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Accessory Publication

for

A synthetic and computational investigation into the direct synthesis of α-hydroxymethylated enones from β-keto phosphonates

Sarah J. Ryan, Christopher D. Thompson and David W. Lupton*

School of Chemistry, Monash University, Clayton Campus 3800, Victoria, AUSTRALIA

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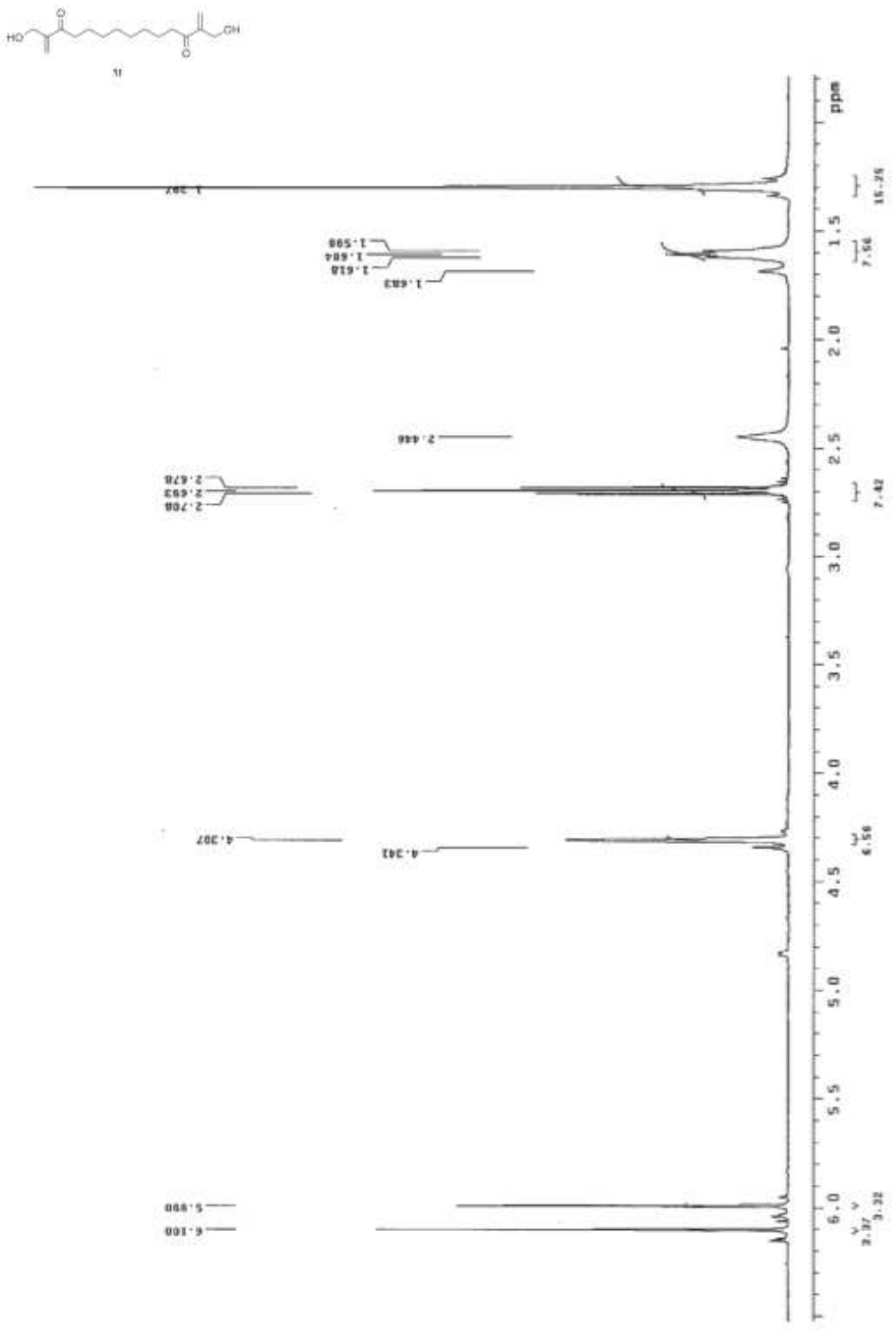
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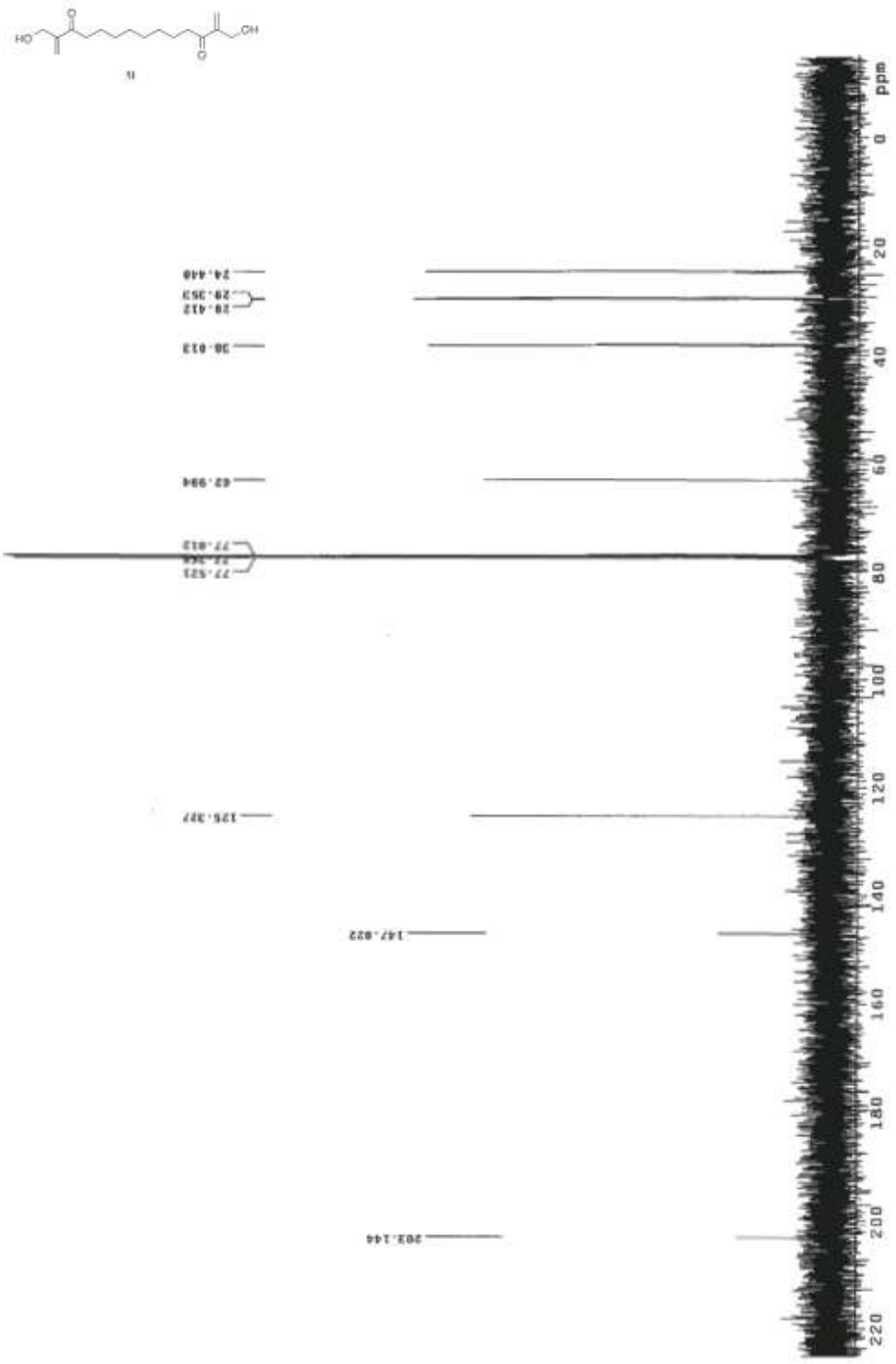
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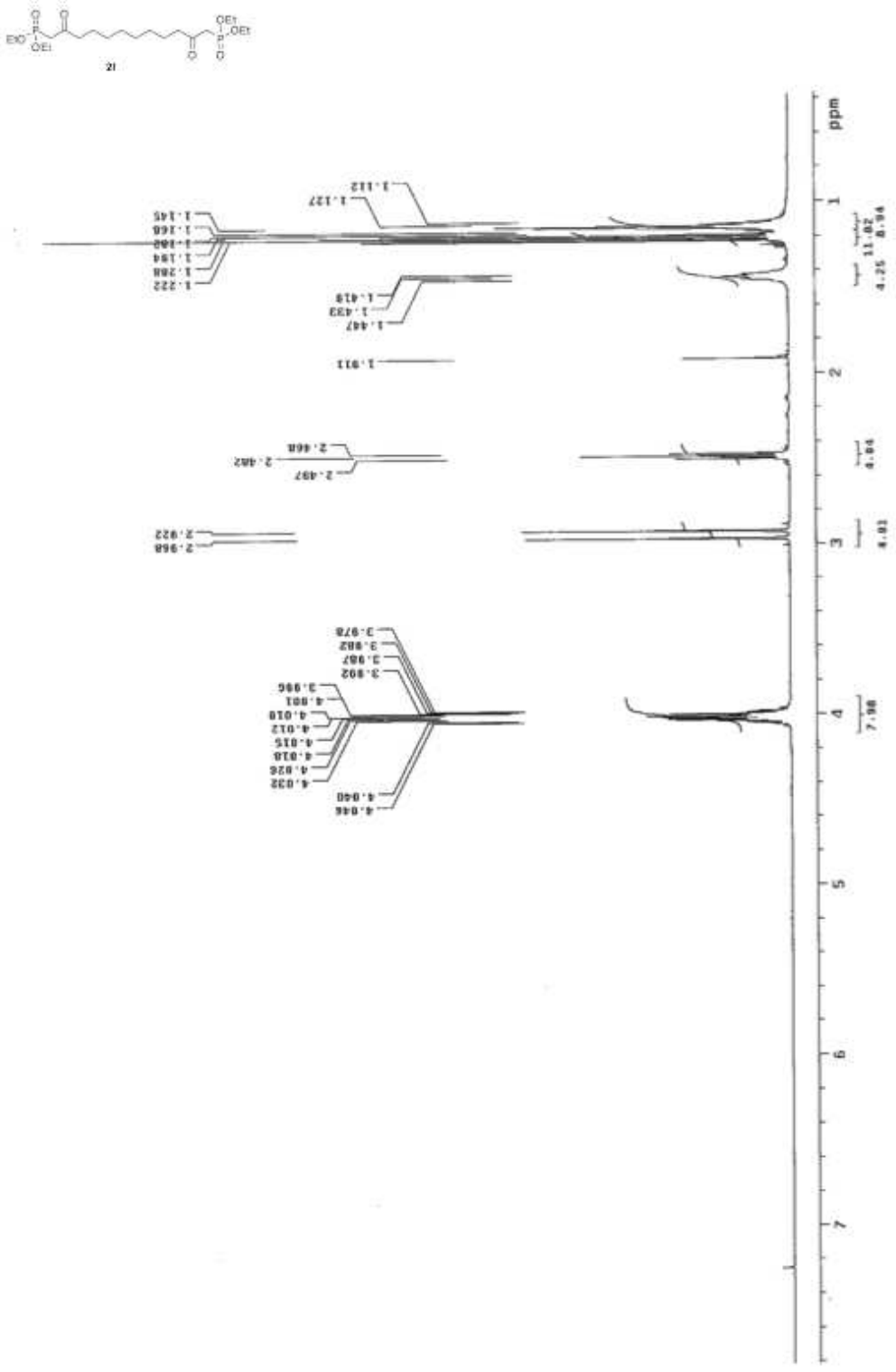

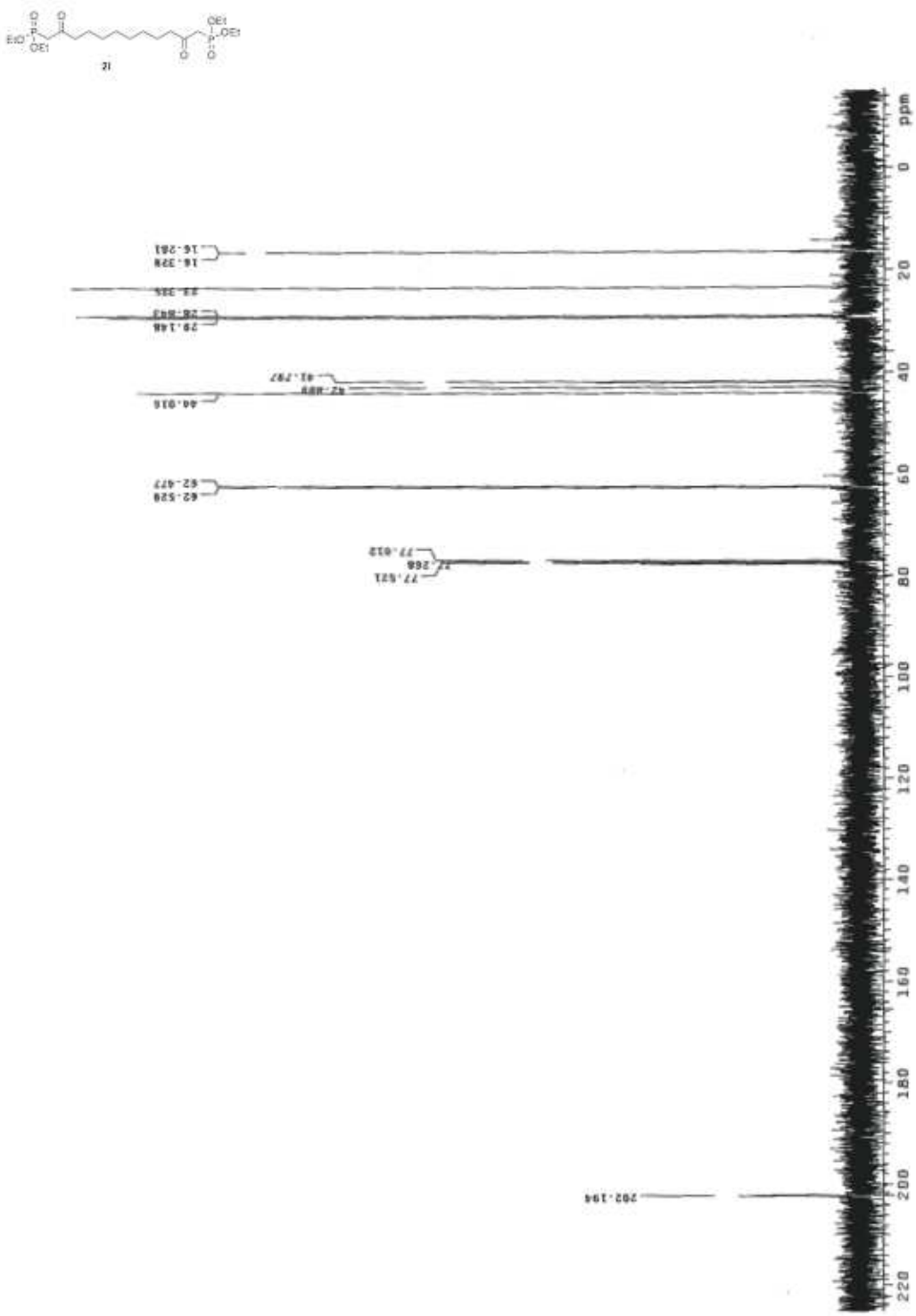
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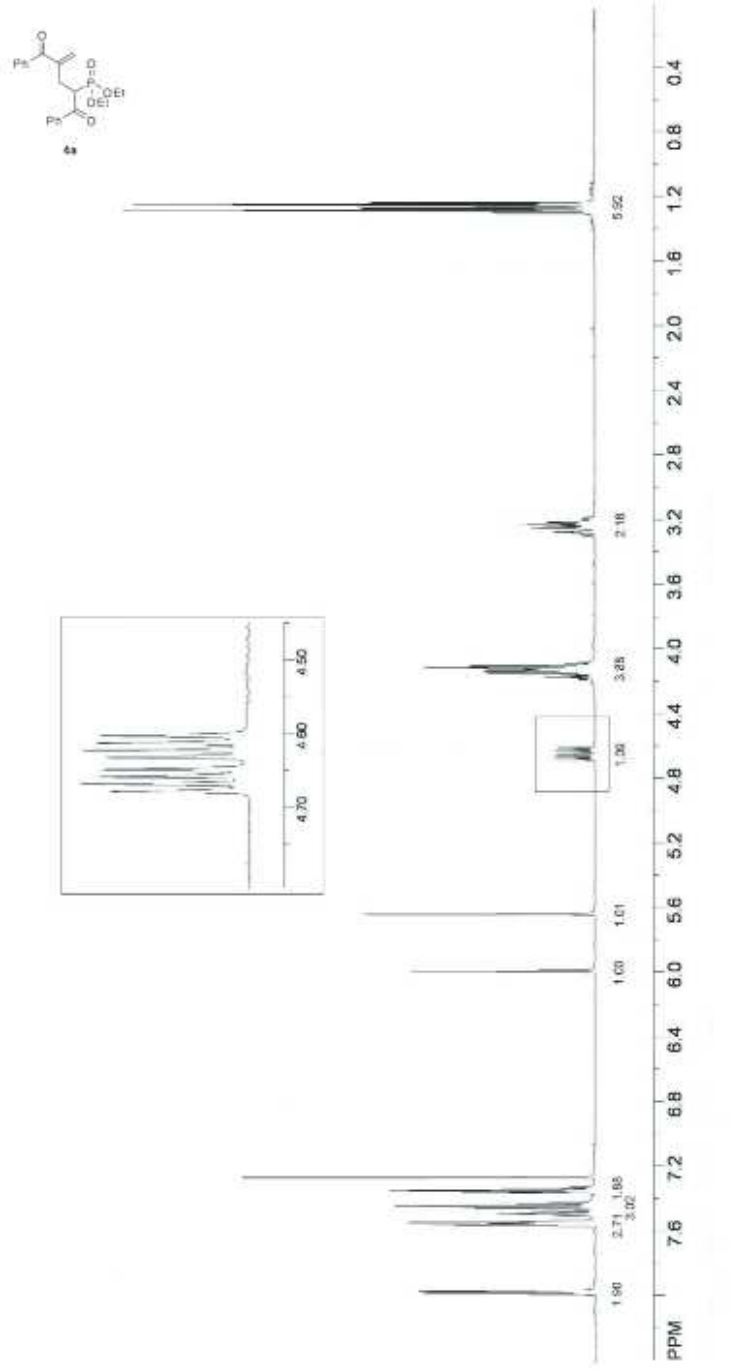
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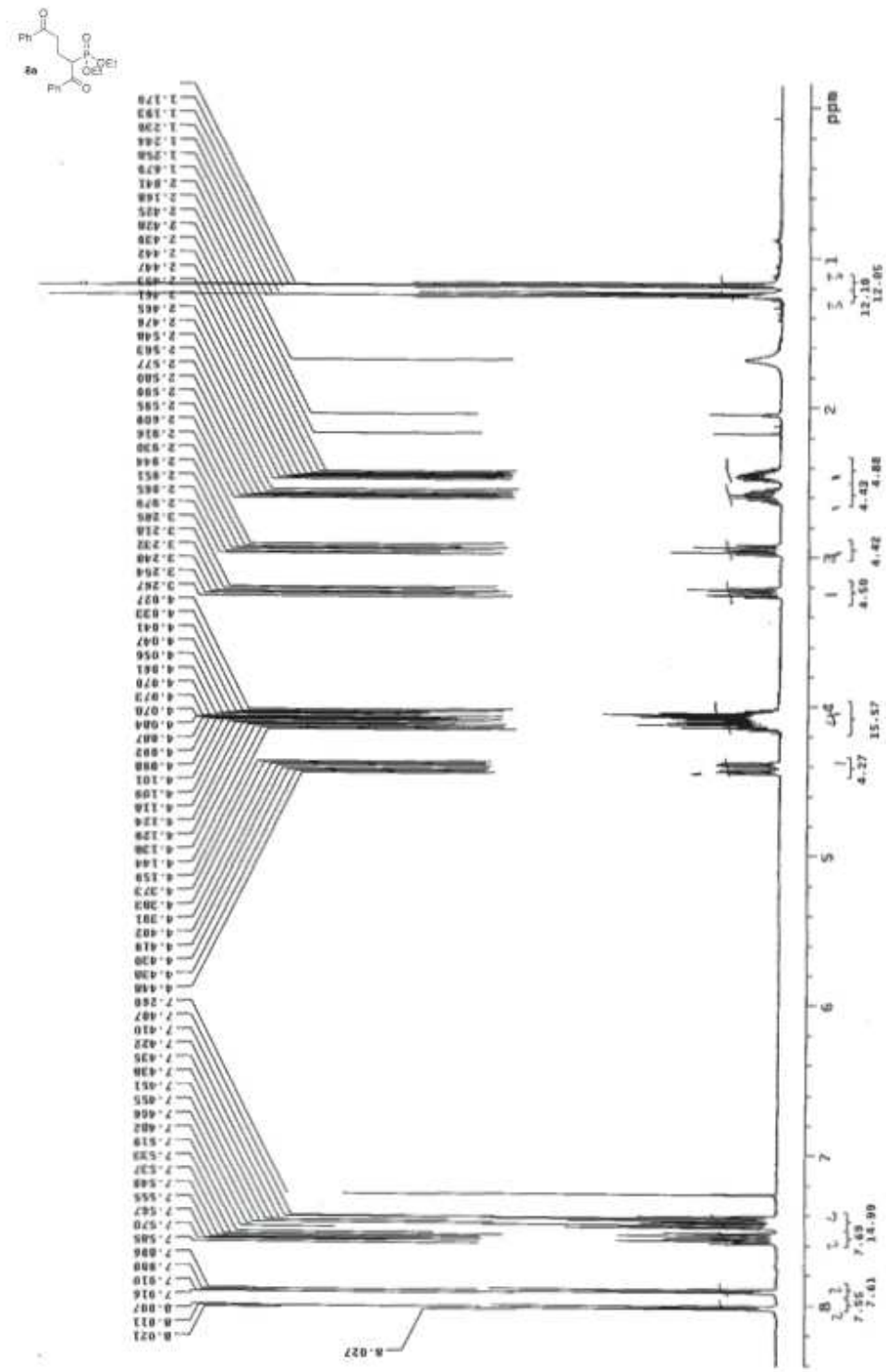
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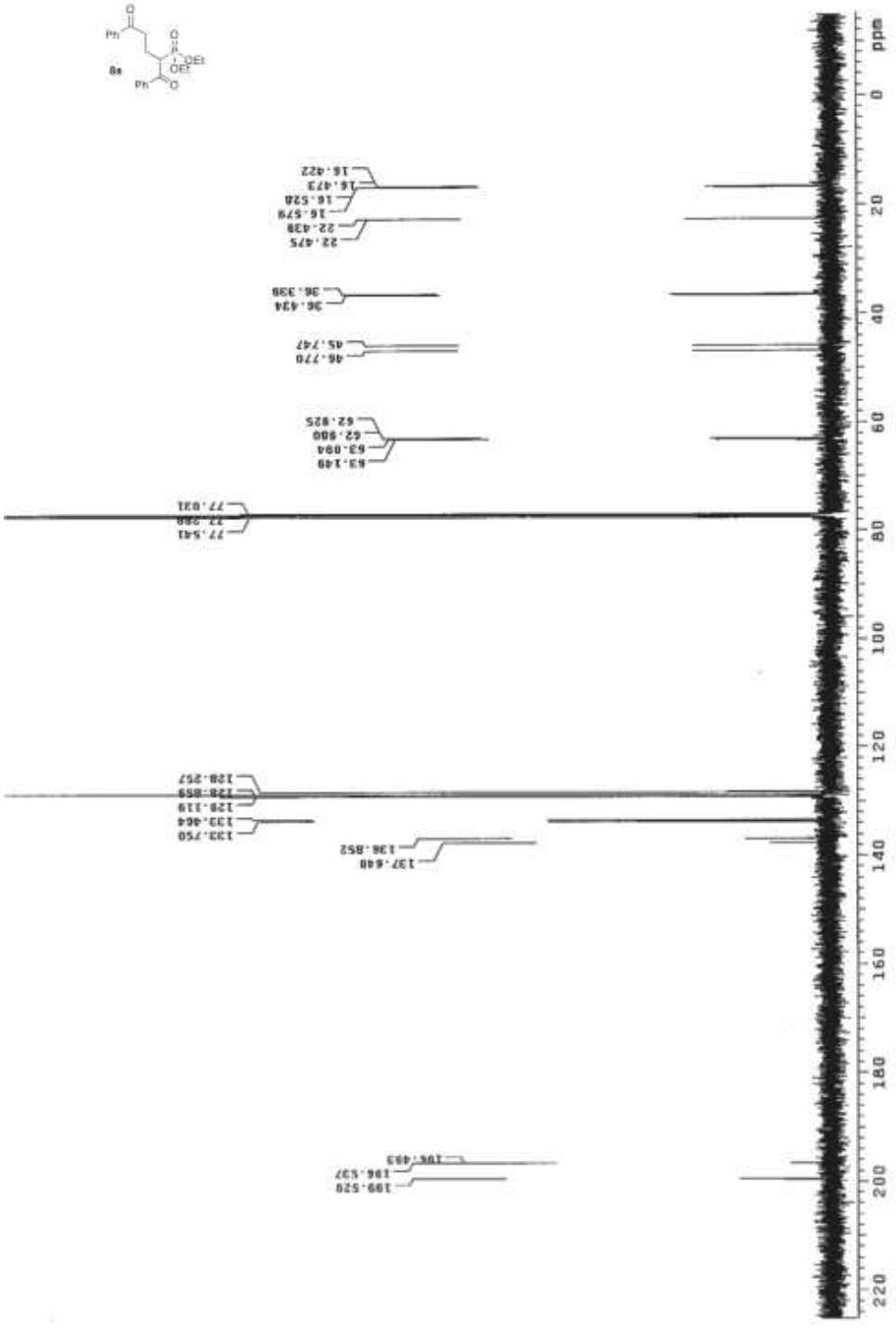
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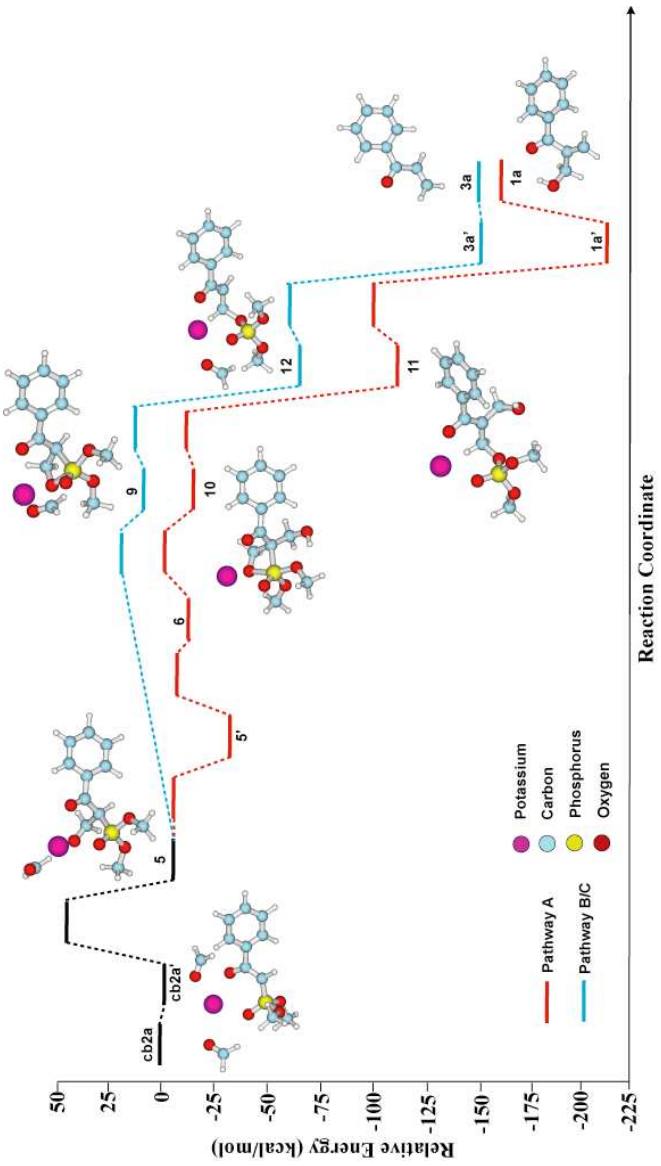

Figure S1. Reaction coordinate calculated using PCM/B3LYP/6-31+G* and computational derived structure.

The following geometry coordinates and vibrational frequencies (wavenumber) correspond to the relevant minima and transition states referred to in the text. All calculations have been performed using software package Gaussian03 at the PCM/B3LYP/6-31+G* level of theory and basis set with e=78.39 (solvent=water).

Cartesian Coordinates for all Minima;

Structure 5; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.646465	-0.612379	-0.031102
2	6	0	3.424691	0.162633	0.848604
3	6	0	4.786232	-0.106319	1.015492
4	6	0	5.387840	-1.156701	0.315813
5	6	0	4.621849	-1.938109	-0.559609
6	6	0	3.266566	-1.664371	-0.734455
7	6	0	1.188565	-0.364921	-0.277620
8	6	0	0.400452	0.483313	0.680370
9	6	0	-0.436840	-0.498019	1.685158
10	8	0	-1.448788	-1.179626	1.124146
11	8	0	0.618204	-0.944440	-1.211010
12	15	0	-0.711909	1.687660	-0.124577
13	8	0	-1.585886	2.349085	1.072381
14	6	0	-2.916838	1.852417	1.369611
15	8	0	0.333816	2.880994	-0.451671
16	6	0	-0.110556	4.074654	-1.138361
17	8	0	-1.549596	1.260806	-1.296587
18	19	0	-2.175664	-1.403605	-1.436284
19	8	0	-4.161493	-3.122409	-0.122566
20	6	0	-4.026920	-2.969335	1.083668
21	1	0	2.987988	0.991317	1.402271
22	1	0	5.376641	0.508969	1.694081

23	1	0	6.448992	-1.366669	0.450733
24	1	0	5.084151	-2.760412	-1.105574
25	1	0	2.668941	-2.267174	-1.414702
26	1	0	1.044915	1.089615	1.326222
27	1	0	-0.569655	3.815562	-2.097018
28	1	0	-0.820466	4.627530	-0.515267
29	1	0	0.784944	4.675789	-1.304222
30	1	0	-3.214117	2.343821	2.298061
31	1	0	-3.603209	2.129969	0.564339
32	1	0	-2.896150	0.765063	1.492694
33	1	0	0.361950	-1.135176	2.133567
34	1	0	-0.743908	0.203805	2.493649
35	1	0	-4.739346	-3.439158	1.789968
36	1	0	-3.194503	-2.361699	1.486287

Structure 9; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.687224	1.166281	-0.192465
2	6	0	3.384986	1.181252	-0.690612
3	6	0	2.518103	0.094199	-0.465621
4	6	0	2.983458	-1.005193	0.278273
5	6	0	4.284553	-1.013375	0.787276
6	6	0	5.140229	0.067782	0.550039
7	6	0	1.137828	0.155970	-1.040716
8	6	0	0.282777	-1.086346	-1.119386

9	6	0	-0.730050	-1.085230
-2.261863				
10	8	0	-1.895440	-0.693000
-1.539659				
11	15	0	-1.170063	-1.025510
0.140373				
12	8	0	-0.060716	-1.538418
1.352183				
13	6	0	-0.468186	-1.574487
2.713247				
14	8	0	0.702415	1.230544
-1.474936				
15	8	0	-1.786029	0.210642
0.797913				
16	8	0	-1.999763	-2.458662
0.300225				
17	6	0	-3.322537	-2.628172
-0.222647				
18	19	0	-2.001396	2.137029
-1.123244				
19	8	0	-2.148260	3.630268
1.403186				
20	6	0	-1.865035	2.952160
2.378618				
21	1	0	2.322255	-1.838854
0.490096				
22	1	0	4.629896	-1.866207
1.371044				
23	1	0	6.157485	0.055293
0.941368				
24	1	0	5.351153	2.009075
-0.383166				
25	1	0	3.028888	2.031824
-1.267719				
26	1	0	0.869970	-2.000622
-1.008060				
27	1	0	-0.775543	-0.580810
3.061560				
28	1	0	-1.299872	-2.276414
2.865131				
29	1	0	0.392800	-1.913006
3.301117				
30	1	0	-3.701523	-3.555824
0.216764				
31	1	0	-3.974238	-1.797018
0.069469				
32	1	0	-3.309645	-2.705639
-1.312994				
33	1	0	-0.504009	-0.372088
-3.064926				
34	1	0	-0.834799	-2.090641
-2.700132				
35	1	0	-1.821469	3.404820
3.387755				

36	1	0	-1.651654	1.875165	2.272564

Structure 12; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.789832	0.083633	0.806008
2	6	0	5.298962	1.177502	0.083348
3	6	0	4.004150	1.148032	-0.443216
4	6	0	3.175959	0.023896	-0.278393
5	6	0	3.681009	-1.065919	0.454883
6	6	0	4.971847	-1.037026	0.992577
7	6	0	1.779262	0.041784	-0.870262
8	8	0	1.225173	1.199154	-1.008198
9	6	0	1.219704	-1.172982	-1.256329
10	6	0	-0.101534	-1.282552	-1.876670
11	8	0	-1.166573	-1.968901	-0.979912
12	15	0	-1.945581	-1.241425	0.194749
13	8	0	-1.266428	-1.630426	1.602471
14	6	0	-0.321810	-0.734552	2.234834
15	8	0	-2.173314	0.227952	0.010897
16	8	0	-3.271525	-2.140227	0.366092
17	6	0	-4.192832	-2.272678	-0.740279
18	19	0	-0.982579	2.592330	-0.608132
19	8	0	-3.519145	3.400597	0.582707
20	6	0	-4.274736	2.568992	1.054999
21	1	0	3.057730	-1.942573	0.621326

22	1	0	5.336510	-1.890141	1.565091
23	1	0	6.796185	0.106008	1.223847
24	1	0	5.925479	2.056714	-0.068991
25	1	0	3.619234	2.003239	-0.994852
26	1	0	1.803144	-2.085574	-1.160239
27	1	0	-0.526137	-0.314721	-2.147689
28	1	0	-0.142062	-1.967865	-2.726348
29	1	0	-3.700825	-2.761001	-1.586393
30	1	0	-4.576132	-1.291867	-1.038761
31	1	0	-5.011915	-2.893565	-0.374371
32	1	0	-0.069524	-1.199205	3.189291
33	1	0	0.573788	-0.631461	1.616713
34	1	0	-0.782089	0.242760	2.402841
35	1	0	-4.020217	1.496293	1.033700
36	1	0	-5.234806	2.866103	1.516641

Structure 3a'; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.147323	-0.293538	-0.022707
2	6	0	5.118944	-1.233287	0.372527
3	6	0	6.437510	-0.831640	0.602763
4	6	0	6.804724	0.506692	0.426938
5	6	0	5.845895	1.449167	0.029875
6	6	0	4.526923	1.053531	-0.185248
7	6	0	2.717904	-0.664634	-0.248611

8	6	0	2.359018	-2.096851
-0.430412				
9	6	0	1.087685	-2.524038
-0.376848				
10	8	0	1.847393	0.216539
-0.297730				
11	19	0	-0.614373	1.415446
-0.148301				
12	8	0	-3.390592	0.853328
-0.633942				
13	15	0	-3.331589	-0.483833
0.081698				
14	8	0	-4.447608	-0.425629
1.278398				
15	6	0	-4.599716	-1.538810
2.176745				
16	8	0	-1.976461	-0.944582
0.591974				
17	8	0	-4.024245	-1.672631
-0.826550				
18	6	0	-3.312521	-2.162141
-1.972631				
19	8	0	-1.819031	4.049156
-0.044255				
20	6	0	-3.026187	4.126119
-0.202982				
21	1	0	4.855807	-2.278039
0.524505				
22	1	0	7.177955	-1.566090
0.919082				
23	1	0	7.835834	0.816590
0.598691				
24	1	0	6.130069	2.491999
-0.110779				
25	1	0	3.777894	1.781732
-0.490513				
26	1	0	3.161897	-2.808773
-0.613321				
27	1	0	0.254608	-1.854042
-0.170165				
28	1	0	0.852866	-3.577716
-0.516960				
29	1	0	-2.344402	-2.582224
-1.677124				
30	1	0	-3.158451	-1.362489
-2.707767				
31	1	0	-3.932474	-2.945767
-2.415556				
32	1	0	-5.318888	-1.226817
2.938163				
33	1	0	-4.985626	-2.413616
1.641668				
34	1	0	-3.643835	-1.786781
2.650611				

35	1	0	-3.632741	3.220006	-0.372023
36	1	0	-3.544256	5.103171	-0.165876

Structure 5'; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.463687	0.298752	-0.005138
2	6	0	3.140228	1.356355	-0.637200
3	6	0	4.536364	1.383688	-0.689252
4	6	0	5.282019	0.363376	-0.084959
5	6	0	4.619441	-0.685723	0.561166
6	6	0	3.220524	-0.722711	0.592207
7	6	0	0.951265	0.342905	0.089878
8	6	0	0.197826	-0.793157	-0.275090
9	6	0	0.776004	-1.954843	-1.047428
10	8	0	1.055712	-3.163457	-0.287078
11	8	0	0.463437	1.451303	0.494357
12	15	0	-1.532353	-0.858030	0.015139
13	8	0	-2.228995	-0.723210	-1.459273
14	6	0	-3.660555	-0.844712	-1.592727
15	8	0	-1.892727	-2.441973	0.310718
16	6	0	-1.965967	-2.891301	1.677938
17	8	0	-2.171661	0.034879	1.048692
18	19	0	-1.609376	2.572581	1.765483
19	8	0	-2.358936	3.157096	-1.023793
20	6	0	-1.665496	2.548191	-1.821829

```
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-1.090386
   22          1             0        5.043977    2.204169
-1.196824
   23          1             0        6.371275    0.388289
-0.115610
   24          1             0        5.191493   -1.479537
1.041903
   25          1             0        2.712508   -1.545829
1.089272
   26          1             0       -2.252532   -3.944688
1.638860
   27          1             0       -0.992295   -2.793639
2.172496
   28          1             0       -2.718066   -2.320365
2.229429
   29          1             0       -3.885253   -0.673666
-2.647681
   30          1             0       -3.988007   -1.847978
-1.301827
   31          1             0       -4.168048   -0.093889
-0.978813
   32          1             0        0.120279   -2.232798
-1.884240
   33          1             0        1.738768   -1.669412
-1.476037
   34          1             0        0.205704   -3.614325
-0.136626
   35          1             0       -1.927085    2.516114
-2.896041
   36          1             0       -0.758946    2.015785
-1.493517

Structure 6; Standard orientation:
 ---------------------------------------------------------------
----------
 Center     Atomic     Atomic              Coordinates
(Angstroms)
 Number     Number      Type              X           Y
Z
 ---------------------------------------------------------------
----------
    1          6             0       -4.437522   -1.316389
0.033682
    2          6             0       -3.047469   -1.284119
-0.122175
    3          6             0       -2.380003   -0.054931
-0.252310
    4          6             0       -3.131081    1.135977
-0.226667
    5          6             0       -4.513992    1.100488
-0.042749
    6          6             0       -5.172874   -0.128488
0.084252
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7	6	0	-0.899311	0.087946	-0.502390
8	6	0	0.114125	-0.468312	0.474459
9	6	0	-0.176851	-1.873485	1.049414
10	8	0	-0.408319	-2.903633	0.086913
11	8	0	-0.542098	0.827486	-1.423400
12	15	0	1.849822	-0.403661	-0.187875
13	8	0	2.777025	-0.811530	1.081123
14	6	0	3.533053	0.192660	1.802934
15	6	0	0.074356	0.570900	1.765915
16	8	0	0.521361	1.807838	1.504840
17	8	0	2.389259	0.776499	-0.937395
18	8	0	1.887027	-1.788041	-1.050466
19	6	0	3.096915	-2.162210	-1.756416
20	19	0	1.124679	3.181767	-0.663335
21	1	0	-0.987699	0.511971	2.093779
22	1	0	0.659921	0.017388	2.534231
23	1	0	-2.622853	2.091755	-0.339135
24	1	0	-5.078342	2.032048	-0.005504
25	1	0	-6.254301	-0.158836	0.216255
26	1	0	-4.945002	-2.277482	0.114295
27	1	0	-2.490675	-2.212899	-0.180748
28	1	0	-1.085853	-1.820726	1.656018
29	1	0	0.645247	-2.157357	1.717555
30	1	0	0.381451	-2.957189	-0.483459
31	1	0	3.366521	-1.384978	-2.476178
32	1	0	3.912486	-2.323982	-1.045573
33	1	0	2.865552	-3.092339	-2.277601

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   34          1             0        3.951867   -0.321290
2.670120
   35          1             0        2.876956    1.009479
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   36          1             0        4.338385    0.576588
1.170881

Structure 10; Standard orientation:
 ---------------------------------------------------------------
----------
 Center     Atomic     Atomic              Coordinates
(Angstroms)
 Number     Number      Type              X           Y
Z
 ---------------------------------------------------------------
----------
    1          6             0       -4.548388   -1.196796
-0.159381
    2          6             0       -3.154853   -1.110228
-0.236310
    3          6             0       -2.518666    0.137764
-0.118523
    4          6             0       -3.304045    1.290692
0.080417
    5          6             0       -4.691591    1.194799
0.186981
    6          6             0       -5.318705   -0.050972
0.062318
    7          6             0       -1.035701    0.347122
-0.251605
    8          6             0       -0.015719   -0.444933
0.566600
    9          6             0        0.383837    0.446479
1.777596
   10          8             0        1.598128    0.981801
1.283151
   11         15             0        1.786800   -0.230380
-0.102531
   12          8             0        1.453110   -1.508697
-1.261060
   13          6             0        2.485044   -1.969287
-2.130039
   14          8             0       -0.646991    1.308588
-0.920585
   15          6             0       -0.380615   -1.876485
0.990233
   16          8             0       -0.547778   -2.785391
-0.094493
   17          8             0        2.762612   -1.252748
0.764802
   18          6             0        3.752947   -0.749232
1.670603
   19          8             0        2.495693    0.755576
-1.031142
```

```
   20          19             0        1.510649    3.216922
-0.464106
   21           1             0       -0.335793    1.240658
2.021076
   22           1             0        0.529799   -0.170599
2.679407
   23           1             0        2.054332   -2.749510
-2.767361
   24           1             0        2.855496   -1.151600
-2.758103
   25           1             0        3.321443   -2.392200
-1.559174
   26           1             0        4.380831    0.007968
1.188012
   27           1             0        4.370402   -1.608354
1.947475
   28           1             0        3.290696   -0.316732
2.562305
   29           1             0        0.406367   -2.237176
1.666345
   30           1             0       -1.319162   -1.871931
1.556497
   31           1             0        0.204321   -2.581240
-0.702004
   32           1             0       -2.565606   -2.002061
-0.422185
   33           1             0       -5.032138   -2.166655
-0.272869
   34           1             0       -6.403574   -0.126483
0.134243
   35           1             0       -5.284247    2.092537
0.360954
   36           1             0       -2.816958    2.260994
0.162641

Structure 11; Standard orientation:
 ---------------------------------------------------------------
----------
 Center     Atomic     Atomic              Coordinates
(Angstroms)
 Number     Number      Type              X           Y
Z
 ---------------------------------------------------------------
----------
    1          6             0        2.764447    0.141407
-0.183240
    2          6             0        2.958609   -0.518099
1.040121
    3          6             0        4.248295   -0.735953
1.541560
    4          6             0        5.364823   -0.306181
0.817329
    5          6             0        5.182582    0.351832
-0.406069
```

6	6	0	3.893195	0.579950	-0.895876
7	6	0	1.373497	0.460151	-0.692839
8	6	0	0.572079	-0.564142	-1.204132
9	6	0	-0.753870	-0.222660	-1.757105
10	8	0	-1.955271	-0.761054	-0.975074
11	15	0	-2.588387	-0.070586	0.305291
12	8	0	-2.011342	-0.758997	1.634954
13	6	0	-1.986636	-2.203378	1.782369
14	8	0	1.050826	1.707295	-0.630423
15	6	0	1.075125	-1.961845	-1.397924
16	8	0	0.677821	-2.952883	-0.390179
17	8	0	-4.101352	-0.634089	0.297502
18	6	0	-4.984639	-0.334272	-0.808602
19	8	0	-2.464721	1.417953	0.403664
20	19	0	-0.643706	3.421133	0.463440
21	1	0	2.095560	-0.843740	1.619557
22	1	0	4.378372	-1.242319	2.498221
23	1	0	6.369340	-0.479659	1.202844
24	1	0	6.046950	0.689071	-0.978577
25	1	0	3.757337	1.100378	-1.844267
26	1	0	0.663581	-2.383834	-2.323827
27	1	0	2.167972	-1.990171	-1.476455
28	1	0	1.173150	-2.772606	0.432401
29	1	0	-0.901850	0.855241	-1.828969
30	1	0	-0.948915	-0.697144	-2.723581
31	1	0	-1.527227	-2.391246	2.754320
32	1	0	-1.383002	-2.645568	0.985964

33	1	0	-3.006961	-2.596619	1.768937
34	1	0	-5.107993	0.747931	-0.915467
35	1	0	-4.590317	-0.765556	-1.733233
36	1	0	-5.942489	-0.793554	-0.559696

Structure 1a'; Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.790189	-0.618382	0.243201
2	6	0	5.954429	-1.453692	-0.509802
3	6	0	4.583250	-1.204606	-0.562582
4	6	0	4.034395	-0.098549	0.112439
5	6	0	4.879589	0.737248	0.864136
6	6	0	6.249490	0.469504	0.936454
7	6	0	2.553115	0.101669	0.064781
8	8	0	1.804787	-0.884336	0.059198
9	6	0	1.969100	1.476360	0.015751
10	6	0	0.542071	1.650772	0.491462
11	8	0	-0.369308	1.299193	-0.556578
12	6	0	2.646957	2.507704	-0.517829
13	8	0	-2.664003	0.400573	0.517260
14	15	0	-3.878090	-0.305459	-0.077395
15	8	0	-4.650849	0.649659	-1.151810
16	6	0	-4.896827	2.033400	-0.837965
17	8	0	-3.644732	-1.638609	-0.756275
18	8	0	-5.054634	-0.401455	1.063109

19	6	0	-4.757024	-1.024298	2.323649
20	19	0	-0.755949	-1.596135	-0.796980
21	1	0	4.467732	1.577393	1.419143
22	1	0	6.893881	1.112363	1.535360
23	1	0	7.860537	-0.818171	0.291337
24	1	0	6.373121	-2.300576	-1.052839
25	1	0	3.928387	-1.856097	-1.138997
26	1	0	0.393982	2.700024	0.783360
27	1	0	0.360482	1.021399	1.373424
28	1	0	-1.255465	1.106117	-0.153120
29	1	0	3.655152	2.407129	-0.909849
30	1	0	2.186252	3.491090	-0.600907
31	1	0	-5.344682	2.477049	-1.729891
32	1	0	-3.959976	2.545999	-0.598528
33	1	0	-5.591583	2.117004	0.004543
34	1	0	-4.500812	-2.081182	2.184216
35	1	0	-3.932534	-0.506206	2.825140
36	1	0	-5.662570	-0.947862	2.929749

Transition States; Geometries and Frequencies.
TS from Structure 5 to Structure 9
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	19	0	-2.090691	2.330361	-0.818573
2	8	0	-1.876371	0.238978	0.963402
3	15	0	-1.301226	-0.979300	0.275184

4	8	0	-0.279190	-1.718964
1.361605				
5	6	0	-0.716644	-1.945265
2.706270				
6	1	0	-1.018375	-1.006033
3.182109				
7	1	0	-1.554438	-2.652598
2.730874				
8	1	0	0.133320	-2.372846
3.244847				
9	8	0	-2.290252	-2.263326
0.083908				
10	6	0	-3.670105	-2.128090
-0.306266				
11	1	0	-4.227975	-1.589251
0.466998				
12	1	0	-4.054533	-3.147084
-0.394568				
13	1	0	-3.728808	-1.593088
-1.256433				
14	8	0	-0.822902	3.633393
1.521080				
15	6	0	-0.381185	2.827360
2.322663				
16	1	0	0.240099	3.156760
3.177067				
17	1	0	-0.594029	1.750542
2.216031				
18	6	0	0.003661	-0.929854
-1.064417				
19	6	0	-0.925441	-0.723599
-2.285961				
20	8	0	-2.095649	-0.189894
-1.767302				
21	1	0	-1.070172	-1.715320
-2.764061				
22	1	0	-0.440955	-0.077698
-3.044123				
23	1	0	0.515632	-1.896726
-1.059365				
24	6	0	0.982363	0.213803
-0.848400				
25	8	0	0.604124	1.380779
-0.989815				
26	6	0	2.415501	-0.063610
-0.511783				
27	6	0	3.328870	1.008101
-0.572031				
28	1	0	2.968853	1.991898
-0.864219				
29	6	0	4.675405	0.814660
-0.269943				
30	1	0	5.370744	1.651585
-0.329402				

```
   31          6             0        5.132833   -0.454475
0.109536
   32          1             0        6.185304   -0.607182
0.348439
   33          6             0        4.235537   -1.524646
0.180299
   34          1             0        4.584102   -2.512582
0.479769
   35          6             0        2.886824   -1.333778
-0.132238
   36          1             0        2.208944   -2.179130
-0.058215

Vibrational frequencies:
          1 -170.8757
          2   18.2953
          3    24.168
          4   32.4502
          5   45.5265
          6   52.5219
          7   68.5829
          8   77.9571
          9   83.7736
         10   92.8208
         11   98.9999
         12  106.0571
         13  116.3607
         14  123.4543
         15  135.3168
         16   144.944
         17  154.6006
         18  161.4339
         19  169.7136
         20  181.9642
         21  190.1496
         22  195.1176
         23  256.9526
         24  272.4123
         25  293.4627
         26  314.3825
         27  338.3823
         28  405.1217
         29  408.3946
         30  413.9569
         31  454.3157
         32  471.2018
         33  480.9432
         34  593.7484
         35  627.3139
         36  645.8458
         37  671.8781
         38   693.818
         39  719.1818
         40  740.3171
```

41 776.2475
42 793.5074
43 835.9988
44 857.9173
45 928.0263
46 956.7714
47 996.8662
48 1010.6844
49 1016.4772
50 1020.5456
51 1047.0528
52 1049.2379
53 1072.0471
54 1080.1497
55 1096.1012
56 1112.5702
57 1144.1973
58 1172.5445
59 1177.6472
60 1177.8218
61 1179.3987
62 1198.8644
63 1201.5543
64 1202.0398
65 1225.1624
66 1230.3154
67 1236.5736
68   1283.02
69 1330.6415
70 1350.4236
71 1364.9462
72 1383.3608
73 1458.0302
74 1478.2436
75 1479.6804
76 1499.8191
77 1506.3275
78 1522.4656
79 1526.2268
80 1527.3501
81 1533.5899
82 1534.5497
83 1618.8774
84 1638.033
85 1686.1113
86 1775.5642
87 2875.082
88 2921.7649
89 2958.1796
90 3041.3512
91 3055.3634
92 3068.9332
93 3085.962
94 3110.079

95	3134.8955
96	3136.2699
97	3138.298
98	3148.5089
99	3157.0575
100	3162.4703
101	3177.3007
102	3195.5073

TS from Structure 9 to Structure 12
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.374657	0.381696	-0.869238
2	6	0	2.276991	-0.443620	-0.558249
3	6	0	2.499828	-1.630108	0.163634
4	6	0	3.791377	-1.980049	0.565136
5	6	0	4.876581	-1.158586	0.240112
6	6	0	4.665384	0.023275	-0.481706
7	6	0	0.917637	-0.021903	-1.019265
8	8	0	0.726283	1.148165	-1.376583
9	6	0	-0.210426	-1.016191	-1.093180
10	15	0	-1.687477	-0.664242	0.081453
11	8	0	-2.205016	0.738776	0.413966
12	6	0	-1.148932	-0.903411	-2.293566
13	8	0	-2.393858	-0.785460	-1.608853
14	8	0	-2.610742	-1.939707	0.612762
15	6	0	-3.940644	-2.171106	0.138658
16	8	0	-0.591327	-0.931594	1.399187
17	6	0	-1.052351	-0.887206	2.742174

```
   18          19             0       -1.310750    2.967119
-0.770069
   19           8             0        0.369815    3.322174
1.506549
   20           6             0        0.665977    2.346086
2.174384
   21           1             0        1.667067   -2.270812
0.436641
   22           1             0        3.950052   -2.896274
1.132879
   23           1             0        5.884208   -1.438728
0.546592
   24           1             0        5.507729    0.663883
-0.740999
   25           1             0        3.204952    1.299349
-1.428147
   26           1             0        0.126844   -2.040081
-0.912245
   27           1             0       -1.539975    0.071451
2.968661
   28           1             0       -1.762195   -1.697643
2.948365
   29           1             0       -0.177607   -1.005958
3.392493
   30           1             0       -4.359402   -2.949014
0.783995
   31           1             0       -4.553870   -1.266119
0.220649
   32           1             0       -3.933813   -2.506109
-0.901420
   33           1             0       -0.940317   -0.016735
-2.907586
   34           1             0       -1.129550   -1.793370
-2.939298
   35           1             0        1.271140    2.449628
3.094712
   36           1             0        0.343423    1.332803
1.884659

Vibrational frequencies:
         1  -33.0789
         2   23.1086
         3   26.1171
         4   36.5478
         5   41.7122
         6   48.4808
         7   53.5704
         8   71.2317
         9   84.2439
        10    86.306
        11   96.1039
        12  115.8795
        13  121.9037
        14  128.7014
```

15	133.997
16	142.4903
17	154.9282
18	164.1399
19	184.3259
20	188.025
21	196.9405
22	236.4565
23	299.0304
24	310.3391
25	323.6336
26	380.1763
27	391.0672
28	412.6142
29	415.8172
30	421.116
31	452.8443
32	494.4776
33	511.8338
34	554.0769
35	597.607
36	627.4913
37	658.8177
38	693.0276
39	699.6947
40	724.6867
41	737.4986
42	808.387
43	832.8374
44	855.987
45	951.7222
46	958.1389
47	993.218
48	1011.6961
49	1013.2925
50	1038.6496
51	1047.9316
52	1054.8225
53	1058.071
54	1078.3026
55	1082.144
56	1102.4118
57	1112.5278
58	1131.4604
59	1174.4022
60	1175.4369
61	1177.193
62	1194.1611
63	1196.9434
64	1201.346
65	1210.603
66	1221.7444
67	1241.7296
68	1279.4789

69	1339.0564
70	1356.7049
71	1360.5312
72	1390.4714
73	1470.2459
74	1475.3613
75	1478.4281
76	1498.71
77	1502
78	1518.8716
79	1527.5638
80	1529.7755
81	1536.1394
82	1544.6895
83	1617.8777
84	1638.9369
85	1677.8473
86	1781.0173
87	2963.426
88	3007.5901
89	3014.151
90	3044.2274
91	3045.4247
92	3074.7842
93	3076.3993
94	3091.9717
95	3094.9028
96	3116.6703
97	3139.0603
98	3141.0442
99	3148.9754
100	3157.9312
101	3174.4487
102	3207.105

TS from Structure 5' to Structure 6
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	19	0	1.236649	3.176067	-0.778932
2	8	0	2.372868	0.691479	-0.956619
3	15	0	1.797281	-0.478824	-0.216896
4	8	0	1.793183	-1.867148	-1.080922

5	6	0	3.009374	-2.320614
-1.726310				
6	1	0	3.368426	-1.561895
-2.427028				
7	1	0	3.774969	-2.539757
-0.976167				
8	1	0	2.743256	-3.230962
-2.265705				
9	8	0	2.724823	-0.920298
1.046728				
10	6	0	3.628092	0.019973
1.673894				
11	1	0	4.382123	0.355900
0.957422				
12	1	0	4.104643	-0.527327
2.489314				
13	1	0	3.079707	0.880812
2.066505				
14	6	0	0.096117	-0.451713
0.417692				
15	6	0	-0.256606	-1.738378
1.164320				
16	8	0	-0.422018	-2.915765
0.353125				
17	1	0	0.360043	-2.987203
-0.225359				
18	1	0	0.508668	-1.932064
1.926098				
19	1	0	-1.210497	-1.607860
1.683094				
20	8	0	0.545632	2.025208
1.547151				
21	6	0	0.147423	0.850860
1.883106				
22	1	0	0.808963	0.235877
2.521876				
23	1	0	-0.911973	0.719486
2.176466				
24	6	0	-0.895725	0.205985
-0.444756				
25	8	0	-0.566507	1.090614
-1.259273				
26	6	0	-2.377312	-0.010339
-0.239654				
27	6	0	-3.176782	1.135581
-0.071542				
28	1	0	-2.703185	2.115491
-0.039750				
29	6	0	-4.561872	1.023800
0.061590				
30	1	0	-5.165550	1.919132
0.209335				
31	6	0	-5.173157	-0.234702
-0.003625				

```
   32          1             0       -6.255642   -0.322984
0.087834
   33          6             0       -4.388075   -1.376448
-0.191039
   34          1             0       -4.857415   -2.358114
-0.254436
   35          6             0       -2.996689   -1.269437
-0.296923
   36          1             0       -2.394640   -2.161561
-0.438404

Vibrational frequencies:
         1 -209.0205
         2   30.3618
         3   36.3317
         4   50.8631
         5    64.574
         6   76.1261
         7   80.0186
         8   92.9974
         9    94.369
        10  104.3629
        11  113.2653
        12  119.8106
        13  132.4704
        14  146.1216
        15  159.2775
        16  170.5753
        17  195.8855
        18  206.4777
        19  212.8902
        20   219.169
        21  232.7727
        22  240.9396
        23  270.4628
        24  301.7577
        25   319.201
        26  379.3463
        27  389.6054
        28  405.6495
        29  416.2751
        30  445.6359
        31   468.536
        32  481.5086
        33  542.3668
        34  568.1087
        35  629.5962
        36  635.9575
        37  664.1383
        38  710.3848
        39  724.1224
        40  742.9409
        41  760.2005
        42  783.1983
```

43 813.3732
44 868.3331
45 931.7178
46 952.8409
47 971.6705
48 996.9316
49 1002.3765
50 1011.7998
51 1016.1031
52 1019.706
53 1049.354
54 1053.2574
55 1102.8657
56 1110.6542
57 1166.7039
58 1175.4754
59 1177.2026
60 1183.2775
61 1191.2457
62 1200.6776
63 1202.3157
64 1205.9377
65 1221.2332
66 1253.1415
67 1270.4688
68 1329.4613
69 1336.4949
70 1362.6416
71 1377.3487
72 1394.2217
73 1437.2209
74 1474.6403
75 1482.0135
76 1490.7463
77 1506.5853
78 1507.0355
79 1514.9252
80 1517.964
81 1523.2134
82 1526.1861
83 1575.3024
84 1607.9976
85 1626.2464
86 1643.4219
87 2914.2699
88 2949.0753
89 3049.9814
90 3065.2322
91 3066.6586
92 3111.6584
93 3135.1684
94 3144.1395
95 3147.0306
96 3148.7444

97	3153.9886
98	3162.741
99	3165.0993
100	3170.3571
101	3209.9936
102	3662.2068

TS from Structure 6 to Structure 10
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	19	0	1.383271	3.158410	-0.609558
2	8	0	2.437595	0.689547	-1.047441
3	15	0	1.791296	-0.342749	-0.155776
4	8	0	1.621661	-1.723641	-1.094715
5	6	0	2.737233	-2.204450	-1.864473
6	1	0	3.127950	-1.411021	-2.508063
7	1	0	3.528790	-2.570058	-1.201218
8	1	0	2.362776	-3.027547	-2.478064
9	8	0	2.755980	-1.007514	0.978118
10	6	0	3.757632	-0.236697	1.670450
11	1	0	3.291193	0.627222	2.148791
12	1	0	4.531623	0.089740	0.968197
13	1	0	4.192947	-0.912261	2.410337
14	6	0	0.020391	-0.438311	0.523672
15	6	0	-0.340441	-1.848371	1.032072
16	8	0	-0.567987	-2.832128	0.024789
17	1	0	0.209950	-2.788451	-0.568451
18	1	0	0.455226	-2.178425	1.712566

```
   19          1             0       -1.263717   -1.784768
1.617585
   20          8             0        1.287953    1.358623
1.387924
   21          6             0        0.239437    0.553409
1.746576
   22          1             0        0.443462   -0.086193
2.631726
   23          1             0       -0.698824    1.098621
1.971007
   24          6             0       -0.987819    0.247695
-0.383922
   25          8             0       -0.612067    1.102124
-1.189908
   26          6             0       -2.471500    0.082337
-0.177805
   27          6             0       -3.223167    1.260535
0.002654
   28          1             0       -2.713694    2.222663
0.034126
   29          6             0       -4.608856    1.200655
0.155994
   30          1             0       -5.175390    2.117798
0.315644
   31          6             0       -5.267252   -0.033927
0.095610
   32          1             0       -6.350768   -0.081606
0.203312
   33          6             0       -4.529722   -1.204374
-0.108364
   34          1             0       -5.037902   -2.166437
-0.170984
   35          6             0       -3.137226   -1.153272
-0.232595
   36          1             0       -2.572552   -2.065301
-0.397627

Vibrational frequencies:
         1 -165.5514
         2   34.6022
         3   37.9031
         4   55.1257
         5   62.7251
         6   77.1723
         7   86.0681
         8  101.6968
         9  110.9366
        10  126.2062
        11  136.0671
        12  141.5593
        13  144.3028
        14  165.2094
        15  177.0965
        16  194.7469
```

17	199.948
18	227.0638
19	241.0773
20	250.6749
21	272.8601
22	294.3978
23	317.7494
24	335.298
25	378.4171
26	392.3877
27	403.3185
28	417.68
29	472.0346
30	479.9307
31	543.0479
32	570.0044
33	600.6966
34	612.3383
35	629.9573
36	654.0615
37	660.833
38	711.9064
39	722.2087
40	740.0587
41	770.3858
42	795.3981
43	869.0687
44	934.1001
45	951.0954
46	968.5257
47	995.1323
48	1001.5789
49	1011.8323
50	1022.4025
51	1033.1799
52	1040.5263
53	1052.0293
54	1071.381
55	1100.052
56	1108.2914
57	1141.0313
58	1158.7182
59	1169.4157
60	1177.2813
61	1178.7519
62	1180.4867
63	1200.0121
64	1202.148
65	1206.5382
66	1233.1059
67	1239.0121
68	1299.8439
69	1335.018
70	1364.5022

71	1365.4109
72	1397.6964
73	1443.5725
74	1464.8973
75	1474.4976
76	1481.2673
77	1501.1773
78	1505.7
79	1520.8275
80	1521.8641
81	1526.0437
82	1529.9945
83	1532.8475
84	1617.523
85	1639.9345
86	1677.0014
87	2875.6276
88	2920.2758
89	3043.8784
90	3051.9548
91	3058.4937
92	3099.2301
93	3127.4849
94	3136.9542
95	3138.3863
96	3146.0139
97	3146.3308
98	3155.0427
99	3162.0759
100	3162.6387
101	3222.7949
102	3592.1692

TS from Structure 10 to Structure 11
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.502309	-0.510578	0.220192
2	8	0	-1.982853	0.244028	1.460004
3	19	0	-2.392193	2.841720	0.766261
4	8	0	-0.354949	-1.589721	0.980504
5	6	0	-0.715282	-2.326309	2.144627

6	1	0	-0.985764	-1.649214
2.962963				
7	1	0	-1.556372	-3.001931
1.944102				
8	1	0	0.157400	-2.919475
2.439562				
9	8	0	-2.395009	-1.818984
-0.258956				
10	6	0	-3.728005	-1.682885
-0.769528				
11	1	0	-4.341450	-1.051211
-0.117805				
12	1	0	-4.143800	-2.694466
-0.787926				
13	1	0	-3.725227	-1.260537
-1.777546				
14	6	0	-0.093787	-0.059673
-1.062679				
15	6	0	-1.161693	0.642544
-1.911791				
16	1	0	-1.386495	0.071008
-2.826006				
17	1	0	-0.903105	1.669701
-2.194291				
18	8	0	-2.256663	0.627044
-0.995147				
19	6	0	0.566068	-1.250195
-1.797444				
20	1	0	-0.236619	-1.797453
-2.314263				
21	1	0	1.244032	-0.863493
-2.569853				
22	8	0	1.323558	-2.136486
-0.989606				
23	1	0	0.816572	-2.207466
-0.146452				
24	6	0	0.840137	0.935343
-0.391894				
25	8	0	0.438578	2.067418
-0.108864				
26	6	0	2.268308	0.576823
-0.068422				
27	6	0	2.627370	0.032218
1.171959				
28	1	0	1.857482	-0.199086
1.902502				
29	6	0	3.971694	-0.223956
1.456589				
30	1	0	4.246644	-0.645511
2.423289				
31	6	0	4.962007	0.060343
0.508403				
32	1	0	6.009285	-0.138561
0.734663				

```
   33          6             0        4.603491    0.609133
-0.727175
   34          1             0        5.368105    0.837832
-1.469529
   35          6             0        3.259617    0.865769
-1.017151
   36          1             0        2.984767    1.294518
-1.981716
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Vibrational frequencies:
          1 -178.4204
          2   20.9494
          3   54.3115
          4   60.7045
          5   83.4198
          6    89.341
          7    94.712
          8  111.9001
          9  126.4846
         10   133.696
         11  141.0326
         12  147.9142
         13  160.8146
         14  173.0927
         15  186.4211
         16  214.7304
         17  226.8673
         18  254.8968
         19  283.3729
         20   319.327
         21  326.7839
         22  366.6683
         23  376.2584
         24  404.8723
         25  415.2895
         26  416.3871
         27  434.5529
         28  460.9033
         29  514.8292
         30  548.1692
         31  555.0275
         32  584.3577
         33  624.2157
         34  628.2516
         35  640.9603
         36  676.2482
         37  693.2952
         38  710.9256
         39  722.5663
         40  731.3231
         41  774.8641
```

42 796.6919
43 857.6186
44 925.8341
45   954.536
46 984.5634
47 989.2424
48 1006.0642
49 1011.9473
50 1025.2095
51 1050.9672
52 1053.0157
53 1054.6479
54 1071.5544
55 1083.1673
56 1095.2139
57 1104.3648
58 1157.7918
59 1169.5835
60   1174.5
61 1177.1588
62 1178.925
63 1197.2944
64 1204.2451
65 1227.2297
66 1240.9695
67 1264.7534
68 1279.3344
69 1330.8062
70 1363.4676
71 1367.9833
72 1406.4613
73 1464.6277
74 1474.3467
75 1482.6346
76 1491.5779
77 1500.0003
78 1508.7426
79 1515.9564
80 1519.1008
81 1525.4843
82 1527.3813
83 1529.5808
84 1620.1625
85 1644.4202
86 1678.3407
87 2993.1821
88 3006.7383
89 3031.0881
90 3052.3519
91 3056.451
92 3080.9328
93 3099.8841
94 3107.3871
95 3134.1612

```
 96 3134.6374
 97 3137.5935
 98  3140.845
 99 3148.7303
100  3157.367
101 3218.6534
102 3469.6796
```

SI-2-2

SI-2-3