**Mechanisms for Formation of Diazocinones, Pyridazines, and Pyrazolines from
Tetrazines—Oxyanion-Accelerated Pericyclic Cascades?**

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Table of Contents

Gaussian03 Full Reference.....	S1
Imaginary Frequencies for TS4→6 and TS 4→7	S2
Pyridazine-Forming Steps	S3 – S5
Relaxed PES Scan of C-C (enolate-tetrazine) distance in 1+2 Complex leading towards structure 3'	S6
Relaxed Potential Energy Surface Scan of C3-C4 distance in 3'	S7
Electrostatic potential maps for model systems lacking the phenyl rings....	S7
Coordinates and Energies.....	S8 – S97
IRC Plots.....	S98 – S104

Gaussian03 Full Reference

GAUSSIAN03, Revision D.01

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
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J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

Imaginary Frequencies for TS4→6 and TS 4→7 (see footnote 20)

As mentioned in footnote 20, the assignment of disrotatory or conrotatory descriptors to the motion of the imaginary frequencies in **TS4→6** and **TS4→7** is somewhat ambiguous. While in **TS4→6**, the hydrogen atom on C7 clearly rotates outwards and in **TS4→7** the same hydrogen atom clearly rotates inwards, the motion of the oxygen atom is much less clear, and appears to correspond mainly to planarization of the carbon center in both structures. Therefore, our assignment of a disrotatory product and a conrotatory product is based on the structures which result from forward IRC calculations, and subsequent optimization of these end points. From this perspective, the oxygen is ultimately rotated outwards in both products, and thus **TS4→6**, with the H rotated outwards can be said to correspond to a disrotatory product while **TS4→7**, with the H rotated inwards can be said to correspond to a conrotatory product. Note that this situation bears a connection to systems which have been described by Borden, et al. as “monorotatory”, see *J. Chem. Soc., Perkin Trans. 2*, **1999**, 2339-2347.

Shown below are images containing frame shots of the equilibrium (center images) and extreme positions of the animated frequencies for both structures. Also included along with this document are animated .gif files for the imaginary frequency of each structure.

TS4→6

TS4→7

Pyridazine-Forming Steps (see footnote 26)

As proposed in Scheme 2, the aromatization pathway likely occurs via a protonation-elimination pathway involving an external proton source and an external base. This involvement of external species presents a challenge in examining the energetics of these processes with computations. Here, we make an attempt to examine plausible steps in a discrete sense.

The first step, protonation of the oxyanion to give **7** is likely to occur intermolecularly, with methanol as the obvious proton source. At this point, a syn-elimination is required to form the corresponding pyridazine. An intramolecular, concerted version of this process would almost certainly face an exceedingly high reaction barrier, and therefore we hypothesize that the elimination may occur via a two-step, E1cb-type mechanism, where the hydrogen at C7 is deprotonated to form a delocalized carbanion prior to elimination of hydroxide. The E1cb mechanism is frequently invoked when the possibility exists for the formation of a stabilized carbanion and when a relatively poor leaving group must be eliminated. For example, the final elimination step in the common aldol condensation reaction is often formulated in this way, and this same mechanism was proposed very recently by Domingo et al, for systems closely related to these (see reference 2f). This process is detailed in the scheme below.

In order to test the feasibility of this hypothesis, we computed the **12**→**pyridazine** step for the system derived from cyclopentanone, as well as the system derived from cyclobutanone for comparison. As shown in the figure below, we were able to find minima for the delocalized carbanions, and transition-state structures for the elimination of hydroxide ion. Product complexes with the hydroxide ion associated with aromatic and aliphatic hydrogen atoms in the systems were also found (vide infra), but these gas-phase structures are likely not meaningful representations of the solution phase where the hydroxide ion is expected to be solvated.

Computed geometries and energies (B3LYP/6-31+G(d,p)) for stationary point structures in the proposed E1cb transformation leading to pyridazines (n=1 and n=2). Energies are in kcal/mol; regular text shows gas-phase free energy values, italicized text in parentheses shows solvent single-point electronic energy values (see methods). Selected distances are in Å.

The scheme below summarizes the energies associated with the potential energy surfaces for the cyclobutanone-derived (n=1) and cyclopentanone-derived (n=2) systems in the regions involved in the ring-opening and aromatization processes. Following the n=1 pathway, we see that **4** can either undergo exothermic ring-opening with a barrier of 10 kcal/mol, or can isomerize via intermolecular proton transfer to **12**. At this point, it faces a barrier ranging from ~4-12 kcal/mol towards the fused pyridazine product. In comparison, the n=2 system can undergo ring-opening with a somewhat higher barrier of ~11-22 kcal/mol, but can isomerize to **12** in a process that is significantly more exergonic than for the n=1 system. From there, the transformation to a pyridazine is essentially barrierless. Beyond the two transition-state structures, intermediate **6** leading towards the diazocinone products represents a more exergonic product for n=1 than it does for n=2. For the fused pyridazines, the n=1 structure is slightly exergonic, while the n=2 product is overall exergonic by ~14-19 kcal/mol. Both values likely underestimate the true exergonicity since the structures involve a non-solvated hydroxide ion. Thus, the

theoretical evidence points to an easier and more exergonic ring-opening for the n=1 system than for the n=2 system.

Energies (B3LYP/6-31+G(d,p)) are in kcal/mol; regular text shows gas-phase free energy values, italicized text in parentheses shows optimized solvent free energy values (*Values for the TS12→pyridazine transitions structures are derived from calculations utilizing ua0 radii instead of uaks, and are relative to structures 4 computed with the same method). Selected distances are in Å. Note that for the pyridazines, the structure includes an associated hydroxide ion (computed as an isolated species), which likely artificially raises the energy compared to the expected solution phase behavior where the hydroxide ion would be dissociated and solvated.

Relaxed Potential Energy Surface Scan of C-C (enolate-tetrazine) distance in 1+2 Complex leading towards structure 3'

The C7-C8 distance here was scanned from 3.01 Å to 1.51 Å in 0.1 Å increments.

Relaxed Potential Energy Surface Scan of C3-C4 distance in 3' (see footnote 17)

The C3-C4 distance here was scanned from 2.79 Å to 1.39 Å in 0.2 Å increments.

Electrostatic potential maps for model systems lacking the phenyl rings

model of 4

model of TS4→6

model of TS4→7

Coordinates and Energies

Coordinates and energies correspond to gas phase optimizations, except where noted.

1+2 complex (n=1, Figure 1)

HF = -989.1655142 hartrees (-620711.251815642 kcal/mol)

Imaginary Frequencies: 1 (-31.9351 1/cm)

Zero-point correction = 0.290735 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -988.923838 hartrees (-620559.59758338 kcal/mol)

Solvent Single Point: HF = -989.2491025 hartrees (-620763.7043 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.565283	2.538473	-0.879359
2	1	2.355787	1.917689	-1.319344
3	1	1.841834	3.595807	-0.984741
4	6	0.101057	2.192777	-1.316347
5	1	0.019841	1.399156	-2.075009
6	1	-0.466927	3.063678	-1.683345
7	6	1.135684	2.150112	0.565355
8	6	0.984026	-1.013504	-0.024830
9	6	-0.161361	1.781106	0.122451
10	1	-1.093216	1.672553	0.670032
11	6	-1.553990	-0.886845	-0.003876
12	8	1.752054	2.224180	1.646838
13	7	0.352664	-1.335770	1.145323
14	7	-0.943926	-1.263243	1.153949
15	7	0.343804	-1.206081	-1.211249
16	7	-0.958904	-1.126030	-1.198799
17	6	2.443371	-0.857057	-0.017784
18	6	3.111290	-0.523204	1.174325
19	6	3.192379	-1.024188	-1.199147
20	6	4.499367	-0.385238	1.184551
21	1	2.532114	-0.342927	2.070999
22	6	4.579372	-0.886871	-1.179479
23	1	2.672380	-1.268151	-2.119050
24	6	5.240519	-0.572039	0.014221
25	1	4.999707	-0.108105	2.108452
26	1	5.146725	-1.024348	-2.096928
27	1	6.321952	-0.458979	0.026854
28	6	-2.982096	-0.533988	0.025832
29	6	-3.678418	-0.259093	-1.165898
30	6	-3.673099	-0.446688	1.248778
31	6	-5.029300	0.085575	-1.132943
32	1	-3.144257	-0.319120	-2.107710
33	6	-5.023807	-0.100347	1.275575
34	1	-3.134639	-0.651931	2.167438
35	6	-5.711484	0.165631	0.086362
36	1	-5.551368	0.297076	-2.062894
37	1	-5.541308	-0.034837	2.229447
38	1	-6.763274	0.439188	0.109803

3' (n=1, Figure 1)

HF = -989.1906031 hartrees (-620726.995351281 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.293790 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -988.944525 hartrees (-620572.57888275 kcal/mol)

Solvent Single Point: HF = -989.2759467 hartrees (-620780.5493 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.605579	2.613045	-0.466499
2	1	1.277264	2.155364	-1.198654
3	1	0.901759	3.655043	-0.302806
4	6	-0.903081	2.319384	-0.731862
5	1	-1.124690	1.894851	-1.712912
6	1	-1.548959	3.182984	-0.546752
7	6	0.463064	1.787885	0.822317
8	6	1.265063	-0.699731	-0.151646
9	6	-0.932589	1.274362	0.433850
10	1	-1.639886	1.494801	1.239716
11	6	-1.240100	-0.231879	-0.001028
12	8	1.046396	1.853554	1.887046
13	7	0.594279	-0.634623	-1.339023
14	7	-0.690101	-0.552403	-1.322787
15	7	-0.666134	-1.169028	0.980366
16	7	0.610640	-1.244478	0.923943
17	6	2.729077	-0.651333	-0.147981
18	6	3.459611	-0.424793	-1.333848
19	6	3.449759	-0.786952	1.056725
20	6	4.852755	-0.355135	-1.315055
21	1	2.914531	-0.318485	-2.266136
22	6	4.842553	-0.718633	1.068627
23	1	2.895485	-0.940601	1.976099
24	6	5.558703	-0.504080	-0.115174
25	1	5.391997	-0.184962	-2.244854
26	1	5.373756	-0.825298	2.012094
27	1	6.644448	-0.446396	-0.101848
28	6	-2.756733	-0.393771	-0.030398
29	6	-3.480965	-0.287353	-1.225746
30	6	-3.462085	-0.619725	1.161740
31	6	-4.875893	-0.392999	-1.227784
32	1	-2.935816	-0.144989	-2.151922
33	6	-4.854523	-0.730400	1.160622
34	1	-2.903148	-0.729715	2.085589
35	6	-5.570776	-0.614271	-0.035586
36	1	-5.419399	-0.307673	-2.166263
37	1	-5.380781	-0.912396	2.095017
38	1	-6.655037	-0.698942	-0.037863

TS3'→4 (n=1, Figure 1)

HF = -989.1512852 hartrees (-620702.322975852 kcal/mol)

Imaginary Frequencies: 1 (-459.9626 1/cm)

Zero-point correction = 0.291285 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -988.907283 hartrees (-620549.20915533 kcal/mol)

Solvent Single Point: HF = -989.2372322 hartrees (-620756.2556 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.888506	2.117658	1.333368
2	1	-1.421913	1.535521	2.092355
3	1	-1.336353	3.112132	1.251669
4	6	0.656394	2.100651	1.456076
5	1	1.044384	1.520131	2.298976
6	1	1.117119	3.094620	1.474439
7	6	-0.776912	1.458405	-0.104997
8	6	-1.205679	-0.175673	0.034321
9	6	0.823008	1.382594	0.078407
10	1	1.306347	1.981502	-0.695599
11	6	1.393508	-0.012652	0.152313
12	8	-1.284642	2.063243	-1.120477
13	7	-0.547014	-0.920338	0.985185
14	7	0.760753	-0.896317	1.006454
15	7	0.643828	-0.608377	-1.522884
16	7	-0.522905	-0.620190	-1.439151
17	6	-2.678217	-0.435798	-0.031405
18	6	-3.340341	-1.121383	1.000871
19	6	-3.432378	0.051237	-1.113545
20	6	-4.721363	-1.324520	0.950425
21	1	-2.755047	-1.495611	1.833598
22	6	-4.813681	-0.155409	-1.159854
23	1	-2.921280	0.613654	-1.885877
24	6	-5.465843	-0.844670	-0.132647
25	1	-5.216096	-1.859815	1.758142
26	1	-5.383705	0.230471	-2.002046
27	1	-6.541211	-1.003959	-0.173441
28	6	2.861092	-0.246034	0.019863
29	6	3.388787	-1.527986	0.267062
30	6	3.752043	0.768245	-0.369439
31	6	4.754180	-1.780351	0.140673
32	1	2.704883	-2.314045	0.568016
33	6	5.119936	0.514115	-0.504157
34	1	3.377978	1.767421	-0.563383
35	6	5.630873	-0.760503	-0.247664
36	1	5.136491	-2.778831	0.340256
37	1	5.786505	1.317999	-0.807463
38	1	6.694982	-0.958147	-0.351076

4 (n=1, Figures 1 and 2, and pyridazine scheme and figure in SI)
(gas phase optimization)

HF = -879.6946968 hartrees (-552017.219188968 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.284080 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.455705 hartrees (-551867.24944455 kcal/mol)

Solvent Single Point: HF = -879.7937401 hartrees (-552079.3699 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.998316	2.203331	0.780429
2	1	-1.941522	2.113645	1.332891
3	1	-0.910765	3.217228	0.372402
4	6	0.303416	1.743616	1.476141
5	1	0.127733	0.946083	2.205791
6	1	0.934395	2.506910	1.946758
7	6	-0.698835	1.184889	-0.401277
8	6	-1.274914	-0.204326	-0.079687
9	6	0.815426	1.171426	0.117966
10	1	1.367009	1.934768	-0.440114
11	6	1.479012	-0.154360	0.075160
12	8	-0.966799	1.486027	-1.661168
13	7	-0.580624	-1.293698	0.114156
14	7	0.814795	-1.274119	0.118286
15	6	2.959368	-0.279821	-0.023468
16	6	3.561978	-1.522346	-0.310271
17	6	3.802774	0.827205	0.182421
18	6	4.946932	-1.648098	-0.384439
19	1	2.911481	-2.375235	-0.469469
20	6	5.193119	0.701112	0.107213
21	1	3.368539	1.795061	0.410859
22	6	5.774738	-0.536326	-0.176743
23	1	5.386868	-2.616692	-0.611212
24	1	5.820733	1.573780	0.272243
25	1	6.855738	-0.635331	-0.238310
26	6	-2.753151	-0.389630	-0.088659
27	6	-3.328189	-1.442367	0.650711
28	6	-3.612829	0.488715	-0.777341
29	6	-4.712683	-1.609740	0.705982
30	1	-2.665560	-2.122883	1.174810
31	6	-4.997848	0.320576	-0.714102
32	1	-3.154227	1.271050	-1.375335
33	6	-5.558498	-0.727418	0.024651
34	1	-5.132719	-2.429603	1.285107
35	1	-5.643729	1.006632	-1.258070
36	1	-6.637774	-0.857526	0.065775

4 (n=1, Figures 1 and 2, and pyridazine scheme and figure in SI)
(solvent optimization, methanol, uaks radii)

HF = -879.7964677 hartrees (-552081.081446427 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.284840 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.556503 hartrees (-551930.50119753 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.011477	2.184779	-0.625505
2	1	1.982941	2.129325	-1.127335
3	1	0.876759	3.190754	-0.209914
4	6	-0.241392	1.720280	-1.410117
5	1	-0.009799	0.941475	-2.144656
6	1	-0.857699	2.485622	-1.891462
7	6	0.667422	1.127501	0.493165
8	6	1.284822	-0.235837	0.141721
9	6	-0.800751	1.125611	-0.079805
10	1	-1.379990	1.889615	0.454111
11	6	-1.485012	-0.196590	-0.051001
12	8	0.855030	1.407922	1.811786
13	7	0.589875	-1.314288	-0.078604
14	7	-0.817310	-1.312854	-0.045237
15	6	-2.967786	-0.292090	0.006136
16	6	-3.608168	-1.476464	0.422115
17	6	-3.767672	0.802544	-0.370256
18	6	-4.998978	-1.561090	0.457912
19	1	-3.001258	-2.324571	0.722174
20	6	-5.162341	0.714661	-0.341835
21	1	-3.304074	1.728352	-0.697649
22	6	-5.783849	-0.465956	0.073679
23	1	-5.474095	-2.481158	0.790554
24	1	-5.761089	1.570609	-0.644081
25	1	-6.868846	-0.533155	0.102172
26	6	2.766576	-0.391396	0.077548
27	6	3.337201	-1.475623	-0.619323
28	6	3.634163	0.550501	0.662244
29	6	4.721761	-1.617348	-0.719554
30	1	2.681682	-2.201790	-1.088742
31	6	5.020132	0.406622	0.563947
32	1	3.208964	1.380874	1.215059
33	6	5.572272	-0.677479	-0.125957
34	1	5.137619	-2.460195	-1.267161
35	1	5.669932	1.142925	1.031612
36	1	6.651484	-0.787830	-0.202780

4 (n=1, Figures 1 and 2, and pyridazine scheme and figure in SI)

(solvent optimization, methanol, ua0 radii)

HF = -879.7904059 hartrees (-552077.277606309 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.283702 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.551618 hartrees (-551927.43581118 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.010133	2.186433	-0.647507
2	1	1.973236	2.116415	-1.164391
3	1	0.898649	3.193176	-0.227601
4	6	-0.260430	1.740747	-1.413141
5	1	-0.049457	0.972035	-2.163827
6	1	-0.879667	2.516952	-1.872298
7	6	0.671771	1.131798	0.477236
8	6	1.282974	-0.232692	0.122695
9	6	-0.805941	1.130555	-0.084076
10	1	-1.386038	1.883526	0.461332
11	6	-1.484864	-0.193317	-0.066458
12	8	0.879402	1.399405	1.785006
13	7	0.590717	-1.315158	-0.095434
14	7	-0.816657	-1.310099	-0.078504
15	6	-2.967626	-0.292875	0.005471
16	6	-3.600557	-1.475769	0.438592
17	6	-3.775607	0.797159	-0.369497
18	6	-4.991415	-1.565498	0.486547
19	1	-2.988851	-2.320419	0.743557
20	6	-5.170153	0.704482	-0.327802
21	1	-3.320160	1.724763	-0.705707
22	6	-5.784155	-0.476174	0.100463
23	1	-5.460672	-2.486137	0.831423
24	1	-5.775399	1.558046	-0.630159
25	1	-6.870388	-0.547269	0.138578
26	6	2.765433	-0.390472	0.075588
27	6	3.342070	-1.416717	-0.700365
28	6	3.627641	0.494944	0.751436
29	6	4.728406	-1.560878	-0.786375
30	1	2.691647	-2.095311	-1.245657
31	6	5.014754	0.348518	0.665982
32	1	3.190348	1.280390	1.358897
33	6	5.573670	-0.680642	-0.100291
34	1	5.149743	-2.358931	-1.396738
35	1	5.661607	1.039927	1.204958
36	1	6.655140	-0.793203	-0.165851

N₂ (Figure 1)

HF = -109.5297794 hartrees (-68731.031871294 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.005592 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -109.542636 hartrees (-68739.09951636 kcal/mol)

Solvent Single Point: HF = -109.5305906 hartrees (-68731.54091 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	0.000000	0.000000	0.552563
2	7	0.000000	0.000000	-0.552563

TS4→6 (n=1, Figure 3 and pyridazine figure and scheme in SI)

HF = -879.6776885 hartrees (-552006.546310635 kcal/mol)

Imaginary Frequencies: 1 (-288.2393 1/cm)

Zero-point correction = 0.282473 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.440350 hartrees (-551857.6140285 kcal/mol)**Solvent Single Point: HF = -879.7648279 hartrees (-552061.2272 kcal/mol)**

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.430325	2.303263	1.327847
2	1	-0.357697	1.639284	2.197120
3	1	-1.056497	3.168791	1.574565
4	6	0.932077	2.589120	0.712941
5	1	1.785832	2.664708	1.403211
6	1	0.889738	3.504606	0.113499
7	6	-0.967509	1.561884	0.057375
8	6	-1.365188	0.130130	0.327286
9	6	0.977464	1.384894	-0.256868
10	1	1.332307	1.631780	-1.262582
11	6	1.465752	0.129991	0.267450
12	8	-1.559740	2.268723	-0.824685
13	7	-0.596566	-0.766368	0.898141
14	7	0.754607	-0.713175	1.024729
15	6	2.842185	-0.340384	-0.042129
16	6	3.228551	-1.677218	0.198581
17	6	3.814000	0.534689	-0.569415
18	6	4.526683	-2.110053	-0.064579
19	1	2.480280	-2.355135	0.594042
20	6	5.109198	0.094515	-0.853516
21	1	3.551252	1.573337	-0.743150
22	6	5.476952	-1.229760	-0.599058
23	1	4.797772	-3.145219	0.132171
24	1	5.835898	0.792687	-1.263008
25	1	6.486255	-1.572389	-0.814324
26	6	-2.735314	-0.362325	-0.003837
27	6	-3.235223	-1.515858	0.642912
28	6	-3.574387	0.286969	-0.932697
29	6	-4.515234	-1.995458	0.376844
30	1	-2.592134	-2.019097	1.356086
31	6	-4.858707	-0.202380	-1.196069
32	1	-3.191288	1.171787	-1.427103
33	6	-5.339822	-1.342503	-0.549493
34	1	-4.873917	-2.882384	0.895323
35	1	-5.484536	0.315979	-1.919646
36	1	-6.338541	-1.718820	-0.760264

TS4→6 (n=1, Figure 2 and pyridazine figure and scheme in SI)

(solvent optimization, methanol, uaks radii)

HF = -879.7769758 hartrees (-552068.850084258 kcal/mol)

Imaginary Frequencies: 1 (-370.7367 1/cm)

Zero-point correction = 0.282639 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.539350 hartrees (-551919.7375185 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.989708	2.425832	-0.275345
2	1	2.028057	2.544620	-0.620505
3	1	0.710558	3.308401	0.314377
4	6	-0.095613	2.110179	-1.312242
5	1	0.268974	1.455287	-2.110587
6	1	-0.567093	2.983201	-1.781199
7	6	0.734779	1.171495	0.597701
8	6	1.242272	-0.077546	-0.114908
9	6	-1.026291	1.377354	-0.346830
10	1	-1.648793	2.055707	0.241590
11	6	-1.535021	0.066966	-0.528844
12	8	0.791079	1.208697	1.873893
13	7	0.572666	-0.920729	-0.865337
14	7	-0.798759	-0.963530	-0.958983
15	6	-2.942074	-0.261074	-0.153298
16	6	-3.281729	-1.538348	0.331591
17	6	-3.965504	0.696969	-0.279002
18	6	-4.598620	-1.847786	0.677194
19	1	-2.497851	-2.281854	0.440012
20	6	-5.283674	0.389921	0.068003
21	1	-3.729810	1.684435	-0.667254
22	6	-5.605659	-0.884098	0.547809
23	1	-4.838880	-2.838832	1.056128
24	1	-6.060241	1.143467	-0.043098
25	1	-6.631298	-1.123825	0.819261
26	6	2.698565	-0.380567	0.030927
27	6	3.375732	-1.074353	-0.996962
28	6	3.457656	0.040810	1.141975
29	6	4.741485	-1.343300	-0.911964
30	1	2.814475	-1.394304	-1.868787
31	6	4.827923	-0.228241	1.223635
32	1	2.959165	0.566978	1.947652
33	6	5.480023	-0.923599	0.201875
34	1	5.233762	-1.876145	-1.723070
35	1	5.384355	0.103613	2.097880
36	1	6.544904	-1.134178	0.268800

TS4→7 (n=1, Figure 2)

HF = -879.6557715 hartrees (-551992.793173965 kcal/mol)

Imaginary Frequencies: 1 (-559.3049 1/cm)

Zero-point correction = 0.281578 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.419445 hartrees (-551844.49593195 kcal/mol)

Solvent Single Point: HF = -879.7404514 hartrees (-552045.9307 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.919943	1.474097	-0.152301
2	6	-1.350388	0.030557	-0.455709
3	6	1.033289	1.422237	-0.735063
4	1	0.693949	1.821927	-1.680850
5	6	1.475209	0.064732	-0.722313
6	8	-1.546057	2.370910	-0.787034
7	7	-0.655118	-0.898551	-1.059018
8	7	0.725046	-0.960242	-1.129513
9	6	2.826695	-0.331501	-0.215598
10	6	3.066654	-1.632548	0.265161
11	6	3.903013	0.573796	-0.239129
12	6	4.335454	-2.012187	0.705842
13	1	2.235713	-2.330121	0.274420
14	6	5.170559	0.200061	0.211165
15	1	3.732413	1.571145	-0.634627
16	6	5.394240	-1.096842	0.686764
17	1	4.499155	-3.023191	1.072683
18	1	5.987794	0.917406	0.182095
19	1	6.381475	-1.390811	1.035690
20	6	-2.743753	-0.345872	-0.103078
21	6	-3.206784	-1.668069	-0.294136
22	6	-3.645938	0.587771	0.450193
23	6	-4.508274	-2.032539	0.039005
24	1	-2.513575	-2.389637	-0.712139
25	6	-4.949221	0.214723	0.791867
26	1	-3.328856	1.615781	0.578536
27	6	-5.393069	-1.094349	0.590166
28	1	-4.835693	-3.057888	-0.121666
29	1	-5.622598	0.958565	1.212558
30	1	-6.406803	-1.382379	0.858997
31	6	1.137885	2.342335	0.479943
32	6	-0.181863	1.886492	1.152202
33	1	0.008681	1.001781	1.776912
34	1	-0.730689	2.639117	1.740428
35	1	2.024519	2.196692	1.109723
36	1	1.090881	3.398520	0.193332

6 (n=1, Figure 2 and pyridazine figure and scheme in SI)

HF = -879.7130114 hartrees (-552028.711783614 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.284251 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.475004 hartrees (-551879.35976004 kcal/mol)

Solvent Single Point: HF = -879.7948079 hartrees (-552080.0399 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.419523	2.935685	0.617206
2	1	-0.220899	2.614257	1.643742
3	1	-1.032214	3.843758	0.646210
4	6	0.896570	3.225877	-0.102966
5	1	1.463254	4.018914	0.415316
6	1	0.664567	3.624359	-1.101438
7	6	-1.243815	1.902753	-0.164454
8	6	-1.298721	0.551702	0.342813
9	6	1.754824	2.007031	-0.259549
10	1	2.580289	2.115625	-0.962737
11	6	1.645914	0.808011	0.357782
12	8	-1.937836	2.350239	-1.108295
13	7	-0.464082	0.124371	1.352287
14	7	0.801928	0.348746	1.425676
15	6	2.663034	-0.253742	0.048766
16	6	2.272264	-1.604560	0.017269
17	6	4.012244	0.044234	-0.212362
18	6	3.184772	-2.611599	-0.301819
19	1	1.241375	-1.855156	0.242253
20	6	4.929209	-0.962093	-0.526483
21	1	4.351026	1.074184	-0.150296
22	6	4.519604	-2.297669	-0.577470
23	1	2.851361	-3.646096	-0.333036
24	1	5.968010	-0.702302	-0.717576
25	1	5.231803	-3.082939	-0.818720
26	6	-2.445690	-0.344241	0.094805
27	6	-2.537619	-1.586333	0.776340
28	6	-3.491374	-0.041858	-0.813459
29	6	-3.616750	-2.447673	0.590381
30	1	-1.745476	-1.852399	1.467162
31	6	-4.562765	-0.917647	-1.002036
32	1	-3.440167	0.887605	-1.365119
33	6	-4.645723	-2.127146	-0.304358
34	1	-3.648875	-3.385059	1.143379
35	1	-5.344423	-0.646396	-1.709843
36	1	-5.480583	-2.806480	-0.461112

6 (n=1, Figure 2 and pyridazine figure and scheme in SI)

(solvent optimization, methanol, uaks radii)

HF = -879.796034 hartrees (-552080.80929534 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.283873 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.558866 hartrees (-551931.98400366 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.454686	2.996261	0.547075
2	1	-0.255391	2.731332	1.591209
3	1	-1.058582	3.912382	0.538979
4	6	0.864379	3.249185	-0.186879
5	1	1.445772	4.039208	0.318712
6	1	0.646103	3.639584	-1.192938
7	6	-1.283112	1.928389	-0.167392
8	6	-1.310523	0.594018	0.356889
9	6	1.705613	2.017724	-0.331159
10	1	2.516422	2.101262	-1.054804
11	6	1.619001	0.840942	0.327156
12	8	-2.017404	2.328621	-1.118953
13	7	-0.472682	0.216332	1.396901
14	7	0.792911	0.446836	1.442864
15	6	2.628102	-0.234961	0.047857
16	6	2.229084	-1.583404	0.014667
17	6	3.982615	0.060248	-0.192488
18	6	3.142934	-2.598825	-0.278427
19	1	1.192019	-1.835328	0.212228
20	6	4.899216	-0.953919	-0.483401
21	1	4.325609	1.090236	-0.138175
22	6	4.483492	-2.288715	-0.530640
23	1	2.806713	-3.632929	-0.309435
24	1	5.942112	-0.700504	-0.661148
25	1	5.197288	-3.078448	-0.753244
26	6	-2.411934	-0.358807	0.102976
27	6	-2.301295	-1.695201	0.561631
28	6	-3.607104	-0.017785	-0.576765
29	6	-3.331875	-2.620987	0.387788
30	1	-1.390595	-2.004389	1.064003
31	6	-4.630005	-0.950567	-0.759728
32	1	-3.716720	0.987351	-0.962145
33	6	-4.508194	-2.259364	-0.277634
34	1	-3.206183	-3.635399	0.761794
35	1	-5.534787	-0.648081	-1.284026
36	1	-5.306400	-2.982816	-0.426905

7 (n=1, Figure 2)

HF = -879.6771575 hartrees (-552006.213102825 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.283554 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.439440 hartrees (-551857.0429944 kcal/mol)

Solvent Single Point: HF = -879.7594723 hartrees (-552057.8665 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.956144	1.556052	0.290628
2	6	-1.294573	0.182188	-0.202785
3	6	1.278161	1.373892	-1.303010
4	1	0.392708	1.502055	-1.926669
5	6	1.559704	0.071909	-1.010745
6	8	-1.833462	2.436345	0.319288
7	7	-0.618227	-0.759391	-0.904091
8	7	0.617984	-0.936812	-1.310521
9	6	2.786504	-0.384813	-0.318460
10	6	2.766155	-1.552168	0.469772
11	6	4.012354	0.296142	-0.458148
12	6	3.918865	-2.000792	1.117755
13	1	1.831233	-2.096123	0.555438
14	6	5.161718	-0.145610	0.197252
15	1	4.053632	1.164794	-1.109142
16	6	5.121606	-1.297769	0.992342
17	1	3.877846	-2.902550	1.724444
18	1	6.096016	0.397749	0.073969
19	1	6.019169	-1.648591	1.495982
20	6	-2.726244	-0.226817	-0.017682
21	6	-3.322015	-1.172808	-0.881895
22	6	-3.527438	0.242338	1.047354
23	6	-4.629222	-1.622818	-0.693323
24	1	-2.723046	-1.557998	-1.699149
25	6	-4.833870	-0.209257	1.238667
26	1	-3.124486	0.978668	1.732911
27	6	-5.403697	-1.147291	0.370491
28	1	-5.047336	-2.348876	-1.388533
29	1	-5.411141	0.176977	2.076836
30	1	-6.423748	-1.494786	0.517616
31	6	1.414952	2.455108	-0.270030
32	6	0.419585	1.971739	0.841598
33	1	0.896856	1.121730	1.341367
34	1	0.227243	2.762570	1.578366
35	1	2.412413	2.555310	0.170618
36	1	1.113640	3.436372	-0.654765

Reactant, X=O (Table 1)

HF = -915.5917094 hartrees (-574542.953565594 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.260198 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -915.377049 hartrees (-574408.25201799 kcal/mol)

Solvent Single Point: HF = -915.6925479 hartrees (-574606.2307 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.800195	2.084417	-0.885828
2	1	1.510078	1.832538	-1.684654
3	1	0.882156	3.147028	-0.616396
4	6	0.717617	1.182853	0.411051
5	6	1.298429	-0.215099	0.155711
6	6	-0.812151	1.157721	0.059293
7	1	-1.358136	1.868097	0.694550
8	6	-1.464288	-0.188706	0.037830
9	8	1.116582	1.620806	1.598451
10	7	0.607665	-1.318214	0.063250
11	7	-0.790391	-1.297497	0.042054
12	8	-0.564289	1.730344	-1.260643
13	6	2.777130	-0.383321	0.089257
14	6	3.317842	-1.494517	-0.588050
15	6	3.665182	0.563957	0.635944
16	6	4.698032	-1.654025	-0.717555
17	1	2.632599	-2.223622	-1.006718
18	6	5.045637	0.402452	0.497741
19	1	3.231391	1.392769	1.188584
20	6	5.572125	-0.704939	-0.175934
21	1	5.092360	-2.519033	-1.246571
22	1	5.715119	1.141833	0.931996
23	1	6.648280	-0.828858	-0.275618
24	6	-2.945175	-0.301499	0.045990
25	6	-3.747783	0.799761	-0.303416
26	6	-3.583315	-1.511371	0.383867
27	6	-5.141601	0.696795	-0.312682
28	1	-3.275551	1.734169	-0.590331
29	6	-4.972722	-1.611593	0.376445
30	1	-2.961129	-2.359618	0.648090
31	6	-5.762233	-0.507044	0.029566
32	1	-5.741664	1.559517	-0.591815
33	1	-5.445691	-2.552890	0.646947
34	1	-6.846607	-0.586201	0.026971

Electrocyclic TS, X=O (Table 1)

HF = -915.5829487 hartrees (-574537.456138737 kcal/mol)

Imaginary Frequencies: 1 (-319.7877 1/cm)

Zero-point correction = 0.259010 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -915.368503 hartrees (-574402.88931753 kcal/mol)

Solvent Single Point: HF = -915.6761506 hartrees (-574595.9413 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.843170	2.392029	-0.628184
2	1	1.766799	2.441292	-1.222362
3	1	0.640998	3.373642	-0.170407
4	6	0.772580	1.297523	0.468850
5	6	1.250921	-0.025144	-0.127908
6	6	-1.009075	1.374044	-0.346684
7	1	-1.618854	2.111908	0.181194
8	6	-1.522124	0.054245	-0.500447
9	8	0.991174	1.564591	1.687464
10	7	0.578790	-0.924621	-0.809414
11	7	-0.782406	-0.977684	-0.890274
12	8	-0.267173	1.947753	-1.417008
13	6	2.694807	-0.362496	0.056568
14	6	3.325735	-1.228058	-0.865672
15	6	3.484249	0.177467	1.092755
16	6	4.680390	-1.534460	-0.759492
17	1	2.722300	-1.650271	-1.661359
18	6	4.844807	-0.131601	1.192184
19	1	3.006753	0.825188	1.818925
20	6	5.454671	-0.988323	0.272784
21	1	5.137340	-2.200705	-1.488518
22	1	5.427297	0.296250	2.005493
23	1	6.511813	-1.229834	0.357507
24	6	-2.923714	-0.267298	-0.113396
25	6	-3.941522	0.703324	-0.146736
26	6	-3.267402	-1.573358	0.286656
27	6	-5.252886	0.385336	0.215810
28	1	-3.705191	1.709571	-0.478407
29	6	-4.577936	-1.894300	0.637722
30	1	-2.480921	-2.319987	0.309135
31	6	-5.578916	-0.915459	0.609605
32	1	-6.022285	1.153108	0.180509
33	1	-4.819938	-2.909099	0.945183
34	1	-6.599343	-1.164516	0.890777

Fragmentation TS, X=O (Table 1)

HF = -915.5467404 hartrees (-574514.735068404 kcal/mol)

Imaginary Frequencies: 1 (-477.7999 1/cm)

Zero-point correction = 0.257439 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -915.334640 hartrees (-574381.6399464 kcal/mol)

Solvent Single Point: HF = -915.6326208 hartrees (-574568.6259 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.077411	1.976851	-1.003212
2	1	-0.057524	1.140573	-1.709129
3	1	0.476381	2.859562	-1.522117
4	6	0.938500	1.555402	0.226660
5	6	1.324730	0.102226	0.537496
6	6	-1.034628	1.495333	0.789686
7	1	-0.737187	2.012713	1.692103
8	6	-1.483121	0.162398	0.839921
9	8	1.581120	2.450944	0.823334
10	7	0.634064	-0.767069	1.237255
11	7	-0.723369	-0.792125	1.431168
12	8	-1.183348	2.295462	-0.377137
13	6	2.662174	-0.342831	0.090213
14	6	3.543739	0.526964	-0.589497
15	6	3.103296	-1.668949	0.315071
16	6	4.800134	0.091991	-1.020491
17	1	3.254364	1.558808	-0.752013
18	6	4.360322	-2.092790	-0.104058
19	1	2.428958	-2.344521	0.829486
20	6	5.222435	-1.217983	-0.782324
21	1	5.455244	0.789241	-1.538507
22	1	4.670723	-3.117818	0.089067
23	1	6.200418	-1.554458	-1.118029
24	6	-2.753422	-0.302321	0.226306
25	6	-3.006785	-1.679056	0.070398
26	6	-3.749823	0.608485	-0.178347
27	6	-4.220091	-2.128783	-0.452887
28	1	-2.231722	-2.372783	0.378535
29	6	-4.953631	0.157784	-0.719497
30	1	-3.564105	1.671705	-0.069858
31	6	-5.199086	-1.214219	-0.856318
32	1	-4.399289	-3.196792	-0.556347
33	1	-5.706379	0.878233	-1.031574
34	1	-6.139835	-1.564367	-1.274874

Electrocyclic product, X=O (Table 1)

HF = -915.6035481 hartrees (-574550.382468231 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.259668 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -915.390761 hartrees (-574416.85643511 kcal/mol)

Solvent Single Point: HF = -915.6843804 hartrees (-574601.1055 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.399105	2.735116	-0.442113
2	1	1.205911	3.250278	-0.979373
3	1	-0.039570	3.442988	0.272983
4	6	1.081822	1.621297	0.377900
5	6	1.336653	0.294711	-0.175083
6	6	-1.643398	1.736825	-0.859345
7	1	-2.508292	2.374788	-0.674207
8	6	-1.660800	0.401018	-0.660243
9	8	1.624855	2.069252	1.409697
10	7	0.559013	-0.462556	-0.998492
11	7	-0.711548	-0.504337	-1.176842
12	8	-0.560165	2.368408	-1.426156
13	6	2.668723	-0.343435	0.059081
14	6	3.050145	-1.477513	-0.706115
15	6	3.620476	0.120661	1.000255
16	6	4.295052	-2.082978	-0.558655
17	1	2.338899	-1.866316	-1.424359
18	6	4.867953	-0.495322	1.144098
19	1	3.367091	0.964535	1.626323
20	6	5.226460	-1.601226	0.370859
21	1	4.539257	-2.945689	-1.176511
22	1	5.563433	-0.100871	1.883187
23	1	6.195584	-2.079959	0.491918
24	6	-2.877821	-0.250787	-0.105355
25	6	-3.279789	-1.520149	-0.563319
26	6	-3.649649	0.366533	0.896238
27	6	-4.426183	-2.132863	-0.056056
28	1	-2.670103	-2.006458	-1.316541
29	6	-4.799777	-0.246362	1.399717
30	1	-3.328112	1.320587	1.302934
31	6	-5.197794	-1.499316	0.924695
32	1	-4.718864	-3.112219	-0.427773
33	1	-5.374253	0.249007	2.178997
34	1	-6.087823	-1.980954	1.322068

Fragmentation product, X=O (Table 1)

HF = -915.5698686 hartrees (-574529.248245186 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.259537 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -915.356186 hartrees (-574395.16027686 kcal/mol)

Solvent Single Point: HF = -915.6522424 hartrees (-574580.9386 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.728605	2.042062	-0.502181
2	1	-1.579804	1.674528	-1.087363
3	1	-0.374497	2.965805	-0.967527
4	6	0.448138	1.022851	-0.671492
5	6	1.102766	0.091662	0.284769
6	6	-1.076439	1.335579	1.656125
7	1	-0.396598	1.483194	2.494287
8	6	-1.445626	0.078543	1.306619
9	8	0.880454	1.112747	-1.837011
10	7	0.648275	-0.758992	1.260050
11	7	-0.536470	-0.919853	1.775759
12	8	-1.166107	2.418212	0.825648
13	6	2.550576	-0.176765	-0.001004
14	6	3.135369	-1.423539	0.311007
15	6	3.416976	0.812702	-0.516257
16	6	4.497223	-1.666036	0.121022
17	1	2.496577	-2.196713	0.721933
18	6	4.777525	0.572670	-0.706053
19	1	3.015301	1.784530	-0.780555
20	6	5.336580	-0.671451	-0.390649
21	1	4.903066	-2.644805	0.370890
22	1	5.407002	1.367140	-1.102651
23	1	6.397026	-0.859532	-0.541942
24	6	-2.540810	-0.328002	0.417386
25	6	-3.641180	0.516194	0.149146
26	6	-2.552265	-1.622765	-0.141695
27	6	-4.697121	0.087601	-0.653178
28	1	-3.661490	1.510404	0.585712
29	6	-3.614195	-2.050190	-0.939784
30	1	-1.714133	-2.279314	0.066241
31	6	-4.693087	-1.200169	-1.204010
32	1	-5.531645	0.758446	-0.844899
33	1	-3.595379	-3.051560	-1.363582
34	1	-5.517789	-1.533556	-1.828927

Reactant, X=S (Table 1)

HF = -1238.5832135 hartrees (-777223.352303385 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.257754 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1238.371576 hartrees (-777090.54765576 kcal/mol)**Solvent Single Point: HF = -1238.678415 hartrees (-777283.0919 kcal/mol)**

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.124295	2.202033	-0.267483
2	1	2.059919	2.119933	-0.827254
3	1	1.100962	3.131339	0.309214
4	6	0.711033	0.989757	0.658391
5	6	1.295226	-0.338272	0.137787
6	6	-0.807075	1.025536	0.237249
7	1	-1.353995	1.663002	0.937243
8	6	-1.455207	-0.298672	0.049253
9	8	0.980624	1.062418	1.954554
10	7	0.608417	-1.413122	-0.135737
11	7	-0.784480	-1.396081	-0.137142
12	16	-0.405152	2.022898	-1.309029
13	6	2.773786	-0.501601	0.077247
14	6	3.646309	0.243843	0.893808
15	6	3.330676	-1.403465	-0.849890
16	6	5.029600	0.093440	0.774464
17	1	3.203096	0.905719	1.631548
18	6	4.713804	-1.552124	-0.963625
19	1	2.656670	-1.981212	-1.473189
20	6	5.572937	-0.802711	-0.152670
21	1	5.687313	0.672202	1.419282
22	1	5.122008	-2.252317	-1.689221
23	1	6.651002	-0.918140	-0.239997
24	6	-2.937019	-0.420817	0.073981
25	6	-3.554523	-1.682547	0.190356
26	6	-3.762755	0.713377	-0.029512
27	6	-4.942049	-1.801097	0.204893
28	1	-2.916125	-2.555683	0.268192
29	6	-5.155402	0.592597	-0.018007
30	1	-3.315685	1.696659	-0.136604
31	6	-5.753818	-0.663466	0.101540
32	1	-5.396113	-2.784581	0.302087
33	1	-5.771212	1.484461	-0.104981
34	1	-6.836874	-0.757529	0.115172

Electrocyclic TS, X=S (Table 1)

HF = -1238.5676217 hartrees (-777213.568292967 kcal/mol)

Imaginary Frequencies: 1 (-310.4953 1/cm)

Zero-point correction = 0.256011 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1238.357251 hartrees (-777081.55857501 kcal/mol)

Solvent Single Point: HF = -1238.651363 hartrees (-777266.1167 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.149317	2.351792	0.208882
2	1	2.201127	2.440919	-0.093126
3	1	0.897013	3.154914	0.907475
4	6	0.807055	0.989247	0.857104
5	6	1.246689	-0.178474	-0.032675
6	6	-1.064199	1.304463	-0.063007
7	1	-1.705292	1.913404	0.571928
8	6	-1.544485	0.006003	-0.394242
9	8	0.851948	0.853947	2.102872
10	7	0.549237	-0.961031	-0.815408
11	7	-0.813272	-0.989742	-0.880827
12	16	-0.055197	2.304626	-1.176882
13	6	2.698691	-0.518041	0.038847
14	6	3.307961	-1.186105	-1.046544
15	6	3.517033	-0.163607	1.131051
16	6	4.668258	-1.485992	-1.038557
17	1	2.682553	-1.462523	-1.888006
18	6	4.882729	-0.464084	1.132753
19	1	3.065352	0.323969	1.987636
20	6	5.470504	-1.127046	0.052748
21	1	5.108202	-1.999213	-1.891194
22	1	5.486369	-0.185302	1.993862
23	1	6.532226	-1.362352	0.059162
24	6	-2.967111	-0.356613	-0.105479
25	6	-3.986235	0.611549	-0.087346
26	6	-3.321072	-1.695258	0.148029
27	6	-5.311513	0.258742	0.181622
28	1	-3.738017	1.645810	-0.305251
29	6	-4.643730	-2.049949	0.411616
30	1	-2.532987	-2.440121	0.128153
31	6	-5.647646	-1.074139	0.433713
32	1	-6.082639	1.025662	0.186142
33	1	-4.893381	-3.090011	0.608883
34	1	-6.678200	-1.350275	0.644028

Fragmentation TS, X=S (Table 1)

HF = -1238.5376677 hartrees (-777194.771858427 kcal/mol)

Imaginary Frequencies: 1 (-465.0351 1/cm)

Zero-point correction = 0.254782 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1238.329054 hartrees (-777063.86467554 kcal/mol)

Solvent Single Point: HF = -1238.620849 hartrees (-777246.9691 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.524819	1.921784	-1.068594
2	1	0.489798	1.121418	-1.818450
3	1	1.124237	2.762831	-1.438246
4	6	1.049272	1.407924	0.305933
5	6	1.413443	-0.065184	0.517697
6	6	-1.014169	1.265979	0.785058
7	1	-0.694950	1.678477	1.732574
8	6	-1.444852	-0.090360	0.748381
9	8	1.594193	2.232942	1.073825
10	7	0.704064	-1.020197	1.058526
11	7	-0.669141	-1.096482	1.163635
12	16	-1.196083	2.414188	-0.591828
13	6	2.794631	-0.453832	0.119656
14	6	3.758008	0.505762	-0.256247
15	6	3.180633	-1.812900	0.096148
16	6	5.047801	0.121530	-0.634097
17	1	3.502310	1.558298	-0.220553
18	6	4.469219	-2.190675	-0.271600
19	1	2.440312	-2.552531	0.380151
20	6	5.415331	-1.225986	-0.645061
21	1	5.770383	0.885049	-0.913629
22	1	4.737415	-3.245121	-0.278110
23	1	6.418709	-1.522465	-0.941435
24	6	-2.784684	-0.511944	0.243789
25	6	-3.003709	-1.830689	-0.196206
26	6	-3.868553	0.383397	0.222587
27	6	-4.262909	-2.239126	-0.637849
28	1	-2.165140	-2.518485	-0.175527
29	6	-5.126222	-0.020129	-0.228412
30	1	-3.715828	1.397963	0.576913
31	6	-5.330831	-1.334848	-0.660845
32	1	-4.411041	-3.263163	-0.973472
33	1	-5.949606	0.690273	-0.237020
34	1	-6.310634	-1.650570	-1.011705

Electrocyclic product, X=S (Table 1)

HF = -1238.5831132 hartrees (-777223.289364132 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.255911 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1238.374370 hartrees (-777092.3009187 kcal/mol)

Solvent Single Point: HF = -1238.662579 hartrees (-777273.1546 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.011863	2.321785	0.022095
2	1	2.060002	2.507942	-0.243858
3	1	0.608856	3.170292	0.579098
4	6	0.920694	1.058403	0.868024
5	6	1.340578	-0.222338	0.184240
6	6	-1.418165	1.369670	-0.946298
7	1	-2.284233	2.020501	-0.998431
8	6	-1.600914	0.065608	-0.511993
9	8	0.541380	1.105781	2.030047
10	7	0.535453	-1.057598	-0.440412
11	7	-0.782231	-1.025149	-0.517183
12	16	0.077942	2.077880	-1.559336
13	6	2.774028	-0.526803	0.184146
14	6	3.303087	-1.568567	-0.618893
15	6	3.692440	0.208074	0.971219
16	6	4.663521	-1.854248	-0.625032
17	1	2.610474	-2.137883	-1.228764
18	6	5.060066	-0.077098	0.951541
19	1	3.330464	0.991505	1.631074
20	6	5.562321	-1.109992	0.155947
21	1	5.034331	-2.662320	-1.252737
22	1	5.734029	0.508001	1.573930
23	1	6.626007	-1.333683	0.142693
24	6	-3.000730	-0.309440	-0.112497
25	6	-3.820389	0.566449	0.620366
26	6	-3.523373	-1.570697	-0.453611
27	6	-5.121528	0.204822	0.982845
28	1	-3.422559	1.527410	0.930718
29	6	-4.823452	-1.930124	-0.096524
30	1	-2.881914	-2.256618	-0.995411
31	6	-5.634172	-1.044023	0.622598
32	1	-5.729593	0.898164	1.559636
33	1	-5.206226	-2.908317	-0.379623
34	1	-6.645559	-1.326966	0.904803

Fragmentation product, X=S (Table 1)

HF = -1238.560542 hartrees (-777209.12571042 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.256386 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1238.350744 hartrees (-777077.47536744 kcal/mol)

Solvent Single Point: HF = -1238.637622 hartrees (-777257.4939 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.276612	1.638172	1.192606
2	1	0.994134	0.891137	1.537807
3	1	0.305177	2.524142	1.831001
4	6	-1.119446	1.123871	1.147113
5	6	-1.470818	-0.122013	0.347002
6	6	0.957455	0.689063	-1.457548
7	1	-0.008014	0.440303	-1.898913
8	6	1.446294	-0.364244	-0.578187
9	8	-2.028939	1.708195	1.754856
10	7	-0.694629	-1.068857	-0.099582
11	7	0.647082	-1.190917	0.056349
12	16	0.913927	2.187546	-0.558913
13	6	-2.926727	-0.369436	0.080838
14	6	-3.423606	-1.684217	0.083111
15	6	-3.813568	0.672609	-0.242083
16	6	-4.758474	-1.952103	-0.224324
17	1	-2.739419	-2.492387	0.319414
18	6	-5.146678	0.404403	-0.559362
19	1	-3.456733	1.695395	-0.243303
20	6	-5.629736	-0.907725	-0.549429
21	1	-5.118126	-2.978439	-0.209711
22	1	-5.810852	1.226933	-0.813843
23	1	-6.669989	-1.112979	-0.790553
24	6	2.901278	-0.521995	-0.273820
25	6	3.859544	0.136366	-1.062175
26	6	3.351454	-1.334288	0.783643
27	6	5.223466	-0.004148	-0.798616
28	1	3.500455	0.752097	-1.880941
29	6	4.715219	-1.486317	1.038853
30	1	2.614438	-1.846580	1.393491
31	6	5.660579	-0.819656	0.250581
32	1	5.948036	0.520368	-1.417565
33	1	5.042208	-2.122806	1.858243
34	1	6.723124	-0.935112	0.452052

Reactant, X=NH (Table 1)

HF = -895.7222041 hartrees (-562074.640294791 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.272824 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -895.494596 hartrees (-561931.81393596 kcal/mol)**Solvent Single Point: HF = -895.8297353 hartrees (-562142.1172 kcal/mol)**

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.922975	2.139998	-0.866586
2	1	1.789191	1.988299	-1.523898
3	1	0.901039	3.179847	-0.506893
4	6	0.710612	1.186157	0.386885
5	6	1.285563	-0.208634	0.111388
6	6	-0.806952	1.170338	-0.088454
7	1	-1.350780	1.924125	0.497068
8	6	-1.473861	-0.165269	-0.043806
9	8	1.022346	1.574732	1.613104
10	7	0.590492	-1.302863	-0.035530
11	7	-0.805161	-1.278700	-0.037039
12	7	-0.365623	1.653799	-1.428900
13	1	-0.964396	2.371764	-1.830728
14	6	2.763904	-0.388689	0.093726
15	6	3.324624	-1.464648	-0.622438
16	6	3.634654	0.515384	0.733081
17	6	4.707889	-1.631058	-0.701262
18	1	2.652197	-2.161146	-1.111643
19	6	5.018588	0.346921	0.647015
20	1	3.185115	1.318132	1.310942
21	6	5.565366	-0.724914	-0.067147
22	1	5.118014	-2.468085	-1.262523
23	1	5.674444	1.052425	1.152776
24	1	6.643852	-0.854581	-0.126751
25	6	-2.955083	-0.287097	0.029685
26	6	-3.791688	0.824344	-0.180033
27	6	-3.567225	-1.529775	0.295752
28	6	-5.183568	0.703222	-0.128078
29	1	-3.352660	1.794119	-0.390937
30	6	-4.953303	-1.650744	0.347301
31	1	-2.922664	-2.386834	0.456775
32	6	-5.773937	-0.534147	0.136267
33	1	-5.805116	1.579699	-0.295516
34	1	-5.400240	-2.619832	0.557494
35	1	-6.856071	-0.629772	0.179515

Electrocyclic TS, X=NH (Table 1)

HF = -895.7151165 hartrees (-562070.192754915 kcal/mol)

Imaginary Frequencies: 1 (-310.9291 1/cm)

Zero-point correction = 0.271517 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -895.488179 hartrees (-561927.78720429 kcal/mol)

Solvent Single Point: HF = -895.814723 hartrees (-562132.6968 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.924862	2.398974	-0.571402
2	1	1.910194	2.469448	-1.058133
3	1	0.704101	3.349513	-0.057341
4	6	0.767124	1.262739	0.485432
5	6	1.250696	-0.059276	-0.107515
6	6	-0.995116	1.359546	-0.373575
7	1	-1.592626	2.084159	0.189537
8	6	-1.522848	0.034263	-0.486147
9	8	0.926088	1.485091	1.723163
10	7	0.573194	-0.974799	-0.755911
11	7	-0.793424	-1.020274	-0.817588
12	7	-0.157577	1.915860	-1.430046
13	1	-0.626732	2.627558	-1.984997
14	6	2.700428	-0.375445	0.058574
15	6	3.329642	-1.248634	-0.856811
16	6	3.497253	0.197299	1.071200
17	6	4.690288	-1.533713	-0.765009
18	1	2.719861	-1.693692	-1.635154
19	6	4.863178	-0.090234	1.156673
20	1	3.020668	0.850911	1.793221
21	6	5.471767	-0.956366	0.244601
22	1	5.146444	-2.207512	-1.487699
23	1	5.451635	0.361662	1.952593
24	1	6.533507	-1.181057	0.318026
25	6	-2.937046	-0.265932	-0.114243
26	6	-3.939077	0.720225	-0.156309
27	6	-3.308778	-1.565983	0.280901
28	6	-5.260710	0.424235	0.188094
29	1	-3.681622	1.725184	-0.476236
30	6	-4.628769	-1.865804	0.614729
31	1	-2.534500	-2.324808	0.312601
32	6	-5.613955	-0.871314	0.575052
33	1	-6.015962	1.205812	0.146623
34	1	-4.890815	-2.877014	0.917899
35	1	-6.641834	-1.103884	0.843098

Fragmentation TS, X=NH (Table 1)

HF = -895.6835484 hartrees (-562050.383456484 kcal/mol)

Imaginary Frequencies: 1 (-545.9559 1/cm)

Zero-point correction = 0.270421 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -895.458648 hartrees (-561909.25620648 kcal/mol)

Solvent Single Point: HF = -895.7737718 hartrees (-562106.9995 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.086635	1.921029	-1.052827
2	1	-0.108880	1.074687	-1.725111
3	1	0.546101	2.744673	-1.622053
4	6	0.917225	1.485540	0.194078
5	6	1.348377	0.043638	0.479561
6	6	-1.018259	1.433981	0.789547
7	1	-0.701099	1.853142	1.735544
8	6	-1.479447	0.090467	0.760176
9	8	1.541014	2.392472	0.813796
10	7	0.650344	-0.870645	1.108681
11	7	-0.721322	-0.918416	1.217666
12	7	-1.186685	2.303395	-0.379188
13	1	-1.111819	3.273875	-0.082774
14	6	2.719768	-0.350407	0.084160
15	6	3.608064	0.569476	-0.514715
16	6	3.184453	-1.671910	0.281931
17	6	4.897272	0.185097	-0.894056
18	1	3.293124	1.597485	-0.650506
19	6	4.472880	-2.046414	-0.087205
20	1	2.503043	-2.384088	0.734025
21	6	5.343027	-1.122125	-0.684278
22	1	5.558865	0.918763	-1.349875
23	1	4.801791	-3.070105	0.080818
24	1	6.346082	-1.419230	-0.981315
25	6	-2.799601	-0.318449	0.197798
26	6	-3.071341	-1.674457	-0.068115
27	6	-3.824509	0.619731	-0.030521
28	6	-4.325487	-2.078556	-0.529728
29	1	-2.278083	-2.392995	0.108052
30	6	-5.072721	0.217766	-0.506057
31	1	-3.621674	1.668080	0.156095
32	6	-5.333396	-1.135285	-0.755810
33	1	-4.514912	-3.132604	-0.721426
34	1	-5.846926	0.961569	-0.681184
35	1	-6.307710	-1.448107	-1.124418

Electrocyclic product, X=NH (Table 1)

HF = -895.7390762 hartrees (-562085.227706262 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.272175 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -895.513667 hartrees (-561943.78117917 kcal/mol)

Solvent Single Point: HF = -895.8285982 hartrees (-562141.4037 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.448774	2.667074	-0.422749
2	1	1.303538	3.173086	-0.896350
3	1	-0.001276	3.380911	0.283506
4	6	1.095983	1.565422	0.436857
5	6	1.368577	0.233334	-0.103102
6	6	-1.653488	1.631400	-1.004067
7	1	-2.581806	2.207116	-1.013563
8	6	-1.675675	0.321426	-0.630099
9	8	1.581072	1.993285	1.502204
10	7	0.563494	-0.581158	-0.831034
11	7	-0.712367	-0.641385	-0.962196
12	7	-0.483116	2.261789	-1.467227
13	1	-0.690283	3.042096	-2.079411
14	6	2.731369	-0.343967	0.082626
15	6	3.114499	-1.497295	-0.652793
16	6	3.719416	0.205018	0.937437
17	6	4.390726	-2.044648	-0.555003
18	1	2.377132	-1.947157	-1.306504
19	6	4.999133	-0.350585	1.029512
20	1	3.468198	1.064177	1.544476
21	6	5.356807	-1.479615	0.288765
22	1	4.633648	-2.926881	-1.145412
23	1	5.721177	0.107850	1.703459
24	1	6.351293	-1.912401	0.370546
25	6	-2.937581	-0.262262	-0.101513
26	6	-3.820468	0.490184	0.697093
27	6	-3.284176	-1.599650	-0.381926
28	6	-5.017912	-0.057220	1.165852
29	1	-3.548406	1.502844	0.978428
30	6	-4.476323	-2.146566	0.092299
31	1	-2.593810	-2.187259	-0.976487
32	6	-5.356750	-1.379172	0.864631
33	1	-5.676715	0.546618	1.785991
34	1	-4.721373	-3.180026	-0.142870
35	1	-6.283440	-1.809256	1.236851

Fragmentation product, X=NH (Table 1)

HF = -895.7095642 hartrees (-562066.708631142 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.272526 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -895.482767 hartrees (-561924.39112017 kcal/mol)

Solvent Single Point: HF = -895.7991577 hartrees (-562122.9294 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.643134	2.055314	0.144547
2	1	-1.561091	1.990400	-0.450408
3	1	-0.225706	3.051890	-0.041517
4	6	0.392177	1.055359	-0.490780
5	6	1.125445	-0.090105	0.130071
6	6	-0.928329	0.595374	1.967354
7	1	-0.218524	0.328813	2.751889
8	6	-1.400120	-0.420123	1.179633
9	8	0.660362	1.412336	-1.651452
10	7	0.668478	-1.229161	0.746416
11	7	-0.524190	-1.544956	1.167023
12	7	-0.952574	1.923641	1.574654
13	1	-0.386897	2.519752	2.164264
14	6	2.592972	-0.179632	-0.137561
15	6	3.370222	-1.123745	0.586176
16	6	3.315454	0.667394	-1.015336
17	6	4.752032	-1.217645	0.438925
18	1	2.853795	-1.787952	1.268670
19	6	4.703599	0.576281	-1.149829
20	1	2.776582	1.385912	-1.617386
21	6	5.444392	-0.365915	-0.431199
22	1	5.295377	-1.962636	1.018209
23	1	5.206691	1.248363	-1.843287
24	1	6.523451	-0.437937	-0.546343
25	6	-2.583933	-0.429783	0.319343
26	6	-3.603211	0.547053	0.411216
27	6	-2.772975	-1.486003	-0.600052
28	6	-4.750782	0.467624	-0.375443
29	1	-3.488070	1.365670	1.115651
30	6	-3.926244	-1.563810	-1.380321
31	1	-1.995999	-2.238988	-0.678595
32	6	-4.925278	-0.589060	-1.278263
33	1	-5.516826	1.234761	-0.282603
34	1	-4.041514	-2.387658	-2.081233
35	1	-5.819883	-0.647201	-1.893219

8 (Figure 4)

HF = -958.3453245 hartrees (-601371.274576995 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.342536 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.049744 hartrees (-601185.79485744 kcal/mol)

Solvent Single Point: HF = -958.4389536 hartrees (-601430.0278 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.781860	0.998712	-0.114234
2	6	-1.467881	-0.397385	-0.051891
3	6	0.625090	0.737491	-0.795935
4	1	0.390587	0.552370	-1.858097
5	6	1.276139	-0.512068	-0.234466
6	8	-1.455467	1.938841	-0.803898
7	7	-0.811444	-1.516849	0.054301
8	7	0.581030	-1.508801	0.212685
9	6	2.753680	-0.719903	-0.184052
10	6	3.348674	-1.317857	0.941814
11	6	3.581615	-0.378599	-1.267861
12	6	4.723052	-1.550908	0.989055
13	1	2.709905	-1.601839	1.771612
14	6	4.956802	-0.623250	-1.226918
15	1	3.142523	0.059626	-2.158618
16	6	5.536818	-1.203583	-0.095498
17	1	5.161484	-2.006584	1.873804
18	1	5.574775	-0.360616	-2.082218
19	1	6.608054	-1.385260	-0.059504
20	6	-2.950478	-0.555242	-0.089644
21	6	-3.539499	-1.702216	0.482855
22	6	-3.792093	0.407571	-0.682640
23	6	-4.920996	-1.890376	0.453931
24	1	-2.890453	-2.437822	0.945448
25	6	-5.176732	0.212800	-0.704937
26	1	-3.302594	1.289268	-1.090783
27	6	-5.749281	-0.932299	-0.143563
28	1	-5.353627	-2.781823	0.903350
29	1	-5.812502	0.964947	-1.167561
30	1	-6.827691	-1.076690	-0.164930
31	6	1.445231	2.040794	-0.706298
32	6	-0.539109	1.424031	1.387400
33	6	1.638584	2.530648	0.738488
34	1	2.417995	1.944640	-1.201444
35	1	0.861234	2.787229	-1.255922
36	6	0.287035	2.714005	1.446191
37	1	-0.035395	0.629129	1.960381
38	1	-1.527384	1.582228	1.835579
39	1	2.198954	3.476949	0.731941
40	1	2.253732	1.810269	1.299321
41	1	0.442089	3.027175	2.489339
42	1	-0.283795	3.501431	0.939794

TS8→9 (Figure 4)

HF = -958.3065158 hartrees (-601346.921729658 kcal/mol)

Imaginary Frequencies: 1 (-250.7803 1/cm)

Zero-point correction = 0.340117 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.013619 hartrees (-601163.12605869 kcal/mol)

Solvent Single Point: HF = -958.3835498 hartrees (-601395.2613 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.211354	1.545909	-0.260400
2	6	1.454594	0.130297	-0.584054
3	6	-0.457630	0.531378	0.788912
4	1	-0.144864	-0.077422	1.650833
5	6	-1.213098	-0.221445	-0.240933
6	8	1.889021	2.211014	0.573522
7	7	0.695021	-0.570463	-1.448728
8	7	-0.633753	-0.576535	-1.390886
9	6	-2.555638	-0.759942	-0.007430
10	6	-3.326800	-1.320305	-1.060921
11	6	-3.151515	-0.737735	1.276868
12	6	-4.607778	-1.810279	-0.839194
13	1	-2.882837	-1.360481	-2.049541
14	6	-4.432271	-1.252620	1.496915
15	1	-2.598413	-0.324358	2.113301
16	6	-5.178909	-1.787491	0.444759
17	1	-5.170840	-2.224733	-1.673492
18	1	-4.849138	-1.227829	2.501917
19	1	-6.179906	-2.176050	0.614358
20	6	2.702831	-0.573624	-0.152149
21	6	2.856702	-1.940095	-0.471257
22	6	3.744897	0.060057	0.555773
23	6	4.006914	-2.640888	-0.113507
24	1	2.055690	-2.426342	-1.017244
25	6	4.894865	-0.649121	0.915630
26	1	3.619317	1.101401	0.824900
27	6	5.036589	-1.999243	0.585199
28	1	4.099121	-3.692409	-0.376665
29	1	5.684664	-0.138168	1.462128
30	1	5.932454	-2.546275	0.870871
31	6	-0.970986	1.875769	1.293182
32	6	0.417877	2.358282	-1.305606
33	6	-1.526028	2.854535	0.244834
34	1	-1.774160	1.677717	2.024864
35	1	-0.157781	2.363839	1.850208
36	6	-0.435241	3.448595	-0.654819
37	1	-0.191950	1.723808	-1.950856
38	1	1.189987	2.819536	-1.939063
39	1	-2.048411	3.667559	0.768871
40	1	-2.278638	2.340987	-0.368807
41	1	-0.891331	4.077115	-1.432663
42	1	0.221635	4.090778	-0.055608

9 (Figure 4)

HF = -958.3657059 hartrees (-601384.064109309 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.342883 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.070627 hartrees (-601198.89914877 kcal/mol)

Solvent Single Point: HF = -958.4476732 hartrees (-601435.4994 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.555119	1.732306	-0.669455
2	6	1.138950	0.263346	-0.462991
3	6	-0.060557	0.074242	0.544634
4	1	0.148934	-0.830280	1.139958
5	6	-1.187535	-0.215623	-0.446821
6	8	2.723593	2.103710	-0.637916
7	7	0.574882	-0.084195	-1.822272
8	7	-0.707721	-0.296625	-1.694754
9	6	-2.539782	-0.607865	-0.145455
10	6	-3.494500	-0.835797	-1.181212
11	6	-3.001538	-0.806218	1.185040
12	6	-4.797846	-1.220438	-0.899497
13	1	-3.170249	-0.701843	-2.207851
14	6	-4.314914	-1.194546	1.457027
15	1	-2.317314	-0.668648	2.015779
16	6	-5.234974	-1.404000	0.425375
17	1	-5.491771	-1.381264	-1.723122
18	1	-4.619354	-1.337766	2.492655
19	1	-6.258224	-1.700897	0.640181
20	6	2.324254	-0.624510	-0.101102
21	6	2.591467	-1.788326	-0.834371
22	6	3.136772	-0.341120	1.009576
23	6	3.631881	-2.648308	-0.466140
24	1	1.970065	-1.997275	-1.698730
25	6	4.174751	-1.197702	1.381443
26	1	2.966718	0.565026	1.582278
27	6	4.428983	-2.359258	0.643995
28	1	3.817084	-3.547228	-1.050226
29	1	4.791156	-0.953774	2.243976
30	1	5.238288	-3.026713	0.931319
31	6	-0.278946	1.200008	1.596571
32	6	0.457335	2.740661	-0.995972
33	6	-0.968021	2.492897	1.127159
34	1	-0.880355	0.781528	2.411915
35	1	0.692018	1.447460	2.052061
36	6	-0.092752	3.418759	0.274660
37	1	-0.358876	2.257440	-1.538706
38	1	0.916496	3.492594	-1.646713
39	1	-1.306463	3.048305	2.013568
40	1	-1.869258	2.223641	0.562038
41	1	-0.684267	4.294877	-0.025420
42	1	0.747630	3.799814	0.872763

10 (Figure 4)

HF = -997.6492986 hartrees (-626034.911364486 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.370942 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.327657 hartrees (-625833.07804407 kcal/mol)

Solvent Single Point: HF = -997.7399346 hartrees (-626091.7864 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.770033	0.819984	-0.173809
2	6	-1.503415	-0.566416	-0.079178
3	6	0.569103	0.445101	-0.951328
4	1	0.199018	0.112190	-1.936744
5	6	1.222634	-0.756817	-0.298427
6	8	-1.449844	1.768401	-0.837463
7	7	-0.879739	-1.703066	0.027075
8	7	0.512560	-1.715722	0.202801
9	6	2.698250	-0.951184	-0.158980
10	6	3.240663	-1.336341	1.079797
11	6	3.572184	-0.816207	-1.251188
12	6	4.610338	-1.559129	1.227020
13	1	2.566936	-1.463761	1.920820
14	6	4.942416	-1.049538	-1.108521
15	1	3.173769	-0.550873	-2.225200
16	6	5.470399	-1.414796	0.133145
17	1	5.007451	-1.847703	2.197333
18	1	5.597185	-0.948776	-1.970781
19	1	6.537661	-1.587963	0.246271
20	6	-2.990756	-0.678948	-0.084321
21	6	-3.601203	-1.780878	0.549810
22	6	-3.815663	0.279275	-0.707169
23	6	-4.988092	-1.930995	0.552497
24	1	-2.964844	-2.513023	1.035128
25	6	-5.204914	0.122717	-0.699186
26	1	-3.312609	1.130362	-1.159523
27	6	-5.799431	-0.978473	-0.075190
28	1	-5.437094	-2.788204	1.049887
29	1	-5.827714	0.870589	-1.185731
30	1	-6.881677	-1.092111	-0.071783
31	6	1.442387	1.683375	-1.207394
32	6	-0.462408	1.223242	1.323833
33	6	1.941505	2.470791	0.022046
34	6	-0.193508	2.721946	1.539366
35	6	0.875455	3.391877	0.643467
36	1	-1.348128	0.970801	1.923332
37	1	0.361635	0.623006	1.736359
38	1	-1.137997	3.254821	1.391263
39	1	0.085491	2.851795	2.596781
40	1	0.363305	3.899071	-0.181718
41	1	1.384334	4.172502	1.229715
42	1	2.361333	1.793838	0.779313
43	1	2.779932	3.101374	-0.309051
44	1	0.819753	2.355999	-1.808461
45	1	2.305812	1.408866	-1.824370

TS10→11 (Figure 4)

HF = -997.6097383 hartrees (-626010.086880633 kcal/mol)

Imaginary Frequencies: 1 (-329.3166 1/cm)

Zero-point correction = 0.368704 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.289405 hartrees (-625809.07453155 kcal/mol)

Solvent Single Point: HF = -997.6859289 hartrees (-626057.8972 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.143349	1.328610	0.316030
2	6	-1.474410	-0.081725	0.601105
3	6	0.372201	0.227195	-0.777746
4	1	-0.048547	-0.448494	-1.539246
5	6	1.168085	-0.504398	0.252869
6	8	-1.797393	2.059251	-0.488397
7	7	-0.748426	-0.850176	1.434537
8	7	0.586654	-0.880355	1.387366
9	6	2.531618	-0.995907	0.033550
10	6	3.351924	-1.402236	1.119002
11	6	3.094740	-1.087099	-1.261628
12	6	4.648378	-1.859038	0.916022
13	1	2.934663	-1.350981	2.118930
14	6	4.394645	-1.560633	-1.460271
15	1	2.500615	-0.801254	-2.122600
16	6	5.189179	-1.945933	-0.378023
17	1	5.249143	-2.155215	1.773946
18	1	4.786930	-1.625783	-2.473292
19	1	6.203988	-2.303461	-0.532855
20	6	-2.762208	-0.701561	0.153193
21	6	-2.997905	-2.062122	0.444339
22	6	-3.763659	0.010290	-0.538222
23	6	-4.187233	-2.684989	0.070758
24	1	-2.227997	-2.605416	0.981403
25	6	-4.953870	-0.620698	-0.913199
26	1	-3.574206	1.048698	-0.781347
27	6	-5.175624	-1.967072	-0.613401
28	1	-4.343602	-3.734242	0.311691
29	1	-5.711837	-0.051346	-1.446861
30	1	-6.102644	-2.452827	-0.910258
31	6	0.914252	1.456657	-1.494465
32	6	-0.317392	2.030560	1.412043
33	6	1.683319	2.546923	-0.708867
34	6	0.033424	3.488988	1.103737
35	6	0.818880	3.722393	-0.207088
36	1	-0.938453	1.996410	2.320546
37	1	0.587716	1.476577	1.663652
38	1	-0.884867	4.085927	1.070424
39	1	0.623835	3.862297	1.953762
40	1	0.108629	3.975865	-1.001316
41	1	1.466599	4.601614	-0.072346
42	1	2.252687	2.099474	0.115972
43	1	2.433783	2.964482	-1.394079
44	1	0.062338	1.929747	-2.004959
45	1	1.582809	1.098406	-2.295736

11 (Figure 4)

HF = -997.6705858 hartrees (-626048.269295358 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.371512 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.348155 hartrees (-625845.94074405 kcal/mol)

Solvent Single Point: HF = -997.7515997 hartrees (-626099.1063 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.499709	1.470719	-0.827141
2	6	1.120195	0.010910	-0.506652
3	6	-0.069182	-0.148771	0.521462
4	1	0.139215	-1.072675	1.089629
5	6	-1.218089	-0.430777	-0.449173
6	8	2.643670	1.904858	-0.743383
7	7	0.545577	-0.441672	-1.831455
8	7	-0.740783	-0.617417	-1.687247
9	6	-2.583723	-0.766696	-0.133934
10	6	-3.538270	-1.009690	-1.166990
11	6	-3.062749	-0.892921	1.199042
12	6	-4.854685	-1.342901	-0.881397
13	1	-3.202575	-0.930253	-2.195526
14	6	-4.390098	-1.228148	1.475338
15	1	-2.383601	-0.740382	2.030444
16	6	-5.308090	-1.455019	0.445986
17	1	-5.546260	-1.518413	-1.704006
18	1	-4.706520	-1.316180	2.513555
19	1	-6.341529	-1.711444	0.664122
20	6	2.327721	-0.824387	-0.099149
21	6	2.595606	-2.040739	-0.743305
22	6	3.163280	-0.442156	0.964175
23	6	3.656297	-2.855309	-0.333546
24	1	1.958365	-2.326951	-1.573270
25	6	4.221703	-1.254388	1.377577
26	1	2.996943	0.505876	1.463868
27	6	4.475028	-2.468245	0.730268
28	1	3.841030	-3.795358	-0.849028
29	1	4.854750	-0.933922	2.202179
30	1	5.300414	-3.100270	1.050165
31	6	-0.235524	0.927316	1.633284
32	6	0.394392	2.366881	-1.380272
33	6	-0.907774	2.295437	1.352450
34	6	0.221821	3.664686	-0.574567
35	6	0.033475	3.451992	0.938656
36	1	0.680044	2.612619	-2.410460
37	1	-0.549553	1.824207	-1.431344
38	1	1.088191	4.317780	-0.735270
39	1	-0.653278	4.192353	-0.979297
40	1	1.015296	3.286826	1.402546
41	1	-0.342622	4.392012	1.365989
42	1	-1.715584	2.170443	0.620535
43	1	-1.398631	2.593771	2.288010
44	1	0.752367	1.107801	2.081821
45	1	-0.815630	0.450151	2.430646

Cyclopentanone reactant (Table 2 and pyridazine figure and scheme in SI)

HF = -919.0300534 hartrees (-576700.548809034 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.313824 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.762647 hartrees (-576532.74861897 kcal/mol)

Solvent Single Point: HF = -919.1305868 hartrees (-576763.6345 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.668581	0.995016	0.587201
2	6	1.260185	-0.321380	0.065598
3	6	-0.837397	1.084840	0.123355
4	1	-1.327267	1.638539	0.933778
5	6	-1.478234	-0.261026	-0.022396
6	8	0.839900	0.935570	1.924722
7	7	0.574373	-1.379878	-0.277845
8	7	-0.818718	-1.353226	-0.263879
9	6	-2.959221	-0.402155	0.056036
10	6	-3.565952	-1.674577	-0.016168
11	6	-3.802630	0.715611	0.197575
12	6	-4.949248	-1.817157	0.046452
13	1	-2.917357	-2.537173	-0.120647
14	6	-5.192132	0.572016	0.261923
15	1	-3.373370	1.709661	0.257696
16	6	-5.776078	-0.693731	0.186375
17	1	-5.388943	-2.810549	-0.009167
18	1	-5.816896	1.455311	0.372534
19	1	-6.856226	-0.806644	0.237967
20	6	2.737118	-0.519227	0.073097
21	6	3.335985	-1.331415	-0.908112
22	6	3.566084	0.094369	1.032101
23	6	4.720249	-1.514362	-0.941604
24	1	2.695411	-1.819389	-1.635370
25	6	4.949572	-0.090829	0.994771
26	1	3.078944	0.683986	1.804187
27	6	5.536733	-0.893243	0.009223
28	1	5.161678	-2.143941	-1.711404
29	1	5.572925	0.385222	1.748769
30	1	6.614727	-1.037533	-0.013555
31	6	-0.876427	1.922959	-1.200170
32	1	-1.485362	2.823968	-1.052049
33	1	-1.330438	1.371519	-2.031521
34	6	0.593626	2.313841	-1.498250
35	1	1.044692	1.581828	-2.181294
36	1	0.669889	3.295326	-1.984561
37	6	1.280278	2.244438	-0.133690
38	1	2.371917	2.205577	-0.192386
39	1	1.010327	3.107545	0.491408

Cyclopentanone reactant (Table 2 and pyridazine figure and scheme in SI)
(solvent optimization, methanol, uaks radii)

HF = -919.133689 hartrees (-576765.58118439 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.314463 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.865732 hartrees (-576597.43548732 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.601758	0.909710	0.721820
2	6	1.245809	-0.366819	0.151250
3	6	-0.808355	1.037337	0.051393
4	1	-1.378033	1.699683	0.716786
5	6	-1.503236	-0.286110	-0.044631
6	8	0.577976	0.792071	2.095852
7	7	0.558315	-1.400476	-0.240105
8	7	-0.847237	-1.398810	-0.179342
9	6	-2.988908	-0.378340	0.009438
10	6	-3.634662	-1.627557	0.118128
11	6	-3.789826	0.776760	-0.057257
12	6	-5.024508	-1.714803	0.158213
13	1	-3.029388	-2.526210	0.173163
14	6	-5.184685	0.688786	-0.023431
15	1	-3.330295	1.756231	-0.141046
16	6	-5.808905	-0.555956	0.085933
17	1	-5.499796	-2.688969	0.248461
18	1	-5.780727	1.596500	-0.081211
19	1	-6.893689	-0.625111	0.117088
20	6	2.725472	-0.524504	0.076757
21	6	3.304392	-1.194749	-1.017699
22	6	3.576183	-0.008383	1.071559
23	6	4.689350	-1.344446	-1.115425
24	1	2.657563	-1.589832	-1.795455
25	6	4.960994	-0.166035	0.976991
26	1	3.136653	0.496669	1.925680
27	6	5.524627	-0.831638	-0.116887
28	1	5.116343	-1.857821	-1.974100
29	1	5.601071	0.230454	1.762010
30	1	6.603323	-0.948194	-0.191327
31	6	-0.596248	1.745908	-1.327499
32	1	-1.323243	2.556554	-1.446282
33	1	-0.748990	1.058509	-2.167218
34	6	0.860192	2.292214	-1.296862
35	1	1.510206	1.661120	-1.915430
36	1	0.928438	3.309274	-1.697357
37	6	1.283396	2.197361	0.172636
38	1	2.367111	2.205633	0.315605
39	1	0.865056	3.031527	0.753386

Cyclopentanone reactant (Table 2 and pyridazine figure and scheme in SI)
(solvent optimization, methanol, ua0 radii)

HF = -919.1277576 hartrees (-576761.859171576 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.313472 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.860247 hartrees (-576593.99359497 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.596020	0.889586	0.743671
2	6	1.242292	-0.364326	0.127717
3	6	-0.806452	1.037381	0.058968
4	1	-1.383595	1.707342	0.708480
5	6	-1.504545	-0.280968	-0.058280
6	8	0.570958	0.705861	2.101752
7	7	0.555741	-1.390371	-0.291049
8	7	-0.849476	-1.389245	-0.232363
9	6	-2.989397	-0.375291	0.003350
10	6	-3.630458	-1.621866	0.160348
11	6	-3.793949	0.774801	-0.108414
12	6	-5.020927	-1.712595	0.199939
13	1	-3.023484	-2.517754	0.255167
14	6	-5.189013	0.682596	-0.075264
15	1	-3.339432	1.754042	-0.227720
16	6	-5.809241	-0.559976	0.079481
17	1	-5.493890	-2.685403	0.328783
18	1	-5.789142	1.586545	-0.169857
19	1	-6.895597	-0.631861	0.110251
20	6	2.722400	-0.522642	0.057175
21	6	3.306203	-1.167051	-1.050627
22	6	3.570016	-0.035938	1.070346
23	6	4.691862	-1.321296	-1.142394
24	1	2.663852	-1.538473	-1.845601
25	6	4.955092	-0.198281	0.981942
26	1	3.126069	0.448386	1.935446
27	6	5.523312	-0.839681	-0.124782
28	1	5.122766	-1.815495	-2.012394
29	1	5.592307	0.174986	1.782799
30	1	6.603449	-0.961690	-0.194196
31	6	-0.552239	1.727661	-1.318160
32	1	-1.337714	2.460445	-1.530310
33	1	-0.575369	0.997402	-2.134567
34	6	0.851468	2.395616	-1.206348
35	1	1.559530	1.894858	-1.877929
36	1	0.826574	3.450503	-1.500937
37	6	1.273313	2.205569	0.257062
38	1	2.357467	2.204453	0.397409
39	1	0.860162	3.002338	0.890659

Cyclopentanone Electrocyclic TS (Table 2 and pyridazine figure and scheme in SI)

HF = -919.0097193 hartrees (-576687.788957943 kcal/mol)

Imaginary Frequencies: 1 (-267.3701 1/cm)

Zero-point correction = 0.311764 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.744425 hartrees (-576521.31413175 kcal/mol)

Solvent Single Point: HF = -919.0960133 hartrees (-576741.9393 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.618767	0.757922	0.934686
2	6	1.171603	-0.180048	-0.143823
3	6	-1.080669	1.430323	-0.272357
4	1	-1.702987	2.023650	0.396269
5	6	-1.564718	0.145660	-0.596038
6	8	0.363349	0.274931	2.066419
7	7	0.520952	-0.779625	-1.113899
8	7	-0.838430	-0.804549	-1.195353
9	6	-2.950591	-0.274254	-0.223086
10	6	-3.246462	-1.636970	-0.033237
11	6	-3.991736	0.655535	-0.058214
12	6	-4.533146	-2.051878	0.310000
13	1	-2.440613	-2.351233	-0.162556
14	6	-5.280085	0.243594	0.292483
15	1	-3.790513	1.709955	-0.221632
16	6	-5.558343	-1.113676	0.478268
17	1	-4.736652	-3.110288	0.456539
18	1	-6.068656	0.983075	0.413338
19	1	-6.560387	-1.436524	0.751162
20	6	2.605904	-0.538872	-0.027812
21	6	3.320400	-1.001623	-1.157003
22	6	3.317594	-0.413301	1.185191
23	6	4.674624	-1.316941	-1.076507
24	1	2.779289	-1.111725	-2.090592
25	6	4.676488	-0.729963	1.260377
26	1	2.783521	-0.100488	2.076467
27	6	5.369266	-1.182788	0.133730
28	1	5.195673	-1.668204	-1.965137
29	1	5.193012	-0.631893	2.213042
30	1	6.426390	-1.430130	0.195511
31	6	-0.232495	2.240503	-1.239245
32	1	-0.828960	3.089249	-1.605146
33	1	0.004319	1.632022	-2.117121
34	6	1.079085	2.762219	-0.575155
35	1	1.954080	2.439392	-1.151637
36	1	1.105426	3.859330	-0.558862
37	6	1.148036	2.203809	0.846323
38	1	2.182799	2.197962	1.220169
39	1	0.558672	2.800115	1.552099

Cyclopentanone Electrocyclic TS (Table 2 and pyridazine figure and scheme in SI)

(solvent optimization, methanol, uaks radii)

HF = -919.096771 hartrees (-576742.41477021 kcal/mol)

Imaginary Frequencies: 1 (-297.4029 1/cm)

Zero-point correction = 0.311308 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.831611 hartrees (-576576.02421861 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.587655	0.627812	0.970972
2	6	1.173661	-0.198752	-0.175075
3	6	-1.101355	1.444331	-0.247406
4	1	-1.734902	2.004649	0.442388
5	6	-1.568792	0.183000	-0.634418
6	8	0.285093	0.011170	2.032044
7	7	0.529990	-0.726388	-1.188788
8	7	-0.833322	-0.730098	-1.309734
9	6	-2.947158	-0.259515	-0.264695
10	6	-3.218543	-1.615402	-0.003411
11	6	-4.008730	0.659924	-0.172474
12	6	-4.503280	-2.037549	0.345474
13	1	-2.405080	-2.331421	-0.070820
14	6	-5.295045	0.240780	0.176966
15	1	-3.827572	1.708705	-0.392562
16	6	-5.547636	-1.110358	0.438403
17	1	-4.689341	-3.089576	0.550975
18	1	-6.102003	0.967877	0.236737
19	1	-6.548724	-1.437769	0.710125
20	6	2.619505	-0.528292	-0.072421
21	6	3.373370	-0.807988	-1.234731
22	6	3.299984	-0.546810	1.164070
23	6	4.733927	-1.104842	-1.161470
24	1	2.874808	-0.783446	-2.198564
25	6	4.664513	-0.842755	1.234530
26	1	2.749118	-0.355115	2.079233
27	6	5.392639	-1.125673	0.075017
28	1	5.286203	-1.312363	-2.075944
29	1	5.157014	-0.858469	2.204678
30	1	6.453984	-1.355662	0.131188
31	6	-0.176642	2.297495	-1.094750
32	1	-0.752076	3.153453	-1.473884
33	1	0.151730	1.734791	-1.973587
34	6	1.053710	2.803214	-0.284101
35	1	1.982666	2.623973	-0.843157
36	1	0.994970	3.888181	-0.117897
37	6	1.082087	2.075579	1.063154
38	1	2.104434	2.039705	1.469789
39	1	0.464148	2.583316	1.812795

Cyclopentanone Fragmentation TS (Table 2)

HF = -918.9956259 hartrees (-576678.945208509 kcal/mol)

Imaginary Frequencies: 1 (-399.9578 1/cm)

Zero-point correction = 0.311324 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.730591 hartrees (-576512.63315841 kcal/mol)

Solvent Single Point: HF = -919.0796645 hartrees (-576731.6803 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.002863	1.318588	-0.166828
2	6	-1.405086	-0.141538	-0.412028
3	6	1.054857	1.211194	-0.847628
4	1	0.536884	1.449603	-1.766083
5	6	1.450787	-0.143101	-0.681224
6	8	-1.561312	2.169413	-0.916178
7	7	-0.692625	-1.123607	-0.900216
8	7	0.676352	-1.206561	-0.909205
9	6	2.824651	-0.530946	-0.209697
10	6	3.010152	-1.668783	0.594717
11	6	3.963279	0.192129	-0.604311
12	6	4.286610	-2.060913	1.002951
13	1	2.131988	-2.239997	0.877444
14	6	5.242370	-0.197979	-0.200881
15	1	3.834427	1.057913	-1.247320
16	6	5.410295	-1.325543	0.609790
17	1	4.406357	-2.942220	1.629259
18	1	6.109106	0.373929	-0.524641
19	1	6.404928	-1.629956	0.927282
20	6	-2.823573	-0.483854	-0.120843
21	6	-3.272475	-1.822224	-0.205665
22	6	-3.766493	0.495156	0.259617
23	6	-4.595867	-2.159885	0.062629
24	1	-2.549832	-2.578407	-0.491520
25	6	-5.092820	0.149998	0.537123
26	1	-3.462653	1.534345	0.301015
27	6	-5.520796	-1.176024	0.441669
28	1	-4.909540	-3.199241	-0.013063
29	1	-5.796356	0.929395	0.822454
30	1	-6.552430	-1.441946	0.660533
31	6	1.626361	2.341463	-0.016811
32	6	-0.505043	1.804003	1.201770
33	6	0.519019	2.915293	0.923899
34	1	2.443618	1.965395	0.608804
35	1	2.045807	3.156960	-0.623794
36	1	-0.051276	0.976766	1.764002
37	1	-1.352248	2.195635	1.783910
38	1	0.954528	3.310265	1.851719
39	1	-0.009075	3.735229	0.425860

Cyclopentanone Electrocyclic product (Table 2)

HF = -919.0190476 hartrees (-576693.642559476 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.311949 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.754786 hartrees (-576527.81576286 kcal/mol)

Solvent Single Point: HF = -919.1029525 hartrees (-576746.2937 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.613144	0.407309	1.139950
2	6	1.209308	-0.232764	-0.095865
3	6	-1.347651	1.711457	-0.582736
4	1	-2.102515	2.315368	-0.082374
5	6	-1.592294	0.372076	-0.731664
6	8	0.115436	-0.271570	2.034116
7	7	0.523675	-0.650216	-1.157452
8	7	-0.769965	-0.550116	-1.372670
9	6	-2.922265	-0.187807	-0.331064
10	6	-3.001157	-1.513080	0.131308
11	6	-4.113244	0.555725	-0.404674
12	6	-4.218964	-2.063122	0.534700
13	1	-2.087527	-2.096468	0.170552
14	6	-5.334103	0.008118	-0.002901
15	1	-4.082538	1.567133	-0.799711
16	6	-5.393704	-1.305714	0.472694
17	1	-4.251205	-3.086968	0.900238
18	1	-6.241925	0.603515	-0.074504
19	1	-6.343449	-1.735836	0.782169
20	6	2.643712	-0.509263	-0.076096
21	6	3.325223	-0.951812	-1.242357
22	6	3.431510	-0.340839	1.091359
23	6	4.691167	-1.209152	-1.231696
24	1	2.741159	-1.089914	-2.145601
25	6	4.805398	-0.590546	1.090765
26	1	2.956404	-0.043881	2.021836
27	6	5.455671	-1.027257	-0.067441
28	1	5.173401	-1.550209	-2.146343
29	1	5.369043	-0.453381	2.011826
30	1	6.524995	-1.222855	-0.066550
31	6	-0.109809	2.417990	-1.059200
32	1	-0.396402	3.348501	-1.571533
33	1	0.384567	1.792369	-1.807188
34	6	0.907618	2.775212	0.071130
35	1	1.928378	2.691477	-0.320258
36	1	0.778904	3.825541	0.366480
37	6	0.762562	1.919313	1.340732
38	1	1.660690	2.052575	1.963109
39	1	-0.084175	2.242844	1.954107

Cyclopentanone Fragmentation product (Table 2)

HF = -919.006867 hartrees (-576685.99911117 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.312441 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.742027 hartrees (-576519.80936277 kcal/mol)

Solvent Single Point: HF = -919.089045 hartrees (-576737.5666 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.023241	1.414222	0.238325
2	6	-1.404671	0.054606	-0.247269
3	6	1.405667	1.346233	-1.302024
4	1	0.533336	1.633783	-1.888528
5	6	1.511599	0.027297	-0.989521
6	8	-1.749018	2.389481	-0.002406
7	7	-0.697810	-0.840888	-0.965730
8	7	0.545648	-0.943935	-1.342513
9	6	2.698205	-0.566528	-0.302734
10	6	2.518892	-1.588201	0.647908
11	6	4.015221	-0.192984	-0.626280
12	6	3.611147	-2.175786	1.288748
13	1	1.508931	-1.920385	0.866493
14	6	5.110732	-0.783093	0.008313
15	1	4.172648	0.552936	-1.399925
16	6	4.914382	-1.773636	0.976233
17	1	3.445304	-2.956077	2.027845
18	1	6.119363	-0.479697	-0.263440
19	1	5.765919	-2.237211	1.468429
20	6	-2.829979	-0.340823	-0.077038
21	6	-3.323897	-1.533778	-0.663708
22	6	-3.749015	0.388488	0.716635
23	6	-4.634366	-1.963435	-0.467977
24	1	-2.641297	-2.113797	-1.273561
25	6	-5.060897	-0.047302	0.912094
26	1	-3.439770	1.321296	1.172257
27	6	-5.525785	-1.228005	0.324383
28	1	-4.964841	-2.885769	-0.943249
29	1	-5.727702	0.551116	1.530738
30	1	-6.549303	-1.563015	0.475200
31	6	2.040216	2.450605	-0.498290
32	6	0.185216	1.695230	1.150812
33	6	1.053273	2.867445	0.638544
34	1	2.974662	2.110555	-0.043992
35	1	2.279518	3.330763	-1.110534
36	1	0.780065	0.797576	1.335300
37	1	-0.266759	1.990868	2.108899
38	1	1.624498	3.299342	1.470937
39	1	0.366520	3.642281	0.281170

Cyclohexanone reactant (Table 2)

HF = -958.3453245 hartrees (-601371.274576995 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.342536 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.049744 hartrees (-601185.79485744 kcal/mol)

Solvent Single Point: HF = -958.4389536 hartrees (-601430.0278 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.781860	0.998712	-0.114234
2	6	-1.467881	-0.397385	-0.051891
3	6	0.625090	0.737491	-0.795935
4	1	0.390587	0.552370	-1.858097
5	6	1.276139	-0.512068	-0.234466
6	8	-1.455467	1.938841	-0.803898
7	7	-0.811444	-1.516849	0.054301
8	7	0.581030	-1.508801	0.212685
9	6	2.753680	-0.719903	-0.184052
10	6	3.348674	-1.317857	0.941814
11	6	3.581615	-0.378599	-1.267861
12	6	4.723052	-1.550908	0.989055
13	1	2.709905	-1.601839	1.771612
14	6	4.956802	-0.623250	-1.226918
15	1	3.142523	0.059626	-2.158618
16	6	5.536818	-1.203583	-0.095498
17	1	5.161484	-2.006584	1.873804
18	1	5.574775	-0.360616	-2.082218
19	1	6.608054	-1.385260	-0.059504
20	6	-2.950478	-0.555242	-0.089644
21	6	-3.539499	-1.702216	0.482855
22	6	-3.792093	0.407571	-0.682640
23	6	-4.920996	-1.890376	0.453931
24	1	-2.890453	-2.437822	0.945448
25	6	-5.176732	0.212800	-0.704937
26	1	-3.302594	1.289268	-1.090783
27	6	-5.749281	-0.932299	-0.143563
28	1	-5.353627	-2.781823	0.903350
29	1	-5.812502	0.964947	-1.167561
30	1	-6.827691	-1.076690	-0.164930
31	6	1.445231	2.040794	-0.706298
32	6	-0.539109	1.424031	1.387400
33	6	1.638584	2.530648	0.738488
34	1	2.417995	1.944640	-1.201444
35	1	0.861234	2.787229	-1.255922
36	6	0.287035	2.714005	1.446191
37	1	-0.035395	0.629129	1.960381
38	1	-1.527384	1.582228	1.835579
39	1	2.198954	3.476949	0.731941
40	1	2.253732	1.810269	1.299321
41	1	0.442089	3.027175	2.489339
42	1	-0.283795	3.501431	0.939794

Cyclohexanone 1,2-shift TS (Table 2)

HF = -958.3065158 hartrees (-601346.921729658 kcal/mol)

Imaginary Frequencies: 1 (-250.7803 1/cm)

Zero-point correction = 0.340117 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.013619 hartrees (-601163.12605869 kcal/mol)

Solvent Single Point: HF = -958.3835498 hartrees (-601395.2613 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.211354	1.545909	-0.260400
2	6	1.454594	0.130297	-0.584054
3	6	-0.457630	0.531378	0.788912
4	1	-0.144864	-0.077422	1.650833
5	6	-1.213098	-0.221445	-0.240933
6	8	1.889021	2.211014	0.573522
7	7	0.695021	-0.570463	-1.448728
8	7	-0.633753	-0.576535	-1.390886
9	6	-2.555638	-0.759942	-0.007430
10	6	-3.326800	-1.320305	-1.060921
11	6	-3.151515	-0.737735	1.276868
12	6	-4.607778	-1.810279	-0.839194
13	1	-2.882837	-1.360481	-2.049541
14	6	-4.432271	-1.252620	1.496915
15	1	-2.598413	-0.324358	2.113301
16	6	-5.178909	-1.787491	0.444759
17	1	-5.170840	-2.224733	-1.673492
18	1	-4.849138	-1.227829	2.501917
19	1	-6.179906	-2.176050	0.614358
20	6	2.702831	-0.573624	-0.152149
21	6	2.856702	-1.940095	-0.471257
22	6	3.744897	0.060057	0.555773
23	6	4.006914	-2.640888	-0.113507
24	1	2.055690	-2.426342	-1.017244
25	6	4.894865	-0.649121	0.915630
26	1	3.619317	1.101401	0.824900
27	6	5.036589	-1.999243	0.585199
28	1	4.099121	-3.692409	-0.376665
29	1	5.684664	-0.138168	1.462128
30	1	5.932454	-2.546275	0.870871
31	6	-0.970986	1.875769	1.293182
32	6	0.417877	2.358282	-1.305606
33	6	-1.526028	2.854535	0.244834
34	1	-1.774160	1.677717	2.024864
35	1	-0.157781	2.363839	1.850208
36	6	-0.435241	3.448595	-0.654819
37	1	-0.191950	1.723808	-1.950856
38	1	1.189987	2.819536	-1.939063
39	1	-2.048411	3.667559	0.768871
40	1	-2.278638	2.340987	-0.368807
41	1	-0.891331	4.077115	-1.432663
42	1	0.221635	4.090778	-0.055608

Cyclohexanone Fragmentation TS (Table 2)

HF = -958.3179839 hartrees (-601354.118077089 kcal/mol)

Imaginary Frequencies: 1 (-374.4852 1/cm)

Zero-point correction = 0.340125 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.025301 hartrees (-601170.45663051 kcal/mol)

Solvent Single Point: HF = -958.3987723 hartrees (-601404.8136 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.960212	1.103627	-0.014276
2	6	-1.534899	-0.311509	-0.233724
3	6	0.885702	0.721934	-1.254273
4	1	0.093716	0.645456	-1.989013
5	6	1.298950	-0.494404	-0.675988
6	8	-1.495458	2.056413	-0.630433
7	7	-0.871871	-1.396713	-0.535802
8	7	0.485367	-1.536412	-0.456472
9	6	2.704288	-0.767037	-0.221976
10	6	2.945215	-1.528021	0.935169
11	6	3.811269	-0.328310	-0.966175
12	6	4.246798	-1.817732	1.347858
13	1	2.089060	-1.896356	1.490933
14	6	5.116110	-0.620317	-0.559934
15	1	3.640761	0.230508	-1.880359
16	6	5.341035	-1.362028	0.603771
17	1	4.409459	-2.403458	2.249926
18	1	5.957299	-0.274153	-1.156290
19	1	6.355648	-1.587664	0.923675
20	6	-3.001483	-0.484330	-0.069045
21	6	-3.602175	-1.746229	-0.293726
22	6	-3.849304	0.573558	0.325791
23	6	-4.971878	-1.934669	-0.140591
24	1	-2.957162	-2.566436	-0.588402
25	6	-5.224938	0.377475	0.482846
26	1	-3.429512	1.559616	0.481857
27	6	-5.801327	-0.873197	0.251879
28	1	-5.399535	-2.918799	-0.322588
29	1	-5.848584	1.216468	0.784783
30	1	-6.871332	-1.022736	0.375919
31	6	1.581445	2.062313	-1.149533
32	6	-0.235368	1.392314	1.304088
33	6	1.896825	2.481078	0.305840
34	1	2.510472	2.140745	-1.741329
35	1	0.896438	2.807335	-1.576232
36	6	0.660964	2.639605	1.211529
37	1	0.333888	0.512486	1.626460
38	1	-1.017054	1.563730	2.064312
39	1	2.440655	3.438147	0.290814
40	1	2.581937	1.749996	0.753910
41	1	0.997500	2.913386	2.221709
42	1	0.043427	3.467577	0.842118

Cyclohexanone 1,2-shift product (Table 2)

HF = -958.3657059 hartrees (-601384.064109309 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.342883 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.070627 hartrees (-601198.89914877 kcal/mol)

Solvent Single Point: HF = -958.4476732 hartrees (-601435.4994 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.555119	1.732306	-0.669455
2	6	1.138950	0.263346	-0.462991
3	6	-0.060557	0.074242	0.544634
4	1	0.148934	-0.830280	1.139958
5	6	-1.187535	-0.215623	-0.446821
6	8	2.723593	2.103710	-0.637916
7	7	0.574882	-0.084195	-1.822272
8	7	-0.707721	-0.296625	-1.694754
9	6	-2.539782	-0.607865	-0.145455
10	6	-3.494500	-0.835797	-1.181212
11	6	-3.001538	-0.806218	1.185040
12	6	-4.797846	-1.220438	-0.899497
13	1	-3.170249	-0.701843	-2.207851
14	6	-4.314914	-1.194546	1.457027
15	1	-2.317314	-0.668648	2.015779
16	6	-5.234974	-1.404000	0.425375
17	1	-5.491771	-1.381264	-1.723122
18	1	-4.619354	-1.337766	2.492655
19	1	-6.258224	-1.700897	0.640181
20	6	2.324254	-0.624510	-0.101102
21	6	2.591467	-1.788326	-0.834371
22	6	3.136772	-0.341120	1.009576
23	6	3.631881	-2.648308	-0.466140
24	1	1.970065	-1.997275	-1.698730
25	6	4.174751	-1.197702	1.381443
26	1	2.966718	0.565026	1.582278
27	6	4.428983	-2.359258	0.643995
28	1	3.817084	-3.547228	-1.050226
29	1	4.791156	-0.953774	2.243976
30	1	5.238288	-3.026713	0.931319
31	6	-0.278946	1.200008	1.596571
32	6	0.457335	2.740661	-0.995972
33	6	-0.968021	2.492897	1.127159
34	1	-0.880355	0.781528	2.411915
35	1	0.692018	1.447460	2.052061
36	6	-0.092752	3.418759	0.274660
37	1	-0.358876	2.257440	-1.538706
38	1	0.916496	3.492594	-1.646713
39	1	-1.306463	3.048305	2.013568
40	1	-1.869258	2.223641	0.562038
41	1	-0.684267	4.294877	-0.025420
42	1	0.747630	3.799814	0.872763

Cyclohexanone Fragmentation product (Table 2)

HF = -958.3256389 hartrees (-601358.921666139 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.340904 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -958.033665 hartrees (-601175.70512415 kcal/mol)

Solvent Single Point: HF = -958.40535 hartrees (-601408.9412 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.137780	1.242816	0.220818
2	6	-1.602738	-0.130254	-0.135051
3	6	1.162682	0.864388	-1.432008
4	1	0.183977	1.014567	-1.877754
5	6	1.359377	-0.344353	-0.831373
6	8	-1.708811	2.252140	-0.206010
7	7	-0.871974	-1.184398	-0.534249
8	7	0.402131	-1.372239	-0.757560
9	6	2.678851	-0.784319	-0.278191
10	6	2.723480	-1.570487	0.887459
11	6	3.895654	-0.494219	-0.919460
12	6	3.938945	-2.003336	1.421077
13	1	1.785374	-1.849189	1.356736
14	6	5.113770	-0.930027	-0.392983
15	1	3.879371	0.060730	-1.851936
16	6	5.143306	-1.680521	0.787096
17	1	3.945748	-2.602880	2.328490
18	1	6.040442	-0.694999	-0.911875
19	1	6.090399	-2.022579	1.197458
20	6	-3.058790	-0.409635	-0.053308
21	6	-3.560432	-1.696530	-0.380108
22	6	-4.014492	0.541355	0.382108
23	6	-4.912488	-2.008154	-0.269004
24	1	-2.850064	-2.441324	-0.719242
25	6	-5.370131	0.222703	0.489765
26	1	-3.695926	1.549068	0.618202
27	6	-5.841498	-1.053477	0.168023
28	1	-5.247387	-3.010540	-0.531237
29	1	-6.065414	0.990052	0.826042
30	1	-6.898394	-1.296410	0.248090
31	6	1.976159	2.128549	-1.236947
32	6	-0.039713	1.441475	1.274524
33	6	2.139997	2.515336	0.253868
34	1	2.979988	2.081231	-1.683302
35	1	1.460691	2.946343	-1.757270
36	6	0.839899	2.696027	1.064682
37	1	0.554283	0.535228	1.409431
38	1	-0.615367	1.571640	2.206069
39	1	2.706857	3.458342	0.307560
40	1	2.762599	1.757653	0.745662
41	1	1.127754	3.082732	2.052084
42	1	0.210104	3.465645	0.601627

2,2,6-Trimethylcyclohexanone reactant (Table 2)

HF = -1076.2851767 hartrees (-675379.711231017 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.426087 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1075.908719 hartrees (-675143.48025969 kcal/mol)

Solvent Single Point: HF = -1076.367877 hartrees (-675431.6062 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.720424	0.836444	0.340995
2	6	1.389906	-0.557569	0.080496
3	6	-0.697440	0.463893	1.038091
4	6	-1.362390	-0.670187	0.268045
5	8	1.433560	1.601587	1.183048
6	7	0.718721	-1.655662	-0.108959
7	7	-0.667824	-1.609981	-0.288064
8	6	-2.840327	-0.827761	0.092579
9	6	-3.350865	-1.254490	-1.148060
10	6	-3.753359	-0.617501	1.140962
11	6	-4.719494	-1.444077	-1.338847
12	1	-2.650934	-1.443548	-1.954817
13	6	-5.123922	-0.817646	0.954713
14	1	-3.389320	-0.322101	2.118172
15	6	-5.616571	-1.224602	-0.287815
16	1	-5.087109	-1.765613	-2.310449
17	1	-5.806278	-0.658144	1.786149
18	1	-6.683579	-1.372264	-0.434623
19	6	2.869548	-0.758974	0.103359
20	6	3.425466	-1.804813	-0.662729
21	6	3.740215	0.044203	0.867177
22	6	4.799877	-2.044463	-0.666172
23	1	2.757499	-2.423348	-1.252315
24	6	5.116275	-0.200146	0.857878
25	1	3.285127	0.851733	1.433224
26	6	5.655616	-1.242003	0.096662
27	1	5.203944	-2.854735	-1.269420
28	1	5.772330	0.430532	1.454259
29	1	6.728216	-1.424887	0.093332
30	6	-1.510948	1.771525	1.153043
31	6	0.513334	1.604630	-1.080732
32	6	-1.711301	2.520316	-0.168474
33	1	-2.477872	1.593148	1.636987
34	1	-0.925638	2.412912	1.822930
35	6	-0.358758	2.850801	-0.807002
36	1	-2.268856	3.448708	0.023198
37	1	-2.333338	1.930004	-0.854958
38	1	-0.504937	3.401715	-1.749687
39	1	0.199442	3.504383	-0.125996
40	6	-0.410400	-0.044370	2.476044
41	1	0.075016	-1.025716	2.473576
42	1	0.264061	0.674748	2.949105
43	1	-1.337986	-0.125300	3.057449
44	6	1.896973	2.091886	-1.553006
45	1	2.404359	2.605947	-0.733255
46	1	2.530484	1.259366	-1.880246
47	1	1.783627	2.778149	-2.404991
48	6	-0.104489	0.790687	-2.240059
49	1	0.445532	-0.137733	-2.425105
50	1	-1.151152	0.525477	-2.078252
51	1	-0.061634	1.388669	-3.162378

2,2,6-Trimethylcyclohexanone 1,2-shift TS (Table 2)

HF = -1076.245302 hartrees (-675354.68945802 kcal/mol)

Imaginary Frequencies: 1 (-160.3784 1/cm)

Zero-point correction = 0.423385 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1075.873117 hartrees (-675121.13964867 kcal/mol)

Solvent Single Point: HF = -1076.31591 hartrees (-675398.9964 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.266653	1.219195	0.192528
2	6	1.368120	-0.106889	-0.443974
3	6	-0.652396	0.148097	1.012320
4	6	-1.379971	-0.354399	-0.173702
5	8	1.890124	1.500278	1.253918
6	7	0.552498	-0.578281	-1.400546
7	7	-0.769547	-0.506161	-1.353805
8	6	-2.777572	-0.806097	-0.132897
9	6	-3.483156	-1.139085	-1.320640
10	6	-3.501391	-0.898798	1.080477
11	6	-4.817834	-1.525261	-1.288480
12	1	-2.946293	-1.086997	-2.261159
13	6	-4.838085	-1.304276	1.107610
14	1	-3.009688	-0.661262	2.016254
15	6	-5.515456	-1.618604	-0.073039
16	1	-5.323510	-1.767378	-2.221542
17	1	-5.352409	-1.370555	2.064368
18	1	-6.556578	-1.930505	-0.051789
19	6	2.556655	-0.985495	-0.185603
20	6	2.607453	-2.255551	-0.802467
21	6	3.645341	-0.613097	0.630771
22	6	3.697560	-3.105549	-0.627042
23	1	1.773600	-2.545718	-1.431968
24	6	4.735558	-1.470643	0.805958
25	1	3.607682	0.343151	1.136025
26	6	4.772889	-2.719936	0.181983
27	1	3.705991	-4.075414	-1.119780
28	1	5.559704	-1.156679	1.442925
29	1	5.620925	-3.385417	0.327434
30	6	-1.069556	1.473973	1.624764
31	6	0.823385	2.479540	-0.659098
32	6	-1.366644	2.667486	0.704892
33	1	-1.978787	1.272590	2.225531
34	1	-0.292619	1.768277	2.345805
35	6	-0.095379	3.364898	0.207879
36	1	-1.962062	3.397239	1.271089
37	1	-1.993587	2.347931	-0.136756
38	1	-0.364022	4.257850	-0.376129
39	1	0.476215	3.708783	1.078535
40	6	-0.248957	-0.834748	2.095745
41	1	-0.130710	-1.852415	1.711733
42	1	0.711576	-0.509107	2.521426
43	1	-0.968123	-0.865090	2.934560
44	6	2.146991	3.251333	-0.908990
45	1	1.935487	4.196636	-1.426842
46	1	2.653349	3.463632	0.035186
47	1	2.827434	2.667019	-1.540858
48	6	0.181098	2.254627	-2.042979
49	1	0.798371	1.614710	-2.678617
50	1	-0.808998	1.801733	-1.995520
51	1	0.083569	3.231521	-2.536900

2,2,6-Trimethylcyclohexanone Fragmentation TS (Table 2)

HF = -1076.257075 hartrees (-675362.07713325 kcal/mol)

Imaginary Frequencies: 1 (-301.5678 1/cm)

Zero-point correction = 0.423634 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1075.883556 hartrees (-675127.69022556 kcal/mol)

Solvent Single Point: HF = -1076.33296 hartrees (-675409.6958 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.954215	0.988007	0.197258
2	6	1.448356	-0.472941	0.277241
3	6	-1.019406	0.532105	1.420045
4	6	-1.411451	-0.620129	0.687478
5	8	1.474330	1.808578	0.992518
6	7	0.748585	-1.552524	0.515964
7	7	-0.606149	-1.661466	0.445115
8	6	-2.803123	-0.854164	0.161616
9	6	-3.012102	-1.655112	-0.976493
10	6	-3.936104	-0.373293	0.839748
11	6	-4.299220	-1.935440	-1.436814
12	1	-2.141218	-2.065518	-1.476155
13	6	-5.227154	-0.651504	0.383097
14	1	-3.802639	0.207602	1.745161
15	6	-5.416285	-1.428959	-0.763122
16	1	-4.432546	-2.553260	-2.322120
17	1	-6.085887	-0.267993	0.929422
18	1	-6.420012	-1.644794	-1.121676
19	6	2.910065	-0.717770	0.116382
20	6	3.388764	-2.037577	-0.064894
21	6	3.869611	0.317398	0.147123
22	6	4.748560	-2.306406	-0.192308
23	1	2.659804	-2.839551	-0.094789
24	6	5.234276	0.042511	0.017255
25	1	3.539633	1.335744	0.308949
26	6	5.689002	-1.267054	-0.153410
27	1	5.079547	-3.333582	-0.333128
28	1	5.946139	0.864573	0.055662
29	1	6.750904	-1.476368	-0.259509
30	6	-1.687481	1.888243	1.299110
31	6	0.414357	1.566216	-1.153815
32	6	-1.890571	2.389072	-0.143062
33	1	-2.644411	1.960412	1.849785
34	1	-1.019355	2.602892	1.803016
35	6	-0.581715	2.723292	-0.877982
36	1	-2.497250	3.307030	-0.114628
37	1	-2.477643	1.663247	-0.717265
38	1	-0.831948	3.175010	-1.850351
39	1	-0.045333	3.487949	-0.302389
40	6	-0.294632	0.330600	2.733025
41	1	0.577369	0.994455	2.816726
42	1	-0.977594	0.575088	3.566603
43	1	0.039840	-0.700385	2.872808
44	6	1.641834	2.185307	-1.877978
45	1	2.130857	2.926567	-1.239267
46	1	2.379113	1.419677	-2.142140
47	1	1.319174	2.677502	-2.805462
48	6	-0.190351	0.516437	-2.100642
49	1	0.488053	-0.333473	-2.231964
50	1	-1.144196	0.127018	-1.749736
51	1	-0.358758	0.966422	-3.088380

2,2,6-Trimethylcyclohexanone 1,2-shift product (Table 2)

HF = -1076.2959135 hartrees (-675386.448680385 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.426414 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1075.919800 hartrees (-675150.433698 kcal/mol)

Solvent Single Point: HF = -1076.37512 hartrees (-675436.1512 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.527370	1.475385	-0.324322
2	6	1.051436	-0.020260	-0.330830
3	6	-0.147571	-0.470452	0.617888
4	6	-1.293314	-0.452904	-0.415117
5	8	2.723216	1.685441	-0.496953
6	7	0.493712	-0.143003	-1.729638
7	7	-0.791568	-0.352354	-1.651080
8	6	-2.698277	-0.732036	-0.228346
9	6	-3.573100	-0.831246	-1.353582
10	6	-3.310919	-0.905244	1.044212
11	6	-4.929964	-1.084536	-1.208896
12	1	-3.142547	-0.702993	-2.340684
13	6	-4.677044	-1.160403	1.178684
14	1	-2.712420	-0.839220	1.944936
15	6	-5.510672	-1.254948	0.060659
16	1	-5.551722	-1.152413	-2.100308
17	1	-5.092472	-1.285711	2.177433
18	1	-6.573895	-1.452421	0.169028
19	6	2.302914	-0.893635	-1.169964
20	6	2.651431	-1.829832	-1.150232
21	6	3.112030	-0.809165	0.974851
22	6	3.762391	-2.665501	-0.988112
23	1	2.037220	-1.881598	-2.042873
24	6	4.218085	-1.642178	1.145251
25	1	2.882492	-0.074036	1.740953
26	6	4.550853	-2.580131	0.161109
27	1	4.010877	-3.384169	-1.766202
28	1	4.825956	-1.553995	2.043110
29	1	5.414859	-3.228335	0.288711
30	6	-0.307881	0.396705	1.895238
31	6	0.598619	2.729889	-0.222541
32	6	-0.907349	1.800152	1.740923
33	1	-0.932477	-0.162288	2.602152
34	1	0.673886	0.473860	2.387719
35	6	0.062071	2.868823	1.229068
36	1	-1.263471	2.129310	2.727712
37	1	-1.793667	1.746523	1.099544
38	1	-0.436108	3.847665	1.287095
39	1	0.923369	2.925595	1.912095
40	6	0.019939	-1.941431	1.094279
41	1	0.251437	-2.602795	0.255869
42	1	0.816931	-2.047913	1.839466
43	1	-0.917438	-2.285431	1.542933
44	6	1.467789	3.976775	-0.502563
45	1	0.841808	4.874932	-0.430586
46	1	2.294108	4.066875	0.208081
47	1	1.902938	3.935237	-1.504875
48	6	-0.566919	2.747568	-1.235215
49	1	-0.187898	2.690094	-2.258957
50	1	-1.268269	1.926698	-1.098321
51	1	-1.115730	3.692125	-1.118035

2,2,6-Trimethylcyclohexanone Fragmentation product (Table 2)

HF = -1076.2629891 hartrees (-675365.788290141 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.424274 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1075.889887 hartrees (-675131.66299137 kcal/mol)

Solvent Single Point: HF = -1076.340123 hartrees (-675414.1903 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.053726	1.079220	0.071453
2	6	1.455507	-0.361727	0.345230
3	6	-1.267926	0.695928	1.647607
4	6	-1.449851	-0.481717	0.955690
5	8	1.481094	1.981272	0.796177
6	7	0.736414	-1.392284	0.794285
7	7	-0.545189	-1.553072	1.042297
8	6	-2.708772	-0.869389	0.240701
9	6	-2.685366	-1.928868	-0.689495
10	6	-3.966871	-0.315552	0.550960
11	6	-3.850858	-2.375758	-1.314376
12	1	-1.732044	-2.404062	-0.892567
13	6	-5.134080	-0.756371	-0.074723
14	1	-4.035882	0.457612	1.307245
15	6	-5.084387	-1.787006	-1.019671
16	1	-3.795228	-3.191749	-2.031502
17	1	-6.087613	-0.303275	0.187756
18	1	-5.993211	-2.134038	-1.505474
19	6	2.891160	-0.668620	0.152009
20	6	3.344103	-2.015145	0.165129
21	6	3.881019	0.322347	-0.063802
22	6	4.684005	-2.339529	-0.017888
23	1	2.606181	-2.791117	0.333253
24	6	5.225096	-0.011208	-0.251320
25	1	3.603196	1.369437	-0.050346
26	6	5.648412	-1.342630	-0.232101
27	1	4.982501	-3.386529	0.001288
28	1	5.949114	0.787350	-0.404045
29	1	6.694998	-1.599101	-0.377091
30	6	-1.908670	2.029621	1.294809
31	6	0.336342	1.530508	-1.239963
32	6	-2.015848	2.350373	-0.213029
33	1	-2.902209	2.155484	1.758732
34	1	-1.287206	2.811213	1.754207
35	6	-0.693417	2.662047	-0.946764
36	1	-2.644671	3.248055	-0.314605
37	1	-2.555181	1.553759	-0.733221
38	1	-0.961905	3.090947	-1.923983
39	1	-0.161662	3.447809	-0.396694
40	6	-0.358493	0.725943	2.852096
41	1	0.581341	1.263698	2.676980
42	1	-0.882265	1.251977	3.666704
43	1	-0.118029	-0.286149	3.187786
44	6	1.466407	2.168904	-2.098467
45	1	1.918597	3.018187	-1.577745
46	1	2.255364	1.442510	-2.319693
47	1	1.051714	2.520227	-3.052058
48	6	-0.266270	0.382820	-2.059994
49	1	0.484935	-0.389763	-2.254678
50	1	-1.107594	-0.093748	-1.562918
51	1	-0.620367	0.763450	-3.027355

Cycloheptanone reactant (Table 2)

HF = -997.6492986 hartrees (-626034.911364486 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.370942 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.327657 hartrees (-625833.07804407 kcal/mol)

Solvent Single Point: HF = -997.7399346 hartrees (-626091.7864 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.770033	0.819984	-0.173809
2	6	-1.503415	-0.566416	-0.079178
3	6	0.569103	0.445101	-0.951328
4	1	0.199018	0.112190	-1.936744
5	6	1.222634	-0.756817	-0.298427
6	8	-1.449844	1.768401	-0.837463
7	7	-0.879739	-1.703066	0.027075
8	7	0.512560	-1.715722	0.202801
9	6	2.698250	-0.951184	-0.158980
10	6	3.240663	-1.336341	1.079797
11	6	3.572184	-0.816207	-1.251188
12	6	4.610338	-1.559129	1.227020
13	1	2.566936	-1.463761	1.920820
14	6	4.942416	-1.049538	-1.108521
15	1	3.173769	-0.550873	-2.225200
16	6	5.470399	-1.414796	0.133145
17	1	5.007451	-1.847703	2.197333
18	1	5.597185	-0.948776	-1.970781
19	1	6.537661	-1.587963	0.246271
20	6	-2.990756	-0.678948	-0.084321
21	6	-3.601203	-1.780878	0.549810
22	6	-3.815663	0.279275	-0.707169
23	6	-4.988092	-1.930995	0.552497
24	1	-2.964844	-2.513023	1.035128
25	6	-5.204914	0.122717	-0.699186
26	1	-3.312609	1.130362	-1.159523
27	6	-5.799431	-0.978473	-0.075190
28	1	-5.437094	-2.788204	1.049887
29	1	-5.827714	0.870589	-1.185731
30	1	-6.881677	-1.092111	-0.071783
31	6	1.442387	1.683375	-1.207394
32	6	-0.462408	1.223242	1.323833
33	6	1.941505	2.470791	0.022046
34	6	-0.193508	2.721946	1.539366
35	6	0.875455	3.391877	0.643467
36	1	-1.348128	0.970801	1.923332
37	1	0.361635	0.623006	1.736359
38	1	-1.137997	3.254821	1.391263
39	1	0.085491	2.851795	2.596781
40	1	0.363305	3.899071	-0.181718
41	1	1.384334	4.172502	1.229715
42	1	2.361333	1.793838	0.779313
43	1	2.779932	3.101374	-0.309051
44	1	0.819753	2.355999	-1.808461
45	1	2.305812	1.408866	-1.824370

Cycloheptanone 1,2-shift TS (Table 2)

HF = -997.6097383 hartrees (-626010.086880633 kcal/mol)

Imaginary Frequencies: 1 (-329.3166 1/cm)

Zero-point correction = 0.368704 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.289405 hartrees (-625809.07453155 kcal/mol)

Solvent Single Point: HF = -997.6859289 hartrees (-626057.8972 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.143349	1.328610	0.316030
2	6	-1.474410	-0.081725	0.601105
3	6	0.372201	0.227195	-0.777746
4	1	-0.048547	-0.448494	-1.539246
5	6	1.168085	-0.504398	0.252869
6	8	-1.797393	2.059251	-0.488397
7	7	-0.748426	-0.850176	1.434537
8	7	0.586654	-0.880355	1.387366
9	6	2.531618	-0.995907	0.033550
10	6	3.351924	-1.402236	1.119002
11	6	3.094740	-1.087099	-1.261628
12	6	4.648378	-1.859038	0.916022
13	1	2.934663	-1.350981	2.118930
14	6	4.394645	-1.560633	-1.460271
15	1	2.500615	-0.801254	-2.122600
16	6	5.189179	-1.945933	-0.378023
17	1	5.249143	-2.155215	1.773946
18	1	4.786930	-1.625783	-2.473292
19	1	6.203988	-2.303461	-0.532855
20	6	-2.762208	-0.701561	0.153193
21	6	-2.997905	-2.062122	0.444339
22	6	-3.763659	0.010290	-0.538222
23	6	-4.187233	-2.684989	0.070758
24	1	-2.227997	-2.605416	0.981403
25	6	-4.953870	-0.620698	-0.913199
26	1	-3.574206	1.048698	-0.781347
27	6	-5.175624	-1.967072	-0.613401
28	1	-4.343602	-3.734242	0.311691
29	1	-5.711837	-0.051346	-1.446861
30	1	-6.102644	-2.452827	-0.910258
31	6	0.914252	1.456657	-1.494465
32	6	-0.317392	2.030560	1.412043
33	6	1.683319	2.546923	-0.708867
34	6	0.033424	3.488988	1.103737
35	6	0.818880	3.722393	-0.207088
36	1	-0.938453	1.996410	2.320546
37	1	0.587716	1.476577	1.663652
38	1	-0.884867	4.085927	1.070424
39	1	0.623835	3.862297	1.953762
40	1	0.108629	3.975865	-1.001316
41	1	1.466599	4.601614	-0.072346
42	1	2.252687	2.099474	0.115972
43	1	2.433783	2.964482	-1.394079
44	1	0.062338	1.929747	-2.004959
45	1	1.582809	1.098406	-2.295736

Cycloheptanone Fragmentation TS (Table 2)

HF = -997.628431 hartrees (-626021.81673681 kcal/mol)

Imaginary Frequencies: 1 (-357.3449 1/cm)

Zero-point correction = 0.369254 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.307166 hartrees (-625820.21973666 kcal/mol)

Solvent Single Point: HF = -997.7080088 hartrees (-626071.7526 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.044427	1.018992	0.000197
2	6	-1.662242	-0.387921	-0.161217
3	6	0.737246	0.469629	-1.267658
4	1	-0.114347	0.292510	-1.916323
5	6	1.170805	-0.676458	-0.577195
6	8	-1.505981	1.979159	-0.664247
7	7	-1.012863	-1.511850	-0.316328
8	7	0.340355	-1.663768	-0.202880
9	6	2.594499	-0.955784	-0.199854
10	6	2.897927	-1.674179	0.970762
11	6	3.656721	-0.579975	-1.037469
12	6	4.217235	-1.980913	1.304682
13	1	2.073760	-1.995927	1.598945
14	6	4.979864	-0.890323	-0.709572
15	1	3.436675	-0.057343	-1.962825
16	6	5.267863	-1.587551	0.466908
17	1	4.428534	-2.531457	2.218732
18	1	5.785111	-0.592135	-1.377191
19	1	6.296576	-1.827401	0.725547
20	6	-3.139109	-0.511425	-0.055262
21	6	-3.763103	-1.773529	-0.201251
22	6	-3.974896	0.599762	0.189536
23	6	-5.144186	-1.913174	-0.112435
24	1	-3.127355	-2.632679	-0.384012
25	6	-5.362590	0.452955	0.281228
26	1	-3.533139	1.584788	0.279107
27	6	-5.961916	-0.799391	0.131801
28	1	-5.590547	-2.898775	-0.230158
29	1	-5.977330	1.331360	0.466778
30	1	-7.041358	-0.910143	0.203938
31	6	1.405826	1.792964	-1.547528
32	6	-0.420242	1.292913	1.370806
33	6	2.331331	2.430432	-0.482204
34	6	0.509723	2.517899	1.437718
35	6	1.967767	2.250302	1.006137
36	1	-1.278496	1.456832	2.044749
37	1	0.092804	0.395522	1.737600
38	1	0.525371	2.869185	2.478735
39	1	0.067040	3.325761	0.841312
40	1	2.243292	1.237851	1.323661
41	1	2.628156	2.924489	1.571977
42	1	2.373037	3.507881	-0.703474
43	1	3.358425	2.063675	-0.603914
44	1	0.564565	2.484038	-1.708309
45	1	1.960050	1.796657	-2.505212

Cycloheptanone 1,2-shift product (Table 2)

HF = -997.6705858 hartrees (-626048.269295358 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.371512 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.348155 hartrees (-625845.94074405 kcal/mol)

Solvent Single Point: HF = -997.7515997 hartrees (-626099.1063 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.499709	1.470719	-0.827141
2	6	1.120195	0.010910	-0.506652
3	6	-0.069182	-0.148771	0.521462
4	1	0.139215	-1.072675	1.089629
5	6	-1.218089	-0.430777	-0.449173
6	8	2.643670	1.904858	-0.743383
7	7	0.545577	-0.441672	-1.831455
8	7	-0.740783	-0.617417	-1.687247
9	6	-2.583723	-0.766696	-0.133934
10	6	-3.538270	-1.009690	-1.166990
11	6	-3.062749	-0.892921	1.199042
12	6	-4.854685	-1.342901	-0.881397
13	1	-3.202575	-0.930253	-2.195526
14	6	-4.390098	-1.228148	1.475338
15	1	-2.383601	-0.740382	2.030444
16	6	-5.308090	-1.455019	0.445986
17	1	-5.546260	-1.518413	-1.704006
18	1	-4.706520	-1.316180	2.513555
19	1	-6.341529	-1.711444	0.664122
20	6	2.327721	-0.824387	-0.099149
21	6	2.595606	-2.040739	-0.743305
22	6	3.163280	-0.442156	0.964175
23	6	3.656297	-2.855309	-0.333546
24	1	1.958365	-2.326951	-1.573270
25	6	4.221703	-1.254388	1.377577
26	1	2.996943	0.505876	1.463868
27	6	4.475028	-2.468245	0.730268
28	1	3.841030	-3.795358	-0.849028
29	1	4.854750	-0.933922	2.202179
30	1	5.300414	-3.100270	1.050165
31	6	-0.235524	0.927316	1.633284
32	6	0.394392	2.366881	-1.380272
33	6	-0.907774	2.295437	1.352450
34	6	0.221821	3.664686	-0.574567
35	6	0.033475	3.451992	0.938656
36	1	0.680044	2.612619	-2.410460
37	1	-0.549553	1.824207	-1.431344
38	1	1.088191	4.317780	-0.735270
39	1	-0.653278	4.192353	-0.979297
40	1	1.015296	3.286826	1.402546
41	1	-0.342622	4.392012	1.365989
42	1	-1.715584	2.170443	0.620535
43	1	-1.398631	2.593771	2.288010
44	1	0.752367	1.107801	2.081821
45	1	-0.815630	0.450151	2.430646

Cycloheptanone Fragmentation product (Table 2)

HF = -997.6350416 hartrees (-626025.964954416 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.369501 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -997.315638 hartrees (-625825.53600138 kcal/mol)

Solvent Single Point: HF = -997.7134972 hartrees (-626075.1966 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.258320	1.165724	0.221288
2	6	-1.763979	-0.208331	-0.091798
3	6	0.982489	0.609997	-1.426782
4	1	-0.028075	0.703039	-1.809913
5	6	1.214288	-0.529542	-0.710473
6	8	-1.695020	2.179207	-0.329059
7	7	-1.036784	-1.308543	-0.329095
8	7	0.249742	-1.521090	-0.459676
9	6	2.569972	-0.969983	-0.256586
10	6	2.705465	-1.762603	0.898610
11	6	3.733430	-0.678943	-0.989679
12	6	3.957610	-2.203030	1.329984
13	1	1.804821	-2.038977	1.436920
14	6	4.988465	-1.122643	-0.565026
15	1	3.647144	-0.118633	-1.914848
16	6	5.109362	-1.881196	0.603255
17	1	4.034894	-2.807155	2.231170
18	1	5.871531	-0.885555	-1.154319
19	1	6.084940	-2.228906	0.934679
20	6	-3.226917	-0.432342	-0.056338
21	6	-3.758221	-1.735827	-0.240385
22	6	-4.166144	0.601582	0.181271
23	6	-5.125799	-1.984333	-0.179021
24	1	-3.058362	-2.541490	-0.429696
25	6	-5.538054	0.344740	0.238137
26	1	-3.819086	1.621037	0.298403
27	6	-6.039868	-0.947836	0.061159
28	1	-5.485876	-3.001688	-0.323715
29	1	-6.221320	1.172918	0.418347
30	1	-7.108737	-1.143217	0.102015
31	6	1.800759	1.868338	-1.622014
32	6	-0.293247	1.320697	1.396636
33	6	2.649847	2.411291	-0.438389
34	6	0.663746	2.535791	1.331992
35	6	2.140806	2.200838	1.004634
36	1	-0.975400	1.436076	2.255174
37	1	0.245320	0.385604	1.570449
38	1	0.642087	3.035509	2.308592
39	1	0.251172	3.258384	0.617541
40	1	2.340531	1.167088	1.304485
41	1	2.788521	2.818398	1.644003
42	1	2.779779	3.489985	-0.613709
43	1	3.658091	1.981469	-0.478129
44	1	1.073551	2.646271	-1.886966
45	1	2.469787	1.809284	-2.499466

Cyclooctanone reactant (Table 2)

HF = -1036.9581996 hartrees (-650701.639830996 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.399563 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1036.608797 hartrees (-650482.38620547 kcal/mol)

Solvent Single Point: HF = -1037.044202 hartrees (-650755.6071 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.776465	0.606339	-0.256291
2	6	-1.434091	-0.801026	-0.085676
3	6	0.720973	0.342746	-0.739302
4	1	0.606261	0.201296	-1.827094
5	6	1.307840	-0.930517	-0.150780
6	8	-1.435279	1.332506	-1.186196
7	7	-0.791485	-1.912486	0.113320
8	7	0.595261	-1.908207	0.304176
9	6	2.781657	-1.178240	-0.077283
10	6	3.354766	-1.716601	1.087898
11	6	3.620432	-0.943504	-1.180671
12	6	4.720428	-1.995701	1.153822
13	1	2.707202	-1.920251	1.934499
14	6	4.985605	-1.234252	-1.121157
15	1	3.195304	-0.550685	-2.099684
16	6	5.544994	-1.755383	0.049075
17	1	5.142635	-2.404411	2.068870
18	1	5.612044	-1.053975	-1.991460
19	1	6.608744	-1.973878	0.099057
20	6	-2.919694	-0.969628	-0.126141
21	6	-3.500663	-1.996916	0.646958
22	6	-3.772647	-0.151540	-0.894166
23	6	-4.880187	-2.205153	0.652879
24	1	-2.846539	-2.627372	1.239400
25	6	-5.154949	-0.362340	-0.880000
26	1	-3.300843	0.638979	-1.468850
27	6	-5.717905	-1.386716	-0.113060
28	1	-5.302044	-3.002880	1.260646
29	1	-5.796192	0.279701	-1.480375
30	1	-6.794429	-1.545313	-0.109069
31	6	1.658593	1.555546	-0.507550
32	6	-0.845765	1.247807	1.203257
33	6	1.092954	2.908347	-1.001909
34	1	-0.032241	0.869966	1.842795
35	1	-1.774254	0.866432	1.645791
36	6	-0.936783	2.789178	1.283933
37	6	1.056290	4.001018	0.078333
38	1	1.689228	3.273092	-1.850725
39	1	0.075348	2.734112	-1.369067
40	6	0.382880	3.584115	1.403331
41	1	-1.512495	3.119133	0.409421
42	1	-1.540377	3.029382	2.170204
43	1	2.075104	4.355949	0.305411
44	1	0.517861	4.867757	-0.333198
45	1	1.090408	3.005698	2.014657
46	1	0.193246	4.503017	1.977894
47	1	1.889656	1.609014	0.563485
48	1	2.622598	1.364565	-0.988504

Cyclooctanone Electrocyclic TS (Table 2)

HF = -1036.9179349 hartrees (-650676.373329099 kcal/mol)

Imaginary Frequencies: 1 (-164.5891 1/cm)

Zero-point correction = 0.397249 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1036.570930 hartrees (-650458.6242843 kcal/mol)

Solvent Single Point: HF = -1036.991444 hartrees (-650722.5011 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.340814	0.999552	0.047748
2	6	1.356222	-0.432632	-0.357866
3	6	-1.016103	0.622171	0.609220
4	1	-1.167743	0.424352	1.679277
5	6	-1.485835	-0.403176	-0.279922
6	8	1.912696	1.432032	1.075738
7	7	0.537040	-1.011474	-1.227307
8	7	-0.784030	-0.886366	-1.338698
9	6	-2.772802	-1.090636	-0.054276
10	6	-3.153482	-2.228332	-0.807802
11	6	-3.690107	-0.623603	0.915782
12	6	-4.387834	-2.842515	-0.615381
13	1	-2.448974	-2.609911	-1.538116
14	6	-4.913602	-1.263085	1.128782
15	1	-3.440758	0.254598	1.502031
16	6	-5.278560	-2.372421	0.360850
17	1	-4.652205	-3.711407	-1.214965
18	1	-5.591108	-0.881308	1.889754
19	1	-6.234819	-2.864815	0.520179
20	6	2.535188	-1.281013	0.003142
21	6	2.794056	-2.465165	-0.728519
22	6	3.422829	-0.962149	1.053629
23	6	3.890939	-3.272195	-0.439560
24	1	2.111612	-2.725948	-1.529182
25	6	4.517327	-1.783586	1.344260
26	1	3.234785	-0.069926	1.636213
27	6	4.765154	-2.941066	0.604498
28	1	4.063227	-4.169771	-1.030121
29	1	5.178282	-1.510980	2.164466
30	1	5.616280	-3.577134	0.836838
31	6	-1.401262	2.054807	0.259432
32	6	1.282510	1.938494	-1.197882
33	6	-0.741658	3.150791	1.118437
34	1	0.417907	1.723586	-1.831372
35	1	2.149369	1.594086	-1.780411
36	6	1.476153	3.453048	-0.950433
37	6	-0.542877	4.479151	0.374266
38	1	-1.347539	3.329391	2.018554
39	1	0.231411	2.798081	1.466843
40	6	0.221628	4.355934	-0.961623
41	1	2.023065	3.572266	-0.006837
42	1	2.143205	3.822225	-1.740766
43	1	-1.514140	4.959202	0.176144
44	1	0.007777	5.165932	1.034061
45	1	-0.458684	4.009354	-1.751587
46	1	0.524702	5.368776	-1.264686
47	1	-1.229081	2.229014	-0.804735
48	1	-2.501397	2.144714	0.363868

Cyclooctanone Fragmentation TS (Table 2)

HF = -1036.9377968 hartrees (-650688.836869968 kcal/mol)

Imaginary Frequencies: 1 (-352.6731 1/cm)

Zero-point correction = 0.397526 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1036.590090 hartrees (-650470.6473759 kcal/mol)

Solvent Single Point: HF = -1037.01594 hartrees (-650737.8726 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.954018	0.746616	0.185651
2	6	-1.629361	-0.630044	-0.066837
3	6	0.724760	0.261356	-1.174389
4	1	-0.123997	0.132917	-1.842204
5	6	1.153983	-0.931166	-0.525605
6	8	-1.507365	1.752146	-0.336593
7	7	-1.016477	-1.757440	-0.279513
8	7	0.343149	-1.899924	-0.112993
9	6	2.586141	-1.209971	-0.160880
10	6	2.913895	-1.667584	1.126347
11	6	3.621134	-1.090405	-1.102411
12	6	4.232388	-1.973504	1.468375
13	1	2.112480	-1.792096	1.847073
14	6	4.940916	-1.407377	-0.768576
15	1	3.383889	-0.761089	-2.109098
16	6	5.254501	-1.843955	0.521905
17	1	4.462931	-2.317745	2.474030
18	1	5.723754	-1.315492	-1.517956
19	1	6.281643	-2.084440	0.785837
20	6	-3.117101	-0.703203	-0.039526
21	6	-3.772597	-1.886309	-0.450562
22	6	-3.922462	0.364914	0.406332
23	6	-5.159845	-1.993197	-0.421667
24	1	-3.158976	-2.714931	-0.786465
25	6	-5.316321	0.252370	0.436276
26	1	-3.451529	1.293303	0.703751
27	6	-5.948199	-0.922347	0.023835
28	1	-5.632716	-2.917710	-0.747048
29	1	-5.909271	1.096036	0.783141
30	1	-7.032273	-1.006106	0.047524
31	1	0.055319	-0.112369	1.892366
32	6	-0.269520	0.879034	1.555555
33	6	0.914305	1.855848	1.673359
34	1	-1.070935	1.197129	2.243497
35	6	0.704418	3.279605	1.097097
36	1	1.791268	1.397039	1.204510
37	1	1.160332	1.931111	2.742271
38	6	1.486260	3.598259	-0.192318
39	1	-0.360644	3.446171	0.912860
40	1	1.022316	4.015967	1.850383
41	6	1.663106	1.376920	-1.602698
42	6	1.132085	2.835318	-1.487914
43	1	1.347200	4.671453	-0.395544
44	1	2.563811	3.470732	0.005626
45	1	1.937948	1.227574	-2.663239
46	1	2.609894	1.321149	-1.051976
47	1	0.047847	2.850081	-1.634479
48	1	1.581124	3.408623	-2.312675

Cyclooctanone Electrocyclic product (Table 2)

HF = -1036.9638777 hartrees (-650705.202895527 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.398322 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1036.617566 hartrees (-650487.88884066 kcal/mol)

Solvent Single Point: HF = -1037.040177 hartrees (-650753.0817 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.007450	-1.234826	0.739440
2	6	-0.924318	-0.851055	-0.342075
3	6	2.470013	1.254198	-0.679693
4	1	2.746177	2.145861	-0.117093
5	6	1.138967	0.999224	-0.822200
6	8	-0.254909	-1.162977	1.950156
7	7	-0.490195	-0.537558	-1.587603
8	7	0.622575	0.111398	-1.794508
9	6	0.173656	1.953449	-0.169726
10	6	0.337370	2.360951	1.163808
11	6	-0.873711	2.530047	-0.910805
12	6	-0.503405	3.320244	1.734328
13	1	1.111895	1.895615	1.765241
14	6	-1.715732	3.485863	-0.342927
15	1	-1.021660	2.215189	-1.938777
16	6	-1.534032	3.891327	0.984012
17	1	-0.364277	3.604093	2.774953
18	1	-2.519625	3.913507	-0.937612
19	1	-2.195501	4.630504	1.429295
20	6	-2.370456	-1.117896	-0.213335
21	6	-3.222539	-0.943331	-1.333943
22	6	-2.979030	-1.558142	0.986775
23	6	-4.584053	-1.228268	-1.267630
24	1	-2.782609	-0.588425	-2.259073
25	6	-4.346961	-1.831042	1.047508
26	1	-2.368372	-1.666226	1.874242
27	6	-5.166906	-1.676010	-0.074813
28	1	-5.199731	-1.088498	-2.154463
29	1	-4.775946	-2.164587	1.990663
30	1	-6.232976	-1.883410	-0.019310
31	6	3.625146	0.454834	-1.227620
32	6	1.239800	-2.044418	0.311335
33	6	4.713445	0.168878	-0.141902
34	1	1.383952	-1.958439	-0.766287
35	1	0.961040	-3.091183	0.512505
36	6	2.555441	-1.711549	1.037934
37	6	5.006908	-1.314674	0.194755
38	1	5.664420	0.635089	-0.434978
39	1	4.412671	0.679740	0.780434
40	6	3.781627	-2.249202	0.261232
41	1	2.621223	-0.625074	1.132102
42	1	2.532441	-2.105050	2.060135
43	1	5.700624	-1.729331	-0.551665
44	1	5.549575	-1.338565	1.151612
45	1	3.471285	-2.464688	-0.768586
46	1	4.102726	-3.216579	0.673117
47	1	3.247559	-0.470317	-1.671938
48	1	4.095632	1.006091	-2.057714

Cyclooctanone Fragmentation product (Table 2)

HF = -1036.9554973 hartrees (-650699.944110723 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.398127 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1036.609316 hartrees (-650482.71188316 kcal/mol)

Solvent Single Point: HF = -1037.032396 hartrees (-650748.199 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.303952	0.934210	-0.729204
2	6	1.780214	-0.359457	-0.220793
3	6	-0.934703	0.343452	1.302833
4	1	0.103216	0.603247	1.494704
5	6	-1.166699	-0.730782	0.495842
6	8	1.879832	2.006274	-0.466782
7	7	1.053693	-1.498788	-0.110596
8	7	-0.225572	-1.672102	0.016581
9	6	-2.553637	-1.199426	0.166744
10	6	-2.872009	-1.571992	-1.151238
11	6	-3.553701	-1.338879	1.143584
12	6	-4.150068	-2.018742	-1.489390
13	1	-2.095319	-1.519683	-1.907266
14	6	-4.834188	-1.792752	0.812185
15	1	-3.316376	-1.112503	2.178274
16	6	-5.142543	-2.127000	-0.508958
17	1	-4.370133	-2.291668	-2.518859
18	1	-5.586981	-1.895672	1.590475
19	1	-6.137284	-2.480466	-0.769354
20	6	3.237093	-0.573230	-0.002468
21	6	3.701297	-1.839976	0.438191
22	6	4.228564	0.413825	-0.224286
23	6	5.056970	-2.107241	0.614043
24	1	2.964429	-2.611366	0.627848
25	6	5.586044	0.140485	-0.040185
26	1	3.925785	1.406644	-0.528580
27	6	6.022243	-1.120074	0.378369
28	1	5.362089	-3.097236	0.949039
29	1	6.310269	0.932239	-0.224245
30	1	7.079828	-1.324746	0.528168
31	1	-0.077066	-0.033307	-2.103593
32	6	0.213831	0.981341	-1.813753
33	6	-1.074329	1.811242	-1.554680
34	1	0.745749	1.424211	-2.668062
35	6	-0.918623	3.182151	-0.848013
36	1	-1.766164	1.196018	-0.982077
37	1	-1.554367	1.959024	-2.532183
38	6	-1.910895	3.435869	0.307865
39	1	0.101238	3.292618	-0.470687
40	1	-1.053204	3.981993	-1.590131
41	6	-1.928236	1.305976	1.901657
42	6	-1.587812	2.804266	1.684469
43	1	-1.956691	4.523511	0.466676
44	1	-2.926901	3.137010	0.004098
45	1	-1.983306	1.154094	2.994674
46	1	-2.940282	1.120887	1.524792
47	1	-0.525960	2.970548	1.913356
48	1	-2.154654	3.371047	2.438412

12 (n=1, pyridazine figure and scheme in SI and footnote 26)

HF = -879.702823 hartrees (-552022.31846073 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.283797 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.464323 hartrees (-551872.65732573 kcal/mol)

Solvent Single Point: HF = -879.7870874 hartrees (-552075.1952 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.778438	2.243697	-0.760265
2	1	1.220673	1.862059	-1.685194
3	1	1.269746	3.179533	-0.471522
4	6	-0.793740	2.269441	-0.807030
5	1	-1.261429	2.178452	-1.796909
6	1	-1.203524	3.166158	-0.318651
7	6	0.694286	1.156518	0.356719
8	6	1.312537	-0.198937	0.311910
9	6	-0.755339	1.022175	0.054839
10	6	-1.433734	-0.141249	0.292803
11	8	0.987240	1.865807	1.633021
12	7	0.575026	-1.280823	0.592596
13	7	-0.750607	-1.280093	0.698790
14	6	-2.887501	-0.321866	0.063946
15	6	-3.448671	-1.611613	-0.021565
16	6	-3.754822	0.780503	-0.066643
17	6	-4.816418	-1.787868	-0.235030
18	1	-2.779753	-2.458089	0.088473
19	6	-5.121847	0.603862	-0.291236
20	1	-3.351735	1.784155	0.024345
21	6	-5.664104	-0.682877	-0.377368
22	1	-5.224376	-2.794830	-0.295884
23	1	-5.767033	1.474340	-0.389770
24	1	-6.729019	-0.821904	-0.548723
25	6	2.738881	-0.412345	0.037578
26	6	3.270515	-1.712389	-0.145049
27	6	3.643109	0.670793	-0.059103
28	6	4.623064	-1.911828	-0.408527
29	1	2.587808	-2.552047	-0.070859
30	6	4.996405	0.466801	-0.335776
31	1	3.281071	1.678591	0.113210
32	6	5.503531	-0.824872	-0.513287
33	1	4.996945	-2.925507	-0.542172
34	1	5.662083	1.325460	-0.401139
35	1	6.558113	-0.983030	-0.726137
36	1	0.764030	1.238935	2.335556

12 (n=1, pyridazine figure and scheme in SI and footnote 26)

HF = -879.7882136 hartrees (-552075.901916136 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.282706 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.551162 hartrees (-551927.14966662 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.776666	2.167289	-0.858072
2	1	1.222934	1.729549	-1.760642
3	1	1.266703	3.123660	-0.628796
4	6	-0.796568	2.184486	-0.916152
5	1	-1.257411	2.026447	-1.899847
6	1	-1.218102	3.105150	-0.488686
7	6	0.690573	1.152992	0.323413
8	6	1.318669	-0.201419	0.353128
9	6	-0.757373	0.994203	0.024283
10	6	-1.438440	-0.148553	0.334139
11	8	0.972370	1.915097	1.565965
12	7	0.591363	-1.257800	0.720884
13	7	-0.752541	-1.251777	0.834000
14	6	-2.892731	-0.332977	0.089019
15	6	-3.446029	-1.609151	-0.129725
16	6	-3.763084	0.774855	0.064957
17	6	-4.813778	-1.771120	-0.366053
18	1	-2.787861	-2.472156	-0.116929
19	6	-5.129269	0.615654	-0.179328
20	1	-3.366061	1.767751	0.255938
21	6	-5.663574	-0.659793	-0.395441
22	1	-5.216151	-2.768009	-0.534583
23	1	-5.779220	1.488138	-0.190592
24	1	-6.727684	-0.785622	-0.581991
25	6	2.749169	-0.415580	0.061233
26	6	3.284760	-1.707546	-0.146308
27	6	3.640962	0.676256	-0.033034
28	6	4.639534	-1.896643	-0.419135
29	1	2.617864	-2.562566	-0.094398
30	6	4.995355	0.486634	-0.318622
31	1	3.271389	1.681449	0.139693
32	6	5.508186	-0.800830	-0.511334
33	1	5.019231	-2.905009	-0.573030
34	1	5.654413	1.350323	-0.382160
35	1	6.562702	-0.948734	-0.732073
36	1	0.668372	1.363343	2.314382

TS12→pyridazines (n=1, pyridazine figure and scheme in SI and footnote 26)

HF = -879.6806217 hartrees (-552008.386922967 kcal/mol)

Imaginary Frequencies: 1 (-123.8210 1/cm)

Zero-point correction = 0.281583 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.444764 hartrees (-551860.38385764 kcal/mol)**Solvent Single Point: HF = -879.787017 hartrees (-552075.151 kcal/mol)**

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.758621	2.191001	-1.046889
2	1	1.083655	2.046756	-2.086395
3	1	1.324430	2.978864	-0.553284
4	6	-0.814788	2.284863	-0.908507
5	1	-1.389014	2.391885	-1.837742
6	1	-1.112588	3.057705	-0.193066
7	6	0.646944	0.885270	-0.272734
8	6	1.299276	-0.332764	-0.004860
9	6	-0.747561	0.889480	-0.306067
10	6	-1.460761	-0.251774	0.035678
11	8	1.257180	2.290239	1.565748
12	7	0.558117	-1.417250	0.306090
13	7	-0.771240	-1.385524	0.347795
14	6	-2.939677	-0.359907	0.043860
15	6	-3.571106	-1.616196	0.119531
16	6	-3.751887	0.787278	-0.019446
17	6	-4.961950	-1.718192	0.124763
18	1	-2.943544	-2.498537	0.178166
19	6	-5.144702	0.683558	-0.016569
20	1	-3.288880	1.767494	-0.055527
21	6	-5.759482	-0.569903	0.053986
22	1	-5.427574	-2.699374	0.183500
23	1	-5.749793	1.585867	-0.062338
24	1	-6.843646	-0.651232	0.057582
25	6	2.768812	-0.494098	-0.030664
26	6	3.368179	-1.704489	-0.420037
27	6	3.583417	0.588589	0.353496
28	6	4.758604	-1.828691	-0.445180
29	1	2.730202	-2.538205	-0.696782
30	6	4.974091	0.454778	0.324610
31	1	3.082398	1.483491	0.736649
32	6	5.568301	-0.746833	-0.078084
33	1	5.211966	-2.768464	-0.753278
34	1	5.597868	1.290559	0.634296
35	1	6.651789	-0.844045	-0.098133
36	1	1.061150	1.842912	2.401843

TS12→pyridazines (n=1, pyridazine figure and scheme in SI and footnote 26)**(solvent optimization, methanol, ua0 radii)**

HF = -879.7738438 hartrees (-552066.884722938 kcal/mol)

Imaginary Frequencies: 1 (-267.4212 1/cm)

Zero-point correction = 0.280250 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -879.540020 hartrees (-551920.1579502 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.767757	2.224893	-0.919044
2	1	1.203819	1.996997	-1.898772
3	1	1.255968	3.099389	-0.487436
4	6	-0.811678	2.245205	-0.939752
5	1	-1.281781	2.208023	-1.929347
6	1	-1.240192	3.082064	-0.377001
7	6	0.659938	0.997463	-0.014009
8	6	1.324911	-0.243883	0.196535
9	6	-0.739342	0.929083	-0.181773
10	6	-1.443553	-0.208980	0.168234
11	8	0.973444	2.041501	1.759209
12	7	0.592312	-1.308897	0.570896
13	7	-0.745709	-1.297656	0.618889
14	6	-2.914605	-0.358785	0.046224
15	6	-3.505613	-1.623506	-0.135859
16	6	-3.755417	0.769017	0.103487
17	6	-4.891168	-1.754788	-0.255117
18	1	-2.867920	-2.501825	-0.189107
19	6	-5.141313	0.637925	-0.018267
20	1	-3.326348	1.754232	0.264393
21	6	-5.716135	-0.625078	-0.198237
22	1	-5.328185	-2.742211	-0.399389
23	1	-5.772834	1.523828	0.034928
24	1	-6.796246	-0.728215	-0.292729
25	6	2.782194	-0.436274	0.028544
26	6	3.339248	-1.718232	-0.153892
27	6	3.650453	0.673046	0.021712
28	6	4.714537	-1.883432	-0.328571
29	1	2.682161	-2.583799	-0.163494
30	6	5.026225	0.507012	-0.158935
31	1	3.243092	1.663894	0.194041
32	6	5.566848	-0.771711	-0.334565
33	1	5.122652	-2.883699	-0.469615
34	1	5.678441	1.379590	-0.154401
35	1	6.639000	-0.901555	-0.475167
36	1	0.594881	1.393286	2.380626

12 (n=2, pyridazine figure and scheme in SI and footnote 26)

HF = -919.0525897 hartrees (-576714.690562647 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.313917 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.784548 hartrees (-576546.49171548 kcal/mol)

Solvent Single Point: HF = -919.1356715 hartrees (-576766.8252 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.687402	1.025489	0.314282
2	6	1.306673	-0.336744	0.212841
3	6	-0.772040	0.905392	0.011233
4	1	0.551479	0.918201	2.304755
5	6	-1.410898	-0.297684	0.195713
6	8	0.892854	1.594269	1.702521
7	7	0.590412	-1.454329	0.346237
8	7	-0.733809	-1.478209	0.433930
9	6	-2.885677	-0.467354	0.091208
10	6	-3.426962	-1.681906	-0.374389
11	6	-3.785066	0.543988	0.476679
12	6	-4.806786	-1.867101	-0.469358
13	1	-2.734382	-2.471204	-0.645666
14	6	-5.167326	0.361341	0.379469
15	1	-3.395116	1.473990	0.877876
16	6	-5.688394	-0.844903	-0.098197
17	1	-5.197897	-2.813792	-0.836352
18	1	-5.838178	1.160160	0.688440
19	1	-6.763740	-0.989062	-0.173413
20	6	2.762828	-0.531473	0.067387
21	6	3.281430	-1.760273	-0.405746
22	6	3.699451	0.472012	0.403989
23	6	4.652088	-1.968015	-0.541556
24	1	2.574148	-2.543624	-0.656251
25	6	5.073272	0.264215	0.258147
26	1	3.342035	1.406942	0.820845
27	6	5.565848	-0.955180	-0.217590
28	1	5.013388	-2.925782	-0.911895
29	1	5.764126	1.058943	0.533538
30	1	6.635564	-1.116220	-0.329163
31	6	-1.256347	2.188908	-0.617868
32	1	-1.467184	2.966284	0.135953
33	1	-2.160974	2.068662	-1.223261
34	6	-0.026814	2.613329	-1.453340
35	1	-0.045642	2.077011	-2.410522
36	1	-0.010026	3.688028	-1.676563
37	6	1.198077	2.167024	-0.619829
38	1	2.021724	1.836994	-1.257843
39	1	1.567058	2.991703	-0.000253

12 (n=2, pyridazine figure and scheme in SI and footnote 26)

(solvent optimization, methanol, uaks radii)

HF = -919.1369028 hartrees (-576767.597876028 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.313139 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.870041 hartrees (-576600.13942791 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.683955	1.018285	0.311575
2	6	1.313286	-0.345182	0.268596
3	6	-0.774430	0.876308	0.007539
4	1	0.509808	1.003079	2.323306
5	6	-1.414834	-0.311875	0.250940
6	8	0.882541	1.630212	1.673531
7	7	0.606907	-1.448945	0.496450
8	7	-0.734331	-1.470987	0.587451
9	6	-2.890427	-0.477164	0.114514
10	6	-3.438292	-1.638970	-0.461278
11	6	-3.779014	0.514708	0.569005
12	6	-4.821047	-1.800308	-0.584647
13	1	-2.766476	-2.415636	-0.814735
14	6	-5.162888	0.356696	0.447030
15	1	-3.382154	1.411108	1.037617
16	6	-5.691567	-0.802038	-0.131938
17	1	-5.219499	-2.705331	-1.038564
18	1	-5.828126	1.136494	0.811796
19	1	-6.767838	-0.926904	-0.226764
20	6	2.773556	-0.530889	0.087917
21	6	3.291638	-1.731558	-0.446315
22	6	3.702330	0.470520	0.445827
23	6	4.664921	-1.926678	-0.603194
24	1	2.597451	-2.511759	-0.743775
25	6	5.076978	0.279448	0.280255
26	1	3.342464	1.396757	0.880827
27	6	5.570709	-0.920685	-0.243223
28	1	5.029396	-2.863291	-1.020716
29	1	5.765489	1.070026	0.572144
30	1	6.640453	-1.069264	-0.370608
31	6	-1.262020	2.126700	-0.684131
32	1	-1.479437	2.932147	0.035925
33	1	-2.166261	1.976035	-1.282603
34	6	-0.030559	2.516989	-1.533112
35	1	-0.041520	1.940275	-2.467116
36	1	-0.016477	3.579913	-1.802211
37	6	1.192987	2.112926	-0.674976
38	1	2.018611	1.753685	-1.294504
39	1	1.564067	2.967102	-0.097882

TS12→pyridazines (n=2, pyridazine and scheme figure in SI and footnote 26)

HF = -919.0383184 hartrees (-576705.735179184 kcal/mol)

Imaginary Frequencies: 1 (-162.3356 1/cm)

Zero-point correction = 0.311640 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.773146 hartrees (-576539.33684646 kcal/mol)**Solvent Single Point: HF = -919.1436739 hartrees (-576771.8468 kcal/mol)**

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.663353	0.835579	-0.151094
2	6	1.289704	-0.430062	0.012753
3	6	-0.746306	0.819589	-0.226631
4	1	0.707529	1.273766	2.482417
5	6	-1.418915	-0.370650	0.035693
6	8	1.031430	1.877366	1.797409
7	7	0.576816	-1.554286	0.190582
8	7	-0.749873	-1.540236	0.230750
9	6	-2.900535	-0.494623	0.073674
10	6	-3.523161	-1.680132	-0.360815
11	6	-3.717281	0.538037	0.567140
12	6	-4.910737	-1.818366	-0.321622
13	1	-2.892617	-2.487254	-0.717731
14	6	-5.107361	0.399344	0.608563
15	1	-3.258421	1.444943	0.946214
16	6	-5.713206	-0.777435	0.159888
17	1	-5.369109	-2.741855	-0.668153
18	1	-5.715958	1.210077	1.002094
19	1	-6.794720	-0.885234	0.190433
20	6	2.764645	-0.590721	0.017763
21	6	3.371891	-1.722576	-0.554606
22	6	3.578506	0.383598	0.626562
23	6	4.760079	-1.870962	-0.538540
24	1	2.738576	-2.481485	-1.003479
25	6	4.967174	0.228920	0.640002
26	1	3.079855	1.214142	1.128045
27	6	5.566261	-0.892401	0.055131
28	1	5.214370	-2.750161	-0.990615
29	1	5.584499	0.982958	1.123704
30	1	6.647950	-1.007772	0.068079
31	6	-1.242911	2.177570	-0.669037
32	1	-1.403961	2.813384	0.211746
33	1	-2.174522	2.141074	-1.243970
34	6	-0.044036	2.717840	-1.487493
35	1	-0.144956	2.389675	-2.530868
36	1	0.001692	3.812672	-1.488737
37	6	1.213543	2.074807	-0.844254
38	1	1.971529	1.813634	-1.592692
39	1	1.663977	2.736018	-0.103535

TS12→pyridazines (n=2, pyridazine and scheme figure in SI and footnote 26)**(solvent optimization, methanol, ua0 radii)**

HF = -919.129248 hartrees (-576762.79441248 kcal/mol)

Imaginary Frequencies: 1 (-306.8545 1/cm)

Zero-point correction = 0.310504 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.865569 hartrees (-576597.33320319 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.664161	0.911872	0.060106
2	6	1.308752	-0.370305	0.187959
3	6	-0.747524	0.831731	-0.145237
4	1	0.404455	1.040674	2.408585
5	6	-1.411608	-0.349047	0.153846
6	8	0.867476	1.711198	1.872852
7	7	0.604057	-1.479321	0.444540
8	7	-0.732817	-1.484010	0.494300
9	6	-2.892697	-0.492513	0.085803
10	6	-3.476482	-1.642576	-0.476719
11	6	-3.742806	0.505383	0.595620
12	6	-4.865280	-1.787004	-0.534143
13	1	-2.831361	-2.422294	-0.875010
14	6	-5.132481	0.360676	0.542768
15	1	-3.316230	1.392649	1.057249
16	6	-5.700049	-0.785294	-0.024750
17	1	-5.296721	-2.682046	-0.980902
18	1	-5.771701	1.142496	0.951180
19	1	-6.782539	-0.897496	-0.068628
20	6	2.779357	-0.549556	0.070523
21	6	3.315329	-1.734181	-0.472881
22	6	3.676389	0.449342	0.495261
23	6	4.695955	-1.915269	-0.583806
24	1	2.636838	-2.511929	-0.814974
25	6	5.058120	0.269330	0.382248
26	1	3.278763	1.352103	0.947451
27	6	5.576400	-0.912874	-0.158283
28	1	5.085581	-2.838178	-1.012150
29	1	5.732259	1.053194	0.725969
30	1	6.652964	-1.052018	-0.247271
31	6	-1.256979	2.119908	-0.750615
32	1	-1.544620	2.833913	0.034652
33	1	-2.129379	1.981151	-1.397262
34	6	-0.014309	2.640481	-1.511863
35	1	-0.006123	2.212926	-2.522274
36	1	-0.009003	3.730603	-1.616645
37	6	1.206643	2.117863	-0.710083
38	1	2.036388	1.838843	-1.367583
39	1	1.576591	2.871344	-0.011609

Pyridazine (n=1, pyridazine scheme in SI and footnote 26)

HF = -803.8381319 hartrees (-504416.466148569 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.271534 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -803.613434 hartrees (-504275.46596934 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.790274	2.589419	0.000277
2	1	-1.248407	3.030951	0.891418
3	1	-1.249396	3.031894	-0.889825
4	6	0.789832	2.589482	-0.000221
5	1	1.248943	3.031605	0.890112
6	1	1.247965	3.031481	-0.891136
7	6	-0.691820	1.070238	-0.000189
8	6	-1.395648	-0.137900	-0.000159
9	6	0.691634	1.070331	-0.000361
10	6	1.395657	-0.137747	-0.000458
11	7	-0.660240	-1.278692	-0.000499
12	7	0.660297	-1.278583	-0.000715
13	6	2.868129	-0.288541	-0.000116
14	6	3.453740	-1.568256	0.005376
15	6	3.712415	0.836248	-0.005295
16	6	4.839641	-1.713130	0.005854
17	1	2.804399	-2.435877	0.009219
18	6	5.100245	0.687866	-0.004856
19	1	3.290499	1.835181	-0.009914
20	6	5.670333	-0.587414	0.000767
21	1	5.274104	-2.708757	0.010257
22	1	5.734900	1.569439	-0.008997
23	1	6.750304	-0.703382	0.001155
24	6	-2.868061	-0.288706	0.000010
25	6	-3.453716	-1.568409	-0.005183
26	6	-3.712232	0.836132	0.005430
27	6	-4.839620	-1.713151	-0.005264
28	1	-2.804430	-2.436080	-0.009248
29	6	-5.100068	0.687901	0.005336
30	1	-3.290008	1.834955	0.009855
31	6	-5.670224	-0.587359	-0.000016
32	1	-5.274190	-2.708735	-0.009467
33	1	-5.734660	1.569515	0.009569
34	1	-6.750198	-0.703278	-0.000094

Pyridazine (n=1, pyridazine scheme in SI and footnote 26)

(solvent optimization, methanol, uaks radii)

HF = -803.8548721 hartrees (-504426.970791471 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.270376 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -803.629075 hartrees (-504285.28085325 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.791228	2.539292	0.326846
2	1	-1.256760	2.820687	1.279889
3	1	-1.246131	3.122980	-0.483016
4	6	0.789560	2.539727	0.327913
5	1	1.253769	2.821758	1.281410
6	1	1.245123	3.123379	-0.481634
7	6	-0.691693	1.042279	0.078121
8	6	-1.395594	-0.158300	-0.069320
9	6	0.691227	1.042559	0.079522
10	6	1.395700	-0.158028	-0.065375
11	7	-0.664257	-1.289836	-0.223056
12	7	0.664821	-1.289717	-0.219498
13	6	2.870105	-0.295080	-0.050076
14	6	3.477191	-1.542532	0.187652
15	6	3.694344	0.824315	-0.268143
16	6	4.866695	-1.664305	0.205938
17	1	2.851075	-2.411349	0.362416
18	6	5.085296	0.699541	-0.251830
19	1	3.254042	1.795717	-0.468000
20	6	5.677355	-0.544469	-0.013922
21	1	5.318630	-2.634999	0.396049
22	1	5.705106	1.575285	-0.428453
23	1	6.760321	-0.641148	0.001050
24	6	-2.869916	-0.295556	-0.053938
25	6	-3.476457	-1.541338	0.193650
26	6	-3.694509	0.822310	-0.278429
27	6	-4.865946	-1.662983	0.215458
28	1	-2.849963	-2.408769	0.373904
29	6	-5.085417	0.697634	-0.258575
30	1	-3.254438	1.792287	-0.485878
31	6	-5.676989	-0.544680	-0.010656
32	1	-5.317536	-2.632221	0.413680
33	1	-5.705612	1.572108	-0.440110
34	1	-6.759926	-0.641152	0.007543

OH⁻ (pyridazine scheme in SI and footnote 26)

HF = -75.8034349 hartrees (-47567.413434099 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.008554 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -75.811143 hartrees (-47572.25034393 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.000000	0.000000	0.107768
2	1	0.000000	0.000000	-0.862143

OH⁻ (pyridazine scheme in SI and footnote 26)

(solvent optimization, methanol, uaks radii)

HF = -76.0389539 hartrees (-47715.203961789 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.013515 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -76.042483 hartrees (-47717.41850733 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	8	0.000000	0.000000	0.162958
2	1	0.000000	0.000000	-1.303667

4 (n=2, pyridazine scheme in SI and footnote 26)

See cyclopentanone reactant in Table 2.

TS4→6 (n=2, pyridazine scheme in SI and footnote 26)

See cyclopentanone Electrocyclic TS in Table 2.

6 (n=2, pyridazine figure and scheme in SI)

HF = -919.0190476 hartrees (-576693.642559476 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.311949 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.754786 hartrees (-576527.81576286 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.613144	0.407309	1.139950
2	6	1.209308	-0.232764	-0.095865
3	6	-1.347651	1.711457	-0.582736
4	1	-2.102515	2.315368	-0.082374
5	6	-1.592294	0.372076	-0.731664
6	8	0.115436	-0.271570	2.034116
7	7	0.523675	-0.650216	-1.157452
8	7	-0.769965	-0.550116	-1.372670
9	6	-2.922265	-0.187807	-0.331064
10	6	-3.001157	-1.513080	0.131308
11	6	-4.113244	0.555725	-0.404674
12	6	-4.218964	-2.063122	0.534700
13	1	-2.087527	-2.096468	0.170552
14	6	-5.334103	0.008118	-0.002901
15	1	-4.082538	1.567133	-0.799711
16	6	-5.393704	-1.305714	0.472694
17	1	-4.251205	-3.086968	0.900238
18	1	-6.241925	0.603515	-0.074504
19	1	-6.343449	-1.735836	0.782169
20	6	2.643712	-0.509263	-0.076096
21	6	3.325223	-0.951812	-1.242357
22	6	3.431510	-0.340839	1.091359
23	6	4.691167	-1.209152	-1.231696
24	1	2.741159	-1.089914	-2.145601
25	6	4.805398	-0.590546	1.090765
26	1	2.956404	-0.043881	2.021836
27	6	5.455671	-1.027257	-0.067441
28	1	5.173401	-1.550209	-2.146343
29	1	5.369043	-0.453381	2.011826
30	1	6.524995	-1.222855	-0.066550
31	6	-0.109809	2.417990	-1.059200
32	1	-0.396402	3.348501	-1.571533
33	1	0.384567	1.792369	-1.807188
34	6	0.907618	2.775212	0.071130
35	1	1.928378	2.691477	-0.320258
36	1	0.778904	3.825541	0.366480
37	6	0.762562	1.919313	1.340732
38	1	1.660690	2.052575	1.963109
39	1	-0.084175	2.242844	1.954107

6 (n=2, pyridazine figure and scheme in SI)

(solvent optimization, methanol, uaks radii)

HF = -919.104032 hartrees (-576746.97112032 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.311605 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -918.839861 hartrees (-576581.20117611 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.599674	0.370569	1.112449
2	6	1.207485	-0.230123	-0.138637
3	6	-1.344938	1.719132	-0.525659
4	1	-2.088254	2.294312	0.023947
5	6	-1.598844	0.394696	-0.736998
6	8	0.106790	-0.364894	1.971911
7	7	0.533268	-0.610360	-1.213038
8	7	-0.772274	-0.495878	-1.446555
9	6	-2.920423	-0.183937	-0.336835
10	6	-3.000293	-1.523751	0.085017
11	6	-4.110108	0.568150	-0.371127
12	6	-4.216208	-2.084322	0.484833
13	1	-2.092451	-2.119377	0.102855
14	6	-5.327932	0.010672	0.027693
15	1	-4.085069	1.593789	-0.730137
16	6	-5.387279	-1.318779	0.460550
17	1	-4.249484	-3.119974	0.816873
18	1	-6.234019	0.611658	-0.012962
19	1	-6.335598	-1.754969	0.766297
20	6	2.652659	-0.502909	-0.101912
21	6	3.368011	-0.860740	-1.273008
22	6	3.399869	-0.408721	1.097281
23	6	4.735745	-1.121056	-1.238978
24	1	2.825335	-0.929436	-2.210112
25	6	4.774470	-0.660126	1.124391
26	1	2.902126	-0.161224	2.030848
27	6	5.458101	-1.020817	-0.040560
28	1	5.248090	-1.395343	-2.159467
29	1	5.309996	-0.580611	2.068482
30	1	6.527301	-1.216552	-0.019348
31	6	-0.122578	2.461834	-0.986262
32	1	-0.431502	3.411595	-1.444701
33	1	0.374165	1.884364	-1.771631
34	6	0.894558	2.776834	0.156007
35	1	1.917636	2.725197	-0.242781
36	1	0.752262	3.810773	0.503948
37	6	0.755223	1.861334	1.383787
38	1	1.658709	1.958124	2.006903
39	1	-0.083678	2.162853	2.020662

Pyridazine (n=2, pyridazine scheme in SI and footnote 26)

HF = -843.1963106 hartrees (-529114.116864606 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.301639 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -842.939321 hartrees (-528952.85332071 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.696962	0.946336	0.063440
2	6	-1.365823	-0.281594	-0.073975
3	6	0.696963	0.946355	0.063413
4	6	1.365815	-0.281586	-0.073999
5	7	-0.659387	-1.432347	-0.142799
6	7	0.659396	-1.432337	-0.142799
7	6	2.842600	-0.441708	-0.097143
8	6	3.426698	-1.587791	0.471804
9	6	3.681874	0.511572	-0.697918
10	6	4.809575	-1.763613	0.454696
11	1	2.780582	-2.334919	0.919118
12	6	5.066487	0.330362	-0.721255
13	1	3.255592	1.385837	-1.177943
14	6	5.636128	-0.804759	-0.140105
15	1	5.243520	-2.651732	0.905198
16	1	5.697721	1.073345	-1.200357
17	1	6.713276	-0.943911	-0.154602
18	6	-2.842600	-0.441714	-0.097129
19	6	-3.426723	-1.587620	0.472120
20	6	-3.681830	0.511416	-0.698218
21	6	-4.809610	-1.763439	0.455000
22	1	-2.780636	-2.334623	0.919679
23	6	-5.066437	0.330206	-0.721558
24	1	-3.255517	1.385543	-1.178452
25	6	-5.636118	-0.804747	-0.140110
26	1	-5.243591	-2.651424	0.905731
27	1	-5.697656	1.073055	-1.200897
28	1	-6.713267	-0.943884	-0.154615
29	6	1.225814	2.346652	0.301886
30	1	1.522486	2.810031	-0.649524
31	1	2.105090	2.365438	0.952257
32	6	-0.000020	3.078401	0.899930
33	1	-0.000028	2.957697	1.989317
34	1	-0.000025	4.150683	0.685304
35	6	-1.225840	2.346644	0.301860
36	1	-2.105158	2.365469	0.952154
37	1	-1.522401	2.809956	-0.649609

Pyridazine (n=2, pyridazine scheme in SI and footnote 26)

(solvent optimization, methanol, uaks radii)

HF = -843.2146474 hartrees (-529125.623389974 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.300117 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -842.959378 hartrees (-528965.43928878 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.696509	0.918685	0.076027
2	6	-1.365744	-0.304797	-0.102843
3	6	0.696152	0.918928	0.076985
4	6	1.366032	-0.304494	-0.099557
5	7	-0.663355	-1.449978	-0.237502
6	7	0.664207	-1.449934	-0.234328
7	6	2.845741	-0.447411	-0.108124
8	6	3.452011	-1.525533	0.561026
9	6	3.662549	0.469691	-0.791340
10	6	4.839630	-1.677385	0.553315
11	1	2.828209	-2.238740	1.092058
12	6	5.050933	0.312098	-0.805214
13	1	3.215814	1.295612	-1.337209
14	6	5.644357	-0.759066	-0.130209
15	1	5.293037	-2.511769	1.083259
16	1	5.667316	1.024861	-1.347837
17	1	6.725193	-0.878126	-0.137320
18	6	-2.845388	-0.448329	-0.111351
19	6	-3.450482	-1.526675	0.558581
20	6	-3.663424	0.469154	-0.792567
21	6	-4.838152	-1.678212	0.553850
22	1	-2.825729	-2.239959	1.088374
23	6	-5.051866	0.311827	-0.803525
24	1	-3.217705	1.295417	-1.338745
25	6	-5.644106	-0.759375	-0.127513
26	1	-5.290623	-2.512565	1.084664
27	1	-5.669318	1.025030	-1.344370
28	1	-6.725005	-0.877981	-0.132018
29	6	1.226825	2.309734	0.349172
30	1	1.529390	2.785991	-0.594966
31	1	2.103385	2.310631	1.005456
32	6	-0.000967	3.032126	0.957574
33	1	-0.001551	2.895002	2.049162
34	1	-0.000968	4.109604	0.750160
35	6	-1.227969	2.309250	0.348122
36	1	-2.104960	2.309593	1.003827
37	1	-1.530177	2.785496	-0.596131

bis-*p*-CN substituted reactant (n=1, footnote 25)

HF = -1064.2063579 hartrees (-667800.131645829 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.281320 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1063.975467 hartrees (-667655.24529717 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.997643	2.355706	0.780222
2	1	-1.940596	2.278057	1.333910
3	1	-0.903195	3.365747	0.365174
4	6	0.300633	1.893312	1.480540
5	1	0.120212	1.104686	2.218198
6	1	0.937416	2.656762	1.940855
7	6	-0.705066	1.324346	-0.384941
8	6	-1.288397	-0.061681	-0.077224
9	6	0.808693	1.302943	0.126351
10	1	1.363593	2.057909	-0.439724
11	6	1.458777	-0.027578	0.094510
12	8	-0.975622	1.595012	-1.650747
13	7	-0.600416	-1.160632	0.103737
14	7	0.785842	-1.145994	0.137363
15	6	2.933311	-0.172656	0.019836
16	6	3.524742	-1.436561	-0.199826
17	6	3.788007	0.935639	0.181331
18	6	4.902150	-1.586711	-0.252733
19	1	2.867164	-2.288878	-0.325664
20	6	5.171936	0.797270	0.127973
21	1	3.365201	1.918144	0.358964
22	6	5.745455	-0.467345	-0.089434
23	1	5.340611	-2.564895	-0.425086
24	1	5.813993	1.663134	0.256176
25	6	-2.761774	-0.242947	-0.113331
26	6	-3.344195	-1.320126	0.587612
27	6	-3.614888	0.661411	-0.779557
28	6	-4.722540	-1.489799	0.631206
29	1	-2.687598	-2.019930	1.092055
30	6	-4.995399	0.503372	-0.732181
31	1	-3.151667	1.457950	-1.354163
32	6	-5.566382	-0.574901	-0.027674
33	1	-5.155999	-2.324204	1.174390
34	1	-5.641840	1.204126	-1.251915
35	6	-6.987750	-0.741956	0.016968
36	6	7.168442	-0.617298	-0.143446
37	7	-8.145679	-0.877887	0.056867
38	7	8.327256	-0.740535	-0.185740

bis-*p*-CN substituted Electrocyclic TS (n=1, footnote 25)

HF = -1064.190798 hartrees (-667790.36765298 kcal/mol)

Imaginary Frequencies: 1 (-286.4770 1/cm)

Zero-point correction = 0.279739 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1063.961649 hartrees (-667646.57436399 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.477815	2.776201	1.118729
2	1	-0.461648	2.257591	2.084312
3	1	-1.103225	3.672440	1.192173
4	6	0.918466	2.954938	0.536059
5	1	1.744898	3.075588	1.249657
6	1	0.938080	3.796668	-0.163252
7	6	-0.954697	1.849681	-0.051563
8	6	-1.366058	0.470786	0.413274
9	6	0.957126	1.643858	-0.289939
10	1	1.291518	1.773299	-1.323098
11	6	1.449748	0.457559	0.370203
12	8	-1.519209	2.406280	-1.053078
13	7	-0.607362	-0.344786	1.109741
14	7	0.736232	-0.285092	1.230537
15	6	2.814706	-0.052547	0.116471
16	6	3.230816	-1.305338	0.626494
17	6	3.757480	0.698820	-0.619908
18	6	4.519765	-1.775166	0.424731
19	1	2.506844	-1.890651	1.181173
20	6	5.043998	0.224651	-0.850522
21	1	3.478297	1.673977	-1.003539
22	6	5.444464	-1.017907	-0.325533
23	1	4.821175	-2.737224	0.828222
24	1	5.750315	0.816371	-1.424801
25	6	-2.727762	-0.055816	0.136855
26	6	-3.238327	-1.115579	0.924796
27	6	-3.556988	0.476723	-0.874246
28	6	-4.513514	-1.618882	0.719493
29	1	-2.603970	-1.527875	1.700541
30	6	-4.839745	-0.024937	-1.082180
31	1	-3.161277	1.286181	-1.476392
32	6	-5.333633	-1.078175	-0.293317
33	1	-4.888464	-2.429626	1.336969
34	1	-5.464646	0.396023	-1.864175
35	6	-6.650183	-1.596378	-0.511620
36	6	6.771198	-1.505101	-0.548833
37	7	-7.723316	-2.019334	-0.686311
38	7	7.853232	-1.901838	-0.729656

bis-*p*-CN substituted Fragmentation TS (n=1, footnote 25)

HF = -1064.168484 hartrees (-667776.36539484 kcal/mol)

Imaginary Frequencies: 1 (-598.6094 1/cm)

Zero-point correction = 0.278871 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1063.940024 hartrees (-667633.00446024 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.907434	1.708277	-0.087592
2	6	-1.349617	0.308052	-0.543008
3	6	1.005103	1.735903	-0.684249
4	1	0.694036	2.242026	-1.588713
5	6	1.462812	0.387675	-0.822456
6	8	-1.555339	2.660925	-0.613069
7	7	-0.657411	-0.552706	-1.248758
8	7	0.715175	-0.597483	-1.322115
9	6	2.825554	-0.047818	-0.397008
10	6	3.101773	-1.406301	-0.141370
11	6	3.882822	0.876220	-0.289834
12	6	4.378987	-1.826738	0.209850
13	1	2.287716	-2.116339	-0.235127
14	6	5.162344	0.471784	0.073699
15	1	3.689509	1.919424	-0.518394
16	6	5.423152	-0.888512	0.327812
17	1	4.579332	-2.876331	0.402735
18	1	5.967630	1.195660	0.152556
19	6	-2.741973	-0.091657	-0.255134
20	6	-3.237826	-1.352301	-0.668088
21	6	-3.621117	0.758605	0.454013
22	6	-4.538508	-1.742047	-0.394369
23	1	-2.564816	-2.008683	-1.207385
24	6	-4.926037	0.370545	0.739032
25	1	-3.281078	1.742856	0.750845
26	6	-5.403832	-0.884778	0.321133
27	1	-4.898802	-2.713622	-0.719547
28	1	-5.585944	1.040747	1.281630
29	6	1.137280	2.523375	0.620030
30	6	-0.169129	1.982430	1.253257
31	1	0.035727	1.037143	1.776501
32	1	-0.719894	2.660730	1.921692
33	1	2.034326	2.321544	1.217673
34	1	1.074849	3.602101	0.445976
35	6	-6.742948	-1.289254	0.618497
36	6	6.739968	-1.313647	0.698594
37	7	-7.835323	-1.621670	0.859972
38	7	7.812113	-1.658645	1.000508

bis-*p*-CN substituted Electrocyclic product (n=1, footnote 25)

HF = -1064.2293092 hartrees (-667814.533816092 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.281704 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1063.999142 hartrees (-667670.10159642 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.448680	3.506648	0.395962
2	1	-0.301539	3.297505	1.459124
3	1	-1.080302	4.396130	0.299544
4	6	0.897790	3.759029	-0.283122
5	1	1.429915	4.595844	0.199302
6	1	0.712103	4.076543	-1.318960
7	6	-1.208024	2.377451	-0.315512
8	6	-1.269931	1.083926	0.338622
9	6	1.777579	2.546945	-0.311677
10	1	2.618004	2.610187	-1.001472
11	6	1.655938	1.397846	0.391157
12	8	-1.847242	2.693424	-1.340811
13	7	-0.457563	0.779386	1.411689
14	7	0.797719	1.033894	1.486227
15	6	2.668663	0.313039	0.184993
16	6	2.285326	-1.034209	0.331234
17	6	4.010725	0.581040	-0.146766
18	6	3.187497	-2.070529	0.116955
19	1	1.263596	-1.261285	0.612394
20	6	4.925685	-0.444653	-0.357821
21	1	4.349340	1.609225	-0.219152
22	6	4.520521	-1.785966	-0.231864
23	1	2.868072	-3.102815	0.219070
24	1	5.957754	-0.216399	-0.605301
25	6	-2.398410	0.168426	0.162794
26	6	-2.550252	-0.955501	1.024185
27	6	-3.380860	0.327562	-0.852439
28	6	-3.614705	-1.832844	0.905256
29	1	-1.810992	-1.111279	1.800814
30	6	-4.441826	-0.558587	-0.979676
31	1	-3.285763	1.161077	-1.535240
32	6	-4.585105	-1.654850	-0.105000
33	1	-3.703685	-2.672578	1.588913
34	1	-5.174984	-0.407500	-1.767185
35	6	-5.674658	-2.566027	-0.242037
36	6	5.461495	-2.845357	-0.443686
37	7	-6.568541	-3.310674	-0.350963
38	7	6.231786	-3.702947	-0.617626

bis-*p*-CN substituted Fragmentation product (n=1, footnote 25)

HF = -1064.1934842 hartrees (-667792.053270342 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.281133 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -1063.963531 hartrees (-667647.75533781 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.920413	1.811865	-0.499596
2	6	1.271935	0.573202	0.280767
3	6	-1.278892	2.051333	1.045500
4	1	-0.404746	2.363994	1.617376
5	6	-1.560227	0.722379	1.141866
6	8	1.769115	2.699437	-0.657609
7	7	0.607817	-0.129649	1.232339
8	7	-0.606593	-0.159967	1.713606
9	6	-2.777952	0.079839	0.614119
10	6	-2.757081	-1.278601	0.233575
11	6	-4.004825	0.772557	0.529774
12	6	-3.900265	-1.908665	-0.245627
13	1	-1.825200	-1.825104	0.327538
14	6	-5.150170	0.157338	0.042630
15	1	-4.051491	1.799230	0.878674
16	6	-5.108661	-1.194749	-0.354629
17	1	-3.867642	-2.952962	-0.540528
18	1	-6.085861	0.704642	-0.018078
19	6	2.663083	0.078004	0.120238
20	6	3.201298	-0.873949	1.026915
21	6	3.504213	0.453870	-0.959626
22	6	4.471549	-1.405870	0.873056
23	1	2.580196	-1.185854	1.857221
24	6	4.774902	-0.078736	-1.124450
25	1	3.160844	1.186626	-1.677891
26	6	5.288935	-1.019758	-0.210136
27	1	4.847010	-2.125692	1.595110
28	1	5.383592	0.233331	-1.968396
29	6	-1.441149	2.812264	-0.238640
30	6	-0.439584	2.052798	-1.176994
31	1	-0.907639	1.098524	-1.440591
32	1	-0.236468	2.623459	-2.091961
33	1	-2.440505	2.776525	-0.682612
34	1	-1.149068	3.862600	-0.135287
35	6	6.598165	-1.563320	-0.374513
36	6	-6.289449	-1.836794	-0.848516
37	7	7.669413	-2.009519	-0.510017
38	7	-7.252546	-2.355845	-1.252210

di-CN substituted reactant (n=1, footnote 25)

HF = -602.0511437 hartrees (-377793.113183187 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.119574 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -601.968342 hartrees (-377741.15428842 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.996332	1.930963	-0.425939
2	1	1.903511	1.898892	-1.039848
3	1	0.995204	2.848427	0.173016
4	6	-0.368514	1.683026	-1.110809
5	1	-0.285366	1.042060	-1.993734
6	1	-0.982168	2.551813	-1.366936
7	6	0.705103	0.719046	0.532896
8	6	1.139082	-0.623417	-0.067842
9	6	-0.841088	0.875447	0.144262
10	1	-1.350643	1.527796	0.860357
11	6	-1.546208	-0.413912	-0.031514
12	8	1.105805	0.658987	1.781961
13	7	0.398224	-1.668436	-0.347181
14	7	-0.984190	-1.560952	-0.307551
15	6	2.563323	-0.854736	-0.122891
16	6	-2.981732	-0.447688	0.104644
17	7	3.709877	-0.996617	-0.276411
18	7	-4.141734	-0.395889	0.213230

di-CN substituted Electrocyclic TS (n=1, footnote 25)

HF = -602.0485234 hartrees (-377791.468918734 kcal/mol)

Imaginary Frequencies: 1 (-306.8685 1/cm)

Zero-point correction = 0.118635 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -601.966182 hartrees (-377739.79886682 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.061791	1.892650	-0.439014
2	1	2.041076	1.871370	-0.933643
3	1	0.953588	2.838739	0.102467
4	6	-0.194482	1.575419	-1.265961
5	1	-0.002442	0.842007	-2.054074
6	1	-0.721264	2.424978	-1.713946
7	6	0.770497	0.744627	0.580876
8	6	1.117785	-0.611103	-0.058159
9	6	-0.939349	0.943781	-0.074336
10	1	-1.482780	1.677584	0.522170
11	6	-1.582863	-0.339456	-0.161331
12	8	1.024960	0.829229	1.822805
13	7	0.356142	-1.554357	-0.563886
14	7	-1.012175	-1.479975	-0.511956
15	6	2.512587	-0.967224	0.025996
16	6	-2.969234	-0.456055	0.235396
17	7	3.656771	-1.194118	0.023533
18	7	-4.093346	-0.483599	0.542849

di-CN substituted Fragmentation TS (n=1, footnote 25)

HF = -602.0161501 hartrees (-377771.154349251 kcal/mol)

Imaginary Frequencies: 1 (-629.2900 1/cm)

Zero-point correction = 0.117120 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -601.936012 hartrees (-377720.86689012 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.872710	0.905175	-0.088625
2	6	-1.319469	-0.578081	-0.023756
3	6	0.976141	0.676280	-0.801400
4	1	0.655433	0.780233	-1.830443
5	6	1.418670	-0.614186	-0.380011
6	8	-1.589286	1.596840	-0.859911
7	7	-0.674295	-1.662248	-0.374304
8	7	0.706469	-1.731893	-0.371926
9	6	1.208735	1.891193	0.089147
10	6	-0.027412	1.630544	0.992410
11	1	0.241402	0.931433	1.796970
12	1	-0.537361	2.505589	1.418884
13	1	2.167695	1.911377	0.622567
14	1	1.101580	2.824083	-0.471073
15	6	-2.697045	-0.787432	0.324109
16	6	2.754232	-0.761639	0.184430
17	7	-3.810441	-0.911720	0.652128
18	7	3.840937	-0.822505	0.603326

di-CN substituted Electrocyclic product (n=1, footnote 25)

HF = -602.0825249 hartrees (-377812.805199999 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.119965 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -602.000406 hartrees (-377761.27476906 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.601492	2.050946	-0.065354
2	1	1.425637	2.582761	-0.563730
3	1	0.273271	2.694884	0.757467
4	6	-0.551712	1.796776	-1.042466
5	1	-0.206361	1.171142	-1.873723
6	1	-0.889783	2.749814	-1.467557
7	6	1.265975	0.812912	0.550454
8	6	1.226264	-0.509786	-0.120222
9	6	-1.676158	1.122072	-0.322956
10	1	-2.442691	1.738986	0.141832
11	6	-1.758777	-0.223666	-0.191309
12	8	2.047256	1.017628	1.485786
13	7	0.311496	-1.260767	-0.787366
14	7	-0.979123	-1.226418	-0.804260
15	6	2.498496	-1.180618	-0.087052
16	6	-2.908699	-0.765595	0.500724
17	7	3.541243	-1.708354	-0.078409
18	7	-3.833531	-1.189726	1.068394

di-CN substituted Fragmentation product (n=1, footnote 25)

HF = -602.0525229 hartrees (-377793.978644979 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.119885 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Sum of electronic and thermal Free Energies = -601.970105 hartrees (-377742.26058855 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.018028	1.032916	-0.240947
2	6	1.246550	-0.433357	-0.044041
3	6	-1.246306	0.382699	1.242787
4	1	-0.467892	0.226583	1.987826
5	6	-1.529276	-0.701545	0.489155
6	8	2.015408	1.768194	-0.299746
7	7	0.569283	-1.585131	0.273804
8	7	-0.676178	-1.848801	0.517984
9	6	-1.353722	1.767812	0.697897
10	6	-0.337940	1.732892	-0.495975
11	1	-0.843189	1.216888	-1.320237
12	1	-0.082314	2.745630	-0.823649
13	1	-2.347844	2.020668	0.312057
14	1	-1.068883	2.523252	1.437297
15	6	2.649556	-0.758045	-0.165016
16	6	-2.582900	-0.710807	-0.486310
17	7	3.772439	-1.063267	-0.266199
18	7	-3.450843	-0.753367	-1.265678

IRC Diagrams

Structures on the following IRC plots correspond to the transition state structures (center images) and to the last structures from the forward and reverse IRC calculations (side images).

3'→4 (Figure 1)

4→6 (Figure 2) / cyclobutanone allowed electrocyclic reaction (Table 2)

4→7 (Figure 2) / cyclobutanone fragmentation reaction (Table 2)

Cyclopentanone allowed electrocyclic reaction (Table 2)

Cyclopentanone fragmentation reaction (Table 2)

Cyclohexanone 1,2-shift reaction (Table 2)

Cyclohexanone fragmentation reaction (Table 2)

Cycloheptanone 1,2-shift reaction (Table 2)

Cycloheptanone fragmentation reaction (Table 2)

Cyclooctanone allowed electrocyclic reaction (Table 2)

Cyclooctonone fragmentation reaction (Table 2)

12 $\rightarrow$ pyridazine (n=1, pyridazine figure and scheme in SI and footnote 26)

12→pyridazine (n=2, pyridazine figure and scheme in SI and footnote 26)