Electronic Supplementary Information

Oxoketene-oxoketene, imidoylketene-imidoylketene and oxoketenimine-imidoylketene rearrangements. 1,3-Shifts of phenyl groups

Lisa George,[a] Klaus-Peter Netsch,[b] Gerhard Penn,[c] Gert Kollenz[c] and Curt Wentrup*[a]

[a]Chemistry Building, School of Molecular and Microbial Sciences, The University of Queensland, Brisbane, Qld 4072, Australia. E-mail: wentrup@uq.edu.au

[b]Fachbereich Chemie, Philipps-Universitaet Marburg, D-3550 Marburg, Germany

[c]Institut fuer Chemie, Karl-Franzens-Universitaet Graz, A-8010 Graz, Austria

Summary of calculated energies (B3LYP/6-31G).**

No.	Structures	Energy+ZPVE	ΔE (+ZPVE)kJ/mol
1	5a	-841.168633	0
2	6a	-841.167108	4.0
3	TS3	-841.118614	131.3
4	13a	-821.276866	0
5	14a	-821.272032	12.7
6	TS4	-821.225179	135.7
7	14b	-821.273235	9.5
8	15a	-821.271875	13.1
9	TS5	-821.212449	169.1
10	32	-821.268717	21.4
11	33	-821.280092	-8.5
12	TS6	-821.266448	27.4
13	TS7	-821.265164	30.7
14	34+35	-821.259298	46.1
15	TS8	-821.196527	210.9
16	21	-1091.545307	0
17	22	-1091.541747	9.3
18	TS9	-1091.496373	128.5
19	23	-1091.546234	-2.4
20	TS10	-1091.486692	153.9
21	23a	-1091.543325	5.2
22	TS11	-1091.541202	10.8
23	24a	-1091.541477	10.1
24	TS12	-1091.488665	148.7
25	24	-1091.544972	0.9
26	TS13	-1091.538241	18.6
27	25	-1091.547423	-5.6
28	TS14	-1091.521397	62.8
29	26	-1091.536030	24.4
30	TS15	-1091.524255	55.2
31	27	-1091.585703	-106.1
32	TS16	-1091.497391	125.8
33	28	-1091.614602	-181.9
34	TS17	-1091.529209	42.3
35	29	- 1091.600836	-145.8

Computational data for all calculated ground states and transition structures (B3LYP/6-31G).**

1: Dibenzoylketene 5a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.729929	2.162673	0.136957
2	8	1.329114	3.127841	0.366899
3	6	0.015121	1.058643	-0.117423
4	6	0.699050	-0.176865	-0.611056
5	8	-1.870906	2.457461	-0.389946
6	6	-1.467385	1.317066	-0.193291
7	6	-2.422393	0.192411	0.032432
8	6	-3.722150	0.340192	-0.475180
9	6	-4.680934	-0.641612	-0.245304
10	1	-3.957788	1.232414	-1.044841
11	6	-3.071906	-1.912213	1.039757
12	6	-4.357374	-1.769063	0.514015
13	1	-5.681084	-0.527295	-0.652329
14	1	-2.821973	-2.782467	1.638935
15	1	-5.106622	-2.533530	0.698321
16	8	0.101203	-0.956864	-1.337057
17	6	2.128448	-0.416486	-0.233252
18	6	2.914607	-1.180443	-1.110144
19	6	2.688822	0.048589	0.965517
20	6	4.246654	-1.443910	-0.808847
21	1	2.459727	-1.551759	-2.022113
22	6	4.021689	-0.227651	1.270996
23	1	2.079764	0.593650	1.679909
24	6	4.803038	-0.966066	0.381833
25	1	4.853378	-2.022960	-1.498426
26	1	4.445352	0.126515	2.205695
27	1	5.842045	-1.175723	0.618249
28	6	-2.104784	-0.940283	0.794055
29	1	-1.110670	-1.056254	1.211046

Energy = -841.3843552
E+ZPVE = -841.168633

2: Dibenzoylketene 6a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000057	-1.142628	-0.000067
2	8	0.000238	-2.308273	0.000090
3	6	0.000021	0.187898	-0.000268
4	6	-1.254202	0.948418	-0.356615
5	8	1.163559	2.044500	0.877154
6	6	1.254176	0.948439	0.356484
7	6	2.586352	0.315555	0.100486
8	6	3.661972	0.711240	0.911335
9	6	4.926183	0.165710	0.714815
10	1	3.480468	1.444701	1.689538
11	6	4.077949	-1.143674	-1.134737
12	6	5.135837	-0.764637	-0.307927
13	1	5.750717	0.465576	1.354539
14	1	4.242935	-1.849028	-1.943370
15	1	6.124266	-1.186764	-0.463853
16	8	-1.163855	2.044594	-0.877094
17	6	-2.586354	0.315476	-0.100517
18	6	-3.661958	0.710992	-0.911440
19	6	-2.806159	-0.607723	0.931772
20	6	-4.926176	0.165490	-0.714880
21	1	-3.480429	1.444247	-1.689835
22	6	-4.077947	-1.143523	1.134917
23	1	-1.998144	-0.880890	1.602648
24	6	-5.135831	-0.764658	0.308029
25	1	-5.750640	0.465117	-1.354801
26	1	-4.242896	-1.848791	1.943634
27	1	-6.124271	-1.186729	0.464034
28	6	2.806133	-0.607887	-0.931587
29	1	1.998133	-0.880931	-1.602533

Energy = -841.3828547
E+ZPVE = -841.167108

3: TS3 connecting 5a and 6a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.183364	1.357962	-0.104628
2	8	-1.576247	2.480298	-0.194868
3	6	0.004967	0.576964	-0.042817

4	6	1.386658	1.107479	-0.037431
5	6	2.607798	0.234719	-0.013366
6	6	2.599105	-1.161317	-0.149364
7	6	3.838784	0.896932	0.137444
8	6	3.798384	-1.874862	-0.132206
9	1	1.670094	-1.704100	-0.266750
10	6	5.030890	0.182403	0.158893
11	1	3.827261	1.976864	0.233175
12	6	5.013744	-1.208890	0.023209
13	1	3.779384	-2.955328	-0.240354
14	1	5.974312	0.706741	0.279808
15	1	5.944064	-1.769645	0.038541
16	6	-0.632046	-0.678056	0.053324
17	8	-0.468376	-1.857199	0.143062
18	6	-2.278680	0.026188	-0.002964
19	6	-2.988408	-0.278599	-1.201343
20	6	-2.983194	-0.088167	1.231187
21	6	-4.312688	-0.682671	-1.165094
22	1	-2.470373	-0.190440	-2.152781
23	6	-4.307487	-0.493002	1.264575
24	1	-2.460826	0.146889	2.154915
25	6	-4.971520	-0.790932	0.067172
26	1	-4.841225	-0.914248	-2.084462
27	1	-4.831474	-0.578878	2.211257
28	1	-6.009826	-1.108536	0.094051
29	8	1.504741	2.331123	-0.046562

Energy = -841.3325991
E+ZPVE = -841.118614
Imaginary frequency: -406.5 cm^{-1}

4: Benzoyl(phenylimidoyl)lketene 13a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.749691	2.183214	0.158789
2	8	-1.390058	3.115818	0.415524
3	7	1.821675	2.565987	-0.441512
4	1	2.841056	2.641550	-0.389075
5	6	-0.012339	1.099936	-0.122429
6	6	1.455498	1.354743	-0.215361
7	6	2.394720	0.220568	0.028237
8	6	2.159666	-0.719650	1.041073
9	6	3.579445	0.135566	-0.717447

10	6	3.098649	-1.711438	1.314785
11	1	1.245890	-0.662704	1.624359
12	6	4.511910	-0.865118	-0.451897
13	1	3.754195	0.840762	-1.524860
14	6	4.276117	-1.788245	0.568233
15	1	2.910092	-2.426894	2.109622
16	1	5.418661	-0.928397	-1.046046
17	1	5.002936	-2.567804	0.776329
18	6	-0.659150	-0.156500	-0.595437
19	8	-0.025813	-0.944890	-1.283731
20	6	-2.090670	-0.425073	-0.241716
21	6	-2.842523	-1.212835	-1.127175
22	6	-2.684824	0.033720	0.942853
23	6	-4.173953	-1.505071	-0.849836
24	1	-2.361382	-1.580891	-2.026932
25	6	-4.016907	-0.270693	1.224674
26	1	-2.103067	0.597684	1.665077
27	6	-4.764398	-1.032337	0.326231
28	1	-4.753480	-2.103045	-1.546749
29	1	-4.466181	0.079910	2.148802
30	1	-5.802762	-1.264228	0.544249

Energy = -821.5051423
E+ZPVE = -821.276866

5: Benzoyl(phenylimidoyl)lketene 14a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.015127	-1.095607	-0.095313
2	8	-0.019428	-2.260657	-0.051698
3	7	-1.135645	2.084755	-1.094750
4	1	-2.056988	2.507596	-1.240160
5	6	-0.007558	0.236462	-0.123379
6	6	-1.261016	0.965722	-0.488670
7	6	-2.567744	0.322562	-0.142036
8	6	-2.768399	-0.308804	1.095371
9	6	-3.632406	0.377811	-1.055579
10	6	-4.008797	-0.860034	1.414772
11	1	-1.958797	-0.342372	1.817786
12	6	-4.867307	-0.184116	-0.739881
13	1	-3.477892	0.842673	-2.025123
14	6	-5.059218	-0.802366	0.497743

15	1	-4.154979	-1.332057	2.381672
16	1	-5.677593	-0.146634	-1.461845
17	1	-6.022107	-1.239653	0.744291
18	6	1.239072	0.973293	0.300282
19	8	1.151065	2.063079	0.835129
20	6	2.569503	0.314712	0.097497
21	6	3.612338	0.667547	0.968567
22	6	2.819852	-0.590733	-0.943435
23	6	4.872335	0.097137	0.822142
24	1	3.408677	1.388598	1.752914
25	6	4.088037	-1.151931	-1.095844
26	1	2.038674	-0.829583	-1.657738
27	6	5.111830	-0.815711	-0.209957
28	1	5.670647	0.363753	1.508279
29	1	4.277143	-1.843463	-1.911201
30	1	6.097260	-1.257181	-0.326758

Energy = -821.5001077
E+ZPVE = -821.272032

6: TS4 connecting 13a and 14a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.209628	1.391947	-0.362597
2	8	1.689316	2.425220	-0.713121
3	7	-1.525662	2.549567	-0.232443
4	1	-2.520383	2.787468	-0.288130
5	6	-0.020994	0.742803	-0.101133
6	6	-1.390749	1.273491	-0.136396
7	6	-2.536215	0.311565	-0.055113
8	6	-2.542450	-0.893792	-0.771619
9	6	-3.659306	0.644733	0.718113
10	6	-3.652852	-1.735530	-0.729526
11	1	-1.683827	-1.167132	-1.375444
12	6	-4.763605	-0.203174	0.770137
13	1	-3.652800	1.564169	1.296726
14	6	-4.764574	-1.394617	0.042297
15	1	-3.648461	-2.660015	-1.299246
16	1	-5.619805	0.062694	1.383084
17	1	-5.625031	-2.056124	0.080615
18	6	0.512416	-0.508470	0.263542
19	8	0.237953	-1.614051	0.620150

20	6	2.209045	0.002901	0.018724
21	6	2.953438	0.117441	1.227676
22	6	2.850318	-0.611326	-1.094992
23	6	4.252151	-0.357939	1.318504
24	1	2.483372	0.586825	2.088033
25	6	4.148783	-1.086375	-1.002888
26	1	2.301610	-0.703906	-2.028777
27	6	4.849676	-0.960139	0.203812
28	1	4.806712	-0.265237	2.247118
29	1	4.624348	-1.553624	-1.859654
30	1	5.867494	-1.332555	0.275296

Energy = -821.4513864
E+ZPVE = -821.225179
Imaginary frequency: -415.6 cm^{-1}

7: Benzoyl(phenylimidoyl)lketene 14b

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.743555	2.097806	-0.234694
2	8	-1.340084	3.022378	-0.602328
3	7	-0.082191	-0.864123	1.572849
4	1	-0.653029	-1.665358	1.855644
5	6	-0.025648	1.032149	0.146723
6	6	-0.721279	-0.147794	0.722718
7	6	-2.133735	-0.399662	0.292191
8	6	-2.529213	-0.261994	-1.047604
9	6	-3.083046	-0.815039	1.239731
10	6	-3.840086	-0.544695	-1.431101
11	1	-1.802722	0.043046	-1.794685
12	6	-4.394428	-1.086372	0.857017
13	1	-2.792529	-0.898408	2.283035
14	6	-4.775540	-0.954467	-0.480388
15	1	-4.128860	-0.446932	-2.473207
16	1	-5.121559	-1.392583	1.603038
17	1	-5.797867	-1.166545	-0.778531
18	6	1.453219	1.309116	0.172971
19	8	1.846987	2.465074	0.285150
20	6	2.425012	0.190300	-0.019566
21	6	3.736322	0.391320	0.435626
22	6	2.110391	-0.986166	-0.712452
23	6	4.710649	-0.579584	0.222705

24	1	3.969519	1.316713	0.950732
25	6	3.091770	-1.947415	-0.943373
26	1	1.104176	-1.145051	-1.083477
27	6	4.390365	-1.750167	-0.469166
28	1	5.720608	-0.422321	0.589414
29	1	2.843619	-2.851622	-1.491153
30	1	5.151563	-2.505707	-0.641367

Energy = -821.273235
E+ZPVE = -821.5013211

8: Ketenimine 15a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.673372	2.249410	-0.236841
2	6	-0.001499	1.157614	0.130588
3	6	1.496672	1.333255	0.234162
4	8	-0.125901	-0.706903	1.557410
5	6	-0.699422	-0.029747	0.714293
6	8	1.965185	2.435980	0.483942
7	6	2.386924	0.162726	-0.029984
8	6	3.708558	0.233239	0.435969
9	6	1.981823	-0.948917	-0.781164
10	6	4.601827	-0.800738	0.174139
11	1	4.011583	1.108551	1.000026
12	6	2.882094	-1.975876	-1.056859
13	1	0.969778	-1.005741	-1.167550
14	6	4.190115	-1.907158	-0.573779
15	1	5.619746	-0.744855	0.548267
16	1	2.562835	-2.829804	-1.646586
17	1	4.888268	-2.712840	-0.781893
18	7	-1.245611	3.215537	-0.696486
19	1	-1.533676	3.976205	-0.082058
20	6	-2.096775	-0.361611	0.287729
21	6	-2.623862	0.001851	-0.960239
22	6	-2.883112	-1.117520	1.171983
23	6	-3.921764	-0.371514	-1.309409
24	1	-2.017651	0.553920	-1.670229
25	6	-4.181424	-1.477779	0.826466
26	1	-2.452368	-1.409372	2.123737
27	6	-4.703682	-1.104146	-0.415605
28	1	-4.319021	-0.094398	-2.281163

29	1	-4.787214	-2.052372	1.520782
30	1	-5.715892	-1.389189	-0.687436

Energy = -821.4990054
E+ZPVE = -821.271875

9: TS5 connecting 14a and 15a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.630554	-0.699056	-0.000084
2	8	-0.430194	-1.887716	0.000107
3	7	-1.589908	2.516355	-0.001500
4	1	-2.583250	2.713495	-0.001578
5	6	0.006992	0.554264	-0.000491
6	6	-1.183250	1.343776	-0.000860
7	6	-2.237107	-0.099288	-0.000068
8	6	-2.955790	-0.268996	1.220695
9	6	-2.956405	-0.270166	-1.220309
10	6	-4.309412	-0.563304	1.219506
11	1	-2.420239	-0.155414	2.159493
12	6	-4.310022	-0.564464	-1.218148
13	1	-2.421334	-0.157497	-2.159492
14	6	-4.987345	-0.708314	0.000922
15	1	-4.845533	-0.684587	2.155603
16	1	-4.846621	-0.686637	-2.153855
17	1	-6.048717	-0.938930	0.001297
18	6	1.374446	1.105574	-0.000326
19	8	1.486373	2.331626	-0.000370
20	6	2.608440	0.245146	-0.000022
21	6	3.836843	0.928850	0.001131
22	6	2.612183	-1.157309	-0.000994
23	6	5.038882	0.230605	0.001307
24	1	3.814016	2.012843	0.001820
25	6	3.821448	-1.854911	-0.000866
26	1	1.683836	-1.715343	-0.001673
27	6	5.034604	-1.167351	0.000275
28	1	5.980108	0.772921	0.002235
29	1	3.811435	-2.941098	-0.001643
30	1	5.972496	-1.715863	0.000383

Energy = -821.4375447

E+ZPVE = -821.212449
Imaginary frequency: - 458.6 cm^{-1}

10: Oxetone 32

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.291565	0.725707	-0.118746
2	6	-0.281297	1.870252	-0.295223
3	6	-0.058209	0.424723	-0.104579
4	6	2.587830	0.112757	-0.015037
5	6	2.726417	-1.285299	0.105921
6	6	3.731177	0.939032	-0.032747
7	6	3.999351	-1.836367	0.212716
8	1	1.829502	-1.899621	0.103954
9	6	4.994918	0.372444	0.074870
10	1	3.607293	2.011983	-0.128125
11	6	5.129878	-1.014444	0.198423
12	1	4.112524	-2.912181	0.304867
13	1	5.875680	1.006797	0.062627
14	1	6.119614	-1.454405	0.281376
15	8	-1.107299	2.713444	-0.419107
16	6	-0.906840	-0.751708	-0.015684
17	6	-2.389267	-0.543328	0.041851
18	6	-2.966463	0.451733	0.843761
19	6	-3.230392	-1.398219	-0.688115
20	6	-4.352628	0.576034	0.925596
21	1	-2.333740	1.121972	1.414307
22	6	-4.615072	-1.264870	-0.614996
23	1	-2.791908	-2.153214	-1.334573
24	6	-5.179939	-0.278985	0.196450
25	1	-4.785775	1.344449	1.558710
26	1	-5.252264	-1.924739	-1.196275
27	1	-6.259251	-0.174176	0.255229
28	8	1.179999	2.102996	-0.289861
29	7	-0.358790	-1.921889	-0.004714
30	1	-1.077917	-2.641932	0.095891

Energy = -821.4979415
E+ZPVE = -821.268717

11: Azetinone 33

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.314133	0.818768	0.012715
2	6	0.186851	2.118072	-0.089713
3	6	0.062273	0.623381	-0.075044
4	6	-2.556642	0.081074	0.022417
5	6	-2.614079	-1.297014	-0.271479
6	6	-3.749297	0.775754	0.320619
7	6	-3.842607	-1.949759	-0.279162
8	1	-1.688121	-1.822963	-0.471338
9	6	-4.969475	0.111450	0.314881
10	1	-3.705815	1.828107	0.581318
11	6	-5.018259	-1.252176	0.009980
12	1	-3.883346	-3.010163	-0.507960
13	1	-5.881048	0.651110	0.551716
14	1	-5.972450	-1.771042	0.004529
15	7	-1.248618	2.240743	0.153168
16	1	-1.799523	2.843892	-0.456469
17	8	0.992487	2.990604	-0.272254
18	8	0.358984	-1.689090	-0.097775
19	6	0.900558	-0.576849	-0.059408
20	6	2.396509	-0.497754	0.002303
21	6	3.130321	0.696767	-0.058842
22	6	3.085685	-1.717458	0.123402
23	6	4.524143	0.664352	0.003083
24	1	2.630878	1.652215	-0.165159
25	6	4.473769	-1.743966	0.189481
26	1	2.503453	-2.631062	0.163840
27	6	5.198536	-0.549834	0.129597
28	1	5.082571	1.594407	-0.048513
29	1	4.993418	-2.692747	0.286921
30	1	6.283633	-0.567912	0.180184

Energy = -821.5097326
E+ZPVE = -821.280092

12: TS6 connecting 13a and 33

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.327493	0.859501	-0.175433

2	6	-0.492758	1.802748	-0.378951
3	6	-0.051468	0.475682	-0.195249
4	6	2.595750	0.156274	-0.020229
5	6	2.681693	-1.245966	0.041624
6	6	3.765781	0.937608	0.068692
7	6	3.928298	-1.849100	0.196688
8	1	1.771574	-1.834105	-0.045718
9	6	5.001804	0.324253	0.224388
10	1	3.678669	2.017150	0.016453
11	6	5.083808	-1.071182	0.289419
12	1	3.997980	-2.931686	0.242526
13	1	5.901711	0.927369	0.295248
14	1	6.051494	-1.550073	0.410401
15	8	-1.270604	2.660325	-0.530931
16	6	-0.874620	-0.727672	-0.134737
17	6	-2.354529	-0.536568	0.023054
18	6	-2.887026	0.299280	1.015186
19	6	-3.231918	-1.257137	-0.801714
20	6	-4.267015	0.402920	1.184550
21	1	-2.220174	0.853414	1.668248
22	6	-4.611256	-1.141801	-0.640129
23	1	-2.825857	-1.892527	-1.583592
24	6	-5.131893	-0.313535	0.355958
25	1	-4.666276	1.044468	1.964318
26	1	-5.279123	-1.694151	-1.294470
27	1	-6.206611	-0.224803	0.483814
28	8	1.306822	2.149204	-0.316949
29	7	-0.333677	-1.895181	-0.224586
30	1	-1.050275	-2.616858	-0.120791

Energy = -821.4944865
E+ZPVE = -821.266448
Imaginary frequency: -228.1 cm^{-1}

13: TS7 connecting 14b and 32

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.537807	1.915445	-0.527552
2	8	1.328835	2.713477	-0.847186
3	7	-1.335481	2.294782	-0.258253
4	1	-2.183288	2.813681	-0.468364
5	6	0.056285	0.632994	-0.223739

6	6	-1.357511	0.987616	-0.141838
7	6	-2.574555	0.178686	0.018099
8	6	-3.734526	0.802019	0.518750
9	6	-2.626856	-1.177030	-0.345641
10	6	-4.922484	0.090619	0.639345
11	1	-3.692568	1.837271	0.843618
12	6	-3.825431	-1.880196	-0.232857
13	1	-1.722342	-1.664515	-0.688885
14	6	-4.971681	-1.252848	0.255614
15	1	-5.806777	0.578093	1.038172
16	1	-3.859472	-2.926086	-0.522104
17	1	-5.899797	-1.809363	0.348508
18	6	0.834292	-0.593278	-0.106966
19	8	0.307766	-1.709159	-0.173122
20	6	2.324777	-0.504346	0.068437
21	6	3.101787	-1.540303	-0.472369
22	6	2.955413	0.511883	0.799142
23	6	4.484445	-1.540839	-0.316031
24	1	2.598282	-2.337094	-1.009157
25	6	4.339895	0.501672	0.969042
26	1	2.368200	1.297632	1.261792
27	6	5.107000	-0.518006	0.405055
28	1	5.078301	-2.339597	-0.750630
29	1	4.817368	1.288031	1.545929
30	1	6.185709	-0.520605	0.532417

Energy = -821.4924535
E+ZPVE = -821.265164
Imaginary frequency: - 319.6cm^{-1}

14: Benzoyl(phenyl)acetylene 34

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.008811	0.837505	-0.000627
2	6	-1.156632	0.487728	-0.000890
3	6	-2.527943	0.100946	-0.000474
4	6	-3.538876	1.082843	-0.000613
5	6	-2.891510	-1.260174	0.000161
6	6	-4.878600	0.707024	-0.000018
7	1	-3.257102	2.130422	-0.001164
8	6	-4.234064	-1.625915	0.000756
9	1	-2.113951	-2.016904	0.000189

10	6	-5.229295	-0.645401	0.000695
11	1	-5.651305	1.469692	-0.000097
12	1	-4.505805	-2.677115	0.001264
13	1	-6.275914	-0.934809	0.001189
14	6	1.370698	1.339234	-0.000035
15	8	1.582009	2.548212	0.000560
16	6	2.481687	0.340331	-0.000045
17	6	3.801553	0.816452	0.000546
18	6	2.243068	-1.040588	-0.000592
19	6	4.866455	-0.078265	0.000607
20	1	3.961195	1.889299	0.000921
21	6	3.311746	-1.935359	-0.000543
22	1	1.220978	-1.405521	-0.001073
23	6	4.622928	-1.455601	0.000085
24	1	5.887037	0.292804	0.001052
25	1	3.123203	-3.004750	-0.000979
26	1	5.455434	-2.153364	0.000144

Energy = -652.8005046
E+ZPVE = -652.599115

15: Isocyanic acid 35

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.477185	-1.071224	0.000000
2	1	1.464563	-1.273247	0.000000
3	6	0.000000	0.049803	0.000000
4	8	-0.600607	1.059124	0.000000

Energy = -168.681499
E+ZPVE = -168.660183

16: TS8 connecting 33 and 34+35

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.186514	0.242690	-0.238278
2	6	0.181342	2.089801	-0.487929
3	6	0.024614	0.466744	-0.560368

4	7	-0.727598	2.494812	0.380931
5	1	-0.770089	3.521221	0.364221
6	8	1.005759	2.615324	-1.217879
7	6	-2.503968	-0.134446	0.051998
8	6	-2.971105	-0.150545	1.387996
9	6	-3.361019	-0.539614	-0.998886
10	6	-4.263059	-0.574907	1.658793
11	1	-2.312356	0.196927	2.175538
12	6	-4.649980	-0.969517	-0.709496
13	1	-2.992268	-0.519253	-2.018589
14	6	-5.100396	-0.987038	0.614040
15	1	-4.626791	-0.583722	2.681234
16	1	-5.306905	-1.287385	-1.512630
17	1	-6.110803	-1.318548	0.833994
18	6	1.133617	-0.440750	-1.043035
19	8	0.985843	-1.075133	-2.071121
20	6	2.369000	-0.488754	-0.219480
21	6	2.481240	0.203710	0.995197
22	6	3.441102	-1.270765	-0.679319
23	6	3.655193	0.112524	1.740707
24	1	1.656409	0.810727	1.354555
25	6	4.610683	-1.356245	0.066928
26	1	3.331596	-1.796964	-1.621422
27	6	4.718630	-0.664532	1.277980
28	1	3.741465	0.651005	2.679331
29	1	5.440148	-1.958447	-0.291268
30	1	5.633687	-0.730917	1.859447

Energy = -821.4216332
E+ZPVE = -821.196527
Imaginary frequency: - 254.0 cm^{-1}

17: Toluoyl(phenylimidoyl)ketene 21

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.811580	-1.881684	0.183344
2	8	1.083469	-2.977016	0.453977
3	7	-1.727269	-1.309894	-0.260253
4	6	0.516122	-0.608814	-0.119520
5	6	-0.939938	-0.296544	-0.136036
6	6	-1.340839	1.133919	0.032775
7	6	-0.778624	1.913966	1.052698

8	6	-2.291827	1.708745	-0.821825
9	6	-1.174516	3.238543	1.228419
10	1	-0.034698	1.477969	1.713083
11	6	-2.673402	3.037636	-0.655278
12	1	-2.723352	1.113891	-1.619325
13	6	-2.120625	3.804392	0.372581
14	1	-0.739003	3.830100	2.028261
15	1	-3.403272	3.475615	-1.329497
16	1	-2.422605	4.839439	0.502724
17	6	1.567321	0.296780	-0.673262
18	8	1.245976	1.215992	-1.413368
19	6	-3.123434	-1.262169	-0.091885
20	6	-3.924640	-1.879975	-1.066553
21	6	-3.735896	-0.741007	1.061089
22	6	-5.307908	-1.932508	-0.913180
23	1	-3.442630	-2.309928	-1.938925
24	6	-5.118384	-0.818712	1.217202
25	1	-3.122281	-0.287600	1.832426
26	6	-5.912908	-1.404631	0.229889
27	1	-5.914396	-2.400868	-1.683232
28	1	-5.576634	-0.416865	2.116587
29	1	-6.990069	-1.459309	0.354831
30	6	3.002381	0.045218	-0.334928
31	6	3.977419	0.480304	-1.246729
32	6	3.418236	-0.553274	0.862033
33	6	5.326523	0.287079	-0.981126
34	1	3.650768	0.968348	-2.158776
35	6	4.775101	-0.733509	1.126735
36	1	2.689552	-0.845879	1.611370
37	6	5.750690	-0.328041	0.208416
38	1	6.068277	0.620225	-1.702558
39	1	5.080256	-1.187098	2.065851
40	6	7.217811	-0.555567	0.477806
41	1	7.581423	-1.441526	-0.057271
42	1	7.821800	0.293410	0.143011
43	1	7.410727	-0.713356	1.542338

Energy = -1091.545307
E+ZPVE = -1091.880874

18: Toluoyl(phenylimidoyl)ketene 22

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z

1	6	-1.021979	1.650874	-0.326653
2	8	-1.410591	2.696956	-0.663196
3	7	1.163320	-1.100319	-0.186843
4	6	-0.587103	0.458205	0.081566
5	6	0.866150	0.134619	-0.026724
6	6	1.817038	1.295019	0.004416
7	6	1.696428	2.291485	0.985982
8	6	2.823219	1.416334	-0.966992
9	6	2.571623	3.377167	1.004308
10	1	0.927408	2.203295	1.747660
11	6	3.685135	2.510235	-0.956190
12	1	2.923615	0.652345	-1.730274
13	6	3.564781	3.491166	0.031080
14	1	2.475484	4.133518	1.777532
15	1	4.452393	2.597311	-1.719637
16	1	4.241159	4.340720	0.039738
17	6	-1.559849	-0.485019	0.749407
18	8	-1.170591	-1.233123	1.628243
19	6	2.468592	-1.615685	-0.150254
20	6	2.875113	-2.470913	-1.188501
21	6	3.333888	-1.405841	0.937560
22	6	4.138042	-3.057456	-1.163522
23	1	2.187638	-2.659743	-2.007050
24	6	4.585688	-2.017296	0.965132
25	1	3.008332	-0.779482	1.761364
26	6	5.000497	-2.835916	-0.087094
27	1	4.443499	-3.704044	-1.981446
28	1	5.240610	-1.851696	1.816073
29	1	5.978340	-3.307146	-0.062187
30	6	-2.998773	-0.441031	0.346957
31	6	-3.956940	-0.865537	1.282270
32	6	-3.427928	-0.047107	-0.927187
33	6	-5.306750	-0.859717	0.959197
34	1	-3.616204	-1.195634	2.257825
35	6	-4.784900	-0.054981	-1.247762
36	1	-2.703697	0.228143	-1.687078
37	6	-5.746694	-0.449936	-0.310980
38	1	-6.036573	-1.180852	1.698144
39	1	-5.099413	0.240896	-2.244844
40	6	-7.217913	-0.429595	-0.645419
41	1	-7.383688	-0.348442	-1.722860
42	1	-7.719951	-1.335161	-0.290108
43	1	-7.716939	0.423091	-0.168909

Energy = -1091.877171
E+ZPVE = -1091.541747

19: TS9 connecting 21 and 22

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.433882	-1.219133	0.236840
2	8	1.471761	-2.382660	0.500343
3	7	-1.511798	-1.258718	-0.053596
4	6	0.544007	-0.139505	0.006418
5	6	-0.921342	-0.112877	-0.032169
6	6	-1.583284	1.233625	-0.083497
7	6	-1.229425	2.244317	0.821266
8	6	-2.558232	1.503136	-1.055748
9	6	-1.850663	3.491355	0.768632
10	1	-0.471974	2.050059	1.574236
11	6	-3.166693	2.754631	-1.117419
12	1	-2.836496	0.727901	-1.761634
13	6	-2.818290	3.750545	-0.202664
14	1	-1.573565	4.261772	1.482106
15	1	-3.914732	2.952095	-1.879533
16	1	-3.296488	4.724603	-0.249149
17	6	1.526879	0.846988	-0.226743
18	8	1.694917	2.000922	-0.486738
19	6	2.878824	-0.274471	0.010680
20	6	3.605767	-0.566202	-1.181604
21	6	3.644660	-0.034336	1.189242
22	6	4.987156	-0.607892	-1.192005
23	1	3.051422	-0.754479	-2.097550
24	6	5.026529	-0.077042	1.172707
25	1	3.121851	0.189404	2.115733
26	6	5.723310	-0.367149	-0.015724
27	1	5.517327	-0.827414	-2.114747
28	1	5.587398	0.114246	2.083402
29	6	7.225700	-0.446977	-0.025810
30	1	7.666346	0.140145	0.784009
31	1	7.553046	-1.486335	0.106163
32	1	7.639094	-0.096890	-0.975963
33	6	-2.899798	-1.439762	0.047615
34	6	-3.520384	-2.305969	-0.869705
35	6	-3.669142	-0.898237	1.093265
36	6	-4.882047	-2.580762	-0.773071
37	1	-2.914535	-2.751081	-1.652722

38	6	-5.026016	-1.198280	1.196475
39	1	-3.192536	-0.255572	1.826010
40	6	-5.643606	-2.030633	0.260963
41	1	-5.347569	-3.240808	-1.499872
42	1	-5.604145	-0.776609	2.014220
43	1	-6.702053	-2.258326	0.343953

Energy = -1091.8298281
E+ZPVE = -1091.496373
Imaginary frequency: -382.8 cm^{-1}

20: Toluoylketenimine 23

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-1.310152	1.267510	1.589070
2	7	2.082374	-0.716122	-0.973014
3	6	-0.158857	-0.096280	0.055499
4	6	1.049007	-0.400824	-0.432479
5	6	-1.083130	-1.283416	0.198502
6	8	-0.612692	-2.395713	0.417402
7	6	3.234119	-1.380831	-0.493231
8	6	4.462421	-1.106695	-1.100105
9	6	3.133040	-2.328892	0.534819
10	6	5.607440	-1.761998	-0.650079
11	1	4.506646	-0.381746	-1.905760
12	6	4.283222	-2.986586	0.962880
13	1	2.156957	-2.553111	0.954414
14	6	5.520845	-2.701298	0.379252
15	1	6.566223	-1.544405	-1.110534
16	1	4.211851	-3.726498	1.754279
17	1	6.413348	-3.217054	0.720025
18	6	-2.550661	-1.096513	0.019651
19	6	-3.404995	-2.105731	0.488684
20	6	-3.105615	-0.004584	-0.660741
21	6	-4.778277	-2.011358	0.299431
22	1	-2.967964	-2.958601	0.996541
23	6	-4.480285	0.075871	-0.860903
24	1	-2.462502	0.775183	-1.054325
25	6	-5.341356	-0.918152	-0.376195
26	1	-5.427496	-2.797793	0.675881
27	1	-4.893393	0.923798	-1.400918
28	6	-6.835364	-0.803657	-0.554695

29	1	-7.089792	-0.244146	-1.459591
30	1	-7.308275	-1.788162	-0.617113
31	1	-7.291655	-0.276720	0.292723
32	6	-0.445855	1.204362	0.722459
33	6	0.345037	2.424061	0.351004
34	6	0.449638	3.444695	1.309037
35	6	0.928207	2.606783	-0.911134
36	6	1.150295	4.611585	1.021409
37	1	-0.027734	3.297630	2.271853
38	6	1.619578	3.783125	-1.201986
39	1	0.822685	1.845881	-1.676963
40	6	1.738181	4.782520	-0.235522
41	1	1.236876	5.390722	1.772945
42	1	2.059096	3.920994	-2.185372
43	1	2.281456	5.695384	-0.462105

Energy = -1091.8819657
E+ZPVE = -1091.546234

21: TS10 connecting 22 and 23

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.569376	-2.618027	-0.089047
2	8	-0.739322	-3.798176	-0.216912
3	7	-0.391908	0.701850	0.358278
4	6	0.462779	-1.648572	0.029368
5	6	-0.378186	-0.518464	0.132291
6	6	-1.870045	-1.529872	-0.057037
7	6	-2.681085	-1.546062	1.120589
8	6	-2.535790	-1.316385	-1.302234
9	6	-4.051756	-1.370137	1.051858
10	1	-2.199480	-1.713097	2.080432
11	6	-3.912401	-1.148529	-1.366111
12	1	-1.944186	-1.319188	-2.214194
13	6	-4.671540	-1.178017	-0.192239
14	1	-4.651059	-1.391479	1.956929
15	1	-4.400178	-0.998402	-2.324392
16	1	-5.748826	-1.050855	-0.242995
17	6	1.910080	-1.891663	0.158565
18	8	2.291509	-3.039118	0.384225
19	6	2.909549	-0.781360	0.029833
20	6	4.185522	-0.997502	0.574255

21	6	2.667346	0.417621	-0.651853
22	6	5.177730	-0.032006	0.462035
23	1	4.375005	-1.940810	1.075176
24	6	3.671907	1.376451	-0.774164
25	1	1.701130	0.604753	-1.104445
26	6	4.938447	1.175494	-0.212815
27	1	6.157332	-0.215293	0.896914
28	1	3.468879	2.295811	-1.317616
29	6	-1.315076	1.726083	0.255534
30	6	-1.632408	2.483294	1.397950
31	6	-1.903122	2.056422	-0.980013
32	6	-2.549328	3.525405	1.308424
33	1	-1.155212	2.233707	2.339649
34	6	-2.819102	3.103201	-1.055444
35	1	-1.624653	1.497151	-1.866455
36	6	-3.148936	3.838322	0.084727
37	1	-2.795908	4.099061	2.196918
38	1	-3.270783	3.350443	-2.011741
39	1	-3.858804	4.657046	0.019156
40	6	6.012443	2.231428	-0.313084
41	1	6.065355	2.828874	0.605743
42	1	7.000167	1.784418	-0.463364
43	1	5.821169	2.920515	-1.140490

Energy = -1091.8198465
E+ZPVE = -1091.486692
Imaginary frequency: - 446.4 cm^{-1}

22: Toluoylketenimine 23a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.379540	0.052206	-0.401872
2	6	-0.509908	-1.197127	0.037422
3	6	0.621398	-2.187393	-0.070437
4	8	-1.755779	-2.436425	1.614170
5	6	-1.797622	-1.659872	0.674707
6	8	0.367072	-3.371607	-0.218674
7	7	-0.290969	1.152518	-0.913539
8	6	-3.105534	-1.127782	0.173630
9	6	-3.285785	-0.646340	-1.130867
10	6	-4.202817	-1.168917	1.048667
11	6	-4.539611	-0.197914	-1.546160

12	1	-2.456620	-0.644982	-1.829717
13	6	-5.449418	-0.710110	0.636214
14	1	-4.051083	-1.566961	2.046266
15	6	-5.619635	-0.221976	-0.662944
16	1	-4.673538	0.164054	-2.561111
17	1	-6.290755	-0.735444	1.322459
18	1	-6.593983	0.132384	-0.986956
19	6	0.019044	2.412662	-0.360213
20	6	0.343018	3.445434	-1.246408
21	6	-0.009582	2.650314	1.022322
22	6	0.657232	4.708936	-0.749683
23	1	0.348817	3.238843	-2.311189
24	6	0.298722	3.918161	1.507886
25	1	-0.287005	1.848591	1.700185
26	6	0.635724	4.948476	0.625603
27	1	0.914106	5.508100	-1.438074
28	1	0.273039	4.103434	2.577434
29	1	0.874624	5.935329	1.009790
30	6	2.037773	-1.703828	-0.049168
31	6	3.013968	-2.519314	-0.644824
32	6	2.443899	-0.518486	0.575990
33	6	4.349584	-2.140547	-0.640441
34	1	2.696899	-3.449197	-1.104714
35	6	3.788404	-0.149533	0.587015
36	1	1.719628	0.105877	1.088320
37	6	4.761738	-0.945924	-0.027006
38	1	5.090379	-2.779736	-1.114410
39	1	4.086352	0.767570	1.088217
40	6	6.213369	-0.533483	-0.042120
41	1	6.870624	-1.378632	0.186490
42	1	6.505372	-0.157286	-1.030333
43	1	6.413051	0.258831	0.684267

Energy = -1091.879022
E+ZPVE = -1091.543325

23: TS11 connecting 23 and 23a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.053505	-2.704261	1.647075
2	7	-0.922566	1.289421	-0.741875
3	6	0.138827	-0.620256	0.558479

4	6	-0.462322	0.368409	-0.088134
5	6	1.431252	-0.281050	1.314391
6	8	1.391020	-0.148375	2.522549
7	6	-1.746704	2.362918	-0.330624
8	6	-2.243830	3.209547	-1.326249
9	6	-2.055524	2.596680	1.017744
10	6	-3.057163	4.286037	-0.975904
11	1	-1.985356	3.009399	-2.360603
12	6	-2.865186	3.676263	1.357296
13	1	-1.655748	1.937594	1.782835
14	6	-3.369120	4.521660	0.363922
15	1	-3.444723	4.941575	-1.749669
16	1	-3.103721	3.859649	2.400563
17	1	-4.000367	5.362041	0.635961
18	6	2.690652	-0.123239	0.536943
19	6	3.852088	0.268823	1.224916
20	6	2.769423	-0.362448	-0.841257
21	6	5.052288	0.424045	0.546668
22	1	3.783901	0.441932	2.293591
23	6	3.979172	-0.206755	-1.514992
24	1	1.886909	-0.682122	-1.384562
25	6	5.137586	0.191836	-0.837010
26	1	5.942671	0.726791	1.091996
27	1	4.026010	-0.401805	-2.583029
28	6	6.442214	0.386118	-1.569433
29	1	6.431441	-0.104192	-2.546477
30	1	6.643233	1.451567	-1.736608
31	1	7.284645	-0.013470	-0.996055
32	6	-0.458730	-1.961711	0.820664
33	6	-1.688009	-2.397534	0.075216
34	6	-2.532120	-3.315469	0.719796
35	6	-1.995951	-1.985143	-1.228753
36	6	-3.679912	-3.783029	0.087412
37	1	-2.265880	-3.648008	1.717242
38	6	-3.139738	-2.466809	-1.866507
39	1	-1.336275	-1.310152	-1.762153
40	6	-3.987123	-3.358324	-1.208236
41	1	-4.333535	-4.482243	0.600552
42	1	-3.363952	-2.149698	-2.880643
43	1	-4.879919	-3.727145	-1.704905

Energy = -1091.8767341
E+ZPVE = -1091.541202
Imaginary frequency: - 15.3 cm^{-1}

24: Benzoyl(tolylimidoyl)ketene 24a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.399790	1.550997	-0.412149
2	8	1.668392	2.628684	-0.764970
3	7	-0.490647	-1.403734	-0.210151
4	6	1.101015	0.322657	0.013719
5	6	-0.316561	-0.144792	-0.054858
6	6	-1.374759	0.915168	0.002207
7	6	-1.322925	1.932885	0.966264
8	6	-2.426783	0.928813	-0.927552
9	6	-2.301404	2.924729	1.006476
10	1	-0.525720	1.934142	1.703791
11	6	-3.389172	1.931795	-0.891283
12	1	-2.486037	0.149290	-1.679394
13	6	-3.346845	2.947241	0.075956
14	1	-2.250795	3.693469	1.773134
15	1	-4.190489	1.927354	-1.625741
16	6	2.180993	-0.513428	0.653255
17	8	1.895885	-1.310371	1.528758
18	6	-1.734511	-2.050199	-0.138556
19	6	-2.075938	-2.948816	-1.163576
20	6	-2.589763	-1.925447	0.970198
21	6	-3.269477	-3.664052	-1.104516
22	1	-1.393294	-3.069675	-1.998851
23	6	-3.769619	-2.664093	1.031626
24	1	-2.311199	-1.263491	1.783305
25	6	-4.123026	-3.527703	-0.007031
26	1	-3.526061	-4.343740	-1.912343
27	1	-4.416522	-2.562975	1.898691
28	1	-5.045192	-4.098510	0.044608
29	6	3.602683	-0.307045	0.228012
30	6	4.611345	-0.606071	1.157626
31	6	3.959035	0.121280	-1.058744
32	6	5.950127	-0.445208	0.816936
33	1	4.319343	-0.960307	2.140389
34	6	5.303091	0.270517	-1.401868
35	1	3.192361	0.302421	-1.805025
36	6	6.298314	-0.004208	-0.463689
37	1	6.724687	-0.665200	1.545504
38	1	5.571331	0.592022	-2.403600
39	1	7.344066	0.116998	-0.730739
40	6	-4.385050	4.042642	0.093314

41	1	-4.436560	4.530008	1.070773
42	1	-4.153178	4.817454	-0.647974
43	1	-5.379785	3.654405	-0.146394

Energy = -1091.8769239
E+ZPVE = -1091.541477

25: TS12 connecting 23a and 24a

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.181697	-2.471236	-0.047772
2	8	0.112646	-3.666283	-0.143973
3	7	0.116376	0.863102	0.335852
4	6	1.139567	-1.421452	0.027875
5	6	0.214942	-0.357379	0.127565
6	6	-1.186189	-1.496044	-0.012774
7	6	-1.979099	-1.544812	1.178402
8	6	-1.896653	-1.363952	-1.245150
9	6	-3.355878	-1.467627	1.131926
10	1	-1.473538	-1.657506	2.133888
11	6	-3.280421	-1.297966	-1.281717
12	1	-1.329200	-1.348901	-2.172306
13	6	-4.035330	-1.347873	-0.098859
14	1	-3.931996	-1.512804	2.052373
15	1	-3.792834	-1.210241	-2.235869
16	6	2.602239	-1.543106	0.131150
17	8	3.086101	-2.649074	0.366031
18	6	3.505425	-0.353749	-0.035161
19	6	4.792778	-0.446416	0.516572
20	6	3.154104	0.795808	-0.755201
21	6	5.700452	0.598354	0.374015
22	1	5.057114	-1.354277	1.048021
23	6	4.070004	1.836469	-0.911227
24	1	2.172692	0.878335	-1.206116
25	6	5.340343	1.743877	-0.341478
26	1	6.690234	0.520498	0.814593
27	1	3.790896	2.719312	-1.479041
28	1	6.049296	2.558799	-0.457802
29	6	-5.536482	-1.252025	-0.132857
30	1	-5.932712	-1.471664	-1.127333
31	1	-5.996047	-1.940091	0.583476
32	1	-5.863276	-0.240066	0.138558

33	6	-0.883500	1.812992	0.236168
34	6	-1.215600	2.581924	1.366545
35	6	-1.535201	2.063069	-0.986194
36	6	-2.205468	3.555403	1.279696
37	1	-0.690155	2.396125	2.297257
38	6	-2.524161	3.041643	-1.059485
39	1	-1.247524	1.497485	-1.865622
40	6	-2.866151	3.788260	0.069634
41	1	-2.460923	4.138706	2.159412
42	1	-3.022855	3.227706	-2.006326
43	1	-3.632289	4.554760	0.005362

Energy = -1091.8218895
E+ZPVE = -1091.488665
Imaginary frequency: -423.6 cm^{-1}

26: Benzoyl(tolylimidoyl)ketene 24

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.358528	-2.067309	0.305007
2	8	1.674085	-3.135224	0.631161
3	7	-1.185982	-1.646376	-0.228320
4	6	1.011893	-0.823486	-0.060016
5	6	-0.458232	-0.586812	-0.123916
6	6	-0.935779	0.823901	-0.022820
7	6	-0.425760	1.685537	0.957092
8	6	-1.913885	1.310646	-0.901097
9	6	-0.895907	2.991437	1.067238
10	1	0.334892	1.327712	1.645086
11	6	-2.365632	2.621897	-0.796409
12	1	-2.316452	0.659935	-1.669701
13	6	-1.868286	3.486154	0.188927
14	1	-0.496392	3.639117	1.843410
15	1	-3.118859	2.982112	-1.492349
16	6	2.032992	0.106343	-0.625142
17	8	1.692483	0.986339	-1.402806
18	6	-2.586161	-1.669433	-0.091492
19	6	-3.333181	-2.352709	-1.065422
20	6	-3.249179	-1.153094	1.035448
21	6	-4.714773	-2.474641	-0.937689
22	1	-2.811338	-2.777919	-1.916967
23	6	-4.628585	-1.300083	1.166536

24	1	-2.676024	-0.648347	1.806079
25	6	-5.370473	-1.951521	0.179271
26	1	-5.279653	-2.993404	-1.707104
27	1	-5.126033	-0.901079	2.046168
28	1	-6.445660	-2.060200	0.284434
29	6	3.473371	-0.071990	-0.250599
30	6	4.442796	0.350513	-1.173615
31	6	3.883394	-0.592790	0.985245
32	6	5.796199	0.221182	-0.879598
33	1	4.109459	0.774043	-2.114917
34	6	5.241341	-0.711010	1.282638
35	1	3.147648	-0.873898	1.731977
36	6	6.198056	-0.312168	0.348974
37	1	6.540351	0.537247	-1.604494
38	1	5.550022	-1.106184	2.245623
39	1	7.254868	-0.409244	0.579643
40	6	-2.343480	4.916081	0.278613
41	1	-2.245311	5.308391	1.294948
42	1	-1.756598	5.567752	-0.380723
43	1	-3.391125	5.009818	-0.022747

Energy = -1091.8804837
E+ZPVE = -1091.544972

27: TS13 connecting 24a and 24

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.489448	-1.295873	1.182546
2	8	-1.736132	-1.975074	2.094218
3	7	0.913833	-1.608841	-0.122986
4	6	-1.138623	-0.484894	0.180683
5	6	0.361637	-0.454137	-0.034661
6	6	1.083151	0.856784	0.102944
7	6	0.987110	1.906522	-0.818333
8	6	1.908278	1.022917	1.228584
9	6	1.706886	3.084699	-0.615387
10	1	0.339651	1.803868	-1.678646
11	6	2.608618	2.207604	1.427548
12	1	1.999726	0.217182	1.950718
13	6	2.525017	3.260571	0.505377
14	1	1.623436	3.885976	-1.345244
15	1	3.233236	2.315465	2.310847

16	6	-2.131094	0.263121	-0.615561
17	8	-1.779526	1.075669	-1.464707
18	6	2.297362	-1.816477	-0.296283
19	6	2.910654	-2.789060	0.509783
20	6	3.048449	-1.190689	-1.304872
21	6	4.260492	-3.089880	0.346092
22	1	2.312702	-3.294102	1.261924
23	6	4.391142	-1.519585	-1.480532
24	1	2.573045	-0.463018	-1.952961
25	6	5.007130	-2.459097	-0.651703
26	1	4.726006	-3.831997	0.988343
27	1	4.959294	-1.034903	-2.269399
28	1	6.055180	-2.706770	-0.790157
29	6	-3.594356	0.032367	-0.365816
30	6	-4.450508	1.139594	-0.465352
31	6	-4.137511	-1.233400	-0.105017
32	6	-5.818760	0.990707	-0.260570
33	1	-4.022799	2.107930	-0.701993
34	6	-5.512230	-1.382302	0.084846
35	1	-3.502966	-2.113887	-0.092484
36	6	-6.352275	-0.271079	0.017679
37	1	-6.471975	1.855952	-0.322829
38	1	-5.925371	-2.368422	0.273696
39	1	-7.421083	-0.388041	0.170614
40	6	3.309738	4.533595	0.713552
41	1	3.220830	4.894195	1.743727
42	1	4.377814	4.376906	0.519132
43	1	2.966543	5.328750	0.046238

Energy = -1091.8738064
E+ZPVE = -1091.538241
Imaginary frequency: -21.7 cm^{-1}

28: Toluoyl(phenylimidoyl)ketene 25

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.032151	-0.740234	1.420426
2	8	0.204827	-1.410631	2.357983
3	7	-2.624006	-0.201012	-0.007914
4	6	-0.184503	0.032687	0.361898
5	6	-1.593620	0.546742	0.122601
6	6	-1.765685	2.024074	0.066633

7	6	-0.761597	2.904061	0.495156
8	6	-2.974721	2.557685	-0.413043
9	6	-0.959256	4.283643	0.449159
10	1	0.174942	2.510097	0.874721
11	6	-3.169536	3.933463	-0.458594
12	1	-3.746268	1.872613	-0.745132
13	6	-2.162364	4.802584	-0.028004
14	1	-0.172271	4.951352	0.786818
15	1	-4.107019	4.331946	-0.835282
16	1	-2.315471	5.877145	-0.067272
17	6	0.841655	0.217710	-0.703910
18	8	0.468400	0.490407	-1.838750
19	6	-2.576290	-1.603431	-0.085737
20	6	-3.375183	-2.356503	0.788797
21	6	-1.840097	-2.261622	-1.086882
22	6	-3.403100	-3.746048	0.690674
23	1	-3.962745	-1.837955	1.539855
24	6	-1.893526	-3.650345	-1.189072
25	1	-1.253597	-1.672466	-1.784748
26	6	-2.665433	-4.399791	-0.298636
27	1	-4.013746	-4.318979	1.382622
28	1	-1.327826	-4.148941	-1.971200
29	1	-2.700264	-5.481808	-0.381633
30	6	2.291512	0.045331	-0.387241
31	6	3.156633	-0.278256	-1.445442
32	6	2.832543	0.231620	0.891700
33	6	4.516377	-0.441708	-1.219123
34	1	2.736087	-0.395992	-2.438261
35	6	4.200801	0.074457	1.109214
36	1	2.200047	0.535906	1.719406
37	6	5.063938	-0.272635	0.063652
38	1	5.170249	-0.701424	-2.047790
39	1	4.604413	0.233952	2.105324
40	6	6.540620	-0.470160	0.302299
41	1	6.799769	-1.535895	0.296537
42	1	7.138359	0.009994	-0.479090
43	1	6.849654	-0.060615	1.267515

Energy = -1091. 8831845
E+ZPVE = -1091.547423

29: TS14 connecting 21 and 25

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	-0.488361	-1.123888	-1.297573
2	8	-0.570603	-1.931356	-2.135534
3	7	2.073966	-0.376918	-0.066694
4	6	-0.327872	-0.190350	-0.368259
5	6	1.088879	0.376021	-0.188459
6	6	1.204970	1.869728	-0.188451
7	6	0.207289	2.692972	-0.727129
8	6	2.373262	2.457811	0.320854
9	6	0.373760	4.076799	-0.757051
10	1	-0.695066	2.250305	-1.134908
11	6	2.534515	3.839280	0.297925
12	1	3.146609	1.819540	0.735265
13	6	1.535143	4.653476	-0.242576
14	1	-0.404359	4.703598	-1.182225
15	1	3.439259	4.283320	0.702258
16	1	1.662339	5.731873	-0.261451
17	6	-1.357286	0.129376	0.658888
18	8	-1.011513	0.681712	1.695456
19	6	3.155393	-1.168203	0.070220
20	6	3.716053	-1.826490	-1.049076
21	6	3.750315	-1.358774	1.339921
22	6	4.841927	-2.628285	-0.893411
23	1	3.263101	-1.687229	-2.025149
24	6	4.859047	-2.188128	1.470825
25	1	3.318808	-0.863811	2.203591
26	6	5.422190	-2.824138	0.361815
27	1	5.262991	-3.115532	-1.768725
28	1	5.293479	-2.329503	2.456825
29	1	6.293895	-3.460443	0.473857
30	6	-2.785380	-0.248997	0.426234
31	6	-3.597834	-0.452503	1.553247
32	6	-3.358706	-0.364132	-0.846669
33	6	-4.934886	-0.796323	1.405410
34	1	-3.155393	-0.335447	2.536640
35	6	-4.705136	-0.698619	-0.986984
36	1	-2.773297	-0.155901	-1.736661
37	6	-5.512941	-0.930401	0.132185
38	1	-5.546552	-0.961398	2.288772
39	1	-5.136096	-0.770864	-1.981825
40	6	-6.961713	-1.324465	-0.018215
41	1	-7.097502	-2.396916	0.167492
42	1	-7.596413	-0.791502	0.696815
43	1	-7.332406	-1.115122	-1.025115

Energy = -1091.8555789
E+ZPVE = -1091.521397
Imaginary frequency: -178.0 cm^{-1}

30: 4aH-quinolone 26

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.508467	-1.483822	0.583046
2	8	-1.297404	-2.573987	1.096199
3	7	-2.214727	1.150842	-0.405898
4	6	-0.571909	-0.357884	0.608228
5	6	-0.954740	0.878630	0.124755
6	6	-0.074303	2.079074	0.139630
7	6	0.807595	2.365274	1.195319
8	6	-0.154342	2.982329	-0.935483
9	6	1.606437	3.507706	1.157392
10	1	0.845413	1.718708	2.062867
11	6	0.657368	4.111840	-0.977266
12	1	-0.862547	2.785296	-1.732367
13	6	1.543124	4.378264	0.069493
14	1	2.273060	3.720182	1.987864
15	1	0.593141	4.790286	-1.823031
16	1	2.169898	5.264922	0.042117
17	6	0.737567	-0.661997	1.309751
18	8	0.779017	-0.675907	2.531883
19	6	-3.095911	0.195119	-0.503679
20	6	-4.449287	0.502172	-0.892545
21	6	-2.755723	-1.254014	-0.276048
22	6	-5.427165	-0.439687	-0.791978
23	1	-4.662388	1.524375	-1.186897
24	6	-3.905295	-2.168890	-0.014156
25	1	-2.358990	-1.559923	-1.271337
26	6	-5.163330	-1.778170	-0.300603
27	1	-6.450586	-0.174768	-1.043135
28	1	-3.665574	-3.151653	0.377187
29	1	-6.000579	-2.452085	-0.147093
30	6	1.932524	-0.997628	0.484248
31	6	3.123078	-1.346005	1.144370
32	6	1.914756	-0.989579	-0.916021
33	6	4.259093	-1.675177	0.419352
34	1	3.124643	-1.355410	2.229080
35	6	3.059966	-1.319240	-1.638426

36	1	1.003487	-0.724807	-1.441896
37	6	4.249173	-1.665933	-0.986280
38	1	5.171872	-1.947294	0.943685
39	1	3.030608	-1.308900	-2.724744
40	6	5.495525	-2.010711	-1.763877
41	1	6.255126	-1.226724	-1.658211
42	1	5.944394	-2.942075	-1.402628
43	1	5.284801	-2.126903	-2.830168

Energy = -1091.8727474
E+ZPVE = -1091.536030

31: TS15 connecting 25 and 26

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.461089	-1.550476	-0.238377
2	8	-0.207376	-2.538275	-0.330592
3	7	2.714566	0.373782	-0.044321
4	6	0.332475	-0.192010	0.046750
5	6	1.444651	0.732548	-0.058210
6	6	-0.862928	0.222034	0.873300
7	8	-0.702827	0.958386	1.838444
8	6	3.057601	-0.927539	-0.092858
9	6	4.163704	-1.407213	0.655064
10	6	2.264727	-1.857463	-0.850632
11	6	4.451877	-2.753426	0.666969
12	1	4.746271	-0.693035	1.226612
13	6	2.625540	-3.248657	-0.835940
14	1	1.871603	-1.479746	-1.797950
15	6	3.675347	-3.687703	-0.075002
16	1	5.285855	-3.115202	1.261935
17	1	2.033243	-3.945161	-1.420585
18	1	3.932998	-4.741343	-0.044150
19	6	-2.232644	-0.246169	0.498315
20	6	-2.564571	-0.686766	-0.789277
21	6	-3.247397	-0.161788	1.464547
22	6	-3.876491	-1.037127	-1.099055
23	1	-1.798613	-0.743155	-1.554935
24	6	-4.550906	-0.527537	1.154002
25	1	-2.988652	0.201600	2.453365
26	6	-4.889125	-0.973851	-0.133418

27	1	-4.119030	-1.366623	-2.106037
28	1	-5.323589	-0.462102	1.916028
29	6	1.194439	2.191564	-0.177293
30	6	0.040187	2.685167	-0.805567
31	6	2.162501	3.102803	0.274953
32	6	-0.144934	4.055746	-0.969928
33	1	-0.705374	1.993172	-1.183029
34	6	1.971834	4.472128	0.117259
35	1	3.054132	2.716539	0.754902
36	6	0.817728	4.953575	-0.505655
37	1	-1.039670	4.422242	-1.464153
38	1	2.722448	5.166504	0.483264
39	1	0.670235	6.022554	-0.629446
40	6	-6.301694	-1.394310	-0.458272
41	1	-7.035163	-0.754985	0.042840
42	1	-6.494462	-1.356673	-1.534085
43	1	-6.490639	-2.423132	-0.127193

Energy = -1091.859442
E+ZPVE = -1091.524255
Imaginary frequency: -396.0 cm^{-1}

32: 3H-quinolone 27

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.842290	-1.525448	-0.916999
2	8	-0.169045	-2.307040	-1.574995
3	7	-2.568638	0.544563	0.146346
4	6	-1.370146	0.877062	-0.191228
5	6	-1.023513	2.319978	-0.214335
6	6	0.280187	2.774972	-0.474775
7	6	-2.028685	3.273903	0.033595
8	6	0.569657	4.139230	-0.487143
9	1	1.086799	2.073172	-0.657384
10	6	-1.738702	4.632610	0.016050
11	1	-3.031487	2.918372	0.238837
12	6	-0.437275	5.072632	-0.245305
13	1	1.584649	4.469977	-0.685872
14	1	-2.527960	5.353733	0.207571
15	1	-0.211557	6.134904	-0.258454
16	6	0.672131	-0.321640	0.660574

17	8	0.224682	-0.243906	1.790364
18	6	-2.961845	-0.797051	0.148562
19	6	-4.235597	-1.099881	0.651644
20	6	-2.173468	-1.843496	-0.381919
21	6	-4.705388	-2.409731	0.634062
22	1	-4.835899	-0.287511	1.046899
23	6	-2.666073	-3.153912	-0.419599
24	6	-3.924828	-3.441798	0.095944
25	1	-5.690727	-2.631013	1.033998
26	1	-2.037134	-3.927148	-0.848859
27	1	-4.301742	-4.459627	0.081030
28	6	2.118286	-0.573918	0.400980
29	6	3.000977	-0.449821	1.489309
30	6	2.634434	-0.938142	-0.851472
31	6	4.361234	-0.663646	1.321085
32	1	2.591744	-0.182537	2.457568
33	6	4.001281	-1.163653	-1.005877
34	1	1.968412	-1.104825	-1.690175
35	6	4.887731	-1.021495	0.068255
36	1	5.030699	-0.556032	2.170787
37	1	4.384467	-1.461532	-1.978055
38	6	6.370728	-1.234448	-0.108602
39	1	6.909084	-0.278871	-0.094540
40	1	6.783805	-1.846694	0.699643
41	1	6.595521	-1.727018	-1.058113
42	6	-0.295301	-0.136253	-0.555280
43	1	0.275492	0.211956	-1.417397

Energy = -1091.9244674
E+ZPVE = -1091.585703

33: TS16 connecting 26 and 27

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.897945	-0.996919	1.325342
2	8	-1.989714	-1.748842	2.268043
3	7	-2.062503	1.318085	-0.419524
4	6	-0.689262	-0.263781	0.817674
5	6	-0.915551	1.015542	0.188627
6	6	0.137680	2.066037	0.130162
7	6	0.988487	2.327306	1.216523
8	6	0.244350	2.862370	-1.022865

9	6	1.935939	3.347982	1.139251
10	1	0.893889	1.753883	2.131136
11	6	1.198537	3.872285	-1.099786
12	1	-0.432145	2.675722	-1.849421
13	6	2.049562	4.116965	-0.018796
14	1	2.580148	3.545398	1.990759
15	1	1.278109	4.471628	-2.002071
16	1	2.791942	4.907630	-0.077613
17	6	0.639175	-0.681752	1.400528
18	8	0.772227	-0.711985	2.616863
19	6	-3.003413	0.358667	-0.511010
20	6	-4.124655	0.553687	-1.366789
21	6	-2.866963	-0.917200	0.165789
22	6	-5.047584	-0.446750	-1.545312
23	1	-4.208788	1.510839	-1.870215
24	6	-3.884677	-1.913398	-0.001372
25	1	-1.521607	-1.111952	-0.265775
26	6	-4.924952	-1.692388	-0.862885
27	1	-5.892921	-0.288134	-2.208276
28	1	-3.804865	-2.824836	0.582160
29	1	-5.684173	-2.454839	-1.008799
30	6	1.737143	-1.113431	0.485524
31	6	2.949661	-1.522505	1.066821
32	6	1.619517	-1.136291	-0.910640
33	6	4.008168	-1.938685	0.272465
34	1	3.030434	-1.506983	2.148368
35	6	2.687828	-1.553070	-1.702505
36	1	0.694438	-0.829011	-1.386098
37	6	3.898298	-1.959098	-1.128388
38	1	4.937757	-2.255227	0.738991
39	1	2.579393	-1.564859	-2.783718
40	6	5.062739	-2.394372	-1.983388
41	1	5.865076	-1.646967	-1.963782
42	1	5.492227	-3.334677	-1.622024
43	1	4.765986	-2.534795	-3.026020

Energy = -1091.8295751
E+ZPVE = -1091.497391
Imaginary frequency: -1551.5 cm^{-1}

34: 4-toloyloxyquinoline 28

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z

1	6	-0.234267	0.576980	0.013161
2	6	-2.557661	-0.053665	0.060886
3	6	-3.609751	-1.103957	0.126335
4	6	-3.349637	-2.436583	-0.231579
5	6	-4.906066	-0.761458	0.545382
6	6	-4.354373	-3.400787	-0.161436
7	1	-2.368381	-2.722295	-0.596931
8	6	-5.906438	-1.726283	0.619126
9	1	-5.106313	0.270928	0.808242
10	6	-5.634697	-3.051194	0.268677
11	1	-4.136667	-4.424814	-0.450602
12	1	-6.901418	-1.445260	0.952442
13	1	-6.416063	-3.803499	0.325834
14	6	-2.032788	2.193845	-0.077926
15	6	-2.479888	3.540104	-0.155692
16	6	-0.624649	1.941024	-0.086475
17	6	-1.577101	4.575461	-0.241474
18	1	-3.551027	3.711784	-0.148160
19	6	0.284967	3.023650	-0.178386
20	6	-0.185091	4.316298	-0.255902
21	1	-1.931178	5.600409	-0.301940
22	1	1.349245	2.817517	-0.192406
23	1	0.514601	5.143362	-0.329955
24	7	-2.965149	1.205482	-0.009110
25	8	1.129644	0.355781	0.109198
26	6	1.743073	-0.742212	-0.455721
27	8	1.159968	-1.575866	-1.110168
28	6	3.197623	-0.750344	-0.163415
29	6	3.815543	0.194153	0.668113
30	6	3.972533	-1.764640	-0.744390
31	6	5.184679	0.120566	0.906846
32	1	3.222042	0.973194	1.131840
33	6	5.339264	-1.826603	-0.501691
34	1	3.483164	-2.494533	-1.380096
35	6	5.970331	-0.884346	0.325014
36	1	5.653180	0.853509	1.558171
37	1	5.929051	-2.618231	-0.956164
38	6	7.459455	-0.939137	0.561535
39	1	7.824540	-1.970239	0.575724
40	1	8.001095	-0.414155	-0.235179
41	1	7.732919	-0.465865	1.508631
42	6	-1.178517	-0.414753	0.093785
43	1	-0.878932	-1.446232	0.193439

Energy = -1091.9538201
E+ZPVE = -1091.614602

34: TS17 connecting 27 and 28

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.023476	-1.456067	-0.227827
2	8	-0.221495	-2.432836	-0.030540
3	7	-2.655886	0.872758	-0.036515
4	6	-1.350958	1.001586	-0.130025
5	6	-0.799999	2.382052	-0.113708
6	6	0.575323	2.627152	0.030504
7	6	-1.666717	3.481054	-0.243906
8	6	1.070497	3.930512	0.036748
9	1	1.265622	1.799543	0.156990
10	6	-1.171381	4.780988	-0.237037
11	1	-2.727531	3.285588	-0.349137
12	6	0.200067	5.012348	-0.098974
13	1	2.137020	4.100214	0.153464
14	1	-1.855474	5.618233	-0.342379
15	1	0.585872	6.027727	-0.094992
16	6	0.847663	-1.111135	1.125963
17	8	0.463477	-1.131428	2.238348
18	6	-3.216480	-0.385563	-0.126828
19	6	-4.624012	-0.488146	-0.086831
20	6	-2.460203	-1.588375	-0.232457
21	6	-5.243479	-1.724828	-0.159911
22	1	-5.196047	0.429364	0.002085
23	6	-3.104305	-2.839562	-0.278203
24	6	-4.486308	-2.908968	-0.257527
25	1	-6.327990	-1.783587	-0.132696
26	1	-2.492075	-3.734124	-0.329258
27	1	-4.987314	-3.871019	-0.301808
28	6	2.193016	-1.128098	0.528617
29	6	3.218513	-0.562462	1.304466
30	6	2.482249	-1.668103	-0.728532
31	6	4.517972	-0.531321	0.808311
32	1	2.991418	-0.161331	2.286371
33	6	3.789177	-1.638027	-1.202092
34	1	1.684799	-2.136628	-1.292900
35	6	4.826326	-1.062762	-0.451732
36	1	5.307094	-0.094140	1.413902
37	1	4.011673	-2.074579	-2.171813

38	6	6.231600	-1.000041	-0.996543
39	1	6.445692	-1.851458	-1.648725
40	1	6.379498	-0.089665	-1.590599
41	1	6.973069	-0.988904	-0.192934
42	6	-0.464434	-0.135284	-0.276301
43	1	0.416111	0.007859	-0.889478

Energy = -1091.8650954
E+ZPVE = -1091.529209
Imaginary frequency: -524.3 cm^{-1}

36: 4-quinolone 29

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.871173	-1.512205	0.799765
2	8	-0.191020	-2.409328	1.308087
3	6	-0.382121	-0.134075	0.673474
4	6	-1.171979	0.855133	0.136393
5	6	-0.794209	2.282469	-0.063079
6	6	-0.325517	3.077877	0.994058
7	6	-0.961894	2.863486	-1.332934
8	6	-0.029352	4.423112	0.776856
9	1	-0.189032	2.632747	1.971426
10	6	-0.659292	4.207356	-1.543727
11	1	-1.301927	2.251474	-2.164049
12	6	-0.194312	4.991593	-0.486892
13	1	0.329667	5.029150	1.603159
14	1	-0.780054	4.638165	-2.533191
15	1	0.040671	6.039404	-0.648821
16	6	1.007036	0.123764	1.211992
17	8	1.164550	0.795795	2.224696
18	6	-2.985168	-0.715920	-0.285993
19	6	-4.281549	-0.954112	-0.778058
20	6	-2.231504	-1.764198	0.274108
21	6	-4.810012	-2.233436	-0.711003
22	1	-4.857097	-0.137256	-1.206012
23	6	-2.790555	-3.051469	0.328803
24	6	-4.065547	-3.290297	-0.157860
25	1	-5.810767	-2.416742	-1.090798
26	1	-2.184421	-3.837197	0.767309
27	1	-4.492707	-4.286986	-0.111787
28	6	2.174882	-0.456991	0.490527

29	6	3.448215	-0.329361	1.067897
30	6	2.059192	-1.090117	-0.753543
31	6	4.569662	-0.829030	0.419609
32	1	3.529849	0.168446	2.028077
33	6	3.188144	-1.585172	-1.401119
34	1	1.085134	-1.189012	-1.220524
35	6	4.459935	-1.469052	-0.825620
36	1	5.548813	-0.724249	0.880499
37	1	3.082143	-2.071143	-2.367521
38	6	5.678991	-2.036967	-1.510206
39	1	6.550625	-1.388143	-1.378756
40	1	5.940921	-3.017590	-1.093652
41	1	5.511794	-2.171242	-2.582544
42	7	-2.426763	0.548587	-0.340530
43	1	-2.995737	1.313994	-0.672053

Energy = -1091.9402795
E+ZPVE = -1091.600836