Supporting Information

Two P, Ten P, White P, Red P: Mechanistic Exploration of the Oligomerization of Red Phosphorus from Diphosphorus with the Ab Initio Nanoreactor

Nathan D. Yoshino[a], Lee-Ping Wang[a]*

[a]Department of Chemistry, University of California, Davis, Davis, California 95616, United States

*Corresponding Author.
E-mail: leeping@ucdavis.edu

Supporting Information

Table S1. ωB97X-D3/TZVP electronic energies. The last column indicates the per-atom reaction energy relative to P_2; i.e., $\boldsymbol{\Delta E_n = \frac{1}{n}E - \frac{1}{2}E(P_2)}$.

n(P)	label	symmetry	E(au)	ΔE(kcal/mol)
2	P_2	$D_{2\infty}$	-682.6786	0.00
4	P_4a	T_d	-1365.4456	-13.88
4	P_4b	C_{2v}	-1365.3577	-0.09
4	P_4c	D_{2d}	-1365.3644	-1.14
6	P_6a	C_{2v}	-2048.1361	-10.50
6	P_6b	C_{2v}	-2048.1062	-7.38
6	P_6c	D_{3h}	-2048.1307	-9.94
6	P_6d	C_1	-2048.0997	-6.70
6	P_6e	C_{2h}	-2048.0977	-6.49
6	P_6f	C_{2v}	-2048.0997	-6.70
8	P_8a	C_{2v}	-2730.8828	-13.22
8	P_8b	C_s	-2730.8540	-10.96
8	P_8c	C_s	-2730.8663	-11.93
8	P_8d	C_{2h}	-2730.8247	-8.67
8	P_8e	C_s	-2730.8643	-11.77
10	$P_{10}a$	C_{2v}	-3413.6283	-14.78
10	$P_{10}b$	C_s	-3413.6175	-14.10

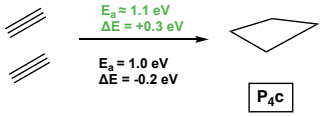

Figure S1. Comparison of P_4c formation with ωB97X-D3 (this work) and CASSCF-RSPT3 (4,9).

Table S2. Energies of small P clusters relative to white phosphorus for ωB97X-D3 (this work) compared to CASSCF-RSPT3 (4,9)[87].

P Cluster	ΔE (eV) ωB97X-D3 /def-TZVP	ΔE (eV) CASSCF-RSPT3/ aug-cc-pVTZ [87]
P_4a (T_d)	0.00	0.00
P_4b (C_2v)	+2.39	+1.8
P_4c (D_2d)	+2.21	+2.5
2 P_2	+2.40	+2.2

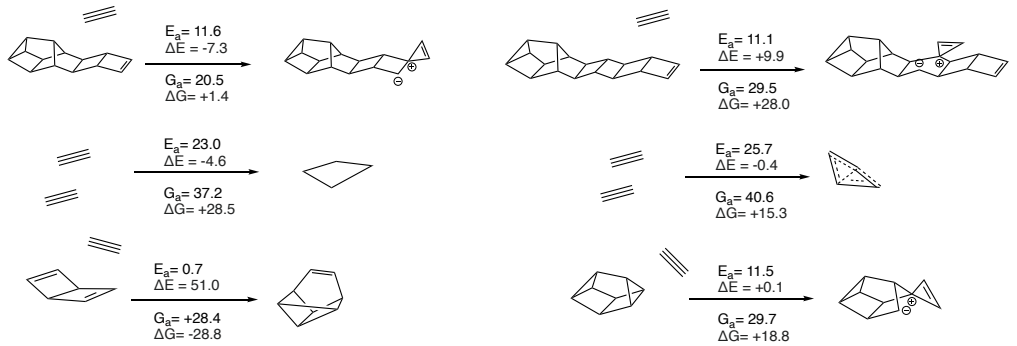

Figure S2. Comparison of electronic and free energies of diphosphorus addition reactions.

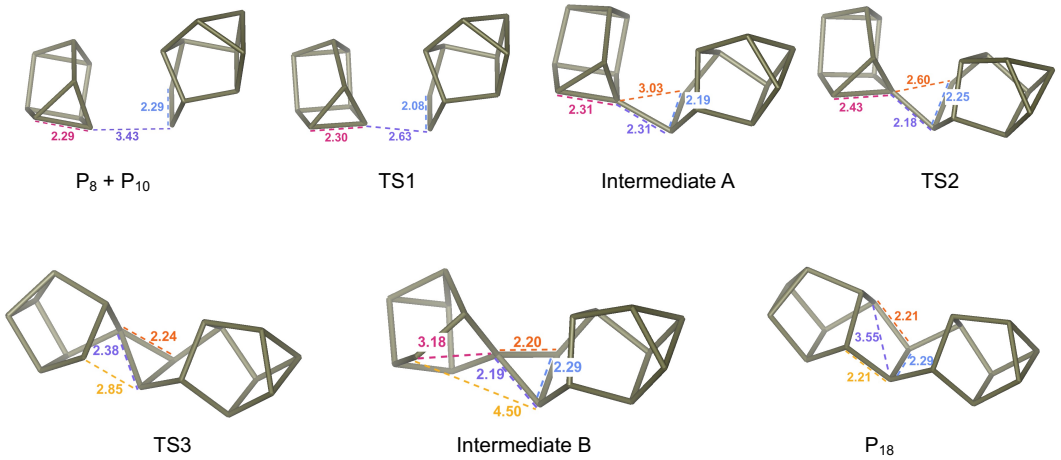

Figure S3. Bond distances (Å) for the reaction in Scheme 3g.

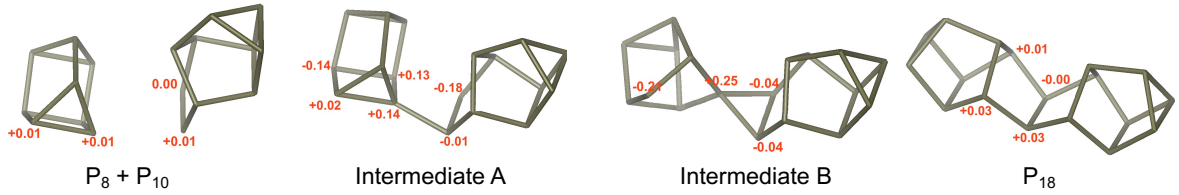

Figure S4. RESP charges for the reaction in Scheme 3g. All atoms without charges listed are smaller in magnitude than 0.05 a. u..

Table S3. List of nanoreactor simulations parameters used to study phosphorus clusters.

Number of Simulations	Species	Number of Species	Method	r1 (Å)	r2 (Å)	k1 (kcal/ (mol Å^2)	k2 (kcal/ (mol Å^2)	t1 (fs)	t2 (fs)	Number of MD Steps (fs)	Temperature (K)	Langevin Damping Time (fs)	Notes
10	P_2	30	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_2; white P	12; 10	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 4	RHF/6-31G*	14	8	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 4	RHF/6-31G*	14	8.5	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 4	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 5	RHF/6-31G*	14	9.5	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 6	RHF/6-31G*	14	10	1	0.5	1500	500	20000	1500	150	
5	P_2; P_6b	16; 7	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	levelshifting a=1.6, b=0.1
4	P_6a	12	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
4	P_6a; P_2	5; 20	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_6c; P_2	6; 12	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_6c; P_2	6; 12	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	
2	$P10_b$; P_3; P_2	2; 2; 17	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	Charge = +1
2	$P10_b$; P_3; P_2	2; 2; 17	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	Charge = -1
5	P_7; P_5; P_3; P_2	1; 1; 1; 22	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_7; P_5; P_3; P_2	1; 1; 1; 22	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_6b; P_2	5; 15	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	
5	P_8b; P_2	5; 15	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_8b; P_6b; P_2	2; 3; 15	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	
5	P_8b; P_6b; P_2	2; 3; 15	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
6	P_{10}b; P_2	3; 20	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	
6	P_{10}b; P_2	3; 20	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
5	P_{10}a; P_2	3; 20	RHF/6-31G*	14	8.5	1	0.3	1500	500	20000	1500	150	
5	P_{10}a; P_2	3; 20	RHF/6-31G*	14	9	1	0.5	1500	500	20000	1500	150	
3	P_{10}b; P_8a; P_2	1; 2; 10	UHF/6-31G*	14	9	1	0.5	1500	500	20000	1000	150	spin multiplicity = 1
4	P_6o; P_2	6; 15	UHF/6-31G*	14	9	1	0.5	1500	500	20000	1000	150	spin multiplicity = 1
5	P_3; P_2	10; 10	UHF/6-31G*	14	9	1	0.5	1500	500	20000	1000	150	spin multiplicity = 2
2	P_3; P_2	1; 20	UHF/6-31G*	13	9	1	0.3	1500	500	20000	1500	150	spin multiplicity = 2
2	P_3; P_2	1; 20	UHF/6-31G*	13	12.9	1	1	1500	1	20000	1500	150	spin multiplicity = 2
2	P_3; P_2	1; 20	UHF/6-31G*	13	9	1	0.5	1500	500	20000	1000	150	spin multiplicity = 2
2	P_3; P_2	1; 20	UHF/6-31G*	13	9	1	0.5	1500	500	20000	800	150	spin multiplicity = 2
2	P_2	20	UHF/6-31G*	13	9	1	0.3	1500	500	20000	1500	150	spin multiplicity = 2
2	P_2	20	UHF/6-31G*	13	12.9	1	1	1500	1	20000	1500	150	spin multiplicity = 2
2	P_2	20	UHF/6-31G*	13	9	1	0.5	1500	500	20000	1000	150	spin multiplicity = 2
2	P_2	20	UHF/6-31G*	13	9	1	0.5	1500	500	20000	800	150	spin multiplicity = 2

XYZ Coordinates for Reaction Structures

Geometries labeled “Transition state” contained one imaginary vibrational mode. The exception to this are barrierless associations in Scheme 1. “Product” or “Reactant” and structures in Figure 3 showed no imaginary vibrational modes.

Cartesian coordinates for structures in Figure 3 and Table S1

2
P2
P 0.0000521024 0.0000431078 0.0115069495
P -0.0000521024 -0.0000431078 1.8884930486

4
P4a
P -2.6021460621 1.9109017082 1.3073552264
P -0.9484773765 3.0847056155 2.1257971402
P -1.7467214795 1.3879069433 3.2507939861
P -2.9338705013 3.2116694587 3.0337289300

4
P4b
P 1.1673756961 -0.5953666454 -1.0545469111
P -0.7711490759 -0.9191539851 -0.2497941487
P -0.7799674904 0.3592527950 1.4462355744
P 0.3837408847 1.1552678320 -0.1418945089

4
P4c
P 0.9698561492 0.8260716167 -0.7966211227
P 0.7607203753 0.2692741965 1.2673229321
P -1.2042262680 -0.4480924451 0.7788905516
P -0.5263502557 -0.6472533584 -1.2495923559

10
P10a
P -1.9081283411 5.7736000563 -1.3042785809
P -1.2199901777 3.8042665039 -2.0315906184
P -1.4676629493 5.6868963288 0.8660095521
P -0.4666769997 2.8266021885 -0.1908221633
P 0.2812857922 4.3747744140 1.2004283029
P -1.7700317965 3.5715306805 1.4319189561
P 0.4614040723 6.3019046044 -3.8455599024
P 1.6278460111 6.0205121740 -1.9834147441
P 0.7184191452 4.2772543949 -2.9963591895
P -0.2805951084 7.1376188654 -1.9383721538

10
P10b
P -2.6900008735 -0.7522014960 0.7220039973
P -4.0485590789 2.2429980956 1.4508887461
P -5.7727369273 0.9401791734 1.0038559426
P -4.8653374741 -1.0599782174 0.5175445746
P -5.1847277791 -1.7189253727 2.6305049928
P -6.0926424522 0.2803411444 3.1165215088
P -2.6481906411 0.7747381198 2.3101244515
P -4.0188667630 -0.2023311277 3.7725332673
P -3.2812008257 2.3455082559 -0.6416168048
P -2.4641174934 0.5434486937 -1.0802297438

6
P6a
P -0.0041976318 2.0575699943 0.5419063277
P -1.7702063129 2.3512711235 1.4372417301
P 0.0731455959 -0.1377324685 0.0896735526
P -2.7386303652 0.3300600826 1.5149474174
P -1.0868575396 -1.1314489733 1.6903992327
P -2.0192535390 -0.7597197136 -0.2711680885

6
P6b
P -3.0762720577 0.0026732893 0.5903287460
P -3.9827050904 1.7709990438 1.0422765272
P -5.9885385914 0.8330732447 1.1137016178
P -4.9998700461 -1.0944178933 0.6184712649
P -5.2664316103 -1.6728173816 2.7397419803
P -6.1742639695 0.0941938697 3.1937567644

6
P6c
P -1.2931140564 -0.4811133437 -0.1985295733
P -0.0534182076 1.2645011358 0.4106969153
P 0.8725694620 -0.4215467274 -0.7094684820
P 0.4381331689 0.2305206216 2.3739332519
P 1.3642691329 -1.4553374356 1.2537469288
P -0.8014394932 -1.5150242782 1.7646209923

6
P6d
P -0.1187321745 -1.1485142871 0.0020586791
P -0.1681106700 1.1395108194 -0.0286723741
P -2.3361407222 1.6284793599 -0.1958687327

P -2.2661803241 -1.7345821773 -0.1103599251
P -1.4218766569 -1.6016929849 1.7036517273
P -1.2596131298 1.5392669407 -1.8852463547

6
P6e
P -0.4557108939 -1.2405393070 -0.0316278981
P -2.6762513775 -0.9758930689 -0.2673184886
P -2.3978138861 1.4824268357 -0.1110881035
P -1.7721271782 -1.2840269688 1.5855306600
P -1.0836409049 1.5231020779 -1.7278877945
P -0.1775057090 1.2142406088 0.1253815156

6
P6f
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P 0.1423348434 -0.8996902674 0.8615821019
P -1.3315716272 0.1893269677 2.1264846637
P -0.8360927448 0.8748705371 0.0665390727
P 0.3858427469 1.4384667393 2.8015343164
P 0.8787689242 2.4170934689 4.3754868315

8
P8a
P -2.9203429302 -0.1844320594 0.5670670010
P -3.8787452200 1.8341825611 1.0390905633
P -5.8790972201 0.8206050399 1.1334412754
P -4.9519957455 -1.1321849074 0.6763689697
P -5.2009238478 -1.7914456884 2.8073382322
P -6.1594354809 0.2270434569 3.2798032056
P -2.7020851098 0.7486113932 2.5446304886
P -4.1156281291 -0.2473729890 3.9333740277

8
P8b
P 1.1874124303 -0.9897130969 -1.0559838705
P 0.5255511538 1.5389906249 -0.9268829143
P -1.4585920804 1.2355605636 -0.1407599896
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P 0.7018044802 0.0662044401 2.2997980387

8
P8c

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P -3.5171274701 1.1125140078 2.0133074924
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8
P8d
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P -3.7660935392 1.7748912554 1.6962520959
P -5.8107471856 1.0597231329 1.0932008840
P -4.9226564928 -0.8890250435 0.3931341780
P -5.4732635791 -1.7259654459 2.3704145078
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P -3.2154761809 2.6119074891 -0.2810010542

8
P8e
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P -3.7641916958 1.8768309652 0.7277784725
P -5.7865448860 0.9360676135 1.3256103486
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P -2.5531186055 1.7985918045 2.5711503169
P -2.0950604403 -0.1927353697 2.3372063966

8
P8f
P -3.0536687372 -0.2047547806 0.3842746849
P -3.7641916958 1.8768309652 0.7277784725
P -5.7865448860 0.9360676135 1.3256103486
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P -2.5531186055 1.7985918045 2.5711503169
P -2.0950604403 -0.1927353697 2.3372063966

Cartesian coordinates for structures in Scheme 1

Reaction (a):

4
Reactant: -1365.3588913573028

P 0.5324985878 1.4345951541 -2.3720546323
P 0.6372206854 -0.6659168667 2.6808594627
P -0.9800136284 -0.5003528982 1.7417919980
P -0.1897073050 -0.2683258992 -2.0505968853

4
Transition state: -1365.32040058
P 0.9075110212 0.9046858328 -1.2942714423
P 0.6392125232 0.0351006341 1.7104894411
P -1.1321393688 -0.3675088464 0.8543013677
P -0.3854295090 -0.6316782816 -1.2727568947

4
Product: -1365.3643651756865
P 0.9698561492 0.8260716167 -0.7966211227
P 0.7607203753 0.2692741965 1.2673229321
P -1.2042262680 -0.4480924451 0.7788905516
P -0.5263502557 -0.6472533584 -1.2495923559

Reaction (b)
6
Reactant: -2047.89890199
P 0.9366015945 0.8121875986 -0.8346097904
P 0.7173955014 0.2467411030 1.2857098581
P -1.1791373461 -0.4213738181 0.8161972995
P -0.4858409348 -0.6205393216 -1.2678820233
P -3.7596554769 4.6316863136 0.3097690233
P -2.6660339349 5.4494859033 -0.6904166973

6
Product: -2048.10621114
P 0.6385871792 1.7071929830 -0.5647539971
P 0.0028963639 1.3995400624 1.3468188856
P -2.1189487965 1.2840775008 0.7205241596
P -1.4250425765 1.6185400550 -1.3633037803
P -2.8081010369 3.3891958884 0.7304038260
P -2.1718247982 3.6958091680 -1.1809863081

Reaction (c)
8
Reactant: -2730.79098431
P 0.5057979042 0.9582013044 -2.3410204968
P 0.2900480755 1.7436169758 -0.4710376737
P -1.6275916286 0.6956908551 -0.0464646800

P -1.4300118512 -0.0646725897 -2.1338211925
P -0.7947114252 -2.0289931516 -1.3758565876
P -1.0696857551 -1.3786576760 0.5378125217
P 2.1694048810 0.8558559103 2.2499164086
P 1.4466852963 -0.7970580847 2.7897466307

8
Transition state: -2730.78981474
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P 0.3599292055 1.7018841412 -0.3134474135
P -1.5731561701 0.6991001148 0.1490520273
P -1.3331714984 -0.0926802473 -1.9446728599
P -0.5570065105 -2.0009898972 -1.2095555054
P -0.9879657758 -1.3779024500 0.6967062603
P 2.0217563878 0.8194575270 2.0188068017
P 1.2942975843 -0.8464973476 2.5641876774

8
Product: -2730.86627252
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P 0.5222021184 1.7193693769 0.1008751758
P -1.4431580150 0.8032106106 0.5142286453
P -1.3320581147 0.0462311999 -1.6504776870
P 0.0313126376 -1.5955233085 -0.9966192788
P -0.7710399740 -1.2263807623 1.0641076699
P 1.8511551692 0.8905807081 1.6766558242
P 1.0713305323 -0.8845713119 2.2574177970

Reaction (d)
8
Reactant: -2730.8662700988
P 0.8209120699 0.0373890617 2.3323283895
P 2.0283906872 0.9865010243 1.0140721942
P -1.1219767496 -0.3235631400 1.3166635623
P -0.6029717394 -1.8793360408 -0.2123059097
P -1.4884431776 -0.4791020039 -1.7075889275
P -1.2293690378 1.2539704312 -0.2237235478
P 0.8812433969 1.2500143324 -0.8706793071
P 0.7122143319 -0.8458736751 -1.6487666196

8
Transition state: -2730.84585194
P 0.9845704616 -0.8372155912 -1.3343675335
P 0.6635714019 1.4643899523 -0.8943533036
P -1.4028992876 1.3092073852 -0.1443014933
P -1.2502183456 -0.3371245510 -1.6882027826

P -0.6099342991 -1.7752982392 -0.1656536867
P -1.1505666060 -0.2488923330 1.4184414312
P 1.8870431363 0.5966459316 0.6321380906
P 0.7833782200 0.0657674728 2.3184200064

8
Product: -2730.8539715508
P 1.1383944401 -1.0198572188 -1.0810070796
P 0.5098248291 1.5206068488 -0.9652801663
P -1.4490108968 1.2503594018 -0.1083170651
P -1.0073027246 -0.1673788902 -1.7854531912
P -0.7031046985 -1.7660692516 -0.2457906993
P -1.1263073687 -0.3453553085 1.4595575532
P 1.8557811021 0.4380744543 0.4535174317
P 0.7817253662 0.0896199297 2.2727720324

Reaction (e)
8
Reactant: -2730.8533649905735
P 2.1933069563 -0.7286077921 -0.6156367361
P 0.0676959156 1.8650987122 0.3510821331
P -0.7170849252 1.0191761673 -1.4313817380
P 0.3413757683 -0.9630382894 -1.6402963098
P -1.1652818050 -1.4970766221 -0.0481482605
P -1.8818034790 0.6294869706 0.5347862766
P 1.5434557871 0.3352017687 1.1103614879
P -0.3816648789 -0.6602407447 1.7392336344

8
Transition state: -2730.83040775
P 2.1543113650 -0.5099734457 -0.6664049496
P 0.5242406062 1.9061139603 0.1504455108
P -0.7166552709 0.9683007215 -1.3267004947
P 0.3145625340 -0.9479256497 -1.6816646241
P -1.2021233486 -1.5739427153 -0.0394793503
P -1.9641578985 0.4631685583 0.5212164263
P 1.4760166561 0.3147854698 1.2063249006
P -0.4851744831 -0.6776798582 1.7735942907

8
Product: -2730.8827720653430
P 2.0197312300 -0.2283444452 -0.6188378527
P 1.0937118615 1.8127377334 -0.1800383537
P -0.7907961805 1.1337294887 -1.1928867727
P 0.1053220186 -0.8407643320 -1.6170616808
P -1.1401680014 -1.7929823301 -0.0107246391

P -2.0664483118 0.2481926741 0.4277041886
P 1.3685827309 0.3184766580 1.4076044027
P -0.5899351021 -0.6510454875 1.7842407340

Reaction (f)
10
Reactant: -3413.56605014
P 0.7806604021 -0.3645111634 -1.0793942561
P -0.8271004153 1.0612262967 -0.3141330083
P -2.1482183749 -0.7078589191 0.0963500126
P -0.5919404035 -2.0877376122 -0.6444102921
P -0.1122170557 -2.7318410090 1.4519896694
P -1.7210222662 -1.3051240893 2.2177837528
P 0.9705806704 0.6258860159 0.8739662285
P 0.4152887500 -0.8416379257 2.4406804531
P 0.9535823209 3.7626548357 -2.2073575902
P 2.2803851331 2.5889442047 -2.8354758249

10
Transition state: -3413.49766546
P 1.4680805094 -0.4348195113 -0.9570470249
P -0.5420299404 1.2322272864 -0.4814559371
P -2.0686539169 -0.2433226188 -0.1158742687
P -0.5004063984 -1.6702784933 -0.8213993722
P -0.2373510207 -2.5111978249 1.2474160621
P -1.7478114171 -1.0150019488 1.9989397234
P 1.1612121986 0.7707841115 0.8302189384
P 0.4072660437 -0.6946124194 2.3334244672
P 0.2335117159 2.8552515848 -1.7814002616
P 1.8261822427 1.7109698400 -2.2528223956

10
Product: -3413.61751248
P 1.6968036154 -0.4198211803 -0.7589978557
P -0.6407507994 1.7726502311 0.2784984822
P -1.7813731910 -0.0171131917 -0.3256449883
P -0.2202753383 -1.4811411541 -1.0185821588
P -0.2122763029 -2.4297916609 1.0063803111
P -1.7726369982 -0.9655630513 1.6994963958
P 1.2254687192 0.8394988520 0.9867349474
P 0.3533602094 -0.7208973689 2.3192929634
P -0.0273660474 2.3704805124 -1.7813958447
P 1.3790463828 1.0516978211 -2.4057824743

Reaction (g)
8

Reactant: -2730.8827714115514
P 0.7885135982 -1.1149621442 -1.6412010963
P 1.0484946844 1.1468925325 -1.4599448058
P -0.9039002282 1.2450251273 -0.3571451426
P -1.1547156692 -0.9431398120 -0.5317899479
P -0.6423039208 -1.2127373828 1.6367415430
P -0.3837290167 1.0492945011 1.8173587572
P 2.2382777635 -0.2405463911 -0.2398927509
P 1.3505474825 -0.3000800964 1.7912538534

8
Transition state: -2730.76058809
P 0.5764519130 -0.4407346606 -1.9541642905
P 0.3254960893 1.5967280462 -1.6556925985
P -1.3299460925 1.2257385632 -0.2867668536
P -1.3815734854 -0.8818110640 -0.9006868045
P -1.3723293258 -1.4938043243 1.1915011486
P -0.9114261690 0.4374793747 1.7937836299
P 2.3396589410 -0.7518408644 0.0651233661
P 1.7611003616 0.0716181172 1.6943580487

8
Product: -1365.3588734437
P -0.4821494687 -0.3290051473 -2.3408520437
P -0.4373643969 1.6143377097 -1.7293652002
P -2.3890335359 1.4318405822 -0.6982155674
P -2.4368583086 -0.6873501679 -1.3637673890
P -1.9228333330 -1.2558166163 0.7142039978
P -1.8819821805 0.6875927994 1.3252133051
P 2.7694316059 -0.7758390605 0.2717173669
P 2.2728888305 0.0093600666 1.9027448961

Reaction (h)
10
Reactant: -3413.5384441502756

P 1.4631251561 -1.2864683309 -2.5016813930
P 0.0798326176 0.4524289476 -2.8023620373
P -1.2504960559 -0.4214136892 -1.2322586264
P 0.1381493125 -2.1782626320 -0.9109315982
P 1.1419853520 -1.7427749075 0.9073702428
P -0.1029984137 1.2605764178 -0.5273369218
P 2.1691966349 0.5444451576 -1.6015323009
P 1.6159019390 0.3147832631 0.5468667906
P -1.8111262866 1.7449424132 2.7365506272
P -1.8134383956 -0.1181562388 2.9891785187

10
Transition state: -3413.53426153
P 1.1915108665 -1.2475208712 -2.0839858553
P 0.0866126672 0.6849448052 -2.4884394463
P -1.4461927200 0.0513127545 -1.0056633292
P -0.3264311783 -1.8694739353 -0.5714675846
P 0.6937527304 -1.5219392169 1.2885853651
P -0.1879383527 1.5678912105 -0.1460218494
P 2.0592814743 0.5442712327 -1.2217606312
P 1.4349734806 0.4567576068 0.9071287521
P -1.7403653357 1.6222592136 2.4053325943
P -1.5850811195 -0.1932940022 2.9494284282

10
Product: -3413.6175076124300
P 0.8182546609 -1.4710481636 -1.6676655868
P 0.2679768099 0.5868168846 -2.3892092722
P -1.4497228825 0.6301190655 -0.9578700877
P -0.8995212330 -1.4285688375 -0.2365953913
P 0.3339474478 -1.0812735731 1.5594771559
P -0.4884325453 2.0016495937 0.4790489070
P 2.0050970623 0.3009958982 -1.0233331307
P 1.2947537990 0.8278603148 1.0235583101
P -1.8221582355 1.5158552886 2.2004554368
P -1.3279823826 -0.3390085334 2.8498562470

Reaction (i)
4
Reactant: -1365.35770883
P 1.1189564907 -0.5748092054 -1.1168978825
P -0.7605969568 -0.9400395115 -0.1976580373
P -0.7036428571 0.3518467586 1.4868867083
P 0.3452833308 1.1630019378 -0.1723307975

4
Transition state: -1365.31618458
P 1.1751677359 -0.9031254977 -1.2307673856
P -0.6328429783 -1.0252754911 -0.5244090811
P -0.6495030665 0.6072148476 1.7255323891
P 0.0888017053 1.3032818169 0.0662548518

4
Product: -1365.3588734437
P 1.4316473938 -1.8623457541 -1.4956584643
P -0.4177237124 -1.6244675032 -1.2768153541

P -0.5769805468 1.4827419628 2.2853279151
P -0.4369424358 2.0040711648 0.4871472133

Reaction (j)
6
Reactant: -2048.03171506
P 1.1936742798 -0.6046985014 -1.0309839298
P -0.7472510107 -0.9260720131 -0.2310859772
P -0.7555014343 0.3475164824 1.4684542916
P 0.4110417371 1.1450079897 -0.1167508485
P 5.1478475623 -1.7885989213 4.6423714086
P 4.0104906345 -1.2047980517 3.3796968225

6
Product: -2048.09973127
P 2.4711517969 -0.9124518278 0.2192029602
P 0.3004995661 -1.1650119817 0.6472485465
P 0.7101601601 -0.0608108563 2.5374414637
P 1.1386837343 0.8414625383 0.5470787227
P 4.1372243261 -1.4397718808 3.6625103251
P 2.7618480815 -0.9243420900 2.4288893112

Reaction (k)
6
Reactant: -2048.09972849
P 1.0215807606 0.4787270347 -1.1127582233
P 0.2191231406 -1.5979197492 -1.1756506706
P -1.2624824595 -0.8981835518 0.3325667240
P -1.0951481282 0.0657903553 -1.6685750083
P 0.3064286311 0.5379982351 0.9970962827
P 0.8104977661 1.4135866242 2.6273210554

Transition state: -2048.06129165
P 0.9575260653 0.6571992801 -0.7641340486
P 0.5032970545 -1.5236424886 -0.7064229748
P -1.3950437262 -0.8784559261 0.3001889060
P -0.9152122249 -0.2264553817 -1.7289475812
P -0.3335783498 1.0529242072 1.0396433906
P 1.3396463722 0.6687922082 2.1267910571

6
Product: -2048.09774886
P 1.3890955865 0.8832989474 -0.2917287891
P 0.4739466238 -1.3390803179 -0.8820445660
P -1.3894375563 -0.8838781710 0.2911413325
P -1.2288185357 -0.5065082984 -1.7531704667

P -0.4732320792 1.3397777406 0.8824127667
P 1.2284457552 0.5063904490 1.7533892988

Reaction (l)
6
Reactant: -2048.09774886
P 1.3890955865 0.8832989474 -0.2917287891
P 0.4739466238 -1.3390803179 -0.8820445660
P -1.3894375563 -0.8838781710 0.2911413325
P -1.2288185357 -0.5065082984 -1.7531704667
P -0.4732320792 1.3397777406 0.8824127667
P 1.2284457552 0.5063904490 1.7533892988

6
Transition state: -2048.09745203
P 1.0231817690 -1.2859023992 -0.0320628205
P -1.2168619561 -1.2021468009 -0.1037005303
P -0.9352514186 1.4662771156 0.0079361897
P -0.2379964719 -1.4532292190 1.6738265719
P 0.2109477744 1.4885267157 -1.6852349699
P 1.2704244272 1.0735903731 0.1130568115

6
Product: -2048.09969290417
P 0.9855322513 -1.2623148940 0.0194743449
P -1.2227505522 -1.5558434478 -0.0505702470
P -0.8472429401 1.7884999874 -0.0280513272
P -0.3250533364 -1.6004142830 1.7418784096
P 0.1696244967 1.6183752660 -1.7476212421
P 1.2398900049 1.0116973394 0.0648898420

Reaction (m)
8
Reactant: -2730.7824897768132
P 3.1074640957 -1.0986136190 -0.2123964346
P 2.3525879021 0.8396503820 -0.9008081042
P 0.9196409171 0.2108089815 -2.5690185455
P -0.4789094165 -1.2049391133 -1.5652796274
P -1.0258532527 0.7198155729 -1.6996089422
P -2.8879023535 0.4221160763 1.6325997618
P 1.6316980394 -0.2907878306 0.8788592391
P -1.6425341270 -0.1080409368 2.9345709414

8
Transition state: -2730.77627704

P 1.8000664798 -1.2483950895 0.0520369474
P 2.1345209112 0.9031283966 -0.4099373337
P 0.5083162920 1.2236686206 -2.0016850923
P -0.3670678731 -0.8216027772 -2.0712908714
P -1.5085059643 0.6837155142 -1.3523426714
P -2.7455840099 0.4197817229 1.4538258822
P 1.3943430922 0.1135033366 1.4898512073
P -1.4077168269 0.1534276591 2.7647695029

8
Product: -2730.8356037810604
P 1.1144782851 -1.6186446669 -0.0356466166
P 1.6727341433 0.5351818829 0.0592442534
P 0.0676466249 1.0189591239 -1.4699643538
P -0.4896312903 -1.1350410563 -1.5658175652
P -1.9535807372 0.3644605314 -0.8824769373
P -2.5220333438 0.4167455925 1.2435327138
P 0.9156425462 -0.4985750991 1.8526750035
P -1.0955176312 -0.0105280329 2.6031468258

Reaction (n)
8
Reactant: -2730.8356052486174
P 1.6011041831 -1.2914835135 -0.2396765705
P 1.8638566275 0.9020268869 0.0410370411
P 0.3285980448 1.2934860219 -1.5835850692
P 0.0656838498 -0.9003158357 -1.8638957246
P -1.6279757557 0.3497642961 -1.2104393937
P -2.3560187812 0.1727910311 0.8596318827
P 1.1165847552 -0.3505139908 1.6938553099
P -0.9918383240 -0.1757580519 2.3030622585

8
Transition state: -2730.79529940
P 1.7219109136 -1.3320966515 -0.0246600711
P 1.8311767092 0.9159914461 0.0864255371
P 0.3346697337 0.9694506028 -1.6132982924
P -0.0121965337 -1.2040671041 -1.5408928279
P -1.5715438500 0.2381830326 -0.7997212731
P -2.2505751166 1.2750830322 1.1483515378
P 0.8892643538 -0.2508888865 1.6659590294
P -1.3021311538 -0.5778966820 1.3856736175

8
Product: -2730.88276674269
P 1.6505830084 -1.3106241313 -0.2704850319

P 1.9095265582 0.9023535846 0.2307908356
P 0.2256286755 1.3802218143 -1.1738494355
P -0.0244136884 -0.7603998937 -1.6592357903
P -1.8957248128 -0.8605409454 -0.4244220346
P -1.6371620224 1.3522996878 0.0786020089
P 0.9848506539 -0.4908472160 1.6568451157
P -1.2132120949 -0.2124482197 1.5617007303

Reaction (o)
Reactant: -2048.03518794
P 1.1905112175 -0.6052377439 -1.0313668444
P -0.7495970608 -0.9285743003 -0.2294736100
P -0.7599549092 0.3495588912 1.4668695733
P 0.4041906554 1.1456072503 -0.1210861598
P 3.2108893245 -1.3328263660 4.3701135438
P 3.9433857362 -1.9149506864 2.8127799840

Product: -2048.13606398
P 2.2083056629 -1.0362920218 0.0780403375
P 0.0522008606 -1.1845749401 0.5523231370
P 0.3059127567 -0.0633278205 2.4431157894
P 1.0390316629 0.7855572594 0.5358169416
P 2.0999384186 -0.9528845673 3.4530506039
P 3.2941862639 -1.5648966285 1.9676664397

Reaction (p)
6
Reactant: -2048.04671834
P -0.3980553360 -1.4577704250 -0.7192977297
P -0.6469224810 0.2785697164 2.0847502935
P 0.6469507667 -0.2780805740 -2.0844789258
P -1.5788846850 0.5024140631 0.2337658635
P 0.3986507852 1.4569611899 0.7176364175
P 1.5782609502 -0.5020939704 -0.2323759192

6
Transition state: -2048.033944
P -0.3083301517 -1.4706860166 -0.2706954468
P -0.7717944318 0.0101243122 1.8336165453
P 0.2821983494 -0.2457913122 -1.9531987549
P -1.3695299577 0.6602699939 -0.1417602771
P 0.5258815868 1.3720264231 0.8656354536
P 1.6415746051 -0.3259434005 -0.3335975201

6

Product: -2048.07984698
P 0.1016401976 -1.7109393167 -0.0170162589
P -0.9425998041 -0.2802520794 1.4071998837
P -0.1892999370 -0.2649687428 -1.6837864265
P -1.2316650517 1.1671004446 -0.2591315278
P 0.6094657308 1.2594553148 0.9890862563
P 1.6524588644 -0.1703956205 -0.4363519268

Reaction (q)
6
Reactant: -2048.13068153
P 0.8782225847 -0.5050939040 1.3844757857
P 0.6233899083 -1.4530464416 -0.6652534748
P 0.6464959210 1.5151331176 0.4787645140
P 0.3919678647 0.5670176065 -1.5709625649
P -1.3972537427 -0.5360572634 -0.8384831247
P -1.1428224730 0.4120468184 1.2114587689

6
Transition state: -2048.05183085
P 0.8200895488 -0.3558216661 1.3365802213
P 0.4917332635 -1.3561420615 -0.7112406090
P 0.5340538011 1.4598461341 0.1264803149
P 0.9458737733 0.5560423786 -1.7433356701
P -1.4289053725 -0.2926843112 -0.5529064682
P -1.3628449623 -0.0112405336 1.5444221163

6
Product: -2048.10621964
P 0.6894187275 -0.2053042774 1.2383733247
P 0.3665449704 -1.1733125320 -0.7353906471
P 1.2805278863 1.6254517233 0.1402702003
P 0.9848305217 0.7373129954 -1.6697662396
P -1.8087610536 -0.9363952501 -0.3916054623
P -1.5125609484 -0.0477527012 1.4181187242

Reaction (r)
6
Reactant: -2048.0913278520779
P 1.7635964055 0.0484650492 -0.4674954185
P 0.9125488822 0.8674645364 1.3213481572
P -1.2277817284 0.1964640358 0.9071925235
P -1.3205760203 -1.7793900883 0.1866734332
P -0.1800918147 -0.8131103046 -1.2951185164
P 0.0523048181 1.4801082513 -0.6525997046

Transition state: -2048.08285372
P 1.8421992072 0.3080484308 -0.4250465894
P 1.0084765650 0.7376064788 1.4234986580
P -1.1871253289 0.3160605829 1.1412525664
P -1.3840624926 -1.5617203011 0.1329282286
P -0.1189478808 -0.9372725006 -1.4418766205
P -0.1712036307 1.1315610062 -0.8330929090

6
Product: -2048.1062107474872
P 1.8829374357 0.8577696264 -0.1439494851
P 1.1117615156 0.4382829106 1.6949803445
P -0.9679837728 0.4879058480 0.9351687982
P -1.3348375581 -1.5731415866 0.2118162942
P -0.5644812736 -1.1548622254 -1.6276676048
P -0.1273966043 0.9440450541 -1.0703484567

Reaction (s)
6
Reactant: -2048.09774827
P 1.0888900095 0.9826608502 -0.8029911816
P -1.0162169820 0.3529449430 -1.2798074059
P 0.6531187992 -0.6764000542 -1.9891110135
P -1.0887684615 -0.9825972269 0.8030008652
P 1.0159724237 -0.3532067049 1.2798975085
P -0.6529949992 0.6765983411 1.9890116325

Transition state: -2048.08480321
P -0.5969615910 0.8875507199 1.4462868217
P 1.0169316094 -0.4828862327 1.3782103188
P -1.0628450495 -1.1058482418 0.9022719859
P 0.6111605843 -0.4377285989 -2.1016280356
P -1.0925046260 0.2386171597 -1.0654260578
P 1.1242199584 0.9002953639 -0.5597148001

6
Product: -2048.09132314
P -0.5650583504 1.0408238099 1.1028384518
P 0.9846784910 -0.5399370592 1.4387397492
P -1.0204138439 -1.1481176988 0.9860512586
P 0.5299056834 -0.1419721749 -2.1547968181
P -1.1991420227 0.0200859356 -0.9652935103
P 1.2700309996 0.7691173808 -0.4075386797

Reaction (t)

6
Reactant: -2048.0913189910161
P 0.0034185956 1.3702315469 -0.8584702310
P 0.1262134468 -0.9945426288 -1.1683851169
P -1.1416697984 -1.8891922111 0.2551285790
P -1.3754336127 0.1589396401 0.6783343385
P 0.5849230497 1.1454796714 1.2935702832
P 1.8025483459 0.2090831574 -0.2001779473

6
Transition state: -2048.09048013
P -0.0705588288 1.3863702658 -0.8140631252
P 0.2215604236 -1.1076561651 -1.1749373138
P -1.1470610845 -1.8540612147 0.1989396744
P -1.3462671159 0.2263865593 0.6938326317
P 0.6063645467 1.1618048793 1.3001260042
P 1.7718254457 0.1925268554 -0.2223094457

6
Product: -2048.1360616241468
P -0.1972874125 1.7001357152 -0.5824385334
P 0.6268355355 -1.7476803384 -0.8874423336
P -1.1941764275 -1.6751334613 -0.0598834868
P -1.3920938575 0.4050576978 0.7553050051
P 0.6496799393 1.0283030551 1.3377192360
P 1.5070422238 0.2893174716 -0.5632599184

<u>Reaction (u)</u>
8
Reactant: -2730.8189665568916
P -0.7368836668 1.0288541328 -1.4681408859
P -1.9227829775 1.2200376648 0.1333495461
P 0.0698987344 -1.0627387836 -1.3640702779
P -1.8124644902 -0.7553944312 1.1888474147
P 0.2118005356 -1.5562036042 0.7853564545
P -1.5079552248 -2.2734483820 -0.3918788030
P 3.0200772863 1.1379838474 1.3020573024
P 2.6766397785 2.2470978640 -0.1743080826

8
Transition state: -2730.79638775
P 0.0761328291 1.0346265306 -0.7414887272
P -1.5625510967 1.3573368393 0.4377538058
P 0.5892502250 -1.1376002321 -0.8539293732
P -1.9900757195 -0.7506656948 0.9677607378
P -0.1473952050 -1.9636924169 1.0638472273

P -1.4212943392 -2.0362872356 -0.7541775212
P 2.4967395974 1.0686722308 0.5938084023
P 1.9575251351 2.4137950606 -0.7023578634

8
Product: -2730.8259494481536
P 0.5409074395 0.8003252810 -0.0427474910
P -1.3059074901 1.3435918947 0.8319697686
P 0.7406336827 -1.3237987016 -0.6023874709
P -2.1042893832 -0.6733369094 0.7124934216
P -0.5468847176 -2.2452816295 0.9461151585
P -1.3728258792 -1.7985846959 -1.0629302456
P 2.3995494241 1.7309354154 0.5389863998
P 1.6471483178 2.1523344827 -1.3102832331

Reaction (v)
8
Reactant: -2730.825952
P 0.5345584501 0.8046972753 -0.0672873888
P -1.2840810742 1.3428487710 0.8677739966
P 0.7303387249 -1.3229700082 -0.6148174463
P -2.0745944369 -0.6791125310 0.7867682314
P -0.5009910893 -2.2407000554 0.9809756956
P -1.3941284757 -1.8129533067 -1.0031880910
P 2.4053972655 1.7561191468 0.4373423822
P 1.5835007933 2.1520714881 -1.3875669152

8
Transition state: -2730.81149292
P 0.9403159435 0.5365251869 0.3772368701
P -0.9605517298 1.3441475833 0.9714664323
P 0.8669552090 -1.5530992299 -0.3390208986
P -2.0795891619 -0.4583623696 0.4893650119
P -0.8431723591 -2.2802145380 0.8734111729
P -1.1603435050 -1.6005987781 -1.2070011671
P 2.4051120680 2.1060414902 0.0821635597
P 0.8312738158 1.9055610041 -1.2476208793

8
Product: -2730.82862904
P 1.2477408723 0.4360387451 0.8108063079
P -0.7493938457 1.3892681714 0.8080838292
P 0.8558998071 -1.5078350700 -0.3576107732
P -2.0567435295 -0.3485666692 0.3879819966
P -0.8899150399 -2.2196943686 0.7917747516
P -1.1327070549 -1.5097995967 -1.2831859831

P 2.2413896918 2.1930220163 -0.1012649548
P 0.4837293692 1.5675671664 -1.0565851197

Reaction (w)
8
Reactant: -2730.82863691
P 1.3085297177 0.6649457736 0.5006435569
P -0.7675550320 1.2832297349 0.9530513394
P 0.9913174952 -1.3644376803 -0.5384081339
P -1.8287861884 -0.6579589388 0.8509152898
P -0.3065603564 -2.2981217826 0.9845631998
P -1.1260619025 -1.7255155353 -0.9824306078
P 1.7639264373 2.5186888928 -0.6225799259
P -0.0348164087 1.5791754885 -1.1457580240

8
Transition state: -2730.82752101
P 1.3580584761 0.6278926658 0.5927922364
P -0.7389007389 1.2779472290 0.9560844470
P 1.0151453247 -1.3470398399 -0.5059390566
P -1.8316763585 -0.6468924663 0.8321538789
P -0.3286233867 -2.2985194093 0.9661904198
P -1.0991247799 -1.6798800447 -1.0059193327
P 1.7479731704 2.4146625231 -0.6914181030
P -0.1228477568 1.6518434210 -1.1439493463

8
Product: -2730.86426161
P 1.4940667365 0.5527439297 0.6808605845
P -0.5862591046 1.2032250392 1.0997550628
P 1.2286012212 -1.4789456556 -0.1218235840
P -1.7859539270 -0.5360012429 0.4843894313
P -0.5227895216 -2.2915027270 0.9638932019
P -0.7314449485 -1.6085925210 -1.1358527571
P 1.4055245462 1.7818032356 -1.1772248214
P -0.5017405867 2.3772840089 -0.7940021304

Reaction (x)
8
Reactant: -2730.7961164300
P -0.2294349015 -1.8658470068 -1.7115440636
P -1.2787714803 0.0672523630 -1.4388462483
P 1.1142230561 1.3222767517 1.8742629991
P 0.2624435917 -0.7138441493 1.5599446330
P 0.8817827000 0.0463124858 -1.8959434239
P 1.3477667451 -1.3493108433 -0.2460869818

P -1.5503069138 0.2692097041 0.7366285360
P -0.5477027973 2.2239506947 1.1215845496

8
Transition state: -2730.7395580000
P -0.1868410037 -1.4687212521 -1.8731512379
P -1.5688942004 0.0461443246 -1.1226696980
P 1.0230781591 1.2408958399 1.8060277414
P 0.2844917599 -0.8040696923 1.7535389422
P 1.0418938389 0.3789270014 -1.4389532137
P 1.2690028107 -1.3863973440 -0.2273687009
P -1.5597712078 0.1878746766 0.9941014167
P -0.3029601568 1.8053464459 0.1084747502

8
Product: -2730.8146583700
P -0.3180554054 -1.1215153944 -1.7752773710
P -1.6262910431 0.3745520444 -0.7335408174
P 0.2063657479 1.2616563855 1.6961854357
P 0.5011122488 -0.9153944559 1.6939452822
P 1.4402068507 0.3135531669 -1.5330383696
P 1.2714896693 -1.4990728856 -0.3022901650
P -1.5528589236 -0.1741477922 1.4413118477
P 0.0780308553 1.7603689312 -0.4872958426

Reaction (y)

8
Reactant: -2730.7223030600
P 2.0819176845 -0.1309408997 0.5505600082
P 1.1428923920 1.6776529891 0.6115033828
P -0.8482564325 0.7369702005 0.3844237514
P 0.1689873139 -1.2372562036 0.3423080348
P -0.5432969800 -1.5231386016 2.4249453052
P -1.4668151993 0.2908971543 2.4648102098
P -1.1296141702 0.4591529203 -3.3129751447
P 0.5941853914 -0.2733375594 -3.4655755476

8
Transition state: -2730.6790790000
P 1.1950783620 -0.5969364704 -0.4294138797
P 0.4099970432 1.3623147709 -0.3115393703
P -1.4511756155 0.6429001138 0.7093395419
P -0.6297293809 -1.4296939315 0.5482991141
P -0.0474804298 -1.2966124306 2.6764953189
P -0.8358507796 0.5774549018 2.8406328663

P -0.0931561241 0.1127088433 -2.4367878290
P 1.4523169246 0.6278642027 -3.5970257622

8
Product: -2730.7237537700
P 1.1274128263 -0.4001712176 -0.6116986860
P 0.3169591457 1.6592520320 -0.4036693657
P -1.4316564027 0.7701745952 0.7193064666
P -0.8266771341 -1.3280180270 0.1862379435
P -0.0927803587 -1.5148734857 2.2858119094
P -0.5450242072 0.4245876850 2.7193182188
P -0.2572063893 0.5032524861 -2.2016704615
P 1.7089725200 -0.1142040681 -2.6936360251

Reaction (z)
8
Reactant: -2730.72376742
P 1.2231334068 -0.2451429777 -0.5086219542
P 0.3627260217 1.6887668283 0.1693197971
P -1.5438727784 0.5779454754 0.6610450301
P -0.8218456479 -1.2931166294 -0.3546788522
P -0.4545025738 -2.1125550361 1.6885030399
P -1.0237067372 -0.3766937539 2.5918005611
P 2.1431754970 0.6208624043 -2.2867059046
P 0.1148928117 1.1399336892 -1.9606617174

8
Transition state: -2730.722178
P 1.3023174712 -0.2841164662 -0.3989571923
P 0.3459824086 1.6692814181 0.1336215815
P -1.5516541803 0.5719815806 0.6596494065
P -0.8000244952 -1.2808123407 -0.3629217473
P -0.4632671459 -2.1136679836 1.6659730133
P -1.0063172682 -0.3742396449 2.5861556284
P 2.0668875983 0.5843599473 -2.2748567528
P 0.1060756114 1.2272134894 -2.0086639373

8
Product: -2730.75738344
P 1.5026705662 -0.4096654537 -0.3339378620
P 0.4630933738 1.4947004630 0.2714204299
P -1.5036181746 0.4072366908 0.3318342069
P -0.4642212082 -1.4979631221 -0.2710153342
P -0.3769267924 -2.0059197559 1.8848466364
P -1.3273822529 -0.2870674921 2.4302238949
P 1.3252896690 0.2886070241 -2.4306434841

P 0.3810948191 2.0100716459 -1.8827284878

Reaction (aa)
10
Reactant: -3413.42410158
P 0.9337354341 -0.5739619335 -0.7737326464
P 0.0179802085 1.4623494706 -0.4852920473
P -2.0333354902 0.5549940012 -0.6778241833
P -1.1131767079 -1.4855910229 -0.9181755121
P -1.4302247156 -1.7623017334 1.2601063732
P -2.2813722458 0.0773764294 1.4728243826
P 2.4948007513 -0.8412936293 2.5848926013
P 1.9443393045 0.8718312427 3.1232101020
P 0.3328844404 1.7756877873 -2.6614285950
P 1.1343690206 -0.0790906121 -2.9245804752

10
Transition state: -3413.397873
P 1.1369641716 -0.2766458104 -0.4370114130
P 0.1937234267 1.6914795655 -0.3627080697
P -1.7837680639 0.6122478290 -0.3804620051
P -0.8673884131 -1.4359921864 -0.6582712100
P -1.5746927567 -1.8650779001 1.3841193870
P -1.9076865864 0.1339790818 1.7566960275
P 2.1887019453 -0.6901668663 1.5535314440
P 0.9118931326 0.5183126837 2.4674886374
P 0.3539259588 1.5338073033 -2.6437584176
P 1.3483271852 -0.2219437000 -2.6796243804

10
Product: -3413.46716135
P 1.0258627876 -0.1190994826 -0.4323994515
P -0.1395538298 1.7388834810 -0.7688104227
P -1.9439925556 0.5120902805 -0.2876520488
P -0.8681005241 -1.4195370263 -0.5312704377
P -1.2030395843 -1.7169689035 1.6640077375
P -1.5590398954 0.5160202365 1.9419446905
P 2.1759663274 -0.3717770460 1.2778169337
P 0.3800581563 -0.4177391813 2.5141144681
P 0.3400851768 1.3316738005 -2.8929212497
P 1.7917539413 -0.0535461588 -2.4848302193

Reaction (ab)
10
Reactant: -3413.4671501500

P	1.5720004526	-0.6500410208	0.3978765282
P	1.1834701740	1.5243205884	0.6373494855
P	-0.9899429581	1.2262716004	1.0640135326
P	-0.7194795898	-0.8227227659	0.2580039869
P	-1.3612330945	-1.6888722688	2.1666693339
P	-1.1088314713	0.1642932135	3.0022187201
P	2.0185341839	-0.1877472779	-1.7470886103
P	0.8784011485	1.7821040917	-1.5893279223
P	-0.0276182360	0.0006643898	-2.5743772989
P	-1.4453006098	-1.3482705501	-1.6153377557

10
Transition state: -3413.422372

P	1.7535547492	-0.7951534126	0.2226375761
P	1.1361754098	1.3261416179	0.6209775389
P	-1.0052361606	1.5605461503	1.3017850612
P	-0.4113734256	-1.0229161427	0.3585061952
P	-1.0809935926	-1.7236533381	2.2559403551
P	-1.7519719515	0.2236085044	2.7165709482
P	2.0090562078	-0.1952638289	-1.9300979793
P	0.8880878513	1.7495555104	-1.5507074591
P	-0.0800845261	0.0220436066	-2.6022568807
P	-1.4572145617	-1.1449086673	-1.3933553556

Product: -3413.5325330900

P	1.7141262584	-0.4000997294	-0.7269005730
P	-0.6612944963	1.7626135865	0.2854760716
P	-1.7729296083	-0.0281081256	-0.3672644497
P	-0.1892594566	-1.4734761647	-1.0453825783
P	-0.2263010090	-2.4438927254	0.9687325017
P	-1.8022267123	-0.9928167589	1.6518800132
P	1.1968157914	0.8347732229	1.0237658688
P	0.3106038302	-0.7528072850	2.3150691414
P	0.0031701540	2.4001274764	-1.7467783724
P	1.4272952486	1.0936865032	-2.3585976234

Cartesian coordinates for structures in Scheme 2

12
Reactant 1: -4096.20001028

P	2.6633247933	-1.0771839264	-1.9132612996
P	2.3499411458	-2.1055467782	0.0622293718
P	1.9898630625	-0.1230385854	1.0335898765
P	-0.1940212690	-0.3758053962	1.2053223983
P	0.2626023510	1.1676506612	-1.7576968084
P	2.2976556044	0.9042184545	-0.9434252509
P	-0.7360311829	-0.6109944243	-0.9192868022
P	0.7597857708	-2.1566515125	-1.4994160796
P	-0.3814217301	2.7152557351	-0.2826094817
P	-0.6551486788	1.7858366791	1.4979170838
P	-4.1323727983	-0.9374407404	1.4215743526
P	-4.2241770685	0.8136998339	2.0950626393

12
Transition state 1: -4096.179825

P	2.8269378559	-0.8354551881	-1.7506736035
P	2.4263437746	-2.0335804784	0.1104804327
P	1.7068305685	-0.1907875924	1.1515231664
P	-0.4186374084	-0.7834400099	1.0627975524
P	0.1147665762	1.0841105940	-1.7035870234
P	2.0780394245	1.0002727521	-0.7199295323
P	-0.7003922294	-0.8852985690	-1.1352701589
P	1.0438620457	-2.1665979158	-1.6432119048
P	-0.9061046601	2.4833967283	-0.3048304024

P -1.2483508771 1.2404780558 1.3107147976
P -3.6143407773 -0.1801815735 1.1827745949
P -3.3089542932 1.2670831968 2.4392120813

12
Reactant 2: -4096.20802058
P 3.0525932416 -0.5182969825 -1.2942918496
P 2.3713399593 -2.0619381649 0.1993773066
P 1.2124816146 -0.4830357466 1.2743499541
P -0.7367552967 -1.1834610999 0.5120217135
P 0.2330294315 1.2093896152 -1.6691869451
P 1.8871475701 1.0512946932 -0.2176645671
P -0.4647321928 -0.8957792073 -1.6655630853
P 1.4641398743 -1.9919003938 -1.8367214242
P -1.4159417758 2.2443432547 -0.7072720155
P -1.7821070964 0.7470902765 0.7841335836
P -3.7099461625 0.6435020788 1.7547777734
P -2.1112491673 1.2387916766 2.8660395558

12
Transition State 2: -4096.193999
P 2.2480606072 -1.8821684087 -1.6865633335
P 1.5171676363 -2.8670735196 0.2029864032
P 1.4447390794 -0.8700407048 1.1995852766
P -0.7593368051 -0.7751380229 1.1247355905
P 0.3245561261 0.8194714241 -1.7067495792
P 2.1513842692 0.1196118039 -0.6996016744
P -1.0905654417 -0.7767662473 -1.0696262473
P 0.1387011724 -2.5715205225 -1.5307864201
P -0.2582873963 2.5429636285 -0.4777618960
P -0.8916890313 1.4099517933 1.2667772967
P -2.8451379071 2.1279453569 0.7977842577
P -1.9795923091 2.7227634191 2.5792203258

12
Reactant 3: -4096.21297503
P 2.1964450865 -1.7896491771 -1.7402738013
P 1.5232120684 -2.8760181568 0.1143314797
P 1.4328520885 -0.9314755707 1.2002124504
P -0.7642128709 -0.7549134584 1.2228142324
P 0.2142662048 0.8161337116 -1.6311970126
P 2.0821205438 0.1663694771 -0.6606434996
P -1.1615477797 -0.7973833352 -0.9557566471
P 0.1029699260 -2.5248827942 -1.5676358399
P -0.3350451945 2.5003145473 -0.2774907404
P -0.6214562099 1.4572680060 1.6865272880

P -2.4096496869 1.9444050184 0.3405826905
P -2.2599541760 2.7898317318 2.2685293998

12
Transition State 3: -4096.210052
P 2.2637294365 -1.4782800246 -1.9217332783
P 2.0308527959 -2.5363110026 0.0535584774
P 1.7287466909 -0.5671145910 1.0557455142
P -0.4421960820 -0.7643080408 1.3585117127
P -0.1186653472 0.7451317220 -1.6600036992
P 1.9408579769 0.4978729225 -0.9245687645
P -1.0866465080 -1.0270201843 -0.7410612424
P 0.3761818995 -2.5561967299 -1.4372274257
P -0.7975093119 2.3688083997 -0.3040850523
P -0.5994672901 1.4668816490 1.7739030114
P -2.7217210227 1.5548318271 0.4078083092
P -2.5741632379 2.2957040530 2.3391524374

12
Product: -4096.2469961
P 2.0682357623 -1.5354200640 -2.0184737539
P 2.0857897661 -2.5178189880 0.0088279205
P 1.9381763651 -0.5111467118 0.9757912405
P -0.1808875357 -0.7059289834 1.5350687398
P -0.2178095793 0.7623336102 -1.5128975062
P 1.9154674594 0.4700968069 -1.0488812471
P -1.0991995655 -0.9833645244 -0.4659132972
P 0.2460293504 -2.5648761549 -1.2513994805
P -0.6077467045 2.3991138457 -0.0933248588
P -0.5569450039 1.4239749782 1.9465214658
P -2.8176104503 2.3085866936 0.0368535704
P -2.7734998641 1.4544494920 1.8878272067

<u>Reaction B:</u>
12
Reactant1: -4096.1971878500
P -0.5648602050 -1.6736757128 0.5743405684
P 0.4601821318 0.6478239302 -1.6441820293
P 2.0807985825 0.5453840364 -0.1511810279
P 1.3969591556 -1.0016903939 1.3327631499
P 2.5883461494 -2.5560472605 0.2475728915
P 3.2643300047 -1.0090697110 -1.2380016878
P -0.2620288369 -1.4341571594 -1.5942465667
P 1.6936193980 -2.4869005125 -1.7926429634
P -1.0281791461 1.6203014262 -0.2972048890
P -1.6469699484 0.2228737617 1.0349441302

P -3.9897003703 3.1098625708 2.5866774578
P -3.9924969147 4.0152950249 0.9411609661

12
Transition State 1: -4096.174037
P -0.6672267865 -1.4772141191 0.7338255800
P 0.2876068160 0.7941121558 -1.5525392894
P 1.9837227323 0.6917958476 -0.1546446408
P 1.3165033704 -0.7902568410 1.3970740134
P 2.4382030341 -2.4086829583 0.3216726571
P 3.0949347974 -0.9174718236 -1.2312139143
P -0.4511640837 -1.2981597714 -1.4437079372
P 1.4787849447 -2.3830231098 -1.6894022843
P -0.9833760987 1.8471168417 -0.0550903290
P -2.0546734510 0.3003697601 0.8390142491
P -3.2493381134 2.3073854905 2.2289232232
P -3.1939771617 3.3340285276 0.6060886722

12
Reactant 2: -4096.2021567
P -0.7184062636 -1.4101919818 0.8721638247
P 0.1831586030 0.9026200844 -1.6138248121
P 1.9288074528 0.7767171805 -0.2683125898
P 1.2644202870 -0.5738568990 1.4179289850
P 2.3590314517 -2.2510925236 0.4151881574
P 2.9955059706 -0.9020229691 -1.2660298449
P -0.5733514766 -1.2119419632 -1.3436075582
P 1.3241910104 -2.3421271035 -1.5733293876
P -0.8385229615 1.8261341008 0.1735014604
P -2.2002439848 0.2498351990 0.6594374592
P -3.1668125104 1.7720141732 1.9518441683
P -2.5577775786 3.1639127024 0.5750401376

12
Transition State 2: -4096.189869
P -0.5789328624 -1.4955716334 0.8787691929
P 0.2923962283 1.0165694566 -1.3852147582
P 1.8887047313 1.0058856949 0.1428147751
P 1.2778716167 -0.5592687009 1.6536657881
P 2.5929277786 -2.0356868224 0.6151639663
P 3.2163836447 -0.4667263321 -0.8691268804
P -0.2694357646 -1.1607424977 -1.3064043600
P 1.7628714277 -2.0441950562 -1.4721319007
P -1.1003407672 1.9373461873 0.1145710045
P -1.9933648441 0.1366467076 0.7737247874
P -3.8780699787 1.0691015966 1.0462505855

P -3.2110112103 2.5966413998 -0.1920822005

12
Product: -4096.24637422
P -0.6721889197 -1.2239364542 0.9744001143
P 0.3066849558 1.2180422925 -1.1472599786
P 1.9877241515 0.9805187593 0.2505636196
P 1.3308843886 -0.6382142063 1.6705784559
P 2.4258770843 -2.1489654885 0.4435893213
P 3.0770337328 -0.5302734844 -0.9798793855
P -0.4715465930 -0.8582269306 -1.2017186842
P 1.4397710395 -1.9363859305 -1.5456795540
P -1.0777085617 2.2070400428 0.2485229942
P -1.7482495295 0.5692260206 1.6597208926
P -3.5994113152 0.4399405689 0.4462005501
P -2.9988704336 1.9212348105 -0.8190383457

Reaction C
12
Reactant 1 (black): -4096.20001028
P 2.6633247933 -1.0771839264 -1.9132612996
P 2.3499411458 -2.1055467782 0.0622293718
P 1.9898630625 -0.1230385854 1.0335898765
P -0.1940212690 -0.3758053962 1.2053223983
P 0.2626023510 1.1676506612 -1.7576968084
P 2.2976556044 0.9042184545 -0.9434252509
P -0.7360311829 -0.6109944243 -0.9192868022
P 0.7597857708 -2.1566515125 -1.4994160796
P -0.3814217301 2.7152557351 -0.2826094817
P -0.6551486788 1.7858366791 1.4979170838
P -4.1323727983 -0.9374407404 1.4215743526
P -4.2241770685 0.8136998339 2.0950626393

12
Transition State 1 (black): -4096.179825
P 2.8269378559 -0.8354551881 -1.7506736035
P 2.4263437746 -2.0335804784 0.1104804327
P 1.7068305685 -0.1907875924 1.1515231664
P -0.4186374084 -0.7834400099 1.0627975524
P 0.1147665762 1.0841105940 -1.7035870234
P 2.0780394245 1.0002727521 -0.7199295323

P -0.7003922294 -0.8852985690 -1.1352701589
P 1.0438620457 -2.1665979158 -1.6432119048
P -0.9061046601 2.4833967283 -0.3048304024
P -1.2483508771 1.2404780558 1.3107147976
P -3.6143407773 -0.1801815735 1.1827745949
P -3.3089542932 1.2670831968 2.4392120813

12
Reactant1 (blue): -4096.1971878500
P -0.5648602050 -1.6736757128 0.5743405684
P 0.4601821318 0.6478239302 -1.6441820293
P 2.0807985825 0.5453840364 -0.1511810279
P 1.3969591556 -1.0016903939 1.3327631499
P 2.5883461494 -2.5560472605 0.2475728915
P 3.2643300047 -1.0090697110 -1.2380016878
P -0.2620288369 -1.4341571594 -1.5942465667
P 1.6936193980 -2.4869005125 -1.7926429634
P -1.0281791461 1.6203014262 -0.2972048890
P -1.6469699484 0.2228737617 1.0349441302
P -3.9897003703 3.1098625708 2.5866774578
P -3.9924969147 4.0152950249 0.9411609661

12
Transition State 1 (blue): -4096.174037
P -0.6672267865 -1.4772141191 0.7338255800
P 0.2876068160 0.7941121558 -1.5525392894
P 1.9837227323 0.6917958476 -0.1546446408
P 1.3165033704 -0.7902568410 1.3970740134
P 2.4382030341 -2.4086829583 0.3216726571
P 3.0949347974 -0.9174718236 -1.2312139143
P -0.4511640837 -1.2981597714 -1.4437079372
P 1.4787849447 -2.3830231098 -1.6894022843
P -0.9833760987 1.8471168417 -0.0550903290
P -2.0546734510 0.3003697601 0.8390142491
P -3.2493381134 2.3073854905 2.2289232232
P -3.1939771617 3.3340285276 0.6060886722

14
Reactant 2 (black): -4778.91379021
P 0.7546242812 -1.1737805732 -3.4473153181
P 0.7830409043 -2.7607064881 -1.8498951357
P 2.0410075111 -1.4414416333 -0.5604542899
P 0.4129151143 -0.8923936344 0.8127275795
P 0.3757776022 1.4955403922 -1.5779805226
P 2.0133762810 0.1444240035 -2.1586807766
P -1.0046022377 0.0624397734 -0.6011082920

P -1.0392813416 -1.5138442018 -2.1650942712
P 1.3592748540 2.4381683633 0.1509768418
P 1.3904886870 0.8441514526 1.7529179860
P -0.3885395734 3.3100581734 1.1951957335
P -0.3462916561 1.8884333102 2.6586743645
P -3.2411223944 -1.7449156403 2.1329507100
P -3.1106680325 -0.6561332981 3.6570853914

14
Transition State 2 (black): -4778.883804
P 1.0477848769 -0.9851231768 -3.5916820538
P 1.0601152659 -2.7418706788 -2.1785449548
P 2.0677155630 -1.4947757064 -0.6227464717
P 0.2487857237 -1.2489933897 0.5917343108
P 0.2795247599 1.4054841184 -1.4859698562
P 2.0659103564 0.2571658675 -2.0415860122
P -1.0829870028 -0.2076666199 -0.8394281709
P -0.8237062657 -1.6040819995 -2.5531261586
P 0.9711862353 2.1971871360 0.4537341809
P 1.0018349177 0.3992279503 1.8565363793
P -0.8837137720 2.9915101322 1.3630133929
P -0.8028786570 1.3983440903 2.6660693829
P -2.6757765447 -0.7784635060 2.4253244176
P -2.4737954567 0.4120557822 3.9566716139

14
Reactant2 (blue): -4778.91237769
P 3.6308467726 -0.2373195874 -1.8360079108
P 3.6330673757 -1.8276738233 -0.2406991367
P 2.8137199962 -0.3563992679 1.2253681146
P 0.7701769201 -1.1722643724 1.2160730422
P 0.7653519879 1.2154634028 -1.1820260005
P 2.8103707008 1.2325907187 -0.3692496641
P 0.2485435478 -0.9243554394 -0.9242012719
P 2.0662635474 -1.8268331200 -1.8278966580
P -0.2173729346 2.1550847026 0.5496349317
P -0.2138477054 0.5622081396 2.1495673046
P -2.3354589917 1.6173180656 0.1727919995
P -2.3293903904 0.1729375520 1.6141104458
P -5.5507959414 0.0023924129 -1.1186450268
P -6.0914748848 -0.6131493838 0.5711798301

14
Transition State 2 (blue): -4778.886542
P 3.5464151636 -0.4727628329 -1.9094067355
P 3.4624333295 -2.0423535042 -0.2977875355

P 2.5517383968 -0.5530715640 1.0993594498
P 0.5302265986 -1.4026689640 0.9811686897
P 0.6297535659 0.9650878587 -1.4533241989
P 2.6263467284 1.0150169518 -0.5207487056
P 0.1175112573 -1.1723134855 -1.1877559873
P 1.9959009614 -2.0706332105 -1.9780248388
P -0.3424704745 1.9586001730 0.2814507584
P -0.6588085240 0.2557409491 1.8339421096
P -2.5080453191 1.7050894935 0.3685048781
P -2.6146513515 -0.3395486127 0.8209751117
P -4.6497967754 1.9395672082 0.4115318675
P -4.6865535569 0.2142495394 1.5501151369

16
Reactant 3 (black): -5461.62081947
P 2.3126609270 -0.8805228549 -3.7423450442
P 1.7469165815 -2.8674203459 -2.8387988174
P 1.8384338762 -1.9640450259 -0.7979313348
P -0.3428057475 -1.8615258864 -0.5273560668
P 0.5115279922 1.1175543627 -1.8879193059
P 2.4060650541 0.0187465651 -1.7004954770
P -0.8986128690 -0.5579084235 -2.2253339450
P 0.2077020702 -1.6088471657 -3.8459185863
P 0.1937549991 1.5576852770 0.2458182237
P -0.3800402232 -0.4438713361 1.1557386062
P -1.9767714978 2.1273669879 0.1252965365
P -2.5425658720 0.1612989352 1.0588022258
P -2.6778219966 1.2345892988 2.9929128609
P -2.1897866474 3.0259927969 2.1406747876
P 1.4820648859 0.5369816465 4.1932903363
P 0.3092784673 0.4039251683 5.6535650003

16
Transition State 3 (black): -5461.594946
P 2.0877345144 -0.8222648684 -3.9866714231
P 1.6538069385 -2.8423343398 -3.0837986500
P 1.9846864407 -1.9978641258 -1.0429788118
P -0.1471161395 -1.9324358515 -0.5033933708
P 0.4945213833 1.0943537474 -1.8742940445
P 2.4120822331 0.0227821637 -1.9449115919
P -0.9231959671 -0.5922963721 -2.0851474132
P -0.0075788599 -1.5744632390 -3.8583563000
P 0.3926650861 1.5043643423 0.2856179095
P 0.0843308689 -0.5463961710 1.2009625927
P -1.8398987819 1.8734254926 0.3896709590
P -2.0653090606 -0.0425984841 1.5467574565

P -1.9661677816 1.3122147768 3.2987523997
P -2.0843510297 3.0765012535 2.2204690757
P 0.7333764940 0.7826807839 4.1345272238
P -0.8095863387 0.6843308915 5.3027939883

16
Reactant 3 (blue): -5461.61950789
P 3.1945600141 -1.7699182365 -3.3202785462
P 3.1887185133 -3.3599147494 -1.7230273052
P 2.9880095440 -1.7819953013 -0.1544490743
P 0.8612751434 -2.1763668066 0.2397029760
P 0.8713843127 0.2068693051 -2.1538873764
P 2.9946122534 -0.1943897178 -1.7494723146
P -0.0072527359 -1.7866897020 -1.7589328371
P 1.3795455464 -3.0209979427 -2.9824452350
P 0.3468259535 1.2844462278 -0.3050942835
P 0.3420192187 -0.3199071952 1.3072375334
P -1.8832661841 1.0706584568 -0.5061841946
P -1.8883256168 -0.5056927558 1.0912283042
P -2.5090034485 1.0761845680 2.5134412504
P -2.5157470286 2.5101027954 1.0554660244
P -3.8240724891 3.7087442726 4.8609498428
P -3.5392829959 5.0588667809 3.5857452354

16
Transition State 3 (blue): -5461.595260
P 3.1618397036 -2.5742215298 -2.5384181554
P 3.0081787326 -3.6771214374 -0.5790446297
P 2.8515603666 -1.7296405348 0.5038102897
P 0.6993514574 -1.9244914877 0.8998188537
P 0.9032635623 -0.2365132264 -2.0300371098
P 2.9928459259 -0.6280208227 -1.4580741523
P -0.0858334831 -2.0191328839 -1.1717394698
P 1.2662848494 -3.5964740036 -1.9704804960
P 0.5383199360 1.3126843617 -0.5025318313
P 0.2398423979 0.1603179009 1.4358622551
P -1.6808175303 1.6197981245 -0.6217855769
P -1.9810183349 0.0689944476 1.0222049077
P -2.8561409836 1.8743555205 1.8803228570
P -1.6197059752 3.2899836117 0.9421477345
P -4.1065588428 3.3650484534 2.7875351023
P -3.3314117818 4.6944335060 1.4004094211

16
Product: -5461.66014817
P 2.3276346772 -3.1852634904 -2.5414951872

P	2.1440830256	-4.1375611342	-0.5066434861
P	2.5912360847	-2.1694117080	0.4494792768
P	0.5170188886	-1.7960973245	1.0742677631
P	0.7803366456	-0.3579243098	-1.9824109534
P	2.7653456235	-1.2158638358	-1.5831130467
P	-0.5077780004	-1.7910732047	-0.8896095075
P	0.3211097885	-3.6839666032	-1.7096982301
P	0.8447776515	1.3267677396	-0.5656144146
P	0.6708259864	0.3603267475	1.4856585065
P	-1.3502398506	1.7662685741	-0.5412074128
P	-1.5228182862	0.8036482360	1.4972882842
P	-1.3971482237	2.8289254638	2.4651199985
P	-1.2251250416	3.7886588166	0.4310670122
P	-3.5578629305	3.2982535514	2.3805668100
P	-3.4013960389	4.1643124817	0.5363445871

Reaction D

12

Reactant: -4096.3145877834

P	2.2489387554	-1.5263951912	-1.9112964450
P	1.8592453121	-2.6774162010	-0.0148774116
P	1.6162101926	-0.7549840973	1.0863398645
P	-0.5796807633	-0.8338435704	1.2761444054
P	-0.0104293591	0.8193837781	-1.6361173344
P	1.9880562257	0.4049252863	-0.8139029704
P	-1.1324456673	-0.9369504541	-0.8646258903
P	0.2788061513	-2.5074944393	-1.5764540297
P	-0.6382135159	2.4405753930	-0.2441293048
P	-0.6564886567	1.3857218389	1.7371640909
P	-2.5829959831	1.6589055807	0.5241772772
P	-2.3910014735	2.5275720845	2.4375764274

12

Transition State: -4096.28079221

P	2.1868034332	-1.7705966765	-1.9748133375
P	1.6529523184	-2.7128668529	-0.0096195611
P	1.5530097329	-0.6742332747	0.9047032487
P	-0.6135547597	-0.9393179944	0.8872998676
P	0.1602867065	0.9614699863	-1.9175115642
P	2.0354528161	0.2949640329	-1.0857619075
P	-1.0815446183	-0.7037688658	-1.2870502360
P	0.1509091293	-2.5359401506	-1.6901852523

P -0.7042175476 2.8146311261 0.0456616970
P -1.1094726395 1.2276845260 1.4077489867
P -2.7575779003 2.0907644874 0.2914043964
P -1.9928184803 3.0862869225 2.1082640437

12
Product: -4096.3086735843
P 1.8503051275 -2.4752669148 -1.6366138668
P 1.5382678786 -2.9301690507 0.5382187120
P 1.4850250334 -0.7162807522 0.8969283256
P -0.4548880527 -1.6399514311 0.9787693343
P -0.1748662776 0.2984977364 -1.9841651048
P 1.7583054486 -0.2449372325 -1.3000562095
P -1.3201156403 -1.2515592593 -1.0470748891
P -0.1424653703 -3.1446804093 -1.1680134774
P 0.1970526796 2.9206779023 1.1228374687
P -1.6661331560 1.8539145247 1.5400971866
P -1.5994493914 3.3686378566 -0.0262692519
P -1.4710177086 3.9611282249 2.0853419793

Cartesian coordinates for structures in Scheme 3

Reaction A
20
Reactant 1: -6827.2029861729
P -0.6566200169 3.5412322605 -2.4564227422
P -1.7186805741 2.1307372762 -3.1024542913
P -3.2962303259 4.5164850074 2.7493140438
P -2.9120574333 3.5951148663 4.5325341716
P -3.3130896765 2.6026279773 1.6420662113
P -2.8983634796 1.5855451798 3.6126281842
P -1.1205777328 2.5368528061 1.1565734022
P -0.7010360256 1.5207948462 3.1416672456
P -0.7140773387 -0.4754368358 2.1301289409
P -1.1526012656 0.5314630247 0.1521468035
P 1.4611978123 -0.5425388778 1.6209416463
P 1.0236576000 0.4912520542 -0.3672619232
P 1.1130281199 -4.4997735262 -1.6827011011
P 0.1745568986 -2.8032495437 -0.5930987022
P 3.0783611660 -1.6394810420 -1.9140448741
P 0.9394029506 -1.1413440034 -1.8387845914
P 1.5821123696 -2.6799721609 1.1113522975
P 3.5054243942 -2.6613100198 0.0471701626
P 3.2036323440 -4.6506303473 -0.9223958079
P 2.7749891437 -3.6274793098 -2.8859830969

20
Transition State 1: -6827.17765260
P 2.8712899773 -3.5801758761 -3.0420205326
P 2.8916410723 -4.7403774200 -1.1080719293
P 3.2802095290 -2.8505386584 0.0160149103
P 1.2409118950 -2.6717151356 0.8091857278
P 1.2047693439 -0.9563935813 -2.1210125765
P 3.2635175806 -1.6907296468 -1.9151312960
P 0.0840308069 -2.5510644081 -1.0736324290
P 0.9634201325 -4.2973853048 -2.1345524891
P 1.2988647201 0.6085393020 -0.5684074543
P 1.2865482656 -0.5563007931 1.4300224181
P -0.8677469285 0.9763970279 -0.2683507154
P -0.8895853951 -0.3139280945 1.7331296139
P -0.8215891737 1.6170913064 2.8045543881
P -0.8906515340 2.8744627492 0.8778409363
P -3.0578913903 1.7990300452 2.9998820003
P -3.1238267894 3.0087649894 1.0996427984
P -3.1373581772 3.7218459474 4.0881986927
P -3.1555679570 4.8197386787 2.3635784615
P -2.1601822166 0.9155952288 -2.0421874183
P -0.9073958909 2.4224416383 -2.4482429333

20
Reactant 2: -6827.1797199594
P 2.9271992876 -3.5086460575 -3.1207337605
P 2.8422626706 -4.7011317686 -1.2096372579
P 3.2600245281 -2.8464298385 -0.0383115849
P 1.2036729456 -2.6063217389 0.6976557006
P 1.3294377186 -0.8369338337 -2.1913070205
P 3.3528674677 -1.6547131340 -1.9480790407
P 0.1155808801 -2.4140793554 -1.2200436171
P 0.9655259262 -4.1699677458 -2.2880829263
P 1.4264440477 0.6709581966 -0.5949502242
P 1.2964188767 -0.5053701748 1.3646626147
P -0.7357932438 1.2183997098 -0.4596085454
P -0.8689662672 -0.1941288147 1.6039309372
P -0.8014492710 1.6968340727 2.7196739190
P -0.7933705759 3.0209879734 0.8595058245
P -3.0449582787 1.8924628632 2.8542261993
P -3.0156397823 3.1906410932 1.0155343092
P -3.1725321997 3.7672346051 4.0219065854
P -3.0827395600 4.9455845490 2.3538419426
P -2.2418782059 0.7741990570 -1.9340762127
P -0.9621119208 2.2604122455 -2.4861044958

20
Transition State 2: -6827.16853581
P 2.8640032185 -3.3828641095 -3.3444367470
P 2.9570624586 -4.4803393443 -1.3785387023
P 3.3241878159 -2.5531859081 -0.3085123981
P 1.3026549700 -2.4297503140 0.5384302931
P 1.1719339550 -0.7500408826 -2.4299646443
P 3.2430954632 -1.4581687262 -2.2784988531
P 0.1175484910 -2.3558823248 -1.3213944207
P 0.9934865457 -4.1103361266 -2.3728194357
P 1.3607250695 0.8174184662 -0.8877533636
P 1.2184379820 -0.3427635860 1.2327761191
P -0.6806129085 1.5739032156 -0.8156469007
P -0.8271186312 -0.2980334664 1.9411923644
P -0.5883789776 1.7397968644 2.6684266664
P -0.5499784003 3.0861015623 0.7791884490
P -2.8097171575 2.1377312083 2.8615195488
P -2.7260934656 3.4591013839 1.0435838272
P -2.7723064326 4.0110970010 4.0446782459
P -2.5956386131 5.2020284633 2.3936679358
P -2.2084788898 0.0464028741 -0.8985045340
P -2.3203332131 1.6308211358 -2.2128778692

20
Reactant 3: -6827.1889484194353
P 3.2484320499 -3.3516821408 -3.2314640943
P 3.2130865709 -4.4842049503 -1.2848134832
P 3.2236726212 -2.5585076806 -0.1557012381
P 1.1010002850 -2.6377504221 0.4150673042
P 1.1565804606 -0.9209277314 -2.5009619382
P 3.2646364507 -1.4239490615 -2.1065774557
P 0.1374970816 -2.6724998225 -1.5836326156
P 1.3620077632 -4.2891624391 -2.5110991289
P 1.1205036147 0.6276396107 -0.9319662636
P 0.9243011346 -0.5394507416 1.0617661599
P -0.9091682368 1.5570955284 -0.8580993947
P -1.2002674642 -0.3734487610 1.7158589745
P -0.9420800132 1.6196212466 2.5852915440
P -0.4005391306 2.9222766600 0.8094851403
P -3.0744040008 2.3611884559 2.5481522411
P -2.4184573779 3.8649807322 1.0096269181
P -2.7845458993 3.9875857955 4.0416797589
P -1.9742984043 5.2628032038 2.6690210562
P -2.0418986943 -0.3238818150 -0.3943195956
P -3.0060566309 1.3722658405 -1.2973013639

20
Transition State 3: -6827.17625751
P 3.7066366675 -3.0512264275 -2.6189217617
P 3.3019616545 -4.2961825342 -0.7850372589
P 3.1404893682 -2.4398158025 0.4436768362
P 0.9484720652 -2.4924208066 0.6187851407
P 1.5544498669 -0.6229814666 -2.1365228595
P 3.5463334495 -1.1923974777 -1.3921301922
P 0.3636216593 -2.3939716365 -1.5180751978
P 1.7083717985 -3.9840672062 -2.3127132526
P 1.1833834642 0.8439715861 -0.5309033730
P 0.7072081726 -0.4180482427 1.3235068425
P -0.7345027120 1.8266615889 -1.0725858963
P -1.4782179437 -0.1802564518 1.5889766980
P -1.2594943071 1.8328497640 2.4458263190
P -0.6152568219 3.1331700031 0.7198194680
P -3.3508458737 2.6628820718 2.3205484964
P -2.6620318461 4.0391137815 0.6941204737
P -3.0280955694 4.3664786870 3.7345972021
P -2.3492834477 5.6000778506 2.2665994752
P -1.9936708635 -0.0124791268 -0.5782087797
P -3.3661467909 1.4865000813 -1.0443697177

20
Reactant 4: -6827.2580146877444
P 3.7451856684 -3.3065863398 -2.7009091544
P 2.8848365616 -4.7356952126 -1.1858197201
P 2.8873259011 -3.1082224896 0.3400849315
P 0.7198984131 -2.7398514032 0.2894118857
P 2.0030288205 -0.6338460999 -2.0263444216
P 3.7432459029 -1.6753089933 -1.1759077261
P 0.4527307685 -2.2052845075 -1.8482557433
P 1.5899139442 -3.8772298020 -2.7810200833
P 1.5458458073 0.6746075789 -0.3098475968
P 0.8343592355 -0.7827859905 1.3070027594
P -0.3232734846 1.5959142433 -1.0560096227
P -1.2682159639 -0.2176643721 1.6278194845
P -0.5963541099 1.7589875532 2.4614148984
P -0.5754175886 3.0276697815 0.6040861426
P -2.7321604778 2.3743157253 2.8051511194
P -2.8429219717 2.8466725108 0.6567721889
P -2.8879104431 4.5731113264 3.0290577481
P -3.6158362619 4.8522362167 1.1307728152
P -1.9031294115 0.1408483335 -0.4964635879
P -3.6611532509 1.4381129414 -0.6709964177

20
Transition State 4: -6827.19643275
P 3.1794933552 -3.4927861430 -2.8503410017
P 2.4013298706 -4.9606769196 -1.3265163526
P 2.6464633704 -3.4249197862 0.2743393255
P 0.5034717985 -2.9699214804 0.4522368619
P 1.6672142965 -0.7757758159 -1.8442047486
P 3.4234707586 -1.9564339573 -1.2489278041
P 0.0592181945 -2.2809809218 -1.6063038337
P 1.0003239534 -3.9519072227 -2.7365049902
P 1.4803749929 0.4153356222 0.0038828574
P 0.7250050486 -1.0762386746 1.5654617322
P -0.2789071363 1.6427836809 -0.4983747158
P -1.3756846401 -0.5117122485 1.8779496699
P -0.9407485395 1.3568753793 2.9713440463
P -0.3218273382 2.8341364386 1.3593055591
P -3.0207635432 2.1000332660 2.7188741482
P -2.4038999529 3.4923424991 0.8815224501
P -3.2003493538 3.8509082090 3.9661681589
P -3.0777394471 5.0519826388 2.2811754229
P -1.9905236988 0.2831377897 -0.1053726403
P -3.6609361473 1.5614740870 0.1865607929

20
Reactant 4: -6827.3070088113163
P 3.2589566767 -3.3842327280 -3.2047810342
P 2.5434781947 -4.8210698005 -1.6223073243
P 2.8527697964 -3.2558327371 -0.0608687668
P 0.7166214733 -2.8020714103 0.1896128067
P 1.7909469675 -0.6444953934 -2.1847969555
P 3.5685272189 -1.8189973107 -1.6432487904
P 0.1964404369 -2.1462130921 -1.8600826866
P 1.0858846449 -3.8397133816 -2.9957682132
P 1.6804370211 0.5670822303 -0.3439317613
P 0.9552627241 -0.8831684527 1.2522674686
P -0.0691650879 1.8188873680 -0.7689375039
P -1.1388301235 -0.3213672301 1.5801313912
P -0.8693777453 1.5791935836 2.6778601070
P -0.1373258347 3.0420479047 1.0721199205
P -3.0862363911 1.7134419593 2.5431868974
P -2.0169502071 3.8509811880 0.1988797858
P -3.4327166777 3.7667020006 3.3105578436
P -2.7862634402 5.0574300262 1.8953063387
P -1.8176200463 0.4810103174 -0.3911742004
P -3.2948404855 2.0403860202 0.3559735701

Reaction B:

18

Reactant: -6144.5224957770

P	2.7024041699	-2.9632365905	-2.9882903386
P	2.7882656671	-4.1484568165	-1.0700123273
P	3.1538650625	-2.2673004269	0.0787319203
P	1.1180173005	-2.1561848180	0.8994672215
P	0.9943758311	-0.3687164021	-1.9720883185
P	3.0730261190	-1.0859179073	-1.8386579296
P	-0.0788340095	-2.0219748879	-0.9588985425
P	0.8313798125	-3.7319909457	-2.0542814645
P	1.2058140961	1.1368382595	-0.3719075809
P	1.0921313377	-0.0628842154	1.5821348470
P	-0.8991112785	1.6519207305	0.0680872824
P	-1.1544412097	0.1028753284	1.6607047179
P	-1.5235034578	1.8271066397	3.0092283709
P	-0.7322211265	3.3379239387	1.5671941361
P	-3.6420770993	2.1390378557	2.2623372420
P	-2.8400386655	4.1152352868	1.4380163077
P	-2.3383903538	1.8823085459	-1.4080290673
P	-3.7506659104	2.6133999099	0.0962766370

18

Transition State : -6144.46761188

P	1.6812899666	-1.4549347391	-2.1425201652
P	1.7321966479	-2.6086767269	-0.2061293844
P	1.8709076347	-0.6965150563	0.9441056292
P	-0.2129693445	-0.7664665696	1.6422395063
P	-0.2774512553	1.0162868911	-1.2450448744
P	1.8339286134	0.4511840502	-0.9960524520
P	-1.2970550916	-0.7145601264	-0.2865397064
P	-0.1842151383	-2.3473571332	-1.3176053500
P	-0.1741966922	2.5079300902	0.3805138613
P	-0.5834337003	1.2752619817	2.3680928676
P	-2.2196241344	3.2710114134	0.3475725521
P	-2.7634208647	1.1359289711	2.2820454489
P	-3.1232658679	3.0511855514	3.2484660633
P	-2.3816513210	4.7938341083	1.8366022543
P	-5.1970240033	3.3663213905	2.5384233369
P	-4.5503903086	5.3255448329	1.6068740717
P	-3.7492873098	2.7890645364	-0.8766200086
P	-5.3341385691	3.7229609994	0.3046649067

18

Product: -6144.5948870690

P	3.3966193114	-2.8787744416	-2.4025705962
P	2.9798179592	-4.0563913353	-0.5260173033
P	2.9812131571	-2.1650127080	0.6607384987
P	0.7978787869	-2.0836709395	0.9044253906
P	1.4245045150	-0.3133563442	-1.9074199525
P	3.3995433859	-0.9876581873	-1.2151198244
P	0.1532603888	-1.9874472960	-1.2111158077
P	1.3537173001	-3.6819215749	-2.0076284506
P	1.0893787665	1.2214626356	-0.3570997545
P	0.6543902745	0.0232750768	1.5444954830
P	-0.8763856794	2.0201990815	-0.9623203292
P	-1.5192146802	0.2504476691	1.8467600018
P	-1.4970927547	2.3512898115	2.4956320055
P	-1.0739550094	3.5322752204	0.6222694897
P	-3.6877240971	2.6700977151	2.2062586371
P	-3.2652354973	3.8521083107	0.3325522916
P	-2.2754923493	0.4703071634	-0.2228870697
P	-4.0352274903	1.7627694829	0.1990501427

<u>Reaction C</u>

10

Reactant 1: -3413.5685080297035

P	1.2983803047	-0.4381008807	-2.3934894334
P	-0.1277468236	1.0651211525	-1.4303182115
P	-1.2856016243	-0.6388420454	-0.5446781685
P	0.0907090318	-2.0955694276	-1.4870667706
P	1.0624343218	-2.5335842180	0.4797834070
P	-0.3640159860	-1.0373613786	1.4609184121
P	1.8985548446	0.7513059146	-0.6442354350
P	1.7529085944	-0.5532847311	1.1436086628
P	-2.6776477931	2.3322794790	0.9314298534
P	-1.6934880203	2.0274771016	2.5054462972

10

Transition State 1: -3413.54302530

P	0.9607513099	-0.7766613599	-1.5218505347
P	-0.3809892433	1.0150742888	-1.1347178778
P	-1.7432992924	-0.2985638270	0.0647394616
P	-0.3614568893	-2.0568012911	-0.2274611274
P	0.5890958863	-2.0697334764	1.7275997331
P	-0.8975671587	-0.0170171564	2.0407096296
P	1.5837020021	0.8145183903	-0.1447402760

P 1.2411509845 0.0401120410 1.9195200373
P -2.0877920870 2.2072716815 2.0762400675
P -2.0180073522 0.9852608600 3.6464180470

10
Reactant 2: -3413.5611140105234
P -1.8742931985 0.7264449952 2.7502721296
P -1.5735889888 2.3904697969 1.6296258869
P 1.4508255455 0.0058661677 1.0906672222
P 1.8561137130 0.8041131060 -1.0000459062
P -0.6856937124 0.5330070323 0.9564020089
P 1.0747453948 -2.0993421510 0.8834312791
P -0.0078831210 -2.0791567365 -0.9768665583
P -1.4686598209 -0.3612370456 -0.8809344089
P -0.0844460392 0.9131246100 -2.1128631127
P 1.3128807470 -0.8332897590 -2.3396888160

10
Transition State 2: -3413.55103190
P 1.2241871091 -1.2533419483 -2.1571139854
P 0.0709981918 0.6594369114 -2.4764447665
P -1.4697999401 -0.0491321559 -1.0359113906
P -0.2285128905 -1.9317285445 -0.5796931616
P 0.9118754673 -1.5973373576 1.2473356092
P -0.6946426134 1.0491168492 0.6835591074
P 1.9632040153 0.6157545272 -1.2776547472
P 1.4535842041 0.4677352236 0.8970610391
P -1.6419738200 2.0471179163 2.3391918793
P -1.6259387205 0.0065399028 2.3524779204

10
Reactant 3: -3413.5655125502349
P 1.1897255067 -1.2686455778 -2.1280220032
P 0.0322378980 0.6305884139 -2.4787190334
P -1.4843236557 0.0333869975 -0.9468102106
P -0.2960394580 -1.8431212270 -0.5607036178
P 0.7547078411 -1.2948976849 1.3053486994
P -0.7230455479 1.3732896431 0.6722145191
P 1.9601986996 0.6406145984 -1.3303181838
P 1.4183778381 0.7528988492 0.8112301181
P -1.4576339520 1.4608894286 2.6960224305
P -1.3942106959 -0.4850075628 1.9597592580

10
Transition State 3: -3413.56458470
P 1.1969183836 -1.4962670868 -1.9530455452

P 0.1074369548 0.3982874464 -2.5077631941
P -1.4565655266 0.0027826916 -0.9578790138
P -0.3551022047 -1.8735752396 -0.3914812513
P 0.6571520067 -1.1849837541 1.4380406207
P -0.6599821798 1.5066325958 0.4852625185
P 2.0073226844 0.4585200763 -1.3188007265
P 1.4132326330 0.7959011224 0.7878964668
P -1.4601369725 1.6766118679 2.4990911574
P -1.4523478621 -0.3362239977 2.0736275860

10
Product: -3413.6175065870580
P 1.0561471288 -1.5469326944 -1.8585777980
P 0.2329016226 0.4116017022 -2.5958242319
P -1.4165818561 0.2854820440 -1.0912533342
P -0.5934493666 -1.6738133686 -0.3536370259
P 0.6637797158 -1.1360630016 1.3780946119
P -0.5698956417 1.7978249299 0.2745047005
P 2.0467054359 0.3697600888 -1.3029944825
P 1.3636047556 0.8602249897 0.7621816783
P -1.7627112662 1.1983153280 2.0615152889
P -1.0204998925 -0.5664000843 2.7259894543

Reaction D
10
Reactant: -3413.56605014
P 0.7806604021 -0.3645111634 -1.0793942561
P -0.8271004153 1.0612262967 -0.3141330083
P -2.1482183749 -0.7078589191 0.0963500126
P -0.5919404035 -2.0877376122 -0.6444102921
P -0.1122170557 -2.7318410090 1.4519896694
P -1.7210222662 -1.3051240893 2.2177837528
P 0.9705806704 0.6258860159 0.8739662285
P 0.4152887500 -0.8416379257 2.4406804531
P 0.9535823209 3.7626548357 -2.2073575902
P 2.2803851331 2.5889442047 -2.8354758249

10
Transition State : -3413.49766546
P 1.4680805094 -0.4348195113 -0.9570470249
P -0.5420299404 1.2322272864 -0.4814559371
P -2.0686539169 -0.2433226188 -0.1158742687
P -0.5004063984 -1.6702784933 -0.8213993722
P -0.2373510207 -2.5111978249 1.2474160621
P -1.7478114171 -1.0150019488 1.9989397234
P 1.1612121986 0.7707841115 0.8302189384

P 0.4072660437 -0.6946124194 2.3334244672
P 0.2335117159 2.8552515848 -1.7814002616
P 1.8261822427 1.7109698400 -2.2528223956

10
Product: -3413.61751248
P 1.6968036154 -0.4198211803 -0.7589978557
P -0.6407507994 1.7726502311 0.2784984822
P -1.7813731910 -0.0171131917 -0.3256449883
P -0.2202753383 -1.4811411541 -1.0185821588
P -0.2122763029 -2.4297916609 1.0063803111
P -1.7726369982 -0.9655630513 1.6994963958
P 1.2254687192 0.8394988520 0.9867349474
P 0.3533602094 -0.7208973689 2.3192929634
P -0.0273660474 2.3704805124 -1.7813958447
P 1.3790463828 1.0516978211 -2.4057824743

Reaction E
10
Reactant: -3413.56843392
P 2.4586301301 -0.7193587677 -0.9122455811
P 0.9279449952 0.9516839104 -1.2188713797
P -0.7072838463 -0.5764114783 -1.0748328617
P 0.7764101500 -2.1935788679 -0.7833321819
P 0.2557306923 -2.3242001644 1.3921787734
P -1.2806232459 -0.6578165624 1.0920529937
P 1.9930494150 0.7143537300 0.6876765114
P 0.6245116722 -0.2829215096 2.1195378980
P -2.0110154434 2.9033773353 0.0501485755
P -3.0373552600 2.1848718738 -1.3523150997

10
Transition State : -3413.53400892
P 2.0220482717 -0.6046093279 -1.2329488612
P 1.1628929058 1.4843397009 -0.7691026759
P -0.8192295272 0.6353291811 -0.3257609347
P 0.2950433463 -1.9237974219 -1.1157758249
P -0.1263300994 -2.2248939233 0.9958357730
P -1.1604882454 -0.2654471160 1.6521963883
P 2.3230731487 0.3428805875 0.7240854286
P 0.9448761223 -0.7011213376 2.1561320078
P -2.1890428694 2.3794631623 -0.3791199996
P -2.4528438274 0.8778573779 -1.7055394111

10
Product: -3413.54161160

P 1.8602308685 -0.5610493466 -1.3167789907
P 1.2053404472 1.5766550113 -0.6274437686
P -0.8105275923 1.0102868635 -0.0446964044
P 0.2934329714 -2.0214457791 -1.1771701600
P -0.2489782571 -2.1552046966 0.8951872814
P -1.0814840808 -0.1521246532 1.7718068189
P 2.3809045940 0.2162873613 0.6760239399
P 1.0072467753 -0.8226358025 2.1167938495
P -2.4175851997 2.3237224554 -0.6286540594
P -2.1885837284 0.5855104146 -1.6650665356

Reaction G

18

Reactant 1: -6144.5146443148087

P -0.3098458472 -1.4137082063 -2.7274187176
P -1.8908887498 -0.6034644285 -4.1584252307
P -3.5389151536 -1.0817991349 -2.7406026621
P -1.8895848784 -1.9676658234 -1.2494395076
P -2.3115867835 -0.1347990585 -0.1716401107
P -3.8919903182 0.7454952596 -1.6099898961
P -0.5770758351 0.7532569592 -3.0356218028
P -1.8231662004 1.5829863703 -1.3910259189
P -1.2925632359 -0.4981176883 1.8700476665
P 0.0458581128 1.2658037159 1.9664656913
P -0.1926408530 -2.0659094452 0.7995781747
P 1.4010904917 0.4310174518 3.4871321681
P 1.7709976880 -1.1483946852 0.3551498242
P 2.5829712105 -1.1481701514 2.4019008773
P 3.0371735833 1.9074467231 3.1109411006
P 4.2193788111 0.3275804396 2.0293219509
P 1.2820010460 0.9900982555 0.1528973238
P 3.1628575640 1.9188459108 0.8827486678

18

Transition State 1: -6144.51299662

P -0.4963230564 -1.5663585837 -2.8207575668
P -2.0273932026 -0.7323955675 -4.3048675680
P -3.6701401375 -1.2792566158 -2.8832702633
P -2.1676181487 -2.1150763707 -1.4366373425
P -2.5290016347 -0.3013522951 -0.2189987946
P -4.0459498513 0.5682370539 -1.7136734424
P -0.7447330554 0.5956211460 -3.1163767821
P -2.0073917850 1.3985017277 -1.4736081569
P -1.0909701139 -0.9452377553 1.8900265897
P -0.0238537043 1.0002440468 2.0215567859
P 0.1034665097 -2.2495783738 0.7955977796

P 1.5255369284 0.3120781865 3.4283193130
P 1.9233167821 -1.0953742783 0.2212962624
P 2.8461134801 -1.0539203087 2.2208392842
P 2.9234672396 2.0096355436 3.0221209955
P 4.2441925897 0.6429447577 1.8192205271
P 1.1310315270 0.9554241273 0.1376015613
P 2.9159934370 2.1071414440 0.7922754949

18
Reactant 2: -6144.5156833491046
P -0.6769275756 -1.5181062783 -2.4391008497
P -1.7938546529 -0.6136714019 -4.2203004767
P -3.7117460480 -0.8984801866 -3.0940930608
P -2.6296485948 -1.7644346230 -1.3679629864
P -2.9227422837 0.1282673375 -0.2048939795
P -4.0332432228 1.0279724982 -1.9924120905
P -0.5970845065 0.6341938084 -2.8656323566
P -1.9931905406 1.6576061740 -1.4765813012
P -0.6990889036 -1.3918233828 1.9162200119
P 0.1166494694 0.6465387097 2.3156938572
P 0.5829372312 -2.3264907649 0.6429960969
P 1.8010979092 -0.0022099326 3.5834155159
P 2.2457880561 -0.9055142230 0.1992913471
P 3.2188707644 -1.0343010380 2.1745389615
P 2.9662447570 1.8941010499 3.3671789570
P 4.3840755083 0.8620775396 1.9580997027
P 1.1782370644 1.0090208679 0.4200800136
P 2.8476562645 2.2739333329 1.1735734441

18
Transition State 2: -6144.50618390
P -0.6069428831 -1.9675590574 -3.2381740461
P -2.4673892801 -1.1439854341 -4.2734007836
P -3.7210213115 -1.6526859271 -2.4756641579
P -1.9030951480 -2.5555098951 -1.5086652315
P -1.6806244033 -0.7561507254 -0.3315444927
P -3.7537101404 0.1455580945 -1.2202117707
P -0.9368367978 0.2056160005 -3.4667280527
P -1.7255502681 1.0038175761 -1.5430677827
P -1.0075768704 -0.9304398998 1.7322588807
P -0.2480732033 1.1242216456 2.0959763778
P 0.5289750879 -1.9131351498 0.4077880173
P 1.1958365702 0.4327767320 3.6094524070
P 2.1672996053 -0.4594816538 0.3406037546
P 2.8339406876 -0.5763469480 2.4361365592
P 2.3734554805 2.3295482955 3.6234074790

P 4.0152330467 1.3172468044 2.4568650464
P 1.1287966275 1.4823600980 0.3858082553
P 2.6261995609 2.7349866085 1.4462093065

18
Reactant 3: -6.1445229778318708
P -1.0055107235 -2.2994059384 -3.3210393754
P -2.7627833947 -1.2255088354 -4.2277724724
P -3.8699830286 -1.3083909828 -2.2511046773
P -2.1574794648 -2.5040652185 -1.4015385254
P -1.0189531824 -0.8498535954 -0.5470531498
P -3.6522194464 0.6843884817 -1.4539309577
P -0.9838670177 -0.0868280469 -3.6657313999
P -1.5629367462 0.9728410819 -1.7384122575
P -0.8163226156 -0.9560862810 1.6259723451
P -0.1391084289 1.0701427601 2.2284482413
P 0.8442543358 -1.7179941781 0.2473231263
P 1.4135722751 0.3002527440 3.5869935412
P 2.3168093002 -0.0602365716 0.1942691960
P 3.0499037792 -0.4539878110 2.2336295938
P 2.4893256028 2.2440033623 3.8065250438
P 4.1271315526 1.4884407924 2.4514449806
P 1.1134878181 1.7647740059 0.5371350149
P 2.6146854805 2.9375137810 1.6948494711

18
Transition State 3: -6144.48963074
P -2.7963450308 -2.7360179921 -3.0844639524
P -4.3745150186 -1.1598557421 -2.7035152405
P -4.0237247705 -1.3055838248 -0.4983755938
P -2.4764460346 -2.9677454497 -0.8960425896
P -0.6910800170 -1.7366883510 -0.8927662572
P -2.9117466743 0.4967205064 -0.1412448957
P -2.3873559568 -0.5706551185 -3.4461774445
P -1.3310165910 0.2542889721 -1.6574527386
P -1.0064051147 -1.0098441759 1.3506432200
P -0.1089381750 0.9506144702 1.8972711298
P 0.7911323412 -2.1767506070 0.7243813201
P 1.1743383846 0.2298544551 3.5423338064
P 2.4469318284 -0.7371072972 0.4179080595
P 2.9018122069 -0.8340183103 2.5708889002
P 2.3976444996 2.0977549946 3.6376416485
P 4.1224233127 1.0323956110 2.6473696897
P 1.4096815802 1.2315059272 0.3191222139
P 2.8636487345 2.4522775236 1.4860145099

18
Product: -6144.5947775873619

P	-2.7591646011	-2.2744211331	-3.5824864011
P	-4.2433961698	-0.8817416859	-2.6148427914
P	-3.4154874210	-1.3944583571	-0.6062821642
P	-1.9312959906	-2.7875036725	-1.5738495316
P	-0.1004650632	-1.5915170639	-1.8001802005
P	-2.3273259148	0.4983999161	-0.3488456195
P	-2.4548667530	-0.0666807646	-3.6690298372
P	-0.9646161383	0.4264678625	-2.0929475069
P	-1.0242754869	-0.1491077985	1.3088427898
P	0.1306052800	1.6870617921	1.7090761395
P	0.4817108799	-1.5635549985	0.3270942516
P	1.3349681309	0.9043481725	3.3736834029
P	2.3572626431	-0.4050775975	0.2598778830
P	2.8184657279	-0.4905392353	2.4077916054
P	2.8456023170	2.5467578640	3.3222374482
P	4.3291368136	1.1522225233	2.3560355243
P	1.6314304448	1.6792278867	0.0808164045
P	3.2917131532	2.7101163792	1.1430094067