689
4	6	0	-0.268914	0.224843	-0.522559
5	7	0	0.875034	1.056923	-0.775465
6	1	0	2.877547	1.018870	-1.262933
7	6	0	0.782339	2.529614	-0.699181
8	1	0	2.186476	-1.412923	-2.087320
9	1	0	2.605446	-1.428431	-0.358357
10	6	0	-1.475652	0.732577	-0.205562

11	1	0	-1.656971	1.796722	-0.123063
12	1	0	0.025249	2.869820	-1.408448
13	1	0	0.492617	2.811730	0.315157
14	6	0	-2.592250	-0.199132	0.036846
15	1	0	1.758036	2.945179	-0.953917
16	8	0	-2.461320	-1.412558	-0.033849
17	8	0	-3.722312	0.442304	0.333423
18	6	0	5.000871	-0.028590	1.602757
19	6	0	5.789416	-0.039170	0.305769
20	1	0	5.299975	-0.873992	2.236213
21	1	0	5.194825	0.895876	2.165430
22	1	0	5.479566	0.783927	-0.348344
23	1	0	6.858523	0.071154	0.513664
24	1	0	5.645121	-0.982344	-0.232028
25	8	0	3.596691	-0.123469	1.288067
26	1	0	3.119221	-0.235388	2.125377
27	6	0	-4.893807	-0.392523	0.587970
28	1	0	-4.657509	-1.062371	1.419819
29	1	0	-5.071613	-1.005093	-0.300605
30	6	0	-6.052291	0.532553	0.897758
31	1	0	-6.949664	-0.063555	1.092857
32	1	0	-5.845693	1.140909	1.783627
33	1	0	-6.260448	1.199383	0.055437

22 (TS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.864975	1.757359	0.458046
2	6	0	-2.110646	0.482917	1.005063
3	16	0	-0.527535	-0.415974	1.106574
4	6	0	0.272007	0.886330	0.206473
5	7	0	-0.638032	1.952728	-0.011379
6	1	0	-2.587207	2.569053	0.364645
7	6	0	-0.224885	3.177682	-0.711747
8	1	0	-2.773758	0.413305	1.866851
9	1	0	-2.856216	-0.252376	-0.065616
10	6	0	1.554295	0.887749	-0.220787
11	1	0	1.976819	1.716390	-0.774362
12	1	0	0.626446	3.619327	-0.187930
13	1	0	0.068365	2.932023	-1.736157
14	6	0	2.401538	-0.263814	0.096812
15	1	0	-1.065828	3.872345	-0.711890
16	8	0	1.995714	-1.236633	0.723153
17	8	0	3.647160	-0.123557	-0.370111
18	6	0	-4.450632	-1.868610	-0.531081
19	6	0	-5.666485	-0.969120	-0.524786
20	1	0	-4.239423	-2.299822	0.452450
21	1	0	-4.540055	-2.671766	-1.266094
22	1	0	-5.840048	-0.539503	-1.515309
23	1	0	-6.544796	-1.560481	-0.246676
24	1	0	-5.565177	-0.158438	0.204131
25	8	0	-3.278160	-1.065251	-0.947965
26	1	0	-2.517954	-1.654668	-1.117083
27	6	0	4.569305	-1.214601	-0.088864
28	1	0	4.154653	-2.133320	-0.514611
29	1	0	4.627588	-1.343323	0.996035
30	6	0	5.906806	-0.847871	-0.699344

31	1	0	6.628274	-1.648377	-0.505669
32	1	0	5.822683	-0.716283	-1.782554
33	1	0	6.296736	0.077808	-0.265015

X, Y, Z Coordinates for the Calculated Protonated Zigzag Conformation 20a and Reactive Conformation 20b of Compounds 13a and 15a-c

13a-zigzag

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.917763	-1.423839	0.536593
2	1	0	-3.827792	-4.392478	0.146733
3	7	0	-1.986196	-1.055816	-0.375533
4	6	0	-3.005733	-2.041348	-0.684434
5	1	0	-2.523800	-2.953362	-1.073291
6	6	0	-2.228666	2.688167	-0.099802
7	1	0	0.472749	-0.184000	-0.548340
8	1	0	-0.883434	1.189934	0.719500
9	6	0	0.464814	-1.190922	-0.113832
10	1	0	-1.045156	-2.476434	0.802363
11	1	0	-1.001255	-0.851552	1.470398
12	8	0	-3.217257	3.004624	-0.746535
13	6	0	-2.398705	0.268494	-0.476342
14	8	0	-3.687378	-2.351428	0.512960
15	16	0	-3.868316	0.417027	-1.446624
16	8	0	-1.438758	3.586889	0.541057
17	6	0	-1.858604	4.968396	0.442021
18	6	0	-0.879877	5.802591	1.246628
19	6	0	1.595247	-1.324036	0.901907
20	1	0	0.601196	-1.904399	-0.936314
21	6	0	-3.880438	-1.397634	-1.764508
22	6	0	-4.462986	-3.553584	0.477014
23	6	0	-1.748972	1.328126	0.083985
24	1	0	-5.284021	-3.457727	-0.248108
25	1	0	-4.906860	-1.765600	-1.718923
26	1	0	-3.475128	-1.600974	-2.759948
27	6	0	-5.013255	-3.801120	1.870473
28	1	0	-5.643982	-2.965279	2.187484
29	1	0	-4.199720	-3.913683	2.594221
30	1	0	-5.616685	-4.714624	1.881012
31	1	0	1.687534	-2.338440	1.300585
32	1	0	-2.880994	5.054714	0.822798
33	1	0	-1.875208	5.258589	-0.613457
34	1	0	0.137376	5.705423	0.852505
35	1	0	-0.875415	5.497044	2.297999
36	1	0	-1.165660	6.858592	1.197999
37	1	0	1.471197	-0.633917	1.741356
38	7	0	2.932707	-0.987820	0.275059
39	1	0	3.108456	-1.609558	-0.523715
40	1	0	2.892302	-0.044007	-0.129704
41	6	0	4.153918	-1.052268	1.205186
42	1	0	4.175253	-2.073350	1.593454
43	1	0	3.934672	-0.363677	2.024779

44	6	0	5.396934	-0.685987	0.447826
45	6	0	6.143240	-1.677978	-0.205416
46	6	0	5.794723	0.656151	0.355099
47	6	0	7.270425	-1.329474	-0.948483
48	1	0	5.857974	-2.724588	-0.116613
49	6	0	6.921907	1.001515	-0.389201
50	1	0	5.237869	1.429574	0.880871
51	6	0	7.657340	0.009492	-1.042414
52	1	0	7.851191	-2.101444	-1.443710
53	1	0	7.231757	2.040125	-0.450247
54	1	0	8.538929	0.278990	-1.616055

13a-reactive conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.213616	-0.597483	1.820269
2	1	0	-5.665861	-1.430430	-0.247570
3	7	0	-2.008945	-0.462715	0.373745
4	1	0	0.442484	-2.454055	3.268296
5	6	0	-3.116172	-0.855173	-0.496242
6	1	0	-3.418005	-1.885775	-0.250782
7	6	0	0.709872	2.091172	-0.123716
8	6	0	0.057326	-1.603584	2.699117
9	1	0	-0.256252	1.222179	1.620879
10	6	0	-1.446356	-1.772078	2.458884
11	1	0	-3.283879	-0.756350	1.971208
12	1	0	-1.981041	0.346059	2.323493
13	8	0	0.748204	2.297950	-1.326810
14	6	0	-1.137637	0.449706	-0.176831
15	8	0	-4.181012	0.025119	-0.242742
16	16	0	-1.287893	0.543353	-1.929566
17	8	0	1.529579	2.699311	0.767892
18	6	0	2.389626	3.741204	0.231020
19	1	0	0.277473	-0.692363	3.262860
20	7	0	0.880980	-1.525637	1.438506
21	1	0	-1.881357	-1.952554	3.449807
22	1	0	-1.628955	-2.687346	1.879698
23	6	0	-2.565122	-0.783026	-1.923657
24	6	0	-5.471463	-0.433753	-0.674897
25	6	0	-0.190849	1.152258	0.539977
26	1	0	-5.490400	-0.531952	-1.769822
27	1	0	-3.349658	-0.529295	-2.638452
28	1	0	-2.109818	-1.732676	-2.219506
29	6	0	-6.507426	0.573899	-0.211564
30	1	0	-6.303938	1.559780	-0.639878
31	1	0	-6.503066	0.661991	0.879270
32	1	0	-7.505739	0.257195	-0.530001
33	6	0	3.153791	4.346884	1.391750
34	1	0	1.762619	4.477295	-0.280366
35	1	0	3.055348	3.297349	-0.516026
36	1	0	3.775564	3.597383	1.892612
37	1	0	2.470286	4.779725	2.128733
38	1	0	3.809676	5.142816	1.024190
39	1	0	0.636385	-0.636713	0.926215
40	1	0	0.641591	-2.297625	0.806828
41	6	0	2.392884	-1.537288	1.658673
42	1	0	2.614788	-0.625650	2.219280

43	1	0	2.605093	-2.403636	2.290497
44	6	0	3.113950	-1.599426	0.341210
45	6	0	3.382210	-0.423373	-0.373290
46	6	0	3.485144	-2.839256	-0.198509
47	6	0	4.004483	-0.489430	-1.618999
48	1	0	3.111597	0.540809	0.049805
49	6	0	4.112479	-2.901952	-1.442586
50	1	0	3.302537	-3.754840	0.360990
51	6	0	4.368170	-1.727577	-2.153808
52	1	0	4.206338	0.424074	-2.169497
53	1	0	4.408215	-3.863398	-1.851313
54	1	0	4.858085	-1.776570	-3.121676

15a-zigzag

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.376823	-0.198032	-0.646575
2	6	0	2.023352	-1.463903	-1.431564
3	16	0	0.272568	-1.873381	-1.025954
4	6	0	-0.022271	-0.224543	-0.475385
5	7	0	1.134117	0.560005	-0.568712
6	8	0	2.819989	-0.421611	0.671724
7	6	0	1.170240	1.852459	0.078443
8	1	0	2.663315	-2.300564	-1.146724
9	1	0	2.123331	-1.291000	-2.506789
10	6	0	4.186657	-0.841538	0.794871
11	6	0	4.524455	-0.919241	2.272643
12	6	0	-1.226855	0.229074	-0.033268
13	1	0	-1.359503	1.235868	0.344879
14	7	0	0.257863	4.196375	-0.130886
15	6	0	0.563193	2.894448	-0.874744
16	1	0	-0.158552	4.901357	-0.751560
17	1	0	2.209183	2.097613	0.315686
18	1	0	0.618423	1.831046	1.031132
19	1	0	-0.387113	2.546150	-1.282167
20	1	0	1.238002	3.153827	-1.692482
21	1	0	1.105312	4.607719	0.280074
22	6	0	-2.394445	-0.645269	-0.000125
23	8	0	-2.392482	-1.815871	-0.350087
24	8	0	-3.485235	0.000705	0.467834
25	6	0	-4.697528	-0.793112	0.555311
26	1	0	3.129101	0.394840	-1.192066
27	6	0	-5.794819	0.105893	1.090841
28	1	0	-4.507519	-1.648203	1.211065
29	1	0	-4.931911	-1.183408	-0.439718
30	1	0	-5.968252	0.956238	0.423243
31	1	0	-5.540633	0.488742	2.084533
32	1	0	-6.728222	-0.460755	1.171423
33	1	0	-0.404551	4.031965	0.638341
34	1	0	4.839052	-0.121729	0.274056
35	1	0	4.326825	-1.821022	0.316724
36	1	0	3.871297	-1.636161	2.778748
37	1	0	4.404780	0.057522	2.752324
38	1	0	5.561700	-1.243807	2.403259

15a-reactive conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.170088	0.801968	-0.221730
2	6	0	-0.032506	0.012408	-0.371379
3	16	0	-0.319022	-1.345005	-1.448024
4	6	0	-2.086158	-0.856693	-1.657992
5	6	0	-2.423310	0.102769	-0.510979
6	6	0	2.356850	-0.534795	-0.088910
7	1	0	1.271937	0.991037	1.029273
8	6	0	1.190458	0.312132	0.184984
9	8	0	2.353216	-1.470968	-0.873261
10	1	0	-2.708076	-1.752609	-1.621513
11	1	0	-2.221532	-0.372959	-2.629615
12	8	0	-2.834536	-0.521090	0.675130
13	6	0	-0.692304	3.209833	0.190090
14	6	0	-1.185216	1.868394	0.777306
15	1	0	-3.178263	0.838083	-0.832030
16	8	0	3.428350	-0.142600	0.622560
17	6	0	4.634675	-0.939591	0.450962
18	1	0	-0.245250	3.840352	0.961379
19	1	0	-1.494035	3.768904	-0.297113
20	1	0	-2.209055	1.999515	1.132993
21	1	0	-0.591078	1.587263	1.651732
22	6	0	-4.212383	-0.932995	0.710415
23	1	0	-4.390278	-1.715432	-0.040352
24	1	0	-4.853958	-0.074074	0.457515
25	6	0	5.700472	-0.354665	1.355774
26	1	0	4.922073	-0.908975	-0.604398
27	1	0	4.399624	-1.977562	0.703397
28	1	0	5.389687	-0.390350	2.404536
29	1	0	5.916913	0.685387	1.091300
30	1	0	6.624637	-0.932556	1.252699
31	6	0	-4.511396	-1.451546	2.104716
32	1	0	-5.554168	-1.778866	2.164722
33	1	0	-3.867618	-2.302485	2.345906
34	1	0	-4.350133	-0.670033	2.853637
35	7	0	0.366986	2.978823	-0.877502
36	1	0	0.933436	3.815588	-1.049899
37	1	0	0.993075	2.168635	-0.616008
38	1	0	-0.073209	2.701458	-1.760502

15b-zigzag

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.132448	1.601411	0.309076
2	1	0	4.877793	-0.249264	0.317812
3	7	0	1.150157	0.359985	-0.440979
4	6	0	2.418043	-0.328268	-0.609308
5	1	0	3.145166	0.358478	-1.072888
6	6	0	-2.322754	-1.036019	-0.040666
7	1	0	-0.492402	2.326214	-0.907426
8	1	0	-1.351507	0.812314	0.564568
9	6	0	0.452455	2.721399	-0.514958
10	1	0	2.164255	1.873029	0.545807

11	1	0	0.613805	1.464036	1.267926
12	8	0	-2.289963	-2.148181	-0.547468
13	6	0	0.030580	-0.467970	-0.450571
14	8	0	2.879802	-0.701492	0.670909
15	16	0	0.384047	-2.023479	-1.209177
16	8	0	-3.437518	-0.500871	0.516113
17	6	0	-4.609605	-1.352037	0.509624
18	6	0	-5.730297	-0.592719	1.193736
19	6	0	0.183772	3.955449	0.334552
20	1	0	1.088931	2.975157	-1.371972
21	6	0	2.119675	-1.502859	-1.545926
22	6	0	4.263807	-1.063173	0.737935
23	6	0	-1.192243	-0.123895	0.044155
24	1	0	4.453024	-1.962936	0.135001
25	1	0	2.790412	-2.343186	-1.358938
26	1	0	2.217678	-1.196941	-2.591479
27	6	0	4.614487	-1.316729	2.193306
28	1	0	4.002472	-2.127458	2.599558
29	1	0	4.443371	-0.419054	2.795978
30	1	0	5.668369	-1.599370	2.282987
31	1	0	1.095897	4.458500	0.665857
32	1	0	-4.369304	-2.285049	1.028573
33	1	0	-4.856040	-1.605136	-0.526440
34	1	0	-5.957648	0.337841	0.662789
35	1	0	-5.464943	-0.347188	2.227178
36	1	0	-6.636960	-1.206513	1.209848
37	1	0	-0.434519	3.733107	1.208125
38	7	0	-0.599533	4.995022	-0.472062
39	1	0	-0.807206	5.838672	0.077133
40	1	0	-0.076689	5.286939	-1.307300
41	1	0	-1.493849	4.605235	-0.796746

15b-reactive conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.231128	1.686251	0.880510
2	1	0	4.935895	-0.037817	0.361340
3	7	0	1.186611	0.592109	-0.095127
4	1	0	-0.537742	4.526533	-0.319586
5	6	0	2.458794	-0.015075	-0.489874
6	1	0	3.150407	0.779187	-0.812597
7	6	0	-2.309771	-0.795589	-0.060403
8	6	0	-0.488495	3.482748	-0.000496
9	1	0	-1.257704	0.712106	1.106250
10	6	0	0.962655	3.081446	0.275627
11	1	0	2.236391	1.679715	1.307311
12	1	0	0.553621	1.479717	1.714921
13	8	0	-2.284355	-1.725866	-0.850997
14	6	0	0.079925	-0.186031	-0.308098
15	8	0	2.973101	-0.665619	0.641115
16	16	0	0.386402	-1.502215	-1.431283
17	8	0	-3.396582	-0.435835	0.650611
18	6	0	-4.572859	-1.277237	0.486081
19	1	0	-1.117122	3.364106	0.886259
20	7	0	-1.149345	2.660166	-1.086035
21	1	0	1.334895	3.828635	0.987323
22	1	0	1.564089	3.208955	-0.634391

23	6	0	2.127350	-0.944681	-1.662900
24	6	0	4.379576	-0.960342	0.591505
25	6	0	-1.174517	0.091346	0.218175
26	1	0	4.584862	-1.682373	-0.211517
27	1	0	2.783164	-1.816790	-1.673224
28	1	0	2.217979	-0.422921	-2.619878
29	6	0	4.788423	-1.527509	1.938114
30	1	0	4.230732	-2.442920	2.156783
31	1	0	4.598130	-0.805341	2.738027
32	1	0	5.856721	-1.766112	1.933255
33	1	0	-2.082842	3.020927	-1.309223
34	6	0	-5.650078	-0.741185	1.407810
35	1	0	-4.296106	-2.307408	0.727533
36	1	0	-4.874558	-1.250925	-0.565597
37	1	0	-5.910793	0.291702	1.154839
38	1	0	-5.325318	-0.772401	2.452447
39	1	0	-6.552275	-1.353860	1.311348
40	1	0	-1.264364	1.630956	-0.752568
41	1	0	-0.601458	2.659552	-1.952524

15c-zigzag

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.488126	-0.427906	-0.611715
2	6	0	2.322071	-1.656665	-1.510001
3	16	0	0.662634	-2.363555	-1.135650
4	6	0	0.133206	-0.826822	-0.438350
5	7	0	1.154269	0.115459	-0.446474
6	8	0	3.006103	-0.711445	0.673039
7	6	0	0.999356	1.377137	0.259608
8	1	0	3.089072	-2.406517	-1.308594
9	1	0	2.372999	-1.371972	-2.565017
10	6	0	4.422795	-0.896171	0.728849
11	6	0	4.820342	-1.058910	2.185481
12	6	0	-1.126921	-0.602013	0.031580
13	1	0	-1.398956	0.340532	0.489156
14	6	0	-0.103302	3.678874	0.198273
15	6	0	0.262781	2.418397	-0.604885
16	1	0	0.808273	4.159808	0.580676
17	1	0	1.996471	1.737525	0.527729
18	1	0	0.461828	1.215500	1.203862
19	1	0	-0.648482	1.961089	-1.006152
20	1	0	0.891598	2.686387	-1.462870
21	1	0	-0.709796	3.390380	1.068592
22	6	0	-2.145587	-1.636107	-0.020767
23	8	0	-1.986033	-2.763247	-0.468687
24	8	0	-3.324539	-1.203042	0.497767
25	6	0	-4.392447	-2.177883	0.514561
26	1	0	3.129574	0.323092	-1.101129
27	6	0	-5.606512	-1.515169	1.138089
28	1	0	-4.064783	-3.052247	1.085736
29	1	0	-4.586937	-2.509316	-0.510522
30	1	0	-5.922290	-0.643997	0.554180
31	1	0	-5.392935	-1.188167	2.161055
32	1	0	-6.440223	-2.224414	1.172201
33	6	0	-0.883453	4.659083	-0.666785
34	1	0	4.927236	-0.026107	0.275865

35	1	0	4.718117	-1.783869	0.150409
36	1	0	4.318292	-1.925940	2.625047
37	1	0	4.545113	-0.171111	2.763875
38	1	0	5.902257	-1.205908	2.267584
39	1	0	-1.813391	4.229083	-1.046667
40	1	0	-0.297605	5.037625	-1.507826
41	7	0	-1.297798	5.894722	0.142711
42	1	0	-1.888958	5.629881	0.940677
43	1	0	-1.825022	6.570506	-0.424463
44	1	0	-0.475864	6.380571	0.522765

15c-reactive conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.151194	0.285603	0.088848
2	6	0	-0.235835	-0.011595	-0.039931
3	16	0	-0.717379	-1.290475	1.084704
4	6	0	0.987020	-1.427519	1.753824
5	6	0	1.899675	-0.845419	0.673882
6	1	0	2.831451	-0.457163	1.113575
7	7	0	0.208952	2.622918	1.421939
8	6	0	-1.087839	0.711214	-0.816754
9	6	0	-2.546442	0.553618	-0.948741
10	1	0	1.216290	-2.477545	1.942351
11	1	0	1.075326	-0.876828	2.696081
12	8	0	2.188472	-1.753773	-0.352073
13	6	0	3.269463	-2.664657	-0.085560
14	1	0	-0.698803	1.462116	-1.494893
15	6	0	1.067237	3.771613	0.940910
16	6	0	1.577095	3.536201	-0.479680
17	6	0	2.512248	2.319233	-0.676793
18	6	0	1.869488	0.966121	-1.028735
19	6	0	3.509193	-3.487755	-1.337270
20	1	0	3.011938	-3.314815	0.762502
21	1	0	0.458555	4.676205	1.008184
22	1	0	1.893988	3.852293	1.652047
23	1	0	2.128580	4.447609	-0.737730
24	1	0	0.732735	3.495876	-1.179982
25	1	0	3.170375	2.205881	0.196677
26	1	0	3.178938	2.554166	-1.514420
27	1	0	2.650135	0.277493	-1.359712
28	1	0	1.192886	1.074120	-1.878146
29	8	0	-3.224069	1.308441	-1.620135
30	8	0	-3.038016	-0.489692	-0.249329
31	6	0	-4.472916	-0.715075	-0.357401
32	6	0	-4.809102	-1.950518	0.452952
33	1	0	-4.718973	-0.832560	-1.416275
34	1	0	-4.989017	0.177317	0.009247
35	1	0	-4.554574	-1.813823	1.508881
36	1	0	-4.273261	-2.826665	0.074944
37	1	0	-5.883515	-2.149934	0.383632
38	1	0	4.166494	-2.089895	0.192968
39	1	0	3.780630	-2.844656	-2.180036
40	1	0	2.611306	-4.051934	-1.605827
41	1	0	4.325414	-4.196692	-1.165840
42	1	0	-0.064479	2.717564	2.404777
43	1	0	0.714468	1.711766	1.268263

44	1	0	-0.646648	2.515474	0.856023