Electronic Supplementary Material (ESI) for RSC Advances.

Direct coupling of unactivated alkynes and C(sp^3)−H bonds catalyzed by Pt(II, IV)-centered catalyst: A computational study

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Supporting Information Index

1. Table S1. Thermodynamic properties at different calculated levels

Table S1. Thermodynamic properties(kcal/mol) at different calculated methods **L*n*/PCM/BS4//L*n*/BS1**.

n	L*n*	1A-*a1*-IN1	1A-*a1*-TS1	1A-*a1*-IN2	1A-*a1*-TS2	1A-*a1*-P		
1	B3LYP	0.0	12.6	-24.2	-11.4	-34.1		
2	wB97XD	0.0	18.0	-27.4	-15.5	-40.3		
3	M062X	0.0	19.8	-22.9	-12.8	-38.9		
n	L*n*	1B-*a1*-IN1	1B-*a1*-TS1	1B-*a1*-IN2	1B-*a1*-TS2	1B-*a1*-P		
1	B3LYP	0.0	10.9	-26.4	-12.1	-34.2		
2	wB97XD	0.0	17.7	-29.6	-22.8	-38.8		
3	M062X	0.0	20.9	-25.2	-17.4	-36.8		
n	L*n*	1C-*a1*-IN1	1C-*a1*-TS1	1C-*a1*-IN2	1C-*a1*-TS2	1C-*a1*-P		
1	B3LYP	0.0	8.9	-28.4	-14.5	-32.7		
2	wB97XD	0.0	15.3	-32.2	-26.3	-37.4		
3	M062X	0.0	19.3	-28.2	-23.3	-36.0		
n	L*n*	1A-*a2*-IN1	1A-*a2*-TS1	1A-*a2*-IN2	1A-*a2*-TS2	1A-*a2*-P		
1	B3LYP	1.7	11.9	-21.4	-9.8	-35.1		
2	wB97XD	-0.9	16.7	-26.5	-14.0	-42.5		
3	M062X	1.1	19.9	-23.2	-19.7	-38.4		
n	L*n*	1B-*a2*-IN1	1B-*a2*-TS1	1B-*a2*-IN2	1B-*a2*-TS2	1B-*a2*-P		
1	B3LYP	0.7	10.6	-24.0	-11.0	-34.8		
2	wB97XD	0.3	15.3	-27.7	-24.0	-41.1		
3	M062X	0.9	20.8	-24.4	-19.6	-37.0		
n	L*n*	1C-*a2*-IN1	1C-*a2*-TS1	1C-*a2*-IN2	1C-*a2*-TS2	1C-*a2*-P		
1	B3LYP	1.4	9.0	-24.9	-12.9	-33.1		
2	wB97XD	0.0	13.2	-28.0	-17.2	-39.5		
3	M062X	1.2	16.5	-24.7	-21.5	-35.0		
n	L*n*	1A-*a2*-IN1	1A-*a3*-TS1	1A-*a3*-IN2	1A-*a3*-TS2	1A-*a3*-IN3	1A-*a3*-TS3	1A-*a3*-P
1	B3LYP	1.7	6.4	-0.4	21.2	-11.0	-2.0	-23.4
2	wB97XD	-0.9	4.6	-2.3	27.2	-15.2	-4.9	-29.7
3	M062X	1.1	5.5	-0.2	29.7	-9.8	-10.5	-25.0

Table S1. continued

n	L*n*	1B-*a2*-IN1	1B-*a3*-TS1	1B-*a3*-IN2	1B-*a3*-TS2	1B-*a3*-IN3	1B-*a3*-TS3	1B-*a3*-P
1	B3LYP	0.7	5.9	-1.5	19.9	-13.8	-3.8	-23.1
2	wB97XD	0.3	4.5	-2.9	26.4	-17.3	-3.9	-28.3
3	M062X	0.9	6.2	-1.0	27.6	-11.8	0.0	-23.5
n	L*n*	1C-*a2*-IN1	1C-*a3*-TS1	1C-*a3*-IN2	1C-*a3*-TS2	1C-*a3*-IN3	1C-*a3*-TS3	1C-*a3*-P
1	B3LYP	1.4	5.5	-1.3	18.6	-16.3	-5.0	-21.6
2	wB97XD	0.0	5.1	-1.5	24.0	-18.1	-7.8	-26.7
3	M062X	1.2	6.1	-0.7	26.9	-13.0	-2.4	-21.9
n	L*n*	1A-*a4*-IN1	1A-*a4*-TS1	1A-*a4*-IN2	1A-*a4*-TS2	1A-*a4*-P		
1	B3LYP	1.3	16.5	-20.1	-3.7	-32.5		
2	wB97XD	0.0	18.6	-25.8	-7.4	-40.9		
3	M062X	1.1	23.4	-20.8	-5.3	-35.6		
n	L*n*	1B-*a4*-IN1	1B-*a4*-TS1	1B-*a4*-IN2	1B-*a4*-TS2	1B-*a4*-P		
1	B3LYP	0.9	15.1	-22.3	-6.1	-31.5		
2	wB97XD	-0.8	17.1	-27.4	-8.6	-40.2		
3	M062X	1.7	21.4	-23.3	-5.1	-33.8		
n	L*n*	1C-*a4*-IN1	1C-*a4*-TS1	1C-*a4*-IN2	1C-*a4*-TS2	1C-*a4*-P		
1	B3LYP	2.1	15.5	-25.5	-6.6	-29.6		
2	wB97XD	0.0	16.6	-28.2	-10.2	-37.2		
3	M062X	2.1	19.7	-22.2	-6.3	-31.7		
n	L*n*	1A-*a1*-IN1	1A-*b*-TS1	1A-*b*-IN1	1A-*b*-TS2	1A-*a2*-IN2	1A-*a2*-TS2	1A-*a2*-P
1	B3LYP	0.0	13.7	2.9	8.9	-21.4	-9.8	-35.1
2	wB97XD	0.0	14.5	3.4	8.4	-26.5	-14.0	-42.5
3	M062X	0.0	15.6	5.5	13.0	-23.2	-19.7	-38.4
n	L*n*	1B-*a1*-IN1	1B-*b*-TS1	1B-*b*-IN1	1B-*b*-TS2	1B-*a2*-IN2	1B-*a2*-TS2	1B-*a2*-P
1	B3LYP	0.0	11.6	-0.8	4.9	-24.0	-11.0	-34.8
2	wB97XD	0.0	13.2	0.4	8.8	-27.7	-24.0	-41.1
3	M062X	0.0	5.9	3.2	10.3	-24.4	-19.6	-37.0

Table S1. continued

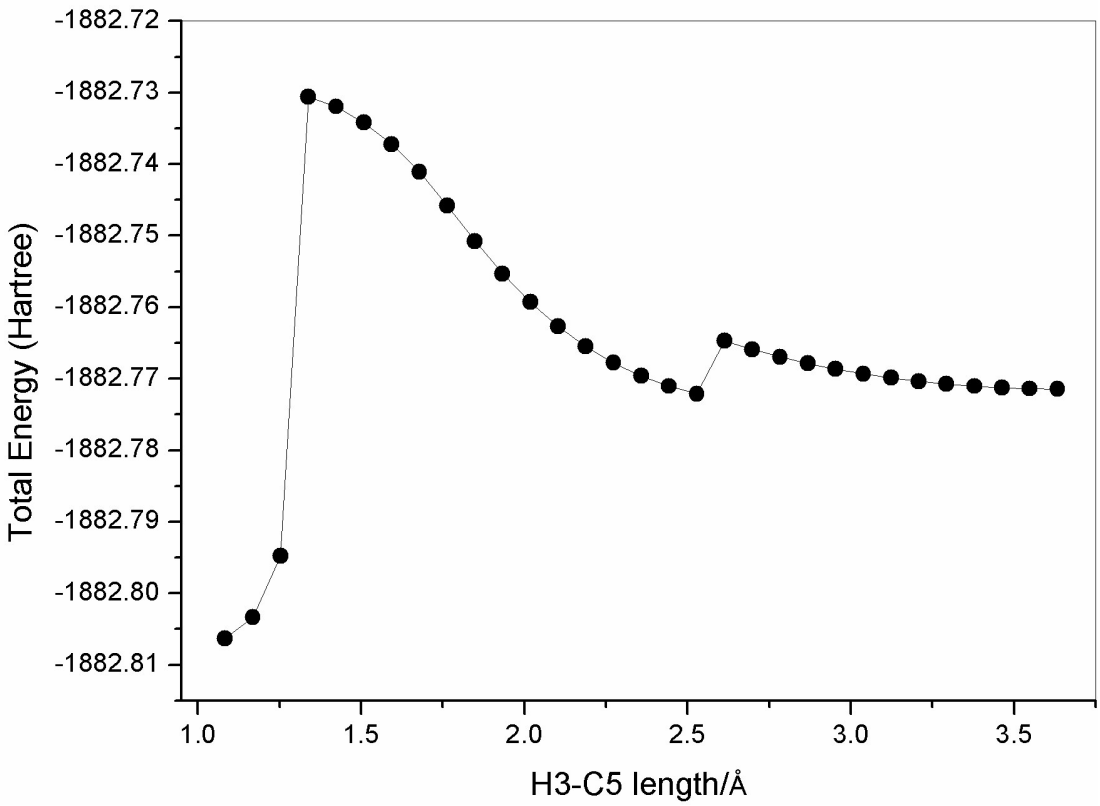
n	L*n*	1C-*a1*-IN1	1C-*b*-TS1	1C-*b*-IN1	1C-*b*-TS2	1C-*a2*-IN2	1C-*a2*-TS2	1C-*a2*-P				
1	B3LYP	0.0	9.7	-2.1	3.2	-24.9	-12.9	-33.1				
2	wB97XD	0.0	11.9	-0.9	4.2	-28.0	-17.2	-39.5				
3	M062X	0.0	13.0	1.2	8.0	-24.7	-21.5	-35.0				
n	L*n*	1D-IN1	1D-*a*-TS1	1D-*a*-IN2	1D-*a*-TS2	1D-P						
1	B3LYP	0.0	2.0	-30.7	-20.0	-22.5						
2	wB97XD	0.0	5.0	-40.9	-26.8	-30.1						
3	M062X	0.0	10.0	-39.5	-27.0	-26.4						
n	L*n*	1D-IN1	1D-*b*-TS1	1D-*b*-IN2	1D-*b*-TS2	1D-*b*-IN3	1D-*b*-TS3	1D-P				
1	B3LYP	0.0	6.6	4.4	14.9	-28.5	-14.2	-22.5				
2	wB97XD	0.0	6.9	4.9	12.4	-39.3	-22.0	-30.1				
3	M062X	0.0	10.1	-12.4	18.5	-36.9	-17.5	-26.4				
n	L*n*	2D-*a*-IN1	2D-*a*-TS1	2D-*a*-IN2	2D-*a*-TS2	2D-*a*-IN3	2D-*a*-IN4	2D-*a*-TS3	2D-P			
1	B3LYP	0.0	12.3	-20.7	-8.7	-3.3	-6.9	2.5	-16.0			
2	wB97XD	0.0	17.6	-22.9	-15.7	-14.5	-16.8	-5.6	-20.9			
3	M062X	0.0	20.0	-19.4	-10.0	-11.8	-15.4	0.0	-15.5			
n	L*n*	2D-*b*-IN1	2D-*b*-TS1	2D-*b*-IN2	2D-*b*-IN3	2D-*b*-TS2	2D-*b*-IN4	2D-*b*-TS3	2D-*b*-IN5	2D-*b*-IN6	2D-*b*-TS4	2D-P
1	B3LYP	-2.6	10.2	7.1	4.4	22.9	-25.9	-16.2	-9.0	-10.6	0.7	-16.0
2	wB97XD	-1.8	15.3	6.0	4.8	25.8	-26.3	-14.2	-18.3	-20.7	-1.1	-20.9
3	M062X	-3.7	16.8	3.8	3.3	27.0	-21.9	-17.6	-16.5	-19.9	-3.0	-15.5
n	L*n*	3D-*a*-IN1	3D-*a*-TS1	3D-*a*-IN2	3D-*a*-TS2	3D-*a*-IN3	3D-*a*-IN4	3D-*a*-TS3	3D-P			
1	B3LYP	0.0	13.1	-18.4	-7.9	-3.0	-5.9	3.7	-14.7			
2	wB97XD	0.0	16.5	-22.7	-15.9	-16.1	-17.3	-3.0	-20.4			
3	M062X	0.0	22.2	-17.2	-9.2	-10.7	-14.9	2.9	-14.7			
n	L*n*	3D-*b*-IN1	3D-*b*-TS1	3D-*b*-IN2	3D-*b*-IN3	3D-*b*-TS2	3D-*b*-IN4	3D-*b*-TS3	3D-*b*-IN5	3D-*b*-IN6	3D-*b*-TS4	3D-P
1	B3LYP	-1.8	11.3	7.7	5.1	23.2	-23.5	-15.4	-8.2	-9.4	1.7	-14.7
2	wB97XD	-1.9	15.9	6.7	3.5	26.0	-24.9	-13.4	-19.7	-21.0	-8.5	-20.4
3	M062X	-2.8	18.5	6.8	7.0	28.8	-19.9	-8.1	-15.0	-18.2	-1.0	-14.7

2. Table S2. Thermodynamic properties at different calculated basis sets

Table S2. Thermodynamic properties (Relative free energy an activation free energy in solution, kcal/mol) in pathway 1X-*a2* at different calculated basis sets.

		1A-*a2*-IN1	1A-*a2*-TS1	1A-*a2*-IN2	1A-*a2*-TS2	1A-*a2*-P
SDD for Pt, 6-31G(d) for other atoms	ΔG_{sol}^{rel}	0.0	10.2	-23.1	-11.5	-36.8
	$\Delta G_{sol}^{\neq}$		10.2		11.6	
SDD for Pt, 6-31G(d,p) for other atoms	ΔG_{sol}^{rel}	0.0	10.5	-23.0	-11.5	-36.6
	$\Delta G_{sol}^{\neq}$		10.5		11.5	
SDD for Pt, Cl, Br and I; 6-31G(d) for other atoms	ΔG_{sol}^{rel}	0.0	9.5	-22.6	-11.9	-37.3
	$\Delta G_{sol}^{\neq}$		9.5		10.7	
		1B-*a2*-IN1	1A-*a2*-TS1	1A-*a2*-IN2	1A-*a2*-TS2	1A-*a2*-P
SDD for Pt, 6-31G(d) for other atoms	ΔG_{sol}^{rel}	0.0	9.9	-24.7	-11.7	-35.5
	$\Delta G_{sol}^{\neq}$		9.9		13.0	
SDD for Pt, 6-31G(d,p) for other atoms	ΔG_{sol}^{rel}	0.0	10.4	-24.3	-11.7	-34.9
	$\Delta G_{sol}^{\neq}$		10.4		12.6	
SDD for Pt, Cl, Br and I; 6-31G(d) for other atoms	ΔG_{sol}^{rel}	0.0	9.7	-24.4	-12.0	-34.5
	$\Delta G_{sol}^{\neq}$		9.7		12.4	
		1C-*a2*-IN1	1C-*a2*-TS1	1C-*a2*-IN2	1C-*a2*-TS2	1C-*a2*-P
SDD for Pt, Cl, Br and I; 6-31G(d) for other atoms	ΔG_{sol}^{rel}	0.0	7.6	-26.3	-14.3	-34.8
	$\Delta G_{sol}^{\neq}$		7.6		12.0	

3. Figure S1. The H3-C5 bond scan energy profile of 1A-a2-IN1



4. The .xyz files of optimized molecular structures and their free energies at L1/BS1

(1). In Path 1A-*a1*

36
1A-a1-IN1,Free Energies= -1882.560271
C -1.456408 3.535574 -0.994664
O -0.977957 2.617851 -1.978627
C -1.897682 1.530042 -1.986932
C -2.452090 1.389587 -0.533559
C -1.900412 2.653100 0.179324
H -0.641446 4.222089 -0.753269
H -2.301198 4.117410 -1.398122
H -2.726363 1.744807 -2.677977
H -2.656060 3.121820 0.813229
H -1.033540 2.423473 0.805228
C -2.159254 0.027602 0.166715
C -0.719828 -0.181073 0.742651
H -0.613091 -1.237763 0.994840
H -0.606569 0.385221 1.674548
C 0.390076 0.216270 -0.138221
C 1.090285 0.833493 -0.987995
H 1.274444 1.460947 -1.840359
C -3.120319 -0.119730 1.370384
O -3.862176 0.741264 1.783071
O -3.006469 -1.344003 1.917523
C -2.461668 -1.125066 -0.810972
O -1.663610 -1.954033 -1.182385
O -3.743856 -1.073647 -1.219293
C -3.843404 -1.598729 3.063429
H -3.618742 -2.621744 3.363690
H -3.607503 -0.897814 3.867743
H -4.896677 -1.495234 2.791961
C -4.144587 -2.107296 -2.141234
H -5.195378 -1.912878 -2.354706
H -3.546535 -2.054447 -3.054129
H -4.016252 -3.091546 -1.684592
H -1.365078 0.650801 -2.359525
H -3.540173 1.458244 -0.574596
Pt 2.444397 -0.229384 0.150201
Cl 2.844338 -1.752984 -1.540446
Cl 2.479867 1.129249 2.042474

36
1A-a1-TS1,Free Energies=-1882.54117
C -1.367295 3.570532 0.312859
O -1.273322 3.243864 -1.100177
C -1.716495 1.963758 -1.324371
C -2.457221 1.453627 -0.091743
C -1.802117 2.286630 1.035104
H -0.393077 3.940901 0.641257
H -2.102835 4.377517 0.404325
H -2.223932 1.889969 -2.292467
H -2.502614 2.477113 1.848845
H -0.929772 1.776239 1.453586
C -2.332594 -0.085520 0.020754
C -0.842850 -0.554040 0.102345
H -0.781280 -1.583966 -0.257938
H -0.509222 -0.535271 1.146010
C 0.116500 0.281880 -0.648952
C 1.280989 0.784586 -0.890484
H 1.579326 1.602813 -1.537577
C -3.088656 -0.593378 1.260048
O -3.715312 0.101054 2.026513
O -2.948262 -1.924119 1.375211
C -2.975825 -0.702834 -1.239513
O -2.356007 -1.127802 -2.187850
O -4.315926 -0.651431 -1.167367
C -3.602539 -2.528568 2.510065
H -3.373448 -3.591499 2.442693
H -3.212985 -2.106080 3.439104
H -4.680436 -2.357982 2.457556
C -5.026287 -1.174326 -2.309953
H -6.082676 -1.058886 -2.069994
H -4.767509 -0.608450 -3.208073
H -4.773456 -2.226169 -2.461031
H -0.805341 1.235254 -1.471337
H -3.520638 1.702051 -0.171038
Pt 2.623297 -0.240655 0.103083
Cl 3.590896 -1.208634 -1.764223
Cl 1.951440 0.531630 2.211751

36
1A-a1-IN2,Free Energies= -1882.607114
C -1.950282 3.368348 -1.589000
O -0.793633 2.583723 -1.923682
C -1.122004 1.206819 -1.806242
C -2.515941 1.095024 -1.122084
C -2.735376 2.525992 -0.583373
H -1.594657 4.320676 -1.189430
H -2.539654 3.562031 -2.497359
H -1.070707 0.711753 -2.782411
H -3.793352 2.785395 -0.523905
H -2.304614 2.645256 0.416807
C -2.355787 -0.027625 -0.050085
C -0.880836 0.126208 0.411686
H -0.436668 -0.755143 0.878802
H -0.774234 0.936756 1.144983
C -0.146871 0.566476 -0.814549
C 1.220913 0.419656 -1.049558
H 1.605259 0.854722 -1.975796
C -3.383859 0.060945 1.076762
O -4.451727 0.625009 0.993129
O -2.942469 -0.579899 2.171157
C -2.455923 -1.375221 -0.782428
O -1.628769 -1.721720 -1.605394
O -3.531506 -2.087537 -0.449460
C -3.848591 -0.601677 3.292181
H -3.322339 -1.141147 4.078896
H -4.082727 0.417047 3.609977
H -4.772789 -1.116264 3.018144
C -3.682778 -3.359674 -1.120732
H -4.602593 -3.785170 -0.721975
H -3.758613 -3.207633 -2.199530
H -2.827007 -4.001864 -0.902057
H 0.597997 -0.574649 -1.399593
H -3.298375 0.845690 -1.843363
Pt 2.532112 -0.132605 0.264209
Cl 3.077893 -2.106626 -0.850207
Cl 2.180881 1.710007 1.651269

36
1A-a1-TS2,Free Energies=-1882.57972
C -1.950282 3.368348 -1.589000
O -0.793633 2.583723 -1.923682
C -1.122004 1.206819 -1.806242
C -2.515941 1.095024 -1.122084
C -2.735376 2.525992 -0.583373
H -1.594657 4.320676 -1.189430
H -2.539654 3.562031 -2.497359
H -1.070707 0.711753 -2.782411
H -3.793352 2.785395 -0.523905
H -2.304614 2.645256 0.416807
C -2.355787 -0.027625 -0.050085
C -0.880836 0.126208 0.411686
H -0.436668 -0.755143 0.878802
H -0.774234 0.936756 1.144983
C -0.146871 0.566476 -0.814549
C 1.220913 0.419656 -1.049558
H 1.605259 0.854722 -1.975796
C -3.383859 0.060945 1.076762
O -4.451727 0.625009 0.993129
O -2.942469 -0.579899 2.171157
C -2.455923 -1.375221 -0.782428
O -1.628769 -1.721720 -1.605394
O -3.531506 -2.087537 -0.449460
C -3.848591 -0.601677 3.292181
H -3.322339 -1.141147 4.078896
H -4.082727 0.417047 3.609977
H -4.772789 -1.116264 3.018144
C -3.682778 -3.359674 -1.120732
H -4.602593 -3.785170 -0.721975
H -3.758613 -3.207633 -2.199530
H -2.827007 -4.001864 -0.902057
H 0.597997 -0.574649 -1.399593
H -3.298375 0.845690 -1.843363
Pt 2.532112 -0.132605 0.264209
Cl 3.077893 -2.106626 -0.850207
Cl 2.180881 1.710007 1.651269

36
1A-a1-P,Free Energies=-1882.619204
C 0.398211 2.775590 -1.984083
O -0.512513 1.955829 -1.251405
C 0.134930 1.584609 -0.040029
C 1.678695 1.590056 -0.345971
C 1.742168 2.070241 -1.818772
H 0.039607 2.823620 -3.014826
H 0.416833 3.795540 -1.567568
H -0.149493 2.276269 0.763519
H 2.608647 2.706192 -2.009472
H 1.795525 1.225096 -2.509470
C 2.157091 0.125777 -0.064570
C 0.883568 -0.735181 -0.294291
H 0.947006 -1.726854 0.150064
H 0.716749 -0.850971 -1.369005
C -0.198742 0.136129 0.322841
C -0.845380 -0.227580 1.555495
H -1.152554 0.547118 2.254851
C 3.349853 -0.334714 -0.914382
O 4.041807 0.361070 -1.620431
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C 2.600690 0.017952 1.408017
O 1.963094 -0.497384 2.301148
O 3.795820 0.605420 1.589261
C 4.650840 -2.226693 -1.462369
H 4.649112 -3.286313 -1.207969
H 4.518867 -2.087354 -2.538122
H 5.585499 -1.753523 -1.150958
C 4.308958 0.584605 2.935835
H 5.274440 1.087086 2.884359
H 3.631191 1.115838 3.608620
H 4.424678 -0.445388 3.281464
H -0.652388 -1.206228 1.983708
H 2.210289 2.295290 0.297215
Pt -2.257274 -0.374909 0.038080
Cl -3.264649 1.616513 0.664037
Cl -1.828494 -2.532236 -0.711757

(2). In Path 1A-*a2*

36
1A-a2-IN1,Free Energies=-1882.556257

C	-3.857314	-2.134344	-1.940874
O	-2.979911	-2.993183	-1.211003
C	-1.928273	-2.191492	-0.695001
C	-2.649823	-0.916307	-0.223321
C	-3.669427	-0.703714	-1.370646
H	-3.615610	-2.164916	-3.014104
H	-4.874055	-2.517368	-1.811137
H	-1.438343	-2.742779	0.109025
H	-4.607385	-0.275343	-1.004889
H	-3.284361	-0.028600	-2.142685
C	-1.797547	0.328438	0.167607
C	-0.847184	0.872214	-0.943561
H	-0.528742	1.882486	-0.674126
H	-1.400740	0.962323	-1.884867
C	0.372429	0.102865	-1.240678
C	1.259826	-0.528162	-1.883742
H	1.646024	-1.133887	-2.684174
C	-2.828435	1.417936	0.552661
O	-3.480090	1.377376	1.571649
O	-2.950884	2.375084	-0.382881
C	-0.978060	0.130393	1.466118
O	-0.106978	0.907865	1.803244
O	-1.350374	-0.938311	2.166854
C	-3.918506	3.404966	-0.092349
H	-3.875941	4.088370	-0.939999
H	-4.915657	2.969713	0.007694
H	-3.654186	3.918367	0.834733
C	-0.657700	-1.145875	3.418111
H	-1.145470	-2.007590	3.872610
H	0.396385	-1.352781	3.224638
H	-0.758611	-0.261372	4.050612
H	-1.184130	-1.976503	-1.477698
H	-3.208385	-1.187005	0.675946
Pt	2.198775	0.032949	-0.149872
Cl	2.009429	-2.098775	0.771741
Cl	2.748847	2.193171	-0.790588

36
1A-a2-TS1,Free Energies=-1882.540268

C	-3.742901	-1.641581	-2.715690
O	-2.607713	-2.451399	-2.325131
C	-2.048216	-1.970590	-1.165597
C	-2.988609	-0.950382	-0.528211
C	-3.757768	-0.436421	-1.770095
H	-3.626472	-1.374846	-3.769383
H	-4.636436	-2.267202	-2.607907
H	-1.681329	-2.782337	-0.536631
H	-4.768515	-0.113690	-1.514911
H	-3.239523	0.412537	-2.229992
C	-2.265185	0.149092	0.291822
C	-1.043734	0.712825	-0.498465
H	-0.513594	1.437729	0.126682
H	-1.377895	1.254967	-1.389512
C	-0.079388	-0.335530	-0.859070
C	1.081309	-0.905959	-0.930264
H	1.328290	-1.887178	-1.325140
C	-3.283691	1.250931	0.644747
O	-4.424903	1.003095	0.968597
O	-2.763401	2.478520	0.561371
C	-1.725713	-0.338995	1.659172
O	-1.477863	0.424021	2.564331
O	-1.530246	-1.663008	1.695049
C	-3.628946	3.557097	0.973740
H	-3.045304	4.465328	0.828996
H	-4.533757	3.571506	0.361649
H	-3.900799	3.432728	2.024158
C	-0.882902	-2.168277	2.892462
H	-0.936969	-3.253185	2.808519
H	0.156326	-1.831903	2.909269
H	-1.412619	-1.815278	3.778732
H	-1.054889	-1.375776	-1.437111
H	-3.680889	-1.475363	0.137434
Pt	2.503631	0.179187	-0.152226
Cl	2.825429	-1.297401	1.628052
Cl	2.484489	1.871654	-1.744067

36

1A-a2-IN2,Free Energies=-1882.604584

C	-2.882933	3.654665	-0.376369
O	-1.472884	3.432456	-0.327250
C	-1.206895	2.140754	-0.868125
C	-2.541063	1.331706	-0.803456
C	-3.497438	2.290504	-0.060408
H	-3.120625	4.434226	0.352237
H	-3.184215	4.006098	-1.376146
H	-0.831666	2.236484	-1.894813
H	-4.532328	2.181994	-0.390272
H	-3.470895	2.120223	1.021993
C	-2.192097	0.008839	-0.060302
C	-1.040513	0.428604	0.898790
H	-0.469978	-0.415423	1.288702
H	-1.467941	0.965535	1.749595
C	-0.185747	1.415005	0.053299
C	0.954449	0.798634	-0.674181
H	1.103286	1.031133	-1.732562
C	-3.405118	-0.617003	0.629231
O	-4.532878	-0.568805	0.188997
O	-3.066149	-1.230313	1.775746
C	-1.614979	-0.971682	-1.090615
O	-0.783404	-0.630045	-1.916464
O	-2.097849	-2.205544	-0.987466
C	-4.138070	-1.907619	2.457701
H	-3.688219	-2.333316	3.354521
H	-4.930894	-1.201768	2.718230
H	-4.551949	-2.693583	1.821504
C	-1.549209	-3.186305	-1.900881
H	-2.066536	-4.114549	-1.662193
H	-1.746481	-2.885315	-2.932086
H	-0.474601	-3.279353	-1.736400
H	0.276601	2.164429	0.716025
H	-2.926876	1.124375	-1.804087
Pt	2.308583	-0.156131	0.109202
Cl	1.662660	-2.371177	0.009136
Cl	3.715977	1.555792	0.749184

36

1A-a2-TS2,Free Energies=-1882.578124

C	-1.579215	3.311004	-1.599223
O	-0.709972	2.344145	-2.237866
C	-1.100309	1.044408	-1.842921
C	-2.407770	1.149434	-1.027325
C	-2.270444	2.573154	-0.448153
H	-0.963794	4.153559	-1.273561
H	-2.304076	3.671136	-2.340918
H	-1.171441	0.388531	-2.719920
H	-3.232661	3.004424	-0.171044
H	-1.636558	2.577788	0.446970
C	-2.359076	-0.052057	-0.037710
C	-0.843396	-0.258124	0.259450
H	-0.553222	-1.310802	0.322935
H	-0.526203	0.192230	1.208816
C	-0.110559	0.403621	-0.862607
C	1.275598	0.573890	-0.953792
H	1.650707	1.018601	-1.878713
C	-3.201117	0.157156	1.222209
O	-4.030839	1.024893	1.374041
O	-2.888900	-0.769129	2.144199
C	-2.863950	-1.279299	-0.819400
O	-2.172066	-1.891005	-1.605301
O	-4.154806	-1.539279	-0.581255
C	-3.629572	-0.699282	3.379041
H	-3.237494	-1.506123	3.997272
H	-3.472303	0.268743	3.860427
H	-4.696063	-0.839063	3.186366
C	-4.720628	-2.643682	-1.319858
H	-5.759392	-2.702887	-0.997172
H	-4.656710	-2.451512	-2.393344
H	-4.185632	-3.566454	-1.084728
H	0.803591	1.508164	-0.340855
H	-3.290561	1.100412	-1.671220
Pt	2.578267	-0.201625	0.256619
Cl	3.411235	-1.819491	-1.167877
Cl	1.920664	1.300768	1.955149

36

1A-a2-P,Free Energies=-1882.622686

C	1.705761	3.710393	0.064328
O	0.528870	3.110872	-0.481900
C	0.274161	1.919878	0.275073
C	1.647451	1.437253	0.839070
C	2.634596	2.531450	0.361452
H	2.093257	4.413012	-0.677859
H	1.457802	4.265912	0.982158
H	-0.463258	2.115932	1.053826
H	3.399360	2.755473	1.109058
H	3.145917	2.232401	-0.561103
C	1.885011	0.022494	0.229157
C	1.062023	0.054010	-1.085633
H	0.870121	-0.923885	-1.522287
H	1.617477	0.646896	-1.826294
C	-0.173519	0.862217	-0.740991
C	-1.294026	1.042889	-1.619930
H	-1.862175	1.968810	-1.566539
C	3.376632	-0.276657	0.074234
O	4.156996	-0.232685	0.999959
O	3.723828	-0.570931	-1.191788
C	1.282437	-1.057150	1.147538
O	0.460567	-0.840669	2.013285
O	1.744428	-2.271438	0.824604
C	5.114374	-0.889826	-1.391264
H	5.214602	-1.097998	-2.456378
H	5.744830	-0.046543	-1.098736
H	5.388722	-1.765109	-0.797607
C	1.179457	-3.381717	1.553517
H	1.747933	-4.254198	1.232702
H	1.285605	-3.220691	2.628410
H	0.124652	-3.492907	1.293138
H	-1.301849	0.533380	-2.581756
H	1.626366	1.377459	1.927153
Pt	-1.947380	-0.257289	-0.138986
Cl	-3.007938	1.379872	1.114789
Cl	-1.420143	-2.253517	-1.223590

(3). In Path 1A-*a3*

36
1A-a2-IN1,Free Energies=-1882.556257

C	-3.857314	-2.134344	-1.940874
O	-2.979911	-2.993183	-1.211003
C	-1.928273	-2.191492	-0.695001
C	-2.649823	-0.916307	-0.223321
C	-3.669427	-0.703714	-1.370646
H	-3.615610	-2.164916	-3.014104
H	-4.874055	-2.517368	-1.811137
H	-1.438343	-2.742779	0.109025
H	-4.607385	-0.275343	-1.004889
H	-3.284361	-0.028600	-2.142685
C	-1.797547	0.328438	0.167607
C	-0.847184	0.872214	-0.943561
H	-0.528742	1.882486	-0.674126
H	-1.400740	0.962323	-1.884867
C	0.372429	0.102865	-1.240678
C	1.259826	-0.528162	-1.883742
H	1.646024	-1.133887	-2.684174
C	-2.828435	1.417936	0.552661
O	-3.480090	1.377376	1.571649
O	-2.950884	2.375084	-0.382881
C	-0.978060	0.130393	1.466118
O	-0.106978	0.907865	1.803244
O	-1.350374	-0.938311	2.166854
C	-3.918506	3.404966	-0.092349
H	-3.875941	4.088370	-0.939999
H	-4.915657	2.969713	0.007694
H	-3.654186	3.918367	0.834733
C	-0.657700	-1.145875	3.418111
H	-1.145470	-2.007590	3.872610
H	0.396385	-1.352781	3.224638
H	-0.758611	-0.261372	4.050612
H	-1.184130	-1.976503	-1.477698
H	-3.208385	-1.187005	0.675946
Pt	2.198775	0.032949	-0.149872
Cl	2.009429	-2.098775	0.771741
Cl	2.748847	2.193171	-0.790588

36
1A-a3-TS1,Free Energies=-1882.548368

C	-4.178840	-2.395973	-0.941635
O	-2.984456	-2.771465	-1.639255
C	-1.968258	-1.795932	-1.435924
C	-2.400072	-1.001089	-0.186385
C	-3.931970	-0.991069	-0.386338
H	-5.027668	-2.435838	-1.634544
H	-4.362817	-3.119753	-0.135213
H	-1.016698	-2.317467	-1.301413
H	-4.480735	-0.796685	0.539058
H	-4.219445	-0.233980	-1.125347
C	-1.704801	0.389563	0.097876
C	-0.742874	0.898073	-1.022386
H	-0.413003	1.909209	-0.767524
H	-1.291600	0.969349	-1.966786
C	0.463298	0.096805	-1.281793
C	1.332626	-0.595281	-1.884304
H	1.722442	-1.211318	-2.674965
C	-2.800367	1.464601	0.309092
O	-3.332331	1.689348	1.371989
O	-3.110095	2.106485	-0.833521
C	-0.926018	0.412466	1.440035
O	-0.011225	1.185755	1.646717
O	-1.393020	-0.453821	2.335435
C	-4.134079	3.116302	-0.717414
H	-4.240031	3.536069	-1.717412
H	-5.072070	2.667043	-0.382792
H	-3.826961	3.883808	-0.003527
C	-0.742385	-0.440107	3.623594
H	-1.295909	-1.156407	4.229944
H	0.299241	-0.748390	3.513555
H	-0.793938	0.560805	4.057310
H	-1.891886	-1.151360	-2.326548
H	-2.194437	-1.634586	0.677602
Pt	2.228799	-0.069561	-0.114368
Cl	1.696858	-2.086704	0.928115
Cl	3.086122	1.951687	-0.857417

36

1A-a3-IN2,Free Energies=-1882.559549

C	-3.815431	-2.444499	-1.203981
O	-3.512201	-1.667383	-2.368416
C	-2.633546	-0.600610	-2.027485
C	-2.175973	-0.848090	-0.569934
C	-3.401018	-1.593786	-0.002964
H	-4.884306	-2.684212	-1.215908
H	-3.252608	-3.389797	-1.234214
H	-1.793509	-0.596575	-2.733809
H	-3.164030	-2.185849	0.880981
H	-4.199162	-0.892071	0.263715
C	-1.669833	0.423635	0.183365
C	-0.672388	1.245241	-0.694047
H	-0.313310	2.104411	-0.120389
H	-1.196502	1.634266	-1.572940
C	0.495984	0.500699	-1.185761
C	1.316644	-0.063919	-1.963484
H	1.668737	-0.471438	-2.894425
C	-2.854661	1.329214	0.584497
O	-3.427390	1.256306	1.648239
O	-3.196256	2.193728	-0.390110
C	-0.953134	0.100965	1.519333
O	-0.101310	0.827378	1.990739
O	-1.375946	-1.026618	2.086829
C	-4.310899	3.059628	-0.088242
H	-4.431737	3.691256	-0.967808
H	-5.211274	2.467868	0.091959
H	-4.090990	3.661004	0.796622
C	-0.757410	-1.365528	3.346151
H	-1.277923	-2.259596	3.688172
H	0.303648	-1.571894	3.192288
H	-0.881030	-0.545909	4.057020
H	-3.166195	0.355988	-2.125438
H	-1.332110	-1.548145	-0.588418
Pt	2.259872	-0.065831	-0.140200
Cl	1.642282	-2.260108	0.344801
Cl	3.207546	2.038965	-0.327432

36

1A-a3-TS2,Free Energies=-1882.518538

C	-3.131679	-0.942892	3.120153
O	-2.432719	-2.084407	2.492010
C	-2.046208	-1.725892	1.264470
C	-2.311872	-0.246813	1.054689
C	-3.556577	-0.062592	1.931988
H	-3.944432	-1.384538	3.697880
H	-2.432423	-0.436735	3.792805
H	-0.718834	-1.812588	1.035248
H	-3.709951	0.981018	2.211517
H	-4.469953	-0.441688	1.462662
C	-2.139708	0.107314	-0.431742
C	-0.805256	-0.622474	-0.888603
H	-0.188386	0.065499	-1.471229
H	-1.061347	-1.456548	-1.546808
C	0.025720	-1.106421	0.255409
C	1.215139	-1.006597	0.815264
H	1.484615	-1.501655	1.747302
C	-3.399194	-0.323502	-1.204885
O	-4.424683	0.320527	-1.181632
O	-3.272931	-1.507985	-1.829661
C	-1.984604	1.617395	-0.701288
O	-1.762948	2.045752	-1.809537
O	-2.102921	2.359047	0.405499
C	-4.437671	-1.952427	-2.559525
H	-4.151320	-2.903060	-3.008056
H	-5.284884	-2.078848	-1.881361
H	-4.696334	-1.221237	-3.328081
C	-1.844860	3.771514	0.229274
H	-2.014027	4.218403	1.208486
H	-0.810097	3.912274	-0.088400
H	-2.527999	4.186091	-0.514916
H	-2.287035	-2.468251	0.497736
H	-1.506731	0.285483	1.573042
Pt	2.607065	0.033897	-0.039354
Cl	1.623095	2.096311	0.484910
Cl	3.873273	-1.784000	-0.734488

36

1A-a3-IN3,Free Energies=-1882.58378

C	-2.088437	-1.774820	2.817531
O	-1.097931	-2.373394	1.927373
C	-1.368163	-1.835183	0.651759
C	-1.766631	-0.395609	0.925326
C	-2.779938	-0.600693	2.047350
H	-2.806014	-2.545544	3.120655
H	-1.551335	-1.428117	3.704913
H	-0.084982	-2.619249	-0.953254
H	-2.922692	0.279758	2.677805
H	-3.755531	-0.911874	1.658139
C	-1.920063	0.244112	-0.478458
C	-0.868499	-0.583083	-1.331252
H	-0.113716	0.087594	-1.743591
H	-1.366334	-1.076106	-2.168556
C	-0.246164	-1.674951	-0.402509
C	1.064312	-1.426586	0.241313
H	1.397024	-2.185108	0.959838
C	-3.339843	0.145461	-1.048863
O	-4.037206	1.093350	-1.330756
O	-3.737401	-1.138275	-1.201386
C	-1.564246	1.740437	-0.481678
O	-0.923491	2.288825	-1.349169
O	-2.055559	2.354176	0.605120
C	-5.061654	-1.312440	-1.744026
H	-5.212921	-2.390449	-1.799423
H	-5.805137	-0.849177	-1.091007
H	-5.126518	-0.860452	-2.736578
C	-1.793650	3.768578	0.685534
H	-2.283742	4.102053	1.600246
H	-0.717154	3.948622	0.735368
H	-2.211064	4.278353	-0.185877
H	-2.189400	-2.382813	0.167611
H	-0.887730	0.086955	1.373197
Pt	2.223552	-0.046572	-0.026276
Cl	1.764622	1.430611	1.685441
Cl	3.377189	-0.693591	-1.907301

36

1A-a3-TS3,Free Energies=-1882.561908

C	-2.249406	3.583564	-0.787892
O	-0.990492	3.194011	-0.154612
C	-1.180580	1.891130	0.309581
C	-2.140877	1.220991	-0.677766
C	-3.180130	2.329552	-0.815086
H	-2.685990	4.412454	-0.221942
H	-2.005222	3.934201	-1.794817
H	0.900534	1.012223	1.458484
H	-3.762318	2.266637	-1.736950
H	-3.872848	2.337506	0.033584
C	-2.256153	-0.217432	-0.117283
C	-0.760375	-0.484591	0.309421
H	-0.234530	-1.121766	-0.407578
H	-0.686117	-0.973427	1.285727
C	-0.084568	0.878808	0.323263
C	1.289389	1.133664	0.302712
H	1.579120	2.182742	0.201601
C	-3.188263	-0.277823	1.099902
O	-2.824433	-0.161029	2.250273
O	-4.467833	-0.419347	0.721913
C	-2.719536	-1.204797	-1.192036
O	-3.057917	-0.894742	-2.311099
O	-2.665710	-2.462373	-0.724927
C	-5.436073	-0.475398	1.790761
H	-6.401123	-0.593427	1.299221
H	-5.225544	-1.325067	2.444209
H	-5.408131	0.446190	2.376835
C	-3.056069	-3.493722	-1.654883
H	-2.936796	-4.431385	-1.113124
H	-4.095091	-3.350513	-1.961282
H	-2.411596	-3.470671	-2.536715
H	-1.639028	1.883480	1.315629
H	-1.624901	1.124118	-1.642118
Pt	2.673544	-0.202353	0.084985
Cl	3.055354	0.119097	-2.177876
Cl	2.462296	-0.819428	2.341045

36
1A-a3-P,Free Energies=-1882.603706

C	-0.604314	3.387044	-0.800086
O	0.227948	2.828944	0.258861
C	-0.379982	1.643506	0.668990
C	-1.233154	1.143843	-0.484897
C	-1.843277	2.458622	-0.962691
H	-0.874089	4.410374	-0.521933
H	0.000527	3.414059	-1.712072
H	1.688573	-0.501531	2.586704
H	-2.204565	2.433362	-1.993643
H	-2.663200	2.788250	-0.313779
C	-1.914830	-0.108757	0.123319
C	-0.848047	-0.600934	1.186942
H	-0.532594	-1.628212	1.020893
H	-1.302923	-0.547770	2.183736
C	0.318562	0.397153	1.138785
C	1.534720	0.322166	1.892348
H	2.056606	1.248547	2.125119
C	-3.230629	0.266417	0.814280
O	-3.351604	0.517712	1.994511
O	-4.233447	0.348879	-0.076318
C	-2.161095	-1.187031	-0.937439
O	-1.851065	-1.102899	-2.103967
O	-2.734503	-2.268787	-0.379692
C	-5.516918	0.727052	0.457388
H	-6.193970	0.735958	-0.396431
H	-5.844780	0.000350	1.204605
H	-5.461674	1.716461	0.918055
C	-2.968764	-3.378003	-1.268499
H	-3.439142	-4.146341	-0.655172
H	-3.628226	-3.076007	-2.085853
H	-2.023074	-3.738369	-1.680589
H	-1.046141	1.860175	1.533477
H	-0.561700	0.776790	-1.269560
Pt	2.068954	-0.296329	-0.016019
Cl	2.794320	1.630358	-1.046302
Cl	1.869190	-2.550926	0.563251

(4). In Path 1A-*a4*

36
1A-a4-IN1,Free Energies=-1882.55532

C	-1.600396	-2.431794	2.608186
O	-0.885449	-1.308362	3.124752
C	-0.630805	-0.441596	2.034104
C	-1.955514	-0.441946	1.249836
C	-2.390257	-1.928018	1.371576
H	-0.898625	-3.230363	2.325616
H	-2.243071	-2.807097	3.409485
H	-0.349503	0.536260	2.426205
H	-3.472430	-2.013637	1.508142
H	-2.129616	-2.510973	0.482075
C	-1.973836	0.141142	-0.195746
C	-0.975370	-0.522683	-1.203208
H	-1.402191	-0.457189	-2.209619
H	-0.864780	-1.588268	-0.985322
C	0.359152	0.082993	-1.337490
C	1.330379	0.677688	-1.885244
H	1.799982	1.318946	-2.609916
C	-3.432054	-0.052116	-0.676489
O	-4.356693	0.594878	-0.239181
O	-3.565283	-1.039102	-1.580027
C	-1.769262	1.672194	-0.263199
O	-1.648802	2.252815	-1.321834
O	-1.748520	2.260884	0.933238
C	-4.913610	-1.291128	-2.026797
H	-4.832209	-2.106298	-2.745339
H	-5.543843	-1.578580	-1.181943
H	-5.327731	-0.396663	-2.497441
C	-1.554214	3.691306	0.922842
H	-1.630876	3.997789	1.965450
H	-0.565725	3.926582	0.522478
H	-2.325648	4.170173	0.316138
H	0.204147	-0.826660	1.420487
H	-2.661107	0.165705	1.821864
Pt	2.154868	-0.104543	-0.181856
Cl	2.402255	-2.310708	-0.863593
Cl	2.235170	1.988915	0.821864

36
1A-a4-TS1,Free Energies=-1882.535383

C	-0.485300	-2.324000	2.005100
O	-0.073300	-1.034600	2.467900
C	-0.730600	-0.087700	1.687300
C	-2.130200	-0.634200	1.360600
C	-1.967900	-2.166200	1.611900
H	0.134800	-2.618000	1.145000
H	-0.311200	-3.034300	2.816000
H	-0.688200	0.889400	2.170800
H	-2.625300	-2.477900	2.427200
H	-2.220900	-2.777900	0.739900
C	-2.614600	-0.245700	-0.060900
C	-1.551400	-0.600900	-1.140500
H	-1.985000	-0.358400	-2.124100
H	-1.326100	-1.671800	-1.138100
C	-0.348000	0.209300	-1.095300
C	0.608200	0.994100	-1.441500
H	0.650400	1.320100	-2.490400
C	-3.957700	-0.956800	-0.315800
O	-4.919500	-0.805100	0.402200
O	-3.932900	-1.755100	-1.395200
C	-2.929500	1.263500	-0.229400
O	-3.164200	1.741900	-1.318800
O	-2.910200	1.933800	0.919700
C	-5.174400	-2.428400	-1.698000
H	-4.969800	-3.024800	-2.586500
H	-5.472800	-3.063700	-0.861100
H	-5.959100	-1.694500	-1.893600
C	-3.138900	3.360800	0.825000
H	-3.212100	3.705400	1.855600
H	-2.290600	3.829100	0.322100
H	-4.062700	3.555100	0.277200
H	-2.857000	-0.220200	2.061100
Pt	2.058800	1.707300	-0.374400
Cl	3.660200	0.239500	-1.193300
Cl	0.787400	3.335900	0.713500
H	-0.162100	0.050000	0.711700

36

1A-a4-IN2,Free Energies=-1882.599897

C	-0.578900	-3.192700	1.864100
O	0.113900	-1.960700	2.085400
C	-0.534200	-0.973600	1.333400
C	-2.054100	-1.311200	1.345400
C	-2.068500	-2.816000	1.745500
H	-0.210900	-3.674600	0.945200
H	-0.349200	-3.848000	2.707100
H	-0.280100	-0.011000	1.778600
H	-2.571600	-2.929000	2.709700
H	-2.587900	-3.447600	1.022000
C	-2.568200	-0.938000	-0.076100
C	-1.409700	-1.363200	-1.005300
H	-1.475300	-0.869300	-1.977500
H	-1.452600	-2.440500	-1.175200
C	-0.110500	-1.017900	-0.229500
C	0.496700	0.260300	-0.642400
H	-0.123000	0.994300	-1.171300
C	-3.928700	-1.566900	-0.417700
O	-4.995100	-1.029500	-0.218200
O	-3.803800	-2.793500	-0.963000
C	-2.785300	0.591400	-0.194800
O	-2.506700	1.228700	-1.191200
O	-3.307100	1.127100	0.911100
C	-5.044800	-3.444000	-1.305900
H	-4.758200	-4.400700	-1.742000
H	-5.656800	-3.591200	-0.412800
H	-5.600400	-2.839300	-2.026100
C	-3.615500	2.534900	0.843600
H	-4.037000	2.783100	1.817000
H	-2.708500	3.113800	0.654100
H	-4.340400	2.719200	0.047700
H	0.643400	-1.807200	-0.306000
H	-2.576200	-0.717800	2.094900
Pt	2.214500	0.780900	-0.301800
Cl	3.413000	-0.286200	-1.956100
Cl	1.981300	2.096700	1.582000

36

1A-a4-TS2,Free Energies=-1882.568757

C	-2.096700	-2.648300	1.479600
O	-0.723200	-2.326700	1.205100
C	-0.556500	-0.914200	1.030500
C	-1.947500	-0.251900	1.229000
C	-2.720900	-1.349700	1.988600
H	-2.593000	-3.006400	0.567200
H	-2.100300	-3.457900	2.214900
H	0.230200	-0.554700	1.693600
H	-2.522900	-1.230900	3.059000
H	-3.804000	-1.302000	1.847700
C	-2.443000	0.114800	-0.232100
C	-1.542100	-0.714700	-1.192600
H	-1.485300	-0.273500	-2.187700
H	-1.917200	-1.739000	-1.263100
C	-0.245800	-0.671600	-0.434500
C	1.014500	-0.410900	-0.986400
H	1.041800	-0.256600	-2.067800
C	-3.948300	-0.128500	-0.414300
O	-4.799700	0.658600	-0.070100
O	-4.211500	-1.326500	-0.969700
C	-2.216200	1.616400	-0.562000
O	-1.956800	1.998300	-1.683200
O	-2.354300	2.406500	0.499500
C	-5.611000	-1.624200	-1.163100
H	-5.634800	-2.606500	-1.633900
H	-6.132300	-1.639800	-0.203000
H	-6.068800	-0.871500	-1.808600
C	-2.138700	3.815700	0.264200
H	-2.342600	4.298700	1.218900
H	-1.103600	3.981800	-0.041900
H	-2.820300	4.174300	-0.509800
H	-1.883700	0.661900	1.815200
Pt	2.614400	0.102600	-0.025800
Cl	3.935400	-1.606800	-0.886300
Cl	1.560400	1.909700	1.017900
H	0.861100	-1.611300	-0.823000

36
1A-a4-P,Free Energies=-1882.617817

C	-2.234000	-2.600600	1.655000
O	-0.838700	-2.312100	1.483400
C	-0.633500	-0.893300	1.329400
C	-2.030700	-0.226500	1.384300
C	-2.856800	-1.291200	2.133500
H	-2.671800	-2.937500	0.702900
H	-2.314100	-3.420300	2.375500
H	0.062100	-0.555800	2.096400
H	-2.683000	-1.169500	3.208500
H	-3.930900	-1.217700	1.957500
C	-2.423800	0.068000	-0.118800
C	-1.349400	-0.670900	-0.971500
H	-1.197000	-0.233900	-1.957000
H	-1.669100	-1.710300	-1.121900
C	-0.118100	-0.722400	-0.096300
C	1.180800	-1.167200	-0.516000
H	1.334100	-1.466600	-1.551000
C	-3.872400	-0.329400	-0.440000
O	-4.827900	0.130200	0.145900
O	-3.964600	-1.241100	-1.423400
C	-2.370800	1.565000	-0.499000
O	-2.910400	1.997900	-1.492100
O	-1.636700	2.312300	0.343100
C	-5.306500	-1.600500	-1.807000
H	-5.193000	-2.326600	-2.611700
H	-5.840900	-2.038300	-0.960300
H	-5.845200	-0.716000	-2.154400
C	-1.515400	3.706000	-0.018600
H	-0.911300	4.154800	0.769300
H	-1.025600	3.797700	-0.990700
H	-2.504200	4.167500	-0.063500
H	1.836800	-1.635100	0.215400
H	-2.006400	0.709600	1.939300
Pt	1.342100	0.894400	-0.359400
Cl	0.920500	1.321200	-2.604700
Cl	2.162600	0.983700	1.810100

(5). In Path 1A-*b*

36
1A-b-TS1,Free Energies=-1882.534918

C	0.479028	-2.029559	2.037248
O	0.945920	-0.796789	1.483224
C	0.003875	0.193045	1.894617
C	-1.366335	-0.463887	1.640678
C	-1.069818	-1.936092	2.049719
H	0.872614	-2.839340	1.416199
H	0.876968	-2.152872	3.054552
H	0.118756	0.408468	2.968313
H	-1.472686	-2.134634	3.046198
H	-1.538479	-2.661165	1.379687
C	-1.862799	-0.316539	0.172543
C	-0.894958	-0.915962	-0.895013
H	-1.402920	-0.954358	-1.863884
H	-0.641722	-1.952025	-0.643690
C	0.360272	-0.195851	-1.076471
C	1.335883	0.532880	-1.367891
H	0.455922	0.955907	-2.029012
C	-3.244609	-1.008288	0.045775
O	-3.874803	-1.475243	0.965068
O	-3.671250	-0.998548	-1.231558
C	-2.106311	1.162099	-0.206769
O	-1.705866	1.676555	-1.230639
O	-2.830465	1.795785	0.720783
C	-4.970505	-1.582031	-1.462448
H	-5.149739	-1.473911	-2.531629
H	-4.968812	-2.635516	-1.172809
H	-5.730003	-1.050621	-0.884447
C	-3.102739	3.191756	0.461065
H	-3.698455	3.529004	1.308356
H	-2.165920	3.749389	0.395401
H	-3.657108	3.298978	-0.473916
H	0.215898	1.107637	1.337593
H	-2.138977	-0.033773	2.278450
Pt	2.982029	1.442086	-1.448142
Cl	4.017594	0.050050	-2.981709
Cl	2.367832	3.082037	0.088566

36
1A-b-IN1,Free Energies=-1882.567059

C	-0.294564	-1.078517	2.791144
O	-0.031573	0.284730	2.465970
C	-1.271853	0.849619	2.068554
C	-2.109653	-0.295747	1.413632
C	-1.252960	-1.558738	1.694971
H	0.660308	-1.608061	2.804794
H	-0.760236	-1.151219	3.788453
H	-1.808985	1.240250	2.947189
H	-1.870669	-2.407286	1.995088
H	-0.668162	-1.864662	0.823097
C	-2.521684	-0.060434	-0.074260
C	-1.382723	-0.171321	-1.133311
H	-1.820967	0.020982	-2.116317
H	-1.000085	-1.193957	-1.142627
C	-0.229575	0.804446	-0.965501
C	0.990047	0.460557	-0.678736
H	-0.430176	1.866126	-1.121168
C	-3.585554	-1.116184	-0.459657
O	-3.920820	-2.058390	0.219193
O	-4.091405	-0.854400	-1.682125
C	-3.190262	1.320817	-0.199199
O	-2.770425	2.247963	-0.859787
O	-4.304976	1.384698	0.548930
C	-5.095089	-1.775276	-2.151946
H	-5.383392	-1.411602	-3.137983
H	-4.683225	-2.785313	-2.216590
H	-5.951825	-1.779245	-1.473699
C	-5.010775	2.641096	0.518645
H	-5.871690	2.504550	1.172502
H	-4.369113	3.445755	0.885563
H	-5.329727	2.871207	-0.500748
H	-1.055110	1.690589	1.405197
H	-3.052140	-0.387815	1.957193
Pt	2.662641	-0.020472	-0.286223
Cl	2.450819	-2.297451	0.011221
Cl	3.807456	1.967321	-0.377575

36

1A-b-TS2,Free Energies=-1882.55276

C	-0.800135	-0.673828	3.379233
O	-0.191312	0.503283	2.802654
C	-0.712540	0.745077	1.540316
C	-2.008085	-0.054198	1.408941
C	-1.685020	-1.283296	2.284204
H	-0.004754	-1.343081	3.719065
H	-1.382718	-0.350850	4.250705
H	-0.778540	1.821693	1.361794
H	-2.585508	-1.757220	2.678603
H	-1.116332	-2.030449	1.721546
C	-2.449841	-0.318468	-0.054544
C	-1.645083	-1.403217	-0.815036
H	-2.028364	-1.433433	-1.838395
H	-1.871989	-2.382843	-0.374296
C	-0.141701	-1.294104	-0.923062
C	0.809662	-0.548664	-0.417091
H	0.317378	-2.018447	-1.609854
C	-3.922261	-0.796026	-0.025440
O	-4.546647	-1.069066	0.974342
O	-4.421347	-0.884488	-1.271214
C	-2.424115	0.991475	-0.875796
O	-1.870067	1.134959	-1.940017
O	-3.118875	1.958652	-0.246390
C	-5.790272	-1.325834	-1.368030
H	-6.018065	-1.329103	-2.433539
H	-5.896405	-2.327845	-0.945292
H	-6.447848	-0.637426	-0.831918
C	-3.173570	3.228692	-0.928935
H	-3.775097	3.874290	-0.289594
H	-2.166859	3.634609	-1.053674
H	-3.638561	3.109925	-1.910413
H	0.025707	0.376692	0.742231
H	-2.808250	0.515023	1.892112
Pt	2.533944	0.017996	-0.243825
Cl	3.502280	-2.004383	-0.804175
Cl	2.343151	2.246877	0.342745

36

1A-a2-IN2,Free Energies=-1882.604887

C	1.383762	3.268063	-1.567840
O	0.348406	2.803851	-0.679924
C	0.789009	1.669397	0.023621
C	2.307472	1.518626	-0.226016
C	2.442004	2.160219	-1.623091
H	0.934210	3.488481	-2.540612
H	1.798021	4.199908	-1.159686
H	0.527948	1.790733	1.078596
H	3.448434	2.533743	-1.813728
H	2.203874	1.437921	-2.411637
C	2.591496	0.004898	-0.101764
C	1.347884	-0.676335	-0.738880
H	1.161622	-1.653142	-0.288919
H	1.509850	-0.842038	-1.806999
C	0.153013	0.321877	-0.563391
C	-0.860167	-0.220031	0.356466
H	-0.292751	0.576566	-1.525671
C	3.896097	-0.447127	-0.764859
O	4.696016	0.265943	-1.325811
O	4.024259	-1.783579	-0.650080
C	2.656760	-0.337692	1.397333
O	1.732817	-0.779777	2.048795
O	3.854507	-0.028079	1.914313
C	5.217083	-2.348603	-1.227149
H	5.146816	-3.420966	-1.046526
H	5.257567	-2.138593	-2.298749
H	6.104707	-1.931268	-0.745249
C	4.012764	-0.266123	3.328623
H	5.033754	0.036414	3.558913
H	3.293851	0.330240	3.895325
H	3.860532	-1.324492	3.552194
H	-0.508078	-0.603509	1.321140
H	2.889705	2.094595	0.500108
Pt	-2.655190	-0.314810	0.046642
Cl	-2.845551	-2.222680	-1.240934
Cl	-3.515410	1.532722	1.116039

(6). In Path 1A-*c*

36
1A-c-IN1,Free Energies=-1882.561849

C	0.759080	-1.609210	2.356441
O	1.081625	-0.245248	1.983268
C	-0.202016	0.432429	1.997002
C	-1.233740	-0.562677	1.405954
C	-0.528380	-1.940763	1.586945
H	1.609793	-2.235175	2.092602
H	0.605609	-1.622581	3.443559
H	-0.449209	0.630254	3.047688
H	-1.164641	-2.643875	2.128716
H	-0.264297	-2.399374	0.632763
C	-1.826329	-0.260293	-0.021137
C	-1.028404	-0.687267	-1.301317
H	-1.667944	-0.473945	-2.164140
H	-0.869867	-1.771177	-1.273716
C	0.273786	-0.055231	-1.582568
C	1.287257	0.363048	-2.217080
H	1.788555	0.764379	-3.078941
C	-3.163807	-1.049630	-0.108638
O	-3.529058	-1.892824	0.678103
O	-3.870190	-0.685966	-1.194787
C	-2.188207	1.233186	-0.161379
O	-1.948536	1.915868	-1.129138
O	-2.832028	1.677466	0.936102
C	-5.126379	-1.367707	-1.381357
H	-5.554492	-0.940941	-2.287923
H	-4.961209	-2.441536	-1.498225
H	-5.780941	-1.195609	-0.523660
C	-3.223159	3.065377	0.902926
H	-3.724848	3.246971	1.853220
H	-2.342331	3.703392	0.799769
H	-3.900485	3.247329	0.065078
H	-0.079083	1.381238	1.481900
H	-2.107145	-0.535172	2.057476
Pt	1.848103	0.098585	-0.233727
Cl	2.341732	-2.182883	-0.546495
Cl	1.816960	2.422546	0.100108

36
1A-c-TS1,Free Energies=-1882.489785

C	0.755085	-1.666427	2.348896
O	1.071017	-0.294702	2.011161
C	-0.208896	0.378300	2.031480
C	-1.239036	-0.605740	1.415916
C	-0.534266	-1.986356	1.575516
H	1.606713	-2.282498	2.064576
H	0.604545	-1.713658	3.435823
H	-0.467266	0.557012	3.083481
H	-1.171001	-2.696711	2.107186
H	-0.271451	-2.432590	0.615137
C	-1.821620	-0.276438	-0.010383
C	-1.014663	-0.670439	-1.289777
H	-1.654886	-0.494949	-2.159013
H	-0.776622	-1.738433	-1.267241
C	0.282341	0.013573	-1.550310
C	1.286060	0.359502	-2.341623
H	0.306860	1.213540	-1.963246
C	-3.163237	-1.053616	-0.128913
O	-3.540111	-1.913703	0.632279
O	-3.854282	-0.653429	-1.212093
C	-2.160263	1.222886	-0.117581
O	-1.788029	1.949851	-1.013395
O	-2.921454	1.625182	0.911175
C	-5.116281	-1.316861	-1.431736
H	-5.527853	-0.862693	-2.332501
H	-4.960125	-2.388843	-1.573701
H	-5.778913	-1.158382	-0.577798
C	-3.290240	3.021758	0.908239
H	-3.895628	3.160778	1.803353
H	-2.395513	3.647388	0.941258
H	-3.864549	3.256978	0.009287
H	-0.084276	1.337865	1.535219
H	-2.119074	-0.589343	2.059391
Pt	1.873548	0.112195	-0.242090
Cl	2.324188	-2.169882	-0.605831
Cl	1.789065	2.417347	0.135858

36

1A-c-IN2,Free Energies=-1882.509683

C	0.525015	-1.356855	2.573079
O	0.932153	-0.064322	2.087869
C	-0.288392	0.672988	1.912905
C	-1.366236	-0.344595	1.436978
C	-0.711081	-1.721525	1.742231
H	1.363909	-2.040223	2.441250
H	0.285567	-1.269777	3.643235
H	-0.582181	1.089763	2.886189
H	-1.399259	-2.380633	2.274197
H	-0.393108	-2.235897	0.833462
C	-1.926665	-0.150501	-0.014806
C	-0.992073	-0.483201	-1.224144
H	-1.603311	-0.385280	-2.129947
H	-0.665315	-1.523224	-1.162614
C	0.201791	0.417565	-1.466770
C	1.380194	0.086362	-2.137293
H	-0.024749	1.491532	-1.469356
C	-3.158577	-1.085466	-0.161466
O	-3.511662	-1.914326	0.643782
O	-3.796131	-0.851354	-1.325335
C	-2.467171	1.288326	-0.156323
O	-2.101898	2.102642	-0.977540
O	-3.408357	1.538964	0.769054
C	-4.964305	-1.659357	-1.572306
H	-5.343349	-1.331375	-2.539820
H	-4.693704	-2.717531	-1.600118
H	-5.707620	-1.497792	-0.788012
C	-3.989032	2.859031	0.733193
H	-4.721506	2.873058	1.539696
H	-3.218309	3.616189	0.895128
H	-4.469635	3.033808	-0.232180
H	-0.079600	1.501836	1.236606
H	-2.241742	-0.227666	2.077527
Pt	2.036108	0.047521	-0.297827
Cl	2.193545	-2.292856	-0.296592
Cl	2.294918	2.332097	0.046650

(7). In Path 1B-*a1*

36
1B-a1-IN1,Free Energies=-6105.004997

C	-1.991949	-1.234520	3.465359
O	-1.454945	0.079478	3.311717
C	-2.311721	0.754129	2.394773
C	-2.873564	-0.325365	1.415520
C	-2.394585	-1.659532	2.047303
H	-1.218898	-1.861161	3.916615
H	-2.865118	-1.211471	4.137759
H	-3.143262	1.227474	2.937695
H	-3.177525	-2.420559	2.027382
H	-1.519776	-2.064778	1.530980
C	-2.520259	-0.115856	-0.088722
C	-1.080724	-0.523165	-0.543915
H	-0.925120	-0.126047	-1.548590
H	-1.007664	-1.614494	-0.617766
C	0.019856	-0.073024	0.324543
C	0.691152	0.231176	1.349713
H	0.838363	0.536387	2.369187
C	-3.488858	-0.969628	-0.941133
O	-4.273034	-1.781562	-0.507392
O	-3.327664	-0.700896	-2.249934
C	-2.749197	1.360603	-0.467545
O	-1.907292	2.108409	-0.908050
O	-4.023784	1.719177	-0.220714
C	-4.165501	-1.451128	-3.151707
H	-3.899547	-1.103922	-4.149665
H	-3.969784	-2.521141	-3.048530
H	-5.219212	-1.255021	-2.939401
C	-4.357693	3.085344	-0.537853
H	-5.411402	3.192578	-0.281364
H	-3.743318	3.772387	0.048993
H	-4.194968	3.277284	-1.601083
H	-1.725669	1.543571	1.916620
H	-3.963218	-0.290745	1.458118
Pt	2.086560	-0.018770	-0.154433
Br	2.590017	2.360336	-0.229128
Br	2.142168	-2.459974	-0.374136

36
1B-a1-TS1,Free Energies=-6104.985998

C	-1.846257	-1.898234	2.990020
O	-1.720868	-0.506885	3.390178
C	-2.120171	0.321489	2.370190
C	-2.873254	-0.486743	1.317465
C	-2.272272	-1.898672	1.513795
H	-0.884247	-2.388571	3.158946
H	-2.595843	-2.351405	3.648164
H	-2.605149	1.220757	2.765593
H	-3.001818	-2.676606	1.286133
H	-1.400727	-2.056361	0.871637
C	-2.701793	0.150724	-0.083287
C	-1.199729	0.249918	-0.507201
H	-1.093581	1.061288	-1.231651
H	-0.893959	-0.684120	-0.992229
C	-0.250724	0.460786	0.605265
C	0.898300	0.369770	1.187744
H	1.174737	0.521901	2.226114
C	-3.469893	-0.663173	-1.138141
O	-4.136476	-1.646061	-0.910049
O	-3.289055	-0.129146	-2.357305
C	-3.294667	1.574891	-0.028504
O	-2.639578	2.587779	0.066580
O	-4.637182	1.535592	-0.042266
C	-3.949411	-0.809238	-3.444673
H	-3.683759	-0.247970	-4.339816
H	-3.596106	-1.840582	-3.514636
H	-5.030861	-0.805851	-3.289090
C	-5.303006	2.813822	0.035442
H	-6.367937	2.586597	0.001056
H	-5.043489	3.320002	0.968317
H	-5.010979	3.442086	-0.809045
H	-1.185291	0.771600	1.818771
H	-3.941859	-0.498061	1.555538
Pt	2.258886	-0.066514	-0.154694
Br	3.351988	2.109523	-0.150158
Br	1.523736	-2.396063	-0.482513

36

1B-a1-IN2,Free Energies=-6105.053564

C	-1.512486	2.825665	-2.071811
O	-0.738660	1.667294	-2.413903
C	-1.471283	0.495562	-2.056396
C	-2.677408	0.942565	-1.179707
C	-2.322894	2.410358	-0.846423
H	-0.813673	3.644513	-1.886182
H	-2.164945	3.100742	-2.914860
H	-1.777849	-0.028929	-2.969219
H	-3.211288	3.020503	-0.678854
H	-1.697610	2.476019	0.049511
C	-2.709885	-0.059796	0.010386
C	-1.215985	-0.376223	0.266079
H	-1.074510	-1.304668	0.820172
H	-0.760927	0.434009	0.842910
C	-0.596729	-0.436837	-1.147578
C	0.839201	-0.129550	-1.299151
H	1.212472	0.048207	-2.313127
C	-3.425469	0.473940	1.254925
O	-4.036805	1.514378	1.338451
O	-3.276272	-0.396559	2.273354
C	-3.437342	-1.334840	-0.453213
O	-2.892882	-2.337104	-0.865239
O	-4.771384	-1.180063	-0.394310
C	-3.914004	-0.024079	3.509299
H	-3.686820	-0.829667	4.207229
H	-3.513934	0.925781	3.872325
H	-4.993175	0.071984	3.365195
C	-5.554198	-2.305413	-0.838343
H	-6.593304	-2.001967	-0.713360
H	-5.338955	-2.528226	-1.886327
H	-5.330720	-3.185506	-0.230660
H	-0.696909	-1.473234	-1.516949
H	-3.615829	0.912442	-1.740940
Pt	2.100534	-0.083671	0.019425
Br	2.098701	2.218403	0.796462
Br	2.870877	-2.383757	0.111616

36

1B-a1-TS2,Free Energies=-6105.024835

C	-2.200970	3.741828	-1.232027
O	-1.036564	2.965643	-1.552542
C	-1.430097	1.602572	-1.680794
C	-2.839486	1.442767	-1.039337
C	-3.072406	2.819993	-0.378211
H	-1.859843	4.641915	-0.715806
H	-2.717269	4.036545	-2.157724
H	-1.383672	1.273909	-2.724406
H	-4.127843	3.099898	-0.370189
H	-2.714684	2.831149	0.658125
C	-2.713395	0.242378	-0.055518
C	-1.229676	0.305276	0.410824
H	-0.818301	-0.623521	0.815296
H	-1.098386	1.065193	1.194373
C	-0.491036	0.791530	-0.791082
C	0.840193	0.505511	-1.111666
H	1.235672	0.995390	-2.004860
C	-3.763321	0.287518	1.051911
O	-4.920955	0.586292	0.855995
O	-3.250768	-0.039237	2.247802
C	-2.828156	-1.064206	-0.857257
O	-2.381676	-1.169730	-1.983431
O	-3.377739	-2.056937	-0.159730
C	-4.190409	-0.075115	3.340794
H	-3.603448	-0.345707	4.217829
H	-4.658024	0.903682	3.471541
H	-4.964068	-0.821353	3.145194
C	-3.381044	-3.353759	-0.802158
H	-3.872629	-4.020664	-0.095248
H	-3.933598	-3.305184	-1.742703
H	-2.353664	-3.672232	-0.991262
H	0.146001	-0.406258	-1.509503
H	-3.600783	1.246265	-1.795667
Pt	2.136227	-0.304047	0.090175
Br	3.279638	1.745679	0.735543
Br	1.212912	-2.572803	-0.244864

36

1B-a1-P,Free Energies=-6105.062851

C	-0.733491	-2.379254	-2.525798
O	0.174919	-1.714483	-1.647861
C	-0.461835	-1.612262	-0.379496
C	-2.009189	-1.583570	-0.664273
C	-2.085133	-1.746266	-2.204102
H	-0.387853	-2.206220	-3.547551
H	-0.732435	-3.463744	-2.330318
H	-0.156711	-2.450643	0.260543
H	-2.944948	-2.342381	-2.515504
H	-2.158772	-0.776400	-2.702284
C	-2.508362	-0.220863	-0.077074
C	-1.252851	0.693336	-0.133558
H	-1.327722	1.567442	0.511099
H	-1.104620	1.035705	-1.161531
C	-0.145599	-0.266119	0.275276
C	0.503866	-0.164927	1.554423
H	0.820607	-1.067116	2.073066
C	-3.719979	0.384002	-0.800409
O	-4.410161	-0.162042	-1.629229
O	-3.929427	1.639705	-0.355559
C	-2.936363	-0.429816	1.389398
O	-2.306674	-0.082976	2.365401
O	-4.109817	-1.082688	1.453589
C	-5.059741	2.323247	-0.929188
H	-5.073255	3.306116	-0.458724
H	-4.939488	2.414524	-2.011468
H	-5.981938	1.777103	-0.715315
C	-4.608263	-1.350386	2.778891
H	-5.557849	-1.864158	2.631705
H	-3.906558	-1.983217	3.327887
H	-4.752758	-0.415526	3.325646
H	0.299030	0.695224	2.183990
H	-2.519474	-2.418171	-0.177855
Pt	1.904758	0.331090	0.096350
Br	3.051526	-1.815363	0.272714
Br	1.480033	2.721179	-0.198541

(8). In Path 1B-*a2*

36
1B-a2-IN1,Free Energies=-6105.000861

C	-4.259396	-1.598117	-2.315510
O	-3.418507	-2.609792	-1.758467
C	-2.344339	-1.958074	-1.097876
C	-3.023537	-0.766873	-0.399045
C	-4.021018	-0.305675	-1.491303
H	-4.013807	-1.439561	-3.376424
H	-5.290464	-1.959697	-2.256431
H	-1.883923	-2.667583	-0.408601
H	-4.945292	0.086647	-1.056762
H	-3.599997	0.483043	-2.124394
C	-2.132156	0.350637	0.221139
C	-1.146050	1.052809	-0.762863
H	-0.797398	1.983304	-0.308688
H	-1.681576	1.334485	-1.676427
C	0.049175	0.302441	-1.185166
C	0.904473	-0.253277	-1.932848
H	1.249482	-0.746176	-2.824446
C	-3.128841	1.387742	0.794337
O	-3.803049	1.178593	1.777516
O	-3.195737	2.511263	0.059883
C	-1.338734	-0.112127	1.467224
O	-0.463696	0.568989	1.962569
O	-1.738459	-1.292035	1.939710
C	-4.128718	3.504932	0.532251
H	-4.043211	4.336562	-0.166652
H	-5.143640	3.100314	0.534238
H	-3.863456	3.818642	1.544258
C	-1.075394	-1.747393	3.140285
H	-1.591567	-2.665760	3.418480
H	-0.022616	-1.942413	2.927413
H	-1.167473	-0.994072	3.925476
H	-1.584692	-1.629195	-1.824065
H	-3.602177	-1.179190	0.431162
Pt	1.890472	-0.005439	-0.151422
Br	2.510811	2.347925	-0.358366
Br	1.756268	-2.390593	0.397776

36
1B-a2-TS1,Free Energies=-6104.984773

C	-4.071085	-1.201460	2.961003
O	-2.977925	-0.339657	3.359544
C	-2.440431	0.294760	2.264447
C	-3.368521	0.118485	1.065348
C	-4.076185	-1.209963	1.429007
H	-3.910849	-2.186440	3.407317
H	-4.988847	-0.771378	3.378466
H	-2.120578	1.307485	2.511702
H	-5.083160	-1.259834	1.011297
H	-3.512557	-2.071239	1.053049
C	-2.638210	0.116198	-0.302106
C	-1.374471	-0.798350	-0.255338
H	-0.840857	-0.716718	-1.207224
H	-1.664540	-1.849045	-0.147853
C	-0.432870	-0.407859	0.803519
C	0.715063	-0.088748	1.312269
H	0.936709	0.216208	2.331102
C	-3.633588	-0.332187	-1.390664
O	-4.791928	0.023982	-1.400052
O	-3.073690	-1.131296	-2.303201
C	-2.162561	1.516407	-0.762424
O	-1.919964	1.766476	-1.920596
O	-2.017637	2.374468	0.255282
C	-3.919369	-1.510285	-3.409359
H	-3.304202	-2.157875	-4.032812
H	-4.802762	-2.040648	-3.046205
H	-4.229247	-0.619845	-3.960595
C	-1.438335	3.660115	-0.088695
H	-1.530370	4.264147	0.813441
H	-0.388652	3.520266	-0.357565
H	-1.988410	4.106224	-0.918847
H	-1.423431	-0.243643	1.971099
H	-4.100836	0.931887	1.061662
Pt	2.168635	-0.157348	0.011405
Br	2.324158	-2.588650	-0.181429
Br	2.392746	2.284339	-0.117071

36

1B-a2-IN2,Free Energies=-6105.050569

C	-3.057413	3.839081	-0.528953
O	-1.662224	3.533994	-0.534943
C	-1.499149	2.194979	-0.997216
C	-2.876853	1.480192	-0.832440
C	-3.733843	2.536365	-0.101053
H	-3.211113	4.673006	0.161079
H	-3.389597	4.149470	-1.532584
H	-1.160167	2.200146	-2.040590
H	-4.789704	2.473870	-0.371851
H	-3.659187	2.426472	0.987225
C	-2.580125	0.175680	-0.038007
C	-1.362357	0.562139	0.850904
H	-0.824739	-0.299491	1.249284
H	-1.718067	1.153974	1.698188
C	-0.487498	1.464735	-0.067482
C	0.604583	0.762127	-0.792613
H	0.702779	0.900465	-1.873618
C	-3.800032	-0.332077	0.731873
O	-4.939137	-0.241256	0.329104
O	-3.454944	-0.895107	1.902480
C	-2.116504	-0.892217	-1.038670
O	-1.325517	-0.646375	-1.933580
O	-2.648433	-2.093275	-0.822013
C	-4.539005	-1.461738	2.661601
H	-4.081973	-1.860588	3.566958
H	-5.277173	-0.693434	2.904870
H	-5.023816	-2.256857	2.089753
C	-2.209862	-3.154007	-1.703005
H	-2.770672	-4.033364	-1.388475
H	-2.437745	-2.897118	-2.739701
H	-1.135807	-3.308273	-1.583508
H	0.022606	2.223065	0.547113
H	-3.321141	1.250031	-1.803332
Pt	1.961102	-0.184127	-0.004635
Br	1.279904	-2.518309	-0.002460
Br	3.500096	1.602456	0.576538

36

1B-a2-TS2,Free Energies=-6105.023184

C	-2.064336	-1.510597	3.323432
O	-1.166387	-0.375973	3.254696
C	-1.493684	0.400731	2.120918
C	-2.803553	-0.145553	1.511681
C	-2.722657	-1.624729	1.944254
H	-1.477347	-2.389596	3.602239
H	-2.805698	-1.319362	4.110146
H	-1.535367	1.463573	2.391606
H	-3.700778	-2.105661	1.968640
H	-2.087824	-2.203005	1.261844
C	-2.703614	0.180371	-0.007980
C	-1.179688	0.112581	-0.327113
H	-0.845414	0.895560	-1.014023
H	-0.879076	-0.835877	-0.792330
C	-0.477135	0.251023	0.984128
C	0.896519	0.099352	1.197055
H	1.253369	0.285950	2.212746
C	-3.548053	-0.741256	-0.889926
O	-4.406606	-1.497057	-0.494873
O	-3.200507	-0.589881	-2.179347
C	-3.164599	1.640842	-0.171271
O	-2.451107	2.590861	0.070402
O	-4.448880	1.729656	-0.538345
C	-3.938723	-1.388510	-3.125404
H	-3.516954	-1.145550	-4.100114
H	-3.813422	-2.450846	-2.903279
H	-5.000477	-1.133138	-3.085844
C	-4.976898	3.068043	-0.659281
H	-6.015230	2.940959	-0.963328
H	-4.912888	3.586922	0.299946
H	-4.415724	3.627185	-1.411289
H	0.374067	-0.995393	1.257856
H	-3.684444	0.319992	1.962954
Pt	2.234042	-0.082189	-0.200603
Br	1.550524	-2.441046	-0.557718
Br	3.113886	2.182600	-0.169539

36

1B-a2-P,Free Energies=-6105.065881

C	1.889503	3.799242	-0.598140
O	0.743866	3.065585	-1.036269
C	0.515370	2.025972	-0.075194
C	1.890791	1.714153	0.592974
C	2.850736	2.731930	-0.071522
H	2.267993	4.363112	-1.454610
H	1.605733	4.508475	0.194999
H	-0.247170	2.332876	0.640647
H	3.593605	3.120490	0.629310
H	3.388597	2.281732	-0.914205
C	2.189113	0.218903	0.272555
C	1.403508	-0.031122	-1.041101
H	1.257728	-1.080669	-1.286390
H	1.961051	0.430338	-1.868733
C	0.130858	0.780139	-0.884753
C	-0.959167	0.762808	-1.817250
H	-1.550191	1.665467	-1.953247
C	3.692970	-0.051118	0.210017
O	4.446257	0.199521	1.125307
O	4.083644	-0.573668	-0.966640
C	1.598000	-0.682737	1.372870
O	0.762300	-0.327427	2.176515
O	2.094318	-1.924154	1.290279
C	5.488196	-0.875723	-1.070818
H	5.624236	-1.282118	-2.072921
H	6.084362	0.029846	-0.934113
H	5.772665	-1.609602	-0.312955
C	1.556240	-2.886530	2.221521
H	2.152893	-3.787249	2.079648
H	1.648390	-2.514496	3.244115
H	0.507345	-3.079355	1.986088
H	-0.915954	0.091499	-2.672791
H	1.846823	1.864834	1.671526
Pt	-1.635982	-0.277025	-0.147495
Br	-2.883509	1.570476	0.848424
Br	-1.056814	-2.549950	-0.872773

(9). In Path 1B-*a3*

36
1B-a3-TS1,Free Energies=-6104.992817

C	-4.608970	-1.850379	-1.538966
O	-3.417977	-2.105952	-2.294391
C	-2.362921	-1.260555	-1.850040
C	-2.780671	-0.779625	-0.445096
C	-4.306266	-0.642790	-0.648151
H	-5.441698	-1.670485	-2.229304
H	-4.848504	-2.740799	-0.940900
H	-1.438596	-1.844675	-1.843960
H	-4.863775	-0.657286	0.292118
H	-4.542636	0.288436	-1.176420
C	-2.027504	0.460313	0.180861
C	-1.019569	1.180700	-0.769953
H	-0.648615	2.078533	-0.268176
H	-1.544826	1.511460	-1.671583
C	0.151645	0.406358	-1.210858
C	0.985583	-0.166565	-1.968462
H	1.336245	-0.603189	-2.886704
C	-3.076888	1.501307	0.644415
O	-3.626992	1.472908	1.721503
O	-3.325734	2.429616	-0.298785
C	-1.275511	0.115775	1.494090
O	-0.349464	0.786429	1.904563
O	-1.777883	-0.940159	2.130950
C	-4.303644	3.428085	0.059167
H	-4.363107	4.094994	-0.800578
H	-5.270393	2.958009	0.254300
H	-3.979764	3.969993	0.950507
C	-1.153827	-1.268823	3.390077
H	-1.735725	-2.099543	3.788274
H	-0.117344	-1.567493	3.220523
H	-1.191252	-0.408284	4.061363
H	-2.241354	-0.420047	-2.552382
H	-2.622383	-1.617238	0.235683
Pt	1.911952	-0.118359	-0.136000
Br	1.363731	-2.449602	0.397481
Br	2.894472	2.108862	-0.316281

36
1B-a3-IN2,Free Energies=-6105.004122

C	-4.235755	-2.138033	-1.369282
O	-3.919112	-1.281416	-2.471620
C	-2.969500	-0.299871	-2.067659
C	-2.534821	-0.660728	-0.625612
C	-3.792652	-1.390499	-0.112038
H	-5.310486	-2.347702	-1.394050
H	-3.698036	-3.093224	-1.472657
H	-2.125494	-0.311147	-2.769550
H	-3.583841	-2.050532	0.729929
H	-4.562770	-0.676257	0.199711
C	-1.980847	0.537621	0.209613
C	-0.937989	1.366076	-0.606466
H	-0.541724	2.164489	0.027033
H	-1.436694	1.839305	-1.458483
C	0.194006	0.597670	-1.145609
C	0.978647	0.044695	-1.967521
H	1.296619	-0.317542	-2.929008
C	-3.129680	1.467102	0.657407
O	-3.720070	1.348374	1.707401
O	-3.420325	2.409118	-0.260266
C	-1.294318	0.104151	1.530078
O	-0.432450	0.773176	2.062683
O	-1.756078	-1.048135	2.013680
C	-4.501664	3.299797	0.086691
H	-4.584008	3.992952	-0.749956
H	-5.428427	2.736386	0.217185
H	-4.268938	3.831266	1.012109
C	-1.172156	-1.482428	3.259968
H	-1.721187	-2.382895	3.533965
H	-0.113304	-1.705809	3.114404
H	-1.290059	-0.706823	4.019536
H	-3.437293	0.693333	-2.112716
H	-1.720263	-1.392561	-0.684209
Pt	1.931138	-0.140746	-0.155836
Br	1.253113	-2.477465	0.152521
Br	3.036653	2.032400	-0.113677

36

1B-a3-TS2,Free Energies=-6104.962431

C	-3.593731	0.363073	3.089414
O	-2.884984	-0.932881	3.056408
C	-2.440323	-1.147772	1.813574
C	-2.665027	0.096296	0.972033
C	-3.947753	0.635874	1.617029
H	-4.440172	0.213129	3.760625
H	-2.919834	1.117510	3.506890
H	-1.107892	-1.345245	1.712016
H	-4.099869	1.695454	1.405991
H	-4.844218	0.080638	1.319203
C	-2.408685	-0.209535	-0.516649
C	-1.124313	-1.139207	-0.535353
H	-0.475593	-0.849828	-1.365364
H	-1.429105	-2.174739	-0.709276
C	-0.332223	-1.037507	0.725359
C	0.807383	-0.597679	1.224621
H	1.024360	-0.583940	2.292396
C	-3.654414	-0.861703	-1.137006
O	-4.512416	-0.242313	-1.722534
O	-3.727484	-2.185186	-0.882119
C	-2.114281	1.049043	-1.359416
O	-1.628615	0.982991	-2.463569
O	-2.445681	2.181091	-0.727364
C	-4.890593	-2.855503	-1.415489
H	-4.774642	-3.902175	-1.135897
H	-5.802472	-2.434672	-0.985231
H	-4.920201	-2.744239	-2.501343
C	-2.098986	3.399970	-1.426046
H	-2.504859	4.206069	-0.815261
H	-1.011778	3.474813	-1.496579
H	-2.544914	3.400076	-2.422452
H	-2.676071	-2.144987	1.433101
H	-1.878212	0.801835	1.259616
Pt	2.201804	0.064370	0.057160
Br	1.412161	2.397642	0.213047
Br	3.303150	-2.067136	-0.387788

36

1B-a3-IN3,Free Energies=-6105.030427

C	-2.592440	0.366385	3.240370
O	-1.542044	-0.617426	2.997666
C	-1.740576	-1.058145	1.671785
C	-2.175510	0.188109	0.921186
C	-3.252319	0.715130	1.864538
H	-3.316607	-0.052952	3.947980
H	-2.115181	1.235444	3.702227
H	-0.352637	-2.634330	1.018565
H	-3.446116	1.784794	1.758023
H	-4.198002	0.176423	1.738933
C	-2.252437	-0.253638	-0.562610
C	-1.133509	-1.376530	-0.626452
H	-0.362659	-1.092904	-1.343885
H	-1.565789	-2.321190	-0.962037
C	-0.558300	-1.567890	0.814367
C	0.710593	-0.900708	1.190438
H	0.996411	-0.982614	2.245834
C	-3.633195	-0.777035	-0.975557
O	-4.338427	-0.271075	-1.818864
O	-3.987822	-1.880267	-0.278165
C	-1.926323	0.892280	-1.535025
O	-1.256236	0.769620	-2.534810
O	-2.481060	2.044047	-1.127525
C	-5.274318	-2.435504	-0.616659
H	-5.394146	-3.304983	0.029664
H	-6.065292	-1.704152	-0.434014
H	-5.295050	-2.728997	-1.668854
C	-2.247905	3.176972	-1.985905
H	-2.794354	4.002808	-1.530258
H	-1.178878	3.398492	-2.031483
H	-2.623162	2.971506	-2.991065
H	-2.523444	-1.829187	1.635350
H	-1.332100	0.889128	0.974531
Pt	1.889778	-0.000337	0.130634
Br	1.335505	2.347822	0.430224
Br	3.220680	-1.775158	-0.847030

36

1B-a3-TS3,Free Energies=-6105.007192

C	2.707672	-0.902238	3.538508
O	1.431559	-0.272459	3.203869
C	1.584876	0.246731	1.916590
C	2.541299	-0.700207	1.185747
C	3.608610	-0.867294	2.263002
H	3.156583	-0.362977	4.378615
H	2.485608	-1.925513	3.854936
H	-0.534867	1.407131	1.126957
H	4.200512	-1.778125	2.149819
H	4.290859	-0.010555	2.288651
C	2.614612	-0.083268	-0.232037
C	1.107432	0.332532	-0.447241
H	0.575541	-0.368017	-1.097807
H	1.012236	1.325612	-0.897446
C	0.464780	0.286752	0.931407
C	-0.901464	0.238614	1.213769
H	-1.167839	0.101540	2.265075
C	3.529117	1.148027	-0.268477
O	3.152819	2.289241	-0.108923
O	4.810988	0.792175	-0.444267
C	3.067732	-1.112589	-1.271199
O	3.429279	-2.237573	-1.013473
O	2.976080	-0.598156	-2.508193
C	5.763999	1.875191	-0.482403
H	6.733106	1.400917	-0.633394
H	5.529867	2.553052	-1.306406
H	5.745165	2.430681	0.458181
C	3.349311	-1.483514	-3.584064
H	3.201744	-0.907252	-4.496828
H	4.394324	-1.784793	-3.478487
H	2.713528	-2.371924	-3.579470
H	2.030318	1.258417	1.940352
H	2.034517	-1.666438	1.063225
Pt	-2.315792	0.044651	-0.096440
Br	-2.431004	-2.390568	-0.117340
Br	-2.391941	2.492202	-0.400586

36

1B-a3-P,Free Energies=-6105.047761

C	-0.962520	-3.526604	0.281402
O	-0.133139	-2.821227	-0.689141
C	-0.740159	-1.585300	-0.915263
C	-1.562907	-1.251479	0.316995
C	-2.181460	-2.615597	0.610746
H	-1.256224	-4.488109	-0.150755
H	-0.344460	-3.708025	1.166294
H	1.277292	0.783717	-2.599366
H	-2.517767	-2.738543	1.643124
H	-3.022089	-2.835610	-0.057740
C	-2.243466	0.081178	-0.087756
C	-1.194131	0.715092	-1.091709
H	-0.859026	1.700792	-0.778254
H	-1.672514	0.820979	-2.072997
C	-0.039169	-0.290766	-1.224331
C	1.143436	-0.122980	-2.013311
H	1.643683	-1.012284	-2.392099
C	-3.576933	-0.180117	-0.797167
O	-3.723840	-0.261429	-1.998214
O	-4.563906	-0.377796	0.093302
C	-2.458473	0.994514	1.123733
O	-2.135232	0.735703	2.260488
O	-3.023253	2.154327	0.740109
C	-5.861453	-0.665040	-0.462362
H	-6.522384	-0.789159	0.395118
H	-6.194985	0.163218	-1.092210
H	-5.826465	-1.579394	-1.059811
C	-3.232418	3.121137	1.787092
H	-3.698755	3.978120	1.301362
H	-3.887079	2.708664	2.558780
H	-2.277552	3.404514	2.236566
H	-1.427141	-1.676600	-1.785559
H	-0.871540	-1.008743	1.131802
Pt	1.760080	0.214866	-0.052922
Br	2.494602	-1.911272	0.845624
Br	1.684359	2.655159	-0.352398

(10). In Path 1B-*a4*

36
1B-a4-IN1,Free Energies=-6104.999976

C	-1.619800	-2.414100	2.624000
O	-0.888700	-1.293600	3.124600
C	-0.629100	-0.439700	2.023900
C	-1.956800	-0.437800	1.245200
C	-2.390500	-1.922700	1.370400
H	-0.930800	-3.231300	2.364600
H	-2.276700	-2.761200	3.426700
H	-0.338600	0.539600	2.406200
H	-3.474600	-2.012400	1.488100
H	-2.111000	-2.510000	0.489500
C	-1.976600	0.144400	-0.200700
C	-0.972900	-0.515200	-1.206400
H	-1.393400	-0.441700	-2.214700
H	-0.866400	-1.581700	-0.994100
C	0.362600	0.095800	-1.321500
C	1.313000	0.743200	-1.845900
H	1.747900	1.451100	-2.529000
C	-3.432200	-0.054100	-0.685100
O	-4.358000	0.603800	-0.266400
O	-3.562300	-1.059400	-1.568500
C	-1.777600	1.675600	-0.266800
O	-1.654100	2.259000	-1.323700
O	-1.762300	2.264900	0.930300
C	-4.908400	-1.319100	-2.016900
H	-4.824800	-2.151800	-2.714800
H	-5.544800	-1.584200	-1.169400
H	-5.317500	-0.435500	-2.512000
C	-1.583300	3.696700	0.918000
H	-1.655800	4.003400	1.960900
H	-0.600800	3.944100	0.509700
H	-2.363600	4.167400	0.316200
H	0.199900	-0.836700	1.411900
H	-2.659800	0.170700	1.819900
Pt	2.197100	-0.166300	-0.235900
Br	2.375000	-2.483800	-0.992400
Br	2.474300	1.983300	0.894200

36
1B-a4-TS1,Free Energies=-6104.980367

C	-1.408400	-2.669100	2.059900
O	-0.569800	-1.610400	2.534000
C	-0.787400	-0.512400	1.708800
C	-2.272200	-0.505600	1.313800
C	-2.699800	-1.985600	1.564500
H	-0.893900	-3.204000	1.248200
H	-1.560200	-3.362200	2.889900
H	-0.402400	0.392900	2.181200
H	-3.482000	-2.020600	2.326700
H	-3.096600	-2.478400	0.670900
C	-2.513200	0.017500	-0.126100
C	-1.608500	-0.718400	-1.155800
H	-1.864500	-0.333700	-2.155900
H	-1.807300	-1.794500	-1.158700
C	-0.191500	-0.427000	-1.031500
C	1.013600	-0.086600	-1.321500
H	1.225000	0.180700	-2.367200
C	-4.011100	-0.150000	-0.447100
O	-4.880800	0.348200	0.230600
O	-4.233500	-0.905800	-1.534300
C	-2.239400	1.534500	-0.298600
O	-2.227200	2.054300	-1.393900
O	-2.033800	2.163000	0.856700
C	-5.620700	-1.076600	-1.898300
H	-5.610400	-1.709800	-2.784900
H	-6.168600	-1.554700	-1.083300
H	-6.071600	-0.106400	-2.117800
C	-1.724500	3.575200	0.767700
H	-1.778700	3.943000	1.791600
H	-0.715200	3.696800	0.368600
H	-2.451700	4.078100	0.128200
H	-2.824300	0.156000	1.983100
Pt	2.578000	0.022700	-0.185700
Br	3.447500	-2.188600	-0.748700
Br	2.113100	2.262100	0.705900
H	-0.165000	-0.629100	0.761800

36

1B-a4-IN2,Free Energies=-6105.045505

C	-1.587900	-2.383900	2.200700
O	-0.495500	-1.469000	2.317400
C	-0.707300	-0.438000	1.390600
C	-2.246100	-0.206900	1.304600
C	-2.826500	-1.511200	1.925800
H	-1.404200	-3.093400	1.378600
H	-1.637800	-2.949800	3.133500
H	-0.137400	0.425000	1.735700
H	-3.337200	-1.267900	2.861600
H	-3.542600	-2.017700	1.275600
C	-2.537800	0.064300	-0.201700
C	-1.568900	-0.887800	-0.936500
H	-1.425000	-0.589100	-1.977400
H	-1.978300	-1.899700	-0.933400
C	-0.260500	-0.858000	-0.103200
C	0.757100	0.065700	-0.647700
H	0.449300	0.812400	-1.389200
C	-4.018900	-0.109800	-0.572500
O	-4.836800	0.782400	-0.539500
O	-4.311800	-1.375300	-0.933500
C	-2.195800	1.528400	-0.575200
O	-1.692100	1.844000	-1.635000
O	-2.513700	2.397600	0.386800
C	-5.689500	-1.610600	-1.290000
H	-5.742200	-2.665600	-1.558000
H	-6.345000	-1.390900	-0.443800
H	-5.972500	-0.980300	-2.136100
C	-2.296000	3.789200	0.074000
H	-2.624800	4.336200	0.956900
H	-1.237400	3.972200	-0.124100
H	-2.886600	4.071100	-0.800400
H	0.193700	-1.849200	-0.004300
H	-2.543900	0.656500	1.897900
Pt	2.519400	0.119600	-0.167000
Br	3.525800	-1.622900	-1.523900
Br	2.583700	1.864400	1.528400

36

1B-a4-TS2,Free Energies=-6105.013739

C	-2.093700	-2.649300	1.463600
O	-0.720900	-2.329100	1.185000
C	-0.553000	-0.916500	1.017500
C	-1.942500	-0.253600	1.226600
C	-2.710400	-1.353600	1.988300
H	-2.596200	-2.996200	0.550300
H	-2.095800	-3.466100	2.190900
H	0.239000	-0.563900	1.679200
H	-2.500300	-1.242100	3.057100
H	-3.794700	-1.301700	1.859300
C	-2.449400	0.115600	-0.230500
C	-1.544400	-0.697800	-1.201100
H	-1.492300	-0.245100	-2.191400
H	-1.912800	-1.723800	-1.284100
C	-0.247200	-0.659200	-0.445200
C	1.012000	-0.387600	-0.991000
H	1.038200	-0.207700	-2.068600
C	-3.953400	-0.142400	-0.402900
O	-4.809800	0.625500	-0.028400
O	-4.208700	-1.328500	-0.985800
C	-2.241800	1.620800	-0.556000
O	-2.011900	2.010800	-1.680700
O	-2.358600	2.404800	0.513100
C	-5.606700	-1.638900	-1.170300
H	-5.623900	-2.606600	-1.670800
H	-6.114600	-1.691200	-0.204300
H	-6.082900	-0.872900	-1.786000
C	-2.143100	3.814400	0.280600
H	-2.332000	4.294000	1.240200
H	-1.111200	3.976100	-0.038800
H	-2.834000	4.178700	-0.482300
H	-1.876200	0.659400	1.814100
Pt	2.615100	0.102100	-0.017000
Br	3.868500	-1.890900	-0.693500
Br	1.651000	2.169200	0.888100
H	0.875500	-1.591300	-0.852900

36
1B-a4-P,Free Energies=-6105.060531

C	2.551000	2.879800	-0.203500
O	1.140900	2.883700	-0.471100
C	0.479200	1.853500	0.289800
C	1.580100	1.093100	1.068300
C	2.706000	2.144400	1.126500
H	3.088700	2.370300	-1.017100
H	2.884200	3.921900	-0.175300
H	-0.281800	2.316900	0.916400
H	2.497600	2.829000	1.956300
H	3.697600	1.718000	1.285900
C	1.861600	-0.220600	0.233500
C	1.081900	-0.027600	-1.101400
H	0.803300	-0.964700	-1.579900
H	1.716300	0.524500	-1.806500
C	-0.072800	0.885800	-0.753100
C	-1.164900	1.217000	-1.622200
H	-1.214400	0.770000	-2.612900
C	3.362200	-0.497200	0.058700
O	4.112100	-0.680500	0.992300
O	3.754400	-0.498200	-1.227500
C	1.332600	-1.512800	0.896100
O	1.674800	-2.612600	0.523600
O	0.435300	-1.295300	1.871500
C	5.144100	-0.809200	-1.448400
H	5.277800	-0.784900	-2.529700
H	5.783200	-0.068800	-0.960900
H	5.373400	-1.800200	-1.050400
C	-0.132600	-2.484400	2.462900
H	-0.826100	-2.123000	3.221700
H	-0.653700	-3.066600	1.699600
H	0.656400	-3.092400	2.911100
H	-1.639000	2.191000	-1.520100
H	1.247900	0.818500	2.067700
Pt	-1.967000	-0.089400	-0.218200
Br	-1.798000	-2.085900	-1.622100
Br	-2.824100	1.497500	1.428900

(11). In Path 1B-*b*

36
1B-a1-IN1,Free Energies=-6105.010291

C	-0.931189	-2.132753	1.859106
O	-0.372689	-0.901431	1.213284
C	-1.196269	0.216078	1.784025
C	-2.593535	-0.350073	1.577507
C	-2.412135	-1.794905	2.130072
H	-0.736256	-2.947007	1.164583
H	-0.324621	-2.258589	2.755899
H	-0.900300	0.289026	2.833080
H	-2.614481	-1.806521	3.204540
H	-3.094296	-2.505621	1.661697
C	-2.934785	-0.340239	0.060025
C	-1.891594	-1.194192	-0.728781
H	-1.974912	-0.967514	-1.792149
H	-2.134494	-2.258516	-0.606617
C	-0.495138	-0.880106	-0.281532
C	0.574279	-0.420846	-0.928798
H	0.486562	-0.342980	-2.013986
C	-4.359108	-0.893475	-0.138323
O	-5.131714	-1.133890	0.764741
O	-4.631942	-1.075447	-1.436956
C	-2.926025	1.092171	-0.535825
O	-2.644081	1.344053	-1.682769
O	-3.293392	2.007206	0.376619
C	-5.951876	-1.571805	-1.739767
H	-5.990919	-1.640606	-2.826212
H	-6.102102	-2.552639	-1.282067
H	-6.710359	-0.879753	-1.366529
C	-3.270356	3.379651	-0.080121
H	-3.619570	3.969611	0.766644
H	-2.251289	3.659136	-0.357406
H	-3.931547	3.501190	-0.940672
H	-0.887675	1.110056	1.244329
H	-3.350308	0.197672	2.137410
Pt	2.236780	0.186781	-0.175552
Br	1.398791	2.466910	0.292934
Br	3.417914	-1.944533	-0.368200

36
1B-b-TS1,Free Energies=-6104.980254

C	-1.859517	-1.304725	3.132309
O	-0.954976	-0.475483	2.398186
C	-1.698657	0.690004	2.044438
C	-3.046824	0.138039	1.543961
C	-3.266090	-1.046047	2.529980
H	-1.513859	-2.337637	3.032078
H	-1.828454	-1.034478	4.197413
H	-1.862918	1.323030	2.930403
H	-3.983317	-0.759082	3.303247
H	-3.681015	-1.930397	2.039961
C	-3.023371	-0.296765	0.049550
C	-1.962100	-1.391906	-0.282678
H	-2.146254	-1.780888	-1.289139
H	-2.066771	-2.245577	0.396185
C	-0.572351	-0.954385	-0.220707
C	0.594185	-0.520450	-0.364491
H	0.096107	-0.340142	-1.416723
C	-4.430396	-0.823228	-0.333769
O	-5.405927	-0.779820	0.378310
O	-4.434615	-1.316855	-1.586755
C	-2.759701	0.898120	-0.895286
O	-1.965785	0.876457	-1.813087
O	-3.529854	1.947452	-0.590850
C	-5.707247	-1.799326	-2.065403
H	-5.521829	-2.142830	-3.082550
H	-6.061814	-2.619282	-1.436363
H	-6.443894	-0.992732	-2.054914
C	-3.345196	3.121736	-1.413691
H	-4.048794	3.856781	-1.024719
H	-2.317179	3.480475	-1.327179
H	-3.562614	2.887105	-2.458069
H	-1.106564	1.257565	1.323911
H	-3.842118	0.876978	1.644471
Pt	2.361081	0.089600	-0.136565
Br	1.721271	2.411613	0.318158
Br	3.493580	-2.033559	-0.511235

36

1B-b-IN1,Free Energies=-6105.014598

C	0.775233	1.025157	2.823035
O	0.485390	-0.335029	2.509941
C	1.706697	-0.920120	2.083803
C	2.550483	0.212273	1.413721
C	1.715220	1.487016	1.703525
H	-0.171500	1.568569	2.855723
H	1.263953	1.096103	3.809496
H	2.255923	-1.323285	2.949236
H	2.348869	2.330497	1.984185
H	1.114789	1.792523	0.842277
C	2.939233	-0.032435	-0.078880
C	1.788556	0.095858	-1.123656
H	2.210091	-0.112710	-2.110706
H	1.428828	1.126905	-1.135709
C	0.616245	-0.850959	-0.931713
C	-0.592965	-0.473774	-0.638492
H	0.790045	-1.919105	-1.073366
C	4.015517	1.004028	-0.480066
O	4.372362	1.944713	0.190045
O	4.504624	0.728580	-1.706500
C	3.581979	-1.425337	-0.208903
O	3.137593	-2.347063	-0.860716
O	4.705589	-1.506519	0.524830
C	5.516699	1.631915	-2.191391
H	5.789357	1.259097	-3.178486
H	5.119317	2.647695	-2.257110
H	6.380528	1.626769	-1.522173
C	5.388733	-2.774951	0.488602
H	6.260629	-2.652022	1.130552
H	4.738178	-3.567488	0.866155
H	5.690038	-3.013343	-0.534279
H	1.460516	-1.754666	1.422699
H	3.501259	0.293280	1.944560
Pt	-2.252288	0.049408	-0.241747
Br	-3.491919	-2.028906	-0.236558
Br	-1.998270	2.457416	-0.036443

36

1B-b-TS2,Free Energies=-6104.99931

C	-1.085301	-1.291124	3.192867
O	-0.524779	-0.011363	2.812811
C	-1.069099	0.410236	1.615835
C	-2.353352	-0.376853	1.375651
C	-1.992435	-1.726115	2.033570
H	-0.261625	-1.983785	3.385503
H	-1.642544	-1.137951	4.124513
H	-1.129878	1.501654	1.589997
H	-2.877174	-2.270736	2.367148
H	-1.431184	-2.363693	1.343366
C	-2.814699	-0.405943	-0.104964
C	-1.989521	-1.317260	-1.049218
H	-2.394227	-1.187568	-2.055940
H	-2.173310	-2.365190	-0.777456
C	-0.492449	-1.131008	-1.157363
C	0.436479	-0.473295	-0.504409
H	-0.029256	-1.677273	-1.988124
C	-4.271518	-0.929771	-0.132879
O	-4.869264	-1.374558	0.820767
O	-4.791050	-0.837867	-1.369439
C	-2.848637	1.022458	-0.699517
O	-2.367063	1.345269	-1.759221
O	-3.509706	1.862874	0.120133
C	-6.147578	-1.303125	-1.515775
H	-6.395397	-1.144940	-2.564937
H	-6.215076	-2.362447	-1.256356
H	-6.815427	-0.730533	-0.867819
C	-3.615695	3.225377	-0.343416
H	-4.179064	3.749682	0.428045
H	-2.621299	3.661827	-0.463338
H	-4.141829	3.258519	-1.300329
H	-0.335103	0.166493	0.753274
H	-3.152055	0.092875	1.958241
Pt	2.147004	0.101183	-0.195032
Br	1.832923	2.494214	0.184283
Br	3.203816	-2.071229	-0.490740

36
1A-a2-IN2, Free Energies=-6105.05102

C	-1.866291	-2.801993	-2.379352
O	-0.816055	-2.602323	-1.414551
C	-1.236404	-1.694009	-0.424836
C	-2.753041	-1.458631	-0.614484
C	-2.902292	-1.699958	-2.131295
H	-1.427899	-2.769044	-3.381233
H	-2.297614	-3.800468	-2.223948
H	-0.977128	-2.103091	0.555970
H	-3.916168	-1.989405	-2.408920
H	-2.649470	-0.797892	-2.699411
C	-3.010634	-0.029388	-0.085971
C	-1.754351	0.777181	-0.519354
H	-1.550562	1.591727	0.178020
H	-1.912261	1.229456	-1.501737
C	-0.577659	-0.253221	-0.625732
C	0.443067	0.012032	0.403786
H	-0.134992	-0.241437	-1.622526
C	-4.305521	0.608216	-0.598509
O	-5.118293	0.087712	-1.327574
O	-4.408675	1.866928	-0.128144
C	-3.073947	-0.103311	1.450040
O	-2.144153	0.127182	2.195402
O	-4.279859	-0.516964	1.866454
C	-5.589601	2.588173	-0.527778
H	-5.499413	3.571108	-0.065959
H	-5.632575	2.674690	-1.616258
H	-6.485770	2.073370	-0.172552
C	-4.438303	-0.666533	3.292577
H	-5.465804	-0.999814	3.434745
H	-3.733172	-1.407796	3.675999
H	-4.266226	0.288869	3.793543
H	0.098257	0.087042	1.441543
H	-3.344090	-2.198858	-0.066067
Pt	2.230152	0.240591	0.115955
Br	2.388070	2.591695	-0.490169
Br	3.205336	-1.944442	0.509227

36
1A-a2-TS2, Free Energies=-6105.023542

C	-2.229792	-1.820056	3.170111
O	-1.213379	-0.790579	3.211371
C	-1.500055	0.173525	2.215962
C	-2.846860	-0.179976	1.554956
C	-2.899486	-1.701672	1.797120
H	-1.738887	-2.781527	3.340439
H	-2.946265	-1.640449	3.982343
H	-1.484714	1.184760	2.644572
H	-3.919477	-2.091582	1.782152
H	-2.318639	-2.248193	1.042427
C	-2.729125	0.306733	0.086785
C	-1.206065	0.217113	-0.250764
H	-0.829480	1.058857	-0.842771
H	-0.960176	-0.670976	-0.848061
C	-0.495789	0.135564	1.061971
C	0.872001	-0.095464	1.234617
H	0.305209	-1.168216	1.147020
C	-3.658525	-0.485317	-0.838611
O	-4.825603	-0.679966	-0.575401
O	-3.042339	-0.928412	-1.942370
C	-3.136548	1.791969	0.021644
O	-3.196349	2.526386	0.983066
O	-3.352109	2.175870	-1.243869
C	-3.869688	-1.658251	-2.871389
H	-3.204508	-1.946845	-3.684293
H	-4.296974	-2.538743	-2.386020
H	-4.676995	-1.018550	-3.235595
C	-3.682539	3.568884	-1.432082
H	-3.822408	3.688585	-2.505746
H	-4.598596	3.814238	-0.890163
H	-2.866798	4.201128	-1.073897
H	1.244735	-0.072332	2.261483
H	-3.676926	0.315823	2.059704
Pt	2.185885	-0.113156	-0.195091
Br	3.046283	2.144970	0.085648
Br	1.485858	-2.407957	-0.815385

36
1A-a2-P,Free Energies=-6105.050611

C	-3.061226	3.834721	-0.537528
O	-1.665751	3.530968	-0.542786
C	-1.501388	2.191119	-1.002215
C	-2.878293	1.475284	-0.835559
C	-3.736397	2.532313	-0.106708
H	-3.215764	4.670046	0.150621
H	-3.393690	4.142514	-1.541865
H	-1.162678	2.194382	-2.045689
H	-4.792171	2.468163	-0.377482
H	-3.661743	2.425001	0.981832
C	-2.580179	0.173074	-0.037836
C	-1.362488	0.562820	0.849732
H	-0.823864	-0.297314	1.250016
H	-1.718439	1.156339	1.695728
C	-0.488784	1.464006	-0.071127
C	0.603890	0.760921	-0.794859
H	0.020835	2.224269	0.541522
C	-3.799733	-0.333475	0.733401
O	-4.938597	-0.246755	0.329055
O	-3.454813	-0.890058	1.907141
C	-2.115886	-0.897023	-1.035806
O	-1.326386	-0.652526	-1.932374
O	-2.645433	-2.098337	-0.814677
C	-4.538770	-1.454233	2.668257
H	-4.082135	-1.846898	3.576511
H	-5.278644	-0.685864	2.906065
H	-5.021419	-2.253592	2.100513
C	-2.206432	-3.161050	-1.693066
H	-2.765228	-4.040385	-1.374906
H	-2.436441	-2.907774	-2.730182
H	-1.131930	-3.313117	-1.574841
H	0.701952	0.897255	-1.876147
H	-3.322371	1.242151	-1.805826
Pt	1.961281	-0.182501	-0.005007
Br	1.287448	-2.518725	-0.006191
Br	3.493860	1.607946	0.581153

(12). In Path 1C-*a1*

36
1C-a1-IN1,Free Energies=-985.031678

C	-2.414351	-1.182766	3.483289
O	-1.836364	0.112710	3.321162
C	-2.655425	0.795903	2.376352
C	-3.219329	-0.282672	1.397397
C	-2.795799	-1.619360	2.062816
H	-1.670707	-1.823595	3.963044
H	-3.302064	-1.123405	4.133978
H	-3.488280	1.294294	2.894230
H	-3.600157	-2.357464	2.035971
H	-1.921566	-2.059381	1.574526
C	-2.818591	-0.107466	-0.099382
C	-1.378558	-0.561267	-0.507663
H	-1.191462	-0.198183	-1.519786
H	-1.332262	-1.656058	-0.549768
C	-0.287988	-0.109538	0.372814
C	0.363121	0.206451	1.407655
H	0.479391	0.506659	2.432922
C	-3.786321	-0.949457	-0.964973
O	-4.603957	-1.732353	-0.539788
O	-3.582015	-0.707574	-2.272863
C	-2.995926	1.367833	-0.508656
O	-2.121419	2.083512	-0.939164
O	-4.265555	1.766211	-0.302254
C	-4.415624	-1.449703	-3.185492
H	-4.113009	-1.126627	-4.181078
H	-4.252531	-2.522744	-3.059731
H	-5.468784	-1.221183	-3.005439
C	-4.552326	3.135499	-0.651433
H	-5.609368	3.275860	-0.426684
H	-3.935637	3.815448	-0.058818
H	-4.354669	3.304283	-1.712633
H	-2.040456	1.565873	1.903102
H	-4.308326	-0.217302	1.408236
Pt	1.791291	-0.021881	-0.071202
I	2.305303	2.575482	-0.193504
I	1.985384	-2.677190	-0.287844

36
1C-a1-TS1,Free Energies=-985.014068

C	-2.592198	-2.296432	2.711836
O	-2.332551	-0.992468	3.296799
C	-2.554161	-0.002811	2.370129
C	-3.317596	-0.578096	1.181822
C	-2.875294	-2.059126	1.221357
H	-1.719436	-2.929368	2.890835
H	-3.452180	-2.719477	3.243123
H	-2.954099	0.897329	2.849056
H	-3.647180	-2.719948	0.825724
H	-1.963733	-2.217139	0.636892
C	-2.998320	0.211931	-0.110321
C	-1.473943	0.193908	-0.453249
H	-1.258293	1.038069	-1.113698
H	-1.235146	-0.728186	-0.995752
C	-0.564358	0.259931	0.709136
C	0.575612	0.142061	1.303895
H	0.827736	0.163055	2.359303
C	-3.783051	-0.369855	-1.299012
O	-4.552533	-1.300773	-1.235862
O	-3.485393	0.300103	-2.423875
C	-3.440620	1.674762	0.106964
O	-2.688597	2.588877	0.356090
O	-4.777485	1.784937	0.038071
C	-4.151649	-0.153471	-3.620720
H	-3.783548	0.491606	-4.417651
H	-3.900329	-1.197815	-3.819536
H	-5.233958	-0.055536	-3.508205
C	-5.309355	3.109561	0.254469
H	-6.389109	3.006574	0.152655
H	-5.045004	3.465029	1.253216
H	-4.911366	3.800998	-0.491574
H	-1.535796	0.380134	1.929270
H	-4.394855	-0.505813	1.364884
Pt	1.981684	-0.078687	-0.047726
I	1.544711	-2.684871	-0.478916
I	2.863346	2.423144	-0.010585

36

1C-a1-IN2,Free Energies=-985.081375

C	-1.977094	2.644403	-2.280663
O	-1.157823	1.498727	-2.552889
C	-1.835476	0.325375	-2.105223
C	-3.044780	0.781112	-1.237017
C	-2.750496	2.282952	-1.014936
H	-1.312138	3.503523	-2.165707
H	-2.652842	2.830109	-3.129707
H	-2.135170	-0.270810	-2.975422
H	-3.662391	2.864714	-0.874970
H	-2.115771	2.439269	-0.136925
C	-3.012257	-0.134540	0.021362
C	-1.501910	-0.372558	0.265368
H	-1.311583	-1.252631	0.880370
H	-1.068950	0.494237	0.773148
C	-0.909325	-0.509549	-1.154218
C	0.512832	-0.174617	-1.360204
H	0.856042	-0.045721	-2.392446
C	-3.725696	0.457636	1.240647
O	-4.384706	1.471752	1.261278
O	-3.513368	-0.325837	2.316722
C	-3.694908	-1.467585	-0.335678
O	-3.117104	-2.471184	-0.696063
O	-5.032218	-1.365910	-0.249356
C	-4.143196	0.107999	3.536829
H	-3.862912	-0.631449	4.286685
H	-3.782412	1.100139	3.818826
H	-5.228434	0.142123	3.411685
C	-5.775877	-2.550630	-0.596283
H	-6.823743	-2.283577	-0.461942
H	-5.577807	-2.833409	-1.633105
H	-5.498303	-3.377887	0.061233
H	-0.983062	-1.572466	-1.447627
H	-3.990552	0.670590	-1.775340
Pt	1.812642	-0.021461	-0.083618
I	1.825376	2.543340	0.573230
I	2.637923	-2.522645	0.177072

36

1C-a1-TS2,Free Energies=-985.050617

C	2.608751	-3.025082	-2.320144
O	1.478061	-2.159389	-2.511230
C	1.826133	-0.849698	-2.081615
C	3.181919	-0.931286	-1.320939
C	3.357927	-2.452035	-1.116871
H	2.223976	-4.035502	-2.165410
H	3.236163	-3.017934	-3.223647
H	1.838586	-0.153204	-2.926659
H	4.408915	-2.742626	-1.074871
H	2.880154	-2.788001	-0.189546
C	2.981253	-0.087201	-0.024423
C	1.475606	-0.290710	0.306992
H	1.020201	0.474777	0.940383
H	1.311634	-1.244224	0.828734
C	0.810098	-0.415094	-1.024399
C	-0.537906	-0.162973	-1.286400
H	-0.881757	-0.370540	-2.303239
C	3.945671	-0.477552	1.094046
O	5.050716	-0.937041	0.909596
O	3.410493	-0.236077	2.301112
C	3.143698	1.393846	-0.402928
O	2.478253	1.901136	-1.286453
O	4.055499	2.039018	0.322326
C	4.261141	-0.518239	3.430478
H	3.663493	-0.279295	4.309434
H	4.551657	-1.571445	3.432461
H	5.158337	0.104024	3.388746
C	4.226926	3.443738	0.021450
H	5.005526	3.787749	0.700794
H	4.533233	3.569076	-1.019193
H	3.291017	3.979150	0.194695
H	0.106447	0.871160	-1.369589
H	4.002755	-0.537733	-1.924841
Pt	-1.918698	0.109470	0.055450
I	-2.249519	-2.463647	0.636432
I	-1.829035	2.780410	-0.097898

36
1C-a1-P,Free Energies=-985.087482

C	-0.964894	-2.385148	-2.621474
O	-0.074052	-1.726671	-1.719540
C	-0.708921	-1.692470	-0.446154
C	-2.257215	-1.711861	-0.724002
C	-2.335295	-1.812254	-2.268843
H	-0.630154	-2.158420	-3.636223
H	-0.925876	-3.475833	-2.470613
H	-0.371136	-2.542689	0.161785
H	-3.175854	-2.423943	-2.601748
H	-2.444600	-0.825449	-2.725703
C	-2.805675	-0.396616	-0.077164
C	-1.587296	0.567626	-0.102376
H	-1.694028	1.409799	0.579808
H	-1.463687	0.959182	-1.115926
C	-0.437437	-0.361614	0.258705
C	0.216654	-0.289848	1.536534
H	0.560274	-1.201506	2.020182
C	-4.044449	0.190229	-0.768919
O	-4.719005	-0.348853	-1.614926
O	-4.297239	1.418458	-0.273447
C	-3.214215	-0.683058	1.381890
O	-2.589373	-0.354127	2.367201
O	-4.361718	-1.381393	1.425690
C	-5.456148	2.082017	-0.813141
H	-5.502134	3.044363	-0.303983
H	-5.346824	2.220189	-1.891572
H	-6.356008	1.494087	-0.615656
C	-4.839717	-1.723638	2.741604
H	-5.772060	-2.263431	2.578388
H	-4.111956	-2.354897	3.257476
H	-5.011929	-0.818953	3.329465
H	-0.014661	0.533877	2.204485
H	-2.731592	-2.585955	-0.271773
Pt	1.593922	0.325725	0.093975
I	3.009149	-1.924066	0.172068
I	1.134342	2.943379	-0.094486

(13). In Path 1C-*a2*

36
1C-a2-IN1,Free Energies=-985.02626

C	-4.535244	-1.306824	-2.453473
O	-3.775902	-2.381919	-1.899694
C	-2.696913	-1.811286	-1.175742
C	-3.342319	-0.614616	-0.453860
C	-4.286324	-0.066701	-1.554802
H	-4.219316	-1.110777	-3.489408
H	-5.583032	-1.621021	-2.471875
H	-2.300218	-2.569563	-0.498733
H	-5.212798	0.331152	-1.130123
H	-3.822088	0.740431	-2.131617
C	-2.419411	0.436640	0.233333
C	-1.390157	1.149584	-0.696661
H	-1.014830	2.038525	-0.184856
H	-1.901496	1.504324	-1.598546
C	-0.218511	0.379527	-1.152075
C	0.611308	-0.162548	-1.938516
H	0.924246	-0.609625	-2.865784
C	-3.387887	1.483608	0.838397
O	-4.080767	1.258171	1.804826
O	-3.406616	2.637744	0.150396
C	-1.670422	-0.113951	1.470710
O	-0.764282	0.496059	2.000905
O	-2.147176	-1.282937	1.898994
C	-4.310999	3.643527	0.652494
H	-4.189300	4.498528	-0.011972
H	-5.338881	3.273938	0.628116
H	-4.046702	3.907881	1.678755
C	-1.552539	-1.799408	3.110163
H	-2.093393	-2.721254	3.321565
H	-0.491541	-1.999777	2.949613
H	-1.678105	-1.078786	3.921299
H	-1.894235	-1.494559	-1.859961
H	-3.962908	-1.029166	0.344231
Pt	1.630031	-0.056988	-0.161603
I	1.520314	-2.692296	0.250884
I	2.409433	2.489703	-0.192751

36
1C-a2-TS1,Free Energies=-985.012801

C	-4.292890	-1.412153	2.911452
O	-3.258191	-0.497448	3.344163
C	-2.768090	0.217360	2.273641
C	-3.686776	0.024364	1.070095
C	-4.296993	-1.364291	1.380040
H	-4.069601	-2.400924	3.320798
H	-5.237659	-1.059027	3.341147
H	-2.527019	1.241251	2.562127
H	-5.297952	-1.471177	0.958100
H	-3.672356	-2.168206	0.974784
C	-2.963643	0.130705	-0.296081
C	-1.649068	-0.710732	-0.306233
H	-1.132834	-0.539203	-1.256233
H	-1.877917	-1.780985	-0.263128
C	-0.713990	-0.340375	0.764338
C	0.425975	-0.065108	1.312032
H	0.632894	0.188720	2.348055
C	-3.939628	-0.322101	-1.401973
O	-5.112303	-0.016775	-1.397256
O	-3.346933	-1.061564	-2.343252
C	-2.579377	1.577718	-0.693025
O	-2.318985	1.885670	-1.833217
O	-2.538941	2.412984	0.353489
C	-4.178830	-1.442161	-3.459778
H	-3.536210	-2.037714	-4.106897
H	-5.034011	-2.026424	-3.112294
H	-4.533428	-0.549026	-3.978710
C	-2.095385	3.761029	0.055481
H	-2.190609	4.306450	0.993720
H	-1.055758	3.738719	-0.278427
H	-2.728563	4.198125	-0.718836
H	-1.723936	-0.230844	1.958492
H	-4.475349	0.782645	1.097912
Pt	1.913512	-0.120684	0.043475
I	2.218224	2.526031	-0.088016
I	2.088217	-2.769191	-0.173927

36

1C-a2-IN2,Free Energies=-985.077447

C	-2.964171	4.177451	-0.458321
O	-1.613329	3.718135	-0.529076
C	-1.618746	2.368007	-0.986667
C	-3.065732	1.819037	-0.788472
C	-3.764732	2.954623	-0.010285
H	-2.992959	5.014889	0.243858
H	-3.302189	4.535479	-1.443864
H	-1.304814	2.330786	-2.036889
H	-4.831584	3.015354	-0.233754
H	-3.654962	2.822085	1.072505
C	-2.904847	0.470398	-0.030038
C	-1.628101	0.689536	0.832177
H	-1.180648	-0.238755	1.189605
H	-1.893895	1.286682	1.708168
C	-0.675079	1.525702	-0.076338
C	0.340313	0.736475	-0.825697
H	0.381279	0.815995	-1.916462
C	-4.153762	0.094127	0.769632
O	-5.285007	0.347453	0.417798
O	-3.842535	-0.556328	1.903845
C	-2.604296	-0.621528	-1.066768
O	-1.793830	-0.464733	-1.963403
O	-3.303668	-1.740564	-0.881937
C	-4.962611	-1.007176	2.688250
H	-4.528244	-1.497338	3.559223
H	-5.583711	-0.159605	2.988536
H	-5.568546	-1.709408	2.110401
C	-3.043337	-2.816549	-1.812822
H	-3.714101	-3.620415	-1.512060
H	-3.260096	-2.489430	-2.832063
H	-1.999541	-3.127652	-1.736464
H	-0.101440	2.220222	0.554351
H	-3.565314	1.667825	-1.748199
Pt	1.680687	-0.267932	-0.079933
I	0.798569	-2.759080	0.091429
I	3.521897	1.575300	0.385593

36

1C-a2-TS2,Free Energies=-985.050617

C	-2.473431	-1.501872	3.305452
O	-1.530730	-0.402632	3.267660
C	-1.811465	0.405631	2.142886
C	-3.124419	-0.088691	1.497161
C	-3.105038	-1.575042	1.911483
H	-1.926715	-2.405542	3.586893
H	-3.223919	-1.289926	4.078076
H	-1.826328	1.463683	2.433045
H	-4.099867	-2.021137	1.908051
H	-2.475782	-2.167184	1.235510
C	-2.981328	0.250538	-0.016460
C	-1.452789	0.139034	-0.303907
H	-1.079296	0.917752	-0.975484
H	-1.178154	-0.813366	-0.776567
C	-0.775545	0.244398	1.024400
C	0.591046	0.065469	1.261340
H	0.929297	0.223555	2.288643
C	-3.837861	-0.634869	-0.923602
O	-4.749604	-1.339312	-0.553547
O	-3.435961	-0.515815	-2.200343
C	-3.388886	1.727775	-0.172129
O	-2.662213	2.646675	0.140648
O	-4.640776	1.868212	-0.622736
C	-4.184467	-1.280091	-3.166977
H	-3.714828	-1.070526	-4.127398
H	-4.128348	-2.345675	-2.932618
H	-5.230440	-0.963934	-3.167467
C	-5.116212	3.226459	-0.745221
H	-6.134793	3.141225	-1.121863
H	-5.101275	3.720227	0.229096
H	-4.487030	3.783254	-1.443139
H	0.029575	-1.014058	1.308581
H	-3.998664	0.401399	1.935071
Pt	1.966400	-0.104390	-0.102039
I	1.470173	-2.731882	-0.435076
I	2.688016	2.442320	-0.161894

36
1C-a2-P, Free Energies=-985.088935

C	-1.925486	-3.894403	-1.115723
O	-0.829853	-3.033957	-1.438175
C	-0.668025	-2.122038	-0.343917
C	-2.052113	-2.012897	0.367648
C	-2.949832	-2.977338	-0.445210
H	-2.270944	-4.351404	-2.046498
H	-1.593675	-4.691075	-0.432010
H	0.120888	-2.468015	0.323360
H	-3.664994	-3.509586	0.186581
H	-3.517092	-2.441858	-1.215837
C	-2.451337	-0.510384	0.288423
C	-1.714141	-0.011214	-0.980786
H	-1.650768	1.070743	-1.067214
H	-2.261869	-0.378618	-1.860693
C	-0.385979	-0.748339	-0.972887
C	0.658354	-0.538555	-1.932962
H	1.290680	-1.376916	-2.215127
C	-3.970562	-0.333759	0.286307
O	-4.687102	-0.782187	1.154308
O	-4.416897	0.350788	-0.782086
C	-1.894507	0.241461	1.512407
O	-1.020005	-0.181641	2.237760
O	-2.473772	1.442755	1.641238
C	-5.839652	0.573872	-0.821356
H	-6.020684	1.131716	-1.739943
H	-6.374728	-0.378850	-0.832793
H	-6.154184	1.151214	0.051302
C	-1.998824	2.263167	2.729742
H	-2.634462	3.148053	2.720023
H	-2.093776	1.724893	3.675376
H	-0.955541	2.537871	2.560377
H	0.539314	0.233355	-2.690788
H	-1.984103	-2.328868	1.408534
Pt	1.348639	0.315737	-0.161587
I	2.947302	-1.655438	0.638229
I	0.686770	2.869708	-0.603423

(14). In Path 1C-*a3*

36
1C-a3-TS1,Free Energies=-985.018576

C	-4.986117	-1.443744	-1.653346
O	-3.792034	-1.782073	-2.371787
C	-2.699454	-1.004751	-1.898063
C	-3.108885	-0.541831	-0.485233
C	-4.617028	-0.292699	-0.711906
H	-5.773318	-1.170057	-2.366270
H	-5.323596	-2.328454	-1.096422
H	-1.808420	-1.638338	-1.902529
H	-5.193889	-0.302048	0.216709
H	-4.776849	0.671729	-1.208074
C	-2.284507	0.621863	0.194632
C	-1.223831	1.313387	-0.719113
H	-0.805418	2.167270	-0.179656
H	-1.720008	1.710390	-1.610683
C	-0.096810	0.488908	-1.186382
C	0.701299	-0.092146	-1.976708
H	1.014658	-0.500887	-2.921256
C	-3.270713	1.709778	0.690482
O	-3.830627	1.676792	1.762356
O	-3.451537	2.686364	-0.218577
C	-1.573016	0.179616	1.500495
O	-0.601243	0.761454	1.939179
O	-2.165275	-0.851159	2.101564
C	-4.366946	3.731610	0.170520
H	-4.376048	4.432418	-0.663861
H	-5.363325	3.317378	0.341571
H	-4.016857	4.218005	1.083679
C	-1.602800	-1.245952	3.370645
H	-2.235098	-2.060888	3.721636
H	-0.574111	-1.585225	3.233185
H	-1.628531	-0.404477	4.066491
H	-2.526520	-0.151070	-2.573762
H	-3.022493	-1.410822	0.168850
Pt	1.645141	-0.192571	-0.155676
I	1.045278	-2.765933	0.247677
I	2.828446	2.191978	-0.165505

36
1C-a3-IN2,Free Energies=-985.030158

C	4.671144	1.835984	-1.392066
O	4.277535	1.008316	-2.492854
C	3.294263	0.069962	-2.069964
C	2.883672	0.470361	-0.632337
C	4.186442	1.124196	-0.128688
H	5.758536	1.963910	-1.426492
H	4.206677	2.828928	-1.491732
H	2.449825	0.103773	-2.770218
H	4.023192	1.801398	0.709713
H	4.910630	0.364727	0.185638
C	2.256717	-0.683132	0.213192
C	1.156005	-1.445280	-0.591032
H	0.716802	-2.214303	0.049859
H	1.617107	-1.953615	-1.444099
C	0.070999	-0.608501	-1.127931
C	-0.668981	-0.009411	-1.959884
H	-0.935037	0.382619	-2.925812
C	3.346121	-1.683249	0.659130
O	3.963829	-1.583513	1.695387
O	3.551130	-2.662522	-0.241753
C	1.611369	-0.204399	1.538506
O	0.735756	-0.833349	2.095931
O	2.124175	0.937406	1.997405
C	4.570913	-3.622742	0.106928
H	4.586587	-4.337754	-0.715069
H	5.538584	-3.126220	0.208825
H	4.316874	-4.115641	1.047921
C	1.598530	1.395827	3.261254
H	2.166819	2.294948	3.497536
H	0.535886	1.626486	3.162542
H	1.744081	0.629610	4.025761
H	3.720363	-0.942978	-2.099279
H	2.118151	1.252943	-0.699780
Pt	-1.667462	0.199209	-0.176162
I	-1.029091	2.776237	0.104916
I	-2.904788	-2.151058	-0.053411

36

1C-a3-TS2,Free Energies=-984.990826

C	-3.974248	0.598876	2.972789
O	-3.171275	-0.628622	3.141314
C	-2.696563	-1.000281	1.946091
C	-2.998791	0.082380	0.923416
C	-4.327167	0.615113	1.475034
H	-4.817021	0.490738	3.656559
H	-3.365015	1.457995	3.270315
H	-1.365084	-1.107975	1.880297
H	-4.557913	1.614560	1.103659
H	-5.173441	-0.049083	1.265982
C	-2.696040	-0.421239	-0.502225
C	-1.355977	-1.257969	-0.375236
H	-0.716767	-1.051428	-1.237427
H	-1.590140	-2.326301	-0.393473
C	-0.586496	-0.920551	0.856223
C	0.533750	-0.385741	1.302862
H	0.727573	-0.214507	2.361638
C	-3.875011	-1.247939	-1.040727
O	-4.689030	-0.830584	-1.830907
O	-3.937666	-2.472560	-0.474805
C	-2.473736	0.720211	-1.516715
O	-1.876495	0.559251	-2.554032
O	-3.013336	1.876738	-1.110747
C	-5.031826	-3.305695	-0.918376
H	-4.916039	-4.245784	-0.379930
H	-5.988365	-2.834375	-0.680789
H	-4.966388	-3.464940	-1.996646
C	-2.808785	2.996217	-2.004358
H	-3.333019	3.832207	-1.542179
H	-1.740468	3.205872	-2.090047
H	-3.225270	2.768471	-2.987656
H	-2.863407	-2.056544	1.721422
H	-2.270009	0.879468	1.107962
Pt	1.947791	0.145179	0.088812
I	1.216034	2.726345	0.089113
I	3.038322	-2.256466	-0.241307

36

1C-a3-IN3,Free Energies=-985.058212

C	-3.013017	0.668122	3.134571
O	-1.872713	-0.238666	3.048396
C	-2.011954	-0.898176	1.808205
C	-2.545866	0.170530	0.871386
C	-3.679183	0.738686	1.719734
H	-3.707292	0.296220	3.896536
H	-2.625440	1.638286	3.458433
H	-0.498061	-2.437179	1.401913
H	-3.966225	1.756731	1.447443
H	-4.571325	0.104011	1.677420
C	-2.561096	-0.503648	-0.523545
C	-1.323015	-1.489623	-0.419057
H	-0.563131	-1.208248	-1.149074
H	-1.631330	-2.512251	-0.643773
C	-0.776542	-1.427777	1.045695
C	0.440391	-0.636510	1.342787
H	0.675532	-0.509873	2.406521
C	-3.872988	-1.235162	-0.835948
O	-4.632879	-0.933954	-1.728413
O	-4.096306	-2.265240	0.010791
C	-2.360130	0.502182	-1.668843
O	-1.674923	0.297620	-2.644759
O	-3.043790	1.634900	-1.443994
C	-5.309808	-3.006509	-0.227154
H	-5.326662	-3.786937	0.533539
H	-6.180426	-2.353143	-0.132501
H	-5.296726	-3.441957	-1.229052
C	-2.957204	2.623479	-2.488520
H	-3.582203	3.452058	-2.155496
H	-1.921313	2.946544	-2.616824
H	-3.330535	2.209844	-3.428254
H	-2.723650	-1.731343	1.893778
H	-1.767878	0.943770	0.814189
Pt	1.649169	0.099059	0.188167
I	1.054817	2.677309	0.081891
I	3.110632	-1.999649	-0.484605

36

1C-a3-TS3,Free Energies=-985.034514

C	-3.076137	0.301118	3.593260
O	-1.757549	-0.204564	3.212825
C	-1.867531	-0.596887	1.877356
C	-2.880066	0.355829	1.234752
C	-3.963673	0.338287	2.308520
H	-3.492574	-0.351266	4.367167
H	-2.925485	1.298512	4.016077
H	0.312324	-1.513402	1.012562
H	-4.614984	1.214487	2.281207
H	-4.586347	-0.560120	2.236144
C	-2.901524	-0.113073	-0.240131
C	-1.367652	-0.398072	-0.477354
H	-0.883524	0.407346	-1.037774
H	-1.203440	-1.326403	-1.033164
C	-0.740309	-0.457854	0.908284
C	0.617224	-0.338718	1.217413
H	0.860867	-0.303664	2.282877
C	-3.724707	-1.395709	-0.417569
O	-3.266288	-2.517381	-0.377313
O	-5.028135	-1.116581	-0.568510
C	-3.421743	0.985441	-1.171910
O	-3.874378	2.043848	-0.801415
O	-3.276489	0.616567	-2.454794
C	-5.899657	-2.255120	-0.733850
H	-6.900130	-1.838273	-0.843956
H	-5.613728	-2.821089	-1.623338
H	-5.843621	-2.906199	0.141666
C	-3.703621	1.583731	-3.436515
H	-3.504938	1.121427	-4.402822
H	-4.768960	1.795400	-3.317601
H	-3.134843	2.509813	-3.325464
H	-2.244056	-1.632734	1.791531
H	-2.438245	1.360805	1.220103
Pt	2.037156	0.118827	-0.020293
I	1.578296	2.738703	-0.010080
I	2.710055	-2.443460	-0.409585

36

1C-a3-P,Free Energies=-985.072214

C	-1.406547	-3.574106	-0.217873
O	-0.527570	-2.753963	-1.046247
C	-1.108417	-1.486139	-1.106761
C	-1.905288	-1.297804	0.170911
C	-2.571828	-2.667237	0.281517
H	-1.759073	-4.419072	-0.817630
H	-0.803253	-3.955210	0.611512
H	0.885271	1.008968	-2.602423
H	-2.886686	-2.925841	1.295309
H	-3.439486	-2.752659	-0.382782
C	-2.550500	0.095116	-0.041372
C	-1.491743	0.832441	-0.960852
H	-1.115204	1.743376	-0.501937
H	-1.979840	1.113125	-1.901885
C	-0.377424	-0.182386	-1.272984
C	0.762696	0.049540	-2.105161
H	1.219143	-0.801383	-2.607630
C	-3.895008	-0.031913	-0.767299
O	-4.048826	0.047021	-1.967651
O	-4.883986	-0.312296	0.098107
C	-2.735499	0.839928	1.284938
O	-2.422656	0.416245	2.374051
O	-3.260207	2.059908	1.066276
C	-6.192554	-0.485487	-0.479063
H	-6.853317	-0.697950	0.360998
H	-6.502042	0.426691	-0.994850
H	-6.189164	-1.316373	-1.188851
C	-3.444543	2.878047	2.237635
H	-3.878967	3.809451	1.875007
H	-4.117849	2.384029	2.942472
H	-2.484180	3.063900	2.724670
H	-1.811375	-1.453260	-1.968917
H	-1.198147	-1.189983	1.000916
Pt	1.492964	0.132041	-0.148770
I	2.255058	-2.233661	0.727397
I	1.690393	2.803240	-0.210001

36
1C-a4-IN1,Free Energies=-985.026175

C	-1.560300	-2.379400	2.611800
O	-0.869900	-1.238700	3.122400
C	-0.635400	-0.374300	2.024100
C	-1.963200	-0.403600	1.246200
C	-2.375700	-1.894900	1.383800
H	-0.841000	-3.158600	2.319100
H	-2.183900	-2.773400	3.419100
H	-0.373200	0.611300	2.412100
H	-3.454400	-1.994000	1.538300
H	-2.121800	-2.480600	0.494700
C	-1.981800	0.166700	-0.204200
C	-0.974600	-0.494700	-1.203500
H	-1.368700	-0.379300	-2.218500
H	-0.911100	-1.568300	-1.018300
C	0.382500	0.083000	-1.262200
C	1.330000	0.787800	-1.714900
H	1.744400	1.594300	-2.294000
C	-3.433700	-0.045100	-0.695700
O	-4.363900	0.626400	-0.309800
O	-3.552500	-1.079600	-1.545900
C	-1.789000	1.698000	-0.278700
O	-1.599600	2.271600	-1.331400
O	-1.862800	2.304400	0.908400
C	-4.894100	-1.362700	-1.994200
H	-4.800200	-2.217100	-2.664000
H	-5.533700	-1.604800	-1.142200
H	-5.306100	-0.498700	-2.520300
C	-1.730100	3.740700	0.884700
H	-1.852700	4.057200	1.919900
H	-0.743100	4.019700	0.508500
H	-2.502600	4.177900	0.248500
H	0.204600	-0.743200	1.411500
H	-2.677400	0.199700	1.812000
Pt	2.262000	-0.413000	-0.335300
I	2.233100	-2.861400	-1.380800
I	2.938300	1.717300	1.109000

36
1C-a4-TS1,Free Energies=-985.005272

C	-1.785600	-2.378100	2.454000
O	-1.095800	-1.158200	2.748700
C	-1.439700	-0.242700	1.761400
C	-2.907600	-0.488200	1.378800
C	-3.146300	-1.952300	1.864500
H	-1.194700	-2.963400	1.734900
H	-1.859700	-2.944100	3.384700
H	-1.183800	0.767700	2.085200
H	-3.928100	-1.965500	2.627900
H	-3.464700	-2.626500	1.063000
C	-3.193800	-0.234600	-0.124600
C	-2.193100	-1.003800	-1.032000
H	-2.474200	-0.806400	-2.079000
H	-2.266600	-2.084600	-0.875500
C	-0.818300	-0.541600	-0.955800
C	0.369700	-0.189400	-1.301200
H	0.558800	-0.057500	-2.377300
C	-4.655500	-0.639600	-0.400200
O	-5.589300	-0.134900	0.180200
O	-4.766900	-1.605000	-1.326100
C	-3.117400	1.256500	-0.541200
O	-3.159400	1.591100	-1.705800
O	-3.009400	2.088600	0.493300
C	-6.117000	-2.014100	-1.637300
H	-6.015400	-2.794000	-2.391300
H	-6.610000	-2.398500	-0.741600
H	-6.683700	-1.166100	-2.027500
C	-2.915200	3.494700	0.161700
H	-2.895500	4.012200	1.119800
H	-1.994700	3.678100	-0.396100
H	-3.780900	3.796200	-0.431200
H	-3.548100	0.195300	1.938400
Pt	1.945300	0.141200	-0.222600
I	2.867800	-2.353200	-0.341600
I	1.498800	2.725300	0.256100
H	-0.792000	-0.425900	0.841300

36

1C-a4-IN2,Free Energies=-985.075251

C	-1.568000	-2.258200	2.349700
O	-0.528800	-1.278400	2.450900
C	-0.753300	-0.323600	1.451900
C	-2.294300	-0.161300	1.312800
C	-2.834700	-1.489000	1.920500
H	-1.294200	-3.025000	1.609700
H	-1.649200	-2.741500	3.325700
H	-0.233700	0.587200	1.755100
H	-3.463000	-1.262700	2.786300
H	-3.435900	-2.067400	1.216200
C	-2.537500	0.095400	-0.202500
C	-1.517900	-0.832000	-0.900900
H	-1.319000	-0.504400	-1.923700
H	-1.914400	-1.847400	-0.948400
C	-0.249700	-0.828400	0.004400
C	0.806300	0.061300	-0.511400
H	0.502800	0.991900	-1.006200
C	-3.997100	-0.125600	-0.635600
O	-4.832900	0.749100	-0.680300
O	-4.246500	-1.410200	-0.958400
C	-2.226300	1.570200	-0.560000
O	-1.653600	1.905600	-1.577400
O	-2.654000	2.427100	0.371400
C	-5.599700	-1.689400	-1.373400
H	-5.615200	-2.752900	-1.610200
H	-6.299800	-1.459900	-0.566500
H	-5.854900	-1.091800	-2.251300
C	-2.486600	3.826000	0.063000
H	-2.901500	4.360000	0.917200
H	-1.428000	4.063400	-0.066800
H	-3.030500	4.073600	-0.851100
H	0.150800	-1.833500	0.150900
H	-2.648200	0.688200	1.895500
Pt	2.610400	-0.215500	-0.392100
I	3.123100	-1.759400	-2.482500
I	3.304000	1.110100	1.793200

36

1C-a4-TS2,Free Energies=-985.040777

C	-2.106700	-2.623300	1.460700
O	-0.731600	-2.330200	1.160900
C	-0.534600	-0.920500	1.004900
C	-1.909400	-0.231000	1.221000
C	-2.690500	-1.314900	1.992300
H	-2.627400	-2.961800	0.555100
H	-2.114000	-3.438200	2.190100
H	0.263300	-0.589400	1.671500
H	-2.465300	-1.207400	3.058500
H	-3.775100	-1.239700	1.877100
C	-2.422400	0.148600	-0.232600
C	-1.512200	-0.642400	-1.214400
H	-1.443600	-0.160700	-2.190200
H	-1.893600	-1.660400	-1.334500
C	-0.216800	-0.659000	-0.454200
C	1.055700	-0.452800	-0.998500
H	1.087800	-0.258800	-2.073600
C	-3.924600	-0.130000	-0.409400
O	-4.793700	0.628700	-0.046100
O	-4.163000	-1.323100	-0.986000
C	-2.248200	1.662000	-0.536100
O	-1.986600	2.075100	-1.645300
O	-2.450200	2.427900	0.534400
C	-5.556800	-1.650600	-1.174600
H	-5.560800	-2.627000	-1.657900
H	-6.070900	-1.690200	-0.211400
H	-6.035600	-0.900200	-1.807400
C	-2.351100	3.852200	0.313800
H	-2.583300	4.306600	1.276100
H	-1.338300	4.109700	-0.003900
H	-3.069700	4.161900	-0.448000
H	-1.820600	0.680200	1.808800
Pt	2.704200	-0.075600	-0.039300
I	3.867400	-2.377600	-0.735100
I	1.899100	2.276200	0.920700
H	0.856000	-1.649200	-0.875200

36
1C-a4-P,Free Energies=-985.083791

C	2.551900	2.884100	-0.220400
O	1.139400	2.892700	-0.475600
C	0.481700	1.857500	0.280800
C	1.584100	1.097200	1.057500
C	2.715400	2.143500	1.105400
H	3.081000	2.375700	-1.040400
H	2.887600	3.925200	-0.191500
H	-0.277600	2.319200	0.910000
H	2.520200	2.826400	1.939800
H	3.706600	1.711500	1.254000
C	1.854900	-0.219400	0.226400
C	1.091400	-0.013500	-1.114700
H	0.829000	-0.947200	-1.608400
H	1.732600	0.549000	-1.805700
C	-0.070300	0.893500	-0.767500
C	-1.152500	1.238400	-1.641900
H	-1.189200	0.817100	-2.644200
C	3.354000	-0.513400	0.069600
O	4.084300	-0.727500	1.012400
O	3.768800	-0.490900	-1.208800
C	1.306500	-1.508100	0.882400
O	1.599200	-2.608200	0.469900
O	0.463300	-1.288300	1.902900
C	5.159200	-0.813000	-1.411400
H	5.314700	-0.759500	-2.488600
H	5.797000	-0.095300	-0.889700
H	5.368100	-1.817900	-1.037800
C	-0.089700	-2.476600	2.510900
H	-0.744200	-2.115700	3.303500
H	-0.650100	-3.050200	1.769300
H	0.713800	-3.094800	2.917400
H	-1.630000	2.209600	-1.527500
H	1.257800	0.829800	2.060600
Pt	-1.971900	-0.095800	-0.265500
I	-1.949400	-2.219400	-1.872300
I	-2.969500	1.485000	1.629300

(16). In Path 1C-*b*

36
1C-a1-IN1,Free Energies=-985.039586

C	-1.046001	-2.089089	1.837805
O	-0.625996	-0.798458	1.195536
C	-1.553814	0.221518	1.779049
C	-2.888560	-0.484182	1.586819
C	-2.551306	-1.908716	2.119519
H	-0.768071	-2.870940	1.134371
H	-0.421238	-2.156061	2.728243
H	-1.253377	0.328105	2.823670
H	-2.745311	-1.954036	3.194642
H	-3.159957	-2.679168	1.645398
C	-3.246806	-0.482490	0.072888
C	-2.126445	-1.197498	-0.744441
H	-2.235545	-0.945934	-1.800005
H	-2.263624	-2.284464	-0.657016
C	-0.756340	-0.781622	-0.295592
C	0.313476	-0.331172	-0.947857
H	0.227861	-0.259582	-2.033743
C	-4.601146	-1.189271	-0.128757
O	-5.302642	-1.601724	0.769460
O	-4.899745	-1.289598	-1.431150
C	-3.414079	0.956527	-0.477356
O	-3.060380	1.313838	-1.574968
O	-4.031719	1.747080	0.418422
C	-6.155143	-1.928719	-1.743152
H	-6.226846	-1.906278	-2.829842
H	-6.157873	-2.957226	-1.374322
H	-6.981925	-1.379369	-1.286960
C	-4.249071	3.112447	-0.005020
H	-4.761041	3.593539	0.827698
H	-3.292409	3.598615	-0.209205
H	-4.865885	3.132301	-0.906184
H	-1.356806	1.143568	1.234291
H	-3.689621	-0.022902	2.163027
Pt	1.998791	0.233881	-0.203607
I	1.284901	2.793594	0.145321
I	3.074744	-2.208281	-0.185219

36
1C-b-TS1,Free Energies=-985.009014

C	-2.144669	-1.274713	3.186220
O	-1.295877	-0.402730	2.434570
C	-2.118604	0.694648	2.043662
C	-3.420485	0.034712	1.551365
C	-3.558827	-1.141014	2.561948
H	-1.721073	-2.280921	3.122084
H	-2.146978	-0.969629	4.242265
H	-2.332685	1.341783	2.908479
H	-4.307282	-0.895619	3.319693
H	-3.895779	-2.065566	2.086788
C	-3.355701	-0.426497	0.065855
C	-2.217299	-1.448252	-0.240429
H	-2.370147	-1.871500	-1.238475
H	-2.264754	-2.293248	0.456114
C	-0.857564	-0.925144	-0.182052
C	0.300359	-0.470130	-0.336140
H	-0.210470	-0.284245	-1.380188
C	-4.717450	-1.061951	-0.315089
O	-5.692418	-1.096925	0.397942
O	-4.682486	-1.554308	-1.568148
C	-3.172410	0.768061	-0.897026
O	-2.340754	0.809540	-1.780186
O	-4.056081	1.739912	-0.649041
C	-5.912115	-2.138490	-2.046477
H	-5.699646	-2.466109	-3.063562
H	-6.198680	-2.984361	-1.417145
H	-6.711562	-1.394126	-2.035878
C	-3.962679	2.907407	-1.496841
H	-4.753304	3.573534	-1.153710
H	-2.981770	3.374464	-1.384176
H	-4.114259	2.626224	-2.541346
H	-1.566369	1.280571	1.306120
H	-4.268020	0.715954	1.632382
Pt	2.075248	0.135845	-0.126376
I	1.476560	2.719930	0.134761
I	3.222289	-2.249720	-0.305577

36

1C-b-IN1,Free Energies=-985.043506

C	1.281738	0.896653	2.940837
O	0.904886	-0.428904	2.577227
C	2.080603	-1.061733	2.094441
C	2.966077	0.049557	1.443125
C	2.214272	1.355301	1.813741
H	0.369354	1.490432	3.030434
H	1.803086	0.894440	3.913047
H	2.630242	-1.526093	2.928444
H	2.903291	2.148067	2.111056
H	1.610587	1.732449	0.983608
C	3.292268	-0.151678	-0.070610
C	2.114296	0.064415	-1.070004
H	2.498559	-0.114934	-2.078044
H	1.793603	1.107614	-1.026835
C	0.914102	-0.846643	-0.885016
C	-0.289619	-0.447014	-0.596672
H	1.057128	-1.917738	-1.041201
C	4.398164	0.854301	-0.470074
O	4.820925	1.749086	0.224082
O	4.829860	0.610240	-1.724261
C	3.872712	-1.563471	-0.273400
O	3.365298	-2.444843	-0.935083
O	5.021232	-1.713235	0.408822
C	5.863389	1.488606	-2.210032
H	6.082156	1.147300	-3.221625
H	5.510331	2.522667	-2.217871
H	6.750170	1.416478	-1.575610
C	5.650626	-3.005520	0.303342
H	6.551879	-2.938411	0.912128
H	4.984250	-3.784305	0.681876
H	5.900626	-3.220605	-0.738343
H	1.772027	-1.856242	1.410850
H	3.936562	0.054964	1.943623
Pt	-1.950798	0.090441	-0.212424
I	-3.270857	-2.194010	-0.165788
I	-1.666519	2.718805	-0.060077

36

1C-b-TS2,Free Energies=-985.026459

C	-1.183857	-2.558032	2.319888
O	-0.678397	-1.215230	2.533398
C	-1.265446	-0.343105	1.640286
C	-2.547480	-0.988167	1.125073
C	-2.128749	-2.474184	1.112165
H	-0.331279	-3.222838	2.160619
H	-1.702964	-2.856128	3.237958
H	-1.341912	0.656806	2.077933
H	-2.986062	-3.143597	1.197354
H	-1.582411	-2.722725	0.196596
C	-3.089442	-0.382080	-0.195464
C	-2.292162	-0.728603	-1.478654
H	-2.775502	-0.205303	-2.306058
H	-2.403541	-1.801538	-1.684212
C	-0.816218	-0.399285	-1.560308
C	0.150575	-0.151543	-0.710559
H	-0.414910	-0.383974	-2.580555
C	-4.529652	-0.917162	-0.397256
O	-5.062581	-1.756490	0.292609
O	-5.117412	-0.329003	-1.453461
C	-3.207897	1.157801	-0.090991
O	-2.814427	1.941366	-0.921695
O	-3.834193	1.511523	1.048310
C	-6.466081	-0.752616	-1.736524
H	-6.775233	-0.170627	-2.604190
H	-6.488632	-1.822322	-1.958349
H	-7.113638	-0.548702	-0.880493
C	-4.022397	2.929680	1.238131
H	-4.547157	3.026487	2.188221
H	-3.055896	3.438006	1.273963
H	-4.616981	3.344084	0.420636
H	-0.555140	-0.188703	0.737009
H	-3.321007	-0.851193	1.887287
Pt	1.871276	0.185176	-0.163288
I	1.698649	2.821638	0.088381
I	2.688174	-2.341732	-0.281121

36

1C-a2-IN2,Free Energies=-985.079638

C	-2.194312	-2.686053	-2.580152
O	-1.135422	-2.541841	-1.614404
C	-1.557993	-1.717551	-0.554766
C	-3.078539	-1.484675	-0.715330
C	-3.238467	-1.615799	-2.244540
H	-1.766806	-2.578629	-3.581391
H	-2.613290	-3.697661	-2.489951
H	-1.287116	-2.197791	0.389938
H	-4.251918	-1.894413	-2.534509
H	-2.998906	-0.672254	-2.747323
C	-3.346344	-0.100912	-0.081240
C	-2.102431	0.748630	-0.464443
H	-1.903224	1.515945	0.285855
H	-2.272237	1.265589	-1.412339
C	-0.914775	-0.257940	-0.650140
C	0.105952	-0.059495	0.393688
H	-0.475635	-0.168187	-1.644567
C	-4.652068	0.558477	-0.536057
O	-5.465788	0.082983	-1.294184
O	-4.763357	1.778545	0.024890
C	-3.396178	-0.287998	1.445629
O	-2.461407	-0.105202	2.198181
O	-4.594940	-0.740878	1.840136
C	-5.955083	2.514484	-0.311326
H	-5.869992	3.462418	0.219429
H	-6.009120	2.678708	-1.390302
H	-6.842681	1.966036	0.013765
C	-4.740426	-0.996182	3.252753
H	-5.764515	-1.346289	3.377906
H	-4.027362	-1.758730	3.574812
H	-4.570359	-0.078981	3.821187
H	-0.236154	-0.069019	1.435193
H	-3.657375	-2.269510	-0.218292
Pt	1.892989	0.213161	0.126095
I	2.028928	2.832745	-0.271444
I	2.965126	-2.196189	0.311138

36

1C-a2-TS2,Free Energies=-985.051236

C	-2.619890	-1.647434	3.230285
O	-1.580367	-0.640233	3.250247
C	-1.823683	0.287099	2.209430
C	-3.160238	-0.068272	1.529239
C	-3.252739	-1.576201	1.836813
H	-2.155880	-2.610701	3.456254
H	-3.351259	-1.414397	4.015107
H	-1.798796	1.314709	2.596648
H	-4.280660	-1.944472	1.813466
H	-2.666465	-2.168853	1.122056
C	-2.996105	0.351515	0.044856
C	-1.467108	0.221647	-0.250245
H	-1.061337	1.035327	-0.862249
H	-1.228174	-0.691015	-0.811200
C	-0.791817	0.182140	1.083330
C	0.569301	-0.053391	1.298926
H	-0.026493	-1.116790	1.254706
C	-3.918538	-0.463889	-0.867421
O	-5.101054	-0.599300	-0.639123
O	-3.278503	-1.000749	-1.914913
C	-3.376610	1.839221	-0.096172
O	-3.472601	2.610914	0.832263
O	-3.523347	2.174705	-1.384805
C	-4.098534	-1.759285	-2.828155
H	-3.415443	-2.122275	-3.595051
H	-4.575731	-2.591298	-2.305333
H	-4.867314	-1.115904	-3.262291
C	-3.820921	3.563947	-1.644674
H	-3.907023	3.641513	-2.727790
H	-4.757685	3.844501	-1.158112
H	-3.012410	4.197665	-1.273045
H	0.915266	0.000436	2.334451
H	-3.991655	0.466965	1.989392
Pt	1.931187	-0.123225	-0.084456
I	2.536432	2.459020	-0.032820
I	1.496337	-2.737118	-0.541257

36
1C-a2-P,Free Energies=-985.078245

C	-3.414937	-1.360411	3.361276
O	-2.123981	-0.713993	3.355990
C	-1.924631	-0.065348	2.119490
C	-3.261123	-0.064783	1.358739
C	-3.916210	-1.345835	1.911189
H	-3.297473	-2.367424	3.773236
H	-4.083813	-0.792712	4.021374
H	-1.532213	0.938378	2.297130
H	-5.005769	-1.319169	1.838719
H	-3.567036	-2.235824	1.372126
C	-2.904204	-0.044163	-0.142252
C	-1.559127	-0.834109	-0.265737
H	-0.880996	-0.359119	-0.977524
H	-1.744824	-1.841473	-0.640517
C	-0.955341	-0.892772	1.156524
C	0.445845	-0.514448	1.376529
H	-1.005427	-1.921012	1.553829
C	-4.065681	-0.567711	-0.994091
O	-5.212574	-0.210383	-0.825979
O	-3.682334	-1.445317	-1.934982
C	-2.660531	1.419984	-0.569557
O	-2.574069	2.355298	0.194000
O	-2.524687	1.511591	-1.901709
C	-4.731296	-1.924410	-2.797947
H	-4.245886	-2.613285	-3.488908
H	-5.500809	-2.436196	-2.214719
H	-5.185973	-1.089982	-3.337285
C	-2.232988	2.829840	-2.412871
H	-2.206871	2.718119	-3.496499
H	-3.013710	3.532191	-2.112211
H	-1.266485	3.171068	-2.034626
H	0.793924	-0.555312	2.417372
H	-3.855167	0.811197	1.626306
Pt	1.716904	-0.008746	0.159836
I	1.642628	2.632231	0.125251
I	2.653646	-2.344493	-0.668106

(17). In Path 1D-*a*

38
1D-IN1,Free Energies=-1007.894117

C	3.409143	-2.717450	-2.462877
O	2.965285	-1.468735	-2.989882
C	3.819775	-0.478723	-2.432586
C	4.234225	-0.978551	-1.011153
C	3.700006	-2.435701	-0.982112
H	2.616490	-3.451090	-2.627761
H	4.317877	-3.053712	-2.989343
H	4.720391	-0.361759	-3.054834
H	4.425690	-3.123662	-0.542990
H	2.770813	-2.519969	-0.411358
C	3.792493	-0.065860	0.172462
C	2.282878	-0.137286	0.589195
H	2.084930	0.702121	1.260986
H	2.103307	-1.061107	1.150104
C	1.339432	-0.102423	-0.525224
C	0.582753	-0.142224	-1.495226
H	0.267290	-0.205726	-2.516346
C	4.599591	-0.461499	1.431845
O	5.360510	-1.397440	1.509474
O	4.327072	0.377963	2.447841
C	4.135246	1.400470	-0.156214
O	3.333255	2.301704	-0.241766
O	5.457774	1.541521	-0.359609
C	5.012973	0.106215	3.686980
H	4.673560	0.875558	4.379787
H	4.751140	-0.889093	4.053793
H	6.094018	0.164109	3.539799
C	5.900195	2.876361	-0.679263
H	6.980445	2.801227	-0.800883
H	5.428540	3.221191	-1.602519
H	5.646807	3.562780	0.132079
H	3.277264	0.470664	-2.441385
H	5.323798	-1.001678	-0.957047
Pt	-1.074246	0.080305	0.074562
I	-3.098421	0.431031	1.771695
I	-0.998486	2.736165	-0.441306
I	-2.835301	-0.549184	-1.880760
I	-0.805426	-2.512610	0.887517

38
1D-a-TS1,Free Energies=-1007.883155

C	3.673265	-2.945433	-2.168034
O	3.438623	-1.777322	-3.001596
C	3.621900	-0.633739	-2.272604
C	4.333233	-0.963447	-0.966080
C	3.877466	-2.423799	-0.739355
H	2.814235	-3.612386	-2.270963
H	4.562813	-3.446246	-2.566181
H	4.013404	0.175830	-2.896517
H	4.618612	-2.995200	-0.180024
H	2.932770	-2.460947	-0.187991
C	3.974320	0.063138	0.136744
C	2.437697	0.135286	0.389561
H	2.210997	1.089376	0.875323
H	2.143419	-0.671484	1.072309
C	1.590090	0.015959	-0.816999
C	0.422740	-0.085471	-1.333107
H	0.134353	-0.249336	-2.362914
C	4.687244	-0.295667	1.451945
O	5.443753	-1.227625	1.601357
O	4.342971	0.571485	2.416865
C	4.466934	1.448395	-0.334546
O	3.755949	2.298020	-0.820246
O	5.796959	1.559591	-0.187901
C	4.941697	0.344549	3.710265
H	4.542590	1.127560	4.353885
H	4.666202	-0.643836	4.085116
H	6.029514	0.415540	3.637915
C	6.374188	2.808707	-0.625919
H	7.440706	2.720031	-0.422336
H	6.192659	2.955592	-1.693233
H	5.938132	3.640156	-0.067765
H	2.565676	-0.195294	-1.934033
H	5.417678	-0.930296	-1.118069
Pt	-1.194442	0.088562	0.035530
I	-3.122173	0.389700	1.902527
I	-1.251141	2.725586	-0.568908
I	-2.931831	-0.675732	-1.861598
I	-0.651232	-2.440139	0.909962

38

1D-a-IN2,Free Energies=-1007.945303

C	2.617857	3.601079	-1.755330
O	1.582298	3.131260	-0.887558
C	2.169343	2.267309	0.082932
C	3.544739	1.796990	-0.495987
C	3.542765	2.399255	-1.921931
H	2.144911	3.937135	-2.681558
H	3.140281	4.455329	-1.296631
H	2.272579	2.810012	1.031939
H	4.546175	2.655288	-2.264978
H	3.113023	1.702423	-2.647565
C	3.527118	0.244038	-0.389239
C	2.028438	-0.124791	-0.513690
H	1.810781	-1.121598	-0.132009
H	1.729792	-0.090506	-1.567729
C	1.304089	0.976838	0.305840
C	-0.115601	1.174130	-0.126097
H	-0.232008	1.650122	-1.095297
C	4.398637	-0.474777	-1.427932
O	5.159427	0.043629	-2.212520
O	4.201066	-1.805391	-1.340005
C	4.055655	-0.170203	0.999898
O	3.378523	-0.548264	1.928952
O	5.393063	-0.023158	1.058788
C	4.978460	-2.612801	-2.243927
H	4.693774	-3.642686	-2.030073
H	4.746157	-2.354675	-3.280084
H	6.045954	-2.459749	-2.066321
C	6.003893	-0.369827	2.316814
H	7.071428	-0.202033	2.175871
H	5.614075	0.264809	3.116555
H	5.803547	-1.416082	2.559810
H	1.356918	0.694407	1.357429
H	4.380897	2.213580	0.071829
Pt	-1.511960	-0.265296	0.162803
I	-0.780337	-1.359473	2.537893
I	-1.386005	2.415028	1.249045
I	-2.955052	0.613958	-1.976729
I	-1.036206	-2.556885	-1.080383

38

1D-a-TS2,Free Energies=-1007.919609

C	2.872153	-3.436612	-2.470029
O	1.666625	-2.663493	-2.358164
C	2.021906	-1.293568	-2.271014
C	3.529340	-1.209003	-1.883256
C	3.899598	-2.687119	-1.621527
H	2.645372	-4.443962	-2.114904
H	3.181565	-3.491758	-3.524014
H	1.774861	-0.762133	-3.196829
H	4.934585	-2.904154	-1.891100
H	3.768382	-2.949971	-0.566083
C	3.583581	-0.270753	-0.637934
C	2.225552	-0.536902	0.073310
H	1.925362	0.222399	0.796833
H	2.254166	-1.491842	0.611628
C	1.263886	-0.706741	-1.065220
C	-0.098780	-0.453712	-1.142713
H	-0.563690	-0.683552	-2.100015
C	4.821488	-0.504317	0.227338
O	5.889688	-0.871367	-0.209399
O	4.570010	-0.242371	1.517675
C	3.528483	1.182827	-1.136193
O	2.653088	1.560722	-1.897138
O	4.490472	1.959444	-0.652248
C	5.691077	-0.374053	2.415585
H	5.297949	-0.138944	3.403833
H	6.083327	-1.393238	2.384377
H	6.480600	0.326398	2.133211
C	4.449687	3.351197	-1.052772
H	5.306277	3.811934	-0.563312
H	4.530649	3.429192	-2.138785
H	3.514663	3.805157	-0.718554
H	0.747350	0.488347	-1.430479
H	4.128011	-0.809010	-2.704225
Pt	-1.369133	0.121239	0.255565
I	-0.069328	2.302568	1.305147
I	-2.537254	1.781842	-1.596740
I	-3.041913	-1.906502	-0.510223
I	-0.579882	-1.400219	2.384177

38
1D-P,Free Energies=-1007.93431

C	-2.237019	3.512985	-0.678951
O	-1.181642	2.573999	-0.466084
C	-1.451118	1.456051	-1.292471
C	-3.020224	1.354061	-1.380496
C	-3.498747	2.649467	-0.677424
H	-2.187906	4.245689	0.129129
H	-2.099290	4.032528	-1.639736
H	-0.973532	1.580737	-2.272012
H	-4.349560	3.105439	-1.189605
H	-3.795904	2.453511	0.358346
C	-3.408773	0.018401	-0.662230
C	-2.182923	-0.291373	0.256101
H	-2.128915	-1.330715	0.577407
H	-2.233935	0.336879	1.147295
C	-1.046503	0.133457	-0.651528
C	-0.259137	-0.811319	-1.375709
H	0.120137	-0.539134	-2.356289
C	-4.759831	0.130453	0.048977
O	-5.773373	0.452849	-0.531208
O	-4.687660	-0.148705	1.358425
C	-3.508568	-1.114254	-1.698094
O	-2.965990	-1.095620	-2.783516
O	-4.204856	-2.154676	-1.220972
C	-5.935279	-0.082034	2.078731
H	-5.686225	-0.326894	3.110714
H	-6.360756	0.921775	2.008109
H	-6.644736	-0.803910	1.667403
C	-4.324705	-3.293346	-2.099422
H	-4.932997	-4.014215	-1.554441
H	-4.811680	-2.999207	-3.031723
H	-3.337717	-3.707397	-2.319316
H	-0.414633	-1.872018	-1.204985
H	-3.344897	1.321756	-2.420439
Pt	1.108218	-0.063551	0.136941
I	0.477289	-2.047998	1.952619
I	2.730556	-1.885595	-1.113633
I	2.182370	1.860822	-1.498903
I	0.855948	1.762470	2.098610

(18). In Path 1D-*b*

38
1D-b-TS1,Free Energies=-1007.876802

C	-3.415630	-2.708298	2.411247
O	-2.877496	-1.499656	2.960954
C	-3.144638	-0.398052	2.096500
C	-4.128654	-0.926189	1.028969
C	-3.719685	-2.407450	0.940545
H	-2.680010	-3.507631	2.542778
H	-4.331609	-2.986108	2.954034
H	-3.580904	0.419052	2.684814
H	-4.508570	-3.039853	0.525359
H	-2.808247	-2.539983	0.345787
C	-4.220243	-0.125686	-0.302970
C	-3.114019	-0.411424	-1.363748
H	-3.356876	0.128751	-2.284150
H	-3.113269	-1.479806	-1.622809
C	-1.737336	-0.126328	-0.995076
C	-0.546347	0.159711	-0.758814
H	-1.098524	1.202510	-0.698220
C	-5.573160	-0.447546	-0.985836
O	-6.368096	-1.274265	-0.607193
O	-5.739392	0.316285	-2.082045
C	-4.179070	1.382351	0.001443
O	-3.247373	2.105979	-0.289958
O	-5.271813	1.782430	0.655498
C	-6.972437	0.115707	-2.805361
H	-6.931142	0.809178	-3.644607
H	-7.040995	-0.916465	-3.156549
H	-7.825709	0.335682	-2.159864
C	-5.310829	3.178174	1.032229
H	-6.260116	3.307974	1.550138
H	-4.471742	3.412449	1.690852
H	-5.262021	3.807818	0.141208
H	-2.202020	-0.042226	1.664642
H	-5.134687	-0.890253	1.457239
Pt	1.444962	0.110485	-0.428483
I	4.115150	0.058458	-0.273534
I	1.379778	2.836483	-0.205796
I	1.120310	-0.436808	2.185789
I	1.352781	-2.492000	-1.243474

38
1D-b-IN2,Free Energies=-1007.894468

C	-2.882061	-1.049312	3.253975
O	-2.656964	0.366193	3.249806
C	-3.177263	0.943309	2.053662
C	-3.922477	-0.190798	1.313405
C	-3.159188	-1.435468	1.800071
H	-1.994610	-1.536986	3.668564
H	-3.742640	-1.287430	3.897850
H	-3.850240	1.770509	2.314890
H	-3.746362	-2.351142	1.700637
H	-2.211596	-1.563886	1.266482
C	-4.105100	-0.013954	-0.222933
C	-2.857051	-0.318442	-1.106011
H	-3.158671	-0.204843	-2.151920
H	-2.551033	-1.356025	-0.959893
C	-1.661218	0.590245	-0.905635
C	-0.412265	0.312695	-0.714277
H	-1.852394	1.666728	-1.013968
C	-5.210064	-0.991739	-0.698505
O	-5.724043	-1.853199	-0.024880
O	-5.517145	-0.763695	-1.990580
C	-4.610655	1.413655	-0.501527
O	-3.984720	2.282833	-1.073713
O	-5.838873	1.594153	0.007116
C	-6.538641	-1.613611	-2.549276
H	-6.652030	-1.288764	-3.583228
H	-6.228080	-2.660146	-2.503363
H	-7.474211	-1.490870	-1.998416
C	-6.406885	2.908985	-0.164765
H	-7.386215	2.863727	0.310442
H	-5.776002	3.659570	0.317027
H	-6.500547	3.143303	-1.227716
H	-2.346868	1.354488	1.466643
H	-4.934959	-0.247192	1.724788
Pt	1.455404	0.003435	-0.432518
I	4.050238	-0.670828	-0.345988
I	1.978580	2.620995	-0.931426
I	1.267057	0.325675	2.239977
I	0.559146	-2.598157	-0.588668

38

1D-b-TS2,Free Energies=-1007.875525

C	2.611665	3.273495	1.160987
O	1.920709	2.228669	1.882577
C	2.236801	0.989426	1.333983
C	3.591257	1.152805	0.643459
C	3.434903	2.575237	0.066644
H	1.868928	3.969459	0.760162
H	3.243335	3.804715	1.882449
H	2.182267	0.220698	2.109180
H	4.396051	3.057512	-0.114913
H	2.868356	2.562950	-0.871143
C	3.995378	0.011683	-0.325852
C	3.122641	-0.133412	-1.600705
H	3.614277	-0.855602	-2.251384
H	3.112179	0.823057	-2.135629
C	1.689134	-0.602731	-1.436823
C	0.652808	-0.245264	-0.727976
H	1.376857	-1.414386	-2.106165
C	5.459562	0.267357	-0.773075
O	6.133783	1.216125	-0.444589
O	5.897855	-0.721839	-1.573025
C	4.013013	-1.352899	0.403346
O	3.474607	-2.358084	0.000633
O	4.727714	-1.281885	1.540462
C	7.259552	-0.599380	-2.030818
H	7.437910	-1.481219	-2.645409
H	7.381101	0.314185	-2.617787
H	7.943415	-0.573712	-1.179163
C	4.828084	-2.510250	2.290657
H	5.437336	-2.267713	3.160832
H	3.834996	-2.850379	2.593674
H	5.304556	-3.284647	1.684893
H	1.448037	0.698970	0.565959
H	4.356283	1.187263	1.425536
Pt	-1.254021	-0.043281	-0.375807
I	-3.940876	0.154897	-0.432588
I	-1.403414	-2.754970	-0.709284
I	-1.254247	-0.247414	2.317973
I	-0.997659	2.655874	-0.727414

38

1D-b-IN3,Free Energies=-1007.939564

C	2.155834	-3.371449	-1.446012
O	1.123273	-2.369546	-1.387152
C	1.686835	-1.100615	-1.145676
C	3.217625	-1.238022	-1.311922
C	3.430173	-2.712873	-0.909409
H	1.832109	-4.236681	-0.860103
H	2.276478	-3.686604	-2.491358
H	1.235352	-0.385472	-1.838694
H	4.345011	-3.130895	-1.329886
H	3.489315	-2.818221	0.180073
C	3.833895	-0.154936	-0.395776
C	2.880656	-0.110470	0.833901
H	2.842341	0.890324	1.267331
H	3.254250	-0.775754	1.617523
C	1.480681	-0.629271	0.359327
C	0.445043	0.441781	0.473268
H	1.178657	-1.509490	0.927688
C	5.286381	-0.438450	0.009641
O	5.983113	-1.330513	-0.414430
O	5.685245	0.458881	0.932300
C	3.884143	1.162348	-1.191401
O	4.821413	1.487655	-1.884170
O	2.749700	1.884374	-1.084407
C	7.057009	0.345457	1.355653
H	7.200588	1.136800	2.091236
H	7.239233	-0.635479	1.801668
H	7.726060	0.483873	0.502940
C	2.703380	3.096266	-1.872508
H	1.708608	3.509356	-1.707949
H	3.477089	3.789518	-1.535227
H	2.859848	2.864031	-2.927976
H	0.735076	1.392058	0.033927
H	3.522228	-1.098651	-2.354097
Pt	-1.524022	0.085126	0.193036
I	-1.876528	-2.387848	1.254876
I	-0.178573	0.997453	2.590790
I	-1.915636	2.661837	-0.630381
I	-2.205119	-0.803781	-2.201805

38

1D-b-TS3,Free Energies=-1007.907249

C	2.887913	3.478391	0.496525
O	1.813856	2.686334	-0.029141
C	1.974941	1.374662	0.505692
C	3.513183	1.163397	0.712050
C	4.105466	2.562181	0.387903
H	2.948591	4.384586	-0.109598
H	2.671088	3.757880	1.537507
H	1.373116	1.233902	1.407885
H	4.922609	2.826023	1.061619
H	4.498531	2.599198	-0.632178
C	3.924441	0.008411	-0.266716
C	2.843435	0.064327	-1.386415
H	2.757848	-0.853889	-1.969028
H	3.083311	0.885285	-2.071842
C	1.587463	0.410508	-0.606551
C	0.338415	-0.115928	-0.928689
H	0.622384	1.028958	-1.399869
C	5.362535	0.123929	-0.786864
O	6.264763	0.659763	-0.188324
O	5.484399	-0.476438	-1.981995
C	3.864249	-1.350093	0.460778
O	4.820685	-2.057843	0.672875
O	2.605440	-1.628990	0.831240
C	6.824902	-0.536060	-2.513036
H	6.733934	-1.045083	-3.472078
H	7.226824	0.471429	-2.643611
H	7.468286	-1.099115	-1.833317
C	2.402434	-2.877677	1.541832
H	1.328948	-2.938296	1.707502
H	2.758848	-3.709005	0.930491
H	2.948944	-2.853190	2.486865
H	0.331574	-0.773625	-1.795299
H	3.735698	0.887284	1.744486
Pt	-1.398123	-0.060303	0.026275
I	-1.786864	2.572641	0.583460
I	-2.536648	0.349403	-2.446773
I	-1.537292	-2.787290	-0.354600
I	-0.781580	-0.500746	2.649323

38

1D-P,Free Energies=-1007.93431

C	-2.237019	3.512985	-0.678951
O	-1.181642	2.573999	-0.466084
C	-1.451118	1.456051	-1.292471
C	-3.020224	1.354061	-1.380496
C	-3.498747	2.649467	-0.677424
H	-2.187906	4.245689	0.129129
H	-2.099290	4.032528	-1.639736
H	-0.973532	1.580737	-2.272012
H	-4.349560	3.105439	-1.189605
H	-3.795904	2.453511	0.358346
C	-3.408773	0.018401	-0.662230
C	-2.182923	-0.291373	0.256101
H	-2.128915	-1.330715	0.577407
H	-2.233935	0.336879	1.147295
C	-1.046503	0.133457	-0.651528
C	-0.259137	-0.811319	-1.375709
H	0.120137	-0.539134	-2.356289
C	-4.759831	0.130453	0.048977
O	-5.773373	0.452849	-0.531208
O	-4.687660	-0.148705	1.358425
C	-3.508568	-1.114254	-1.698094
O	-2.965990	-1.095620	-2.783516
O	-4.204856	-2.154676	-1.220972
C	-5.935279	-0.082034	2.078731
H	-5.686225	-0.326894	3.110714
H	-6.360756	0.921775	2.008109
H	-6.644736	-0.803910	1.667403
C	-4.324705	-3.293346	-2.099422
H	-4.932997	-4.014215	-1.554441
H	-4.811680	-2.999207	-3.031723
H	-3.337717	-3.707397	-2.319316
H	-0.414633	-1.872018	-1.204985
H	-3.344897	1.321756	-2.420439
Pt	1.108218	-0.063551	0.136941
I	0.477289	-2.047998	1.952619
I	2.730556	-1.885595	-1.113633
I	2.182370	1.860822	-1.498903
I	0.855948	1.762470	2.098610

(19). In Path 2D-*a*

39
2D-a-IN1,Free Energies=-822.514404

C	-2.390300	5.466100	-0.233800
C	-3.348300	4.272200	-0.440900
C	-2.615300	2.924800	-0.671300
C	-1.284500	2.920900	0.117800
C	-0.334000	3.999800	-0.486200
C	-1.086200	5.246300	-1.007300
H	-2.876800	6.396000	-0.548100
H	-3.994800	4.146000	0.435800
H	-1.520900	3.191900	1.157200
H	0.381400	4.298600	0.288800
H	-1.317200	5.123900	-2.073500
H	-4.003900	4.466300	-1.297800
H	-2.161800	5.585900	0.833500
H	-0.434500	6.123900	-0.933700
H	0.249800	3.550700	-1.297400
H	-2.374400	2.805500	-1.741200
O	-3.405900	1.820700	-0.259000
C	-4.560400	1.575700	-1.067500
H	-5.295900	2.380000	-0.914700
C	-0.639700	1.564900	0.154300
C	-0.982600	0.343600	-0.206400
H	-4.280800	1.583100	-2.132600
H	-1.931500	0.046000	-0.635300
C	-5.149800	0.238700	-0.689800
C	-5.402000	-0.730600	-1.666400
C	-5.464100	-0.043200	0.647400
C	-5.966000	-1.960700	-1.317900
H	-5.156600	-0.524700	-2.705900
C	-6.016700	-1.273800	0.998100
H	-5.260100	0.700700	1.412400
C	-6.272100	-2.235000	0.015400
H	-6.158100	-2.703800	-2.087000
H	-6.248700	-1.484400	2.038500
H	-6.704300	-3.193300	0.289900
Pt	0.353900	-1.108900	0.133900
I	-0.505400	-1.715900	2.633800
I	-0.960000	-3.201600	-0.858500
I	1.685600	-0.789600	-2.212800
I	1.388500	1.416500	1.078500

39
2D-a-TS1,Free Energies=-822.486048

C	-1.006600	5.330700	-0.318300
C	-2.269100	4.514800	-0.668300
C	-1.950600	3.130200	-1.249700
C	-0.611800	2.572700	-0.586700
C	0.563000	3.487400	-1.099600
C	0.145400	4.965000	-1.260700
H	-1.232200	6.400400	-0.375100
H	-2.894500	4.362600	0.218000
H	-0.747000	2.684600	0.496200
H	1.368200	3.384700	-0.367100
H	-0.157700	5.165800	-2.296700
H	-2.881400	5.049200	-1.403400
H	-0.705400	5.134200	0.718600
H	1.018600	5.597300	-1.068000
H	0.941400	3.084600	-2.042400
H	-1.768900	3.175800	-2.332900
O	-3.047200	2.288600	-0.989900
C	-2.967800	1.065600	-1.650100
H	-2.998200	1.183400	-2.743900
C	-0.350800	1.180400	-0.860300
C	0.158900	-0.000000	-0.963000
H	-0.331800	-0.857700	-1.414000
C	-3.941200	0.052100	-1.146500
C	-4.476500	-0.889700	-2.036900
C	-4.285500	-0.003500	0.212600
C	-5.351100	-1.873000	-1.576400
H	-4.212000	-0.849700	-3.091000
C	-5.164800	-0.982600	0.667800
H	-3.869500	0.724500	0.901600
C	-5.696300	-1.920100	-0.224100
H	-5.764000	-2.597800	-2.271800
H	-5.431700	-1.020100	1.719800
H	-6.375900	-2.687100	0.136300
Pt	1.978200	-0.472000	-0.253500
I	2.122100	1.290900	1.850300
I	0.757300	-2.282000	1.410400
I	2.228800	-2.422300	-2.155800
I	3.622600	1.127800	-1.734800
H	-1.902000	0.690000	-1.443900

39

2D-a-IN2,Free Energies=-822.5371

C	-1.673600	5.227000	0.168200
C	-2.995200	4.425800	0.137500
C	-2.878600	3.182600	-0.753400
C	-1.447800	2.608200	-0.788800
C	-0.552100	3.668300	-1.501900
C	-0.945100	5.131600	-1.178300
H	-1.888800	6.269800	0.424400
H	-3.254500	4.093300	1.148000
H	-1.111800	2.487200	0.243500
H	0.475500	3.463800	-1.187700
H	-1.596800	5.533800	-1.967200
H	-3.820700	5.050900	-0.222700
H	-1.024800	4.836600	0.960900
H	-0.049200	5.761400	-1.173500
H	-0.587100	3.503500	-2.586300
H	-3.230000	3.372400	-1.775600
O	-3.818500	2.180800	-0.195200
C	-4.234600	1.220500	-0.934400
H	-4.027500	1.267300	-2.003500
C	-1.385400	1.285300	-1.488800
C	-1.000000	0.071800	-1.065900
H	-1.639700	1.318400	-2.555200
H	-1.001800	-0.755200	-1.768200
C	-5.026500	0.162400	-0.417100
C	-5.541700	-0.787100	-1.332800
C	-5.306800	0.045600	0.966100
C	-6.334000	-1.826900	-0.873700
H	-5.308500	-0.698600	-2.390600
C	-6.099400	-1.000600	1.411200
H	-4.875500	0.756500	1.660900
C	-6.611200	-1.930700	0.496500
H	-6.729400	-2.561100	-1.567900
H	-6.307800	-1.108300	2.470400
H	-7.226100	-2.751100	0.855800
Pt	-0.290800	-0.542900	0.704200
I	-1.789900	0.769800	2.617200
I	-2.118700	-2.601200	0.698400
I	1.494800	-2.148800	-0.610200
I	1.690100	1.314000	1.006600

39

2D-a-TS2,Free Energies=-822.517926

C	-3.662400	3.348400	-0.558100
C	-2.267500	3.979700	-0.835700
C	-1.293200	3.556900	0.257600
C	-1.559300	2.117300	0.726700
C	-2.863400	2.096300	1.547700
C	-3.900700	3.088700	0.943100
H	-4.446800	4.002000	-0.953800
H	-1.882700	3.637700	-1.802800
H	-1.684500	1.505200	-0.171300
H	-3.263600	1.078500	1.559700
H	-3.858000	4.044900	1.482000
H	-2.331400	5.072700	-0.876900
H	-3.748500	2.399700	-1.101300
H	-4.912900	2.699400	1.095900
H	-2.656600	2.368600	2.591700
H	-1.359800	4.240200	1.119800
O	0.076800	3.551500	-0.178600
C	0.842900	3.056600	0.829500
H	0.759300	3.640600	1.754200
C	-0.282300	1.674800	1.421900
C	0.366000	0.429200	1.234600
H	-0.249900	1.901400	2.495700
H	1.234100	0.248700	1.864200
C	2.257300	2.784200	0.476200
C	3.218100	2.781600	1.500000
C	2.658800	2.585700	-0.851800
C	4.562300	2.569600	1.202500
H	2.913600	2.956100	2.530400
C	4.006300	2.389000	-1.146600
H	1.917400	2.587600	-1.642200
C	4.958000	2.375500	-0.123800
H	5.299700	2.567600	1.999800
H	4.312500	2.237500	-2.177300
H	6.006700	2.217000	-0.359200
Pt	-0.025600	-1.017000	0.007200
I	0.030500	0.017600	-2.505000
I	2.667300	-1.523700	-0.137700
I	-2.711100	-1.435200	-0.288000
I	-0.165000	-2.379700	2.424000

39

2D-a-IN3,Free Energies=-822.524786

C	2.569400	4.483500	-0.585800
C	3.741100	3.468700	-0.731000
C	3.552900	2.327900	0.264400
C	2.069900	1.978800	0.437600
C	1.361300	3.093600	1.223100
C	1.953300	4.480600	0.829000
H	2.918400	5.491500	-0.835600
H	3.759200	3.053900	-1.745400
H	1.643600	1.921600	-0.568200
H	0.285800	3.066500	1.019700
H	2.725800	4.770300	1.553800
H	4.707500	3.957200	-0.563200
H	1.784400	4.241800	-1.313000
H	1.173200	5.247100	0.893800
H	1.484300	2.935200	2.303500
H	3.970600	2.616500	1.246300
O	4.164700	1.102600	-0.130800
C	3.666900	0.141000	0.778400
H	4.136900	0.309900	1.762700
C	2.121200	0.547100	1.013300
C	1.141400	-0.499100	0.543800
H	1.982000	0.583400	2.102600
H	1.477300	-1.516700	0.722900
C	3.999600	-1.265400	0.342100
C	4.039900	-2.288200	1.301300
C	4.295500	-1.569900	-0.991100
C	4.347300	-3.597800	0.931700
H	3.845700	-2.056300	2.347400
C	4.615500	-2.878400	-1.357900
H	4.286400	-0.777800	-1.730600
C	4.637100	-3.895400	-0.402000
H	4.375100	-4.379800	1.685500
H	4.847300	-3.102000	-2.395500
H	4.886000	-4.912500	-0.691900
Pt	-0.006100	-0.391700	-1.131900
I	1.368200	-0.069400	-3.376400
I	0.167500	-3.095600	-1.353600
I	-1.288400	1.969600	-1.571700
I	-0.904200	-0.512400	1.592800

39

2D-a-IN4,Free Energies=-822.530364

C	2.717200	4.536700	-1.085100
C	3.909700	3.533900	-1.106700
C	3.694100	2.493200	-0.015300
C	2.211400	2.113000	0.105200
C	1.476200	3.269700	0.803400
C	2.044100	4.635100	0.301800
H	3.059800	5.528300	-1.400300
H	3.966700	3.030900	-2.079400
H	1.815400	2.002300	-0.911100
H	0.402500	3.207700	0.611600
H	2.776100	5.019300	1.024300
H	4.863800	4.050400	-0.952800
H	1.965300	4.225500	-1.820600
H	1.238500	5.376300	0.264200
H	1.608700	3.196100	1.891100
H	4.030300	2.904300	0.953100
O	4.377400	1.257700	-0.216400
C	3.841100	0.401100	0.770100
H	4.168700	0.751800	1.764000
C	2.251700	0.711300	0.756300
C	1.443600	-0.412800	0.181000
H	1.913900	0.747100	1.802900
H	1.670100	-1.371000	0.639200
C	4.316500	-1.020900	0.591300
C	4.085600	-1.959500	1.607800
C	5.013300	-1.418500	-0.555800
C	4.515300	-3.279300	1.467300
H	3.575200	-1.656900	2.520600
C	5.454200	-2.737600	-0.690000
H	5.223300	-0.686100	-1.327400
C	5.199800	-3.672700	0.314400
H	4.323900	-3.995700	2.261200
H	6.001500	-3.031800	-1.581500
H	5.540500	-4.698500	0.205900
Pt	-0.565500	-0.242900	-0.146600
I	-0.849300	-2.806300	0.713500
I	-1.752600	0.676700	2.042800
I	-1.362700	1.915700	-1.585300
I	1.548400	-0.879300	-2.008400

39

2D-a-TS3,Free Energies=-822.5069

C	2.947600	4.370900	-1.164300
C	4.125500	3.562200	-0.548100
C	3.584700	2.505600	0.413300
C	2.226100	1.967600	-0.049900
C	1.119500	3.029700	0.070500
C	1.722400	4.433800	-0.230900
H	3.282900	5.385100	-1.405200
H	4.695900	3.057700	-1.336300
H	2.335300	1.683600	-1.110200
H	0.309100	2.799200	-0.629500
H	2.015300	4.914400	0.711600
H	4.821100	4.223900	-0.021200
H	2.646600	3.916400	-2.117000
H	0.948900	5.071600	-0.670900
H	0.677200	3.024600	1.072600
H	3.473400	2.930800	1.425800
O	4.409400	1.340600	0.492100
C	3.634500	0.309700	1.089900
H	3.671400	0.397100	2.189400
C	2.167800	0.634500	0.647000
C	1.096300	-0.243800	0.773200
H	1.348000	-1.194800	1.249800
C	4.120400	-1.060000	0.679200
C	4.127000	-2.104600	1.610500
C	4.527100	-1.306500	-0.638200
C	4.519700	-3.389000	1.227000
H	3.838000	-1.914300	2.642100
C	4.926000	-2.587400	-1.017300
H	4.545300	-0.491400	-1.354300
C	4.917800	-3.631700	-0.088200
H	4.522900	-4.192900	1.957400
H	5.243200	-2.771100	-2.039900
H	5.226500	-4.629000	-0.388100
Pt	-0.831100	-0.015100	0.133200
I	0.098700	-0.549200	-2.371900
I	-1.379600	-2.583000	0.714800
I	-1.412000	0.928900	2.638400
I	-3.299700	0.578600	-0.794800
H	1.334800	0.646800	1.699100

39

2D-P,Free Energies=-822.533239

C	3.324000	4.542400	-1.132100
C	4.468900	3.579200	-0.702800
C	3.962200	2.598400	0.353200
C	2.486300	2.238000	0.126900
C	1.536000	3.424100	0.343300
C	2.269600	4.745100	-0.025200
H	3.745600	5.509900	-1.425200
H	4.828300	3.007000	-1.565600
H	2.421500	1.922000	-0.934300
H	0.644100	3.296600	-0.280300
H	2.761000	5.153700	0.867600
H	5.323900	4.140000	-0.309900
H	2.824900	4.144600	-2.025500
H	1.535700	5.494900	-0.340100
H	1.194100	3.465800	1.385200
H	4.076200	3.033000	1.362000
O	4.619100	1.332700	0.318100
C	3.786500	0.424800	1.042900
H	3.988500	0.532800	2.126700
C	2.358100	0.962900	0.874300
C	1.220500	0.433700	1.437100
H	0.410600	1.131700	1.645300
H	1.317200	-0.404100	2.120100
C	4.089600	-1.003600	0.646700
C	4.253300	-1.984300	1.630400
C	4.255600	-1.344800	-0.701600
C	4.566400	-3.297500	1.274100
H	4.152100	-1.719800	2.680600
C	4.574700	-2.654200	-1.056800
H	4.151700	-0.581000	-1.464800
C	4.729100	-3.634000	-0.071200
H	4.699400	-4.049600	2.046800
H	4.705600	-2.910200	-2.104400
H	4.987700	-4.651800	-0.350900
Pt	-0.406700	-0.611600	-0.060100
I	0.648500	0.248200	-2.404000
I	0.636000	-3.057100	0.000500
I	-1.754600	-1.010200	2.273600
I	-2.551400	-1.453300	-1.419700

(20). In Path 2D-*b*

39
2D-b-IN1,Free Energies=-822.517596

C	3.070500	5.326600	0.529100
C	3.224700	4.138200	1.483900
C	2.694200	2.831600	0.852500
C	1.492500	3.103900	-0.099100
C	0.699100	4.348700	0.357600
C	1.576900	5.618600	0.252800
H	3.561900	6.216300	0.937800
H	4.273400	3.994700	1.766700
H	1.924400	3.316700	-1.086900
H	-0.202400	4.464700	-0.252700
H	1.199100	6.361600	0.965000
H	2.679000	4.334700	2.416300
H	3.590600	5.090900	-0.408000
H	1.466300	6.060400	-0.744400
H	0.364100	4.197500	1.391500
H	2.374000	2.142200	1.648600
O	3.676100	2.182900	0.042900
C	4.621300	1.392300	0.763100
H	5.199000	2.032000	1.449100
C	0.598700	1.911900	-0.242400
C	-0.669000	1.677900	0.045600
H	-1.380600	2.374100	0.475700
H	4.094600	0.646600	1.377900
C	5.545400	0.706600	-0.214500
C	5.836800	-0.655300	-0.078100
C	6.145700	1.429800	-1.254400
C	6.718600	-1.285700	-0.959800
H	5.373500	-1.226900	0.723200
C	7.018800	0.799800	-2.140500
H	5.915200	2.484800	-1.371300
C	7.310100	-0.559400	-1.993900
H	6.936100	-2.343700	-0.840800
H	7.474600	1.369900	-2.945800
H	7.992200	-1.048700	-2.684000
Pt	-1.352700	-0.155200	-0.370500
I	-3.878100	0.090400	0.458800
I	-2.099100	0.415100	-2.917700
I	1.407300	0.045300	-1.110000
I	-0.646000	-1.259400	2.011100

39
2D-b-TS1,Free Energies=-822.478586

C	4.896900	8.008100	1.217000
C	5.070300	7.003200	2.361500
C	4.631200	5.588400	1.947300
C	3.357700	5.662400	1.019000
C	2.544100	6.970600	1.224600
C	3.401400	8.203300	0.865600
H	5.350300	8.969200	1.480500
H	6.115700	6.935700	2.677900
H	3.728300	5.655000	-0.019500
H	1.632500	6.941000	0.619500
H	2.993100	9.068200	1.400700
H	4.490600	7.322300	3.236900
H	5.447100	7.636900	0.344000
H	3.296300	8.422300	-0.203300
H	2.226600	7.014000	2.274100
H	4.387000	4.994900	2.842800
O	5.709600	4.992200	1.258700
C	5.661300	3.568600	1.140400
H	5.410300	3.136400	2.123600
C	2.512300	4.480200	1.091200
C	1.740500	3.509700	1.218000
H	4.869300	3.257000	0.443400
C	6.994000	3.048600	0.653600
C	7.037400	1.901400	-0.147500
C	8.192900	3.666700	1.027400
C	8.261300	1.372600	-0.560800
H	6.110100	1.417800	-0.447700
C	9.415800	3.144100	0.604900
H	8.161900	4.563000	1.638600
C	9.454100	1.994300	-0.187200
H	8.280700	0.480800	-1.181300
H	10.340600	3.635200	0.896200
H	10.407400	1.587700	-0.513800
Pt	0.729700	1.889100	1.151100
I	-0.505200	2.551500	3.523300
I	-1.351800	2.994900	-0.230700
I	1.821800	1.038700	-1.194400
I	2.563000	0.404700	2.530900
H	1.526000	4.272800	2.125600

39

2D-b-IN2,Free Energies=-822.498884

C	2.919400	5.489400	-0.267600
C	3.346900	4.738900	0.998100
C	2.892300	3.266200	0.968600
C	1.452100	3.146000	0.351500
C	0.666700	4.471600	0.440700
C	1.375900	5.584000	-0.364000
H	3.364100	6.490200	-0.285400
H	4.435400	4.738400	1.113100
H	1.579000	2.882200	-0.703900
H	-0.351900	4.323100	0.067600
H	1.026700	6.553300	0.010700
H	2.929200	5.228600	1.887100
H	3.322500	4.956100	-1.136600
H	1.065500	5.528000	-1.413900
H	0.573500	4.760300	1.496100
H	2.884400	2.868500	1.997400
O	3.846700	2.557200	0.200700
C	3.899100	1.145500	0.410400
H	3.889900	0.947700	1.496900
C	0.647300	2.034700	1.038400
C	0.033600	1.092800	0.405100
H	0.537900	2.053100	2.126100
H	3.021200	0.646700	-0.018400
C	5.156700	0.588700	-0.214800
C	5.114500	-0.621600	-0.916300
C	6.382800	1.249700	-0.068600
C	6.281500	-1.170800	-1.453400
H	4.164500	-1.135200	-1.045500
C	7.546500	0.706600	-0.612000
H	6.416300	2.197200	0.460900
C	7.500000	-0.507500	-1.303000
H	6.234300	-2.111500	-1.995400
H	8.491900	1.230400	-0.496100
H	8.407900	-0.930300	-1.724900
Pt	-0.805300	-0.229400	-0.545900
I	-2.708300	-0.669400	1.374500
I	-2.510600	1.526500	-1.786600
I	0.798200	-0.211500	-2.754700
I	0.700600	-2.271900	0.491800

39

2D-b-IN3,Free Energies=-822.511279

C	1.392100	3.534800	-1.836600
C	1.925200	2.996400	-3.184300
C	2.719500	1.700300	-3.015800
C	3.985400	1.927700	-2.113700
C	3.805600	3.130800	-1.148300
C	2.352700	3.229300	-0.663700
H	1.238200	4.617100	-1.927900
H	1.101400	2.826400	-3.885800
H	4.115800	1.023000	-1.515300
H	4.499700	3.016500	-0.308400
H	2.268200	3.999900	0.111100
H	2.586600	3.738200	-3.653000
H	0.412000	3.095300	-1.627500
H	2.071600	2.277400	-0.199300
H	4.086600	4.064800	-1.655900
H	3.038800	1.329000	-4.002700
O	1.847500	0.744500	-2.424600
C	2.186000	-0.611900	-2.691500
H	2.210400	-0.766300	-3.784800
C	5.217600	2.131100	-2.966100
C	6.362900	1.483600	-2.875100
H	5.150300	2.912600	-3.724900
H	3.190600	-0.853300	-2.315600
C	1.168500	-1.529800	-2.054300
C	1.562700	-2.788000	-1.583100
C	-0.179600	-1.162100	-1.965200
C	0.625200	-3.669100	-1.040300
H	2.609200	-3.080000	-1.641800
C	-1.115300	-2.038600	-1.414700
H	-0.485400	-0.182400	-2.318100
C	-0.717200	-3.295700	-0.953600
H	0.946000	-4.642700	-0.679100
H	-2.158200	-1.739600	-1.346100
H	-1.447500	-3.977600	-0.526000
Pt	7.227000	0.078400	-1.808300
I	8.155400	1.753200	-4.091700
I	8.399400	1.763700	-0.044500
I	5.775000	-0.984800	0.129900
I	6.558400	-1.936500	-3.490700

39

2D-b-TS2,Free Energies=-822.483442

C	4.059000	4.582200	-0.977500
C	3.899100	3.872600	0.371500
C	2.866600	2.729400	0.314000
C	1.792900	2.978700	-0.776200
C	1.494200	4.486900	-0.893500
C	2.734400	5.258200	-1.404200
H	4.862900	5.324300	-0.923700
H	4.846100	3.444500	0.715500
H	2.228300	2.642200	-1.727200
H	0.643100	4.647300	-1.565700
H	2.695400	6.284200	-1.020100
H	3.582100	4.598000	1.131600
H	4.370600	3.848300	-1.731400
H	2.698500	5.335500	-2.497300
H	1.183100	4.861900	0.090500
H	2.378700	2.626700	1.293600
O	3.576100	1.514000	0.024300
C	2.958900	0.351000	0.489900
H	2.806800	0.369500	1.580000
C	0.507900	2.192800	-0.573900
C	0.235500	0.980000	-0.181800
H	-0.437500	2.696800	-0.826700
C	3.687100	-0.872000	0.035900
C	3.868100	-1.948500	0.917100
C	4.190600	-0.959300	-1.272300
C	4.549100	-3.092600	0.499900
H	3.484000	-1.884300	1.931400
C	4.867200	-2.102600	-1.686600
H	4.058700	-0.122700	-1.951100
C	5.046900	-3.172200	-0.801600
H	4.691600	-3.917800	1.191600
H	5.255500	-2.163900	-2.699200
H	5.575000	-4.063800	-1.128100
Pt	-0.783400	-0.529600	0.290600
I	-3.021400	1.039900	0.123400
I	-1.048800	-1.233700	-2.349300
I	0.164000	-3.006100	0.819100
I	-0.505900	0.131700	2.955600
H	1.883200	0.304600	0.079100

39

2D-b-IN4,Free Energies=-822.545644

C	2.781700	5.352900	-1.508600
C	3.434400	4.612800	-0.334900
C	2.688300	3.317900	0.012300
C	1.206000	3.297100	-0.439500
C	0.627800	4.717300	-0.247800
C	1.323800	5.746900	-1.172900
H	3.369600	6.241500	-1.762000
H	4.486900	4.380600	-0.532200
H	1.192900	3.061100	-1.511900
H	-0.448700	4.688000	-0.439500
H	1.306900	6.730400	-0.689000
H	3.420500	5.250800	0.557400
H	2.805700	4.708100	-2.396500
H	0.757000	5.852000	-2.104900
H	0.740300	5.004900	0.806300
H	2.769100	3.089500	1.079800
O	3.380500	2.209100	-0.694400
C	3.306100	1.009000	-0.234900
H	2.810200	0.837700	0.723800
C	0.457400	2.232400	0.320000
C	-0.051000	1.144100	-0.266000
H	0.367200	2.381000	1.392900
H	-0.009700	0.975200	-1.338900
C	3.884600	-0.076600	-0.941200
C	3.776100	-1.366000	-0.364800
C	4.558500	0.102200	-2.178100
C	4.356700	-2.454300	-1.008100
H	3.228700	-1.494900	0.564500
C	5.123400	-0.990900	-2.806600
H	4.625700	1.093500	-2.613400
C	5.025100	-2.266800	-2.219100
H	4.271900	-3.445200	-0.574900
H	5.641700	-0.869400	-3.752500
H	5.472500	-3.119600	-2.722100
Pt	-0.976700	-0.344800	0.693700
I	-2.364700	1.170400	2.487600
I	-3.087500	-0.184100	-1.021800
I	0.164800	-2.259500	-0.931500
I	1.004700	-0.751800	2.589900

39

2D-b-TS3,Free Energies=-822.524676

C	2.938100	4.294700	-0.470400
C	4.140300	3.355900	-0.184300
C	3.694700	2.140600	0.631500
C	2.242100	1.734300	0.338500
C	1.258600	2.829700	0.805800
C	1.890400	4.241500	0.655200
H	3.299100	5.319700	-0.605800
H	4.580000	3.000500	-1.123000
H	2.166200	1.611400	-0.749500
H	0.336900	2.752300	0.220600
H	2.367600	4.536100	1.599500
H	4.928200	3.891600	0.356000
H	2.462500	4.010200	-1.417900
H	1.100000	4.976900	0.471400
H	0.972200	2.658900	1.849500
H	3.810600	2.319500	1.711500
O	4.440600	0.971700	0.278600
C	3.955900	-0.134000	0.903800
H	4.042400	-0.121900	1.994400
C	2.072100	0.360800	0.999700
C	1.312200	-0.588200	0.302600
H	1.895400	0.405100	2.072100
H	1.416600	-0.658000	-0.779700
C	4.397500	-1.392500	0.270200
C	4.634000	-2.522300	1.067100
C	4.649800	-1.451400	-1.111300
C	5.118200	-3.695400	0.492100
H	4.430000	-2.484100	2.132800
C	5.129400	-2.626200	-1.681500
H	4.487200	-0.570900	-1.724300
C	5.364600	-3.749700	-0.880800
H	5.297300	-4.566200	1.115300
H	5.324500	-2.668000	-2.749100
H	5.740100	-4.665200	-1.329200
Pt	0.015000	-1.785400	1.062400
I	-1.404500	-0.037200	2.622200
I	-1.671900	-1.208500	-1.039000
I	1.004900	-3.908600	-0.358700
I	1.326700	-2.642800	3.312000

39

2D-b-IN5,Free Energies=-822.532163

C	-4.768600	-3.518500	-1.153700
C	-5.179200	-2.321100	-0.253400
C	-3.950600	-1.746600	0.454000
C	-2.702500	-1.788800	-0.432200
C	-2.260600	-3.249900	-0.659200
C	-3.487900	-4.206000	-0.646700
H	-5.588000	-4.243300	-1.210600
H	-5.639300	-1.526800	-0.852400
H	-2.957600	-1.320200	-1.392600
H	-1.742400	-3.337300	-1.619200
H	-3.659000	-4.575000	0.372800
H	-5.921300	-2.628800	0.491700
H	-4.600100	-3.168100	-2.180900
H	-3.266000	-5.088900	-1.256500
H	-1.543000	-3.559600	0.109700
H	-3.742600	-2.329300	1.368400
O	-4.117600	-0.379200	0.796200
C	-2.838700	0.246200	0.938100
H	-2.608600	0.385200	2.002400
C	-1.783800	-0.826600	0.373700
C	-0.646800	-0.169500	-0.347500
H	-1.396200	-1.394200	1.222100
H	-0.911700	0.679900	-0.971900
C	-2.893600	1.606100	0.265600
C	-2.365100	2.732900	0.905200
C	-3.497200	1.764000	-0.991700
C	-2.414500	3.988400	0.295400
H	-1.911400	2.630000	1.886800
C	-3.544800	3.016300	-1.603500
H	-3.959000	0.909000	-1.475500
C	-3.000300	4.132600	-0.962400
H	-1.998200	4.851200	0.807400
H	-4.018200	3.123600	-2.575900
H	-3.042300	5.109000	-1.437100
Pt	1.102500	0.128800	0.640500
I	1.472500	-2.178000	2.071300
I	1.587400	2.402200	-0.767900
I	0.970300	1.495700	2.906700
I	0.686000	-1.379100	-1.748600

39

2D-b-IN6,Free Energies=-822.533898

C	5.092400	-1.435400	-1.262000
C	5.110700	0.098500	-1.529400
C	3.767400	0.519300	-2.115900
C	2.613400	-0.266400	-1.479400
C	2.631500	-1.702400	-2.026100
C	4.108100	-2.185100	-2.185100
H	6.100500	-1.846200	-1.383700
H	5.280500	0.647800	-0.595800
H	2.796700	-0.292900	-0.397300
H	2.079900	-2.370700	-1.361500
H	4.429000	-2.052100	-3.226600
H	5.920500	0.369800	-2.215800
H	4.812100	-1.621800	-0.217800
H	4.164000	-3.260800	-1.986000
H	2.125600	-1.741100	-2.998800
H	3.760100	0.325500	-3.203200
O	3.436400	1.885400	-1.911800
C	2.080900	1.992100	-2.305100
H	2.007800	1.885700	-3.400200
C	1.368100	0.648200	-1.743300
C	0.605200	0.883700	-0.481700
H	0.723800	0.220500	-2.513500
H	1.099000	1.527500	0.243200
C	1.535900	3.343000	-1.914500
C	0.600300	3.983500	-2.737100
C	1.960000	3.981400	-0.741200
C	0.075100	5.228300	-2.381800
H	0.287200	3.511500	-3.666000
C	1.437500	5.226300	-0.387000
H	2.720800	3.512700	-0.125000
C	0.489600	5.850200	-1.202000
H	-0.644500	5.716300	-3.033500
H	1.777000	5.712100	0.523500
H	0.087400	6.821100	-0.926600
Pt	-0.406200	-0.592300	0.500700
I	0.910500	-2.671800	1.493800
I	-0.073600	0.709000	2.882700
I	-1.343200	-2.112300	-1.563100
I	-1.464800	1.756900	-0.677300

39

2D-b-TS4,Free Energies=-822.503437

C	5.583600	-1.752700	-0.268500
C	5.609700	-0.251500	-0.681000
C	4.217100	0.158400	-1.142800
C	3.129500	-0.533500	-0.303400
C	3.044800	-2.018500	-0.716700
C	4.484800	-2.545700	-1.005600
H	6.560900	-2.207100	-0.461300
H	5.902800	0.376300	0.168200
H	3.416000	-0.477200	0.758900
H	2.569800	-2.600000	0.073200
H	4.682000	-2.510200	-2.084600
H	6.335000	-0.073500	-1.481900
H	5.417900	-1.834800	0.813000
H	4.537300	-3.601400	-0.720600
H	2.423200	-2.129200	-1.612000
H	4.071600	-0.124700	-2.199200
O	3.943700	1.553200	-1.017600
C	2.547000	1.692500	-1.197500
H	2.282300	1.545100	-2.259900
C	1.984400	0.440000	-0.416200
C	0.697200	0.477100	0.115600
H	0.160300	1.400400	-0.096300
C	2.056700	3.039300	-0.732300
C	1.066400	3.709000	-1.460500
C	2.566900	3.616000	0.438100
C	0.575900	4.938500	-1.015300
H	0.682700	3.276800	-2.382400
C	2.082700	4.848000	0.874500
H	3.348000	3.106000	0.992500
C	1.083600	5.508000	0.152900
H	-0.194100	5.450300	-1.584900
H	2.483600	5.292300	1.780900
H	0.705200	6.465200	0.499900
Pt	-0.298800	-0.699800	1.358600
I	1.512100	-2.114400	2.843700
I	-0.158900	1.300800	3.228000
I	-2.648800	0.373400	0.408300
I	-0.653500	-2.804300	-0.352400
H	0.847400	-0.072000	-1.030600

(21). In Path 3D-*a*

39
3D-a-IN1,Free Energies=-835.300903

C	4.846900	-3.550200	-0.084300
C	4.859300	-2.029300	-0.352900
C	3.447200	-1.430200	-0.584900
C	2.405400	-2.223700	0.237700
C	2.323600	-3.681400	-0.312700
C	3.681700	-4.213800	-0.825000
H	5.802900	-3.991000	-0.387400
H	5.304500	-1.496800	0.496100
H	2.764300	-2.251300	1.276900
H	1.952800	-4.329300	0.489900
H	3.779500	-4.015000	-1.900200
H	5.481600	-1.814100	-1.229300
H	4.748400	-3.742700	0.992100
H	3.714300	-5.302900	-0.710600
H	1.580300	-3.719800	-1.116800
H	3.172600	-1.512100	-1.649900
O	3.392800	-0.060600	-0.208000
C	4.137500	0.817800	-1.047900
H	5.213200	0.600500	-0.957500
C	1.057000	-1.562400	0.254000
C	0.560100	-0.423100	-0.187000
H	3.861800	0.657700	-2.102600
H	1.112300	0.366200	-0.681400
C	3.862400	2.248200	-0.647000
C	3.766300	3.247200	-1.621100
C	3.741900	2.603700	0.702400
C	3.566900	4.583300	-1.265400
H	3.845800	2.988200	-2.674400
C	3.531700	3.931500	1.076200
H	3.799100	1.835200	1.466400
C	3.454200	4.904100	0.083100
H	3.492700	5.351700	-2.026800
H	3.430000	4.199200	2.121900
Pt	-1.385700	-0.093800	0.146300
I	-1.068400	1.095000	2.562200
I	-1.657800	2.282100	-1.024000
I	-2.251200	-1.341700	-2.105000
Br	3.175100	6.772800	0.597700
I	-0.604300	-2.643600	1.275200

39
3D-a-TS1,Free Energies=-835.27014

C	-0.999900	5.327500	-0.307500
C	-2.269600	4.522300	-0.659300
C	-1.954600	3.140400	-1.246600
C	-0.626300	2.569200	-0.589800
C	0.555100	3.474600	-1.102300
C	0.149000	4.957200	-1.252300
H	-1.217600	6.399100	-0.360100
H	-2.893400	4.369800	0.228200
H	-0.752800	2.677200	0.494600
H	1.362900	3.360100	-0.374800
H	-0.152200	5.167900	-2.286900
H	-2.880100	5.064400	-1.390000
H	-0.699600	5.124700	0.728300
H	1.027300	5.581100	-1.055300
H	0.924900	3.074600	-2.049600
H	-1.778300	3.190200	-2.330400
O	-3.056100	2.294900	-0.991800
C	-2.960700	1.071700	-1.635900
H	-2.960800	1.170100	-2.731800
C	-0.385800	1.170500	-0.873500
C	0.143700	-0.004800	-0.969300
H	-0.350200	-0.869400	-1.403700
C	-3.929500	0.054300	-1.137900
C	-4.415100	-0.924500	-2.016000
C	-4.327500	0.033100	0.207000
C	-5.295100	-1.908400	-1.568200
H	-4.112400	-0.918600	-3.060300
C	-5.211200	-0.939900	0.665800
H	-3.952400	0.786400	0.891800
C	-5.683200	-1.899700	-0.230300
H	-5.673000	-2.661900	-2.249700
H	-5.523100	-0.954300	1.703900
Pt	1.974100	-0.466300	-0.289000
I	2.134100	1.279200	1.827500
I	0.781100	-2.294900	1.375900
I	2.204900	-2.399900	-2.212800
I	3.604900	1.144300	-1.772300
Br	-6.919500	-3.263100	0.406600
H	-1.884500	0.704600	-1.402300

39

3D-a-IN2,Free Energies=-835.31991

C	-1.672900	5.228800	0.170700
C	-2.996700	4.431200	0.135400
C	-2.881200	3.189400	-0.757100
C	-1.451700	2.611000	-0.790600
C	-0.550900	3.669800	-1.499000
C	-0.940900	5.133500	-1.174000
H	-1.886100	6.271800	0.427700
H	-3.259200	4.097800	1.144800
H	-1.118400	2.486400	0.242100
H	0.475200	3.461800	-1.181800
H	-1.589200	5.538700	-1.964000
H	-3.819600	5.059100	-0.225600
H	-1.027300	4.835800	0.964800
H	-0.043300	5.760800	-1.165600
H	-0.582600	3.507000	-2.583800
H	-3.230200	3.381200	-1.779700
O	-3.822700	2.187800	-0.202300
C	-4.230200	1.223400	-0.942100
H	-4.025600	1.271100	-2.011400
C	-1.393100	1.289500	-1.493000
C	-1.016400	0.072600	-1.070400
H	-1.641900	1.326200	-2.560700
H	-1.019200	-0.752600	-1.775000
C	-5.014100	0.161800	-0.421700
C	-5.525400	-0.797400	-1.328300
C	-5.293300	0.045900	0.961600
C	-6.314400	-1.839300	-0.872000
H	-5.295500	-0.719900	-2.387500
C	-6.081100	-0.996500	1.420500
H	-4.865100	0.757600	1.657500
C	-6.586000	-1.921400	0.499400
H	-6.708100	-2.580500	-1.557300
H	-6.288800	-1.104200	2.478500
Pt	-0.316900	-0.548900	0.700700
I	-1.815100	0.764800	2.615400
I	-2.151200	-2.602500	0.683500
I	1.466000	-2.157300	-0.612300
I	1.669700	1.298800	1.015100
Br	-7.692100	-3.368700	1.141200

39

3D-a-TS2,Free Energies=-835.302225

C	-3.655900	3.355300	-0.567600
C	-2.257200	3.981600	-0.836400
C	-1.290600	3.553700	0.261800
C	-1.564400	2.114900	0.729700
C	-2.874400	2.101000	1.542800
C	-3.903600	3.097700	0.932200
H	-4.435100	4.012000	-0.968400
H	-1.868300	3.639400	-1.801700
H	-1.686700	1.502800	-0.168500
H	-3.278800	1.084800	1.551800
H	-3.859700	4.054000	1.470800
H	-2.316600	5.074800	-0.876100
H	-3.742000	2.406900	-1.111100
H	-4.918200	2.712900	1.079900
H	-2.672700	2.372000	2.588100
H	-1.355900	4.237400	1.123500
O	0.082000	3.543100	-0.170400
C	0.846100	3.051600	0.836800
H	0.761400	3.630000	1.764400
C	-0.297200	1.664800	1.436100
C	0.349500	0.419000	1.254600
H	-0.267300	1.902100	2.507200
H	1.201200	0.228600	1.903500
C	2.257800	2.777600	0.480800
C	3.226000	2.784000	1.496700
C	2.655100	2.573000	-0.847400
C	4.571700	2.581000	1.200400
H	2.932600	2.960100	2.529500
C	3.999600	2.382400	-1.158600
H	1.912500	2.562600	-1.636600
C	4.938900	2.386800	-0.129900
H	5.317800	2.586500	1.986700
H	4.305700	2.223700	-2.186200
Pt	-0.024200	-1.020800	0.016200
I	0.005100	0.044400	-2.487400
I	2.678700	-1.473600	-0.141300
I	-0.129000	-2.450100	2.391800
I	-2.708500	-1.449700	-0.261000
Br	6.822200	2.124000	-0.561100

39

3D-a-IN3,Free Energies=-835.310225

C	-3.800600	3.123300	-0.586300
C	-2.449200	3.852600	-0.843000
C	-1.469000	3.517400	0.277000
C	-1.638200	2.069700	0.751600
C	-2.951000	1.929100	1.538500
C	-4.047800	2.841100	0.910600
H	-4.625900	3.718300	-0.992200
H	-2.019700	3.528600	-1.797900
H	-1.691100	1.451300	-0.149200
H	-3.276500	0.883800	1.534800
H	-4.085900	3.796300	1.451100
H	-2.592700	4.937200	-0.903300
H	-3.811600	2.171500	-1.131400
H	-5.032100	2.378400	1.041700
H	-2.797000	2.210100	2.589500
H	-1.631200	4.198200	1.132300
O	-0.097300	3.609200	-0.103600
C	0.615500	3.025100	0.967900
H	0.592800	3.717100	1.827300
C	-0.291300	1.778000	1.447700
C	0.378100	0.436100	1.279000
H	-0.407300	1.891700	2.534300
H	1.441200	0.453400	1.501800
C	2.061900	2.790100	0.604100
C	3.021600	2.695100	1.621400
C	2.477200	2.698200	-0.728300
C	4.369400	2.489600	1.324400
H	2.722900	2.798900	2.663000
C	3.823500	2.503700	-1.043800
H	1.745800	2.791900	-1.522200
C	4.749700	2.398000	-0.011500
H	5.105400	2.418300	2.117400
H	4.138700	2.434700	-2.078900
Pt	-0.044900	-0.930400	-0.167300
I	0.196500	-0.022200	-2.646900
I	2.570000	-1.670500	-0.132200
I	-2.678400	-1.453000	-0.614100
Br	6.638800	2.133000	-0.445100
I	-0.341800	-1.235800	2.674500

39

3D-a-IN4,Free Energies=-835.315186

C	0.939400	5.017700	0.281300
C	2.349700	4.355800	0.232700
C	2.312600	3.069000	1.046700
C	0.976800	2.334200	0.863900
C	-0.096200	3.088100	1.667500
C	0.137900	4.627200	1.543100
H	1.038700	6.107300	0.230200
H	2.624700	4.121700	-0.802600
H	0.717900	2.378900	-0.200300
H	-1.093900	2.821900	1.310900
H	0.672400	4.992900	2.429500
H	3.117500	5.030500	0.627300
H	0.366800	4.721600	-0.606100
H	-0.826900	5.145700	1.536300
H	-0.048500	2.795300	2.724900
H	2.436700	3.310400	2.117100
O	3.312600	2.108800	0.707700
C	2.923600	0.946700	1.409400
H	3.046400	1.125200	2.491700
C	1.321900	0.866200	1.209100
C	0.902200	-0.242000	0.287900
H	0.881700	0.567900	2.172300
H	1.332200	-1.201100	0.560900
C	3.780500	-0.237800	1.031000
C	3.706000	-1.419100	1.782400
C	4.686900	-0.169900	-0.032700
C	4.496900	-2.524600	1.467300
H	3.031500	-1.483600	2.634200
C	5.494700	-1.263800	-0.354300
H	4.775400	0.751400	-0.597400
C	5.382800	-2.429000	0.397100
H	4.428100	-3.435300	2.051300
H	6.200800	-1.201200	-1.175000
Pt	-1.040500	-0.479600	-0.291600
I	-0.706800	-3.165000	-0.047200
I	-2.612700	-0.426900	1.845800
I	-2.252700	1.708300	-1.340200
Br	6.509700	-3.964400	-0.046500
I	1.337200	-0.115600	-1.905900

39

3D-a-TS3,Free Energies=-835.291224

C	3.106600	4.318300	-1.135100
C	4.230500	3.477900	-0.462900
C	3.614200	2.440000	0.473000
C	2.263900	1.940200	-0.052500
C	1.184300	3.034300	0.014900
C	1.841400	4.419400	-0.260500
H	3.482400	5.321600	-1.361500
H	4.822900	2.955500	-1.222700
H	2.413400	1.650600	-1.106600
H	0.400800	2.825100	-0.721400
H	2.103200	4.894500	0.693800
H	4.919000	4.120500	0.095800
H	2.837800	3.869900	-2.100200
H	1.108100	5.077600	-0.737700
H	0.696200	3.044900	0.995400
H	3.469000	2.869700	1.479000
O	4.400600	1.250700	0.591200
C	3.568500	0.242400	1.147000
H	3.558300	0.320800	2.247700
C	2.133500	0.610800	0.640900
C	1.027700	-0.228600	0.728000
H	1.225200	-1.186400	1.216500
C	4.039100	-1.136700	0.748500
C	3.975200	-2.191300	1.665000
C	4.515600	-1.380600	-0.545200
C	4.366400	-3.481500	1.299500
H	3.632400	-2.012100	2.681700
C	4.916500	-2.661300	-0.923200
H	4.591600	-0.562300	-1.253500
C	4.831900	-3.696100	0.006300
H	4.317700	-4.295200	2.014200
H	5.288100	-2.847500	-1.924500
Pt	-0.862600	0.060100	0.003900
I	0.158700	-0.516600	-2.455600
I	-1.522800	-2.485000	0.571100
I	-1.517000	1.034400	2.479500
I	-3.268100	0.723600	-1.030100
Br	5.395800	-5.491400	-0.515600
H	1.248800	0.653700	1.658700

39

3D-P,Free Energies=-835.318462

C	-5.023800	-3.125200	-0.036600
C	-5.513800	-1.650700	0.057200
C	-4.545200	-0.829200	0.905900
C	-3.097300	-1.313100	0.738700
C	-2.864600	-2.721200	1.305000
C	-4.175300	-3.549200	1.179300
H	-5.884600	-3.794300	-0.140500
H	-5.567700	-1.203600	-0.941900
H	-2.921700	-1.339400	-0.355800
H	-2.052200	-3.207300	0.753400
H	-4.773200	-3.431200	2.092600
H	-6.520100	-1.600200	0.486800
H	-4.424700	-3.256100	-0.947200
H	-3.929300	-4.614300	1.110800
H	-2.553400	-2.673000	2.356200
H	-4.825800	-0.891400	1.971900
O	-4.478900	0.545300	0.526100
C	-3.278700	1.065400	1.099000
H	-3.467900	1.342400	2.154400
C	-2.318600	-0.131900	1.187600
C	-1.051400	-0.115900	1.715500
H	-0.683600	-1.050100	2.137300
H	-0.683500	0.795600	2.175400
C	-2.838400	2.307400	0.356400
C	-2.422100	3.439900	1.062100
C	-2.889000	2.352600	-1.042000
C	-2.043500	4.604400	0.390400
H	-2.404300	3.428500	2.149300
C	-2.519200	3.508200	-1.728700
H	-3.235000	1.487200	-1.596400
C	-2.098800	4.618300	-0.999400
H	-1.727300	5.482000	0.943200
H	-2.559400	3.540300	-2.811700
Br	-1.589100	6.247100	-1.954800
Pt	0.831200	-0.404900	0.153500
I	-0.614200	-1.135800	-2.018300
I	1.185900	2.164300	-0.435000
I	2.286900	-0.194900	2.444800
I	3.044300	-1.110600	-1.167800

(22). In Path 3D-*b*

39
3D-b-IN1,Free Energies=-835.30324

C	-3.830300	4.072000	-1.108000
C	-3.695000	2.837600	-2.005600
C	-2.914300	1.706800	-1.299800
C	-1.826400	2.273200	-0.340800
C	-1.309800	3.640500	-0.842600
C	-2.444000	4.692400	-0.815200
H	-4.488800	4.814900	-1.570900
H	-4.679000	2.457500	-2.302000
H	-2.319400	2.428800	0.628800
H	-0.472100	3.975400	-0.222600
H	-2.214400	5.469700	-1.553300
H	-3.176600	3.106600	-2.935300
H	-4.316600	3.771200	-0.171400
H	-2.461500	5.188400	0.162300
H	-0.921600	3.521800	-1.862100
H	-2.431200	1.067200	-2.053400
O	-3.763200	0.898700	-0.479700
C	-4.471000	-0.119100	-1.180600
H	-5.092500	0.329800	-1.972200
C	-0.698600	1.311100	-0.129800
C	0.591300	1.340600	-0.413200
H	1.136700	2.150200	-0.885800
H	-3.760900	-0.800700	-1.673300
C	-5.343900	-0.882800	-0.213100
C	-5.490200	-2.268600	-0.336200
C	-6.051700	-0.215100	0.794300
C	-6.332600	-2.983600	0.518800
H	-4.942800	-2.805000	-1.107900
C	-6.890800	-0.913000	1.663400
H	-5.936200	0.858300	0.906400
C	-7.021500	-2.290600	1.508300
H	-6.439600	-4.057700	0.416600
H	-7.432800	-0.391100	2.444400
Pt	1.652800	-0.276700	0.092700
I	4.064600	0.463600	-0.774100
I	2.254700	0.574300	2.597700
I	-1.095100	-0.632100	0.848100
I	1.200400	-1.629300	-2.221400
Br	-8.201200	-3.278700	2.720200

39
3D-b-TS1,Free Energies=-835.263979

C	3.999600	4.593400	-0.574800
C	3.861800	3.828900	0.746700
C	3.132700	2.487700	0.556300
C	1.988000	2.635600	-0.517300
C	1.477200	4.098400	-0.642900
C	2.615500	5.028900	-1.115100
H	4.644700	5.468300	-0.444200
H	4.840100	3.605300	1.183100
H	2.426900	2.348200	-1.487000
H	0.629600	4.139100	-1.334100
H	2.380600	6.047200	-0.785500
H	3.316200	4.436700	1.479600
H	4.504200	3.944700	-1.301100
H	2.635700	5.054300	-2.210700
H	1.102000	4.414400	0.338700
H	2.688600	2.163700	1.510700
O	4.089000	1.538400	0.130000
C	3.708700	0.170300	0.268500
H	3.281600	0.012600	1.273000
C	0.895700	1.690800	-0.335400
C	-0.074200	0.936800	-0.126300
H	2.925300	-0.098400	-0.455800
C	4.911000	-0.721700	0.059400
C	4.722700	-2.038900	-0.375400
C	6.207600	-0.274500	0.331400
C	5.806300	-2.905200	-0.529700
H	3.720700	-2.400100	-0.596300
C	7.304100	-1.124300	0.172600
H	6.363100	0.747900	0.658400
C	7.084800	-2.430300	-0.253500
H	5.653100	-3.924500	-0.866000
H	8.308600	-0.771500	0.379200
Pt	-1.387300	-0.444900	0.002500
I	-2.718500	0.993400	1.938000
I	-3.023500	0.622300	-1.905000
I	-0.233900	-2.030800	-1.889000
I	-0.066200	-1.831100	1.954700
Br	8.617800	-3.630400	-0.477900
H	-0.217700	1.923200	0.552600

39

3D-b-IN2,Free Energies=-835.284799

C	2.937700	5.495700	-0.234900
C	3.345800	4.733000	1.030000
C	2.885300	3.263300	0.982500
C	1.449500	3.153400	0.354300
C	0.671600	4.483900	0.439700
C	1.395800	5.595400	-0.352500
H	3.385400	6.495300	-0.237200
H	4.432700	4.728000	1.159800
H	1.582900	2.891500	-0.700800
H	-0.343500	4.342700	0.054800
H	1.044400	6.564900	0.019500
H	2.918600	5.216400	1.917900
H	3.351500	4.969400	-1.103000
H	1.099900	5.542800	-1.406600
H	0.568300	4.768900	1.495200
H	2.871200	2.853700	2.006300
O	3.843500	2.558200	0.212200
C	3.880700	1.145100	0.396900
H	3.862000	0.924000	1.478700
C	0.631200	2.046900	1.032500
C	0.034700	1.096000	0.395800
H	0.495800	2.076000	2.117000
H	3.003700	0.659700	-0.048600
C	5.139000	0.588400	-0.227900
C	5.111400	-0.653900	-0.870700
C	6.352700	1.279800	-0.139900
C	6.274700	-1.211500	-1.407900
H	4.173400	-1.196500	-0.960300
C	7.522900	0.743400	-0.677900
H	6.379600	2.252400	0.341000
C	7.464700	-0.500100	-1.301400
H	6.245500	-2.174600	-1.905100
H	8.460100	1.284800	-0.611200
Pt	-0.775200	-0.241700	-0.557300
I	-2.707500	-0.687300	1.330600
I	-2.471500	1.492900	-1.838300
I	0.857200	-0.237000	-2.745000
I	0.736100	-2.257100	0.528200
Br	9.105000	-1.264100	-2.057000

39

3D-b-IN3,Free Energies=-835.297843

C	-3.233200	4.418700	0.142800
C	-2.797400	3.829800	-1.218500
C	-2.409100	2.354300	-1.115200
C	-1.187500	2.156400	-0.148000
C	-1.074100	3.304700	0.891400
C	-2.464900	3.786000	1.326500
H	-3.071000	5.503300	0.122800
H	-3.593900	3.942400	-1.961900
H	-1.356600	1.221100	0.390800
H	-0.489400	2.950500	1.747300
H	-2.371900	4.503600	2.149600
H	-1.928400	4.378500	-1.606800
H	-4.307800	4.265800	0.282900
H	-3.028500	2.929200	1.713200
H	-0.512700	4.146500	0.461200
H	-2.149600	1.968300	-2.113500
O	-3.549600	1.649800	-0.633900
C	-3.586100	0.273200	-0.984000
H	-3.540700	0.177900	-2.083400
C	0.100100	2.039700	-0.932200
C	0.998800	1.078600	-0.842700
H	0.309100	2.849700	-1.633100
H	-2.715300	-0.266000	-0.584300
C	-4.857200	-0.353900	-0.459300
C	-4.882300	-1.716000	-0.138100
C	-6.031700	0.394500	-0.325700
C	-6.057100	-2.331200	0.300100
H	-3.975500	-2.310000	-0.228100
C	-7.213700	-0.200800	0.118600
H	-6.017000	1.453500	-0.560500
C	-7.207500	-1.558900	0.421600
H	-6.068300	-3.386900	0.547400
H	-8.120100	0.385100	0.225000
Pt	1.345400	-0.578100	0.154600
I	2.861800	0.875000	-1.959300
I	2.845600	0.583800	2.083400
I	-0.465000	-1.279700	1.950900
I	0.217500	-2.200600	-1.699700
Br	-8.864100	-2.405500	1.044500

39

3D-b-TS2,Free Energies=-835.269089

C	-5.401900	-3.079700	-0.445000
C	-4.854400	-2.437800	0.834500
C	-3.496600	-1.744100	0.609200
C	-2.715500	-2.372800	-0.570900
C	-2.971600	-3.892400	-0.624700
C	-4.454200	-4.192100	-0.952700
H	-6.402800	-3.487300	-0.266400
H	-5.545500	-1.690200	1.237100
H	-3.120300	-1.926400	-1.489700
H	-2.315300	-4.354400	-1.371400
H	-4.728600	-5.153100	-0.502600
H	-4.733000	-3.207600	1.607000
H	-5.520900	-2.303600	-1.211600
H	-4.577600	-4.311200	-2.035500
H	-2.692500	-4.330900	0.342500
H	-2.893900	-1.809200	1.525700
O	-3.753600	-0.355800	0.329700
C	-2.713900	0.510200	0.659300
H	-2.431700	0.445200	1.721100
C	-1.225200	-2.078600	-0.550700
C	-0.512700	-1.024300	-0.261100
H	-0.546200	-2.885300	-0.866100
C	-3.017600	1.908000	0.230700
C	-2.675800	2.988200	1.056400
C	-3.649800	2.156800	-0.997700
C	-2.968300	4.298000	0.675000
H	-2.186500	2.808400	2.009300
C	-3.945400	3.458000	-1.393000
H	-3.924100	1.324600	-1.637600
C	-3.599700	4.512200	-0.546400
H	-2.710100	5.130100	1.320000
H	-4.435700	3.649700	-2.340700
Pt	1.049800	-0.006100	-0.000700
I	2.513200	-2.312800	-0.165200
I	1.323700	0.384500	-2.701300
I	1.069500	2.680200	0.347200
I	0.813700	-0.348500	2.728900
Br	-4.022500	6.338300	-1.090300
H	-1.746600	0.166200	0.120400

39

3D-b-IN4,Free Energies=-835.328811

C	3.832100	4.565700	-1.356100
C	3.977100	3.950100	0.040800
C	2.987600	2.799300	0.266500
C	1.736200	2.848600	-0.646500
C	1.325700	4.329200	-0.813000
C	2.411000	5.141000	-1.563500
H	4.585800	5.347200	-1.498600
H	4.995600	3.591500	0.226100
H	2.031300	2.459600	-1.630100
H	0.370900	4.372200	-1.344800
H	2.378200	6.182100	-1.221800
H	3.774800	4.712900	0.802900
H	4.043900	3.796900	-2.110400
H	2.185200	5.161100	-2.635600
H	1.138800	4.757500	0.180900
H	2.694200	2.731100	1.318900
O	3.706400	1.534500	-0.037500
C	3.315700	0.430600	0.498800
H	2.520200	0.454500	1.247300
C	0.648800	1.981400	-0.067000
C	0.210500	0.869200	-0.665300
H	0.243800	2.294800	0.891700
H	0.566400	0.541400	-1.638700
C	3.929300	-0.799500	0.152100
C	3.458500	-1.975600	0.785300
C	4.988600	-0.875400	-0.789700
C	4.053600	-3.200700	0.507200
H	2.624300	-1.918300	1.479200
C	5.575300	-2.093200	-1.069500
H	5.337400	0.026300	-1.281700
C	5.102500	-3.242600	-0.409900
H	3.693900	-4.105300	0.982800
H	6.386800	-2.168500	-1.783800
Pt	-1.163400	-0.370800	0.088900
I	-2.831400	1.511900	1.141000
I	-2.576900	-0.272700	-2.237300
I	0.166100	-2.600900	-0.845700
I	0.038100	-0.674100	2.570100
Br	5.941000	-4.939200	-0.801700

39

3D-b-TS3,Free Energies=-835.308903

C	-4.712400	-3.652600	-1.036700
C	-5.209900	-2.298800	-0.463700
C	-4.081600	-1.578500	0.276800
C	-2.696400	-1.887000	-0.312500
C	-2.333500	-3.375600	-0.111500
C	-3.603600	-4.268900	-0.166000
H	-5.556600	-4.344500	-1.123700
H	-5.564600	-1.648900	-1.271600
H	-2.757200	-1.664800	-1.385700
H	-1.617000	-3.672400	-0.883900
H	-3.992400	-4.422600	0.849600
H	-6.054200	-2.454300	0.216400
H	-4.330200	-3.506300	-2.055100
H	-3.335000	-5.261600	-0.542200
H	-1.822000	-3.512300	0.847800
H	-4.083900	-1.826600	1.349100
O	-4.190100	-0.157000	0.137900
C	-3.125000	0.480100	0.686100
H	-3.009900	0.350300	1.765800
C	-1.745700	-0.880900	0.343500
C	-0.748600	-0.320200	-0.464000
H	-1.437900	-1.151400	1.351100
H	-0.984300	-0.066900	-1.497100
C	-2.982100	1.870900	0.215700
C	-2.467300	2.848700	1.078900
C	-3.422900	2.245000	-1.065100
C	-2.393900	4.181200	0.679400
H	-2.110600	2.569800	2.065500
C	-3.352000	3.571500	-1.476800
H	-3.840300	1.497300	-1.731200
C	-2.838700	4.523600	-0.594500
H	-1.992200	4.933400	1.348200
H	-3.693300	3.861600	-2.464000
Pt	1.075800	0.003400	0.047800
I	1.693200	-2.407000	1.191800
I	1.885300	-0.996800	-2.386900
I	1.015100	2.517400	-1.042300
I	0.751800	1.050100	2.562600
Br	-2.751100	6.384800	-1.162300

39

3D-b-IN5,Free Energies=-835.316831

C	6.044100	-0.286700	-0.096600
C	5.461000	0.651500	-1.188700
C	3.980900	0.338400	-1.416300
C	3.265700	-0.046800	-0.118400
C	3.782500	-1.410700	0.385500
C	5.273500	-1.616600	-0.009900
H	7.104300	-0.478200	-0.294100
H	5.555900	1.701000	-0.887200
H	3.474700	0.731200	0.628500
H	3.685100	-1.465500	1.474400
H	5.331400	-2.128400	-0.979100
H	6.008100	0.541300	-2.131600
H	6.001600	0.212300	0.880700
H	5.751800	-2.283900	0.715500
H	3.176200	-2.227900	-0.022800
H	3.886400	-0.504200	-2.122300
O	3.263500	1.455300	-1.926600
C	1.883600	1.367100	-1.560700
H	1.278500	1.145600	-2.448600
C	1.792600	0.091100	-0.596000
C	0.717800	0.240300	0.437400
H	1.579200	-0.780700	-1.218200
H	0.630800	1.224900	0.889700
C	1.448500	2.709000	-0.993100
C	0.200400	3.249600	-1.322800
C	2.298500	3.448500	-0.158000
C	-0.210800	4.484900	-0.816600
H	-0.467900	2.705900	-1.984000
C	1.906300	4.683700	0.358100
H	3.292200	3.075000	0.064900
C	0.650500	5.183200	0.021900
H	-1.181900	4.889200	-1.078500
H	2.573100	5.250200	0.998700
Pt	-1.098700	-0.597200	0.074200
I	-0.520200	-3.038900	-1.020900
I	-2.356600	1.387100	1.437500
I	-2.293700	0.114500	-2.182200
Br	0.096700	6.920300	0.731700
I	0.670800	-1.119700	2.257100

39

3D-b-IN6,Free Energies=-835.318729

C	-0.551300	4.844700	-1.492700
C	0.975300	4.576200	-1.643500
C	1.439000	3.684300	-0.497200
C	0.376200	2.635300	-0.145600
C	-0.775900	3.330100	0.597200
C	-1.029000	4.738400	-0.028600
H	-0.795500	5.835400	-1.891000
H	1.183300	4.073000	-2.595200
H	-0.002900	2.227400	-1.091700
H	-1.681800	2.722300	0.550000
H	-0.515900	5.504200	0.567700
H	1.543100	5.513200	-1.642300
H	-1.111800	4.125100	-2.102300
H	-2.096800	4.976000	0.027800
H	-0.527100	3.439200	1.660100
H	1.628300	4.300700	0.399200
O	2.616400	2.935500	-0.768300
C	2.715300	2.021200	0.307000
H	2.974200	2.566800	1.229700
C	1.201000	1.513200	0.575400
C	0.921900	0.177300	-0.032200
H	0.996500	1.503100	1.647500
H	1.333800	0.029000	-1.028400
C	3.804200	1.016800	0.023400
C	4.587300	0.516200	1.070600
C	4.068600	0.586800	-1.283300
C	5.599600	-0.416200	0.832100
H	4.417500	0.861800	2.087800
C	5.078100	-0.342400	-1.540900
H	3.501400	1.003900	-2.109200
C	5.826700	-0.835900	-0.475600
H	6.205100	-0.793700	1.648700
H	5.278700	-0.668200	-2.555400
Pt	-0.893000	-0.744200	0.094900
I	-3.033200	0.386700	-0.990500
I	-0.435500	-2.053700	-2.260700
I	-1.724000	-0.028100	2.592900
Br	7.247200	-2.131900	-0.826400
I	1.593700	-1.643000	1.121000

39

3D-b-TS4,Free Energies=-835.287365

C	-2.980600	4.543500	0.217400
C	-4.062300	3.459700	-0.066300
C	-3.432400	2.336600	-0.879800
C	-1.982600	2.077300	-0.436600
C	-1.087000	3.221200	-0.960200
C	-1.873800	4.565100	-0.857000
H	-3.452400	5.529300	0.282700
H	-4.449500	3.047100	0.872300
H	-1.945200	2.074500	0.664600
H	-0.163200	3.267200	-0.384100
H	-2.323900	4.805600	-1.828600
H	-4.913200	3.882100	-0.610900
H	-2.522900	4.359600	1.197300
H	-1.165800	5.371700	-0.640900
H	-0.804600	3.036000	-2.002400
H	-3.425000	2.604500	-1.949900
O	-4.087000	1.074600	-0.746500
C	-3.206500	0.121200	-1.309900
H	-3.197900	0.211200	-2.410900
C	-1.799500	0.627600	-0.804600
C	-0.747600	-0.274100	-0.659600
H	-0.994500	-1.292400	-0.955400
C	-3.593100	-1.281900	-0.918200
C	-3.516900	-2.317400	-1.855900
C	-4.021800	-1.563800	0.385000
C	-3.852100	-3.626400	-1.502900
H	-3.205600	-2.109400	-2.877200
C	-4.368100	-2.863800	0.749100
H	-4.100600	-0.763400	1.113300
C	-4.275600	-3.878900	-0.201900
H	-3.791300	-4.426000	-2.232300
H	-4.702300	-3.080500	1.757300
Pt	1.039900	-0.147400	0.183200
I	1.049600	1.903700	1.991800
I	0.105800	-1.795600	2.165500
I	1.817100	-2.352700	-1.267700
I	2.189200	1.433100	-1.731400
Br	-4.764500	-5.698900	0.301400
H	-0.796000	0.393600	-1.747200

5. The .xyz files of optimized molecular structures and their free energies at L2/BS1

(1). In Path 1A-*a1*

36
1A-a1-IN1,Free Energies= -1882.560271
C,0,-1.3639158672,3.46923687,-0.9769557265
O,0,-0.9958446882,2.5646135043,-2.0052698168
C,0,-1.9233740605,1.499807108,-1.9636433765
C,0,-2.4101760715,1.3710233926,-0.4911203332
C,0,-1.7575938785,2.5836062101,0.2064447913
H,0,-0.5052413039,4.1122491916,-0.7756195282
H,0,-2.2096369357,4.093448135,-1.3060779069
H,0,-2.7801592562,1.7176051126,-2.6172486763
H,0,-2.4473824188,3.0695075159,0.8986904552
H,0,-0.8563912766,2.3099017142,0.7612540667
C,0,-2.1574882192,-0.0092251258,0.170980747
C,0,-0.7271502664,-0.2643846859,0.7139968094
H,0,-0.6168954269,-1.3283453829,0.9344177514
H,0,-0.5842393454,0.2831055721,1.6524065703
C,0,0.3534750902,0.1526541132,-0.1891912449
C,0,1.0001183394,0.712230176,-1.1104199591
H,0,1.1671701366,1.2190512357,-2.042481327
C,0,-3.1005873792,-0.1569722162,1.3769822515
O,0,-3.8008521901,0.7141708809,1.8266650593
O,0,-3.0194056334,-1.3921194256,1.883318834
C,0,-2.5012727227,-1.114583716,-0.8327903093
O,0,-1.7209700501,-1.9246246474,-1.2667240956
O,0,-3.7856315996,-1.0370142757,-1.1963176333
C,0,-3.8389169914,-1.6487152594,3.027578922
H,0,-3.6351488117,-2.6817951883,3.3046610155
H,0,-3.5755978316,-0.9701206488,3.8418495924
H,0,-4.8933229317,-1.5165026334,2.7748596875
C,0,-4.2125997085,-2.0111128434,-2.1534698686
H,0,-5.273533588,-1.8221506075,-2.30991692
H,0,-3.6579972681,-1.8928567548,-3.0871790141
H,0,-4.0515276937,-3.0189089638,-1.7647970921
H,0,-1.4228040886,0.6075487794,-2.3537108423
H,0,-3.4935085555,1.5011040633,-0.4776318671
Pt,0,2.3949541309,0.1095829612,0.275112255
Cl,0,3.0548492018,-1.6815699482,-0.9914145131
Cl,0,2.0976811599,1.8420287869,1.7781692422

36
1A-a1-TS1,Free Energies=-1882.54117
C,0,-0.9570268922,3.282680304,0.2945703474
O,0,-1.1977678777,3.1318484823,-1.1154184153
C,0,-1.764709758,1.913450395,-1.3662557125
C,0,-2.4827770199,1.4195543027,-0.1143905091
C,0,-1.8073168182,2.2244014978,1.0183408545
H,0,0.1097485486,3.139636203,0.4953051329
H,0,-1.2308387288,4.3088598094,0.547307264
H,0,-2.3519036929,1.9497755985,-2.2888160275
H,0,-2.5633650727,2.6693492724,1.6653773412
H,0,-1.168287654,1.5992481753,1.6465654783
C,0,-2.3620325222,-0.1138779868,-0.0084126838
C,0,-0.8799666284,-0.578891468,0.0344024777
H,0,-0.797896567,-1.5893585117,-0.3704771781
H,0,-0.525949995,-0.588086823,1.071729387
C,0,0.0428041151,0.3200724691,-0.678058583
C,0,1.128799054,0.9809751079,-0.8645919957
H,0,1.3335305954,1.8188192539,-1.523089325
C,0,-3.0900967707,-0.6190351144,1.2390541375
O,0,-3.7094142783,0.0729644698,2.006180306
O,0,-2.9339403528,-1.9392610652,1.3604108531
C,0,-3.0289752394,-0.7195343387,-1.2516644602
O,0,-2.4294855204,-1.1130199963,-2.2221250342
O,0,-4.3570990525,-0.6915981992,-1.1424661452
C,0,-3.5631685807,-2.5351923275,2.50023747
H,0,-3.3258860153,-3.5961330133,2.4419296222
H,0,-3.1668028865,-2.1005685819,3.4203257496
H,0,-4.6429394398,-2.3761540701,2.4596932774
C,0,-5.0840670098,-1.1927790708,-2.270526527
H,0,-6.1351324007,-1.1014381418,-2.0021122307
H,0,-4.8584108523,-0.5997928534,-3.159586204
H,0,-4.8197209239,-2.2358959299,-2.4556962085
H,0,-0.9515552075,1.1227428584,-1.6336794693
H,0,-3.5451907356,1.6680757616,-0.1747968285
Pt,0,2.5093236208,0.192647531,0.2657911844
Cl,0,3.667747006,-0.7127128411,-1.4967568937
Cl,0,1.6022905538,0.948036841,2.2687205482

36
1A-a1-IN2,Free Energies= -1882.607114
C,0,1.4299697515,3.2711248871,-0.8704829922
O,0,0.8269372907,2.9445503909,0.3839482067
C,0,1.5242101734,1.8687641608,0.9867001027
C,0,2.6414855445,1.4305852687,0.017017934
C,0,2.144974941,2.004480033,-1.3197904854
H,0,0.634652139,3.5844896556,-1.5484492981
H,0,2.1330530348,4.1034968575,-0.7275947055
H,0,1.8973993199,2.1839673156,1.9651058361
H,0,2.9611463537,2.1878534028,-2.0182219949
H,0,1.4288293271,1.3314142601,-1.8025522114
C,0,2.6850454669,-0.1084967892,0.1280814478
C,0,1.2037392234,-0.5068714846,0.2814268983
H,0,1.0787449194,-1.4872758128,0.7416241122
H,0,0.734880573,-0.5426532081,-0.7058805966
C,0,0.5893494904,0.6162942646,1.1343580223
C,0,-0.7927705219,1.0384795131,0.8401758708
H,0,-1.1955784642,1.8734648254,1.4217923478
C,0,3.3624633369,-0.7859310746,-1.0560691119
O,0,3.9811823071,-0.2304375826,-1.9290894297
O,0,3.1723359178,-2.1093758143,-0.9950683156
C,0,3.4454904628,-0.4601112151,1.4089640842
O,0,2.9322200028,-0.5804252489,2.4971881654
O,0,4.7579083954,-0.5561731594,1.1904332902
C,0,3.7773342953,-2.8673905236,-2.0448095196
H,0,3.5015644327,-3.9031682437,-1.8521928594
H,0,3.39862377,-2.5417063423,-3.0161944344
H,0,4.8629404903,-2.7454607755,-2.0221498188
C,0,5.5619047312,-0.8308896538,2.3412208822
H,0,6.5801948199,-0.9273768363,1.9680081992
H,0,5.4893765172,-0.0090353667,3.057339201
H,0,5.2352007765,-1.7558563139,2.8209588318
H,0,0.578066216,0.3036860252,2.1898282863
H,0,3.604826003,1.8781483236,0.2783171404
Pt,0,-1.9276829621,0.2878469039,-0.3528213897
Cl,0,-2.9121430165,-1.3323773457,0.9280746093
Cl,0,-1.5146362024,1.4351007648,-2.2916302036

36
1A-a1-TS2,Free Energies=-1882.57972
C,0,-0.9524043621,3.4055279364,-1.252293358
O,0,-0.2342941481,2.3487166935,-1.8930541149
C,0,-0.9466392535,1.1457028116,-1.7504306239
C,0,-2.2033582618,1.4170083204,-0.8898309388
C,0,-1.8275278705,2.7367969324,-0.1968701235
H,0,-0.219999444,4.0993667812,-0.8364956337
H,0,-1.5614142598,3.9335854074,-1.9984228854
H,0,-1.1676258133,0.7077514868,-2.7297217778
H,0,-2.7053066139,3.3221095563,0.0765565843
H,0,-1.2455495944,2.557059862,0.7132947103
C,0,-2.3283753934,0.1744668054,0.0260105595
C,0,-0.8637014539,-0.2001992958,0.3263400263
H,0,-0.6932355731,-1.2364150406,0.626431696
H,0,-0.4349856354,0.4167924692,1.1282337598
C,0,-0.1242172441,0.1720537,-0.9098650957
C,0,1.1360612932,-0.295291613,-1.2670760409
H,0,1.5818202193,0.1442933291,-2.1624583716
C,0,-3.1733872439,0.4125727735,1.2682941831
O,0,-3.9204207027,1.3451637084,1.4303456208
O,0,-2.971645673,-0.5637302861,2.1551797026
C,0,-2.9169141451,-0.952617432,-0.8253017441
O,0,-2.2633903556,-1.5385264314,-1.6611258184
O,0,-4.203135565,-1.1675995972,-0.59078853
C,0,-3.7390681705,-0.4763145179,3.3597241321
H,0,-3.4448405544,-1.3383636852,3.9560577545
H,0,-3.5129331387,0.4528122799,3.8871946496
H,0,-4.8062519628,-0.5104839856,3.1291177288
C,0,-4.8223361095,-2.1899560286,-1.3846574769
H,0,-5.8663206309,-2.2009600772,-1.0771443195
H,0,-4.7319517354,-1.9495939493,-2.4457463049
H,0,-4.3472313007,-3.1531024949,-1.1886474874
H,0,0.3083078859,-1.0772562912,-1.6715727079
H,0,-3.0967768374,1.5562860825,-1.5036410281
Pt,0,2.3073967029,-1.2349023081,-0.0468544476
Cl,0,2.1898502456,-3.2291738382,-1.2108808981
Cl,0,2.5101425493,0.6118870566,1.3448144093

36
1A-a1-P,Free Energies=-1882.619204
C,0,-0.7275329371,3.3020364764,-1.0365737361
O,0,0.1941057357,2.2332736124,-1.159133014
C,0,-0.5439271026,1.0673048093,-1.4602326736
C,0,-1.9764164258,1.2848149438,-0.8700818506
C,0,-1.8869192036,2.6981054477,-0.258046973
H,0,-0.2182927189,4.1184147565,-0.5217147437
H,0,-1.0453220395,3.6513361077,-2.0312689632
H,0,-0.5403130786,0.8868380844,-2.5422881803
H,0,-2.8242774079,3.2481494301,-0.345594706
H,0,-1.6250017787,2.6526024458,0.802638198
C,0,-2.180321858,0.1190843142,0.1385685787
C,0,-0.7492498571,-0.2219770414,0.6076369384
H,0,-0.6698541696,-1.196738471,1.0859686173
H,0,-0.4084059578,0.5390175477,1.3152818684
C,0,0.0247511897,-0.1242556165,-0.6930722651
C,0,0.5419414714,-1.2913835644,-1.3421005073
H,0,0.5663529291,-1.342171314,-2.4285875655
C,0,-3.1261193204,0.4439646961,1.2938016533
O,0,-3.8362720355,1.4128661093,1.3857084831
O,0,-3.0722855648,-0.5345919619,2.2063006595
C,0,-2.7915969939,-1.0790666253,-0.6003596346
O,0,-2.1984232302,-2.0747971732,-0.9404077912
O,0,-4.0854995517,-0.8654155564,-0.8512775402
C,0,-3.9362144514,-0.3732379086,3.3336717838
H,0,-3.754436757,-1.2399126949,3.9675479786
H,0,-3.6969559697,0.5502023265,3.865685638
H,0,-4.9792371313,-0.3414737728,3.0101988737
C,0,-4.7637953931,-1.9055713255,-1.5603448373
H,0,-5.7979157899,-1.5741854724,-1.6405952587
H,0,-4.3242031846,-2.037936226,-2.5516870866
H,0,-4.7002536538,-2.8466436608,-1.0097615072
H,0,0.5030479085,-2.2431016854,-0.820723292
H,0,-2.7419843387,1.2624797786,-1.6486462264
Pt,0,2.1335479609,-0.1644884133,-0.6635726636
Cl,0,2.5732497636,0.6116102775,-2.782500272
Cl,0,2.2736894524,-0.9287340602,1.5064215378

(2). In Path 1A-*a2*

36
1A-a2-IN1,Free Energies=-1882.556257
C,0,3.9165617707,2.6131170362,-1.7465398397
O,0,3.4113936797,3.1165335525,-0.5228746279
C,0,2.4170842487,2.2166402721,-0.0879104117
C,0,3.0509019458,0.8436625771,-0.3473219005
C,0,3.751886167,1.0751701978,-1.7028987594
H,0,3.3567504808,3.0387605992,-2.5928558993
H,0,4.9580057109,2.9331604468,-1.8296956139
H,0,2.2043454339,2.4086951738,0.9639696827
H,0,4.7103006663,0.5506796448,-1.7506713898
H,0,3.1500517056,0.7244240038,-2.5470005729
C,0,2.1453446156,-0.4111522579,-0.2672370184
C,0,0.9252323869,-0.4156643173,-1.2242732299
H,0,0.5152917183,-1.4279703896,-1.2805365568
H,0,1.2457185313,-0.1469966546,-2.2350765722
C,0,-0.1947095196,0.472888054,-0.8796974043
C,0,-1.1110498188,1.3323457458,-0.9714475064
H,0,-1.6266529731,2.1893602044,-1.3647808381
C,0,3.0692037746,-1.5942041361,-0.6077334074
O,0,3.8654993845,-2.0551773227,0.1720330145
O,0,2.9300327214,-2.0075891808,-1.8699533341
C,0,1.6653298923,-0.7168380098,1.1643683025
O,0,0.7698354239,-1.5022055668,1.3925955653
O,0,2.3416187086,-0.06380011,2.0921377736
C,0,3.8040357018,-3.069186414,-2.267501993
H,0,3.5659284663,-3.2653124522,-3.3117931015
H,0,4.8463034735,-2.7613138885,-2.1589915574
H,0,3.6232827302,-3.9555902702,-1.6561648501
C,0,1.9678656599,-0.3390172507,3.4480462984
H,0,2.6569578003,0.2431005423,4.0573452037
H,0,0.9381828317,-0.0195820419,3.6190161765
H,0,2.071076436,-1.40638344,3.652744536
H,0,1.4901212633,2.3556543599,-0.6643147222
H,0,3.8225289464,0.7064478326,0.4138136351
Pt,0,-1.5352455146,0.2478381593,0.713058318
Cl,0,-0.6784145539,1.8859534343,2.1047141037
Cl,0,-2.6176299548,-1.4729244797,-0.3623064932

36
1A-a2-TS1,Free Energies=-1882.540268
C,0,-3.8086513276,-2.0508275541,-2.3547785143
O,0,-2.5925137536,-2.7246354074,-1.9998272514
C,0,-1.9680759132,-2.0787019866,-0.9628144698
C,0,-2.9217644546,-1.0478129479,-0.370371656
C,0,-3.805813676,-0.7299292837,-1.5898132358
H,0,-3.8309766729,-1.9279036363,-3.4398380308
H,0,-4.6429571821,-2.6945712969,-2.0549610915
H,0,-1.512514382,-2.7849168396,-0.2680917369
H,0,-4.8061540634,-0.4099196816,-1.294954894
H,0,-3.3620092339,0.0634507317,-2.2020035763
C,0,-2.2179361392,0.175965087,0.2515258363
C,0,-1.0813458926,0.6704734578,-0.6748337431
H,0,-0.5468950729,1.5079006564,-0.2117169882
H,0,-1.4663491759,1.0388367302,-1.6298927489
C,0,-0.0859020664,-0.3800893783,-0.8785459038
C,0,1.0503445355,-0.9806553121,-0.7496088331
H,0,1.2861909346,-2.0094005744,-1.0044080253
C,0,-3.2619092528,1.2649965603,0.5226334621
O,0,-4.3517467451,1.0200327927,0.981224332
O,0,-2.8259025917,2.4783950438,0.2058453807
C,0,-1.5695627865,-0.1079603718,1.6203501116
O,0,-1.2775076133,0.7742446322,2.3882772161
O,0,-1.3327289685,-1.4012017438,1.8144095278
C,0,-3.7101291811,3.5592111374,0.5226838073
H,0,-3.1889857114,4.4613595094,0.2074955883
H,0,-4.6536719915,3.446554399,-0.0158343118
H,0,-3.9035179989,3.5789943842,1.5968930262
C,0,-0.5939432302,-1.7227084336,3.0078121488
H,0,-0.5364103551,-2.8094925404,3.0256798701
H,0,0.4066894347,-1.2905588125,2.9468845328
H,0,-1.1215850976,-1.3434857149,3.8846239458
H,0,-1.0499494658,-1.4924434689,-1.405071233
H,0,-3.525581888,-1.531784135,0.4025060788
Pt,0,2.3903098916,0.1323719726,0.1110046333
Cl,0,2.9107352964,-1.5382046926,1.6260877029
Cl,0,2.1507147912,1.996941718,-1.2287549561

36
1A-a2-IN2,Free Energies=-1882.604584
C,0,-3.1687709224,3.388082938,-0.7628269231
O,0,-1.7588954135,3.2780677202,-0.6635273724
C,0,-1.3878803532,1.9888584143,-1.1112626187
C,0,-2.6472123597,1.0821526492,-0.9850702114
C,0,-3.6870907747,2.0167623713,-0.3440964569
H,0,-3.4859422216,4.2044662215,-0.1108123006
H,0,-3.4660872807,3.6261955979,-1.7958383516
H,0,-1.018648542,2.0394789909,-2.1434892006
H,0,-4.7014104931,1.8008336845,-0.682303895
H,0,-3.6729630505,1.9408201985,0.7490299011
C,0,-2.203764236,-0.1180982606,-0.1129653194
C,0,-1.1164192658,0.4921508741,0.8033337402
H,0,-0.5037045738,-0.2564693578,1.3071627705
H,0,-1.6026762691,1.1010841085,1.5696436922
C,0,-0.3246397526,1.4185782304,-0.1456352931
C,0,0.8277049232,0.7774861608,-0.8272484751
H,0,0.9747513382,0.9501264726,-1.8967468709
C,0,-3.3631135818,-0.7711020711,0.6272838377
O,0,-4.4849000793,-0.8516248237,0.1880028047
O,0,-2.9825390362,-1.250480017,1.8128795015
C,0,-1.5418367409,-1.1418164637,-1.0338581138
O,0,-0.7233066983,-0.8180770725,-1.8759622781
O,0,-1.9462559314,-2.3816956983,-0.8389441341
C,0,-3.9886514218,-1.9554441042,2.5427241474
H,0,-3.5070956834,-2.2799700173,3.4638911039
H,0,-4.8341920834,-1.2981269273,2.7583937339
H,0,-4.3383176809,-2.8145602796,1.9657136271
C,0,-1.3288921415,-3.3855545747,-1.6606586279
H,0,-1.7826943198,-4.3253447859,-1.351774419
H,0,-1.5355484292,-3.1821891438,-2.7132584985
H,0,-0.2520405182,-3.393236291,-1.4844153457
H,0,0.1221166323,2.2515966901,0.419534973
H,0,-2.9982466412,0.7482637572,-1.9634374679
Pt,0,2.2008710798,-0.0558051824,0.0320561284
Cl,0,1.4727149203,-2.2036580829,0.3844932387
Cl,0,3.6169581508,1.7415058244,0.2026226412

36
1A-a2-TS2,Free Energies=-1882.578124
C,0,-2.6666872722,3.0981718149,-1.3273494324
O,0,-1.439500587,2.6601313279,-1.9401518235
C,0,-1.2350465407,1.3117420956,-1.6340125911
C,0,-2.5472325414,0.7301011436,-1.0833829245
C,0,-3.1173745949,1.9762775868,-0.3877316751
H,0,-2.4759594745,4.0412482011,-0.8095854341
H,0,-3.3982997203,3.2754430552,-2.1236416213
H,0,-0.8326247848,0.7786076238,-2.504250805
H,0,-4.1984831724,1.9264990931,-0.2640777819
H,0,-2.6798081516,2.1046922898,0.6105205287
C,0,-2.1044462077,-0.4478141012,-0.1828599168
C,0,-0.7369822683,-0.0028697351,0.3930973493
H,0,0.0141964601,-0.7988474678,0.4120964046
H,0,-0.7976585315,0.3677047284,1.4256916206
C,0,-0.2638609084,1.1000935896,-0.4799850876
C,0,0.7865618668,1.9755984436,-0.1917729618
H,0,1.0577828159,2.6777161724,-0.9834963124
C,0,-3.1195034028,-0.8025057713,0.8966537287
O,0,-4.2540918466,-0.3974881984,0.9470306351
O,0,-2.5684281592,-1.6320346202,1.7844915491
C,0,-1.8808915451,-1.6492398812,-1.1078110601
O,0,-0.8664741173,-1.8158303983,-1.7426666207
O,0,-2.9531670986,-2.4325656887,-1.1767964056
C,0,-3.4224212551,-2.0555934093,2.8520448333
H,0,-2.8099274434,-2.7065066711,3.4736049894
H,0,-3.7694922732,-1.192030267,3.4233322685
H,0,-4.2831444099,-2.5968058487,2.4528744905
C,0,-2.8497597752,-3.552559251,-2.0648014204
H,0,-3.8035046354,-4.0716991869,-1.9881307662
H,0,-2.6762685504,-3.2090001208,-3.086797175
H,0,-2.0278819183,-4.2021378718,-1.7569495835
H,0,-0.1769829,2.4616215986,0.3163417502
H,0,-3.2188300059,0.4045307488,-1.8818823534
Pt,0,2.0274221234,1.7040862095,1.2756500635
Cl,0,3.768053712,0.9724491866,-0.031002011
Cl,0,0.3820976634,2.3620713297,2.8083392022

36
1A-a2-P,Free Energies=-1882.622686
C,0,1.9189785873,-2.8607186439,-2.2359276624
O,0,0.6603176347,-2.2716582984,-1.9515200433
C,0,0.8719097383,-0.8689210219,-1.8699518088
C,0,2.3399172603,-0.6602062775,-1.4012044491
C,0,2.90298029,-2.0955308609,-1.3558918008
H,0,1.8463232846,-3.9259606326,-2.0077855142
H,0,2.163356623,-2.7406955542,-3.302217566
H,0,0.6598286864,-0.3939589265,-2.8281587426
H,0,3.9360161023,-2.1482693819,-1.7049407632
H,0,2.8684587018,-2.5034097853,-0.3389963033
C,0,2.2464350026,0.0354208287,-0.0189895867
C,0,0.863136458,-0.4004136118,0.5077024396
H,0,0.4981960529,0.177409292,1.3543625904
H,0,0.9239225194,-1.4531212002,0.81341636
C,0,-0.0139744574,-0.3769104762,-0.7247122849
C,0,-1.4354089653,-0.5215957369,-0.7138291684
H,0,-1.9226220573,-0.990416132,-1.5660886191
C,0,3.4368986618,-0.3273189179,0.8570457413
O,0,4.5780746115,-0.0923945114,0.5405871058
O,0,3.0843749698,-0.9537465959,1.9832894822
C,0,2.2362135617,1.5581667906,-0.1849532347
O,0,2.0108478274,2.1337152597,-1.2254608849
O,0,2.4455278498,2.1622889572,0.9797802289
C,0,4.1673807185,-1.3138344003,2.8445896503
H,0,3.7084029248,-1.801688199,3.7033127279
H,0,4.8516559303,-1.9945114997,2.332712245
H,0,4.7149732529,-0.4212149723,3.1547710054
C,0,2.3519989967,3.5914537591,0.9697805921
H,0,2.5880481714,3.9030393784,1.9858126439
H,0,3.0667044096,4.0095357136,0.2580206258
H,0,1.3366947378,3.8920968955,0.703301607
H,0,-1.9528519282,-0.6027447771,0.2402234912
H,0,2.8947122655,-0.0362538386,-2.1014027589
Pt,0,-1.0432497423,1.4623652293,-1.1345449848
Cl,0,-1.2850241402,1.2361529967,-3.4095224182
Cl,0,-1.1306055407,2.2374961517,1.0445750573

(3). In Path 1A-*a3*

36
1A-a2-IN1,Free Energies= -1882.294088
C,0,3.9165617707,2.6131170362,-1.7465398397
O,0,3.4113936797,3.1165335525,-0.5228746279
C,0,2.4170842487,2.2166402721,-0.0879104117
C,0,3.0509019458,0.8436625771,-0.3473219005
C,0,3.751886167,1.0751701978,-1.7028987594
H,0,3.3567504808,3.0387605992,-2.5928558993
H,0,4.9580057109,2.9331604468,-1.8296956139
H,0,2.2043454339,2.4086951738,0.9639696827
H,0,4.7103006663,0.5506796448,-1.7506713898
H,0,3.1500517056,0.7244240038,-2.5470005729
C,0,2.1453446156,-0.4111522579,-0.2672370184
C,0,0.9252323869,-0.4156643173,-1.2242732299
H,0,0.5152917183,-1.4279703896,-1.2805365568
H,0,1.2457185313,-0.1469966546,-2.2350765722
C,0,-0.1947095196,0.472888054,-0.8796974043
C,0,-1.1110498188,1.3323457458,-0.9714475064
H,0,-1.6266529731,2.1893602044,-1.3647808381
C,0,3.0692037746,-1.5942041361,-0.6077334074
O,0,3.8654993845,-2.0551773227,0.1720330145
O,0,2.9300327214,-2.0075891808,-1.8699533341
C,0,1.6653298923,-0.7168380098,1.1643683025
O,0,0.7698354239,-1.5022055668,1.3925955653
O,0,2.3416187086,-0.06380011,2.0921377736
C,0,3.8040357018,-3.069186414,-2.267501993
H,0,3.5659284663,-3.2653124522,-3.3117931015
H,0,4.8463034735,-2.7613138885,-2.1589915574
H,0,3.6232827302,-3.9555902702,-1.6561648501
C,0,1.9678656599,-0.3390172507,3.4480462984
H,0,2.6569578003,0.2431005423,4.0573452037
H,0,0.9381828317,-0.0195820419,3.6190161765
H,0,2.071076436,-1.40638344,3.652744536
H,0,1.4901212633,2.3556543599,-0.6643147222
H,0,3.8225289464,0.7064478326,0.4138136351
Pt,0,-1.5352455146,0.2478381593,0.713058318
Cl,0,-0.6784145539,1.8859534343,2.1047141037
Cl,0,-2.6176299548,-1.4729244797,-0.3623064932

36
1A-a3-TS1,Free Energies=-1882.280402
C,0,4.3211810686,2.4754418409,-1.3420113969
O,0,3.0363940564,3.0651760953,-1.4916745658
C,0,2.0233001074,2.1323835328,-1.1679837697
C,0,2.7296073294,0.9961211432,-0.4103898059
C,0,4.0838613704,0.9834240783,-1.1381310914
H,0,4.9201211695,2.6943135344,-2.2321342831
H,0,4.8244184189,2.9178689884,-0.4711718371
H,0,1.2676544421,2.6344710988,-0.5588122572
H,0,4.8741886384,0.5005008813,-0.5580482806
H,0,3.9967078669,0.4763849146,-2.1060368714
C,0,1.990519055,-0.3826017582,-0.2752636616
C,0,0.6812448243,-0.5164944132,-1.0963101894
H,0,0.2933202061,-1.5334761258,-0.9873404436
H,0,0.8958058846,-0.3595488973,-2.1567714796
C,0,-0.4021012143,0.4050900751,-0.7263417557
C,0,-1.3013107762,1.2832317589,-0.7879739105
H,0,-1.8766763539,2.0842162676,-1.2146099045
C,0,2.9484287058,-1.5023038893,-0.7259796498
O,0,3.7382466344,-2.0502244935,0.0016746623
O,0,2.8228329136,-1.7764751788,-2.029013674
C,0,1.6840887134,-0.7474070771,1.1935222156
O,0,0.7690029044,-1.4799938156,1.5058411825
O,0,2.5389943122,-0.2214007218,2.0509840528
C,0,3.7225742617,-2.7686542548,-2.5337727658
H,0,3.4773747849,-2.8736310849,-3.5895441407
H,0,4.7561980844,-2.4383727895,-2.4073231015
H,0,3.5788171974,-3.7137328284,-2.0062330117
C,0,2.3136378829,-0.5414267459,3.4275041949
H,0,3.1230533709,-0.0576609499,3.9715040465
H,0,1.3465467144,-0.1446305716,3.7434147534
H,0,2.3400768775,-1.6234514318,3.5702060504
H,0,1.5492863527,1.7742679364,-2.09530997
H,0,2.910050977,1.3559745858,0.6036227444
Pt,0,-1.4709770164,0.4375061464,1.0751205829
Cl,0,-0.1480979189,2.0379839284,2.0999709175
Cl,0,-2.9354019045,-1.1993461254,0.409081424

36
1A-a3-IN2,Free Energies= -1882.295830
C,0,-3.6548929115,-2.5858375206,-1.0068077362
O,0,-3.1792449221,-2.0414971076,-2.2335862168
C,0,-2.426468476,-0.8720830634,-1.987740345
C,0,-2.0930998939,-0.8877209972,-0.4862599526
C,0,-3.3600792493,-1.547430733,0.072761874
H,0,-4.7232496814,-2.8040824275,-1.1066587303
H,0,-3.128847403,-3.5283485776,-0.8031392766
H,0,-1.5317362831,-0.897858158,-2.6199171338
H,0,-3.2125273179,-1.9840484182,1.0598942824
H,0,-4.1791684774,-0.8218150883,0.1400041369
C,0,-1.6679856977,0.480426476,0.1128076312
C,0,-0.6707185428,1.2165693199,-0.8196353071
H,0,-0.3345705191,2.1436328938,-0.3467166574
H,0,-1.1670694454,1.4774243959,-1.7587676172
C,0,0.5155635893,0.4194693111,-1.1597425118
C,0,1.3708538416,-0.2434709816,-1.8026934678
H,0,1.8037157322,-0.7530052906,-2.6441148645
C,0,-2.8937130069,1.3735278766,0.3477323123
O,0,-3.4446598083,1.4973861559,1.4133058271
O,0,-3.3004632456,1.9762464617,-0.7752119638
C,0,-1.0057860711,0.335795425,1.4971443642
O,0,-0.1573218233,1.1016337878,1.8993046463
O,0,-1.458630395,-0.699121212,2.1839828168
C,0,-4.4739101927,2.7867866945,-0.6476483782
H,0,-4.6359706694,3.2201680774,-1.6332570362
H,0,-5.326200398,2.1715033746,-0.3507559725
H,0,-4.3152085544,3.5674044361,0.0990202633
C,0,-0.8645570813,-0.8948353054,3.4711336349
H,0,-1.3704266477,-1.7614956214,3.8933189343
H,0,0.2035436483,-1.091777853,3.358323666
H,0,-1.0187828347,-0.0119347327,4.0945557104
H,0,-3.0137378591,0.0186241839,-2.2545245344
H,0,-1.2511739483,-1.5729279864,-0.3309938388
Pt,0,2.1077384208,-0.087745674,0.1051738662
Cl,0,1.3693880535,-2.1982517233,0.703950228
Cl,0,3.1152130708,1.9529476013,-0.1937846531

36
1A-a3-TS2,Free Energies= -1882.245817
C,0,-3.0570871697,-0.9047763598,3.0017433125
O,0,-2.3059290902,-2.0378677165,2.4750356846
C,0,-1.9400800028,-1.7605847249,1.2067768308
C,0,-2.1951182867,-0.2851129622,0.9470683513
C,0,-3.4668908948,-0.0936511257,1.7643281368
H,0,-3.8851914822,-1.3293122241,3.5699998672
H,0,-2.4085646755,-0.3301174594,3.6700127714
H,0,-0.7240115152,-2.0072981602,1.0146666994
H,0,-3.6625186582,0.9550408037,1.9896285369
H,0,-4.3461706216,-0.5338720508,1.2809189933
C,0,-1.9847360833,0.0373478738,-0.5411910178
C,0,-0.7881339292,-0.875207372,-0.9795131074
H,0,-0.1418950026,-0.3373955875,-1.6802928883
H,0,-1.1491899808,-1.7755516437,-1.4835150659
C,0,0.040292344,-1.2289472661,0.1968270441
C,0,1.0717255963,-0.870725513,0.9246506395
H,0,1.2571823051,-1.238549024,1.9321324815
C,0,-3.2513369051,-0.228801002,-1.3523639887
O,0,-3.9079899351,0.6212108965,-1.8957810549
O,0,-3.5756257302,-1.5325735114,-1.3472232954
C,0,-1.6032162247,1.5072386761,-0.7757821305
O,0,-0.9016600301,1.8632761662,-1.6874881345
O,0,-2.1491903192,2.3059771218,0.1336908193
C,0,-4.7668600491,-1.8710682974,-2.0685797541
H,0,-4.8758669474,-2.9492106877,-1.9612120133
H,0,-5.6275112411,-1.348253859,-1.6458960217
H,0,-4.6597248176,-1.5964527216,-3.1197634028
C,0,-1.7932912791,3.6914178706,0.019375141
H,0,-2.3388758703,4.1969486023,0.814811365
H,0,-0.7158950119,3.800594957,0.1584273755
H,0,-2.0899115365,4.0734771764,-0.9593923348
H,0,-2.322218132,-2.4827496335,0.4771996072
H,0,-1.4129301222,0.2655404607,1.4811504328
Pt,0,2.2462393884,0.4736670888,0.2146254773
Cl,0,1.1879450499,2.0693185886,1.5576791232
Cl,0,3.4171138607,-0.8500683798,-1.2525344806

36
1A-a3-IN3,Free Energies= -1882.324591
C,0,-3.0348388039,-1.1119971806,2.9636475627
O,0,-1.8823033192,-1.8319706174,2.4614614132
C,0,-1.8917344425,-1.6256352677,1.0768795754
C,0,-2.3502319151,-0.1929335657,0.9160392733
C,0,-3.5721694257,-0.1987759983,1.8172799585
H,0,-3.787058096,-1.8344951612,3.2967403232
H,0,-2.6990904012,-0.5301117506,3.8256235535
H,0,-0.2604643674,-2.6693069134,0.0282012029
H,0,-3.8554952907,0.7915407397,2.1776853237
H,0,-4.4341415736,-0.6572485118,1.3222552228
C,0,-2.204785947,0.1006982008,-0.5913521525
C,0,-1.0674269499,-0.9011913334,-1.0227439296
H,0,-0.2632705464,-0.3674406847,-1.5314788821
H,0,-1.4673261198,-1.6438803106,-1.7162552378
C,0,-0.5891919553,-1.6425359262,0.2544109445
C,0,0.5247389282,-1.0656336852,1.0396002306
H,0,0.7901652762,-1.5946310237,1.9622589322
C,0,-3.4884187043,-0.1255395559,-1.3816278036
O,0,-4.0342607484,0.7025156188,-2.0667851965
O,0,-3.9520786763,-1.3765802992,-1.2217606369
C,0,-1.7766771028,1.5499565628,-0.8401215696
O,0,-0.9139935283,1.886783583,-1.6133409067
O,0,-2.4741808642,2.3851260838,-0.0732101309
C,0,-5.1583601565,-1.6775555592,-1.9282310815
H,0,-5.3867688183,-2.7149279953,-1.6868904808
H,0,-5.9658688675,-1.0182557244,-1.6019775975
H,0,-5.0098200022,-1.5559319913,-3.0034499271
C,0,-2.1251035983,3.7663563072,-0.196691093
H,0,-2.7992433282,4.2964807378,0.4746847337
H,0,-1.0857179018,3.9140401796,0.1052130934
H,0,-2.2640592454,4.1002163093,-1.2270117105
H,0,-2.5915351527,-2.316504909,0.5835819693
H,0,-1.6000065795,0.4304377545,1.4178710674
Pt,0,1.5062894989,0.3992769172,0.6473936494
Cl,0,0.5943283893,2.0383565716,1.9687660922
Cl,0,2.9572040935,-0.4347740111,-0.9057459755

36
1A-a3-TS3,Free Energies= -1882.299510
C,0,1.7274889501,-0.5163899723,3.6965274906
O,0,0.484658216,-0.1264453956,3.0590788302
C,0,0.8268532992,0.2875346014,1.7811898542
C,0,2.0192156358,-0.5655931114,1.3609452941
C,0,2.8556059854,-0.4620805319,2.6237534312
H,0,1.9213371111,0.1606345104,4.5331505986
H,0,1.5859429973,-1.5280507313,4.0852898592
H,0,-1.2072485684,1.1125409452,0.4837942304
H,0,3.574384868,-1.275247957,2.7354046092
H,0,3.393955486,0.490926051,2.6681553514
C,0,2.2983042507,-0.0688594666,-0.0685894724
C,0,0.8363299734,0.0684227165,-0.6116817693
H,0,0.5472552907,-0.795535093,-1.219339287
H,0,0.6743149171,0.9560453061,-1.2314578004
C,0,-0.0588625894,0.085748101,0.6078875576
C,0,-1.4447275715,-0.0651066363,0.6109381436
H,0,-1.9130070912,-0.1616760655,1.5934775237
C,0,3.0103182055,1.2816653898,-0.0524775938
O,0,2.4456191279,2.3496971753,-0.036692618
O,0,4.3322849539,1.1276722071,0.0049171451
C,0,3.1062488463,-1.0826538192,-0.8694860737
O,0,3.5909256173,-2.0859844748,-0.4101676843
O,0,3.174821918,-0.7145844765,-2.1493473693
C,0,5.0986997207,2.3367816024,0.0530741691
H,0,6.1396887809,2.0190494372,0.0741691055
H,0,4.8959482733,2.946714623,-0.8295665665
H,0,4.8500194851,2.906690046,0.9511451506
C,0,3.9058278905,-1.5955062441,-3.0093996308
H,0,3.841962233,-1.1525720752,-4.0018155798
H,0,4.9453199461,-1.6622018246,-2.6806708834
H,0,3.458103156,-2.5914862047,-3.0004722599
H,0,1.1252903304,1.3519816568,1.7626229245
H,0,1.678171543,-1.6045861273,1.2612795425
Pt,0,-2.461052099,-0.5782230579,-0.9527608988
Cl,0,-2.5521003342,-2.8170396638,-0.4097088732
Cl,0,-2.3941733359,1.6035020851,-1.7629526518

36
1A-a3-P,Free Energies= -1882.346818
C,0,-1.9521693522,3.4642680588,-0.8622019211
O,0,-0.7777953114,3.1051426398,-0.1000864228
C,0,-0.9822248007,1.8192638459,0.3723073121
C,0,-2.0023837148,1.1616843436,-0.5325787467
C,0,-2.9790775505,2.3112218899,-0.7091007309
H,0,-2.3255956996,4.4205688822,-0.4870496086
H,0,-1.6469244518,3.5837981382,-1.9069612226
H,0,1.9716465904,0.1049849742,1.3303828223
H,0,-3.6263453521,2.2177370075,-1.5831715113
H,0,-3.6022953343,2.4574559539,0.1810695777
C,0,-2.1968797759,-0.2192837227,0.1262544325
C,0,-0.8337939819,-0.4509800011,0.8787126016
H,0,-0.3837909655,-1.4143347118,0.6525745659
H,0,-1.0220027818,-0.4110906339,1.9579009487
C,0,0.0536109833,0.7381785989,0.5113466565
C,0,1.4436660381,0.8874352998,0.7883802536
H,0,1.8444608256,1.8952295106,0.8789065001
C,0,-3.3641384302,-0.1738613642,1.1034457644
O,0,-3.2687908385,0.0464328598,2.2877017613
O,0,-4.524721416,-0.3240485472,0.4615999563
C,0,-2.3963657975,-1.313902288,-0.9183084105
O,0,-2.3307759484,-1.1549059916,-2.1120263003
O,0,-2.5879320773,-2.4932344174,-0.3222978471
C,0,-5.6981874157,-0.2346336299,1.272839605
H,0,-6.5356553597,-0.3643395863,0.588892196
H,0,-5.6937650923,-1.0201905865,2.0318091295
H,0,-5.7480292078,0.7398949974,1.7641672801
C,0,-2.6679453961,-3.6211451421,-1.1980745093
H,0,-2.8557181222,-4.4780196142,-0.5525957026
H,0,-3.4815682731,-3.4902175226,-1.9147513088
H,0,-1.7248017451,-3.7437553289,-1.7356409739
H,0,-1.3977040603,1.871845432,1.4002606982
H,0,-1.5277190202,0.9779466005,-1.5032247217
Pt,0,1.3339843804,0.3680736956,-1.2095178657
Cl,0,1.3362909737,2.4110799529,-2.2284103221
Cl,0,1.6840244815,-1.883222593,-0.7913939362

36
1A-a4-IN1,Free Energies= -1882.290221
C,0,-1.5361497875,-2.5139898591,2.4773316506
O,0,-0.8396957481,-1.4139525057,3.0388301613
C,0,-0.5953670434,-0.5210206289,1.9811998781
C,0,-1.9318788009,-0.4730549759,1.2317673901
C,0,-2.3833830564,-1.9501812415,1.3129560529
H,0,-0.8196228092,-3.2619415732,2.1081807059
H,0,-2.1340790916,-2.9666864254,3.271218216
H,0,-0.2809226217,0.4399124933,2.3888083449
H,0,-3.4572893662,-2.0223612508,1.5060351259
H,0,-2.183960294,-2.4976896126,0.3862083394
C,0,-1.9685436228,0.1403406553,-0.1907537154
C,0,-0.9866319778,-0.4991150414,-1.2150140621
H,0,-1.4276525487,-0.4465337322,-2.2144503051
H,0,-0.829666448,-1.5582907883,-0.9939340988
C,0,0.3233926439,0.1534415314,-1.3556997753
C,0,1.2753634519,0.7769400655,-1.8930265075
H,0,1.756458338,1.4169706814,-2.6100258473
C,0,-3.4251971807,-0.0482729745,-0.6473000957
O,0,-4.3399620678,0.5939004317,-0.1938755339
O,0,-3.5709679936,-1.0338769219,-1.5373202106
C,0,-1.7634940912,1.664434547,-0.2238430128
O,0,-1.7089296908,2.273649506,-1.2668980225
O,0,-1.6571878676,2.2097131299,0.9783898947
C,0,-4.9189116782,-1.3053003173,-1.9342992004
H,0,-4.8522654758,-2.1206938884,-2.652852411
H,0,-5.5146141154,-1.6006304456,-1.0675558595
H,0,-5.3641470619,-0.4198450136,-2.3925648642
C,0,-1.4449356005,3.6260184256,0.9977539583
H,0,-1.3597361885,3.8890484646,2.0505853077
H,0,-0.523743361,3.8691172152,0.4655107531
H,0,-2.291909317,4.1362430791,0.5343500908
H,0,0.2067833197,-0.915665374,1.3306446697
H,0,-2.6137210879,0.1291389463,1.8371725711
Pt,0,2.0395430843,0.0810845927,-0.1278040663
Cl,0,2.3878331303,-2.1118734343,-0.7432778069
Cl,0,1.9732980262,2.1824952397,0.8101582843

36
1A-a4-TS1,Free Energies= -1882.265126
C,0,-0.4795439519,-2.2712527204,1.8446810148
O,0,-0.0893316123,-1.0204382825,2.3871478385
C,0,-0.7846231057,-0.0533086062,1.6850918623
C,0,-2.1739405813,-0.6118843792,1.3525973052
C,0,-1.9867746794,-2.1351608841,1.5864335765
H,0,0.0761017947,-2.4558178117,0.9119797221
H,0,-0.2166303051,-3.0454149008,2.5663973559
H,0,-0.7493038635,0.9019681357,2.2084755994
H,0,-2.5571180166,-2.4461030441,2.4644184347
H,0,-2.3173955264,-2.7508424876,0.7441974252
C,0,-2.6335308715,-0.2306018365,-0.0725152615
C,0,-1.5670191698,-0.6222235529,-1.1214363313
H,0,-1.9674269223,-0.3857494271,-2.1197905193
H,0,-1.3438275861,-1.6917738924,-1.0940445861
C,0,-0.3656695669,0.1851157479,-1.0555820508
C,0,0.6016380593,0.9642439041,-1.3749809728
H,0,0.6780345058,1.2461059481,-2.433092487
C,0,-3.9769876024,-0.9197586179,-0.3300940969
O,0,-4.9666346936,-0.6682237446,0.3102351717
O,0,-3.915619963,-1.8327381272,-1.3018140715
C,0,-2.9039341225,1.2758287255,-0.2609790592
O,0,-3.1237714274,1.7416473126,-1.3544132964
O,0,-2.8542130295,1.9580092504,0.8690033593
C,0,-5.1437033628,-2.5190226783,-1.5774533766
H,0,-4.9107263592,-3.2219346838,-2.3754841898
H,0,-5.4898764863,-3.0445404418,-0.6850909172
H,0,-5.9070026819,-1.8073228338,-1.8979798527
C,0,-3.033587306,3.3785929418,0.7484299781
H,0,-3.0002011884,3.758823079,1.7674478477
H,0,-2.2181065915,3.7992886157,0.158063155
H,0,-3.9960192281,3.5920270007,0.2797091414
H,0,-0.2433779488,0.1444464137,0.7071013343
H,0,-2.9149228192,-0.2073702466,2.0433361637
Pt,0,1.9773319526,1.6728217194,-0.225463021
Cl,0,3.5940011453,0.2295459649,-1.0057024478
Cl,0,0.6315011114,3.2477794399,0.8138062523

36
1A-a4-IN2,Free Energies= -1882.342758
C,0,-2.3455224598,2.6932572722,-1.1891681959
O,0,-0.9528929276,2.530772062,-0.9181473935
C,0,-0.5945678151,1.1595043541,-0.9121740067
C,0,-1.8819503135,0.3384838915,-1.1564538591
C,0,-2.7922540429,1.3799359011,-1.8213640118
H,0,-2.8901110319,2.8941754372,-0.2576188366
H,0,-2.4537457306,3.5568933508,-1.8494656734
H,0,0.2118267037,0.9784072107,-1.6227918748
H,0,-2.5821774195,1.384491473,-2.8950241614
H,0,-3.8584850223,1.1771719362,-1.6932090796
C,0,-2.3087362163,-0.1809223496,0.2732068342
C,0,-1.5037912127,0.6784324639,1.2821353785
H,0,-1.393036405,0.1898804107,2.248989134
H,0,-1.9689113613,1.6594927089,1.3998358706
C,0,-0.2345483332,0.7811515833,0.5051022825
C,0,1.041807505,0.4915528677,0.9881692444
H,0,1.0973309441,0.1919062103,2.0368819439
C,0,-3.8221709345,-0.1180123454,0.4746373857
O,0,-4.5838522306,-0.9801286879,0.1168463451
O,0,-4.2061303995,1.0249072904,1.0551471771
C,0,-1.8889656408,-1.6549698661,0.4823517718
O,0,-1.4740485655,-2.0622885888,1.5419880058
O,0,-2.0482296214,-2.3868011705,-0.6047761506
C,0,-5.6196994635,1.1774941653,1.2282900849
H,0,-5.750623594,2.1421007155,1.7161400635
H,0,-6.1236999317,1.1615989003,0.259151672
H,0,-6.012700658,0.3712868141,1.8507897826
C,0,-1.6239057694,-3.7523942058,-0.4989044244
H,0,-1.8452807915,-4.1972595395,-1.4673197324
H,0,-0.5519100955,-3.7846483912,-0.2935308631
H,0,-2.1764860918,-4.255643741,0.2968222513
H,0,0.933355443,1.6906412342,0.9844949664
H,0,-1.7021878964,-0.5163782945,-1.8044243141
Pt,0,2.5652319535,0.0269423835,-0.1161665126
Cl,0,3.9438132278,1.6293879037,0.801549654
Cl,0,1.3646521987,-1.6321673605,-1.2185777581

36
1A-a4-TS2,Free Energies= -1882.303989
C,0,0.0385578893,-3.0522826745,1.9232926034
O,0,0.5471340374,-1.7350251658,2.0381936826
C,0,-0.3145123193,-0.8878800126,1.3302006349
C,0,-1.7499079517,-1.4585054216,1.4929725733
C,0,-1.4897359159,-2.9137328266,1.9579765602
H,0,0.3757436513,-3.5116689235,0.9796213697
H,0,0.4488174953,-3.6373198738,2.7484850367
H,0,-0.191884789,0.1139452139,1.7420325952
H,0,-1.8703619329,-3.0436786774,2.9728918461
H,0,-1.9852717663,-3.6577208425,1.3330231711
C,0,-2.3930673504,-1.2962221655,0.1000105187
C,0,-1.2401717993,-1.620992176,-0.8647426004
H,0,-1.4490038992,-1.305038374,-1.888263002
H,0,-1.0620713406,-2.7008272367,-0.8711089602
C,0,-0.0409978607,-0.8935148428,-0.2189849241
C,0,0.2332064764,0.4270699008,-0.8344337085
H,0,-0.0107226014,0.5630486999,-1.8913827303
C,0,-3.6463096703,-2.1357495676,-0.1251847783
O,0,-4.2044560713,-2.8160643526,0.6980146395
O,0,-4.0598257924,-2.0018437542,-1.3927299876
C,0,-2.7908120735,0.1702168451,-0.1101396478
O,0,-2.2469630587,0.9130118287,-0.9002957043
O,0,-3.785277683,0.5348793824,0.6845550994
C,0,-5.2528877151,-2.7139310137,-1.7307150184
H,0,-5.4526474979,-2.4708218563,-2.7732921415
H,0,-5.1010691437,-3.7888324241,-1.6084061408
H,0,-6.0798401952,-2.393250595,-1.0932699833
C,0,-4.1742182563,1.9158272152,0.6009743665
H,0,-4.9390565267,2.0448339512,1.3646609108
H,0,-3.3111416151,2.5562627659,0.7932389768
H,0,-4.5768508243,2.1284873493,-0.3915952811
H,0,0.9040566945,-1.4377028598,-0.3892405263
H,0,-2.319895463,-0.9118751991,2.2448015982
Pt,0,1.1635116343,1.783176223,-0.0608778009
Cl,0,3.2544528692,1.2461123842,-0.8338670584
Cl,0,-0.4028911175,2.9486091492,1.1473759417

36
1A-a4-P,Free Energies= -1882.364194
C,0,-2.2881870845,-2.6008825277,1.5439099018
O,0,-0.8973745805,-2.3348240276,1.3894195739
C,0,-0.66331553,-0.9303471196,1.3005360874
C,0,-2.0403912155,-0.2376736983,1.3576663016
C,0,-2.8866987961,-1.3021575101,2.069068978
H,0,-2.7302300626,-2.8862338801,0.5779962793
H,0,-2.3925834228,-3.4436817956,2.2319766362
H,0,0.0234849635,-0.6355811091,2.0925512703
H,0,-2.7116181863,-1.2212596751,3.1466580027
H,0,-3.9590789714,-1.2048678426,1.894265898
C,0,-2.4162462126,0.0782561182,-0.1368176624
C,0,-1.3526805777,-0.6639105323,-0.9864186115
H,0,-1.20779068,-0.2336229351,-1.9760000178
H,0,-1.6603100435,-1.7075574038,-1.1184276689
C,0,-0.1283981963,-0.6931994001,-0.1051664061
C,0,1.1895291399,-1.0637791856,-0.5127710747
H,0,1.3751474575,-1.3192859104,-1.5541781998
C,0,-3.8620926266,-0.2998154108,-0.4518254519
O,0,-4.8087959345,0.2426576601,0.0641580101
O,0,-3.9651896317,-1.3092313755,-1.320921098
C,0,-2.3279427862,1.5669597319,-0.5087263262
O,0,-2.8279226594,2.0103183581,-1.5117178896
O,0,-1.5959050431,2.2909425976,0.3443423757
C,0,-5.3019926028,-1.6910265101,-1.6563436576
H,0,-5.2008811275,-2.5194773,-2.355962408
H,0,-5.8458178554,-2.0028354014,-0.7616130294
H,0,-5.8252681784,-0.8531957607,-2.1215802527
C,0,-1.3870279144,3.6566557236,-0.038147469
H,0,-0.7658004221,4.0831311284,0.7485317745
H,0,-0.8799782923,3.6967697177,-1.0055507412
H,0,-2.3429753742,4.1795682263,-0.1051360048
H,0,1.8552763056,-1.5179819081,0.2185984065
H,0,-2.0009320603,0.6876605832,1.9290354588
Pt,0,1.2120090118,0.9888057076,-0.2805395135
Cl,0,0.8212793278,1.4440911474,-2.5056854353
Cl,0,1.9534968626,1.0719525199,1.8969189637

(5). In Path 1A-*b*

36
1A-b-TS1,Free Energies= -1882.267834
C,0,0.211576003,-2.171646238,1.6632358353
O,0,0.7550758535,-0.9183182668,1.2750916184
C,0,-0.1064249356,0.072891689,1.8138391162
C,0,-1.5095368872,-0.455873561,1.4990546223
C,0,-1.3189113145,-1.9617083636,1.7954768959
H,0,0.491384725,-2.9036600605,0.9004228544
H,0,0.6520486187,-2.4864251305,2.6179014836
H,0,0.0249624425,0.1467151074,2.9034422423
H,0,-1.6543602027,-2.1841957367,2.8115042478
H,0,-1.8881479914,-2.6074299119,1.120142028
C,0,-1.956590757,-0.1834342389,0.0344439564
C,0,-1.0166677771,-0.8029492886,-1.0322522857
H,0,-1.4865594509,-0.7555856387,-2.0188355103
H,0,-0.8211048205,-1.8601571351,-0.8404262108
C,0,0.256041904,-0.0972354015,-1.1247267794
C,0,1.1676618645,0.7443411461,-1.2593920529
H,0,0.3576992926,1.0582695594,-2.0583399424
C,0,-3.3824270995,-0.7376100994,-0.0990136785
O,0,-4.335530259,-0.248906878,0.4534464963
O,0,-3.4374527016,-1.8361687419,-0.8598003841
C,0,-2.061058387,1.3202380521,-0.2849077448
O,0,-1.9532880658,1.7413978988,-1.4169640926
O,0,-2.2684482847,2.066744571,0.7821614328
C,0,-4.7377514123,-2.4225910561,-0.996320742
H,0,-4.5949841819,-3.305353816,-1.6175095032
H,0,-5.1330316117,-2.6974919342,-0.0161375784
H,0,-5.4201702612,-1.717614658,-1.475459441
C,0,-2.3118606475,3.4847584226,0.5541146811
H,0,-2.5116673086,3.9231920646,1.5300369032
H,0,-1.3474153903,3.8207208504,0.1676308041
H,0,-3.108089667,3.7259682671,-0.1523386694
H,0,0.1550551257,1.0344075678,1.3704410734
H,0,-2.2620055374,-0.0072021194,2.148954482
Pt,0,2.6692885223,1.8429007731,-1.0111641977
Cl,0,4.1152103855,0.6519480276,-2.332622545
Cl,0,1.5347925851,3.295735418,0.3988772139

36
1A-b-IN1,Free Energies= -1882.299749
C,0,1.9848359775,2.7916142927,-1.2735924262
O,0,1.6780242955,2.6573951694,0.10277874
C,0,2.8606687726,2.2272360334,0.7378855573
C,0,3.6544636846,1.3796651552,-0.2994791879
C,0,2.8415141041,1.5688373826,-1.5972451014
H,0,1.0442105775,2.8261954896,-1.8264463725
H,0,2.5423721266,3.7257373221,-1.4500992458
H,0,3.4648170011,3.0956095804,1.040177882
H,0,3.4883162734,1.7046937272,-2.4650456535
H,0,2.1823981008,0.7218082231,-1.8035662539
C,0,3.9387748749,-0.0882684882,0.1181820232
C,0,2.727547486,-1.0541116176,0.0835405304
H,0,3.0546459736,-2.0315118171,0.4452872289
H,0,2.395152843,-1.1813634889,-0.9493674997
C,0,1.5595207585,-0.6209819283,0.9440233198
C,0,0.457584419,-0.1589236807,0.4467040332
H,0,1.6447420794,-0.6835555828,2.028253973
C,0,4.9970937482,-0.672990401,-0.8323544816
O,0,5.3991188384,-0.1490443721,-1.8399206489
O,0,5.4080638443,-1.8718358913,-0.3987699157
C,0,4.5388518355,-0.0924094552,1.5278382755
O,0,4.0386469791,-0.6119250452,2.4980986482
O,0,5.6852124574,0.5909119562,1.5599085872
C,0,6.3910299769,-2.5169365632,-1.2130894142
H,0,6.6110279442,-3.4601822838,-0.7153060301
H,0,5.9956935124,-2.6920082703,-2.2161516982
H,0,7.2884788458,-1.8983173619,-1.2839171288
C,0,6.3196557226,0.6803500556,2.8387561419
H,0,7.2158903917,1.2772338734,2.677630654
H,0,5.655920373,1.166257187,3.5573733026
H,0,6.5790498848,-0.3157376512,3.2040646737
H,0,2.5751746254,1.6843055101,1.6427821379
H,0,4.6376164979,1.8349490131,-0.4361176977
Pt,0,-1.0249578585,0.4858713338,-0.2792776349
Cl,0,-0.5874078254,0.218400196,-2.5114403372
Cl,0,-2.2447731615,1.0561432578,1.5571510493

36
1A-b-TS2,Free Energies= -1882.284167
C,0,-0.2064527416,-1.4391381249,2.4469349276
O,0,-0.4504695161,-0.0920845724,2.8557197947
C,0,-1.2198032788,0.5075654997,1.8934882744
C,0,-2.1692596178,-0.5400635737,1.3189849974
C,0,-1.4345631234,-1.8686671437,1.6216373522
H,0,0.7133625505,-1.4669903857,1.8500970615
H,0,-0.0559551074,-2.0261053011,3.3539875582
H,0,-1.6680005425,1.4219782896,2.2860229061
H,0,-2.0922373144,-2.5347975492,2.1816019349
H,0,-1.127038214,-2.4039112751,0.7211627721
C,0,-2.5381333559,-0.2597513126,-0.156018187
C,0,-1.4597932784,-0.6119199046,-1.2005517168
H,0,-1.801157748,-0.2346422292,-2.1681593565
H,0,-1.3951761931,-1.7016892073,-1.2984482978
C,0,-0.0571422901,-0.1038562507,-1.0009913288
C,0,0.569436605,0.6042435611,-0.1011324921
H,0,0.6495212169,-0.3507492839,-1.8015067282
C,0,-3.7748605292,-1.1034531098,-0.5036794717
O,0,-4.2133449608,-1.9962198063,0.1776235359
O,0,-4.2879569229,-0.7344832109,-1.6808623656
C,0,-2.9238905736,1.2198224967,-0.331578935
O,0,-2.4584909934,1.9624633685,-1.1577487784
O,0,-3.8490816324,1.5764361136,0.5659227823
C,0,-5.4423408969,-1.4622656202,-2.1104812183
H,0,-5.7284916443,-1.018878752,-3.0629645334
H,0,-5.2006657185,-2.5204272127,-2.2334644227
H,0,-6.247085966,-1.3599044992,-1.379210962
C,0,-4.2662492434,2.9450418372,0.5042657413
H,0,-4.9996195771,3.0621262564,1.3005390505
H,0,-3.4123675795,3.6075823223,0.6632176403
H,0,-4.7122017622,3.1600508073,-0.4691995376
H,0,-0.555843705,0.8898751565,1.0322912113
H,0,-3.0973654396,-0.5084979872,1.8926033442
Pt,0,2.0123813959,1.4064017184,0.6610032226
Cl,0,3.4999834628,-0.2156867176,-0.0009717773
Cl,0,1.0304933749,3.2770153731,1.5694483812

36
1A-a2-IN2,Free Energies= -1882.344921
C,0,-3.1687709224,3.388082938,-0.7628269231
O,0,-1.7588954135,3.2780677202,-0.6635273724
C,0,-1.3878803532,1.9888584143,-1.1112626187
C,0,-2.6472123597,1.0821526492,-0.9850702114
C,0,-3.6870907747,2.0167623713,-0.3440964569
H,0,-3.4859422216,4.2044662215,-0.1108123006
H,0,-3.4660872807,3.6261955979,-1.7958383516
H,0,-1.018648542,2.0394789909,-2.1434892006
H,0,-4.7014104931,1.8008336845,-0.682303895
H,0,-3.6729630505,1.9408201985,0.7490299011
C,0,-2.203764236,-0.1180982606,-0.1129653194
C,0,-1.1164192658,0.4921508741,0.8033337402
H,0,-0.5037045738,-0.2564693578,1.3071627705
H,0,-1.6026762691,1.1010841085,1.5696436922
C,0,-0.3246397526,1.4185782304,-0.1456352931
C,0,0.8277049232,0.7774861608,-0.8272484751
H,0,0.9747513382,0.9501264726,-1.8967468709
C,0,-3.3631135818,-0.7711020711,0.6272838377
O,0,-4.4849000793,-0.8516248237,0.1880028047
O,0,-2.9825390362,-1.250480017,1.8128795015
C,0,-1.5418367409,-1.1418164637,-1.0338581138
O,0,-0.7233066983,-0.8180770725,-1.8759622781
O,0,-1.9462559314,-2.3816956983,-0.8389441341
C,0,-3.9886514218,-1.9554441042,2.5427241474
H,0,-3.5070956834,-2.2799700173,3.4638911039
H,0,-4.8341920834,-1.2981269273,2.7583937339
H,0,-4.3383176809,-2.8145602796,1.9657136271
C,0,-1.3288921415,-3.3855545747,-1.6606586279
H,0,-1.7826943198,-4.3253447859,-1.351774419
H,0,-1.5355484292,-3.1821891438,-2.7132584985
H,0,-0.2520405182,-3.393236291,-1.4844153457
H,0,0.1221166323,2.2515966901,0.419534973
H,0,-2.9982466412,0.7482637572,-1.9634374679
Pt,0,2.2008710798,-0.0558051824,0.0320561284
Cl,0,1.4727149203,-2.2036580829,0.3844932387
Cl,0,3.6169581508,1.7415058244,0.2026226412

(6). In Path 1A-*c*

36
1A-c-IN1,Free Energies= -1882.304484
C,0,-0.4019138478,-1.1452807643,2.9777910201
O,0,-0.0169472239,0.1768227555,2.5569821772
C,0,-1.2678087691,0.7971244756,2.2012974165
C,0,-2.0933341351,-0.2791034085,1.4624642475
C,0,-1.4457912539,-1.6001155978,1.9518727721
H,0,0.4934614486,-1.7634250434,3.0046184434
H,0,-0.82740126,-1.0567656615,3.9851509131
H,0,-1.7735536003,1.0628992933,3.1371361937
H,0,-2.1891260438,-2.270414151,2.3862790384
H,0,-0.941208858,-2.1382308434,1.1480539638
C,0,-2.290082378,-0.1301503347,-0.0860165394
C,0,-1.2192421582,-0.6945290825,-1.0688801858
H,0,-1.6220426387,-0.5949262923,-2.0813218122
H,0,-1.0749246746,-1.7625057561,-0.8746753716
C,0,0.1095396572,-0.0609799604,-1.0901656793
C,0,1.2441950134,0.3301192194,-1.4791931806
H,0,1.9600092799,0.653785018,-2.2115718344
C,0,-3.5761087146,-0.9155020398,-0.4321701162
O,0,-4.1178754374,-1.7108064113,0.2942688125
O,0,-4.0034677302,-0.6218291588,-1.6638184894
C,0,-2.5425570373,1.3372802186,-0.4624357929
O,0,-2.0557343631,1.8972793241,-1.4104382045
O,0,-3.3876954299,1.9145878688,0.3999596068
C,0,-5.1751212327,-1.3190348537,-2.0966201769
H,0,-5.3715707988,-0.9593702085,-3.1053796282
H,0,-4.9955192957,-2.3964090081,-2.0981064545
H,0,-6.0148427269,-1.0947723743,-1.4352896098
C,0,-3.6392087115,3.3045732088,0.167096422
H,0,-4.3254376411,3.6112570738,0.955163241
H,0,-2.7044912835,3.8670571426,0.2241443174
H,0,-4.0903089911,3.4499866914,-0.8167967222
H,0,-1.046779769,1.7098963741,1.6547505722
H,0,-3.106855688,-0.2234178433,1.8598302925
Pt,0,1.2369070849,0.3170508141,0.589339082
Cl,0,1.8372955004,-1.9354423643,0.6771665941
Cl,0,1.0401877079,2.6369526799,0.5972906716

36
1A-c-TS1,Free Energies= -1882.234740
C,0,0.7833165306,-1.4866609759,2.3742446549
O,0,1.0433952546,-0.138552842,1.9499044055
C,0,-0.2510744778,0.4833151869,1.963346628
C,0,-1.246055775,-0.5614237752,1.4079070167
C,0,-0.4976038464,-1.8988919601,1.6385650536
H,0,1.6520769248,-2.091722538,2.1209839114
H,0,0.6423072287,-1.4706766639,3.4624655465
H,0,-0.5013135748,0.6961459481,3.0099051261
H,0,-1.1026995383,-2.5974897435,2.2185632007
H,0,-0.2257972091,-2.3915370871,0.7039963368
C,0,-1.8400766946,-0.3312907119,-0.0254078509
C,0,-1.0646504048,-0.8190887049,-1.2829146221
H,0,-1.7230429046,-0.7190636281,-2.1497304082
H,0,-0.8031578486,-1.876598773,-1.1845972286
C,0,0.2044411634,-0.1247853658,-1.6163932733
C,0,1.2032173956,0.2016159012,-2.4124311818
H,0,0.1810295455,1.0370152434,-2.1169755661
C,0,-3.1785012416,-1.104261569,-0.0734226868
O,0,-3.52009183,-1.9442060092,0.7199162315
O,0,-3.9039807883,-0.7374521582,-1.1339241507
C,0,-2.1658560553,1.1532543216,-0.2339881298
O,0,-1.8558983734,1.7908393028,-1.2119593047
O,0,-2.830912086,1.6545567025,0.8058121997
C,0,-5.1560704128,-1.4127952567,-1.2943604158
H,0,-5.5964522004,-0.9977802978,-2.1994173113
H,0,-4.9941814516,-2.4876186316,-1.4000728888
H,0,-5.7981442843,-1.227330939,-0.4307048293
C,0,-3.1225934483,3.0563379855,0.732095325
H,0,-3.6284496163,3.2955468702,1.6659980691
H,0,-2.1951829378,3.624835679,0.6343853506
H,0,-3.7686679729,3.2633300752,-0.1235207151
H,0,-0.175743019,1.426242848,1.4268780695
H,0,-2.122612141,-0.5374791673,2.055803012
Pt,0,1.7588900228,0.1376232707,-0.3110831584
Cl,0,2.297123837,-2.1226962561,-0.5230326665
Cl,0,1.5484966696,2.4397050391,-0.1141848497

36
1A-c-IN2,Free Energies= -1882.249448
C,0,0.5270812284,-1.4896630815,2.4737058203
O,0,0.9534512906,-0.2280909872,1.9437123531
C,0,-0.240195641,0.5605219836,1.8784650574
C,0,-1.3858709992,-0.3997760765,1.4746624098
C,0,-0.7871543118,-1.798732418,1.7547767437
H,0,1.3155350049,-2.2172875425,2.2846540016
H,0,0.3819849141,-1.3732825178,3.5562187712
H,0,-0.4328064683,0.9638272386,2.880344216
H,0,-1.4612320339,-2.4071576836,2.3584468185
H,0,-0.5767498751,-2.3464744529,0.8350963713
C,0,-2.0172545382,-0.1886457923,0.0626846659
C,0,-1.2114627623,-0.6056129974,-1.2027800148
H,0,-1.8778489391,-0.4731851991,-2.0624445765
H,0,-0.955001006,-1.6655890096,-1.1446577785
C,0,0.0211292717,0.2057201498,-1.5376019439
C,0,1.1413582432,-0.1990908437,-2.2653621241
H,0,-0.1462274729,1.2907575856,-1.5821801561
C,0,-3.3127746676,-1.0298602422,0.0177265376
O,0,-3.640171796,-1.8554350975,0.8312809526
O,0,-4.0342980222,-0.7232216192,-1.0667380781
C,0,-2.4613468733,1.276307013,-0.0658890425
O,0,-2.1231143017,2.0405155063,-0.938333446
O,0,-3.2809650663,1.6127696363,0.9328172656
C,0,-5.2610225672,-1.4424291212,-1.2215541475
H,0,-5.7116400229,-1.054700326,-2.133904919
H,0,-5.0645431766,-2.5129441562,-1.3130163141
H,0,-5.913722112,-1.2674181308,-0.3634950035
C,0,-3.7645635097,2.9598761472,0.9113795914
H,0,-4.4303262795,3.0426122513,1.7689464633
H,0,-2.932420608,3.6620658886,0.9976246453
H,0,-4.3040224038,3.1522672121,-0.0183662134
H,0,-0.0561040669,1.3964052691,1.2031947263
H,0,-2.2142865055,-0.2329879166,2.1645654318
Pt,0,1.7767734594,-0.2160487168,-0.3995850649
Cl,0,1.7978948989,-2.5491142947,-0.4627205405
Cl,0,2.158965716,2.0485043419,-0.1512964794

(7). In Path 1B-*a1*

36
1B-a1-IN1,Free Energies= -6104.822242
C,0,-1.268184041,3.3926191903,-1.1645109307
O,0,-0.9723431653,2.4203457796,-2.1534507887
C,0,-1.9437364455,1.4030172971,-2.0291048368
C,0,-2.391695276,1.3720343772,-0.5388820671
C,0,-1.6654648865,2.5880146307,0.0744076069
H,0,-0.3756052371,4.0043031093,-1.0213220541
H,0,-2.0947333153,4.0378510546,-1.5022107285
H,0,-2.8094940388,1.6251022638,-2.6693485243
H,0,-2.3117516847,3.1391384156,0.759773629
H,0,-0.7601532031,2.303976682,0.6172821589
C,0,-2.1804651485,0.0161045297,0.1866623527
C,0,-0.7489014716,-0.266104566,0.7123184786
H,0,-0.6751411402,-1.3176855503,0.9980384906
H,0,-0.5621005968,0.3323514551,1.6107234851
C,0,0.3234170227,0.0490226258,-0.2408608355
C,0,0.963266442,0.503186717,-1.2228240557
H,0,1.1175285167,0.9080571682,-2.2054784184
C,0,-3.0979856168,-0.0338932529,1.4191137567
O,0,-3.7318325622,0.8929508385,1.8558381618
O,0,-3.0748730046,-1.2533761831,1.9680088738
C,0,-2.5894881084,-1.1215980964,-0.7539843502
O,0,-1.8528945452,-1.9823340344,-1.166370251
O,0,-3.877971398,-1.0078349645,-1.0929341904
C,0,-3.869211108,-1.417880493,3.1461143676
H,0,-3.7465295156,-2.4598715512,3.4376115553
H,0,-3.5149363862,-0.7526815165,3.9369425498
H,0,-4.9169021182,-1.1965145062,2.9312105665
C,0,-4.3679520551,-1.9999621062,-1.9991512081
H,0,-5.4237966081,-1.7717765155,-2.1367713611
H,0,-3.8331867203,-1.9413796662,-2.949989132
H,0,-4.2397210959,-2.9986088828,-1.576123149
H,0,-1.4944330458,0.4702049602,-2.384817097
H,0,-3.4672876384,1.5528301837,-0.5040144042
Pt,0,2.3789080521,0.0094299031,0.1848068441
Br,0,3.086100661,-1.9241006341,-1.0593938598
Br,0,2.1367547628,1.8932831079,1.6982991554

36
1B-a1-TS1,Free Energies= -6104.798424
C,0,-0.9660549702,3.2910872233,0.0747373239
O,0,-1.1961553184,3.0416345577,-1.3222845207
C,0,-1.7723775483,1.8123877307,-1.4922534
C,0,-2.4933362618,1.4073030166,-0.2104237093
C,0,-1.8103607622,2.2784472459,0.8669903906
H,0,0.1008152491,3.1739133612,0.2919066241
H,0,-1.2510472829,4.3297593572,0.2545751523
H,0,-2.3629715119,1.7942957327,-2.4133328639
H,0,-2.5611264257,2.7610128642,1.4927492481
H,0,-1.1646754792,1.6925566042,1.5259211828
C,0,-2.3844557133,-0.11691963,-0.0056305519
C,0,-0.906666161,-0.5923311512,0.0666655637
H,0,-0.8336835166,-1.6251794687,-0.2786793218
H,0,-0.5518781242,-0.5437733436,1.1029041604
C,0,0.0248389724,0.2554528579,-0.6937623445
C,0,1.1115371427,0.9040753616,-0.9174558254
H,0,1.3097709033,1.7083493501,-1.618952579
C,0,-3.1130970335,-0.5359570304,1.2731804157
O,0,-3.7123486166,0.209985243,2.0046904448
O,0,-2.979886527,-1.8499975558,1.4683080529
C,0,-3.0600080716,-0.7995329556,-1.2038282806
O,0,-2.4680548134,-1.2942410907,-2.1312495418
O,0,-4.3876484125,-0.715636096,-1.1116521499
C,0,-3.5980763866,-2.3675728743,2.6514957108
H,0,-3.3914943394,-3.436480457,2.6433817242
H,0,-3.1661235095,-1.8976842674,3.5376050681
H,0,-4.6737243069,-2.1799794537,2.6291170598
C,0,-5.1226847836,-1.2900503776,-2.1986096174
H,0,-6.171484929,-1.1138895689,-1.9658089718
H,0,-4.847996446,-0.8075392305,-3.1391076869
H,0,-4.914979629,-2.3598341737,-2.2675789684
H,0,-0.9662381819,1.0024781141,-1.7097639943
H,0,-3.5537483485,1.6600668655,-0.2855295312
Pt,0,2.4984355909,0.1670931618,0.2384690364
Br,0,3.6812741037,-0.9130334549,-1.5621802709
Br,0,1.6250129586,1.0896392422,2.3206147616

36
1B-a1-IN2,Free Energies= -6104.877793
C,0,-0.7423414353,3.0890523157,-1.3020439614
O,0,-0.2237261079,2.0025955998,-2.0722489585
C,0,-1.0360945728,0.8558841164,-1.8950059933
C,0,-2.1500703832,1.2202866011,-0.8920592953
C,0,-1.5520366156,2.4467358529,-0.1841334526
H,0,0.1061618835,3.6731029108,-0.9411502137
H,0,-1.370198946,3.7219770279,-1.944588924
H,0,-1.4167042937,0.5309680907,-2.8674778469
H,0,-2.3207082583,3.0987634496,0.2301557304
H,0,-0.8815672187,2.1509485764,0.6294347345
C,0,-2.3369336768,-0.0448433081,-0.0270203846
C,0,-0.9044053999,-0.5881856715,0.1397230129
H,0,-0.8829203374,-1.6482807593,0.3935521512
H,0,-0.4024537565,-0.0448503705,0.9452474136
C,0,-0.2260311034,-0.3004272126,-1.2108556335
C,0,1.2027210369,0.0637039285,-1.2067780749
H,0,1.652849242,0.3339191685,-2.1669926555
C,0,-3.0274980453,0.2231444575,1.3039317334
O,0,-3.549002276,1.2584159707,1.6353461309
O,0,-2.9744443806,-0.8710926582,2.0729940532
C,0,-3.1757828128,-1.0397789653,-0.8326126144
O,0,-2.7204780761,-1.8670587712,-1.5877037141
O,0,-4.4822154674,-0.8398564659,-0.6485693886
C,0,-3.611870116,-0.7599159972,3.3472370531
H,0,-3.4509363331,-1.718672527,3.8380363302
H,0,-3.165473899,0.0509812947,3.9271431762
H,0,-4.6794604748,-0.5658995333,3.2190802212
C,0,-5.3528696168,-1.6857451522,-1.4050245188
H,0,-6.3620006031,-1.4030632081,-1.1091675407
H,0,-5.203548802,-1.5209233219,-2.4745822636
H,0,-5.1594223805,-2.7351057844,-1.1726535076
H,0,-0.2856389954,-1.2009218083,-1.8419860792
H,0,-3.0784473357,1.5001348739,-1.3983592936
Pt,0,2.3190025756,0.0531761114,0.2180635483
Br,0,2.1881801614,2.2981802525,1.0777154055
Br,0,3.0291581505,-2.245943534,0.2085133395

36
1B-a1-TS2,Free Energies= -6104.847573
C,0,-1.6416777117,3.5502207405,-1.1821520835
O,0,-0.563509646,2.6739947186,-1.5018906074
C,0,-1.0969918623,1.3853030083,-1.7284008223
C,0,-2.5171156387,1.3325527143,-1.1082909901
C,0,-2.6311104511,2.694116479,-0.3987621914
H,0,-1.2256319281,4.3848470666,-0.6158219513
H,0,-2.0935063943,3.9348507465,-2.1072653136
H,0,-1.0641941475,1.1140991454,-2.7883298549
H,0,-3.6513652804,3.0806961916,-0.4140441641
H,0,-2.31287428,2.6259831704,0.6480082388
C,0,-2.4973873987,0.1117601489,-0.1580793673
C,0,-1.0287201983,0.0451230668,0.3202007988
H,0,-0.7071002734,-0.9108424953,0.7429257107
H,0,-0.816604506,0.8096094676,1.0824315382
C,0,-0.2599920643,0.4434559477,-0.8810404544
C,0,0.9851075847,-0.0688560051,-1.2634616171
H,0,1.4516726398,0.4122917827,-2.1261796253
C,0,-3.5520287409,0.2070280103,0.9309702292
O,0,-4.6886190003,0.5519973142,0.7155554355
O,0,-3.0700128255,-0.123452024,2.1278017758
C,0,-2.6701875869,-1.1697450317,-0.9764172488
O,0,-2.2424235376,-1.2668054922,-2.1068469418
O,0,-3.2136552819,-2.1529270275,-0.2815026978
C,0,-4.016650657,-0.1037628062,3.2013769657
H,0,-3.4629854514,-0.4197161428,4.0839960898
H,0,-4.4156651595,0.9043000987,3.3343407638
H,0,-4.83719103,-0.7926072741,2.9905443732
C,0,-3.1989970928,-3.4452848239,-0.911475441
H,0,-3.6732400597,-4.1161988133,-0.1978653326
H,0,-3.7575218472,-3.4126905868,-1.8486108943
H,0,-2.1655598194,-3.7436480218,-1.0997326743
H,0,0.2592350498,-0.8889203099,-1.695601523
H,0,-3.2878569858,1.2225691259,-1.8716919682
Pt,0,2.1462874678,-1.027666347,-0.0233166236
Br,0,3.5200012147,0.892916576,0.4686823132
Br,0,0.8794071005,-3.1161232786,-0.245728845

36
1B-a1-P,Free Energies= -6104.888220
C,0,-0.3659193097,-2.6080653705,-2.14231573
O,0,0.521421879,-1.8636257961,-1.3270268776
C,0,-0.1539854715,-1.5730075738,-0.1217995662
C,0,-1.6812361042,-1.5578372261,-0.4630113601
C,0,-1.7028563114,-1.9027658765,-1.9664399015
H,0,0.0238132356,-2.5834290455,-3.1613046958
H,0,-0.4117984771,-3.65497004,-1.8040436674
H,0,0.111309357,-2.3095103237,0.6476679585
H,0,-2.5694475078,-2.5046673206,-2.2414456438
H,0,-1.7181359958,-0.9982581119,-2.5799437959
C,0,-2.1678089568,-0.1312946408,-0.0830494416
C,0,-0.908360418,0.7470814654,-0.2456306105
H,0,-0.984394558,1.7099752777,0.2569348136
H,0,-0.7250945395,0.9241711192,-1.3091603694
C,0,0.1658942161,-0.1521209787,0.3354551223
C,0,0.7723851329,0.1316007801,1.6013165441
H,0,1.0503460584,-0.6861417653,2.262561702
C,0,-3.3526139773,0.3794189818,-0.9020231435
O,0,-4.0200975054,-0.260129173,-1.674591478
O,0,-3.565900182,1.670984354,-0.6189048943
C,0,-2.6260611892,-0.1253490035,1.3818818751
O,0,-2.0201418894,0.3554924139,2.3093452101
O,0,-3.7994343306,-0.7509515758,1.5084485265
C,0,-4.6679795906,2.2778815552,-1.2969709041
H,0,-4.6955560229,3.3080208259,-0.9448922582
H,0,-4.5130447419,2.2453334507,-2.3777363594
H,0,-5.5980002282,1.7601121044,-1.0510099367
C,0,-4.3357539292,-0.8041756969,2.8330558477
H,0,-5.2902523788,-1.319751192,2.7396011513
H,0,-3.6630011137,-1.3540530332,3.4951070782
H,0,-4.4786387218,0.2058443097,3.2234270378
H,0,0.5647352833,1.0826170105,2.0822313559
H,0,-2.2267707206,-2.316710299,0.1019903427
Pt,0,2.2018892142,0.3678658412,0.1252540175
Br,0,3.2578437175,-1.7385412874,0.6488156203
Br,0,1.8186103175,2.6665079604,-0.5263307993

(8). In Path 1B-*a2*

36
1B-a2-IN1,Free Energies= -6104.819334
C,0,-3.8378594006,-2.0995188256,-1.901692466
O,0,-2.9413855095,-2.9455940297,-1.200703745
C,0,-1.8909929176,-2.1397508917,-0.7159892079
C,0,-2.6154850752,-0.885955244,-0.2127015273
C,0,-3.6550712403,-0.6736750295,-1.3308288069
H,0,-3.6172290662,-2.1192518244,-2.9787103491
H,0,-4.8465496792,-2.4935434703,-1.7523164465
H,0,-1.3616588854,-2.6853212705,0.0657406436
H,0,-4.5879296241,-0.2544049175,-0.9436169066
H,0,-3.2892579766,0.0083218086,-2.1055090127
C,0,-1.7735422279,0.3579613575,0.1646951012
C,0,-0.8428104271,0.9004095724,-0.9497599112
H,0,-0.496406137,1.8999543536,-0.6729024233
H,0,-1.402582521,1.0034802816,-1.8841032101
C,0,0.3570383965,0.1055860757,-1.253193712
C,0,1.2338872539,-0.533560937,-1.8924037025
H,0,1.6412401769,-1.1101902793,-2.702721576
C,0,-2.8052023696,1.4335576776,0.5478056796
O,0,-3.4092071264,1.4241967942,1.5917660853
O,0,-2.9959945562,2.3315595697,-0.4218489461
C,0,-0.9526252328,0.1640162424,1.4540998689
O,0,-0.094611894,0.9487620389,1.7954632096
O,0,-1.3028576898,-0.9082581972,2.1434815544
C,0,-3.9893556951,3.3253541246,-0.1494950995
H,0,-3.999986703,3.9739480397,-1.0240432
H,0,-4.9642897186,2.854644323,-0.003893759
H,0,-3.7240313039,3.8892403311,0.7469844993
C,0,-0.6115597021,-1.1030024696,3.3830756518
H,0,-1.0517864149,-1.9983627749,3.8186272826
H,0,0.4533939199,-1.2507419476,3.1951166601
H,0,-0.762337363,-0.2388981269,4.0333152844
H,0,-1.1793660458,-1.9037453671,-1.5218588597
H,0,-3.1496497096,-1.1762589921,0.6952236772
Pt,0,2.0745804632,-0.1311729639,-0.0660929884
Br,0,2.7992991018,2.1270622532,-0.5240589386
Br,0,1.7509555402,-2.4076183149,0.7118131482

36
1B-a2-TS1,Free Energies= -6104.796450
C,0,-3.7928150204,-1.6589292277,-2.6556176843
O,0,-2.6168282156,-2.4188164946,-2.3410227243
C,0,-2.0093625287,-1.9209758021,-1.2155344
C,0,-2.9521223136,-0.9377121816,-0.533864946
C,0,-3.77308419,-0.4394603487,-1.7373334311
H,0,-3.7660833046,-1.4070470574,-3.7180969228
H,0,-4.6608054044,-2.2996067865,-2.4651420253
H,0,-1.597021185,-2.7200737686,-0.5990552058
H,0,-4.772280807,-0.11480346,-1.4433924731
H,0,-3.2737520517,0.4013541333,-2.2320269368
C,0,-2.2320760275,0.1723257424,0.25790845
C,0,-1.0552205884,0.7473488721,-0.5655106102
H,0,-0.5121182418,1.4926483631,0.0257715165
H,0,-1.4008617026,1.2569158219,-1.4693231171
C,0,-0.0857768457,-0.2993721701,-0.8896386062
C,0,1.037498731,-0.9358957429,-0.8447986151
H,0,1.2483338595,-1.930657967,-1.2248547476
C,0,-3.2553758559,1.2482515278,0.6390763586
O,0,-4.3562366051,0.9772994883,1.054798718
O,0,-2.7911097281,2.4799036955,0.4641675395
C,0,-1.6345650753,-0.3016036126,1.5974102579
O,0,-1.2981874403,0.4732706005,2.457429022
O,0,-1.5008394118,-1.6220672819,1.6620806385
C,0,-3.660489726,3.5378122839,0.8831944101
H,0,-3.1168169751,4.4578416593,0.6761618515
H,0,-4.5962839969,3.5034801532,0.3209948677
H,0,-3.8723260466,3.445290065,1.9501072845
C,0,-0.8358378612,-2.1180930822,2.838716295
H,0,-0.8519529896,-3.202140869,2.7406581338
H,0,0.1920744555,-1.7507112652,2.8606137844
H,0,-1.374842402,-1.7983483349,3.7322891356
H,0,-1.0656316606,-1.3108447161,-1.5572299141
H,0,-3.6024995288,-1.488377305,0.1514938765
Pt,0,2.4107920689,0.0567859224,0.1057574775
Br,0,2.3168694476,2.0994484345,-1.1914887954
Br,0,2.8391237575,-1.7918964996,1.619990728

36
1B-a2-IN2,Free Energies= -6104.874344
C,0,-3.0636947317,3.81698624,-0.5125878457
O,0,-1.6770824588,3.5208795303,-0.4987274654
C,0,-1.4999184158,2.2030044802,-0.9821171464
C,0,-2.8660971327,1.4741436866,-0.8328527255
C,0,-3.7358623188,2.5114827379,-0.1041793703
H,0,-3.2338389017,4.6435954051,0.1805085414
H,0,-3.3828896377,4.1293800033,-1.518934164
H,0,-1.1578428738,2.2273163649,-2.0241998422
H,0,-4.7873810549,2.4424455078,-0.386246963
H,0,-3.6696072417,2.3930124698,0.9834155975
C,0,-2.5616990761,0.1858550543,-0.0318169111
C,0,-1.3724036112,0.6003728208,0.8678076406
H,0,-0.8458778827,-0.2475702834,1.3080878672
H,0,-1.7481572977,1.2221034804,1.6841918673
C,0,-0.4950191416,1.4701881197,-0.0626961052
C,0,0.5683354769,0.7323566397,-0.7906683875
H,0,0.6851524316,0.8903291186,-1.86643876
C,0,-3.7771677883,-0.3345917995,0.7230141302
O,0,-4.9099866964,-0.2550011756,0.3127239793
O,0,-3.4352138001,-0.8927292042,1.8859545342
C,0,-2.0758970572,-0.8758798076,-1.0176520279
O,0,-1.271382473,-0.6257949798,-1.8949849619
O,0,-2.614751575,-2.0666106302,-0.8255130451
C,0,-4.5085202757,-1.4749447291,2.6280047376
H,0,-4.052402785,-1.883541237,3.5284725975
H,0,-5.2528397979,-0.7165597083,2.8814708481
H,0,-4.9849200261,-2.2651060593,2.0433037826
C,0,-2.1723509563,-3.1103061016,-1.7067545609
H,0,-2.7224964136,-3.9971629533,-1.3972059123
H,0,-2.4056463557,-2.8496334207,-2.740978605
H,0,-1.0969871854,-3.2566389397,-1.5910601588
H,0,0.0492364384,2.2221078379,0.5290254115
H,0,-3.302413237,1.2385782017,-1.8055503653
Pt,0,1.8715037952,-0.2556948879,0.005780435
Br,0,0.9690344761,-2.4735656607,0.2676179603
Br,0,3.5103265811,1.4880358785,0.2875863936

36
1B-a2-TS2,Free Energies= -6104.846990
C,0,-1.4884922221,3.2325023405,-1.6071351224
O,0,-0.773657621,2.2367290992,-2.3628815805
C,0,-1.1259909441,0.969631944,-1.8919855636
C,0,-2.4073302326,1.0995365649,-1.0522690009
C,0,-2.1928275889,2.5013515801,-0.4594274894
H,0,-0.7738538231,3.9833068527,-1.2611487631
H,0,-2.2068672776,3.7139338824,-2.2797846659
H,0,-1.2007111556,0.2592931603,-2.7248066142
H,0,-3.1278510904,2.9731083559,-0.1600547811
H,0,-1.5496430757,2.4583504701,0.4289406113
C,0,-2.3562831717,-0.0991243608,-0.0740933748
C,0,-0.8454309846,-0.3184425088,0.1887096228
H,0,-0.5420991595,-1.3705086755,0.1881120811
H,0,-0.5059143249,0.0814763109,1.1552870513
C,0,-0.1312020543,0.4008659088,-0.891893118
C,0,1.226846311,0.7324132292,-0.8839637336
H,0,1.6128980758,1.1946222287,-1.7953716752
C,0,-3.156712976,0.1263807939,1.2030181735
O,0,-3.9554367134,1.012482657,1.377708766
O,0,-2.8451056539,-0.8046466868,2.1065986875
C,0,-2.9066510438,-1.3118006458,-0.8320846144
O,0,-2.2430660103,-1.9711391056,-1.5965150449
O,0,-4.2027272974,-1.4996341424,-0.6003263884
C,0,-3.5360017675,-0.713358277,3.3566210849
H,0,-3.1294296105,-1.5140695194,3.9719924308
H,0,-3.354308423,0.2592466938,3.8186342458
H,0,-4.6092121063,-0.8473731098,3.2033192571
C,0,-4.8111335577,-2.584234626,-1.3119033655
H,0,-5.8580064665,-2.5763575744,-1.0133953288
H,0,-4.7146352509,-2.4320001255,-2.3890000833
H,0,-4.3361665739,-3.5280293083,-1.0362399104
H,0,0.7150653887,1.6260629926,-0.2921445224
H,0,-3.3070402092,1.0852181844,-1.6724994917
Pt,0,2.4932774059,-0.0172501192,0.3858309314
Br,0,1.7049924032,1.5328574579,2.1206945877
Br,0,3.375751012,-1.6946319426,-1.1016017389

36
1B-a2-P,Free Energies= -6104.894841
C,0,1.723322284,3.6845515997,0.0228937128
O,0,0.5589985073,3.0813299022,-0.5180081282
C,0,0.2920748824,1.9233681656,0.2612671546
C,0,1.6541058497,1.4369814629,0.8307253097
C,0,2.6457949378,2.5117537883,0.3414140046
H,0,2.1182573511,4.3741439463,-0.7257583855
H,0,1.4713580201,4.251194488,0.9317759158
H,0,-0.4373023437,2.1451722836,1.0402641176
H,0,3.4097384663,2.742303681,1.0863238944
H,0,3.1536361147,2.1939624747,-0.5767957119
C,0,1.8831698309,0.0295863629,0.226424898
C,0,1.081841756,0.0739761255,-1.0910769892
H,0,0.9135896586,-0.8970174608,-1.5511323329
H,0,1.6271603518,0.7009827349,-1.8090596798
C,0,-0.1659854856,0.8497492033,-0.7283271089
C,0,-1.3004932051,1.0069548134,-1.580859202
H,0,-1.883009294,1.9233421905,-1.5183504225
C,0,3.3677614712,-0.2758332591,0.0882299367
O,0,4.1315399048,-0.2508710894,1.0231442935
O,0,3.7293078037,-0.5452261178,-1.1692153664
C,0,1.2689369673,-1.0432587897,1.1317558656
O,0,0.4666497835,-0.8211540706,2.0094131869
O,0,1.6926233058,-2.2550959031,0.7866880036
C,0,5.1145149961,-0.847182974,-1.3541495374
H,0,5.2273966416,-1.0615223612,-2.4159632657
H,0,5.7310094406,0.0065398185,-1.0631649335
H,0,5.395892866,-1.7142409758,-0.7528098509
C,0,1.1113034488,-3.3482999792,1.5062890216
H,0,1.6016374793,-4.2408686767,1.1212620232
H,0,1.2954392249,-3.2350722486,2.5766351639
H,0,0.037423708,-3.3892003688,1.3125821793
H,0,-1.3148650764,0.4958936835,-2.5414775783
H,0,1.6315471147,1.3845683316,1.9187821134
Pt,0,-1.869475727,-0.30362751,-0.0828137648
Br,0,-3.0083685644,1.3348670213,1.2767496991
Br,0,-1.3623202409,-2.380566723,-1.238217197

(9). In Path 1B-*a3*

36
1B-a3-TS1,Free Energies= -6104.813572
C,0,-4.0335815975,-2.4089936082,-1.1194562356
O,0,-2.8111585742,-2.7446939905,-1.7650529813
C,0,-1.8286763767,-1.7636374285,-1.499777846
C,0,-2.3249842069,-1.0146759075,-0.2532825731
C,0,-3.8383612857,-1.017380047,-0.52449584
H,0,-4.8485977669,-2.4470203056,-1.8502657018
H,0,-4.2394233318,-3.1500810142,-0.3356701223
H,0,-0.873104174,-2.2672958917,-1.3369610673
H,0,-4.4320270557,-0.853219619,0.3782199826
H,0,-4.0981529207,-0.2477211326,-1.2604485506
C,0,-1.6757601778,0.3712582025,0.0952753509
C,0,-0.7169830803,0.9434976226,-0.981343136
H,0,-0.3827348358,1.9372118644,-0.6694618394
H,0,-1.2532998525,1.0583710871,-1.9272130657
C,0,0.485591281,0.1445187792,-1.2563988616
C,0,1.3605298719,-0.520072775,-1.8706905751
H,0,1.7986055214,-1.061059831,-2.6893754551
C,0,-2.7999743617,1.3992559986,0.3263358086
O,0,-3.34535409,1.5769174521,1.3867956022
O,0,-3.1228477565,2.0527883417,-0.7952008258
C,0,-0.9309893403,0.357536136,1.4479378616
O,0,-0.0330812942,1.1313668992,1.701742033
O,0,-1.4022431415,-0.5375459025,2.2979936561
C,0,-4.1993529891,2.9875676754,-0.6702733177
H,0,-4.3304921174,3.4130708475,-1.6640050016
H,0,-5.1080180059,2.4753782076,-0.3458686634
H,0,-3.9443977567,3.7642473021,0.0535707616
C,0,-0.7653359172,-0.5679123718,3.5789438511
H,0,-1.2765407285,-1.3505493939,4.1368713939
H,0,0.2929241791,-0.809087219,3.4596262634
H,0,-0.8743967975,0.3992536093,4.0738729088
H,0,-1.732843291,-1.0924376145,-2.3684135825
H,0,-2.1451262688,-1.6706890509,0.5998439006
Pt,0,2.1025292243,-0.2356360405,0.0216362333
Br,0,1.3293545855,-2.3819709556,0.8613026161
Br,0,3.2117264297,1.8508360743,-0.4648559822

36
1B-a3-IN2,Free Energies= -6104.824701
C,0,-3.6492558454,-2.5885828314,-0.996989732
O,0,-3.2480802415,-2.0031303632,-2.2298547909
C,0,-2.4347454205,-0.8717358231,-1.9894150166
C,0,-2.1004547686,-0.8865472754,-0.4863434909
C,0,-3.362455016,-1.5486852371,0.0801795496
H,0,-4.708057087,-2.8562270278,-1.0671437337
H,0,-3.0714537097,-3.5068540914,-0.8192019923
H,0,-1.5376055044,-0.9418752333,-2.6159101866
H,0,-3.2081248511,-1.9790651651,1.0690580498
H,0,-4.1870121916,-0.8290838617,0.1440693121
C,0,-1.6763135551,0.4832052522,0.1090168764
C,0,-0.6765437568,1.2181804134,-0.8220643351
H,0,-0.3428528874,2.1451541135,-0.3474351672
H,0,-1.1698002041,1.4788695379,-1.7627408273
C,0,0.5092857316,0.4197901145,-1.1606946141
C,0,1.3611722388,-0.2435401822,-1.8069465749
H,0,1.7858722544,-0.7552523797,-2.651195882
C,0,-2.9036939656,1.3751125734,0.3392536677
O,0,-3.4635107195,1.4897820641,1.4013987764
O,0,-3.301441479,1.987249569,-0.7815464764
C,0,-1.0181764754,0.3477121028,1.4966482907
O,0,-0.2021585537,1.1396158382,1.9127053623
O,0,-1.4394596648,-0.7101761746,2.1704403069
C,0,-4.4722675213,2.8016971256,-0.6546771531
H,0,-4.6561527802,3.201995815,-1.650450734
H,0,-5.3179738631,2.198356578,-0.317725662
H,0,-4.2952645126,3.6071902811,0.0609445492
C,0,-0.8514068552,-0.8938973176,3.4618757994
H,0,-1.3220098371,-1.7877425637,3.8679932403
H,0,0.2259815362,-1.0407945856,3.3610444792
H,0,-1.0525785654,-0.0263607952,4.0935097987
H,0,-2.9811193736,0.0399001449,-2.2683110738
H,0,-1.2572100801,-1.5693046749,-0.3286885814
Pt,0,2.1011901843,-0.116484979,0.1045780901
Br,0,1.4030436869,-2.3698119695,0.68312971
Br,0,3.1464486541,2.0455990078,-0.108051834

36
1B-a3-TS2,Free Energies= -6104.775262
C,0,-3.0367599618,-0.8862031485,3.0071274525
O,0,-2.3010024539,-2.0300469078,2.4843987337
C,0,-1.939522424,-1.7650235208,1.209301312
C,0,-2.1821351397,-0.2878768326,0.9450042127
C,0,-3.4476596824,-0.0792200751,1.7673324945
H,0,-3.8648680089,-1.2966670189,3.5857051634
H,0,-2.3767271428,-0.312540312,3.6651781282
H,0,-0.738257883,-2.0287356762,1.0118472361
H,0,-3.6315793917,0.9724570659,1.9882374177
H,0,-4.3350385441,-0.5131419587,1.2933068544
C,0,-1.9737207234,0.0312606441,-0.5442600885
C,0,-0.7836971988,-0.8873636209,-0.9853385187
H,0,-0.133850336,-0.3497544673,-1.6835150587
H,0,-1.14908787,-1.7844086981,-1.4921523231
C,0,0.0461756303,-1.2487002943,0.1854931519
C,0,1.069685757,-0.9021237496,0.9288419576
H,0,1.2433193099,-1.2858189749,1.9324060924
C,0,-3.2387962536,-0.2275737615,-1.3606371364
O,0,-3.8698575524,0.6206156482,-1.9362935417
O,0,-3.5892269271,-1.524215261,-1.326825344
C,0,-1.58503294,1.4998630112,-0.7755489547
O,0,-0.8432016805,1.853122739,-1.6559154056
O,0,-2.1803621463,2.3038020738,0.0980989526
C,0,-4.7813927267,-1.8565768245,-2.0491154479
H,0,-4.9158482492,-2.9285960874,-1.9131349799
H,0,-5.633436587,-1.3043692379,-1.6469288079
H,0,-4.6613904659,-1.6133942537,-3.1066813996
C,0,-1.8406492384,3.6921165878,-0.0224920643
H,0,-2.4392127001,4.2028208261,0.7305095467
H,0,-0.7748583615,3.8218211732,0.1761392177
H,0,-2.0853576023,4.0517627835,-1.023754326
H,0,-2.3460070411,-2.482345458,0.4876377684
H,0,-1.394633167,0.2605006318,1.4747874039
Pt,0,2.2496321705,0.4569219789,0.2501418549
Br,0,1.156644746,2.0857209174,1.7242401833
Br,0,3.4805897859,-0.8651809412,-1.3429217376

36
1B-a3-IN3,Free Energies= -6104.855451
C,0,-3.0303245594,-1.0943228679,2.9691417691
O,0,-1.8930065122,-1.8322140295,2.4598113366
C,0,-1.9010745253,-1.6225442384,1.0752173285
C,0,-2.354793713,-0.1887661631,0.9159340456
C,0,-3.5749090973,-0.1906669857,1.8198717495
H,0,-3.7837896398,-1.8044321192,3.3246351637
H,0,-2.6754226937,-0.5026532239,3.8170092085
H,0,-0.2757751576,-2.6699766683,0.0236512151
H,0,-3.8598854876,0.8008737351,2.1756086365
H,0,-4.438051026,-0.654177666,1.3310913019
C,0,-2.2108872605,0.104645093,-0.5909928193
C,0,-1.0669690726,-0.8903378847,-1.0200911736
H,0,-0.2601401891,-0.3501857247,-1.5174800555
H,0,-1.4566352852,-1.6272969328,-1.7251356879
C,0,-0.5976505943,-1.6418483795,0.255218266
C,0,0.5218186655,-1.0843172945,1.0468153607
H,0,0.7688435651,-1.618754913,1.9713507015
C,0,-3.4991110365,-0.1250175877,-1.3732960063
O,0,-4.0748932502,0.7143986051,-2.0192561177
O,0,-3.9332966675,-1.390696965,-1.2513637867
C,0,-1.7928736619,1.5563380531,-0.8425231393
O,0,-0.952400897,1.897565129,-1.6377060267
O,0,-2.4740494717,2.3883762444,-0.0569758069
C,0,-5.1444064612,-1.6911790526,-1.9495422876
H,0,-5.3349278593,-2.747428578,-1.7637218339
H,0,-5.9654316598,-1.0788456979,-1.5694900925
H,0,-5.0237374994,-1.503188641,-3.0185693473
C,0,-2.1416503087,3.7716112275,-0.1988408505
H,0,-2.8147377637,4.3033254265,0.4725376851
H,0,-1.1011391861,3.9340921126,0.0917794278
H,0,-2.2917044233,4.092472967,-1.231808736
H,0,-2.6018739981,-2.3105644674,0.5799031691
H,0,-1.6023985739,0.4336777255,1.4151317998
Pt,0,1.5391814523,0.3585668692,0.660704195
Br,0,0.6333910119,2.1061857058,2.0516164109
Br,0,3.0518165949,-0.5687852229,-0.9593151933

36
1B-a3-TS3,Free Energies= -6104.826676
C,0,1.5794955888,-0.406068214,3.6661398201
O,0,0.3802463996,0.0820436335,3.0103005762
C,0,0.7726707311,0.5318034069,1.7602324855
C,0,1.9476146804,-0.3657269858,1.3485586829
C,0,2.7443450535,-0.332028849,2.6401985834
H,0,1.7659052581,0.2039208104,4.5540725388
H,0,1.3815706694,-1.4354587985,3.9761166218
H,0,-1.3670147044,0.9562627372,0.3842717154
H,0,3.4403810108,-1.1662406593,2.7391851905
H,0,3.2982536739,0.6078643923,2.7422808128
C,0,2.3094369381,0.1366356331,-0.0644648139
C,0,0.8988346175,0.5326217353,-0.6261155485
H,0,0.6111891837,-0.0580356772,-1.494669343
H,0,0.8819585161,1.594434654,-0.89284176
C,0,-0.0303172838,0.2769990827,0.5428383617
C,0,-1.3151298535,-0.2593599981,0.501393802
H,0,-1.7752765856,-0.4505701551,1.4741781196
C,0,3.2281144418,1.3532807277,0.0188997449
O,0,2.8385102859,2.493996588,0.1126574298
O,0,4.5080787273,0.9913648989,0.0480454617
C,0,2.9615989651,-0.9863303808,-0.8690553282
O,0,3.4165209615,-1.988135561,-0.3788748047
O,0,2.9438064381,-0.7063177792,-2.1710753181
C,0,5.4557446702,2.0566867323,0.1772220045
H,0,6.4318431806,1.5750138561,0.1970679591
H,0,5.3766090124,2.7359970706,-0.6740489719
H,0,5.279394614,2.6125570755,1.1007375122
C,0,3.4246730841,-1.7487752634,-3.0275076351
H,0,3.3604264594,-1.3490762724,-4.0382075551
H,0,4.4562912876,-2.0018125022,-2.7739115444
H,0,2.7905916728,-2.6316675485,-2.9205901859
H,0,1.0963896539,1.5856888966,1.7736021777
H,0,1.5603059385,-1.3842979827,1.2132756469
Pt,0,-2.0976849274,-1.1113976891,-1.043475848
Br,0,-0.3776317492,-2.8412572325,-1.0937622459
Br,0,-3.8640211913,0.5311691429,-1.2624605458

36
1B-a3-P,Free Energies= -6104.874273
C,0,-1.9456182297,3.4839489595,-0.8442479664
O,0,-0.748839547,3.1027423384,-0.1284505791
C,0,-0.9698681044,1.8290993667,0.3712356679
C,0,-2.0184762165,1.1808670959,-0.5086121253
C,0,-2.9834358407,2.3428402057,-0.6696446712
H,0,-2.2950680618,4.4406716794,-0.4473709953
H,0,-1.6732952348,3.6108135223,-1.8971934194
H,0,1.954519915,0.0308706279,1.2844541375
H,0,-3.6464737132,2.257142957,-1.5326377126
H,0,-3.5890307972,2.4984542585,0.2311200043
C,0,-2.2204382563,-0.1990505842,0.154037657
C,0,-0.870202212,-0.4244912328,0.9273144663
H,0,-0.4437617709,-1.4086014222,0.7547644121
H,0,-1.065051646,-0.3223197713,2.0012683971
C,0,0.0439157878,0.7260027081,0.5082142426
C,0,1.4443425802,0.8275815261,0.7466609142
H,0,1.8875451447,1.8187725169,0.8191556111
C,0,-3.4034101175,-0.1519691774,1.1103213492
O,0,-3.3299456282,0.1107938429,2.2875538627
O,0,-4.5505850591,-0.3510853171,0.4581983369
C,0,-2.3955107454,-1.2936069231,-0.8968046661
O,0,-2.3562999458,-1.1217285729,-2.0899584679
O,0,-2.5298079342,-2.4844064468,-0.3091548681
C,0,-5.7378746819,-0.2570528107,1.2484803823
H,0,-6.5608428636,-0.4450404947,0.5606211928
H,0,-5.7218711001,-1.0032712971,2.0459853723
H,0,-5.8233951673,0.7387807615,1.6897275742
C,0,-2.5418858748,-3.6071795524,-1.1953017232
H,0,-2.6579784095,-4.4817391385,-0.5565922022
H,0,-3.3731228657,-3.5287911285,-1.8993587179
H,0,-1.598649253,-3.6536304623,-1.7448131245
H,0,-1.3687980008,1.9099516019,1.4032506549
H,0,-1.5668419703,0.9891322678,-1.4882683587
Pt,0,1.2633830565,0.2958625469,-1.2476187052
Br,0,1.402431497,2.4288219888,-2.3315043563
Br,0,1.5228282663,-2.09810944,-0.8936715762

36
1B-a4-IN1,Free Energies= -6104.821091
C,0,-1.5711866126,-2.4536047889,2.5071524801
O,0,-0.9270004305,-1.3309075517,3.0832994682
C,0,-0.6642741234,-0.4517054016,2.0179603647
C,0,-1.9784349546,-0.4354675504,1.2274877879
C,0,-2.4272712523,-1.9129564645,1.338019542
H,0,-0.8198940337,-3.1657107398,2.1351988611
H,0,-2.1563543595,-2.9399235448,3.2903111729
H,0,-0.3751390961,0.5206207946,2.41656213
H,0,-3.4993725227,-1.9802742091,1.542622029
H,0,-2.2372210586,-2.480786874,0.4219224509
C,0,-1.9756411798,0.1403718543,-0.2116246528
C,0,-0.9834005592,-0.5392150789,-1.1999531044
H,0,-1.4026887784,-0.5040749026,-2.2092767635
H,0,-0.8489370933,-1.5944162872,-0.9489160392
C,0,0.3389901421,0.0926262277,-1.3238435986
C,0,1.2968057172,0.7172392429,-1.8498865783
H,0,1.7782861646,1.3636414083,-2.5607908159
C,0,-3.4252072867,-0.0402435084,-0.6934095652
O,0,-4.3378619063,0.6350040653,-0.2858543232
O,0,-3.5699410161,-1.0569000774,-1.5481025822
C,0,-1.7495743492,1.6601794926,-0.2783626231
O,0,-1.6579976982,2.24353042,-1.3333776158
O,0,-1.670771372,2.2351593511,0.9130594863
C,0,-4.9140463558,-1.3181126213,-1.9650833265
H,0,-4.849620831,-2.1728881463,-2.6366953966
H,0,-5.5382038552,-1.5512660786,-1.0996203217
H,0,-5.324666388,-0.4484737542,-2.4821701566
C,0,-1.4502292513,3.6497168105,0.9024186319
H,0,-1.4112878283,3.9433349366,1.9500834516
H,0,-0.5035948539,3.8729964136,0.406847919
H,0,-2.2709979312,4.1525615123,0.3868943607
H,0,0.1631715927,-0.8466463707,1.4023666545
H,0,-2.6805867584,0.180464178,1.7946212072
Pt,0,2.0433004912,0.0060841618,-0.0805112679
Br,0,2.3418436971,-2.3328424728,-0.6263244555
Br,0,2.0975389312,2.2334315536,0.8570691889

36
1B-a4-TS1,Free Energies= -6104.795165
C,0,-1.3231007686,-2.5986285126,1.8497405956
O,0,-0.5587989931,-1.5589961767,2.4390653302
C,0,-0.8478380066,-0.4122158428,1.7252566664
C,0,-2.3238414706,-0.4607570364,1.3124959354
C,0,-2.6817558461,-1.9535652102,1.5393292145
H,0,-0.8189741784,-2.9473340853,0.9348323623
H,0,-1.3700824135,-3.4254597279,2.5590245983
H,0,-0.5113686244,0.4725942728,2.2655456919
H,0,-3.351565403,-2.0446554899,2.3973486491
H,0,-3.1778803929,-2.4220784086,0.6836771235
C,0,-2.5367962209,0.0414279109,-0.1332444813
C,0,-1.6349611684,-0.727476632,-1.1254242171
H,0,-1.8564245112,-0.3609903025,-2.1400955869
H,0,-1.8380203949,-1.8012348829,-1.1050268639
C,0,-0.2222088556,-0.4405922287,-0.9747876889
C,0,1.0032248003,-0.1585327086,-1.230629536
H,0,1.2660964818,0.0339654579,-2.2781935523
C,0,-4.0232028358,-0.1112086966,-0.4705427237
O,0,-4.8867034778,0.4770304167,0.1305345341
O,0,-4.2456598553,-0.9719403788,-1.4657016176
C,0,-2.2260514221,1.5398257315,-0.3254869885
O,0,-2.2134344987,2.0431464657,-1.4239384638
O,0,-1.974642973,2.1686949948,0.8096461571
C,0,-5.6220335576,-1.1537640469,-1.8230130545
H,0,-5.6177574122,-1.8733180135,-2.6400462419
H,0,-6.1853710068,-1.5367600598,-0.9696394677
H,0,-6.0529164578,-0.2039134199,-2.1451919677
C,0,-1.616444995,3.5547142064,0.6892290431
H,0,-1.461840591,3.8987687019,1.7099294639
H,0,-0.6949817841,3.645406464,0.111790416
H,0,-2.4251728704,4.1065762542,0.206694909
H,0,-0.2262576174,-0.4103786202,0.7753897084
H,0,-2.9189996886,0.1815497837,1.9631062337
Pt,0,2.453776643,-0.0658050909,0.0366033883
Br,0,3.2502572451,-2.2973177082,-0.448341679
Br,0,1.9346411213,2.1683976193,0.8427061103

36
1B-a4-IN2,Free Energies= -6104.872246
C,0,-1.29078292,-2.3948255855,2.4712024297
O,0,-0.1917818186,-1.5078332886,2.3671231099
C,0,-0.5184348617,-0.5541023174,1.3948651778
C,0,-2.0453825282,-0.2927172424,1.5083919503
C,0,-2.5433544121,-1.523605433,2.3084194409
H,0,-1.2374353518,-3.1638535809,1.6828452895
H,0,-1.2211864666,-2.8971674111,3.4376410867
H,0,0.0945811398,0.3266679356,1.5872517731
H,0,-2.918797704,-1.1953100033,3.279584846
H,0,-3.3565050181,-2.0567789802,1.8141255605
C,0,-2.5338547481,-0.1875651734,0.0489466907
C,0,-1.7033730942,-1.2523778229,-0.686257474
H,0,-1.7294236365,-1.1254692219,-1.76982004
H,0,-2.093517846,-2.2471843539,-0.4495523971
C,0,-0.2974915658,-1.0790126815,-0.0729299525
C,0,0.6152064576,-0.2700608612,-0.9158714338
H,0,0.4550819776,-0.2712769889,-1.9974934291
C,0,-4.0413723337,-0.3390252383,-0.1260205578
O,0,-4.8561352343,-0.4029121555,0.7595527861
O,0,-4.3475116194,-0.3748429785,-1.4301417024
C,0,-2.1557931674,1.1862646369,-0.5210356681
O,0,-1.3382706865,1.3541687755,-1.4002083629
O,0,-2.8188694124,2.1689774213,0.0723285786
C,0,-5.7415166377,-0.4699930045,-1.7330922842
H,0,-5.803588575,-0.4908206497,-2.8202141788
H,0,-6.1633345126,-1.3823595172,-1.3054715315
H,0,-6.2761849223,0.3944398556,-1.3325814185
C,0,-2.4776229763,3.496094202,-0.3569862367
H,0,-3.0748115683,4.1615843142,0.2639056646
H,0,-1.4097810073,3.6704871539,-0.2093390097
H,0,-2.7266411812,3.6233396017,-1.4126266598
H,0,0.2355528108,-2.0429030362,-0.0022386862
H,0,-2.2587775244,0.6282031961,2.0517276965
Pt,0,2.1226598969,0.5633702758,-0.3396196666
Br,0,3.6574748191,-1.275764299,-0.5993451245
Br,0,1.4200102285,2.7759304561,0.3085357335

36
1B-a4-TS2,Free Energies=-6104.833073
C,0,-2.1888853338,-2.647332665,1.4094776841
O,0,-0.8193617946,-2.4040492419,1.0857322739
C,0,-0.563355106,-1.0140040322,0.9817902013
C,0,-1.9035585833,-0.2747908304,1.1995964881
C,0,-2.7153160029,-1.3286305589,1.9646804624
H,0,-2.739384617,-2.9513269221,0.5099746861
H,0,-2.2163494644,-3.4682959583,2.1298092375
H,0,0.2390373539,-0.7273937553,1.6619975382
H,0,-2.4757909004,-1.241845439,3.0286660073
H,0,-3.7967423115,-1.2120343809,1.8581623057
C,0,-2.4033544567,0.1007345292,-0.2517009451
C,0,-1.5386680136,-0.7459229197,-1.2200400383
H,0,-1.4806469028,-0.3082911333,-2.215620666
H,0,-1.9239152695,-1.7668835325,-1.273998747
C,0,-0.2536406991,-0.7069371346,-0.4637130661
C,0,0.9945836423,-0.3742708124,-0.989439499
H,0,1.0132607597,-0.135541464,-2.0549558842
C,0,-3.9075769828,-0.12135084,-0.4111361326
O,0,-4.7435409732,0.6787755649,-0.0754076735
O,0,-4.1888049051,-1.3232303585,-0.9273489878
C,0,-2.1420787709,1.59042898,-0.5732519864
O,0,-1.8024973668,1.963093092,-1.6714466163
O,0,-2.3525837779,2.3781613114,0.466003828
C,0,-5.5835363661,-1.6215365,-1.0580755706
H,0,-5.6281662884,-2.6169385981,-1.4971619263
H,0,-6.0669090124,-1.6078777929,-0.0784684727
H,0,-6.0666484931,-0.8888564922,-1.7074361941
C,0,-2.0968123551,3.7713522883,0.2467687848
H,0,-2.3365262661,4.2590288089,1.1899369776
H,0,-1.0439691589,3.9129506222,-0.0066685978
H,0,-2.7312849324,4.1467089913,-0.5584342171
H,0,0.9679300495,-1.5739767574,-0.9123437294
H,0,-1.7742106792,0.637855382,1.777190055
Pt,0,2.5077772747,0.2496585745,0.0529882124
Br,0,3.9976674834,-1.4998449257,-0.7127636527
Br,0,1.2116492006,2.0759665909,1.0230351904

36
1B-a4-P,Free Energies= -6104.893016
C,0,2.5892468787,2.8170836561,-0.2434379544
O,0,1.1917005834,2.8381413672,-0.521540088
C,0,0.510229935,1.8610291084,0.2631845158
C,0,1.5855909087,1.0916715737,1.0550432875
C,0,2.7184858591,2.1243516678,1.1074807671
H,0,3.1227058558,2.2658340924,-1.031893912
H,0,2.9467775394,3.8500628102,-0.2456695597
H,0,-0.2337119937,2.3603653333,0.88239263
H,0,2.5044262376,2.8344160756,1.9127065591
H,0,3.7020207021,1.6906140184,1.2924246871
C,0,1.8602895094,-0.2170021089,0.226289423
C,0,1.0898881055,-0.0215798569,-1.1050787879
H,0,0.8268434377,-0.9569823629,-1.5953821121
H,0,1.7113887015,0.5551685513,-1.7993677822
C,0,-0.0711417099,0.8690554248,-0.7352104611
C,0,-1.2029124639,1.158192768,-1.555815694
H,0,-1.2891056595,0.6888630967,-2.5334346625
C,0,3.3533951334,-0.4942675485,0.0596843599
O,0,4.0893837861,-0.7060478115,0.9929613038
O,0,3.7583297306,-0.4524214869,-1.2122903998
C,0,1.3169069397,-1.4988681904,0.8780788208
O,0,1.6590108302,-2.5978755236,0.5194214718
O,0,0.3967373475,-1.2720568643,1.8197042354
C,0,5.1460551062,-0.729147443,-1.419366184
H,0,5.2967744929,-0.6715912261,-2.4963804057
H,0,5.7621203573,0.0101434873,-0.9017482087
H,0,5.3903418257,-1.7254012678,-1.0452549262
C,0,-0.2254885671,-2.4431051237,2.363639835
H,0,-0.9602515296,-2.0716735706,3.0768927377
H,0,-0.7071472917,-3.0122491336,1.5646667771
H,0,0.5196217307,-3.0676579877,2.8604840993
H,0,-1.6969448932,2.1212541847,-1.443961039
H,0,1.2363433643,0.8283072249,2.0515808812
Pt,0,-1.8694740428,-0.1346415322,-0.0818075931
Br,0,-1.6965453066,-2.1338349743,-1.434982672
Br,0,-2.6638794402,1.4424415719,1.5663830505

(11). In Path 1B-*b*

36
1B-a1-IN1,Free Energies= -6104.822242
C,0,-1.268184041,3.3926191903,-1.1645109307
O,0,-0.9723431653,2.4203457796,-2.1534507887
C,0,-1.9437364455,1.4030172971,-2.0291048368
C,0,-2.391695276,1.3720343772,-0.5388820671
C,0,-1.6654648865,2.5880146307,0.0744076069
H,0,-0.3756052371,4.0043031093,-1.0213220541
H,0,-2.0947333153,4.0378510546,-1.5022107285
H,0,-2.8094940388,1.6251022638,-2.6693485243
H,0,-2.3117516847,3.1391384156,0.759773629
H,0,-0.7601532031,2.303976682,0.6172821589
C,0,-2.1804651485,0.0161045297,0.1866623527
C,0,-0.7489014716,-0.266104566,0.7123184786
H,0,-0.6751411402,-1.3176855503,0.9980384906
H,0,-0.5621005968,0.3323514551,1.6107234851
C,0,0.3234170227,0.0490226258,-0.2408608355
C,0,0.963266442,0.503186717,-1.2228240557
H,0,1.1175285167,0.9080571682,-2.2054784184
C,0,-3.0979856168,-0.0338932529,1.4191137567
O,0,-3.7318325622,0.8929508385,1.8558381618
O,0,-3.0748730046,-1.2533761831,1.9680088738
C,0,-2.5894881084,-1.1215980964,-0.7539843502
O,0,-1.8528945452,-1.9823340344,-1.166370251
O,0,-3.877971398,-1.0078349645,-1.0929341904
C,0,-3.869211108,-1.417880493,3.1461143676
H,0,-3.7465295156,-2.4598715512,3.4376115553
H,0,-3.5149363862,-0.7526815165,3.9369425498
H,0,-4.9169021182,-1.1965145062,2.9312105665
C,0,-4.3679520551,-1.9999621062,-1.9991512081
H,0,-5.4237966081,-1.7717765155,-2.1367713611
H,0,-3.8331867203,-1.9413796662,-2.949989132
H,0,-4.2397210959,-2.9986088828,-1.576123149
H,0,-1.4944330458,0.4702049602,-2.384817097
H,0,-3.4672876384,1.5528301837,-0.5040144042
Pt,0,2.3789080521,0.0094299031,0.1848068441
Br,0,3.086100661,-1.9241006341,-1.0593938598
Br,0,2.1367547628,1.8932831079,1.6982991554

36
1B-b-TS1,Free Energies= -6104.792344
C,0,-1.6930899835,-2.4224714556,2.0487527874
O,0,-0.6372720292,-1.5203872126,1.7514646614
C,0,-1.132449734,-0.2209643696,2.0346369046
C,0,-2.5363836444,-0.2253411843,1.4207578025
C,0,-3.0126108318,-1.6445868378,1.8081242095
H,0,-1.5724277551,-3.2964834589,1.4025954541
H,0,-1.61433584,-2.7538624156,3.09210795
H,0,-1.2031538366,-0.0638046228,3.121172204
H,0,-3.6089615451,-1.5989928528,2.7227216866
H,0,-3.6369462015,-2.1114996467,1.0403268723
C,0,-2.5374420767,0.0084358552,-0.1167058437
C,0,-1.7147677942,-1.0387772437,-0.9104699721
H,0,-1.9180896172,-0.9405529871,-1.9807227492
H,0,-1.9913531244,-2.0610733984,-0.643190797
C,0,-0.2778473546,-0.8774449742,-0.7260284087
C,0,0.9026028427,-0.4746296402,-0.6767537189
H,0,0.465442589,0.0194804166,-1.6548175945
C,0,-4.0080402395,0.0027815478,-0.5602705421
O,0,-4.7962700496,0.858785291,-0.2463071528
O,0,-4.3182020771,-1.068831813,-1.2976432965
C,0,-1.9900925627,1.3943607164,-0.5074165902
O,0,-1.4973584046,1.6036212157,-1.5953593583
O,0,-2.1178859035,2.2938780796,0.4491171053
C,0,-5.6851142199,-1.1476075013,-1.7203246175
H,0,-5.7582239041,-2.0678268315,-2.2977886204
H,0,-6.3471691017,-1.1798347103,-0.8524901212
H,0,-5.9389206292,-0.2823854682,-2.335988586
C,0,-1.58450554,3.5950841251,0.1568626608
H,0,-1.8164110405,4.2009459885,1.0308618119
H,0,-0.5046146378,3.5213940975,0.0110155981
H,0,-2.0597540823,4.0024595625,-0.7372800992
H,0,-0.4330703095,0.5103537324,1.6275755884
H,0,-3.1683523125,0.5476519899,1.8599279146
Pt,0,2.6445148034,-0.03350172,-0.1336986295
Br,0,1.943212707,2.0361182743,0.9439015625
Br,0,3.7369479707,-1.9686067078,-1.062400536

36
1B-b-IN1,Free Energies= -6104.831181
C,0,-0.2625225949,-1.067014159,2.6668123408
O,0,-0.0574755519,0.3067623044,2.3896105863
C,0,-1.3113633378,0.8343208677,2.0204626076
C,0,-2.1097452443,-0.3161888327,1.3398329957
C,0,-1.2056372482,-1.545587172,1.564303063
H,0,0.7109687737,-1.5612479952,2.6546528295
H,0,-0.7184035362,-1.1911812378,3.6624869987
H,0,-1.8545781589,1.1778541252,2.9134947093
H,0,-1.7825054809,-2.4303600262,1.8364740037
H,0,-0.6149453054,-1.792981215,0.6788445089
C,0,-2.5423011926,-0.0504007357,-0.1277221255
C,0,-1.4174568181,-0.1042353517,-1.1928383974
H,0,-1.8483192398,0.1567495714,-2.1621317092
H,0,-1.036716465,-1.1256829522,-1.2677057034
C,0,-0.2698793053,0.8476933197,-0.9344903701
C,0,0.8965346451,0.4467554474,-0.5408963984
H,0,-0.4260701015,1.9182181533,-1.0617093292
C,0,-3.5828748528,-1.1083009587,-0.5312865436
O,0,-3.8707600295,-2.0872817936,0.1092271425
O,0,-4.1230792767,-0.8079413555,-1.7196554984
C,0,-3.2275738397,1.3178371315,-0.1976506236
O,0,-2.8323313455,2.2648582568,-0.8366668741
O,0,-4.315107944,1.3467465197,0.5763967218
C,0,-5.0994449115,-1.7339770077,-2.2038203878
H,0,-5.4430553067,-1.3274555101,-3.1538788939
H,0,-4.6488179789,-2.7187763875,-2.3463522022
H,0,-5.9270111889,-1.816458773,-1.4958696154
C,0,-5.0181985134,2.5916801078,0.6133328261
H,0,-5.850203314,2.435629949,1.2981477966
H,0,-4.3624499822,3.3858705522,0.9771180641
H,0,-5.3814950989,2.8523232532,-0.3832451994
H,0,-1.1328638116,1.7029076444,1.381183028
H,0,-3.0408453892,-0.4626196196,1.891340763
Pt,0,2.4745621004,-0.1410158047,0.0116466092
Br,0,3.6514905831,1.9095323134,0.3975213674
Br,0,2.158090972,-2.5241093688,-0.1213512804

36
1B-b-TS2,Free Energies= -6104.812249
C,0,-0.7059994035,-2.6835650197,1.6275689365
O,0,-0.1823822735,-1.5390385174,2.302330609
C,0,-0.7697934052,-0.4315854886,1.7505699871
C,0,-2.174985709,-0.7956144048,1.2603343445
C,0,-2.1766348843,-2.3398477301,1.3726492184
H,0,-0.148451611,-2.8370733612,0.6942863179
H,0,-0.5506489092,-3.5438676307,2.2793576717
H,0,-0.6698527814,0.4254742519,2.4177165452
H,0,-2.7928000435,-2.6371999317,2.2235922378
H,0,-2.5800472929,-2.8445294723,0.49285935
C,0,-2.4806114646,-0.2112000595,-0.1381654664
C,0,-1.7276429534,-0.8647068502,-1.3166008682
H,0,-2.0928040958,-0.3999143508,-2.2349118952
H,0,-1.9869573573,-1.9281497005,-1.3777253168
C,0,-0.2258640514,-0.7440103889,-1.3450011902
C,0,0.671327295,-0.3478269619,-0.4814988874
H,0,0.2591413745,-1.000815648,-2.2916777911
C,0,-3.9892090231,-0.3970160626,-0.3934933929
O,0,-4.7393666905,-0.9868940773,0.3446884839
O,0,-4.363231106,0.1714804003,-1.5408728001
C,0,-2.1928408201,1.3065455088,-0.1932461613
O,0,-1.7975697433,1.8862768332,-1.1718008945
O,0,-2.4437049356,1.8920979091,0.9800658328
C,0,-5.7497999653,0.0514463541,-1.871287695
H,0,-5.8686100581,0.5771088728,-2.8173397204
H,0,-6.0243297417,-1.0006362413,-1.9767099811
H,0,-6.3662875965,0.5085956157,-1.094255726
C,0,-2.1144310536,3.2864030699,1.0515284866
H,0,-2.429348303,3.6067925008,2.0435271428
H,0,-1.0364652628,3.4150780769,0.9272960128
H,0,-2.6442860443,3.8418894919,0.2752754167
H,0,-0.1624172649,-0.08794795,0.8250295904
H,0,-2.9112133025,-0.3782672935,1.9475734435
Pt,0,2.3497343701,0.0520446605,0.1048758577
Br,0,1.8907963125,2.118994471,1.2911026105
Br,0,3.3789937251,-1.8791745956,-0.8979814188

(12). In Path 1C-*a1*

36
1C-a1-IN1,Free Energies= -984.817336
C,0,-1.5898045475,3.4140019074,-0.4700895008
O,0,-0.8568844794,2.5386420002,-1.3067836958
C,0,-1.803113105,1.6314577344,-1.8406164339
C,0,-2.6995336888,1.2463036363,-0.6549731825
C,0,-2.7171373088,2.5651278269,0.1616434706
H,0,-0.8958515836,3.8358346084,0.2612162808
H,0,-2.0103636826,4.2378560464,-1.0651729285
H,0,-2.412844284,2.1251296366,-2.6134219231
H,0,-3.6861755719,3.0614303735,0.0698047961
H,0,-2.5448842797,2.3974823632,1.2291346277
C,0,-2.1960082503,0.0286906776,0.1668337739
C,0,-0.7604489852,0.1740754904,0.7294890018
H,0,-0.5895569578,-0.5997519814,1.4802136591
H,0,-0.6533733817,1.1406756852,1.2311675021
C,0,0.3291614804,0.0910677562,-0.2549572382
C,0,1.3157418934,0.4153786445,-0.9665558558
H,0,1.9567202759,1.1022217473,-1.4886821177
C,0,-3.2073793565,-0.1455365701,1.3145708443
O,0,-4.3596649059,-0.4493917915,1.1244658159
O,0,-2.6896329151,0.1085230385,2.5181249607
C,0,-2.2953395488,-1.3087811956,-0.5890712535
O,0,-1.8446654529,-2.33665773,-0.1366153375
O,0,-2.9390371263,-1.214851952,-1.7440127989
C,0,-3.5936649583,-0.0381277638,3.6185346619
H,0,-3.0073131254,0.1864930038,4.5081372664
H,0,-4.4291030521,0.6580247483,3.5170559372
H,0,-3.9766614453,-1.0597822006,3.6556955511
C,0,-3.1212981251,-2.4490713804,-2.4498325973
H,0,-3.6239613628,-2.1798686524,-3.3771615898
H,0,-2.1537201783,-2.9088262931,-2.6571331855
H,0,-3.7376309521,-3.1269860132,-1.8554086928
H,0,-1.2681414275,0.8022072764,-2.3036030333
H,0,-3.702250401,0.9893580933,-0.9982944511
Pt,0,1.2105979428,-1.6236509087,-1.1334922605
I,0,0.5673586537,-1.4678279957,-3.6937582632
I,0,2.1658518636,-2.3844874668,1.1960321506

36
1C-a1-TS1,Free Energies= -984.792460
C,0,-1.0201284126,3.3285728768,0.144605442
O,0,-1.2741659927,3.1243916952,-1.2535513486
C,0,-1.798625804,1.8748663142,-1.4481320441
C,0,-2.5231109511,1.4313556597,-0.1812292319
C,0,-1.8725916242,2.3046947111,0.9155785045
H,0,0.0480708992,3.1877681466,0.3431370442
H,0,-1.2834755761,4.3655303629,0.3609981606
H,0,-2.374076256,1.8469100409,-2.3779979453
H,0,-2.6425201605,2.7784822809,1.5243818447
H,0,-1.242592137,1.7214221212,1.5922164045
C,0,-2.3841799715,-0.0929866211,0.0009435498
C,0,-0.8987621338,-0.5384668269,0.1002692152
H,0,-0.8020906375,-1.5739079016,-0.2338039317
H,0,-0.5670847169,-0.4804243394,1.143304353
C,0,0.0345179613,0.3053338955,-0.6621467876
C,0,1.1390179591,0.9071155198,-0.9203803687
H,0,1.3638673237,1.717020893,-1.6062779292
C,0,-3.126420077,-0.5474275914,1.2600363654
O,0,-3.7482671769,0.176770103,1.9947256714
O,0,-2.9752227783,-1.8619767338,1.4349095861
C,0,-3.0161625717,-0.7700163258,-1.2232723377
O,0,-2.3901041581,-1.2056307505,-2.1578410252
O,0,-4.3467027967,-0.7535828156,-1.1439947193
C,0,-3.6118192321,-2.4109630451,2.5944351844
H,0,-3.3994683057,-3.478245363,2.563869908
H,0,-3.1980509646,-1.9599019435,3.4988632627
H,0,-4.6874750458,-2.2265787295,2.5565377877
C,0,-5.0412854211,-1.3259069321,-2.2588754464
H,0,-6.0984509266,-1.2606987552,-2.0075373512
H,0,-4.8243139136,-0.7622078121,-3.1689394825
H,0,-4.7386029806,-2.3656717586,-2.3972305724
H,0,-0.9602642513,1.1011379925,-1.6544854958
H,0,-3.5882161087,1.6611419695,-0.2629760941
Pt,0,2.5059890074,0.0523147527,0.1815313108
I,0,2.0045904953,1.4305123933,2.3882991745
I,0,3.3306497569,-1.5746447036,-1.707039728

36
1C-a1-IN2,Free Energies= -984.871884
C,0,-0.7974480327,3.1294397148,-1.3052792296
O,0,-0.217242236,2.0428971259,-2.026847476
C,0,-1.025070344,0.8880220783,-1.880224367
C,0,-2.1634551373,1.2320028826,-0.8943636086
C,0,-1.6127774387,2.4849456408,-0.1932393433
H,0,0.0175185534,3.7584532767,-0.941856978
H,0,-1.4328863894,3.7190298874,-1.9812967446
H,0,-1.385940158,0.5738480984,-2.8642504285
H,0,-2.4059993778,3.1229947224,0.1953129088
H,0,-0.9529336635,2.2194311745,0.6396041641
C,0,-2.3274771871,-0.028480297,-0.0176824425
C,0,-0.8860569236,-0.5411088063,0.1614576487
H,0,-0.8438872836,-1.5959251797,0.4341176194
H,0,-0.3930454875,0.0281095338,0.9549944807
C,0,-0.2165177011,-0.2638299576,-1.1954983179
C,0,1.2183811149,0.0655087242,-1.2066916345
H,0,1.6542070067,0.3929019709,-2.156027664
C,0,-3.0297736443,0.2363984842,1.3084462189
O,0,-3.5579871051,1.2689355505,1.6372245668
O,0,-2.9792185743,-0.8594343782,2.0751967872
C,0,-3.1434233041,-1.0540758889,-0.8096926744
O,0,-2.6694500375,-1.917536028,-1.510333997
O,0,-4.4537757541,-0.8381462221,-0.6776152107
C,0,-3.6297474126,-0.7547074458,3.3435654153
H,0,-3.4851979746,-1.7200888134,3.8264502913
H,0,-3.1800343995,0.0436565086,3.9380497782
H,0,-4.6932220507,-0.5458641412,3.2058086283
C,0,-5.3065648119,-1.719028762,-1.4141952035
H,0,-6.321377467,-1.3857622202,-1.2026098449
H,0,-5.0919575896,-1.6502706005,-2.482971246
H,0,-5.1613546001,-2.7501531302,-1.0844981918
H,0,-0.2890221792,-1.1712719776,-1.8182135105
H,0,-3.0931011592,1.4789258868,-1.4148537955
Pt,0,2.3703631731,-0.083338899,0.1840028565
I,0,2.35074018,2.3056634654,1.2649433758
I,0,2.955539906,-2.6337303489,-0.0235799611

36
1C-a1-TS2,Free Energies= -984.843806
C,0,-1.6278019926,3.5299616135,-1.2432068534
O,0,-0.5624268153,2.6485189016,-1.5927418271
C,0,-1.0942167981,1.3515848279,-1.7596584164
C,0,-2.5029564733,1.3152556772,-1.1138073785
C,0,-2.5906860764,2.6842343739,-0.4164308151
H,0,-1.1902968844,4.368043366,-0.6987814785
H,0,-2.1099184044,3.9063862317,-2.1561782981
H,0,-1.0804689763,1.0398613062,-2.8086689102
H,0,-3.6104883344,3.0716385008,-0.3996473387
H,0,-2.2349224168,2.6282260618,0.6189143314
C,0,-2.4799701928,0.101562244,-0.1537084879
C,0,-1.0064927678,0.030544884,0.3073029141
H,0,-0.6780783074,-0.9260566959,0.7239237116
H,0,-0.7808254991,0.7857950864,1.0751075959
C,0,-0.243981537,0.4366356668,-0.8956210252
C,0,1.0233331928,-0.0375939408,-1.2434389497
H,0,1.4975696987,0.4366635433,-2.1064610934
C,0,-3.5186400627,0.2179231769,0.9495458274
O,0,-4.6441175335,0.6086001602,0.7558181451
O,0,-3.033895975,-0.1558753128,2.132311077
C,0,-2.6816450325,-1.18125758,-0.9636046442
O,0,-2.2212497791,-1.3078159738,-2.0782333788
O,0,-3.3009369973,-2.131177709,-0.2854114994
C,0,-3.9652551201,-0.1288849844,3.2190749029
H,0,-3.4026123244,-0.4530243842,4.0928246151
H,0,-4.3537496492,0.8819648122,3.3604432826
H,0,-4.7946046072,-0.810135304,3.0176807239
C,0,-3.3607103584,-3.4185426007,-0.9230263682
H,0,-3.903904527,-4.0563256823,-0.228569465
H,0,-3.8867367464,-3.341177915,-1.8761523626
H,0,-2.3476713676,-3.7923406586,-1.0863211427
H,0,0.2992225761,-0.8620990142,-1.6902969804
H,0,-3.287294566,1.2083546113,-1.863871685
Pt,0,2.1816468469,-0.9566693637,0.028740761
I,0,3.1574144641,1.2909937708,0.985215542
I,0,1.2330909337,-3.3751943068,-0.5469880716

36
1C-a1-P,Free Energies= -984.879389
C,0,-0.3718639244,-2.603440343,-2.1402365855
O,0,0.5159394506,-1.8692449334,-1.3142613929
C,0,-0.1672494418,-1.5699088307,-0.1150246456
C,0,-1.6913728777,-1.5538769086,-0.464569537
C,0,-1.7049958984,-1.8897565968,-1.9697136042
H,0,0.0253660233,-2.5762971747,-3.1561721868
H,0,-0.4265248916,-3.6511288831,-1.8064995023
H,0,0.0902860405,-2.3036200779,0.6605465952
H,0,-2.5738406819,-2.4839468508,-2.253787055
H,0,-1.7097748719,-0.9816607209,-2.5786511359
C,0,-2.1801655075,-0.1300096849,-0.0795496558
C,0,-0.9219602241,0.7495097154,-0.242162446
H,0,-1.0014311723,1.7105852322,0.2646216357
H,0,-0.7442553866,0.9309110533,-1.3058539707
C,0,0.1574580569,-0.1474325989,0.3359836075
C,0,0.7665215455,0.1379847011,1.5996045597
H,0,1.0257776537,-0.6767155953,2.2718127025
C,0,-3.3668295576,0.3770031095,-0.8975085307
O,0,-4.0436024011,-0.2722238764,-1.6537513649
O,0,-3.5679641454,1.674617487,-0.6359316437
C,0,-2.6310977803,-0.1341910771,1.3873871967
O,0,-2.0056034156,0.3166190252,2.3172021481
O,0,-3.8154022247,-0.737227399,1.5132568198
C,0,-4.6692101949,2.2784291342,-1.3189686153
H,0,-4.6713196384,3.3210477134,-1.004678011
H,0,-4.5322230654,2.2024932924,-2.3998940088
H,0,-5.6044999203,1.7880363114,-1.0390890372
C,0,-4.3324045763,-0.82285755,2.8442012467
H,0,-5.306749975,-1.29910508,2.7473416086
H,0,-3.6693748198,-1.4252323655,3.4695940191
H,0,-4.4300513726,0.1741815233,3.27888464
H,0,0.5675021043,1.0929315121,2.076591572
H,0,-2.2397762376,-2.3162137487,0.0929352131
Pt,0,2.2020041426,0.3591785273,0.1192558537
I,0,3.4269477844,-1.8868187468,0.7317878628
I,0,1.8930736713,2.8690083946,-0.6262128818

(13). In Path 1C-*a2*

36
1C-a2-IN1,Free Energies= -984.812340
C,0,-3.8208609243,-2.0958095075,-1.9168834453
O,0,-2.9576176941,-2.9475942311,-1.1829180518
C,0,-1.9090469244,-2.1524990588,-0.6775240578
C,0,-2.6269647212,-0.8825896613,-0.2051458156
C,0,-3.646602241,-0.670217506,-1.342239152
H,0,-3.561631342,-2.1192163911,-2.9852885924
H,0,-4.8374777064,-2.4810548376,-1.803632794
H,0,-1.4138382791,-2.6989776074,0.1255808155
H,0,-4.5855027515,-0.2510089142,-0.9699990906
H,0,-3.2695754483,0.011946493,-2.1110771682
C,0,-1.7771769742,0.3573221018,0.1701052975
C,0,-0.8484254326,0.8987079652,-0.9459995141
H,0,-0.5046853837,1.8989780713,-0.6693683368
H,0,-1.4105822429,1.0021097634,-1.8788320307
C,0,0.3504475914,0.1052133607,-1.258403778
C,0,1.2131867939,-0.5322532969,-1.9197156873
H,0,1.5950668982,-1.1051784029,-2.74532545
C,0,-2.8058564664,1.4364248529,0.5536776762
O,0,-3.4026504944,1.4334866506,1.601807191
O,0,-3.00255571,2.328416669,-0.4200164114
C,0,-0.9540799999,0.1647318853,1.4577378277
O,0,-0.0942431916,0.9474647498,1.797095928
O,0,-1.3061171349,-0.906728502,2.1492831035
C,0,-3.9940207043,3.3244643043,-0.1471228663
H,0,-4.0236241742,3.9561805275,-1.0334129064
H,0,-4.9640002859,2.8532924577,0.0267812697
H,0,-3.7120553273,3.9056516977,0.7331019333
C,0,-0.6326913797,-1.08809347,3.4008775846
H,0,-1.0464528449,-2.0043277828,3.8182557805
H,0,0.4418931256,-1.1908320145,3.2388825731
H,0,-0.8315173604,-0.2362547028,4.0546273187
H,0,-1.1707142831,-1.9370981065,-1.4650053685
H,0,-3.1788697591,-1.1538609811,0.6981011622
Pt,0,2.1002602621,-0.1491791229,-0.1131333582
I,0,1.9238451121,-2.6684298593,0.66489715
I,0,2.8531030186,2.3391603466,-0.5383081258

36
1C-a2-TS1,Free Energies= -984.786803
C,0,-1.5113248841,3.2427935201,-1.6078200504
O,0,-0.7779994553,2.2508848858,-2.3519552069
C,0,-1.1269013748,0.9819696735,-1.8833072627
C,0,-2.4082292526,1.1055529013,-1.0424521992
C,0,-2.2029831553,2.5105266126,-0.454005706
H,0,-0.8090641795,4.0087245974,-1.2700323154
H,0,-2.23755198,3.7045448997,-2.2858523232
H,0,-1.1987345346,0.271685509,-2.7161699991
H,0,-3.1404745978,2.9743485213,-0.1496697056
H,0,-1.5541389413,2.4768082347,0.4307862877
C,0,-2.3498495568,-0.091777903,-0.0639310046
C,0,-0.8384205943,-0.2975965519,0.2052242864
H,0,-0.5267945164,-1.3475654945,0.2158181973
H,0,-0.5091803777,0.1120694839,1.1707859101
C,0,-0.1289519136,0.4159382209,-0.8836676008
C,0,1.2307561274,0.7358452279,-0.8846162209
H,0,1.6183817479,1.1990816892,-1.7951602301
C,0,-3.1606481386,0.1227061031,1.2080652553
O,0,-3.9613170532,1.0068166582,1.3832103627
O,0,-2.8551776022,-0.8160604217,2.1057243625
C,0,-2.883245108,-1.3086271735,-0.8285071719
O,0,-2.2076509091,-1.9571597632,-1.5915349992
O,0,-4.1786504647,-1.5097745987,-0.606333659
C,0,-3.5614223741,-0.7413776172,3.3484703649
H,0,-3.1860169102,-1.5701208375,3.9462099398
H,0,-3.3584572137,0.2112133391,3.8424861713
H,0,-4.6355260134,-0.8401187441,3.1769022253
C,0,-4.77283532,-2.5945677726,-1.3306007741
H,0,-5.82179233,-2.5964610462,-1.0396827727
H,0,-4.6689381276,-2.4316175995,-2.4053522567
H,0,-4.2917654076,-3.5362033408,-1.058196261
H,0,0.7069423909,1.6403879376,-0.3126502376
H,0,-3.308397356,1.0839975312,-1.6618920058
Pt,0,2.5037387671,-0.0177417676,0.378014414
I,0,1.9304343284,1.82645315,2.2194436224
I,0,3.1327939609,-2.0409235146,-1.1732434268

36
1C-a2-IN2,Free Energies= -984.867317
C,0,-2.8532756174,3.6294279199,-0.3975534847
O,0,-1.4527516125,3.4103068242,-0.3683691359
C,0,-1.1909466272,2.114697664,-0.8720335622
C,0,-2.5227114612,1.3151345871,-0.7978625315
C,0,-3.4604529483,2.2754875211,-0.0489052197
H,0,-3.0808240989,4.4187834946,0.3219206746
H,0,-3.1725130783,3.9613126413,-1.3975158363
H,0,-0.8082679366,2.1806168995,-1.8979296525
H,0,-4.5015597225,2.1618220582,-0.3534252288
H,0,-3.4061269891,2.1196838523,1.0345739161
C,0,-2.177236413,0.0028738343,-0.0545146385
C,0,-1.0426212655,0.4270782401,0.9080709064
H,0,-0.4782129021,-0.41274504,1.3153896034
H,0,-1.4801645798,0.9702631978,1.7494988299
C,0,-0.1862334616,1.4090713971,0.0709511825
C,0,0.969753219,0.7910973877,-0.6274116542
H,0,1.1001707088,0.9613048783,-1.7002595165
C,0,-3.3869903722,-0.6159944916,0.633941784
O,0,-4.5158751247,-0.5416349372,0.2123239231
O,0,-3.0423241804,-1.2570005935,1.7524615899
C,0,-1.6155076773,-0.9785332495,-1.0830553716
O,0,-0.7724022776,-0.6547736772,-1.8965997649
O,0,-2.1428937485,-2.1887445303,-1.0083657457
C,0,-4.1057380809,-1.935275179,2.4243040804
H,0,-3.6512196448,-2.3940308351,3.3009613575
H,0,-4.8849329712,-1.2277549129,2.7174040519
H,0,-4.5391744484,-2.6953848658,1.7703818237
C,0,-1.6612450213,-3.1479090794,-1.9616001885
H,0,-2.2146155602,-4.0612366775,-1.7513368643
H,0,-1.8611869472,-2.7967397301,-2.9759235296
H,0,-0.5888840585,-3.3005076319,-1.8264126781
H,0,0.2573267632,2.1672235804,0.7328797652
H,0,-2.9198439261,1.1097833236,-1.7941809366
Pt,0,2.3370686622,-0.0850429521,0.1928605222
I,0,1.6703967223,-2.618576541,0.3115666182
I,0,3.8412742276,1.9999742532,0.7307386638

36
1C-a2-TS2,Free Energies= -984.841694
C,0,-1.5113248841,3.2427935201,-1.6078200504
O,0,-0.7779994553,2.2508848858,-2.3519552069
C,0,-1.1269013748,0.9819696735,-1.8833072627
C,0,-2.4082292526,1.1055529013,-1.0424521992
C,0,-2.2029831553,2.5105266126,-0.454005706
H,0,-0.8090641795,4.0087245974,-1.2700323154
H,0,-2.23755198,3.7045448997,-2.2858523232
H,0,-1.1987345346,0.271685509,-2.7161699991
H,0,-3.1404745978,2.9743485213,-0.1496697056
H,0,-1.5541389413,2.4768082347,0.4307862877
C,0,-2.3498495568,-0.091777903,-0.0639310046
C,0,-0.8384205943,-0.2975965519,0.2052242864
H,0,-0.5267945164,-1.3475654945,0.2158181973
H,0,-0.5091803777,0.1120694839,1.1707859101
C,0,-0.1289519136,0.4159382209,-0.8836676008
C,0,1.2307561274,0.7358452279,-0.8846162209
H,0,1.6183817479,1.1990816892,-1.7951602301
C,0,-3.1606481386,0.1227061031,1.2080652553
O,0,-3.9613170532,1.0068166582,1.3832103627
O,0,-2.8551776022,-0.8160604217,2.1057243625
C,0,-2.883245108,-1.3086271735,-0.8285071719
O,0,-2.2076509091,-1.9571597632,-1.5915349992
O,0,-4.1786504647,-1.5097745987,-0.606333659
C,0,-3.5614223741,-0.7413776172,3.3484703649
H,0,-3.1860169102,-1.5701208375,3.9462099398
H,0,-3.3584572137,0.2112133391,3.8424861713
H,0,-4.6355260134,-0.8401187441,3.1769022253
C,0,-4.77283532,-2.5945677726,-1.3306007741
H,0,-5.82179233,-2.5964610462,-1.0396827727
H,0,-4.6689381276,-2.4316175995,-2.4053522567
H,0,-4.2917654076,-3.5362033408,-1.058196261
H,0,0.7069423909,1.6403879376,-0.3126502376
H,0,-3.308397356,1.0839975312,-1.6618920058
Pt,0,2.5037387671,-0.0177417676,0.378014414
I,0,1.9304343284,1.82645315,2.2194436224
I,0,3.1327939609,-2.0409235146,-1.1732434268

36
1C-a2-P, Free Energies= -984.884171
C,0,1.7552183474,3.6707606462,-0.0103018204
O,0,0.5948042127,3.0653956678,-0.5582807252
C,0,0.3051972921,1.9279760026,0.2416514135
C,0,1.6567620617,1.4325890891,0.8275322886
C,0,2.6635044677,2.497607697,0.3468903623
H,0,2.1668787383,4.3437076625,-0.7649002741
H,0,1.4921335071,4.2559577718,0.8834996594
H,0,-0.4212019187,2.1796042072,1.0138340997
H,0,3.4083198028,2.7382717135,1.1078364823
H,0,3.1945880586,2.1646857966,-0.5523409396
C,0,1.8783878122,0.0207569491,0.2275430364
C,0,1.0842107766,0.0689131418,-1.0935303921
H,0,0.921871433,-0.9000733443,-1.5591571612
H,0,1.6350607001,0.6975076046,-1.8058192999
C,0,-0.1645262612,0.8467214211,-0.7349689394
C,0,-1.2995870331,1.0117264077,-1.5848025889
H,0,-1.8803149086,1.9287845882,-1.5142000834
C,0,3.3619603859,-0.2934135328,0.0961413889
O,0,4.1121435449,-0.3216576644,1.0415971859
O,0,3.7396642592,-0.4978356027,-1.1689480624
C,0,1.2569933382,-1.0433672073,1.1388187851
O,0,0.472820979,-0.8123487684,2.0302056725
O,0,1.6591390313,-2.2607476701,0.7864278813
C,0,5.1272067344,-0.7909383401,-1.352649938
H,0,5.2582949655,-0.9184981157,-2.4262362826
H,0,5.7412608706,0.0327159026,-0.9813408928
H,0,5.3936676915,-1.7062833399,-0.8198276671
C,0,1.1060321352,-3.3461578745,1.5393040721
H,0,1.5392823821,-4.2467121645,1.1076883469
H,0,1.3786460196,-3.247919856,2.5922955784
H,0,0.0191791755,-3.3597845857,1.4359599879
H,0,-1.3181573365,0.5168837471,-2.5536162333
H,0,1.6217783219,1.3793708503,1.9151243412
Pt,0,-1.8646999959,-0.3149522814,-0.0939360276
I,0,-3.1504791461,1.3576482908,1.4773686983
I,0,-1.4957750349,-2.5631937616,-1.4450495632

(14). In Path 1C-*a3*

36
1C-a3-TS1,Free Energies= -984.805410
C,0,-4.0538531868,-2.4015436064,-1.1325576784
O,0,-2.8162463999,-2.7742667494,-1.7285526004
C,0,-1.8400364896,-1.7827256692,-1.4893426069
C,0,-2.3327428442,-1.0231915438,-0.2478999896
C,0,-3.845187377,-1.0141124602,-0.5280651994
H,0,-4.8423297866,-2.4134864739,-1.8931204837
H,0,-4.3087650192,-3.1395669474,-0.3614773451
H,0,-0.8810661436,-2.2825069319,-1.3345874694
H,0,-4.4415900903,-0.8493657966,0.3725745673
H,0,-4.0940125021,-0.2356980526,-1.2586394547
C,0,-1.6756794117,0.3609816696,0.0918221023
C,0,-0.72772698,0.9240304919,-0.9983657103
H,0,-0.3976377426,1.9244128018,-0.7044584848
H,0,-1.2710627849,1.0239203773,-1.9421355916
C,0,0.4759618072,0.1255184526,-1.271746443
C,0,1.3490985678,-0.5425960525,-1.8857367915
H,0,1.7702308349,-1.1008370711,-2.7021025691
C,0,-2.7970914123,1.3901409966,0.3348516593
O,0,-3.3488616869,1.5476891472,1.3951788329
O,0,-3.1094106027,2.0677855445,-0.774834524
C,0,-0.9186795737,0.3529863426,1.437577409
O,0,-0.017788479,1.1266490579,1.6805843439
O,0,-1.3900843689,-0.5335360509,2.2964947559
C,0,-4.1861004694,3.0011771107,-0.6369622871
H,0,-4.281105534,3.482095289,-1.6092966502
H,0,-5.1066082867,2.4751256891,-0.3733408549
H,0,-3.9549704921,3.7347693974,0.1378385406
C,0,-0.7766138084,-0.5344807841,3.5897002662
H,0,-1.295566339,-1.3082074891,4.1527898451
H,0,0.2853267772,-0.7723062457,3.4997885164
H,0,-0.9016102519,0.441969455,4.0622364899
H,0,-1.7564390035,-1.1194368692,-2.3657187379
H,0,-2.1625294661,-1.676219782,0.60962349
Pt,0,2.1263327491,-0.2256344792,-0.0137439476
I,0,1.5091672274,-2.6353186399,0.8956048807
I,0,3.2287005692,2.1071818719,-0.5325232799

36
1C-a3-IN2,Free Energies= -984.816160
C,0,-3.6351347814,-2.6035943524,-0.9858757876
O,0,-3.2667973492,-2.0020838378,-2.2213652957
C,0,-2.45945115,-0.8652233401,-1.9862387969
C,0,-2.1108857401,-0.8814570487,-0.4861437124
C,0,-3.3587405667,-1.5606363358,0.0908511337
H,0,-4.6872781904,-2.8983470392,-1.0433732178
H,0,-3.0308456584,-3.5069912254,-0.8189433106
H,0,-1.5675735467,-0.925685305,-2.621400356
H,0,-3.1892070864,-1.9900924967,1.0776906709
H,0,-4.1940174295,-0.8543294664,0.1617879152
C,0,-1.6867055848,0.488191075,0.1066854254
C,0,-0.6822835006,1.2162913536,-0.8242827995
H,0,-0.346410703,2.1429357146,-0.3506916261
H,0,-1.1729581274,1.4763172094,-1.7666128759
C,0,0.4987523098,0.4093998722,-1.161350317
C,0,1.3403877747,-0.2543791547,-1.8216967324
H,0,1.7434032479,-0.7659381837,-2.6769725087
C,0,-2.9154536019,1.3794600442,0.3321445486
O,0,-3.4928922616,1.4729226837,1.3869398782
O,0,-3.2935063587,2.0131131012,-0.7831743389
C,0,-1.0301088953,0.3635272381,1.4961180254
O,0,-0.2388688932,1.1770034383,1.9169951373
O,0,-1.4229042315,-0.7090554738,2.1650333113
C,0,-4.466934162,2.8249094665,-0.662834369
H,0,-4.6360995335,3.2379423702,-1.6559793568
H,0,-5.3171928501,2.2166565975,-0.3470856528
H,0,-4.3014882453,3.621209459,0.065713916
C,0,-0.8498617096,-0.8704884943,3.4664264966
H,0,-1.2729854367,-1.7954234361,3.854574483
H,0,0.2366797645,-0.9501542584,3.3900221749
H,0,-1.1162370836,-0.0224806339,4.1006984269
H,0,-3.0162918902,0.0422497687,-2.2580085452
H,0,-1.2623002803,-1.560201066,-0.3416484618
Pt,0,2.1055270773,-0.1602934261,0.0820052126
I,0,1.519310552,-2.6749059623,0.6486914206
I,0,3.2031691216,2.2238891446,-0.0382421151

36
1C-a3-TS2,Free Energies=-984.769581
C,0,-3.0593180208,-0.8725808672,3.0222286961
O,0,-2.3036829125,-2.0057692922,2.5066649847
C,0,-1.9348879352,-1.7376468539,1.2330931377
C,0,-2.1891224533,-0.2622813859,0.9673214336
C,0,-3.4622542663,-0.0653838173,1.7802783216
H,0,-3.8918045364,-1.2934923554,3.5871229815
H,0,-2.4168972387,-0.2937451278,3.6931889269
H,0,-0.7373369762,-1.9807163316,1.048026737
H,0,-3.657591052,0.9843253797,2.0006107938
H,0,-4.3405667031,-0.5052771385,1.2946462297
C,0,-1.9846425013,0.0523994516,-0.5231453959
C,0,-0.7810289427,-0.8478980203,-0.962306808
H,0,-0.1351020478,-0.2997521895,-1.6566535537
H,0,-1.131724507,-1.7466908859,-1.4764101367
C,0,0.054948981,-1.208348774,0.2018819611
C,0,1.1136959745,-0.9276034908,0.9206223876
H,0,1.2922644385,-1.3302863918,1.9160083733
C,0,-3.2527018162,-0.2325457138,-1.3286499036
O,0,-3.9384842162,0.613835376,-1.8413404557
O,0,-3.5401885848,-1.5432986447,-1.3547635678
C,0,-1.6313298895,1.5258115133,-0.7739991482
O,0,-0.9337078538,1.8855051285,-1.6875113644
O,0,-2.2024084479,2.3263986805,0.1186149773
C,0,-4.7330141782,-1.8963213803,-2.0670024743
H,0,-4.8195403531,-2.9775578323,-1.9715145772
H,0,-5.598782639,-1.3965537475,-1.6271200139
H,0,-4.6439342872,-1.6069089852,-3.1159182245
C,0,-1.9342053554,3.7246840139,-0.0571952891
H,0,-2.4400307236,4.2225147269,0.768549035
H,0,-0.8581782366,3.9036122824,-0.0161935357
H,0,-2.3336403197,4.058841847,-1.0170608035
H,0,-2.3335915255,-2.4567596503,0.5086842064
H,0,-1.4057070658,0.2907298519,1.4983183467
Pt,0,2.3861115797,0.332698885,0.2094153902
I,0,1.4341173348,2.2441034185,1.8033074706
I,0,3.5171442774,-1.2851326793,-1.5215791386

36
1C-a3-IN3,Free Energies=-984.849116
C,0,-3.0233517519,-1.0840747367,2.9724389207
O,0,-1.8981097019,-1.8362872032,2.4554799997
C,0,-1.9053354118,-1.6243346012,1.0715738427
C,0,-2.3602780347,-0.1903547782,0.9128572041
C,0,-3.5771643253,-0.1907697305,1.8205990612
H,0,-3.776022001,-1.7845121067,3.3480750684
H,0,-2.6512137401,-0.4836929015,3.8068813865
H,0,-0.2823220037,-2.6697002037,0.0137239752
H,0,-3.8621861164,0.8022650445,2.1724073955
H,0,-4.4409583813,-0.6592304392,1.3378926706
C,0,-2.210828158,0.1085658137,-0.5919072335
C,0,-1.0617485,-0.881104984,-1.0176243141
H,0,-0.2527872315,-0.3350318575,-1.5047276001
H,0,-1.4445826927,-1.6143475343,-1.7304479059
C,0,-0.6000106148,-1.6417612783,0.2544281201
C,0,0.525923304,-1.1082968296,1.0525917109
H,0,0.7712241727,-1.6678286844,1.963082227
C,0,-3.4889937859,-0.1252669529,-1.3890881267
O,0,-4.0352791262,0.7013364362,-2.0759156928
O,0,-3.9464445605,-1.3785975345,-1.2338819584
C,0,-1.7961501001,1.5617568729,-0.8380250037
O,0,-0.9355524383,1.9067321708,-1.6097343798
O,0,-2.5037842108,2.392491902,-0.0744058587
C,0,-5.1480163884,-1.68458142,-1.9465297565
H,0,-5.37805006,-2.7201412691,-1.6991749027
H,0,-5.957180537,-1.0226643575,-1.6304001101
H,0,-4.9919737038,-1.5710910044,-3.0216360671
C,0,-2.1910340348,3.7793804713,-0.2284688964
H,0,-2.8436991728,4.3044446407,0.4675990875
H,0,-1.1420866594,3.9564661046,0.0202315775
H,0,-2.3849911943,4.096481315,-1.2554873529
H,0,-2.6044296262,-2.312650263,0.5741700153
H,0,-1.6066020499,0.4277389705,1.4149646381
Pt,0,1.5650019729,0.332181526,0.7031834696
I,0,0.6978271655,2.1842789479,2.3519838699
I,0,3.1282934563,-0.6938719554,-1.1357892709

36
1C-a3-TS3,Free Energies=-984.824249
C,0,1.6126891135,-0.4189739056,3.6743486978
O,0,0.4087477577,0.0664092845,3.0249844585
C,0,0.7901027986,0.4955155904,1.7651123908
C,0,1.9550712517,-0.4094867046,1.3488492696
C,0,2.7656988195,-0.3744515657,2.632227159
H,0,1.815921374,0.206545362,4.5476133736
H,0,1.4090121697,-1.4400086061,4.0068352487
H,0,-1.3555060283,1.0133544746,0.4260743477
H,0,3.4489524692,-1.2190265379,2.7319322363
H,0,3.3372006688,0.5566120395,2.7174459321
C,0,2.3023716278,0.0883858723,-0.0682955381
C,0,0.8783244299,0.4394049205,-0.6260591666
H,0,0.5746635823,-0.208413767,-1.4493006091
H,0,0.8385946477,1.4783317723,-0.9705476638
C,0,-0.0389373491,0.2500823766,0.5641292722
C,0,-1.3589431913,-0.1963138547,0.5433099129
H,0,-1.8133158029,-0.3680046659,1.52266922
C,0,3.1864142933,1.3317547468,-0.0013529539
O,0,2.7640775325,2.4618456516,0.0771117775
O,0,4.4761322035,1.0068992125,0.0307124985
C,0,2.9855868624,-1.0173948293,-0.8696014166
O,0,3.4357328515,-2.0232274368,-0.3829358172
O,0,2.9999248174,-0.7174472004,-2.167594838
C,0,5.3919252053,2.1016267095,0.1483838003
H,0,6.3832463729,1.6519551319,0.1533125963
H,0,5.2788436598,2.7812748386,-0.6986774797
H,0,5.2103266576,2.6479152319,1.0766299355
C,0,3.5535561733,-1.7229287003,-3.0251364852
H,0,3.5291840754,-1.296501758,-4.0265436345
H,0,4.5776680237,-1.9529653108,-2.7241616157
H,0,2.9438866085,-2.6278714566,-2.975637908
H,0,1.1211145377,1.5480648193,1.7609310963
H,0,1.5643614586,-1.428086179,1.2218245611
Pt,0,-2.220360104,-1.0015073557,-0.9924996559
I,0,-0.7117207151,-3.1769290235,-0.8665218166
I,0,-3.7268234341,1.1093443483,-1.4793573864

36
1C-a3-P,Free Energies=-984.864693
C,0,-1.9711488418,3.4950639533,-0.8115469061
O,0,-0.751336019,3.1002374618,-0.1404913029
C,0,-0.9711929212,1.8293507045,0.3658802927
C,0,-2.0178385052,1.1786604224,-0.5127401561
C,0,-2.9928503985,2.3343339549,-0.6609297447
H,0,-2.3238398332,4.4287871004,-0.3658186252
H,0,-1.7227230531,3.6716837038,-1.862787164
H,0,1.9495909785,0.0619163236,1.3322344304
H,0,-3.6498154675,2.2544559318,-1.5289738035
H,0,-3.606089787,2.4672339432,0.238234833
C,0,-2.2163208244,-0.2011687467,0.1516754213
C,0,-0.8700960277,-0.4192366017,0.9325344544
H,0,-0.4464711775,-1.406942679,0.7753078547
H,0,-1.0717545211,-0.308978103,2.0046190541
C,0,0.0460357948,0.7311198795,0.5122764304
C,0,1.4413029403,0.8446071957,0.7726546991
H,0,1.8773002242,1.8392116047,0.8407237395
C,0,-3.4037750071,-0.1513879383,1.1027329442
O,0,-3.3356497218,0.1261926128,2.2769466089
O,0,-4.5468657574,-0.3625971277,0.4480732101
C,0,-2.3897737245,-1.2977721335,-0.897609527
O,0,-2.3514895939,-1.1279362067,-2.0910590091
O,0,-2.5266651799,-2.4869437757,-0.3075179697
C,0,-5.7393861374,-0.2587545925,1.2294378392
H,0,-6.5575860732,-0.4549787768,0.5382857043
H,0,-5.7296327447,-0.9947113866,2.0363617217
H,0,-5.8275776951,0.7430386893,1.6564658829
C,0,-2.5691968883,-3.6111590581,-1.1916536078
H,0,-2.6676604539,-4.4838918641,-0.5478376377
H,0,-3.4226062191,-3.5297172187,-1.8684091124
H,0,-1.6447191925,-3.6627059592,-1.7716465288
H,0,-1.372632966,1.91508917,1.3967622197
H,0,-1.5670422746,0.991203252,-1.4936458173
Pt,0,1.2902837308,0.2932128618,-1.2232096766
I,0,1.4590213092,2.5415371429,-2.5371396247
I,0,1.7327890285,-2.2969767403,-0.8770311274

36
1C-a4-IN1,Free Energies= -984.812515
C,0,-1.4465996798,-1.9921006503,2.4762006602
O,0,-0.9846101629,-0.7955702895,3.0672122284
C,0,-1.2305021792,0.2307906729,2.1321516707
C,0,-2.5503109332,-0.1321603805,1.4072646657
C,0,-2.7786462802,-1.6084936742,1.824727562
H,0,-0.7272064449,-2.3549218521,1.7251544645
H,0,-1.536836166,-2.7462778747,3.2604968327
H,0,-1.2859681686,1.1787986136,2.6673811811
H,0,-3.5845954076,-1.6604251516,2.5612656663
H,0,-3.0497434408,-2.2670486167,0.9940512604
C,0,-2.5654879396,0.1011752274,-0.130165031
C,0,-1.5887363051,-0.7861327478,-0.9585925614
H,0,-2.0207182493,-0.946898155,-1.9504789934
H,0,-1.4823583667,-1.7720168818,-0.5010678293
C,0,-0.2541394292,-0.2292707881,-1.2363082296
C,0,0.6732223363,0.2765571783,-1.9221353288
H,0,1.0988230326,0.7915591743,-2.7645722
C,0,-4.0196820524,-0.1787197238,-0.5499043455
O,0,-4.9306454997,0.5648307056,-0.2814312629
O,0,-4.1701118457,-1.3457913134,-1.1830665001
C,0,-2.3391077864,1.5651702922,-0.5398271816
O,0,-2.2497787533,1.8998040726,-1.6981882583
O,0,-2.2529199366,2.3919715351,0.4935840034
C,0,-5.5155084003,-1.680045374,-1.5412973734
H,0,-5.4506750858,-2.643613886,-2.0443724492
H,0,-6.1372239802,-1.7500740432,-0.6461220478
H,0,-5.9269796765,-0.9203221966,-2.2088923385
C,0,-2.0367200052,3.7697105342,0.1678113334
H,0,-2.0105157401,4.2902574464,1.1236186352
H,0,-1.0861094559,3.8834912125,-0.3573768187
H,0,-2.8528041666,4.1391853883,-0.4564480187
H,0,-0.3983083396,0.3000651847,1.4186589147
H,0,-3.3563858747,0.4892951056,1.80178498
Pt,0,1.5601513947,-0.1887273897,-0.1363542979
I,0,1.7807266021,-2.8091862977,-0.2639692268
I,0,1.9135593864,2.372174943,0.381811234

36
1C-a4-TS1,Free Energies= -984.788207
C,0,-1.6001513033,-2.3065462674,2.1383120037
O,0,-1.0356713912,-1.0814621428,2.5807082084
C,0,-1.5350131643,-0.1004302819,1.7500270403
C,0,-2.9736269014,-0.4680774963,1.3668408693
C,0,-3.0563561909,-1.9565701046,1.7980393927
H,0,-1.0427968793,-2.6647152348,1.2588650167
H,0,-1.4884042578,-3.0364937263,2.9403598388
H,0,-1.3734332822,0.8864817055,2.1831715916
H,0,-3.6838558861,-2.046058398,2.6875881114
H,0,-3.4757096471,-2.6150743691,1.0312519187
C,0,-3.2487230224,-0.2159175283,-0.1334223279
C,0,-2.2368411384,-0.976421926,-1.0194629149
H,0,-2.4891228183,-0.7733267146,-2.0723237643
H,0,-2.2989970661,-2.0565963328,-0.8636887243
C,0,-0.8708323027,-0.502876953,-0.9037548774
C,0,0.3590449954,-0.2511359115,-1.1775804727
H,0,0.6564234315,-0.2067260934,-2.2320864158
C,0,-4.694169837,-0.6331742172,-0.4223391995
O,0,-5.6373516554,-0.0969381568,0.1029343818
O,0,-4.7817718786,-1.6512271249,-1.279502007
C,0,-3.160133499,1.2666268373,-0.5475280926
O,0,-3.2500620793,1.6029330867,-1.704417905
O,0,-2.9551508066,2.0835658274,0.4728272938
C,0,-6.1138437232,-2.0864195259,-1.5820165978
H,0,-5.9991320253,-2.893329556,-2.3038119382
H,0,-6.6083267511,-2.4431233642,-0.6760130734
H,0,-6.6895164418,-1.2628247153,-2.0085794632
C,0,-2.7834139357,3.4696531157,0.1365400546
H,0,-2.6124487316,3.9754328773,1.0846649292
H,0,-1.9192084221,3.5837487811,-0.5204562667
H,0,-3.6820359175,3.8477639921,-0.3545460998
H,0,-0.9253077717,-0.0870826134,0.7908090357
H,0,-3.684159623,0.141191419,1.9276313587
Pt,0,1.7587121035,0.0298008257,0.1222334355
I,0,2.4276005778,-2.5202132675,0.2144731573
I,0,1.3419122425,2.6244495544,0.4000245019

36
1C-a4-IN2,Free Energies= -984.866034
C,0,-2.2920511818,-2.5401349237,1.7437853703
O,0,-0.9153707104,-2.4091732896,1.4095920538
C,0,-0.5844790785,-1.0688159568,1.1065818379
C,0,-1.8837023929,-0.2335242884,1.2238682026
C,0,-2.7674618312,-1.1331581349,2.0966481113
H,0,-2.8486654769,-2.9445290949,0.8898104666
H,0,-2.371948407,-3.2419947084,2.5783671944
H,0,0.2038692415,-0.735560162,1.7886195843
H,0,-2.5479159834,-0.912966607,3.1459565947
H,0,-3.8393860997,-0.9914168773,1.9437853925
C,0,-2.3379835783,0.0546159498,-0.2599377487
C,0,-1.4805192822,-0.88676962,-1.1289125584
H,0,-1.3853792306,-0.5245539645,-2.1541469599
H,0,-1.9284445642,-1.8814108995,-1.1452960855
C,0,-0.1475974305,-0.9678565156,-0.3711814056
C,0,0.7999966177,0.1208776959,-0.7047273826
H,0,0.7580525616,0.5529396606,-1.7101731082
C,0,-3.8345377342,-0.1278949159,-0.5246695579
O,0,-4.6247977133,0.7665225889,-0.6965192579
O,0,-4.1743506403,-1.4242043249,-0.5691299086
C,0,-2.0055923096,1.5129243729,-0.6172635841
O,0,-1.3479887317,1.8309466239,-1.5859338605
O,0,-2.5079809044,2.3702076754,0.2553448404
C,0,-5.5591326296,-1.6866388954,-0.8087845072
H,0,-5.6532805313,-2.7716831864,-0.815472458
H,0,-6.1732026256,-1.2501569185,-0.0175659745
H,0,-5.8639650031,-1.267030534,-1.7698713769
C,0,-2.3202172359,3.7565588247,-0.0470548217
H,0,-2.7641248915,4.295481241,0.7882500249
H,0,-1.2561470962,3.9853582584,-0.1315841837
H,0,-2.8298779828,4.0030792433,-0.9809781984
H,0,0.4169122092,-1.8794698954,-0.6349522264
H,0,-1.7006620463,0.7191666191,1.7211055209
Pt,0,2.1260595307,0.7438940152,0.3643555291
I,0,3.9934575095,-0.9890865328,-0.2526657622
I,0,1.0774496528,2.7072234765,1.7463522031

36
1C-a4-TS2,Free Energies= -984.830371
C,0,-2.1543207183,-2.6244787895,1.377472071
O,0,-0.7823476899,-2.3572099511,1.0851811293
C,0,-0.5524679528,-0.9616675395,0.9822303249
C,0,-1.9049585073,-0.2466625317,1.2023438899
C,0,-2.7034394996,-1.3238834795,1.9513131634
H,0,-2.6857377094,-2.9130445854,0.4616277416
H,0,-2.1827946294,-3.462434755,2.077465039
H,0,0.2477213337,-0.6655430671,1.6618008768
H,0,-2.4678987623,-1.2509855796,3.0171690042
H,0,-3.7861356927,-1.2231942966,1.8436249827
C,0,-2.4071358996,0.1424385253,-0.2425393501
C,0,-1.518804591,-0.6603254882,-1.2234695855
H,0,-1.451666001,-0.1902009025,-2.2042691608
H,0,-1.8982480395,-1.6813565028,-1.3234035058
C,0,-0.234087371,-0.6692218161,-0.4658746723
C,0,1.0374470313,-0.4492200103,-0.9959370256
H,0,1.0773799515,-0.2167592636,-2.06265128
C,0,-3.905847896,-0.1159106548,-0.4116980147
O,0,-4.7605037996,0.662520134,-0.0717067755
O,0,-4.1579994254,-1.3185921195,-0.9395895928
C,0,-2.2063824597,1.6449500997,-0.5447052223
O,0,-1.9379069898,2.0473244001,-1.6515618983
O,0,-2.3937750072,2.4083714614,0.5179760994
C,0,-5.5455047544,-1.6480264721,-1.0781485921
H,0,-5.5648332977,-2.6472354238,-1.5100247906
H,0,-6.03565688,-1.6376075143,-0.1020288398
H,0,-6.0385776998,-0.9298877547,-1.7361396374
C,0,-2.2540896835,3.8181835286,0.2998805051
H,0,-2.4277223381,4.2775057497,1.2713009628
H,0,-1.2472925903,4.0402067522,-0.0601672004
H,0,-2.9935288738,4.1560164394,-0.4290483426
H,0,0.92537254,-1.6397784346,-0.913986903
H,0,-1.7968681607,0.6585353595,1.7963583841
Pt,0,2.6073965984,0.0495325463,0.0384529569
I,0,3.9287106862,-2.162624549,-0.5311939572
I,0,1.5093017785,2.3056074853,0.8860522154

36
1C-a4-P,Free Energies= -984.880462
C,0,2.6097385982,2.7974179142,-0.2764580572
O,0,1.2111979331,2.8230026412,-0.551341664
C,0,0.5243651102,1.8575623221,0.2421745987
C,0,1.5949098312,1.0851687565,1.0368671035
C,0,2.74096444,2.1038111054,1.074357834
H,0,3.1387795073,2.2447382492,-1.0659794687
H,0,2.9694464175,3.8295098091,-0.2772238615
H,0,-0.2114773656,2.3709082383,0.8592225441
H,0,2.5463139461,2.8173602789,1.8815090937
H,0,3.7216547734,1.658966477,1.2504398374
C,0,1.8507870941,-0.232782219,0.2169524998
C,0,1.0937204457,-0.0284808486,-1.119864565
H,0,0.8359668859,-0.9623469,-1.6155583569
H,0,1.7240478302,0.5475475539,-1.8066703901
C,0,-0.0669522661,0.8656594518,-0.7519594733
C,0,-1.1958386054,1.1670658416,-1.570964307
H,0,-1.2769409369,0.7244489417,-2.5613892021
C,0,3.3416201916,-0.5271229344,0.0684102101
O,0,4.0501294049,-0.8086707017,1.0042780291
O,0,3.7814062078,-0.400290829,-1.1866530589
C,0,1.2798632861,-1.5029665046,0.8689233411
O,0,1.5623375942,-2.6065385755,0.4736070287
O,0,0.4117984975,-1.2594223536,1.8528673037
C,0,5.1755035398,-0.6608376128,-1.373301878
H,0,5.3604969235,-0.5088396452,-2.4356800687
H,0,5.7737015712,0.0278912717,-0.7721977452
H,0,5.4081005445,-1.687469438,-1.0833508224
C,0,-0.2232191385,-2.4151714589,2.4142286078
H,0,-0.926106642,-2.0262784248,3.1494805153
H,0,-0.7430676411,-2.9730191232,1.631160285
H,0,0.5215685292,-3.0596413097,2.8853486075
H,0,-1.6913590803,2.127553601,-1.4429879871
H,0,1.2491305757,0.8333217436,2.0374087751
Pt,0,-1.8683081796,-0.1506335914,-0.114975071
I,0,-1.8765747248,-2.2670385509,-1.681573069
I,0,-2.7296930987,1.3962088239,1.8312898313

(16). In Path 1C-*b*

36
1C-a1-IN1,Free Energies= -984.817336
C,0,-1.5898045475,3.4140019074,-0.4700895008
O,0,-0.8568844794,2.5386420002,-1.3067836958
C,0,-1.803113105,1.6314577344,-1.8406164339
C,0,-2.6995336888,1.2463036363,-0.6549731825
C,0,-2.7171373088,2.5651278269,0.1616434706
H,0,-0.8958515836,3.8358346084,0.2612162808
H,0,-2.0103636826,4.2378560464,-1.0651729285
H,0,-2.412844284,2.1251296366,-2.6134219231
H,0,-3.6861755719,3.0614303735,0.0698047961
H,0,-2.5448842797,2.3974823632,1.2291346277
C,0,-2.1960082503,0.0286906776,0.1668337739
C,0,-0.7604489852,0.1740754904,0.7294890018
H,0,-0.5895569578,-0.5997519814,1.4802136591
H,0,-0.6533733817,1.1406756852,1.2311675021
C,0,0.3291614804,0.0910677562,-0.2549572382
C,0,1.3157418934,0.4153786445,-0.9665558558
H,0,1.9567202759,1.1022217473,-1.4886821177
C,0,-3.2073793565,-0.1455365701,1.3145708443
O,0,-4.3596649059,-0.4493917915,1.1244658159
O,0,-2.6896329151,0.1085230385,2.5181249607
C,0,-2.2953395488,-1.3087811956,-0.5890712535
O,0,-1.8446654529,-2.33665773,-0.1366153375
O,0,-2.9390371263,-1.214851952,-1.7440127989
C,0,-3.5936649583,-0.0381277638,3.6185346619
H,0,-3.0073131254,0.1864930038,4.5081372664
H,0,-4.4291030521,0.6580247483,3.5170559372
H,0,-3.9766614453,-1.0597822006,3.6556955511
C,0,-3.1212981251,-2.4490713804,-2.4498325973
H,0,-3.6239613628,-2.1798686524,-3.3771615898
H,0,-2.1537201783,-2.9088262931,-2.6571331855
H,0,-3.7376309521,-3.1269860132,-1.8554086928
H,0,-1.2681414275,0.8022072764,-2.3036030333
H,0,-3.702250401,0.9893580933,-0.9982944511
Pt,0,1.2105979428,-1.6236509087,-1.1334922605
I,0,0.5673586537,-1.4678279957,-3.6937582632
I,0,2.1658518636,-2.3844874668,1.1960321506

36
1C-b-TS1,Free Energies= -984.787540
C,0,-2.1211808442,-1.3731095083,3.0540536291
O,0,-1.2914174891,-0.4793193066,2.3241125667
C,0,-2.1026269152,0.638313396,1.9995368214
C,0,-3.4187538846,0.0133135469,1.5254581116
C,0,-3.5622394821,-1.1508968206,2.5329988167
H,0,-1.7404774484,-2.3845262566,2.8866298307
H,0,-2.0478485549,-1.1525902203,4.1267449464
H,0,-2.2809395542,1.256355795,2.8915694721
H,0,-4.2329800718,-0.8562566233,3.343137249
H,0,-3.9933872294,-2.0503075367,2.0856250755
C,0,-3.370647928,-0.4641787645,0.0545277978
C,0,-2.275752254,-1.5267794482,-0.2279677151
H,0,-2.4179762826,-1.947877457,-1.2272394079
H,0,-2.3433743014,-2.3636573914,0.4735980436
C,0,-0.9214329031,-0.9908011751,-0.1681243728
C,0,0.1616843137,-0.3915848963,-0.3274773888
H,0,-0.3234343651,-0.4245542654,-1.4034608665
C,0,-4.7523210893,-1.0412585049,-0.3181198641
O,0,-5.7443693269,-0.9336923554,0.3570177986
O,0,-4.7169145569,-1.6542077919,-1.5048688291
C,0,-3.1284161686,0.6971836834,-0.9302405232
O,0,-2.4289117012,0.6018347302,-1.9131428689
O,0,-3.7875751409,1.792046558,-0.5811867407
C,0,-5.9653892892,-2.1811053342,-1.9677995973
H,0,-5.7507154245,-2.6276641784,-2.9372187608
H,0,-6.3417339577,-2.931666084,-1.2693262971
H,0,-6.6997892736,-1.3788153928,-2.0650237488
C,0,-3.5732151376,2.9379954043,-1.4209155114
H,0,-4.1725804258,3.7323517773,-0.9799950404
H,0,-2.5134079957,3.2021531422,-1.4216089174
H,0,-3.9001592167,2.7226169253,-2.4401406471
H,0,-1.5678954306,1.2452995411,1.2664651148
H,0,-4.2501331059,0.7121277767,1.6121618356
Pt,0,1.7796624925,0.5321159194,-0.0820306179
I,0,0.6865443659,2.9437095738,-0.1484968872
I,0,3.2622523672,-1.6320682177,0.0530431826

36
1C-b-IN1,Free Energies= -984.826020
C,0,-0.741657453,-2.5402746746,2.2110823691
O,0,-0.0965114636,-1.2731660745,2.4304192947
C,0,-0.6274820885,-0.322690048,1.5954447208
C,0,-1.9630770745,-0.8295865497,1.0800224619
C,0,-1.6895845673,-2.3405772105,1.0252866103
H,0,0.0312572972,-3.2876234624,2.0208417502
H,0,-1.2777775271,-2.7993074831,3.130358274
H,0,-0.6107097518,0.6620598889,2.0709774557
H,0,-2.6053117827,-2.9276040269,1.1082448935
H,0,-1.1778706676,-2.6186781046,0.0989606942
C,0,-2.4107179421,-0.1373038391,-0.2261760446
C,0,-1.7106798347,-0.6154401897,-1.514411844
H,0,-2.0517821438,0.0237108358,-2.3319448669
H,0,-2.0554035165,-1.631215632,-1.7454919344
C,0,-0.2053634952,-0.643120657,-1.5734858619
C,0,0.7736157314,-0.5337935913,-0.7188154226
H,0,0.2157093265,-0.8382883585,-2.5653230912
C,0,-3.9128408915,-0.4080210891,-0.4175091199
O,0,-4.5611943672,-1.1943400177,0.226721475
O,0,-4.405983169,0.3323457924,-1.4140641884
C,0,-2.2319552316,1.385614406,-0.1048608595
O,0,-1.6274997356,2.0747730913,-0.8854239101
O,0,-2.837748458,1.8449266836,0.9960709529
C,0,-5.8000156718,0.1566941793,-1.6853079915
H,0,-6.0212625314,0.8240822366,-2.5166231283
H,0,-6.0059000805,-0.8811804009,-1.9564144188
H,0,-6.3910006565,0.4234213921,-0.8064016196
C,0,-2.7100376934,3.2529965444,1.2233604267
H,0,-3.2454835956,3.4478129366,2.1512838012
H,0,-1.6563599716,3.524900527,1.3202725584
H,0,-3.1512682429,3.8116320502,0.3952718021
H,0,0.0571134797,-0.1845736764,0.6819843746
H,0,-2.7248874387,-0.6327838042,1.8399326538
Pt,0,2.4799429317,-0.6071516139,-0.078300531
I,0,2.8050945036,1.9839173157,0.2293665847
I,0,2.6345454237,-3.2306402056,-0.2168097112

36
1C-b-TS2,Free Energies= -984.808055
C,0,-0.2712683849,-1.0752538153,2.6729892883
O,0,-0.0495735499,0.2915170706,2.3764247447
C,0,-1.2997462967,0.8309353447,2.0113011833
C,0,-2.1142829486,-0.3156590693,1.3431769991
C,0,-1.2293843396,-1.5563482126,1.5842430734
H,0,0.6962301518,-1.5814045803,2.6635697551
H,0,-0.7224268547,-1.1800195992,3.6729264604
H,0,-1.833966716,1.1853683446,2.9053529187
H,0,-1.8202270096,-2.4254907084,1.8762040866
H,0,-0.6531354268,-1.8313690996,0.6973987083
C,0,-2.5412493212,-0.061445516,-0.1281695383
C,0,-1.4159458654,-0.1353533121,-1.1921564302
H,0,-1.8461479974,0.1142270285,-2.1647794715
H,0,-1.0392009519,-1.1592832165,-1.2534059314
C,0,-0.2676664873,0.816793574,-0.9449756149
C,0,0.9043930742,0.4336492661,-0.5503968511
H,0,-0.4271425276,1.8864746941,-1.0805694025
C,0,-3.5907496608,-1.1144372167,-0.5218853875
O,0,-3.8838203461,-2.0867597731,0.1263574619
O,0,-4.1331701769,-0.8171212445,-1.709781561
C,0,-3.214687514,1.3121008528,-0.2131854937
O,0,-2.8131271183,2.2464818801,-0.8668312636
O,0,-4.2980565594,1.3628508337,0.5651184955
C,0,-5.1213365748,-1.7364730779,-2.1830636521
H,0,-5.4612951522,-1.3356128112,-3.1368176552
H,0,-4.6831699285,-2.7282934584,-2.3155347707
H,0,-5.9488381792,-1.8011408587,-1.4729950234
C,0,-4.9866577044,2.6164998924,0.5886770598
H,0,-5.8117491497,2.4820302541,1.2862551911
H,0,-4.3170643526,3.4092768738,0.929523591
H,0,-5.3593987602,2.8633938256,-0.4079037768
H,0,-1.1143963163,1.6935926833,1.3659281027
H,0,-3.0484952603,-0.441230606,1.8944837324
Pt,0,2.4961202124,-0.1077454104,0.0190709117
I,0,3.5848673149,2.2148285796,0.5324021425
I,0,2.2830904886,-2.7094024922,-0.2500673527

(17). In Path 1D-*a*

38
1D-IN1,Free Energies= -1007.688633
C,0,5.0282616096,2.6064724365,-1.6565352149
O,0,4.1068414463,2.7282873559,-0.5876243195
C,0,4.4689853984,1.7606041988,0.3725631101
C,0,5.0963932515,0.5612361622,-0.3956651077
C,0,5.2362104091,1.1004528433,-1.8352074294
H,0,4.5889992669,3.0901326718,-2.5314515814
H,0,5.9743599389,3.1109817317,-1.4032382672
H,0,5.2134783174,2.1750070082,1.0684163426
H,0,6.2048139595,0.846800078,-2.2694308439
H,0,4.4594848752,0.7121848928,-2.4987969109
C,0,4.3401012222,-0.7861162685,-0.2541199821
C,0,3.0531006375,-0.9495021494,-1.1100888065
H,0,2.4954930455,-1.8179371527,-0.7510593782
H,0,3.3333212525,-1.1384236816,-2.1530497244
C,0,2.1814461164,0.2244201587,-1.0830766358
C,0,1.5650253953,1.2834995175,-1.0410640268
H,0,1.2640147678,2.2866763907,-0.8190554535
C,0,5.2778024693,-1.9305458478,-0.6736157393
O,0,6.3716362382,-1.793873668,-1.1592129633
O,0,4.6976275361,-3.1136184393,-0.4458920165
C,0,3.9686554556,-0.996291854,1.2178349378
O,0,2.844007978,-1.0650798622,1.646306469
O,0,5.0685731664,-1.0542385333,1.9746552156
C,0,5.4683301562,-4.2634676702,-0.8088113194
H,0,4.8476359695,-5.1212105158,-0.5548928545
H,0,5.6903880554,-4.249020444,-1.8781590795
H,0,6.4040830437,-4.2817434284,-0.2459945331
C,0,4.8418650519,-1.2228728942,3.3774484322
H,0,5.8306683685,-1.2384100038,3.8333182514
H,0,4.2486649531,-0.3926406071,3.767008959
H,0,4.3149065672,-2.1611009347,3.5643613851
H,0,3.5722158457,1.5105391324,0.9477338344
H,0,6.0913193978,0.3733021506,0.0110141077
Pt,0,0.3812031888,0.1221744314,-2.6312580353
I,0,-1.0577947049,-0.9959192505,-4.5292490274
I,0,-0.8806268541,-1.3223317439,-0.7610957595
I,0,-1.4295573732,2.0902374869,-2.523749147
I,0,1.9725644204,1.2695524921,-4.469534208

38
1D-a-TS1,Free Energies= -1007.671522

C	2.836397804	-2.52336571	-2.09880198
O	3.097898954	-1.42967156	-2.99397979
C	3.591277695	-0.36549648	-2.29191771
C	4.270397832	-0.86414785	-1.02030109
C	3.634732652	-2.25668029	-0.81063614
H	1.760963863	-2.57483671	-1.90056679
H	3.143240223	-3.43218871	-2.61988765
H	4.180816364	0.28292339	-2.94676739
H	4.411215949	-3.00247837	-0.64018486
H	2.970479316	-2.27903397	0.05676425
C	4.063422329	0.14966641	0.12417713
C	2.559589750	0.41887672	0.40773743
H	2.438205169	1.42695214	0.81101498
H	2.189382755	-0.30244558	1.14788116
C	1.689904143	0.24798805	-0.76304223
C	0.593921105	-0.04374566	-1.34050716
H	0.411497060	-0.19781776	-2.39753543
C	4.740957126	-0.34617453	1.40385299
O	5.376554899	-1.36495785	1.49902027
O	4.516805315	0.50894406	2.40353776
C	4.717771618	1.47087931	-0.30645447
O	4.112389742	2.41672731	-0.74759305
O	6.043296640	1.40668933	-0.18930243
C	5.089845892	0.15139483	3.66671925
H	4.804613682	0.94841094	4.35121511
H	4.691360585	-0.80797700	4.00343816
H	6.176404563	0.08338643	3.58062198
C	6.761932359	2.57343990	-0.60863551
H	7.812241854	2.34385790	-0.43796730
H	6.575409448	2.77212686	-1.66624227
H	6.452312136	3.43818288	-0.01832054
H	2.726423280	0.34012891	-1.96096843
H	5.346102856	-0.95997316	-1.18671362
Pt	-1.064384859	-0.16263476	-0.04501407
I	-3.105598500	-0.15322850	1.66248312
I	-1.647443592	2.30673963	-0.88593234
I	-2.469721655	-1.42815219	-1.90687015
I	-0.090014368	-2.43103234	1.05084489

38
1D-a-IN2,Free Energies= -1007.755610
C,0,3.3423717262,-2.6079539984,-2.4276121096
O,0,2.3817027878,-1.5770676015,-2.6153100216
C,0,2.8794413497,-0.3715736165,-2.0632127034
C,0,4.111848082,-0.7395079458,-1.1911851417
C,0,4.0138225099,-2.272328733,-1.1052482224
H,0,2.8112746357,-3.5622197528,-2.429520745
H,0,4.0656166964,-2.6048331181,-3.2566292263
H,0,3.1267597812,0.3202530857,-2.8767063087
H,0,4.9876055265,-2.7421407118,-0.9702453843
H,0,3.3727945394,-2.5829100845,-0.2736829976
C,0,3.9177542654,0.0333596333,0.1317849626
C,0,2.3911366572,0.0719991577,0.319083878
H,0,2.0725632476,0.855736442,1.0069273862
H,0,2.045787761,-0.8876365898,0.7206807519
C,0,1.8433847734,0.3072316713,-1.1045285273
C,0,0.4792969307,-0.2780175138,-1.279564694
H,0,0.4683463794,-1.3618609492,-1.3634828267
C,0,4.6375123876,-0.5820965517,1.3282507428
O,0,5.4141627943,-1.5038930489,1.2978178405
O,0,4.2805583352,0.0603027025,2.4467646786
C,0,4.4617198582,1.4559835515,-0.0511963338
O,0,3.7990638711,2.4324031175,-0.3022244039
O,0,5.7945267623,1.4676298673,0.0572808787
C,0,4.906278255,-0.3959913986,3.6477078306
H,0,4.4811217115,0.2096408244,4.4466509328
H,0,4.6932944212,-1.4548692699,3.809998671
H,0,5.9877119947,-0.2520354367,3.5875266454
C,0,6.4186178559,2.7409059307,-0.1254197354
H,0,7.4877330112,2.559030722,-0.0260892854
H,0,6.1855736751,3.1407513707,-1.1148792032
H,0,6.0739220291,3.4449231506,0.6352835308
H,0,1.837583841,1.3817782277,-1.2866145237
H,0,5.0508980635,-0.4618751579,-1.6772100077
Pt,0,-1.063765612,0.3916092537,-0.1701246638
I,0,-0.4651125268,2.9968471724,0.0789105602
I,0,-0.6844373884,0.4646992388,-2.9836489725
I,0,-2.2940607987,-1.9959972284,-0.345311728
I,0,-0.7847828603,0.0591623278,2.4170292967

38
1D-a-TS2,Free Energies= -1007.725415
C,0,2.5354202261,3.2139786068,-2.7271902924
O,0,1.5064491146,2.8803809894,-1.7985665654
C,0,2.1170257438,2.3996405113,-0.6265231838
C,0,3.5574491594,1.9408181868,-0.986143869
C,0,3.6118920674,2.1562590962,-2.5100477102
H,0,2.0904486125,3.20167514,-3.7230028576
H,0,2.915054462,4.2237481436,-2.5168805784
H,0,2.0831077755,3.141556957,0.1788617468
H,0,4.60335282,2.4617669905,-2.8466281984
H,0,3.3407177863,1.2419788659,-3.0497536768
C,0,3.6404405098,0.4593370954,-0.5399862264
C,0,2.1902288475,-0.0524635149,-0.714089912
H,0,1.9716913662,-0.9932349375,-0.2093114464
H,0,1.9516712942,-0.1891963711,-1.7751953231
C,0,1.3805131706,1.1123768309,-0.2405139846
C,0,0.1769495792,1.1641285804,0.4342045363
H,0,-0.1976496771,2.1635173764,0.654422269
C,0,4.6989836761,-0.3214660175,-1.3045827341
O,0,5.7694004299,0.1429548016,-1.6130903084
O,0,4.2937099729,-1.5581446106,-1.5818062349
C,0,3.9052834277,0.403741317,0.9657324587
O,0,3.3422535761,1.159135372,1.7354846142
O,0,4.7205175577,-0.5657618832,1.3289638021
C,0,5.2431636344,-2.3880802454,-2.2595279898
H,0,4.75349983,-3.3536099876,-2.3729051655
H,0,5.4895963663,-1.9604910743,-3.2339503786
H,0,6.153545101,-2.4805394891,-1.6637688621
C,0,4.8862539817,-0.7486120872,2.7466515508
H,0,5.5634074424,-1.5940126866,2.8489661294
H,0,5.3147609091,0.1518174415,3.1902049663
H,0,3.9177951058,-0.9632654084,3.2030677071
H,0,1.3050304392,1.1167220508,1.0969888846
H,0,4.3083396946,2.5490763824,-0.4802919934
Pt,0,-1.0013748654,-0.3082673828,0.9646836693
I,0,0.7511569388,-1.9643004308,2.2141219676
I,0,-1.384143892,0.9668176703,3.324456077
I,0,-3.0494589139,1.0730240589,-0.1253855838
I,0,-0.9327063306,-1.8575749072,-1.2436986243

38
1D-P,Free Energies= -1007.738960
C,0,2.0600829219,3.4426615408,-0.2943682073
O,0,1.1048374928,2.4348652067,-0.0132999025
C,0,1.6096875493,1.6604832672,1.0409023027
C,0,3.1703115279,1.704404368,0.905879272
C,0,3.3908251802,2.7014462756,-0.2494021337
H,0,1.8111732831,3.8651460799,-1.2686411327
H,0,2.0129889362,4.2381297042,0.4641357301
H,0,1.2516481393,2.0371879331,2.0066005304
H,0,4.2561839569,3.3449299777,-0.0805212062
H,0,3.5354300108,2.1764523558,-1.2002352897
C,0,3.6182136449,0.2510808029,0.5923072594
C,0,2.356506579,-0.407039525,-0.0225588331
H,0,2.3897087885,-1.4951698024,-0.0294392899
H,0,2.2232072418,-0.0589125723,-1.0482664166
C,0,1.2993854796,0.1756992053,0.8891807635
C,0,0.8014171932,-0.5578380993,2.0101853474
H,0,0.5452787589,-0.0168531999,2.9168930509
C,0,4.8640908566,0.2315653567,-0.2848675184
O,0,5.8959320333,0.7638655293,0.0458357624
O,0,4.6755605148,-0.4064017497,-1.4386432106
C,0,3.939758324,-0.4907995123,1.8913176259
O,0,3.5528012792,-0.1486388756,2.9851610902
O,0,4.626501061,-1.6054867298,1.6532338478
C,0,5.8135881349,-0.4612820188,-2.3044194152
H,0,5.4831102827,-1.0082378028,-3.185855665
H,0,6.1352276856,0.54780865,-2.5716572625
H,0,6.6369994244,-0.9823259076,-1.8111812311
C,0,4.926296179,-2.4133749788,2.797130052
H,0,5.5116416997,-3.2483805197,2.4163150797
H,0,5.4997237636,-1.8378934626,3.5263430007
H,0,4.0030517552,-2.7700838056,3.2596714593
H,0,1.1092072151,-1.5911560114,2.1429432965
H,0,3.6326125257,2.0511506033,1.8297306382
Pt,0,-0.8200827294,-0.4661666484,0.597289799
I,0,-0.1859698617,-2.8613499143,-0.540638952
I,0,-1.935968651,-1.8531750126,2.6326811012
I,0,-1.9149313904,1.7733398373,1.645009806
I,0,-0.9666467867,0.6007694551,-1.8267611487

(18). In Path 1D-*b*

38
1D-b-TS1,Free Energies= -1007.670293
C,0,-2.9351080218,-2.7541869409,1.9114282767
O,0,-3.0973828521,-1.6264181798,2.7672422592
C,0,-3.2725092283,-0.487526565,1.9649502736
C,0,-4.1515488429,-0.9882159405,0.8071536958
C,0,-3.5515535098,-2.379830792,0.5439184769
H,0,-1.8703865654,-2.9952557769,1.8031363682
H,0,-3.4400368584,-3.5977554981,2.3886273485
H,0,-3.7601164491,0.2800098657,2.5735022757
H,0,-4.3143276338,-3.086233687,0.2094236242
H,0,-2.7579924193,-2.3587131487,-0.2091309923
C,0,-4.3093594868,-0.0381174453,-0.4082069779
C,0,-3.2136561572,-0.1284183704,-1.498111743
H,0,-3.4117331488,0.5981247347,-2.2911180722
H,0,-3.2242093329,-1.1206029294,-1.9712694125
C,0,-1.8521004009,0.015736894,-1.0288380284
C,0,-0.6897462867,0.1545384272,-0.6101760249
H,0,-1.1577368649,1.2150548353,-0.411467966
C,0,-5.6475884633,-0.3220682374,-1.1117265857
O,0,-6.3899482286,-1.2329247144,-0.8524166263
O,0,-5.8615870643,0.5744949845,-2.0812527703
C,0,-4.3006161427,1.4028140468,0.1066442551
O,0,-3.3539253574,2.149045206,-0.0158914941
O,0,-5.4198559218,1.7038620172,0.7494968531
C,0,-7.0851981849,0.4193694548,-2.8100315295
H,0,-7.107968432,1.2450194046,-3.5194454729
H,0,-7.0949721318,-0.5396799599,-3.3324502467
H,0,-7.9365789978,0.4693496207,-2.1284571231
C,0,-5.4665014659,3.0044106115,1.3532807502
H,0,-6.4443161571,3.0675954186,1.8269689308
H,0,-4.6696136485,3.1020173241,2.0936285256
H,0,-5.3524801453,3.7779124556,0.5914292774
H,0,-2.3083665151,-0.0948079899,1.6140428866
H,0,-5.1579448531,-1.1238363764,1.2108577174
Pt,0,1.2095327272,-0.3018948147,-0.1215616683
I,0,3.7528979111,-0.9334699773,0.2530188934
I,0,1.707114759,2.3287477329,0.1427989262
I,0,0.6380293965,-0.7212529475,2.4403205497
I,0,0.5984239754,-2.8133707439,-0.9011174239

38
1D-b-IN2,Free Energies= -1007.688065
C,0,-3.4019368481,-2.6568049387,2.0527416305
O,0,-3.1394500362,-1.4834018676,2.8210850987
C,0,-3.4730109084,-0.3251184027,2.0786571427
C,0,-4.3183774588,-0.8247498764,0.8972690031
C,0,-3.6668936114,-2.1824306999,0.6272022545
H,0,-2.5392780817,-3.3264483078,2.1214885054
H,0,-4.2778772912,-3.1716773392,2.470064885
H,0,-4.0275981442,0.3625452917,2.7272771397
H,0,-4.3104293467,-2.8573905148,0.0597561181
H,0,-2.7162718486,-2.0696782167,0.0957985985
C,0,-4.4804481655,0.1324008491,-0.3068760338
C,0,-3.2883506812,0.1974379778,-1.2942574944
H,0,-3.5548990357,0.8834397239,-2.1030174326
H,0,-3.1221694426,-0.7894612385,-1.7316335399
C,0,-1.9984368208,0.7090727234,-0.7027871649
C,0,-0.8361924149,0.1560943347,-0.6682878211
H,0,-2.0126266125,1.7140484339,-0.2624683267
C,0,-5.6930764942,-0.3342119653,-1.1373924826
O,0,-6.3062857664,-1.3562911556,-0.9664726519
O,0,-5.9668065692,0.5515930348,-2.1024389306
C,0,-4.8030722682,1.533959464,0.2211286818
O,0,-4.0766598958,2.4976176006,0.1352385855
O,0,-5.9871854208,1.5496913422,0.8317788507
C,0,-7.0796524269,0.2278541288,-2.9413170958
H,0,-7.1187497626,1.0151855987,-3.6925051185
H,0,-6.9317924466,-0.747366178,-3.4099199904
H,0,-8.0004843587,0.2092906862,-2.3539602583
C,0,-6.3753715292,2.8021417125,1.4066935854
H,0,-7.3461621371,2.6225440334,1.8655143071
H,0,-5.6447474622,3.1160778389,2.1553597094
H,0,-6.4489714029,3.5663425572,0.6300134005
H,0,-2.5552922577,0.1794090235,1.7470291847
H,0,-5.3297816379,-1.010041883,1.2720828207
Pt,0,0.8947288246,-0.6227674394,-0.5077454572
I,0,3.3021095682,-1.746609942,-0.5629004416
I,0,1.8090847394,1.7211016853,0.4211142118
I,0,0.3657722023,-1.5613270655,1.9311545522
I,0,-0.2964589523,-2.583486357,-1.9573234187

38
1D-b-TS2,Free Energies= -1007.671414
C,0,2.6712718623,3.3099555782,0.9050546637
O,0,2.0034295862,2.3239432661,1.7062648283
C,0,2.3252697066,1.0591526475,1.2517756894
C,0,3.6411153537,1.1886267253,0.4998940468
C,0,3.4134422162,2.5389189775,-0.1901308992
H,0,1.9242258447,4.003181448,0.5106248628
H,0,3.3594287114,3.8591388081,1.5573085364
H,0,2.3114196588,0.3452630058,2.0786851459
H,0,4.343556074,3.0183569992,-0.4963614956
H,0,2.7620424862,2.4290068508,-1.0649833072
C,0,4.0263471606,-0.0223309421,-0.3718756982
C,0,3.1731237838,-0.2451736306,-1.6370228638
H,0,3.6326619064,-1.0535934107,-2.2054196054
H,0,3.2132710038,0.652798974,-2.2633007313
C,0,1.7243633446,-0.6167894144,-1.4424082066
C,0,0.7233677743,-0.2105529086,-0.7214313877
H,0,1.3372163204,-1.4141113232,-2.0898209181
C,0,5.4873035665,0.1690339548,-0.8282618733
O,0,6.1505865321,1.1570332726,-0.6384739062
O,0,5.9289893063,-0.9160127395,-1.4714614963
C,0,3.9945356087,-1.3148822271,0.4618319028
O,0,3.404754333,-2.3191208051,0.1518599839
O,0,4.7141237787,-1.1785816633,1.5788780818
C,0,7.2794330609,-0.8530242397,-1.9409063489
H,0,7.4656074886,-1.8134986559,-2.4187456228
H,0,7.3929315909,-0.0360397899,-2.6569360566
H,0,7.9641908497,-0.6973189877,-1.1045515468
C,0,4.7455144207,-2.3261688995,2.4346496287
H,0,5.3511779678,-2.0336762723,3.2909725916
H,0,3.7330940005,-2.5909459553,2.7478772046
H,0,5.1944751367,-3.1745832226,1.9135963822
H,0,1.5261616266,0.6987289044,0.5294356744
H,0,4.4353485657,1.3133720434,1.2428925002
Pt,0,-1.1589913352,0.0764233273,-0.3276428906
I,0,-3.8028667231,0.393701611,-0.2462761196
I,0,-1.4169838589,-2.6000639363,-0.5203757569
I,0,-1.0584598176,-0.0244419098,2.3360608473
I,0,-0.7959528923,2.7041795399,-0.7851068401

38
1D-b-IN3,Free Energies= -1007.751379
C,0,2.8538036277,3.2268919557,-0.2833993985
O,0,2.1530352922,2.4558397474,0.6895988798
C,0,2.6524416204,1.1575916107,0.6736270554
C,0,4.153426395,1.2760203374,0.3748021607
C,0,4.1783752747,2.4889230582,-0.5809086633
H,0,2.2353670959,3.3318607869,-1.1838542647
H,0,3.0026475771,4.2206032315,0.1444940331
H,0,2.4245239727,0.7044844729,1.6406665912
H,0,5.0585005897,3.107317828,-0.4059883526
H,0,4.2190754815,2.1727645737,-1.6273961534
C,0,4.5467117589,-0.0789886206,-0.2365198975
C,0,3.3294602404,-0.4542099011,-1.1190244242
H,0,3.2028508552,-1.5371443272,-1.1824352205
H,0,3.4861149464,-0.0977791247,-2.1405594106
C,0,2.0954810213,0.2735819808,-0.5112252958
C,0,1.0867371219,-0.711091719,-0.0239001381
H,0,1.6426951537,0.9471410599,-1.2411453974
C,0,5.8535923032,-0.0377989764,-1.0210279277
O,0,6.6177902131,0.8927717489,-1.0651143013
O,0,6.0354630639,-1.1934949927,-1.670708406
C,0,4.7814113699,-1.0601636411,0.9168729946
O,0,5.8571726337,-1.2572389865,1.4235922558
O,0,3.6432342229,-1.6250182539,1.3445558622
C,0,7.2666205528,-1.3054361532,-2.3884103074
H,0,7.2543395181,-2.2975573833,-2.8377540404
H,0,7.3304736346,-0.5336883967,-3.1590825505
H,0,8.1111787267,-1.2031222608,-1.7034406553
C,0,3.7534641501,-2.4713664725,2.4969098672
H,0,2.7346181945,-2.7837102303,2.7242508266
H,0,4.3859899591,-3.3318696539,2.2701083856
H,0,4.1828086995,-1.9145329199,3.3319908801
H,0,1.5142925303,-1.5004049258,0.5896504527
H,0,4.7259356409,1.4946207729,1.279343101
Pt,0,-0.6891323869,-0.1064971995,0.6946425287
I,0,-1.2677670297,1.9800096232,-0.8908314481
I,0,-0.1215579266,-1.7487408258,-1.5617780725
I,0,-0.7738454403,-2.2586499913,2.3188551273
I,0,-0.6103846026,1.4699377603,2.78135563

38
1D-b-TS3,Free Energies= -1007.713837
C,0,-2.4492413603,3.677194686,-0.6330801474
O,0,-1.5386700494,2.7490794702,-0.0485518611
C,0,-1.6490003166,1.5598799633,-0.8020631308
C,0,-3.1260480166,1.4702832211,-1.2960955163
C,0,-3.7017749838,2.8492927731,-0.8977640697
H,0,-2.5892463487,4.4887153444,0.0823260822
H,0,-2.021052529,4.0829992826,-1.5594976718
H,0,-0.9018603739,1.5117519891,-1.5966148821
H,0,-4.343892588,3.2605986294,-1.6771406607
H,0,-4.2980048809,2.7830703089,0.01631019
C,0,-3.7154511622,0.2454027344,-0.5424792737
C,0,-2.9058552392,0.197213628,0.7775419006
H,0,-3.0069143312,-0.7329753724,1.3318400022
H,0,-3.1917972915,1.0466790744,1.4071723817
C,0,-1.5379482446,0.4319072889,0.2037273173
C,0,-0.4356691134,-0.3282001023,0.572887921
H,0,-0.4803829154,0.7431915511,1.1789407612
C,0,-5.2268202447,0.3169972734,-0.3193180365
O,0,-5.9799675164,1.050848476,-0.9036068048
O,0,-5.5980361666,-0.5851692307,0.5943308138
C,0,-3.5099092679,-1.0220945667,-1.4034201693
O,0,-3.9423726024,-1.1105739143,-2.5238819194
O,0,-2.8384068778,-1.9722366738,-0.7599212508
C,0,-7.0075988821,-0.6714128918,0.8377256267
H,0,-7.1254400336,-1.4456474183,1.5940102411
H,0,-7.3886706333,0.285493905,1.2007504555
H,0,-7.5311328769,-0.943938846,-0.0810493867
C,0,-2.6193605305,-3.1906829925,-1.4935689465
H,0,-1.9537387878,-2.9947081654,-2.3358073361
H,0,-2.144866504,-3.8684154364,-0.7873541365
H,0,-3.5745325992,-3.5833942962,-1.8467577993
H,0,-0.6295535134,-1.0881419808,1.3274227486
H,0,-3.1858209056,1.3088569103,-2.3724775813
Pt,0,1.2944012661,-0.5462678291,-0.3454111007
I,0,1.999997662,2.0002458885,-0.8589963117
I,0,2.4668452896,-0.3330488339,2.0883567657
I,0,1.1314477388,-3.2333290496,-0.0236092329
I,0,0.3720951604,-0.8265683278,-2.8678216616

38
1D-P,Free Energies= -1007.738961
C,0,2.0600812327,3.4426608874,-0.2943703253
O,0,1.1048360902,2.4348646162,-0.0132998839
C,0,1.6096886172,1.6604825335,1.0409011823
C,0,3.1703125503,1.704405625,0.9058762885
C,0,3.3908240184,2.7014462703,-0.2494058742
H,0,1.8111697767,3.8651450338,-1.2686429577
H,0,2.0129882104,4.2381291318,0.4641334883
H,0,1.2516516633,2.0371868349,2.006600375
H,0,4.2561826323,3.3449305391,-0.0805261591
H,0,3.5354283067,2.1764511407,-1.2002384759
C,0,3.6182154528,0.2510830946,0.5923044116
C,0,2.356509562,-0.4070391851,-0.0225615376
H,0,2.3897148578,-1.4951692222,-0.029442628
H,0,2.2232095379,-0.0589116061,-1.0482687909
C,0,1.299388918,0.1756978955,0.8891790559
C,0,0.8014186891,-0.5578403233,2.0101828197
H,0,0.5452820977,-0.0168570287,2.9168920079
C,0,4.8640926513,0.2315689816,-0.2848697821
O,0,5.895932735,0.7638713712,0.045833277
O,0,4.6755649648,-0.4064053454,-1.4386416064
C,0,3.9397605306,-0.4907958293,1.8913151474
O,0,3.5528045737,-0.1486340449,2.9851584045
O,0,4.6265011394,-1.6054841923,1.6532308749
C,0,5.8135943464,-0.461286301,-2.3044147811
H,0,5.4831180691,-1.0082428409,-3.1858511049
H,0,6.1352347309,0.547804211,-2.5716521432
H,0,6.6370039942,-0.9823302935,-1.8111738384
C,0,4.9262907972,-2.4133724018,2.7971281876
H,0,5.5116267317,-3.2483847446,2.4163135529
H,0,5.4997260505,-1.8378943514,3.5263379585
H,0,4.0030436512,-2.7700699569,3.2596727921
H,0,1.1092067817,-1.5911590355,2.1429404856
H,0,3.6326145184,2.0511529568,1.8297268636
Pt,0,-0.8200839429,-0.4661680175,0.5972959895
I,0,-0.1859745466,-2.8613504554,-0.5406406525
I,0,-1.9359701724,-1.8531807838,2.6326806464
I,0,-1.9149295828,1.7733348334,1.6450277007
I,0,-0.966661235,0.6007770023,-1.8267509687

39
2D-a-IN1,Free Energies= -822.362207
C,0,-2.2571525491,5.5641446933,-0.4851026841
C,0,-3.3261722112,4.4581072079,-0.5609589465
C,0,-2.7268127919,3.0386866914,-0.5961664624
C,0,-1.4334042686,2.9928296443,0.2317671852
C,0,-0.3577362908,3.8953768584,-0.4312790352
C,0,-0.9661103721,5.1067414412,-1.1630393957
H,0,-2.631756695,6.4832912563,-0.9457079396
H,0,-3.9882772613,4.5042253998,0.3106590346
H,0,-1.6715402267,3.3744578595,1.2344538823
H,0,0.332631382,4.2419090962,0.3460576481
H,0,-1.1813960798,4.8428173921,-2.2059832999
H,0,-3.954341505,4.5941425334,-1.448981515
H,0,-2.0441068561,5.8075998892,0.5635473587
H,0,-0.2329044408,5.9186058447,-1.1947628767
H,0,0.2306423959,3.294798441,-1.1340621688
H,0,-2.4698911271,2.7605102711,-1.6327059427
O,0,-3.6238819839,2.0900397182,-0.0759858097
C,0,-4.6778849368,1.6996133823,-0.9308680849
H,0,-5.5520967666,2.3474794582,-0.766340949
C,0,-0.937151635,1.5889641662,0.389186174
C,0,-1.3569605329,0.4195840515,-0.0451676015
H,0,-4.3779169458,1.8209615882,-1.9833329743
H,0,-2.2554705602,0.2005008145,-0.6080204651
C,0,-5.0298086207,0.2516264264,-0.6707521044
C,0,-5.6880231879,-0.4886886667,-1.6543067098
C,0,-4.71036445,-0.3593066199,0.5428923097
C,0,-6.029169486,-1.8183854921,-1.4259859353
H,0,-5.9311783458,-0.0260752302,-2.6085639089
C,0,-5.0434429435,-1.6922076577,0.7672533776
H,0,-4.1805615285,0.203414054,1.3044776542
C,0,-5.7068775084,-2.4235405469,-0.2133044461
H,0,-6.5381064812,-2.3849887391,-2.2002786036
H,0,-4.7644227363,-2.1601465783,1.7061359042
H,0,-5.9625899121,-3.4640454008,-0.0373106689
Pt,0,-0.2202917064,-1.1317811767,0.4575039913
I,0,0.8915789568,1.2632779308,1.5313696299
I,0,-1.4362740206,-1.6324495923,2.7939589211
I,0,-1.5866187205,-3.0555982444,-0.7068615985
I,0,1.3510397578,-0.9031860793,-1.7032604758

39
2D-a-TS1,Free Energies= -822.323060
C,0,-0.9252672772,5.3496338893,-0.3367582103
C,0,-2.231944963,4.6157784958,-0.6947890442
C,0,-1.980994845,3.2528634694,-1.3357889286
C,0,-0.6737460849,2.6244668949,-0.688748144
C,0,0.5478555607,3.4632169194,-1.1622566261
C,0,0.1974001329,4.9560381121,-1.2985847964
H,0,-1.0921130091,6.4300765864,-0.3573613417
H,0,-2.8455317128,4.4518362085,0.196725334
H,0,-0.8260260564,2.7156060783,0.3938637028
H,0,1.3348138002,3.3133066734,-0.417365403
H,0,-0.1099930635,5.1856705949,-2.3266497166
H,0,-2.8292083446,5.2080358862,-1.3954084874
H,0,-0.6230614345,5.1028908412,0.6886144022
H,0,1.0959113275,5.5485005931,-1.1040113016
H,0,0.9231127978,3.0584844257,-2.1061239772
H,0,-1.7808237658,3.3428215893,-2.4138556681
O,0,-3.0821459528,2.4282581812,-1.1158513651
C,0,-3.040933567,1.2752630871,-1.8910106244
H,0,-3.3278953439,1.4763610045,-2.9331452448
C,0,-0.5310073323,1.2211076746,-0.9488019177
C,0,-0.2516524256,-0.035242998,-0.9013260218
H,0,-1.9407774336,0.985957611,-1.9736304782
H,0,-0.8160806846,-0.8187379006,-1.4003338612
C,0,-3.7813589657,0.1316888125,-1.2816732176
C,0,-4.5427271567,-0.7181699492,-2.0854106152
C,0,-3.6500656825,-0.1359529308,0.0837024709
C,0,-5.1762546961,-1.8239652265,-1.5264145102
H,0,-4.6425754054,-0.5154766509,-3.1489167447
C,0,-4.2860557012,-1.2376618829,0.6402840618
H,0,-3.0445485901,0.5136750555,0.7089097073
C,0,-5.0488367138,-2.0830329476,-0.1644520133
H,0,-5.7679417723,-2.4818763198,-2.1549563565
H,0,-4.1728587767,-1.4439645294,1.6994817625
H,0,-5.538741676,-2.9480370127,0.2716460323
Pt,0,1.3123528598,-0.638072584,0.1588659631
I,0,1.3518051388,1.2345048753,2.1283216193
I,0,-0.356765802,-2.1347792324,1.6718617241
I,0,1.6294347116,-2.7167934962,-1.5266247611
I,0,3.2431976154,0.6961306717,-1.1683393032

39
2D-a-IN2,Free Energies= -822.387956
C,0,-1.6124442715,5.1558608004,0.2252119178
C,0,-2.9601747648,4.4121585888,0.1753856995
C,0,-2.8935821391,3.2071317041,-0.7630848973
C,0,-1.4786338911,2.6185410114,-0.8383464812
C,0,-0.5875881395,3.6648489755,-1.5492097262
C,0,-0.9232464301,5.1155825508,-1.1403553417
H,0,-1.7811147151,6.1875271281,0.5475106393
H,0,-3.2177658202,4.0423202253,1.1727619766
H,0,-1.1263435774,2.4863545513,0.1862492568
H,0,0.447010977,3.4176334146,-1.2953840383
H,0,-1.5847230254,5.5774318141,-1.8859741039
H,0,-3.7634158539,5.0823161274,-0.1486617182
H,0,-0.9622172106,4.6917509102,0.9756398974
H,0,-0.0098560494,5.7169145771,-1.1243793071
H,0,-0.6827658599,3.5477023086,-2.6359903144
H,0,-3.2597878991,3.4415734428,-1.7712871445
O,0,-3.8284078722,2.209651358,-0.2215780302
C,0,-4.2116551527,1.2414668657,-0.9501521772
H,0,-3.9859305102,1.2740061992,-2.0162795033
C,0,-1.4488872127,1.3017249418,-1.5423274975
C,0,-1.1308759717,0.0825580658,-1.1008730684
H,0,-1.6862520546,1.3387063808,-2.6109738499
H,0,-1.1556407793,-0.7552707154,-1.7900968876
C,0,-4.9842173579,0.1755625297,-0.4262638546
C,0,-5.3931251217,-0.8394036919,-1.314726636
C,0,-5.3157299036,0.1085775802,0.9420291009
C,0,-6.1314902372,-1.9066751804,-0.839059674
H,0,-5.113594676,-0.7881992883,-2.3633885386
C,0,-6.0549158293,-0.9638072056,1.4048680721
H,0,-4.9699411563,0.8818774473,1.6171253715
C,0,-6.4577012017,-1.9648020337,0.5181950164
H,0,-6.4410202568,-2.6996688309,-1.5104636624
H,0,-6.2991972608,-1.0383306363,2.4583656003
H,0,-7.028275691,-2.8095036002,0.8919815803
Pt,0,-0.4902641856,-0.4929545273,0.6974399252
I,0,-1.9483765777,0.9013731706,2.5303631597
I,0,-2.3537365507,-2.4647457839,0.7063581289
I,0,1.2410488481,-2.1561434142,-0.5391148372
I,0,1.5153915248,1.2945594484,0.9596052355

39
2D-a-TS2,Free Energies= -822.368714
C,0,-3.635856157,3.2391162405,-0.6006035815
C,0,-2.2560718458,3.8880983551,-0.8717181828
C,0,-1.2990324066,3.5370627204,0.2570393388
C,0,-1.58467104,2.1309675961,0.796199899
C,0,-2.8887089777,2.1666460767,1.6008118904
C,0,-3.9173845009,3.0938625924,0.9031386826
H,0,-4.420411219,3.8370371117,-1.073384187
H,0,-1.8374351028,3.5050679574,-1.8081299033
H,0,-1.7170864818,1.4858285314,-0.0748447793
H,0,-3.2772441645,1.1481009828,1.6864950625
H,0,-3.8972124032,4.0891133581,1.3662507201
H,0,-2.3438373828,4.9751072142,-0.9647004747
H,0,-3.6737416078,2.2486144461,-1.069152508
H,0,-4.9278847,2.7042929465,1.0566157196
H,0,-2.6938488834,2.5234167804,2.6206181276
H,0,-1.3613809082,4.2706132693,1.0765149668
O,0,0.0617811083,3.4947580688,-0.1812107779
C,0,0.8465561507,3.0793798622,0.810478694
H,0,0.7472961344,3.6499884329,1.7395603059
C,0,-0.3462694825,1.68609221,1.5248310445
C,0,0.3600579782,0.5053141566,1.3173591058
H,0,-0.275892398,1.9861394393,2.5746713089
H,0,1.1991312786,0.3199698666,1.9854061653
C,0,2.2416770483,2.7679047002,0.4586529963
C,0,3.1750443679,2.6200192213,1.4907558318
C,0,2.6498385434,2.6791148802,-0.8732077127
C,0,4.5069656092,2.3712765191,1.192698587
H,0,2.8564637291,2.6996363308,2.5283504228
C,0,3.9883492736,2.4489529925,-1.166178153
H,0,1.9216722221,2.7886978764,-1.6676973746
C,0,4.9140923665,2.2899713838,-0.1387673629
H,0,5.2282368298,2.2475681503,1.9938505275
H,0,4.3047575052,2.3770520614,-2.2013974981
H,0,5.956798296,2.0999550695,-0.3736724772
Pt,0,0.0812443005,-0.885793783,0.0081491017
I,0,-0.0362710788,0.3653702792,-2.3771503124
I,0,2.7640437992,-1.1306408121,-0.2282823337
I,0,0.132127107,-2.5219059149,2.1857968788
I,0,-2.5834084068,-1.32934522,-0.14991251

39
2D-a-IN3,Free Energies= -822.390201
C,0,2.4710912413,4.4013909901,-0.6430085559
C,0,3.6777377207,3.435782204,-0.773470287
C,0,3.5654308089,2.3361086301,0.2724889964
C,0,2.1037663129,1.9619515733,0.4956063842
C,0,1.3768015595,3.0685229968,1.2568634069
C,0,1.9081508218,4.449002989,0.7883500353
H,0,2.7649490547,5.4072323578,-0.958419677
H,0,3.6811360943,2.9684709275,-1.7642739207
H,0,1.6673572518,1.8766158638,-0.5020018492
H,0,0.2990823979,2.9919136061,1.078837657
H,0,2.6987601969,4.7903284689,1.4689654997
H,0,4.6253188987,3.9716670513,-0.6583699459
H,0,1.6722121853,4.0847836342,-1.3246045383
H,0,1.1084639498,5.1936689134,0.8473828431
H,0,1.5333953169,2.9547822064,2.3377311473
H,0,4.0081316987,2.6702376168,1.2288143911
O,0,4.1844867285,1.1225777703,-0.1083788731
C,0,3.7203239969,0.1673613088,0.8111283817
H,0,4.2362554827,0.3214161844,1.7744009263
C,0,2.1982795409,0.5541159934,1.0930653555
C,0,1.2173093307,-0.4997457935,0.6457266323
H,0,2.0791176956,0.5991397081,2.1837572913
H,0,1.5622787726,-1.5120267641,0.8404313926
C,0,4.0053183975,-1.2364150426,0.3459560916
C,0,3.9158056205,-2.2893224081,1.2612069838
C,0,4.3521407576,-1.5081549261,-0.9749588323
C,0,4.1405944816,-3.5999484052,0.8547670991
H,0,3.6730164731,-2.08171631,2.3024606438
C,0,4.5877860928,-2.8195105713,-1.379257918
H,0,4.441453007,-0.6885008178,-1.6773838863
C,0,4.4766631938,-3.8671888898,-0.4708804781
H,0,4.0622979791,-4.4105440345,1.5727521327
H,0,4.8527587531,-3.0204916587,-2.4127383108
H,0,4.6559955418,-4.8891043498,-0.7905410771
Pt,0,0.1709155588,-0.3803611864,-1.083571014
I,0,1.657653764,0.0218207756,-3.2065015875
I,0,0.4781103157,-3.0278537255,-1.3012352052
I,0,-0.8008693223,-0.4658215688,1.573732659
I,0,-1.1259155227,1.927699812,-1.5846922247

39
2D-a-IN4,Free Energies= -822.365551
C,0,2.9369635947,4.2905858772,-1.1848461073
C,0,4.1193995302,3.5505512192,-0.5082365592
C,0,3.5866784664,2.5208312382,0.4793993959
C,0,2.26358458,1.9325417152,-0.0035135307
C,0,1.1228618151,2.9519985901,0.0386804383
C,0,1.6947866759,4.356236995,-0.2825779244
H,0,3.2465774624,5.3018739561,-1.463987978
H,0,4.7227602438,3.0274036486,-1.2576277412
H,0,2.4176667043,1.6006215127,-1.0444800141
H,0,0.3513454774,2.6767889624,-0.6898422994
H,0,1.9576386412,4.8654157834,0.65286862
H,0,4.7791129489,4.2549215357,0.0068540911
H,0,2.6687122581,3.7831316435,-2.1197607014
H,0,0.9178892994,4.9627187552,-0.7563176167
H,0,0.6410385855,2.9633201788,1.0219444693
H,0,3.4330284119,2.9802429844,1.4710676433
O,0,4.4342570313,1.3901993186,0.6173433846
C,0,3.6754722657,0.3470785468,1.189664586
H,0,3.7162760531,0.3978033614,2.2900134524
C,0,2.2228110295,0.6394737158,0.7428915829
C,0,1.1613166924,-0.234501552,0.9010812391
H,0,1.3574444007,0.6803986557,1.790549181
H,0,1.4114461831,-1.1666350603,1.4159773517
C,0,4.1304319274,-1.0087622583,0.7158743141
C,0,4.1829896642,-2.0769652947,1.6090198446
C,0,4.4030313452,-1.2192333798,-0.6363786742
C,0,4.4978820116,-3.3551508281,1.1532258742
H,0,3.9860899026,-1.9124639673,2.6661028843
C,0,4.7204193019,-2.4942132949,-1.0890353622
H,0,4.3696238984,-0.3834581111,-1.3282558295
C,0,4.7635121588,-3.5642237449,-0.1963025652
H,0,4.5393450466,-4.1827570898,1.8542429736
H,0,4.926883797,-2.6551639517,-2.1423617946
H,0,5.0053576771,-4.5601825798,-0.5540627786
Pt,0,-0.7016790742,-0.008754528,0.1198700283
I,0,0.4194055587,-0.6663249366,-2.2394224057
I,0,-1.2915638446,-2.5173073918,0.7370256925
I,0,-1.4630993408,0.9947343685,2.5063230665
I,0,-3.0437603806,0.586553407,-1.0221792382

39
2D-a-TS3,Free Energies= -822.393488
C,0,2.6310628862,4.4729913151,-1.0998310995
C,0,3.8520136148,3.5133169523,-1.1314782236
C,0,3.699100759,2.4981700386,-0.0116686414
C,0,2.2325649923,2.0987366264,0.1497634097
C,0,1.4964957627,3.2365311696,0.8572145693
C,0,2.0057546756,4.5968495797,0.3026818937
H,0,2.926809621,5.4633263039,-1.4594894226
H,0,3.8909630381,2.9826666045,-2.0895665726
H,0,1.8179440833,1.9836867392,-0.8582385906
H,0,0.4182296974,3.1395758233,0.7131078868
H,0,2.7520585287,5.0202455486,0.986621988
H,0,4.7923506615,4.0626650471,-1.0214610535
H,0,1.8638746496,4.1106411253,-1.7943700453
H,0,1.1799592604,5.313912995,0.2689291502
H,0,1.6799627167,3.1843773329,1.9380871891
H,0,4.0529775123,2.9383620414,0.9376279238
O,0,4.3906053508,1.2784053348,-0.2067517039
C,0,3.8814068368,0.4348540064,0.7944889186
H,0,4.2323166616,0.7905766547,1.7780372154
C,0,2.3091545633,0.708424054,0.7957153128
C,0,1.536990876,-0.4202875322,0.1795766827
H,0,1.9576216835,0.7200304848,1.8368075619
H,0,1.7482996368,-1.3764779109,0.6501988516
C,0,4.3384073212,-0.9883512252,0.6118191607
C,0,4.0306823823,-1.9340234078,1.5941376069
C,0,5.0466619583,-1.3852944882,-0.520749037
C,0,4.3958740715,-3.2657344728,1.4313268967
H,0,3.4957212719,-1.6282441854,2.4918055091
C,0,5.4252897531,-2.7174959866,-0.6763688988
H,0,5.3034644238,-0.6448591563,-1.2706003182
C,0,5.0935031291,-3.6610464257,0.2914180269
H,0,4.1397718702,-3.9931559538,2.1953538746
H,0,5.9828412978,-3.0173454854,-1.5587660759
H,0,5.3835295031,-4.6992867793,0.163027024
Pt,0,-0.4416572913,-0.2084863849,-0.2026663853
I,0,1.6902619746,-0.8426937849,-1.9634036579
I,0,-0.7531264567,-2.7264257322,0.6599082127
I,0,-1.5908119593,0.7277374549,1.9657039991
I,0,-1.1751488139,1.9472345752,-1.6176757363

39
2D-P,Free Energies= -822.387385
C,0,3.3075055832,4.4493851163,-1.1755653597
C,0,4.4671668193,3.5563740751,-0.6649045892
C,0,3.9631431767,2.6058764997,0.4150355343
C,0,2.5045311606,2.2214635479,0.1659046328
C,0,1.5214612156,3.3783811183,0.3077040635
C,0,2.2334059882,4.6906816693,-0.102781882
H,0,3.7062771267,5.4063464425,-1.525070755
H,0,4.8735477244,2.9567850909,-1.486206919
H,0,2.4860456844,1.8615526563,-0.8825031824
H,0,0.6513994131,3.1945396619,-0.332460152
H,0,2.7028828972,5.1448597891,0.7790435522
H,0,5.285218082,4.1674553768,-0.2717570786
H,0,2.8345812125,3.9771395867,-2.0461377528
H,0,1.4954219363,5.4117716113,-0.4665064776
H,0,1.1540102224,3.4556726328,1.3380869983
H,0,4.0533561895,3.0709626895,1.411891828
O,0,4.6309041247,1.3557645138,0.4179909712
C,0,3.7972690308,0.4437191735,1.1120359101
H,0,3.9873800983,0.5209317437,2.1991125164
C,0,2.3782571486,0.9744510153,0.9361035195
C,0,1.2450418705,0.4565290276,1.5129198323
H,0,0.4550482892,1.1769352785,1.7309579208
H,0,1.3646467316,-0.3529374512,2.2285082549
C,0,4.0678048709,-0.9709677764,0.6668198551
C,0,4.2098866398,-1.9909763474,1.6043442626
C,0,4.2012952715,-1.2541861077,-0.6930699122
C,0,4.4774501454,-3.2927306065,1.1873798745
H,0,4.1232335605,-1.7697095428,2.665455265
C,0,4.4672463643,-2.5524342826,-1.1091955274
H,0,4.1066261978,-0.4526225027,-1.4176024187
C,0,4.6065079664,-3.5740681787,-0.1700447812
H,0,4.5951995966,-4.0824431218,1.9230735788
H,0,4.5653377332,-2.7681228034,-2.1684690134
H,0,4.8237577542,-4.5866828369,-0.4967774692
Pt,0,-0.2315899991,-0.5757748589,-0.0140846691
I,0,0.8876070677,0.2004415372,-2.3293391319
I,0,0.7809808754,-3.0033174263,0.1392472792
I,0,-1.6670116054,-0.9778646006,2.2288373288
I,0,-2.2730150389,-1.4786525894,-1.4371927049

39
2D-b-IN1,Free Energies= -822.362793
C,0,3.000359206,5.4300160809,0.5652860132
C,0,3.2008884389,4.2439647357,1.5066966392
C,0,2.7336898079,2.9322351859,0.8525591706
C,0,1.5677876487,3.1720598138,-0.1355754379
C,0,0.6927412933,4.3420187057,0.3350329798
C,0,1.4997752473,5.6563287981,0.2913837935
H,0,3.4494787023,6.3360339314,0.9833720909
H,0,4.2528947975,4.1384818698,1.7921792197
H,0,2.0182544697,3.4387075815,-1.1007691902
H,0,-0.1986385198,4.4257877246,-0.2943461399
H,0,1.0831715619,6.3483675964,1.0312753741
H,0,2.6395198488,4.4083076642,2.4348977665
H,0,3.5312291445,5.2247160558,-0.3723183544
H,0,1.3736636744,6.131437168,-0.6874552224
H,0,0.3449516682,4.1366942827,1.355470262
H,0,2.3964723892,2.2316396946,1.6326181911
O,0,3.7520800691,2.320363987,0.0837391835
C,0,4.6289882766,1.4807114995,0.8124563354
H,0,5.2597462291,2.0827191642,1.4848467588
C,0,0.7691682712,1.9262686178,-0.3280266593
C,0,-0.470309557,1.6062988003,-0.0170108349
H,0,-1.2290470153,2.2388182894,0.4290516136
H,0,4.0492500166,0.7836733129,1.4368931094
C,0,5.4761222673,0.7160679581,-0.1702441905
C,0,5.5338473126,-0.6765245685,-0.1309845469
C,0,6.2002074111,1.4013977599,-1.1488355105
C,0,6.3104840318,-1.3778614903,-1.0517729365
H,0,4.964785438,-1.218338675,0.6209968155
C,0,6.9691592707,0.7034430552,-2.0731104681
H,0,6.1463514274,2.4855873895,-1.1888134249
C,0,7.0273049808,-0.6888308228,-2.0252610243
H,0,6.3506947776,-2.462229258,-1.0100810622
H,0,7.5265907154,1.245430854,-2.8313190862
H,0,7.6293229853,-1.2336693537,-2.746289916
Pt,0,-0.9680098922,-0.2762317742,-0.4162510769
I,0,-3.4551459859,-0.272308276,0.4682639671
I,0,-1.8229554522,0.2467474404,-2.9029417259
I,0,1.6914055311,0.1633193675,-1.2008528299
I,0,-0.0997323412,-1.2191071478,1.9498348882

39
2D-b-TS1,Free Energies= -822.313230
C,0,3.9815650161,4.6929515289,-0.2573978091
C,0,3.8009184928,3.7583587193,0.9372598596
C,0,3.094069347,2.4554576365,0.5435125459
C,0,2.0327301267,2.7614121549,-0.6042323767
C,0,1.486604272,4.1973988686,-0.4903323103
C,0,2.6171617321,5.2060503428,-0.7617623134
H,0,4.6247493209,5.5353368545,0.0121625045
H,0,4.7621617095,3.4704025122,1.3709472282
H,0,2.5576195501,2.6235206095,-1.5571468079
H,0,0.6618825526,4.3474344578,-1.1946912116
H,0,2.361432594,6.1496036351,-0.2691232334
H,0,3.2266114301,4.2597905927,1.7245312864
H,0,4.5031646001,4.1470448298,-1.0525174881
H,0,2.6732580319,5.4169143345,-1.8349617394
H,0,1.0699919833,4.3287515612,0.5146041555
H,0,2.5632700965,2.0409955109,1.4147916623
O,0,4.0583586078,1.5555883558,0.0946601375
C,0,3.6143677909,0.2158307511,-0.0444421298
H,0,2.9541138725,-0.0503960277,0.7942216291
C,0,1.0019739866,1.7550932512,-0.4738051579
C,0,0.0941870747,0.9208918662,-0.336531457
H,0,-0.2445432749,1.7115079976,-1.1815958606
H,0,3.025355347,0.1088137092,-0.9694393176
C,0,4.7866229494,-0.7298334009,-0.0861124736
C,0,4.5609725924,-2.0864996127,0.1570177026
C,0,6.0733092886,-0.290432109,-0.389746222
C,0,5.6121463554,-2.9948315856,0.0894115149
H,0,3.5583383111,-2.4302023365,0.40226714
C,0,7.1256026317,-1.2012564322,-0.4507652436
H,0,6.2499920376,0.7649350605,-0.5681062711
C,0,6.8984317359,-2.5538254529,-0.2147484186
H,0,5.426703077,-4.0472103625,0.2825545242
H,0,8.1269432731,-0.8505731959,-0.6836236158
H,0,7.7204280102,-3.2618477691,-0.2629174403
Pt,0,-0.9988309195,-0.556729322,0.1367287878
I,0,-2.6320349467,1.0179375841,1.604527145
I,0,-2.5703742209,-0.1628032386,-2.0341069661
I,0,0.4718766793,-2.3397084296,-1.2569326392
I,0,0.4029622751,-1.1542772897,2.3607820897

39
2D-b-IN2,Free Energies= -822.356945
C,0,2.799605423,5.3374355559,0.0236460415
C,0,3.2780078938,4.4474869455,1.1708070439
C,0,2.61732481,3.0545046552,1.1127231051
C,0,1.235488163,3.1223998929,0.4381168554
C,0,0.5278991089,4.4386873832,0.7803231936
C,0,1.288081925,5.6202884925,0.1428100769
H,0,3.3610985262,6.2769060454,0.0078858917
H,0,4.36601216,4.3245943008,1.1437463741
H,0,1.4093220027,3.0965335036,-0.6409036031
H,0,-0.5062918768,4.4118204521,0.422988626
H,0,1.1210048479,6.5213002309,0.7434213176
H,0,3.0391120863,4.9245657616,2.1300224598
H,0,3.0153020375,4.8309496574,-0.925492213
H,0,0.8771045578,5.8230434191,-0.8519752871
H,0,0.483845125,4.5494585935,1.8728050504
H,0,2.5019127689,2.6662632945,2.139094687
O,0,3.3668721402,2.1337076002,0.3500626511
C,0,4.402498511,1.4901855314,1.0565141163
H,0,5.0798853446,2.236391613,1.505106044
C,0,0.4100126616,1.9251856127,0.8137737639
C,0,0.0846797388,0.9486300717,-0.0028422612
H,0,0.0519938132,1.8711441264,1.8414004006
H,0,3.9832165436,0.8946703592,1.8829193592
C,0,5.1682838621,0.6010199557,0.1124668345
C,0,5.5909103929,-0.663175645,0.5181780849
C,0,5.4691076103,1.038907928,-1.1776296133
C,0,6.3031837874,-1.4841157164,-0.3526103987
H,0,5.3479656835,-1.0171458083,1.5173863734
C,0,6.1705241114,0.2170977967,-2.052589116
H,0,5.1269131145,2.0175310898,-1.4988340671
C,0,6.5901696505,-1.0467842697,-1.6427174175
H,0,6.6236084779,-2.4690611251,-0.0257315023
H,0,6.3872648964,0.56101749,-3.0597810466
H,0,7.1381221465,-1.6882697105,-2.3265181272
Pt,0,0.3767778192,0.4277980311,-1.8611576624
I,0,-1.2106846767,-0.7266233765,0.3230757639
I,0,-1.6570175427,2.0177305647,-2.5976982595
I,0,2.0632693869,1.8516822607,-3.267956693
I,0,2.2465637832,-1.4414242649,-1.535988477

39
2D-b-IN3,Free Energies= -822.358802
C,0,1.2130695369,3.5695399539,-2.1200815509
C,0,2.0020092983,3.2959617907,-3.4128009344
C,0,2.5882525994,1.8909471011,-3.4331244942
C,0,3.5884913287,1.6892020236,-2.2514675816
C,0,3.3726901362,2.7044281062,-1.1087849871
C,0,1.8808214511,2.9382987117,-0.8789962181
H,0,1.1244713425,4.6539241662,-1.9908077986
H,0,1.3611697835,3.4326223111,-4.2890903285
H,0,3.4192342964,0.6863126162,-1.8494471657
H,0,3.8599517871,2.3261139125,-0.2039342882
H,0,1.7331201432,3.5731418981,0.0003928222
H,0,2.831883723,4.0080772072,-3.5107577635
H,0,0.1968909911,3.1803607344,-2.2296652995
H,0,1.4167458392,1.9729128059,-0.6507384891
H,0,3.8664963545,3.6547989561,-1.3533182502
H,0,3.1210247,1.7290280714,-4.3842656553
O,0,1.5002473043,0.9941942831,-3.3643647773
C,0,1.8074559181,-0.3625871355,-3.6110214264
H,0,1.2454333545,-0.6761434974,-4.5017165182
C,0,5.0079174867,1.7835367751,-2.7455270899
C,0,6.0171095166,1.0523864102,-2.3289200299
H,0,5.2233418311,2.5541883954,-3.4857731065
H,0,2.8745663336,-0.4888316583,-3.8449854753
C,0,1.4467807412,-1.253917663,-2.4421061386
C,0,1.8846131529,-2.5798131545,-2.4284368015
C,0,0.6722651756,-0.7836352316,-1.3842603138
C,0,1.5680711034,-3.4180163802,-1.3659322458
H,0,2.4951050961,-2.9546176113,-3.2463819465
C,0,0.3587587751,-1.6200238417,-0.3143270875
H,0,0.3157212871,0.2399886333,-1.4062980566
C,0,0.8082152332,-2.9381004838,-0.2996308395
H,0,1.9256970967,-4.4432733774,-1.3637104733
H,0,-0.2443619574,-1.2408029787,0.5058632915
H,0,0.5608572778,-3.5919604234,0.5316398348
Pt,0,6.3334088919,-0.3709198113,-1.0304476705
I,0,8.0692834028,1.0819583984,-2.9290353656
I,0,7.0666912153,1.2722580841,0.9454865798
I,0,4.2604362821,-1.1398682233,0.3669591795
I,0,5.9144621599,-2.3058241643,-2.82742516

39
2D-b-TS2,Free Energies= -822.320454
C,0,-5.4445755613,-3.1087596747,-0.2364261203
C,0,-4.7949408643,-2.5010419444,1.0054832668
C,0,-3.4977814124,-1.7508442123,0.6701362126
C,0,-2.8300572594,-2.3165498349,-0.6000890426
C,0,-3.0311496908,-3.8373404758,-0.6658465371
C,0,-4.5233373694,-4.1753838001,-0.8616802568
H,0,-6.4136069469,-3.5487973324,0.0176721769
H,0,-5.4636200309,-1.7943331382,1.5049069486
H,0,-3.342796232,-1.8615355824,-1.4582987277
H,0,-2.4354586611,-4.2633392492,-1.4805049924
H,0,-4.7265258036,-5.1540448022,-0.4140536517
H,0,-4.570780703,-3.2972969576,1.7255484501
H,0,-5.6492623239,-2.309550889,-0.9590036441
H,0,-4.743636389,-4.2680824076,-1.9307233022
H,0,-2.6490415383,-4.2817691713,0.2620227961
H,0,-2.8000435355,-1.8342278954,1.5163371897
O,0,-3.8106470736,-0.3763326997,0.4594398848
C,0,-2.7753349135,0.4798210898,0.8087632156
H,0,-2.5546126654,0.4557999577,1.8873318112
C,0,-1.3648691555,-1.9650129649,-0.7416638317
C,0,-0.6372443152,-0.9601870573,-0.3628659401
H,0,-0.7228776404,-2.6644235279,-1.2946252352
H,0,-1.8117933212,0.0944982661,0.3344707868
C,0,-2.9827945608,1.8588330518,0.2843287685
C,0,-3.0410714596,2.9490129557,1.1522132284
C,0,-3.0788021134,2.0645853365,-1.0948047991
C,0,-3.2059072393,4.2354368827,0.6471103066
H,0,-2.9516900916,2.7906268859,2.2234775129
C,0,-3.2318655803,3.3485866918,-1.5992848749
H,0,-3.0152546405,1.2146584535,-1.7688592868
C,0,-3.2969249746,4.4352671704,-0.7273502247
H,0,-3.2535512427,5.0808026434,1.3263840345
H,0,-3.2901382692,3.5053796392,-2.6716803208
H,0,-3.412417228,5.4399861221,-1.1224850614
Pt,0,0.798836627,0.1982077123,-0.0475818508
I,0,2.3394767948,-1.8922638193,-0.8114370483
I,0,0.675584152,1.1029459321,-2.5977934207
I,0,0.6875293492,2.7136735606,0.8110255035
I,0,0.8351977636,-0.675085015,2.5306499859

39
2D-b-IN4,Free Energies= -822.392259
C,0,2.7810935376,5.3470798856,-1.4930110557
C,0,3.4372910171,4.5999680766,-0.3317143782
C,0,2.6791845106,3.3177931885,0.0122303129
C,0,1.2090587193,3.3172228071,-0.4465908025
C,0,0.6410933006,4.7266857927,-0.2230670641
C,0,1.3393121387,5.759676854,-1.1340343693
H,0,3.3757346492,6.2280014109,-1.7524936258
H,0,4.4837428357,4.356238585,-0.5406165609
H,0,1.1990171061,3.1029539683,-1.5234290148
H,0,-0.436327936,4.708516858,-0.4060170974
H,0,1.3480622364,6.7328380944,-0.6315953867
H,0,3.4359665386,5.2362600858,0.5609059628
H,0,2.7828561092,4.7028493759,-2.3809581661
H,0,0.7643371216,5.8904615469,-2.0564540594
H,0,0.7670100301,4.9936361059,0.8345899167
H,0,2.7482617799,3.0903807888,1.0814643182
O,0,3.345519946,2.2063939261,-0.6877185435
C,0,3.2755791311,1.024007755,-0.2108198239
H,0,2.807086959,0.8691328382,0.7660333304
C,0,0.4629239272,2.2404934104,0.2847275236
C,0,0.0345678464,1.1373300342,-0.323477065
H,0,0.3249887617,2.3857918779,1.3532270001
H,0,0.1341553846,0.9761298942,-1.394359227
C,0,3.8309313862,-0.0722513833,-0.9148504535
C,0,3.8031350399,-1.3311762335,-0.2836216227
C,0,4.4028349972,0.0777040445,-2.199217206
C,0,4.3691895026,-2.4263312457,-0.920635269
H,0,3.3235115772,-1.4383748391,0.6852774123
C,0,4.9483109242,-1.0222571672,-2.825206253
H,0,4.4051382703,1.0512367283,-2.6776293738
C,0,4.9343645439,-2.2698332979,-2.181768584
H,0,4.3437058856,-3.4001459651,-0.445188649
H,0,5.3876627962,-0.9270462406,-3.8121824061
H,0,5.3679986746,-3.1296265176,-2.6834840889
Pt,0,-0.8539326963,-0.3803410288,0.6005624014
I,0,-2.3184732052,1.0748450308,2.3358727515
I,0,-2.8858253363,-0.2495895286,-1.1545782138
I,0,0.3751539401,-2.2080792021,-0.994435178
I,0,1.0539664853,-0.7163070995,2.5343781675

39
2D-b-TS3,Free Energies= -822.376869
C,0,2.9756106497,4.3008077206,-0.4297173799
C,0,4.1494659926,3.3372909702,-0.140556624
C,0,3.6645792463,2.1304048205,0.6549751246
C,0,2.210272941,1.7708166117,0.3398951682
C,0,1.2594389757,2.8826800833,0.8173657171
C,0,1.9316867152,4.2701066741,0.693948316
H,0,3.3620495737,5.3149964103,-0.5651645115
H,0,4.5892378464,2.9782863017,-1.0767989443
H,0,2.1419479481,1.6659994197,-0.7503345916
H,0,0.3412736236,2.8370058356,0.2244962704
H,0,2.4222956885,4.5320526536,1.6403071303
H,0,4.9417509218,3.8498004058,0.4134960392
H,0,2.4920345672,4.0253503323,-1.374826547
H,0,1.1678568312,5.0339349054,0.5220140551
H,0,0.9620006079,2.6988007552,1.8554627218
H,0,3.7767338566,2.2870923218,1.7380058828
O,0,4.3771991611,0.9523718514,0.2882657558
C,0,3.9225537321,-0.1369394587,0.9113331683
H,0,3.9262962597,-0.1155625376,2.0039672247
C,0,1.9652660883,0.4242652466,0.9825794514
C,0,1.3514117942,-0.570265623,0.250987311
H,0,1.7687678313,0.4485472665,2.0522546259
H,0,1.4956198287,-0.6100959363,-0.8286902961
C,0,4.3452464192,-1.3950316191,0.2878716428
C,0,4.6593119216,-2.4902880499,1.0953942981
C,0,4.5061143089,-1.4768019091,-1.1013812612
C,0,5.1400382506,-3.6595797718,0.5186105072
H,0,4.5216356946,-2.4301243199,2.1699989486
C,0,4.9772141292,-2.648192338,-1.6722004194
H,0,4.2685768879,-0.6179617026,-1.7213568663
C,0,5.2964542249,-3.739182103,-0.8614163191
H,0,5.3778359704,-4.5115054211,1.1463776316
H,0,5.0960541284,-2.7162379059,-2.7486025173
H,0,5.6631322911,-4.6562918979,-1.3119004818
Pt,0,0.1541467302,-1.8941142204,0.9571402525
I,0,-1.3882153222,-0.1711378248,2.3700918588
I,0,-1.4735867108,-1.5161403148,-1.1785682897
I,0,1.3438737885,-3.931480181,-0.3493165699
I,0,1.4823127057,-2.5185309127,3.2362959868

39
2D-b-IN5,Free Energies= -822.394107
C,0,-4.7392820952,-3.4771021791,-1.1646535959
C,0,-5.1656598006,-2.3103759614,-0.2409155586
C,0,-3.9460080821,-1.7496504614,0.479757403
C,0,-2.7124106905,-1.7527379713,-0.4167318527
C,0,-2.2492922586,-3.1966345223,-0.6693684654
C,0,-3.4598487596,-4.1628478034,-0.6639965967
H,0,-5.5506922554,-4.2064077432,-1.2482750977
H,0,-5.6254079929,-1.5037937986,-0.8224350736
H,0,-2.9831994742,-1.268721416,-1.3655785229
H,0,-1.738228136,-3.2633188865,-1.6344756493
H,0,-3.6299019051,-4.5428235639,0.3507785236
H,0,-5.9072798794,-2.6417646347,0.4927228988
H,0,-4.5600610485,-3.0982278642,-2.1789905676
H,0,-3.2320671127,-5.0357203461,-1.2836623945
H,0,-1.5209752631,-3.5028262266,0.091046802
H,0,-3.7247755454,-2.3631303449,1.3702741558
O,0,-4.1212458885,-0.4066313989,0.8720505669
C,0,-2.8572120108,0.2286069665,0.9895234344
H,0,-2.6111004228,0.3800077264,2.0484837718
C,0,-1.8091290347,-0.8069201481,0.3973201176
C,0,-0.6991620299,-0.1183459979,-0.3379475737
H,0,-1.3965757861,-1.3905544353,1.223370572
H,0,-0.9991555099,0.7618711262,-0.9032953804
C,0,-2.9150897562,1.5717103124,0.295151865
C,0,-2.3010374594,2.6857723079,0.863167308
C,0,-3.5551837568,1.7057657845,-0.9410825673
C,0,-2.2958893627,3.9093458504,0.1984082852
H,0,-1.8121830049,2.5963564362,1.8284068507
C,0,-3.5498688304,2.9262194623,-1.6072802534
H,0,-4.0793573263,0.8551632774,-1.3659605653
C,0,-2.9142837283,4.0306709863,-1.0411200037
H,0,-1.8020192999,4.7637390386,0.650387553
H,0,-4.0516852247,3.0199609574,-2.5658286531
H,0,-2.9084991856,4.9828250707,-1.5628302186
Pt,0,1.0315898768,0.1665674576,0.6606626828
I,0,1.4518404351,-2.1753247591,1.9506978079
I,0,0.5918346632,-1.2191282532,-1.753874973
I,0,1.4108888956,2.4995468194,-0.5990541407
I,0,0.7995898061,1.3751615359,2.9736734256

39
2D-b-IN6,Free Energies= -822.397003
C,0,4.9794689097,-1.4945022044,-1.2042836405
C,0,5.0694591608,0.040154078,-1.4215405479
C,0,3.785915386,0.5164854731,-2.0820050556
C,0,2.5872668639,-0.2544368715,-1.5319687895
C,0,2.5834014169,-1.6582185592,-2.136909976
C,0,4.0455822084,-2.1798217765,-2.2188894587
H,0,5.9781776004,-1.9377352075,-1.2633067902
H,0,5.1865143757,0.5544634076,-0.4611282123
H,0,2.7323453974,-0.3361099684,-0.4470900866
H,0,1.9673900456,-2.331335207,-1.5373889778
H,0,4.4417473833,-2.0168027173,-3.2290967962
H,0,5.9332777775,0.3025115198,-2.0404936396
H,0,4.6113562413,-1.7011254284,-0.1919253154
H,0,4.0588540558,-3.2617725461,-2.0565439989
H,0,2.137971999,-1.6330543636,-3.1389239896
H,0,3.8432145753,0.3463509416,-3.1718273078
O,0,3.4719048574,1.8761389411,-1.8674980371
C,0,2.1486707507,2.002072229,-2.3285487324
H,0,2.130375871,1.9035292832,-3.4266859756
C,0,1.3922733933,0.7042778921,-1.7904541538
C,0,0.6820612231,0.979312447,-0.5028769668
H,0,0.7075733791,0.3106269778,-2.5442115245
H,0,1.2415040245,1.6128299894,0.1840054777
C,0,1.5776493359,3.3409015572,-1.9492353265
C,0,0.6191172127,3.9398956533,-2.7670963789
C,0,1.9503439645,3.9686837544,-0.7590798194
C,0,0.0147809309,5.1356797377,-2.3870217937
H,0,0.3397487401,3.4665381007,-3.7058022199
C,0,1.3466499872,5.16349188,-0.3784100374
H,0,2.7238989905,3.5236136864,-0.1408132531
C,0,0.3722307615,5.7453568363,-1.186467981
H,0,-0.7282919742,5.5946580317,-3.0322935151
H,0,1.6390146898,5.6410211789,0.5516439653
H,0,-0.0985335714,6.6768253551,-0.8873649176
Pt,0,-0.2479992987,-0.4838283195,0.5445863718
I,0,1.1833484527,-2.502606813,1.4258875697
I,0,0.2544475989,0.8265362948,2.847564002
I,0,-1.341482494,1.8272775328,-0.5819192933
I,0,-1.2589263919,-2.0027039614,-1.4359422868

39
2D-b-TS4,Free Energies= -822.357744
C,0,5.4799953122,-1.4934835153,-1.5961520235
C,0,5.1192170629,-0.025840784,-1.9631735689
C,0,3.6287988897,0.2021541781,-1.9113604659
C,0,3.0802796898,-0.2676478432,-0.5707918652
C,0,3.0481068999,-1.7830210851,-0.4703456391
C,0,4.3759780437,-2.4149667705,-0.9820927007
H,0,5.8543514195,-1.9935836148,-2.4937138331
H,0,5.5692998749,0.6684275834,-1.2436954209
H,0,3.7282816628,0.1475514066,0.2213746037
H,0,2.8572299731,-2.0969190116,0.563404304
H,0,4.1058515187,-3.1674589808,-1.7276638182
H,0,5.5158783359,0.2371181188,-2.9476573783
H,0,6.327950314,-1.4599710234,-0.9067353222
H,0,4.8295323279,-2.9714957728,-0.157932272
H,0,2.2080385331,-2.1625429149,-1.0629262148
H,0,3.11638734,-0.3373908824,-2.7275653868
O,0,3.2924157872,1.5808272787,-1.9646080743
C,0,2.0070785292,1.7487407555,-1.4071462899
H,0,1.232203935,1.6831784258,-2.1880224668
C,0,1.8371936497,0.551547891,-0.4507090568
C,0,0.760192953,0.3693618368,0.3986913413
H,0,0.703120312,-0.2028127314,-0.7282538283
H,0,0.0019453628,1.1558890611,0.3492552494
C,0,1.879741466,3.0523149639,-0.6597348143
C,0,2.9041104034,3.4714990771,0.1895700248
C,0,0.6993767215,3.7884925404,-0.7403519937
C,0,2.7421537667,4.6187272511,0.9572010072
H,0,3.8265158123,2.9014930913,0.2421924218
C,0,0.5372194601,4.9360695586,0.0321254082
H,0,-0.0938042597,3.4728543959,-1.4144692817
C,0,1.5572625591,5.3493655206,0.8833593229
H,0,3.5392187351,4.9396804492,1.6202885231
H,0,-0.3832054818,5.507149352,-0.037258107
H,0,1.4311496999,6.241554381,1.4887482127
Pt,0,0.6034444036,-1.0604049993,1.8436956238
I,0,2.4085850056,0.3872249748,3.2170910725
I,0,-1.4713695735,0.1967894248,2.9077065026
I,0,-0.8749357952,-2.4980352045,0.1002142361
I,0,0.6731639207,-3.056379893,3.6202302546

39
3D-a-IN1,Free Energies= -3393.205135
C,0,4.7422422902,-3.7807734748,-0.4082700925
C,0,4.9809661364,-2.2590424839,-0.3926864067
C,0,3.6754341537,-1.4407795058,-0.4342130891
C,0,2.567532299,-2.1855238757,0.3239664307
C,0,2.2295526336,-3.511467076,-0.4118892234
C,0,3.4438340959,-4.1113894327,-1.1438467399
H,0,5.5911982546,-4.2915591562,-0.8728912463
H,0,5.5157640788,-1.9637190145,0.5165904187
H,0,2.9521173626,-2.4060081293,1.3295001448
H,0,1.8503007226,-4.2295095272,0.3240457311
H,0,3.4976081571,-3.7142857339,-2.1653181223
H,0,5.6062140685,-1.9635721018,-1.2433092075
H,0,4.6768918469,-4.1610577666,0.6190778862
H,0,3.3140090647,-5.1937731181,-1.239813642
H,0,1.4173712916,-3.3288079999,-1.1242217936
H,0,3.3417344593,-1.3105463744,-1.4778596291
O,0,3.8470306264,-0.173385957,0.1528024591
C,0,4.5517364489,0.7744894658,-0.6237372122
H,0,5.5933216997,0.8304810888,-0.2760183084
C,0,1.34428771,-1.3380550595,0.4846254942
C,0,0.9938500412,-0.1471912457,0.0478778498
H,0,4.5785242335,0.4653066239,-1.6789560154
H,0,1.5910496576,0.5562149859,-0.5192637214
C,0,3.8788554723,2.1240066032,-0.5157311618
C,0,3.960336885,3.0333779605,-1.5701420784
C,0,3.1682672847,2.4796126487,0.6320597643
C,0,3.3429294632,4.2774854832,-1.4892523919
H,0,4.5030339308,2.7701975029,-2.475040586
C,0,2.5380450566,3.7159977372,0.7224074268
H,0,3.0761815352,1.7740264085,1.4515608952
C,0,2.6311250165,4.6050065196,-0.3414676552
H,0,3.3996302987,4.9770036525,-2.3156421491
H,0,1.9581896561,3.9696595237,1.6025527282
Pt,0,-0.8417475989,0.4323590202,0.5468543857
I,0,-0.3231703962,-2.1589757808,1.6245296115
I,0,-0.1628915393,1.548642309,2.8890015449
I,0,-0.9194761201,2.7990274774,-0.5994462329
I,0,-1.9504532551,-0.6805721315,-1.6269654294
Br,0,1.7371846478,6.2727395746,-0.2453994564

39
3D-a-TS1,Free Energies= -3393.162704
C,0,-0.9255025733,5.3472933196,-0.3099519612
C,0,-2.2392677825,4.6168142108,-0.6501894281
C,0,-1.995973698,3.2628728481,-1.3109979427
C,0,-0.6806672232,2.6282192834,-0.6959095003
C,0,0.5321665101,3.4692278238,-1.1852977638
C,0,0.1801027656,4.9642072437,-1.2960379537
H,0,-1.0934411936,6.4277036215,-0.3174577647
H,0,-2.8341357176,4.4422474062,0.2520470354
H,0,-0.808280064,2.7097262829,0.3907621144
H,0,1.3352611928,3.309694801,-0.4600265518
H,0,-0.1440338105,5.2072273923,-2.3158577859
H,0,-2.8513527143,5.2166418658,-1.331302329
H,0,-0.6052612974,5.0907037505,0.7074203052
H,0,1.0821437567,5.5538935973,-1.1096787768
H,0,0.8856733246,3.0752048051,-2.1422057762
H,0,-1.8172453414,3.3676261341,-2.3915347324
O,0,-3.091623135,2.4282380211,-1.0845655198
C,0,-3.0490965809,1.2871278144,-1.8712802744
H,0,-3.3281651863,1.4958922087,-2.9140266205
C,0,-0.5487544281,1.2240448084,-0.9697596871
C,0,-0.2613293398,-0.0314021317,-0.918108697
H,0,-1.9438195924,0.998034029,-1.953227451
H,0,-0.8223909284,-0.8184144659,-1.4154227648
C,0,-3.7847039784,0.1339283824,-1.2775652291
C,0,-4.5672354021,-0.6932242634,-2.0835351253
C,0,-3.6281121822,-0.1709535377,0.0772020336
C,0,-5.1962507464,-1.8107620639,-1.546563022
H,0,-4.6928181243,-0.4671384497,-3.1391558757
C,0,-4.2523830922,-1.2824808959,0.6239048568
H,0,-3.0040028381,0.4538410695,0.7091508764
C,0,-5.032024245,-2.0958596691,-0.194921228
H,0,-5.8055963774,-2.4543105953,-2.1704731547
H,0,-4.1186677674,-1.5255431595,1.6714809515
Pt,0,1.3049909751,-0.6282796759,0.1419420321
I,0,1.3479873607,1.2388772809,2.1155994735
I,0,-0.3684995891,-2.1256210964,1.6523279037
I,0,1.6232362897,-2.7071718219,-1.5462789863
I,0,3.2363345787,0.70724745,-1.1848552043
Br,0,-5.8707868744,-3.6199952145,0.5406362441

39
3D-a-IN2,Free Energies= -3393.229690
C,0,-1.6011575713,5.1499195536,0.2324588164
C,0,-2.9565120997,4.4208861999,0.1753112995
C,0,-2.901259314,3.2217493716,-0.7719576416
C,0,-1.4930128626,2.615928806,-0.8406226356
C,0,-0.5832617214,3.6545042607,-1.539658517
C,0,-0.9082356516,5.1075722807,-1.1309723863
H,0,-1.7591341374,6.1818356213,0.5594013013
H,0,-3.2193282304,4.0468202519,1.1697475939
H,0,-1.1509997371,2.4755246766,0.1862767455
H,0,0.4454048689,3.3957850763,-1.2734141096
H,0,-1.5639282747,5.575716085,-1.8776341942
H,0,-3.7523333136,5.1017193703,-0.1450930941
H,0,-0.9579950195,4.6758033775,0.9826230541
H,0,0.0096986335,5.701853191,-1.1107680226
H,0,-0.6666667618,3.5406113036,-2.6277376611
H,0,-3.2599763659,3.4679605452,-1.7799500662
O,0,-3.8508049918,2.232531993,-0.2410632609
C,0,-4.2284177874,1.2616909392,-0.969936797
H,0,-3.9989652706,1.2897825612,-2.0350071634
C,0,-1.470805925,1.301019154,-1.5484167634
C,0,-1.1609922325,0.0783271952,-1.1095525495
H,0,-1.7045193575,1.3419231206,-2.6177059052
H,0,-1.1870208886,-0.7572488494,-1.8017275893
C,0,-4.9949163389,0.1957898956,-0.4408346082
C,0,-5.3824223638,-0.8411956208,-1.3125048565
C,0,-5.3308757208,0.1370935599,0.9269986143
C,0,-6.0922913188,-1.9212213285,-0.8296556592
H,0,-5.1025923081,-0.8055765916,-2.3614663101
C,0,-6.0411616895,-0.9427613553,1.410042224
H,0,-5.0074560743,0.9258356747,1.5953128557
C,0,-6.4099905603,-1.9644870377,0.531181329
H,0,-6.3815854224,-2.7356044446,-1.4825282086
H,0,-6.2865707534,-1.0143255303,2.4624929165
Pt,0,-0.5309544806,-0.507102892,0.6892795942
I,0,-1.9969925542,0.8852462192,2.5171318405
I,0,-2.3946483843,-2.4806872753,0.685407823
I,0,1.2030877188,-2.1647880801,-0.5451149763
I,0,1.4756233159,1.2752344891,0.9745060783
Br,0,-7.3416250132,-3.4494368072,1.1986810202

39
3D-a-TS2,Free Energies= -3393.211593
C,0,2.9692941704,4.4174313902,-0.132072672
C,0,1.4401886885,4.644578837,-0.0422240578
C,0,0.7347502798,3.7683998026,-1.0658919878
C,0,1.4751186652,2.4387034954,-1.2504347777
C,0,2.7741676674,2.7026512657,-2.0213947162
C,0,3.4101131073,4.0369807086,-1.5538823059
H,0,3.4925542505,5.3206322625,0.1948261362
H,0,1.076846945,4.3697436778,0.9534051032
H,0,1.7169877601,2.0755712617,-0.2492121945
H,0,3.4570597586,1.8652899325,-1.8537101382
H,0,3.1299520531,4.8457399376,-2.2415302966
H,0,1.1879406456,5.6960289968,-0.21160997
H,0,3.2630134852,3.6191448887,0.5596233582
H,0,4.5003025913,3.9605349439,-1.5979920707
H,0,2.5717873946,2.7413245622,-3.0996660651
H,0,0.6405310965,4.2814450145,-2.035883928
O,0,-0.5833191412,3.4028054966,-0.642705394
C,0,-1.1295587372,2.5594303867,-1.5109248699
H,0,-1.1306421559,2.9018589399,-2.5502497347
C,0,0.502041268,1.4789810038,-1.8750158622
C,0,0.1625125533,0.2144556737,-1.409457035
H,0,0.4275694712,1.5159025427,-2.9658343129
H,0,-0.5177947983,-0.3638775754,-2.031650343
C,0,-2.3790693152,1.9072936027,-1.095170067
C,0,-3.1383824882,1.2296278602,-2.054627881
C,0,-2.83630206,1.9919853059,0.2207561168
C,0,-4.3319367652,0.6198322123,-1.7024810154
H,0,-2.7926350059,1.169815387,-3.0842961947
C,0,-4.0390018542,1.3987130501,0.5773806725
H,0,-2.2474182838,2.515140628,0.9639962428
C,0,-4.7710494143,0.7092419845,-0.3831067127
H,0,-4.9167773047,0.0804290131,-2.4381491874
H,0,-4.3925293961,1.4519627646,1.6002094663
Pt,0,0.7202271566,-0.7037182758,0.1957038648
I,0,0.2431093935,1.0014672687,2.2295061234
I,0,-1.7733217645,-1.7252554575,0.4314814114
I,0,1.3608874784,-2.6984617854,-1.5449280292
I,0,3.3687624674,-0.2427968571,0.5022966074
Br,0,-6.3854863031,-0.1354666669,0.1102438363

39
3D-a-IN3,Free Energies= -3393.234469
C,0,-3.7436186782,2.9978240611,-0.6301638468
C,0,-2.444666838,3.8177087403,-0.8452416841
C,0,-1.4809651405,3.5580758685,0.3042555825
C,0,-1.6008570133,2.1174224322,0.7881836949
C,0,-2.9121396195,1.9155321041,1.5441700716
C,0,-4.0353581353,2.7372932739,0.8577349921
H,0,-4.5903516323,3.5199796593,-1.0863640429
H,0,-1.9583049807,3.5148587605,-1.7788709189
H,0,-1.6100754628,1.5023900304,-0.1152814266
H,0,-3.1713053558,0.8519499345,1.5623348974
H,0,-4.1520379435,3.7013688731,1.3695324615
H,0,-2.6634357026,4.8876876134,-0.919840704
H,0,-3.6591787083,2.03451197,-1.1478213714
H,0,-4.9920614748,2.2160578567,0.9604922634
H,0,-2.8002475453,2.2370369208,2.5881570385
H,0,-1.6929865838,4.24422983,1.1444727102
O,0,-0.1177532603,3.6938897805,-0.0531134535
C,0,0.6056105604,3.1268393606,1.0091325162
H,0,0.6126577081,3.8333595326,1.8560661133
C,0,-0.2680254248,1.8868861765,1.5064908134
C,0,0.4273313739,0.5567950968,1.3589387822
H,0,-0.4024498374,2.0107817357,2.5892018667
H,0,1.4882908267,0.6039290193,1.5897014517
C,0,2.0308327628,2.8452306827,0.6154382476
C,0,2.9854375795,2.6211912192,1.6105491321
C,0,2.4151167085,2.7728610269,-0.7204025036
C,0,4.2933940346,2.2856891507,1.282696424
H,0,2.7074972003,2.7058504856,2.6596419658
C,0,3.722918202,2.4453706922,-1.0629651545
H,0,1.6834106995,2.9699257476,-1.4939423614
C,0,4.6482657648,2.1916430209,-0.059004856
H,0,5.0285962716,2.1007921232,2.0575961831
H,0,4.0131081877,2.3714180586,-2.1048362872
Pt,0,0.0414833843,-0.7411749932,-0.1454857596
I,0,0.2183233934,0.2967201743,-2.5483929226
I,0,2.6525469285,-1.3206102016,-0.1449115118
I,0,-0.2884688037,-1.1111918344,2.6409488715
I,0,-2.5385491676,-1.3407887514,-0.6263855688
Br,0,6.4166947819,1.697559138,-0.5198057359

39
3D-a-IN4,Free Energies= -3393.236351
C,0,0.8755044722,4.9413875864,0.239513413
C,0,2.3057064638,4.3356683368,0.2107796708
C,0,2.3165263873,3.0812114632,1.0671734267
C,0,1.0031675476,2.3156808965,0.9063266198
C,0,-0.0806705292,3.0452363737,1.7005628587
C,0,0.101028296,4.5787697445,1.5210685901
H,0,0.9316597417,6.0296107409,0.139364129
H,0,2.5842645012,4.0675262187,-0.8146174146
H,0,0.7405658411,2.3464089003,-0.1571267886
H,0,-1.0729804558,2.7336710481,1.3668552582
H,0,0.6342010609,4.9935649773,2.3858117061
H,0,3.0471478009,5.0528735981,0.5767906552
H,0,0.3075084797,4.5820622373,-0.6270636556
H,0,-0.878869613,5.0651721956,1.5026192249
H,0,-0.0051640743,2.7838069628,2.763856612
H,0,2.437549111,3.3582269894,2.1294776277
O,0,3.3288862383,2.1425541891,0.7481673848
C,0,2.9611131457,0.9914361303,1.4629385316
H,0,3.0979774891,1.1766815826,2.541923682
C,0,1.383450277,0.8714776066,1.2618276915
C,0,1.013353326,-0.2298468313,0.311735726
H,0,0.9347138926,0.5511790469,2.2122333368
H,0,1.4317633361,-1.189711091,0.6029265374
C,0,3.8006828964,-0.1958272696,1.0739081481
C,0,3.669049582,-1.3894214123,1.7876166334
C,0,4.6932096963,-0.1391892062,0.0057224736
C,0,4.3867217678,-2.5220600326,1.4236369038
H,0,2.9919601387,-1.4439009849,2.6378265155
C,0,5.4277989609,-1.2637240751,-0.3616218042
H,0,4.8150509532,0.7926100351,-0.5356771742
C,0,5.260688086,-2.4497635991,0.3431038189
H,0,4.2705534449,-3.4494460633,1.9726783716
H,0,6.1228046016,-1.2173542423,-1.1926126005
Pt,0,-0.8983522597,-0.4193302941,-0.3240151541
I,0,1.4908318289,-0.0731190568,-1.8229011089
I,0,-0.6012225228,-3.068026671,-0.0586789756
I,0,-2.4555810095,-0.3319923117,1.7881311662
I,0,-2.0473002539,1.7675440376,-1.3632075067
Br,0,6.2388229627,-3.9877084061,-0.1674234707

39
3D-a-TS3,Free Energies= -3393.203573
C,0,3.1534185016,4.1036007975,-1.2426386835
C,0,4.2402255907,3.4228768672,-0.3728626221
C,0,3.5889543553,2.4661591784,0.6189246415
C,0,2.3169134028,1.8567055296,0.0376435513
C,0,1.1973390177,2.8888612333,-0.1067022347
C,0,1.8180841816,4.2550529959,-0.4982274924
H,0,3.5070316937,5.084246021,-1.5739054018
H,0,4.9290456024,2.8495639659,-1.002525738
H,0,2.5694534913,1.4491523757,-0.9563156674
H,0,0.4833042362,2.5571397916,-0.869622051
H,0,1.9791830871,4.854495179,0.406193112
H,0,4.8357560085,4.167820234,0.1629575968
H,0,2.987319944,3.5155621014,-2.1539923609
H,0,1.1066428723,4.811551144,-1.114466628
H,0,0.6365100963,2.9918224949,0.8279535442
H,0,3.3351050544,2.9935535041,1.5538033619
O,0,4.4095872245,1.3458561637,0.9233300034
C,0,3.5954275447,0.2881413831,1.3802830221
H,0,3.5815859275,0.2502825136,2.4803799685
C,0,2.1787590855,0.6215636475,0.8649530855
C,0,1.0708618208,-0.189091411,1.0397104132
H,0,1.2780318692,0.7906049168,1.8632380244
H,0,1.2516006351,-1.0838596031,1.6420025796
C,0,4.0454376489,-1.0392833285,0.8168241787
C,0,3.8978228926,-2.2067634577,1.5631113193
C,0,4.5198068217,-1.114787194,-0.4915968903
C,0,4.2055183499,-3.4447403672,1.0076025563
H,0,3.5465348781,-2.1597502235,2.5913347543
C,0,4.8359904816,-2.3441866426,-1.0550595904
H,0,4.6517759681,-0.2060756222,-1.0694061823
C,0,4.6700448769,-3.5023160923,-0.3013831755
H,0,4.0916736578,-4.352731993,1.5883536907
H,0,5.2048087342,-2.4043599109,-2.0725428002
Pt,0,-0.7366122678,0.0355182849,0.1421050335
I,0,0.4881608931,-0.8863157231,-2.0718086762
I,0,-1.4764097278,-2.3788246652,0.9524274367
I,0,-1.5844181175,1.2793329764,2.3823665574
I,0,-2.9852718302,0.5972957698,-1.1824902873
Br,0,5.089679547,-5.1793347048,-1.0672236593

39
3D-P,Free Energies= -3393.229466
C,0,-4.9436397731,-3.0999643144,-0.0830010343
C,0,-5.4911107552,-1.6571211387,0.0661432656
C,0,-4.5590532769,-0.8299776942,0.9437192016
C,0,-3.1093614156,-1.2850220574,0.7796122435
C,0,-2.8339190982,-2.6902968856,1.3037811298
C,0,-4.113861428,-3.5443476761,1.1325689558
H,0,-5.7745033883,-3.7944284608,-0.2387510677
H,0,-5.5568455857,-1.1734102847,-0.9141990282
H,0,-2.9379056732,-1.2739973348,-0.3152122351
H,0,-1.9994622332,-3.1274989701,0.7440086379
H,0,-4.731332365,-3.4646503452,2.0362844992
H,0,-6.4982743743,-1.6645777597,0.493679546
H,0,-4.3155858245,-3.1656106304,-0.9805179084
H,0,-3.8416802063,-4.5995582425,1.0356966751
H,0,-2.536107165,-2.6627468891,2.3587614996
H,0,-4.8535033996,-0.9111539479,2.0042150676
O,0,-4.5101527356,0.5396249811,0.5770749153
C,0,-3.3252892227,1.0694046886,1.1421459722
H,0,-3.5126026616,1.356557693,2.1943424464
C,0,-2.356503302,-0.1060968014,1.2365359718
C,0,-1.0923960855,-0.0740643195,1.7668922907
H,0,-0.7407941692,-1.0052036897,2.2131314824
H,0,-0.7567653891,0.843031976,2.2443958297
C,0,-2.8601962634,2.2832743885,0.3815742792
C,0,-2.4065905389,3.4101389944,1.0619780317
C,0,-2.8862727962,2.284454959,-1.012798381
C,0,-1.9603022566,4.5275754564,0.3631232165
H,0,-2.4042509944,3.4278225177,2.148781982
C,0,-2.441360065,3.3913515192,-1.7225268781
H,0,-3.259685355,1.4161175778,-1.5439556617
C,0,-1.9747407714,4.5027225513,-1.0260933177
H,0,-1.6045017128,5.4040724862,0.8926652301
H,0,-2.4440377159,3.3867644466,-2.806390657
Pt,0,0.6260409719,-0.315110612,0.1420136322
I,0,-0.8547367967,-0.94370743,-2.0093285877
I,0,1.0180848381,2.2373006584,-0.3865699678
I,0,2.1874236977,-0.1527013248,2.3289850808
I,0,2.7596767317,-0.955416951,-1.2880928745
Br,0,-1.3315174652,6.0018084256,-1.9883064536

39
3D-b-IN1,Free Energies= -3393.205962
C,0,-3.7524394727,4.2638687567,-1.2452392824
C,0,-3.6986556706,2.9947288797,-2.0939415867
C,0,-3.0127207435,1.8464129767,-1.3325139119
C,0,-1.9629851475,2.3734372806,-0.3263247485
C,0,-1.2957516995,3.6456550629,-0.8679130083
C,0,-2.3303559476,4.786543859,-0.9612831455
H,0,-4.3469694366,5.0360791039,-1.7427657359
H,0,-4.702774514,2.6705958184,-2.3871936378
H,0,-2.4989499723,2.6253624547,0.5982235181
H,0,-0.4635235083,3.941361907,-0.2220491626
H,0,-2.0208951607,5.4776638269,-1.7525788492
H,0,-3.1491575625,3.193948063,-3.0223681575
H,0,-4.2683119219,4.0337643035,-0.3049700727
H,0,-2.3308828275,5.3591407606,-0.0276374596
H,0,-0.8720065017,3.4281119861,-1.8565804965
H,0,-2.5056415204,1.1805292691,-2.0477191311
O,0,-3.9276502038,1.0893614865,-0.5614992662
C,0,-4.552663698,0.0281609587,-1.2524530761
H,0,-5.2656267519,0.4209466354,-1.9946738391
C,0,-0.9587475183,1.3161091986,-0.0063468623
C,0,0.3288080411,1.2084773526,-0.2642865072
H,0,0.9714745316,1.9351065957,-0.7481331586
H,0,-3.7994522406,-0.5602788472,-1.7989550861
C,0,-5.2609343193,-0.8508402255,-0.2541676848
C,0,-5.2930500115,-2.2335978138,-0.4306674234
C,0,-5.8984840935,-0.2953187059,0.8562606868
C,0,-5.9553053577,-3.0549908094,0.4769645757
H,0,-4.7894062497,-2.6840537084,-1.2822836502
C,0,-6.556478745,-1.1042398813,1.776212506
H,0,-5.8672437205,0.7784251365,1.0093299256
C,0,-6.5819735518,-2.4807148156,1.5764874786
H,0,-5.9759492113,-4.1295721958,0.3347032693
H,0,-7.0460303429,-0.6695635955,2.6406053091
Pt,0,1.1479239821,-0.5114087375,0.3008516541
I,0,3.6217728704,-0.1241574729,-0.5333992436
I,0,1.8118070197,0.3503341057,2.7502127299
I,0,-1.574660318,-0.5090858279,0.9992316791
I,0,0.5453514369,-1.7801296012,-1.9943058016
Br,0,-7.4767171507,-3.5899483104,2.8252094329

39
3D-b-TS1,Free Energies= -3393.155818
C,0,2.0051384726,5.6244198508,-0.3892993293
C,0,2.0333395409,4.7223488117,0.8431334612
C,0,1.6557044118,3.2748971918,0.5041361328
C,0,0.5757012936,3.2749017523,-0.6655303662
C,0,-0.2980274082,4.5429298033,-0.6146357123
C,0,0.5652368085,5.7803330111,-0.9197455097
H,0,2.4277739586,6.6048200158,-0.1525667921
H,0,3.0292771837,4.6863021003,1.2923533832
H,0,1.136408161,3.2313433101,-1.6069643043
H,0,-1.1229225029,4.4650712108,-1.3302641887
H,0,0.0867440757,6.653672907,-0.4652015135
H,0,1.3470676118,5.1065896277,1.6062500014
H,0,2.6516472779,5.1865342258,-1.1591670262
H,0,0.5847408107,5.9591471511,-1.9999690082
H,0,-0.7503678415,4.6096125639,0.3811691665
H,0,1.2193755552,2.7863121948,1.3890911113
O,0,2.8119528968,2.60414958,0.1064969236
C,0,2.6961475424,1.1934953192,0.0363840457
H,0,2.1048858536,0.8201889205,0.8855256527
C,0,-0.1884034543,2.0573004772,-0.505290264
C,0,-0.8743665359,1.0358277099,-0.3463823091
H,0,-1.3813301294,1.6917327181,-1.2202328513
H,0,2.1647694655,0.9021596818,-0.883591361
C,0,4.0589875991,0.552243831,0.0481619866
C,0,4.1606351449,-0.8077232554,0.3468857311
C,0,5.2108820749,1.2719433772,-0.2588630127
C,0,5.3952706818,-1.446211731,0.3327249562
H,0,3.2673054768,-1.3757536509,0.5958864571
C,0,6.4535466161,0.6444730289,-0.2708176173
H,0,5.1395919353,2.3309052291,-0.4812259486
C,0,6.53465554,-0.711032188,0.0224577646
H,0,5.4715399115,-2.5018791716,0.5674674756
H,0,7.3509685569,1.2057401871,-0.5062162282
Pt,0,-1.5842029179,-0.6457836932,0.1743462077
I,0,-3.5979959334,0.5480211004,1.5246344842
I,0,-3.1324347189,-0.7474295149,-2.0446542027
I,0,0.3189137533,-2.0771283991,-1.0972385745
I,0,-0.1519002945,-0.7814792244,2.4554794127
Br,0,8.2248179261,-1.5705281305,0.0069166254

39
3D-b-IN2,Free Energies= -3393.199184
C,0,2.7724892452,5.3035977221,-0.5479922221
C,0,3.2900294201,4.7806755293,0.7916613446
C,0,2.8941899407,3.3139644384,0.9930747169
C,0,1.4459324141,3.0450124913,0.4871858756
C,0,0.6196487415,4.3442791222,0.4382799257
C,0,1.2283028098,5.3314848006,-0.5701928181
H,0,3.1753378775,6.3006240013,-0.7508784046
H,0,4.3811267474,4.8349604699,0.8448581235
H,0,1.5274307959,2.6647136703,-0.5353776548
H,0,-0.4133326738,4.1100608938,0.1629104028
H,0,0.8608751589,6.3380340955,-0.3423609849
H,0,2.8935795304,5.3870979611,1.6150561087
H,0,3.1517647401,4.645734787,-1.3379769836
H,0,0.8675391642,5.0853009289,-1.5750689883
H,0,0.586934841,4.7879743739,1.4423561964
H,0,2.9604652093,3.0580602737,2.0658528634
O,0,3.8468403207,2.5560560075,0.2809375309
C,0,3.7753691722,1.1570793927,0.4602008028
H,0,3.7053995495,0.9262022946,1.5375808301
C,0,0.710690711,2.0400243627,1.3332654147
C,0,0.0426224017,0.9948870115,0.8973554015
H,0,0.667064123,2.2450650015,2.4030232038
H,0,2.8854486419,0.7340482876,-0.0219902411
C,0,5.0190598026,0.5445886702,-0.1289531287
C,0,4.9431034795,-0.4201911679,-1.1308615115
C,0,6.2754310944,0.9524341769,0.323529387
C,0,6.0979992572,-0.9853566856,-1.6677275406
H,0,3.9732515363,-0.7390684494,-1.5014674953
C,0,7.436663279,0.4027126399,-0.2037693474
H,0,6.3446126228,1.7179703666,1.0909160803
C,0,7.3353196959,-0.5676909532,-1.1967879638
H,0,6.0324374135,-1.7371200715,-2.4463009167
H,0,8.4110745385,0.7207614992,0.1497331141
Pt,0,-0.3006710647,0.0509777056,-0.7796946724
I,0,-1.312401865,-0.2981258346,1.9381175917
I,0,-2.2269706735,1.7933164431,-1.3992562714
I,0,1.138471535,0.8320775078,-2.8242925207
I,0,1.2568586659,-2.104074028,-0.4661539518
Br,0,8.9167092904,-1.3261005863,-1.9194964567

39
3D-b-IN3,Free Energies= -3393.203060
C,0,-3.2577877155,4.5158343362,-0.3660459022
C,0,-2.6695946965,3.979477806,-1.682460053
C,0,-2.5878107977,2.4589555193,-1.6886510354
C,0,-1.6603611469,1.9453065205,-0.5428781692
C,0,-1.4562305141,2.9921666686,0.5734785901
C,0,-2.7641276024,3.7241556257,0.8654281622
H,0,-2.9866154191,5.572754415,-0.268200676
H,0,-3.2700607888,4.3115318886,-2.534778743
H,0,-2.1416423368,1.0677401073,-0.1012017345
H,0,-1.0782104939,2.4843811941,1.4669107201
H,0,-2.633830602,4.3922565775,1.7225828941
H,0,-1.655930633,4.3724850638,-1.8351621386
H,0,-4.3495770608,4.4740123158,-0.415892612
H,0,-3.5118150748,2.9796594011,1.1603756373
H,0,-0.681707917,3.711637735,0.2752805994
H,0,-2.1872406171,2.1154973142,-2.6560303211
O,0,-3.911938022,1.9831379261,-1.5568052381
C,0,-4.0917329933,0.5985043847,-1.7639688127
H,0,-4.795225608,0.474935361,-2.5986992648
C,0,-0.3209205364,1.5371443396,-1.0980172504
C,0,0.4120649688,0.5332538822,-0.6722998895
H,0,0.0953358896,2.1551336614,-1.8935751344
H,0,-3.1500810284,0.116237853,-2.0641556025
C,0,-4.6351075144,-0.0943163976,-0.5332211392
C,0,-4.6301030344,-1.4877564495,-0.4598508679
C,0,-5.1569684511,0.6358603677,0.5314665914
C,0,-5.1103741948,-2.1457401618,0.6655802916
H,0,-4.2232360876,-2.0724942007,-1.2805369205
C,0,-5.638659473,-0.0075923492,1.6683662357
H,0,-5.1815356392,1.7178558994,0.4687812611
C,0,-5.6024323646,-1.395505387,1.728737282
H,0,-5.0819398956,-3.2278004317,0.725901305
H,0,-6.0352579489,0.5650331906,2.4996751109
Pt,0,0.32455769,-0.8430499684,0.7098277426
I,0,2.3216772025,-0.1535672109,-1.347094342
I,0,1.6809403908,0.5560217409,2.5363668778
I,0,-1.7884737637,-0.814974077,2.2510895714
I,0,-0.8197507754,-2.6163783365,-0.9346040843
Br,0,-6.2173513546,-2.279582815,3.2905162485

39
3D-b-TS2,Free Energies= -3393.163481
C,0,-5.4296452822,-3.1527942741,-0.3001337291
C,0,-4.827205123,-2.5205750939,0.9533812193
C,0,-3.5158113442,-1.7789536449,0.6552287205
C,0,-2.8095014887,-2.3554964073,-0.587239348
C,0,-3.0002170829,-3.8781780783,-0.6350959562
C,0,-4.4839822842,-4.2278251234,-0.8719243073
H,0,-6.4059507923,-3.5910906736,-0.0724948555
H,0,-5.5136982563,-1.8037645384,1.4127013049
H,0,-3.3021551722,-1.9175853711,-1.4659970765
H,0,-2.3772918615,-4.3128801581,-1.42426422
H,0,-4.6978771734,-5.1975893213,-0.4102611631
H,0,-4.6327932891,-3.3026985262,1.6970824152
H,0,-5.610989477,-2.3681338565,-1.0445761952
H,0,-4.6691766042,-4.344259212,-1.9452352767
H,0,-2.6447237126,-4.3062257846,0.3109220283
H,0,-2.845862501,-1.8594641694,1.5237898081
O,0,-3.8146813573,-0.4017829963,0.4289099754
C,0,-2.7856482781,0.4453672568,0.8071322196
H,0,-2.5757878186,0.4023225914,1.8870283673
C,0,-1.3442950541,-1.9917205156,-0.699935213
C,0,-0.6404491796,-0.9589224836,-0.3505272963
H,0,-0.681976569,-2.701310563,-1.2142251013
H,0,-1.8133915174,0.0673152883,0.3382883028
C,0,-2.9771186128,1.8337173876,0.3051896328
C,0,-2.9908869397,2.9135736319,1.1865938609
C,0,-3.0894954734,2.0645360471,-1.0684292677
C,0,-3.1275785432,4.2129162976,0.7095961
H,0,-2.8869033013,2.7437507134,2.2544045307
C,0,-3.21303883,3.3560054449,-1.5582178831
H,0,-3.0600510841,1.2272933591,-1.7595994987
C,0,-3.2317408519,4.4210537422,-0.6604653952
H,0,-3.1394707018,5.053666788,1.3935251195
H,0,-3.2808688567,3.5386673453,-2.6243080784
Pt,0,0.7597317525,0.2689087507,-0.1223857223
I,0,2.3490444021,-1.8194236389,-0.7750445605
I,0,0.5462799564,0.9983043801,-2.7244241692
I,0,0.691209707,2.8348064188,0.5647433377
I,0,0.8542214265,-0.4297362045,2.5066711863
Br,0,-3.3903190208,6.1863756018,-1.321692586

39
3D-b-IN4,Free Energies= -3393.232969
C,0,3.8337920286,4.5464085164,-1.3408190092
C,0,3.9718226872,3.9481396451,0.0596771092
C,0,2.9794568699,2.806643516,0.2834731861
C,0,1.751259737,2.8576026297,-0.6444035979
C,0,1.3365493131,4.3281692528,-0.8008038788
C,0,2.4219511528,5.131061885,-1.5496194688
H,0,4.5922365005,5.320061924,-1.4918199897
H,0,4.9872953686,3.5877411575,0.2523084958
H,0,2.0632400085,2.4790122146,-1.6267076243
H,0,0.3813868057,4.3736750701,-1.3303106318
H,0,2.3989280638,6.1717481026,-1.2091508487
H,0,3.7652803367,4.7202283412,0.8096721147
H,0,4.037595872,3.766657338,-2.0849924462
H,0,2.1957953508,5.1481872979,-2.6206203391
H,0,1.1543506996,4.7523848389,0.1953838448
H,0,2.6686670231,2.7492152666,1.332163656
O,0,3.6807164521,1.5445629964,-0.0062799602
C,0,3.2841906081,0.4583601491,0.5370227396
H,0,2.4980226323,0.4942695797,1.2976133368
C,0,0.6720002413,1.97654451,-0.0888173029
C,0,0.3140105713,0.8388186872,-0.6793706851
H,0,0.2202055204,2.2926845266,0.8484697868
H,0,0.7245531799,0.5129940925,-1.6321864024
C,0,3.8783205866,-0.7759531986,0.1809363573
C,0,3.4655600782,-1.9326437291,0.8703543691
C,0,4.8537868881,-0.8635610889,-0.8386478146
C,0,4.0356784585,-3.1581669582,0.5658049188
H,0,2.6880007027,-1.865007047,1.6260768826
C,0,5.4083008341,-2.0834883843,-1.1491651359
H,0,5.1585275636,0.0295310596,-1.37314587
C,0,4.9948299752,-3.223639462,-0.4398275802
H,0,3.7147911971,-4.0555970769,1.0803643387
H,0,6.1527385932,-2.174595433,-1.9308825309
Pt,0,-1.0220524696,-0.4346259373,0.0539272449
I,0,-2.7553577362,1.3899304015,1.0169185086
I,0,-2.3427361561,-0.3828982234,-2.2864927241
I,0,0.3860926495,-2.5934423693,-0.8195501926
I,0,0.0987899067,-0.6446775126,2.5440401702
Br,0,5.7552379353,-4.8824289984,-0.8782258467

39
3D-b-TS3,Free Energies= -3393.217966
C,0,-4.7474473481,-3.6394293051,-1.0031068184
C,0,-5.2117142138,-2.2862065584,-0.4179975921
C,0,-4.0575884393,-1.5892795838,0.2937596926
C,0,-2.6975995563,-1.9288518134,-0.3228420956
C,0,-2.3646928616,-3.4180605527,-0.1178247561
C,0,-3.6492404098,-4.278776223,-0.144027444
H,0,-5.6054950326,-4.3121420964,-1.0891750589
H,0,-5.5718446899,-1.6294381576,-1.2166027835
H,0,-2.7749006282,-1.7085241734,-1.3951642341
H,0,-1.6673317898,-3.730798165,-0.9003561186
H,0,-4.0295922557,-4.4122809777,0.8770496055
H,0,-6.0407857108,-2.4322035001,0.2809295301
H,0,-4.3657908832,-3.4927832349,-2.0210096548
H,0,-3.412568977,-5.2798490504,-0.5158115768
H,0,-1.8385137032,-3.5552356094,0.8330576744
H,0,-4.0413464257,-1.8250234675,1.3679893386
O,0,-4.1395465461,-0.1738205467,0.1385963912
C,0,-3.1093919288,0.4639480348,0.6933764303
H,0,-2.9333559269,0.2869395473,1.7570344991
C,0,-1.7047933922,-0.9805056187,0.308343115
C,0,-0.8127483375,-0.2991427643,-0.4912060506
H,0,-1.3753891666,-1.2491951653,1.3095150177
H,0,-1.0960404767,-0.0421045787,-1.5119285876
C,0,-2.9425642888,1.8426379041,0.2273726664
C,0,-2.5195701146,2.8262957783,1.1230179339
C,0,-3.2670093103,2.1910955132,-1.0896931342
C,0,-2.4163356846,4.1483967892,0.7131851404
H,0,-2.2569844593,2.5608063084,2.1412129495
C,0,-3.1601715106,3.5063282093,-1.5079772065
H,0,-3.6062688405,1.4282933472,-1.7832134095
C,0,-2.7324603264,4.4754712943,-0.5999934322
H,0,-2.0770617208,4.9119958646,1.4026008432
H,0,-3.3987034504,3.7834701729,-2.5280152908
Pt,0,0.9771224863,0.1926845737,0.0014039865
I,0,1.6768743632,-2.2283525117,1.0007931736
I,0,1.8334227401,-0.625529184,-2.4379658086
I,0,0.7602948518,2.706687162,-0.9537951598
I,0,0.5267148265,1.0607036715,2.5288532148
Br,0,-2.5647095623,6.2649158575,-1.1734378017

39
3D-b-IN5,Free Energies= -3393.238587
C,0,6.0444787642,-0.3452985671,-0.1214094368
C,0,5.4859763989,0.6296510732,-1.1867888728
C,0,4.0076559269,0.3477279776,-1.4222447698
C,0,3.2949813931,-0.0356549917,-0.129821524
C,0,3.7735090455,-1.4155099812,0.3501419469
C,0,5.2445926768,-1.6549235246,-0.0702722331
H,0,7.0993730137,-0.5555096986,-0.321683718
H,0,5.589692656,1.6682175357,-0.8539669032
H,0,3.5301419932,0.7290275299,0.6238979723
H,0,3.6952789261,-1.4790841172,1.4396524231
H,0,5.2764105573,-2.133423581,-1.0568249968
H,0,6.0346807198,0.5374807832,-2.1292681
H,0,6.0082585528,0.1275287481,0.8684618103
H,0,5.7124804505,-2.357555141,0.6262360155
H,0,3.1323977983,-2.2059984764,-0.0575298803
H,0,3.8939134659,-0.4852886255,-2.137190402
O,0,3.3150352147,1.4768455598,-1.9069736266
C,0,1.9374056879,1.3654572341,-1.5871492109
H,0,1.3603986037,1.1114606682,-2.4857313684
C,0,1.8336018231,0.1338064854,-0.5887348888
C,0,0.8091691916,0.3628509336,0.4796485406
H,0,1.5703352142,-0.7546759945,-1.1665168754
H,0,0.776310242,1.3765003828,0.8740715831
C,0,1.4551304287,2.6929171756,-1.0463804253
C,0,0.2341219436,3.2227690515,-1.4539934451
C,0,2.2119828891,3.3939279894,-0.1027140559
C,0,-0.2542908918,4.4053068528,-0.9068311502
H,0,-0.3586703343,2.7031833808,-2.1995632474
C,0,1.737409306,4.5739308739,0.4557724935
H,0,3.1902920488,3.020890275,0.1840745119
C,0,0.4977967382,5.0653891644,0.0546541514
H,0,-1.214324125,4.7990741053,-1.2197424916
H,0,2.324304931,5.112900049,1.1910077127
Pt,0,-1.0292980958,-0.4093572488,0.168412182
I,0,-0.5550172099,-2.8926869837,-0.8029046302
I,0,0.7502856096,-0.8985579632,2.2922364117
I,0,-2.1250228607,1.7049422707,1.3943396629
I,0,-2.1871319255,0.2185981589,-2.0969667982
Br,0,-0.1673352885,6.6587877058,0.8307993632

39
3D-b-IN6,Free Energies= -3393.239399
C,0,-0.6482709771,4.7420633677,-1.4518357896
C,0,0.866499301,4.5041682389,-1.7001498208
C,0,1.4225787877,3.6815187753,-0.5504329112
C,0,0.4029286359,2.635603832,-0.1017859361
C,0,-0.69140655,3.3323817012,0.705777812
C,0,-1.0165120074,4.70112127,0.0431687099
H,0,-0.9467592322,5.7043380855,-1.878769689
H,0,1.0173402723,3.9559276917,-2.6367528175
H,0,-0.0420201846,2.2127115458,-1.0118203753
H,0,-1.5862714666,2.7092256894,0.756469237
H,0,-0.476636744,5.5027326768,0.5624533264
H,0,1.4064110349,5.4524257697,-1.7841514438
H,0,-1.2316510568,3.9777408353,-1.9791952508
H,0,-2.0814263819,4.92152641,0.1636861698
H,0,-0.355361374,3.4856559981,1.7385773214
H,0,1.6450977243,4.3437064573,0.304682346
O,0,2.5923455987,2.9454474204,-0.8451234847
C,0,2.7420080474,2.0929954828,0.2631792189
H,0,3.0060543967,2.6895288351,1.1523088024
C,0,1.2789245156,1.5386692608,0.5660828555
C,0,1.0356723957,0.228014268,-0.1141232757
H,0,1.1007297986,1.465762192,1.6405486737
H,0,1.4383217824,0.1744685296,-1.1250901584
C,0,3.8269200142,1.0822525473,0.0183465882
C,0,4.5420789475,0.5627617141,1.0972480327
C,0,4.0954751701,0.6075119873,-1.2660081601
C,0,5.4874493019,-0.440558531,0.9108674887
H,0,4.3561291551,0.9372613532,2.1011055455
C,0,5.0401099067,-0.3936323617,-1.4674484376
H,0,3.5703502905,1.032809306,-2.1153944337
C,0,5.7211445016,-0.9190376084,-0.3742820846
H,0,6.037791399,-0.8438975646,1.7534261998
H,0,5.2426950412,-0.7650590197,-2.4656329564
Pt,0,-0.77575974,-0.6738566356,-0.0524225703
I,0,-2.8496577897,0.5853129322,-1.0573098793
I,0,-0.3278111017,-1.7827076645,-2.4670918208
I,0,1.6816289217,-1.6176034359,0.8855743523
I,0,-1.5790931887,-0.0851592289,2.4496115508
Br,0,6.9909304937,-2.2978046433,-0.6362356453

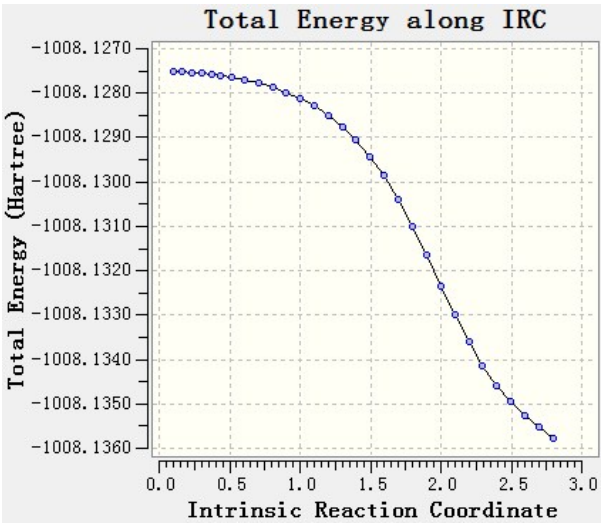
39
3D-b-TS4,Free Energies= -3393.203824
C,0,-2.9926881432,4.4261530226,0.3287478697
C,0,-4.0837191285,3.4479723573,-0.1750027726
C,0,-3.4320474146,2.3723684214,-1.0307692717
C,0,-2.0429737097,2.0167037836,-0.4918828453
C,0,-1.0663753381,3.1583326395,-0.8055028133
C,0,-1.8067521431,4.5130016009,-0.6441184019
H,0,-3.4253933604,5.4190618019,0.4802230182
H,0,-4.5874172752,2.9650994662,0.6693201877
H,0,-2.1131986397,1.8802274879,0.5998740938
H,0,-0.2058180822,3.1085923427,-0.1387296601
H,0,-2.1704034686,4.8597666344,-1.6191734812
H,0,-4.8473999882,3.9734844283,-0.7557852024
H,0,-2.6244040715,4.0987366483,1.3087945877
H,0,-1.0936439536,5.2650422358,-0.295749904
H,0,-0.685000043,3.0603276574,-1.8275239205
H,0,-3.3211109832,2.7254243253,-2.0699465903
O,0,-4.14637455,1.1498206466,-1.0400426266
C,0,-3.277088343,0.1544738076,-1.511097508
H,0,-3.2587482179,0.129502876,-2.6133590334
C,0,-1.8716896635,0.6235161514,-1.0060448524
C,0,-0.8341803751,-0.2961415491,-0.9894781695
H,0,-0.8953600456,0.5151314447,-1.9827671255
H,0,-1.0975700642,-1.2599398053,-1.4231182109
C,0,-3.6380358812,-1.1969792848,-0.9511406203
C,0,-3.4186226265,-2.3520158433,-1.6997020663
C,0,-4.0840268828,-1.3009262895,0.3655138607
C,0,-3.619120365,-3.6072541139,-1.1342337549
H,0,-3.0842077074,-2.2829824049,-2.7326239565
C,0,-4.3007872651,-2.5484003242,0.9348029838
H,0,-4.2630442497,-0.4021893372,0.9459994639
C,0,-4.0553104376,-3.6934186971,0.1827119731
H,0,-3.4362665459,-4.5065602394,-1.7106195343
H,0,-4.6427738277,-2.6331263932,1.9598039816
Pt,0,0.9038506747,-0.3243471445,-0.0874240501
I,0,0.6696086556,1.3077688654,2.050682317
I,0,-0.1602951034,-2.3225094214,1.4079669219
I,0,1.7038913746,-2.1443884344,-1.9359235848
I,0,2.2174868347,1.5671924382,-1.4858402938
Br,0,-4.3167033253,-5.393234261,0.9655755019

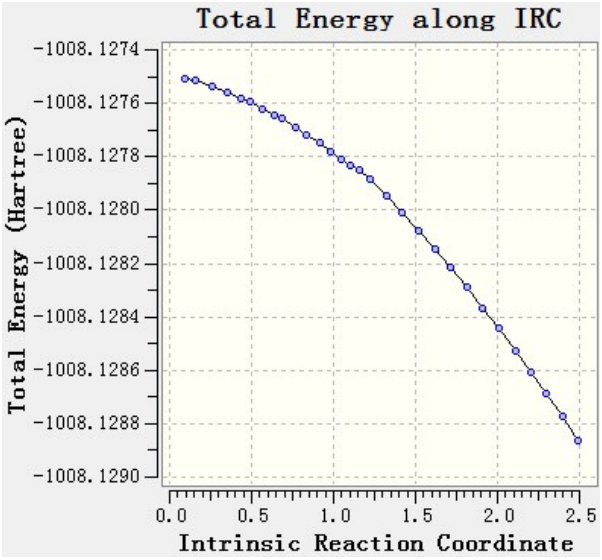
6. The .xyz files of optimized transition states and their free energies at L1/BS3

(1). Transition state 1D-b-TS2

38
1D-b-TS2, Free Energies=-1007.925396

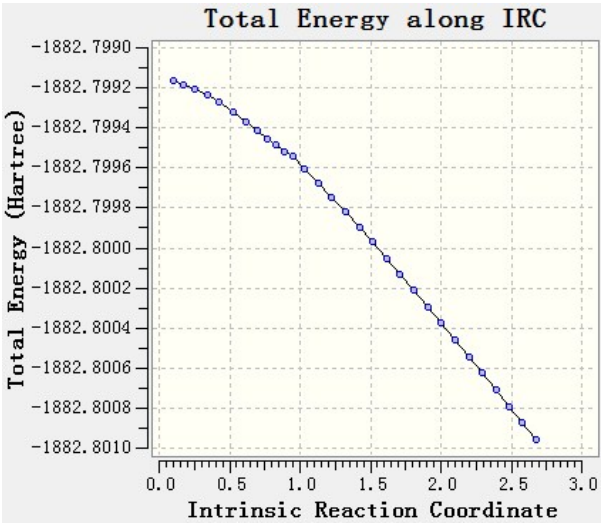
C	2.584600	3.281900	1.114500
O	1.921300	2.236700	1.869400
C	2.237700	0.992000	1.328600
C	3.583200	1.163000	0.622300
C	3.399700	2.572700	0.021200
H	1.821700	3.954600	0.713200
H	3.218100	3.834600	1.817000
H	2.192900	0.232200	2.112300
H	4.351100	3.065400	-0.181700
H	2.819600	2.535400	-0.906900
C	4.000300	0.011300	-0.330300
C	3.132200	-0.151700	-1.606100
H	3.608500	-0.904800	-2.232600
H	3.150700	0.788500	-2.168900
C	1.686400	-0.574400	-1.442600
C	0.658800	-0.222400	-0.718600
H	1.342000	-1.352600	-2.136800
C	5.463400	0.272800	-0.782800
O	6.124100	1.240900	-0.477300
O	5.916700	-0.726200	-1.560500
C	4.026400	-1.344300	0.418400
O	3.505600	-2.362200	0.020800
O	4.726400	-1.253200	1.563600
C	7.279200	-0.604600	-2.027300
H	7.460800	-1.501800	-2.617300
H	7.388600	0.293200	-2.639700
H	7.963400	-0.550700	-1.177700
C	4.844200	-2.472100	2.333100
H	5.431000	-2.201500	3.209900
H	3.854300	-2.832000	2.621500
H	5.352300	-3.239100	1.744300
H	4.352100	1.223300	1.399000
Pt	-1.253100	-0.040400	-0.370800
I	-3.939700	0.140600	-0.447100
I	-1.387900	-2.746800	-0.725500
I	-1.259200	-0.273300	2.317700
I	-1.015700	2.662100	-0.694400
H	1.438700	0.691300	0.571700

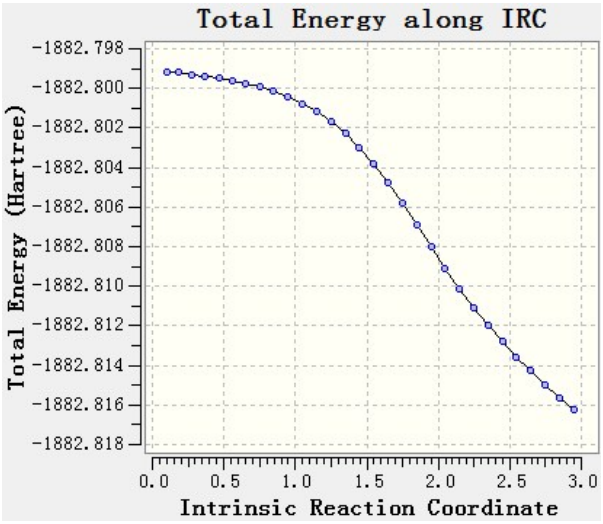




(2). Transition state 1A-a4-TS1

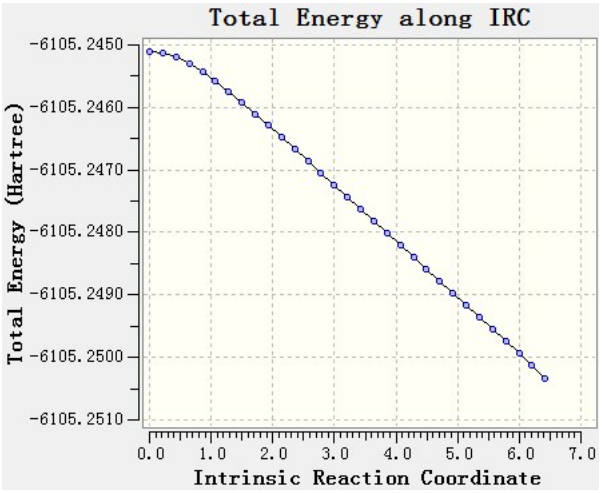
36
1A-a4-TS1, Free Energies=-1882.587974
C -0.49643287 -2.33123164 2.04704590
O -0.07787674 -1.03345315 2.49048229
C -0.72277015 -0.09151543 1.68837589
C -2.12475132 -0.63413537 1.36771858
C -1.97079450 -2.16635201 1.62795583
H 0.13746232 -2.64456676 1.20459073
H -0.34205692 -3.02491110 2.87558998
H -0.67300894 0.89266216 2.15558614
H -2.64443245 -2.47408864 2.43082322
H -2.20760220 -2.78117830 0.75394341
C -2.61771643 -0.25299893 -0.05476457
C -1.54717547 -0.60756800 -1.12770545
H -1.96688891 -0.37355428 -2.11916988
H -1.31784127 -1.67709102 -1.11512585
C -0.34672230 0.20581310 -1.07269339
C 0.60681646 0.99145140 -1.42526716
H 0.62064615 1.30598821 -2.47989632
C -3.95550385 -0.97705309 -0.31075530
O -4.90869111 -0.86407369 0.42919104
O -3.94350549 -1.73344217 -1.41920893
C -2.94698350 1.25420441 -0.22732503
O -3.21921066 1.72227062 -1.31481477
O -2.89520635 1.93752103 0.91159518
C -5.18406039 -2.40883561 -1.73892410
H -4.98058065 -2.96189899 -2.65462845
H -5.46391872 -3.08362453 -0.92740497
H -5.97638509 -1.67395975 -1.89394778
C -3.13336743 3.36642834 0.81830984
H -3.14866009 3.71732618 1.84864102
H -2.31543079 3.83124766 0.26511296
H -4.08761387 3.55167340 0.32241090
H -0.14352090 0.02455184 0.71466845
H -2.84312987 -0.21327106 2.07271913
Pt 2.07907827 1.73343398 -0.41229635
Cl 3.68591231 0.30393087 -1.28981701
Cl 0.79971183 3.32506131 0.72162084

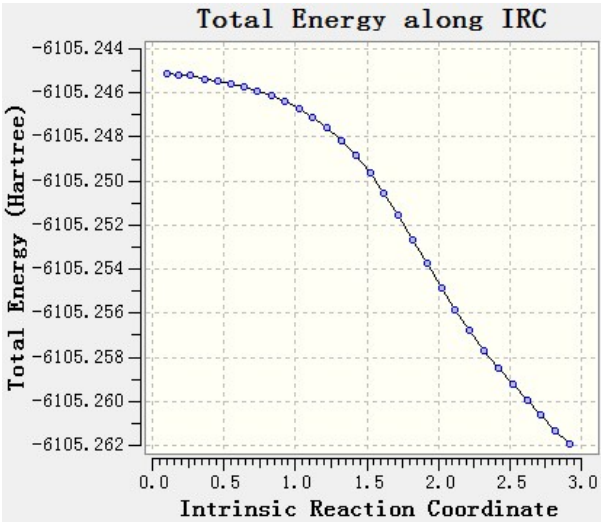




(3). Transition state 1B-a4-TS1

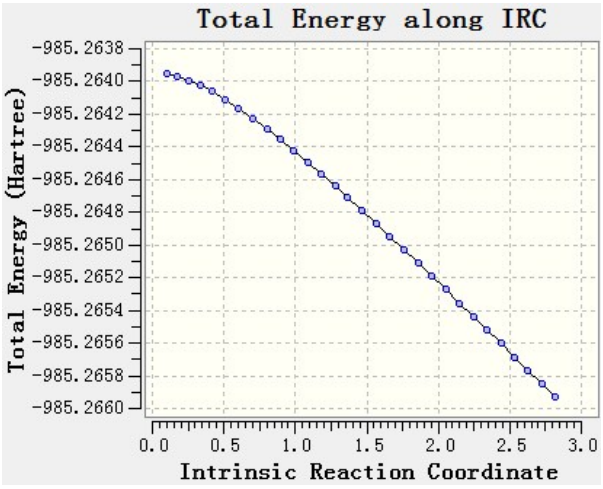
36
1B-a4-TS1, Free Energies=-6105.037061
C -1.4295287 -2.66613077 2.0986672
O -0.5819693 -1.60731247 2.5646715
C -0.7854911 -0.51310468 1.7242994
C -2.2703061 -0.49979495 1.3283062
C -2.7116288 -1.97430971 1.5935922
H -0.9132466 -3.21114048 1.2949493
H -1.5896155 -3.34849896 2.9354490
H -0.3935943 0.39228412 2.1894805
H -3.4954016 -1.99436751 2.3540996
H -3.1100926 -2.47437930 0.7052650
C -2.5130413 0.01277407 -0.1174275
C -1.6021294 -0.73460768 -1.1333385
H -1.8473074 -0.37141090 -2.1441934
H -1.7978760 -1.81082752 -1.1184596
C -0.1873219 -0.43881198 -1.0058935
C 1.0160964 -0.10012666 -1.3041438
H 1.1959989 0.17315735 -2.3554706
C -4.0105090 -0.16236431 -0.4447138
O -4.8876525 0.31262719 0.2436572
O -4.2273946 -0.88787492 -1.5525599
C -2.2472694 1.53091079 -0.3024687
O -2.2519397 2.04593273 -1.4026472
O -2.0287244 2.17124623 0.8422094
C -5.6129675 -1.05643156 -1.9386896
H -5.5858207 -1.66166924 -2.8435362
H -6.1649189 -1.56326877 -1.1445322
H -6.0642086 -0.08166101 -2.1337980
C -1.7384893 3.58939324 0.7395632
H -1.6616782 3.93650954 1.7684898
H -0.7924612 3.72777465 0.2132696
H -2.5481400 4.09534274 0.2106344
H -0.1568933 -0.64689399 0.7837179
H -2.8139721 0.17078136 1.9953447
Pt 2.6191361 0.00689351 -0.2257869
Br 3.5830915 -2.10147015 -1.0099604
Br 2.0701766 2.13600505 0.8745956

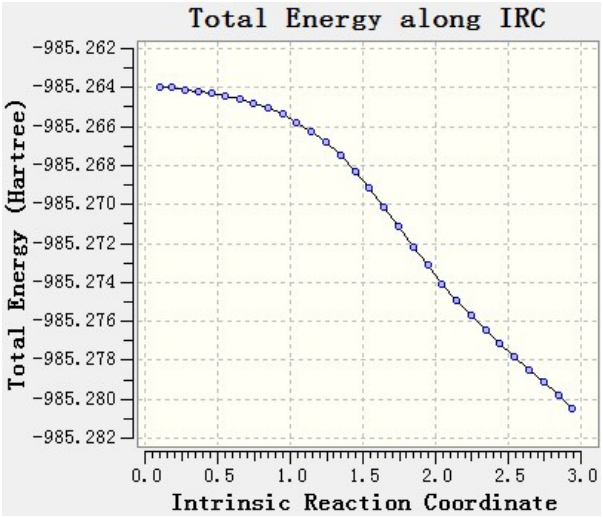




(4). Transition state 1C-a4-TS1

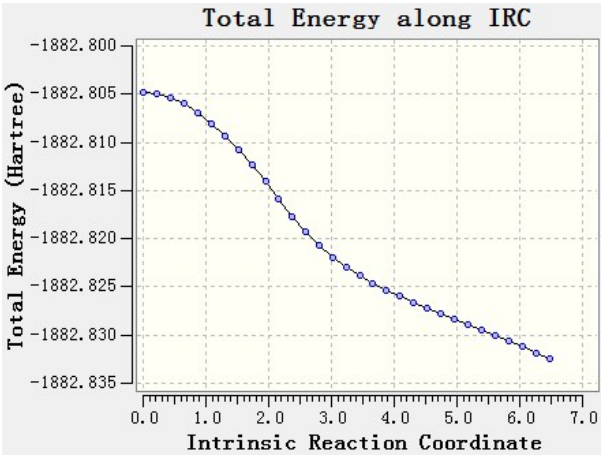
36
1C-a4-TS1, Free Energies=-985.058157
C -1.8160080 -2.3823615 2.50839905
O -1.1028933 -1.1660404 2.77600646
C -1.4268702 -0.2640376 1.76561654
C -2.8999855 -0.4903821 1.39239221
C -3.1628548 -1.9447370 1.89767789
H -1.2274315 -2.9949286 1.81062759
H -1.9075740 -2.9203855 3.45361816
H -1.1469560 0.7469785 2.06535166
H -3.9540937 -1.9373175 2.65056112
H -3.4786055 -2.6281556 1.10333285
C -3.1966496 -0.2506825 -0.11302244
C -2.1917576 -1.0284136 -1.00895024
H -2.4618078 -0.8510483 -2.06202195
H -2.2631888 -2.1062514 -0.83447295
C -0.8198959 -0.5588847 -0.92411741
C 0.3561706 -0.1772068 -1.27998611
H 0.5003462 -0.0423782 -2.36435790
C -4.6581078 -0.6638076 -0.38574136
O -5.5920408 -0.1973843 0.23015710
O -4.7747788 -1.5803516 -1.35835306
C -3.1286560 1.2384948 -0.54375057
O -3.2156454 1.5659378 -1.71017555
O -2.9752236 2.0785240 0.47690543
C -6.1255356 -1.9817633 -1.69280878
H -6.0162163 -2.7179521 -2.48769350
H -6.6147042 -2.4176671 -0.81937166
H -6.6943668 -1.1159841 -2.03735292
C -2.8872773 3.4874346 0.14020187
H -2.8309078 4.0032127 1.09715254
H -1.9858619 3.6653580 -0.44883994
H -3.7737775 3.7893677 -0.42028179
H -0.7794119 -0.4827990 0.85077668
H -3.5222851 0.2091638 1.95249649
Pt 1.9701875 0.1958793 -0.28252078
I 3.0011923 -2.2452223 -0.49929868
I 1.4415986 2.7446780 0.28761598

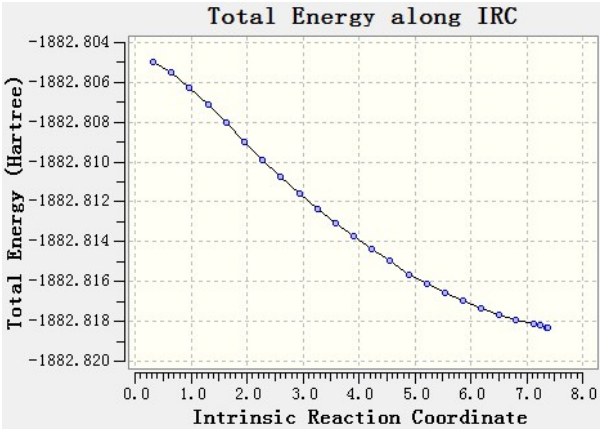




(5). Transition state 1A-a2-TS1

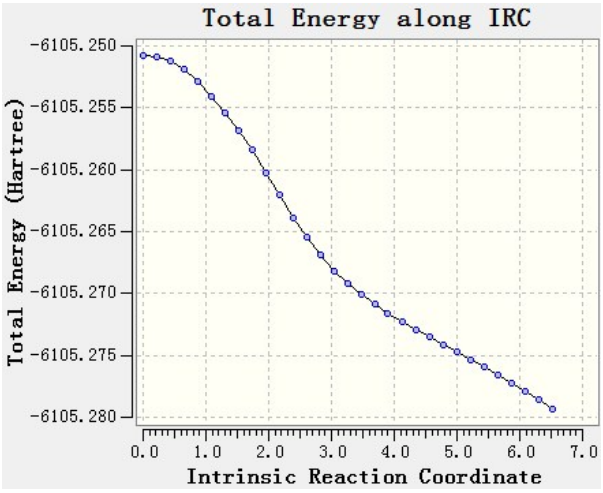
36
1A-a2-TS1, Free Energies=-1882.593740
C -3.7190381 -1.9917800 -2.44231080
O -2.5549633 -2.7294891 -1.98535596
C -1.9908054 -2.1152727 -0.88632355
C -2.9493800 -1.0548185 -0.35100486
C -3.7470699 -0.6940027 -1.62922777
H -3.6213767 -1.8369341 -3.51955696
H -4.5933943 -2.6240677 -2.25181406
H -1.6032445 -2.8501580 -0.18060314
H -4.7628511 -0.3705876 -1.39553498
H -3.2555920 0.1111792 -2.18558986
C -2.2418091 0.1462552 0.33398965
C -1.0464962 0.6474641 -0.53707598
H -0.5182446 1.4449811 -0.00614669
H -1.4111348 1.0850036 -1.47161475
C -0.0643435 -0.4099160 -0.81259863
C 1.1097477 -0.9498029 -0.89544689
H 1.3714744 -1.9604533 -1.19434115
C -3.2871229 1.2543640 0.57776256
O -4.3935956 1.0168519 1.01626207
O -2.8401879 2.4724391 0.26017691
C -1.6731311 -0.1747198 1.73889009
O -1.4491740 0.6885357 2.55853073
O -1.4151520 -1.4765488 1.91008246
C -3.7277076 3.5769379 0.55485388
H -3.1903558 4.4675869 0.23320094
H -4.6646301 3.4640232 0.00540216
H -3.9307626 3.6090702 1.62704573
C -0.7263483 -1.8314588 3.14128314
H -0.6976570 -2.9200310 3.14561283
H 0.2837043 -1.4168832 3.12049138
H -1.2803519 -1.4484657 3.99961323
H -1.0163418 -1.5377402 -1.23253236
H -3.6197438 -1.5192062 0.37915989
Pt 2.5291480 0.2649616 -0.32976037
Cl 2.9804544 -0.9655897 1.60377180
Cl 2.3594711 1.7407974 -2.11947469

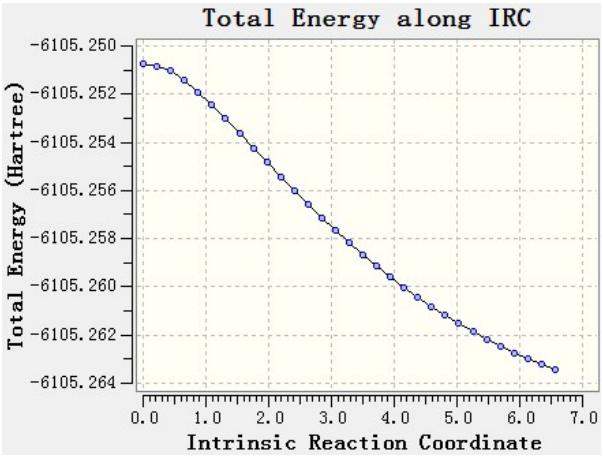




(6). Transition state 1B-a2-TS1

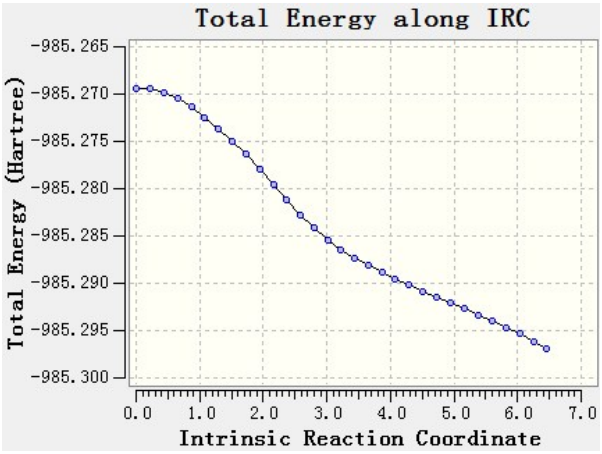
36
1B-a2-TS1, Free Energies=-6105.042350
C -3.7268926 -1.6021413 -2.719268406069
O -2.5960391 -2.4253763 -2.330868303470
C -2.0396310 -1.9631098 -1.154986092423
C -2.9811747 -0.9460162 -0.515874171696
C -3.7361863 -0.4095923 -1.757807050176
H -3.5997130 -1.3234220 -3.768163403998
H -4.6238240 -2.2241587 -2.622962223974
H -1.6916959 -2.7889280 -0.534168940231
H -4.7475548 -0.0835940 -1.508589663095
H -3.2075377 0.4395389 -2.203817859048
C -2.2564957 0.1404532 0.324197791382
C -1.0281553 0.7092796 -0.453582580433
H -0.4915505 1.4168192 0.185525881385
H -1.3575000 1.2712491 -1.332893695346
C -0.0687979 -0.3347412 -0.837723840523
C 1.0892369 -0.9023510 -0.956944576415
H 1.3222405 -1.8810459 -1.365961515348
C -3.2771897 1.2408416 0.681474552085
O -4.3927536 0.9835916 1.084349502105
O -2.7996417 2.4752130 0.501203837534
C -1.7298878 -0.3647054 1.690996365936
O -1.4625132 0.3918013 2.598357661768
O -1.5641187 -1.6920330 1.728754632718
C -3.6657357 3.5620576 0.905078146621
H -3.1049163 4.4692714 0.686269784741
H -4.5984371 3.5308517 0.338019108238
H -3.8807002 3.4835665 1.972540209777
C -0.9319409 -2.2178958 2.928430561206
H -0.9748094 -3.3005771 2.819490488636
H 0.1029982 -1.8717009 2.970396021340
H -1.4813057 -1.8888223 3.811776048790
H -1.0441065 -1.3790893 -1.411524503262
H -3.6821501 -1.4734925 0.138573612598
Pt 2.5380080 0.1961655 -0.243163407777
Br 2.4607260 1.9606223 -1.941882825307
Br 2.9612351 -1.3159866 1.649438040200

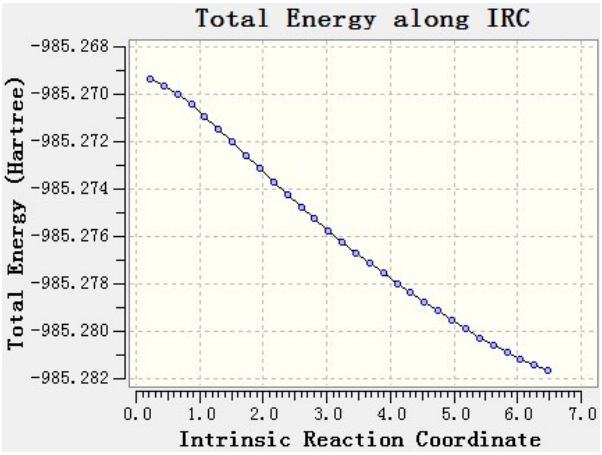




(7). Transition state 1C-a2-TS1

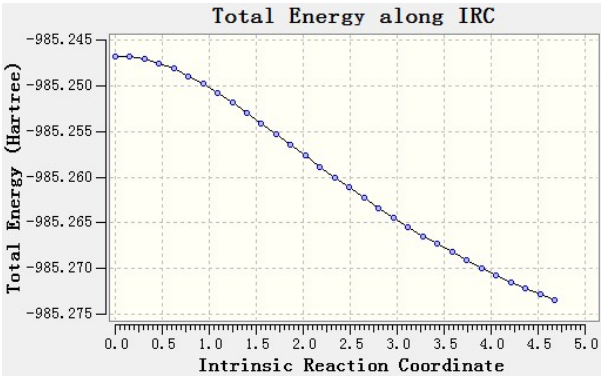
36
1C-a2-TS1, Free Energies=-985.063116
C -3.6889955 -1.5922175 -2.7289928
O -2.5775785 -2.4307099 -2.3195272
C -2.0366641 -1.9746536 -1.1321751
C -2.9777800 -0.9457815 -0.5125673
C -3.6978320 -0.3976837 -1.7697537
H -3.5393700 -1.3165740 -3.7757617
H -4.5971881 -2.2000826 -2.6479024
H -1.7154720 -2.8059344 -0.5041735
H -4.7084747 -0.0538703 -1.5420998
H -3.1451648 0.4409936 -2.2062147
C -2.2564874 0.1281696 0.3449790
C -1.0146080 0.7030830 -0.4083083
H -0.4822186 1.3882580 0.2587073
H -1.3332757 1.2932507 -1.2731530
C -0.0528155 -0.3290112 -0.8184245
C 1.1073717 -0.8702746 -1.0128254
H 1.3325270 -1.8429504 -1.4412543
C -3.2768203 1.2318929 0.6975884
O -4.3981782 0.9761598 1.0849470
O -2.7920821 2.4654948 0.5327304
C -1.7590282 -0.3905975 1.7174142
O -1.4957955 0.3572565 2.6330828
O -1.6181082 -1.7212546 1.7561337
C -3.6593912 3.5530188 0.9327042
H -3.0928934 4.4595726 0.7260302
H -4.5852143 3.5282752 0.3542101
H -3.8874322 3.4688042 1.9970315
C -1.0498070 -2.2601173 2.9803523
H -1.0597886 -3.3406757 2.8460232
H -0.0292430 -1.8913777 3.1004549
H -1.6619230 -1.9641898 3.8339522
H -1.0339418 -1.4038074 -1.3656388
H -3.7007923 -1.4624367 0.1263436
Pt 2.5875742 0.2620794 -0.4226735
I 3.1540764 -1.1885811 1.7407974
I 2.4989219 2.0272731 -2.4126676

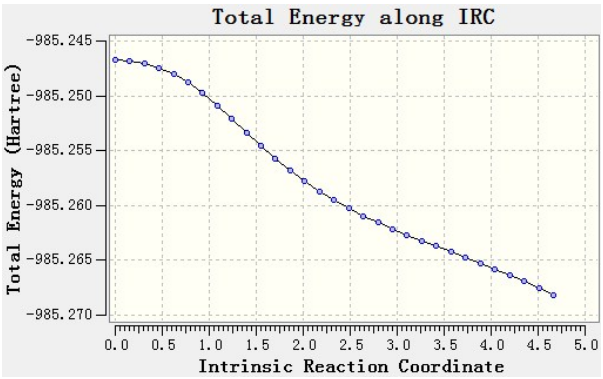




(8). Transition state 1C-a3-TS2

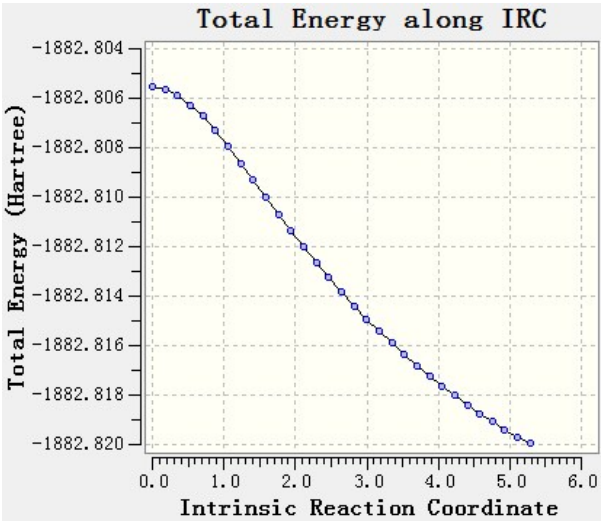
36
1C-a3-TS2, Free Energies=-985.041026
C -3.1740268 -0.8135786 3.09382763
O -2.4379489 -1.9737131 2.54065828
C -2.0326374 -1.6750107 1.29938592
C -2.3132997 -0.2098705 1.01606107
C -3.5851365 -0.0061957 1.85043034
H -3.9920325 -1.2406635 3.67443868
H -2.4992049 -0.2591911 3.75297493
H -0.7024696 -1.7781356 1.10517779
H -3.7679903 1.0462335 2.07233213
H -4.4797804 -0.4318440 1.38312624
C -2.0957933 0.0975748 -0.48012542
C -0.7926229 -0.7140137 -0.88729213
H -0.1657503 -0.1028185 -1.54037336
H -1.0833033 -1.5993046 -1.45844609
C 0.0282425 -1.1098241 0.29445203
C 1.2030210 -0.9377008 0.87462747
H 1.4397288 -1.3519996 1.85480576
C -3.3494855 -0.2983343 -1.28042200
O -4.2407304 0.4755972 -1.55277074
O -3.3882406 -1.6144601 -1.56996172
C -1.8564858 1.5945358 -0.77158471
O -1.4310117 1.9823413 -1.83562479
O -2.1574428 2.3824125 0.26764485
C -4.5509462 -2.0667828 -2.30622325
H -4.3928554 -3.1325969 -2.46463769
H -5.4586831 -1.8865467 -1.72648532
H -4.6155705 -1.5366626 -3.25818207
C -1.8945042 3.7960654 0.07796065
H -2.2257042 4.2740892 0.99874074
H -0.8245804 3.9481531 -0.07573839
H -2.4569583 4.1649277 -0.78170614
H -2.2534372 -2.4571999 0.56894446
H -1.5332317 0.3534507 1.53910407
Pt 2.6256265 0.0535249 0.01370345
I 2.1119432 2.3292089 1.33153207
I 3.5161811 -1.9087578 -1.54013475

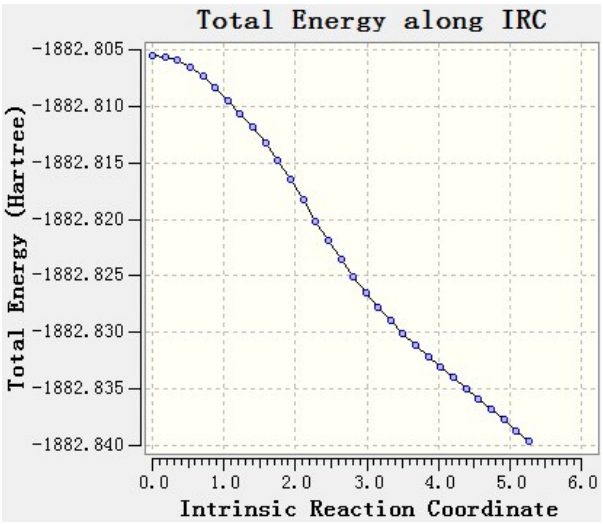




(9). Transition state 1A-a1-TS1

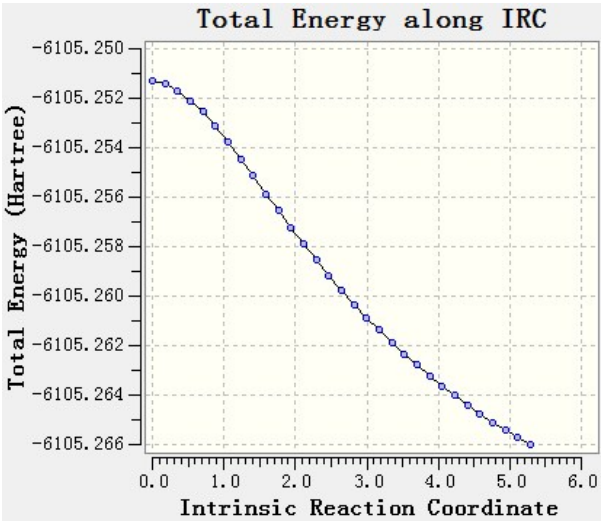
36
1A-a1-TS1, Free Energies=-1882.594237
C -1.3968978 3.5890030 0.3124249
O -1.3062319 3.2626166 -1.1051652
C -1.7164297 1.9666209 -1.3237853
C -2.4586844 1.4563052 -0.0933798
C -1.8112959 2.2974175 1.0329524
H -0.4247447 3.9702766 0.6334073
H -2.1423591 4.3859879 0.4049753
H -2.2089907 1.8752933 -2.2974023
H -2.5119329 2.4785735 1.8484348
H -0.9311856 1.7986397 1.4481463
C -2.3283232 -0.0831481 0.0222323
C -0.8360921 -0.5418296 0.1112458
H -0.7657097 -1.5717875 -0.2466897
H -0.5076292 -0.5164203 1.1562332
C 0.1243587 0.2936847 -0.6391872
C 1.2952687 0.7757057 -0.8913228
H 1.6053485 1.5872280 -1.5408778
C -3.0828324 -0.5955623 1.2630673
O -3.7102533 0.0983582 2.0320743
O -2.9436354 -1.9261019 1.3781409
C -2.9729630 -0.7121692 -1.2345746
O -2.3523459 -1.1859070 -2.1608720
O -4.3117541 -0.6190779 -1.1871611
C -3.5954280 -2.5434131 2.5123266
H -3.3688199 -3.6052538 2.4292538
H -3.1968172 -2.1324670 3.4421985
H -4.6723391 -2.3679420 2.4655828
C -5.0311986 -1.1601744 -2.3200240
H -6.0842229 -1.0039172 -2.0908283
H -4.7482798 -0.6319092 -3.2330526
H -4.8086082 -2.2234542 -2.4305614
H -0.7840070 1.2618483 -1.4509972
H -3.5225097 1.7014278 -0.1770447
Pt 2.6267114 -0.2736244 0.0966217
Cl 3.5780523 -1.2440021 -1.7790792
Cl 1.9653021 0.4989824 2.2097079

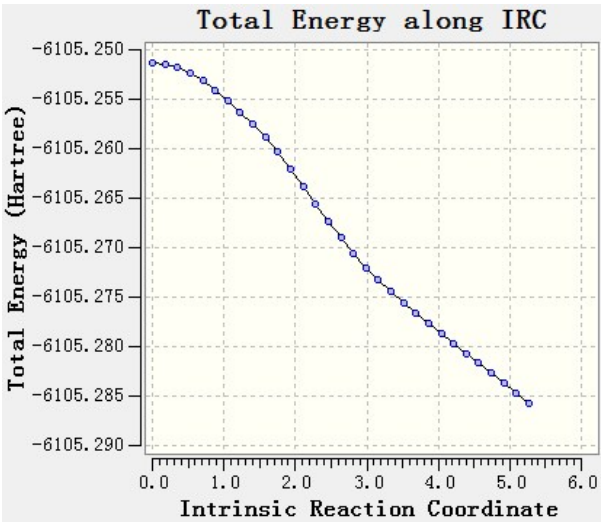




(10). Transition state 1B-a1-TS1

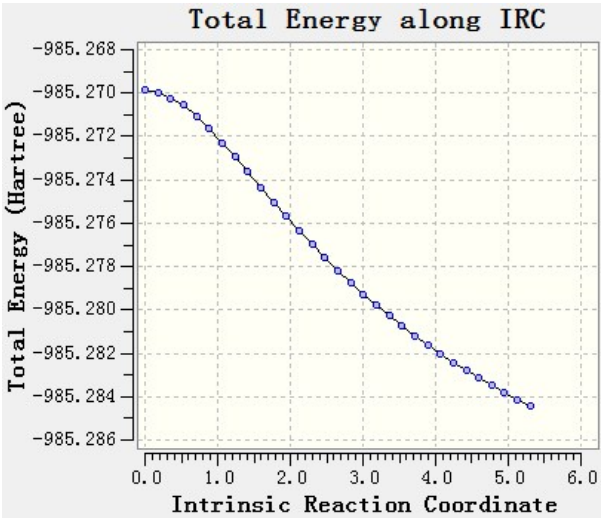
36
1B-a1-TS1, Free Energies=-6105.043120
C -1.4132612 3.6066568 0.1248993
O -1.3153550 3.2048644 -1.2725764
C -1.7258898 1.8990849 -1.4230736
C -2.4744248 1.4566436 -0.1706401
C -1.8268432 2.3538295 0.9109971
H -0.4437892 4.0080922 0.4291303
H -2.1618339 4.4048181 0.1719179
H -2.2136402 1.7556884 -2.3927820
H -2.5259873 2.5758915 1.7175831
H -0.9457392 1.8766361 1.3490176
C -2.3503600 -0.0750426 0.0261072
C -0.8607468 -0.5329899 0.1466251
H -0.7951858 -1.5843912 -0.1438733
H -0.5340630 -0.4436070 1.1886948
C 0.1041606 0.2457545 -0.6570642
C 1.2810748 0.6884076 -0.9509542
H 1.5939200 1.4654873 -1.6402066
C -3.1106123 -0.5194115 1.2895340
O -3.7327303 0.2167158 2.0228596
O -2.9825594 -1.8437104 1.4702140
C -2.9919499 -0.7681639 -1.1978781
O -2.3696716 -1.2982323 -2.0918384
O -4.3304126 -0.6626983 -1.1642898
C -3.6401940 -2.3990852 2.6326474
H -3.4236399 -3.4657869 2.6012540
H -3.2376422 -1.9473274 3.5416621
H -4.7153834 -2.2158620 2.5770043
C -5.0467476 -1.2634812 -2.2686867
H -6.1000922 -1.0879709 -2.0552912
H -4.7552522 -0.7902702 -3.2088549
H -4.8302909 -2.3327163 -2.3167449
H -0.7938178 1.1879792 -1.5060823
H -3.5369866 1.7013422 -0.2704186
Pt 2.6096555 -0.3483759 0.0560775
Br 3.5035740 -1.5525483 -1.8685973
Br 2.0620200 0.6236851 2.2588551

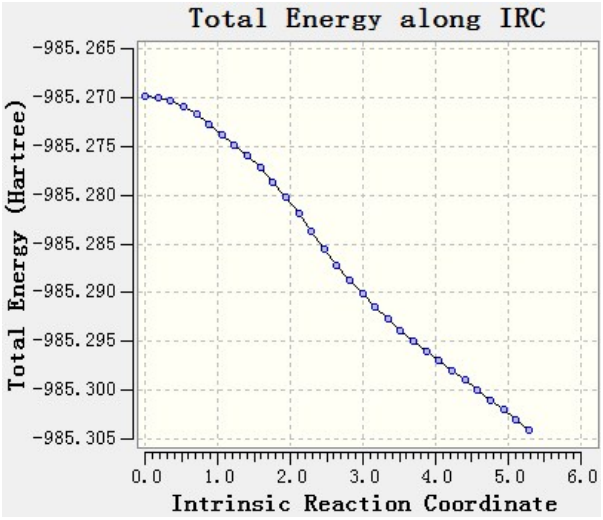




(11). Transition state 1C-a1-TS1

36
1C-a1-TS1, Free Energies=-985.064036
C -1.4589462 3.6261140 0.1522698
O -1.3482575 3.2314939 -1.2458047
C -1.7345536 1.9184365 -1.4024141
C -2.4899335 1.4630104 -0.1592188
C -1.8637584 2.3652027 0.9305230
H -0.4957669 4.0362435 0.4649702
H -2.2162751 4.4159381 0.1984059
H -2.2096716 1.7690754 -2.3773786
H -2.5718514 2.5752594 1.7324887
H -0.9799194 1.8985317 1.3748173
C -2.3501692 -0.0676811 0.0340967
C -0.8568600 -0.5083436 0.1746407
H -0.7804837 -1.5658348 -0.0909138
H -0.5434328 -0.3962192 1.2187531
C 0.1071859 0.2551145 -0.6441385
C 1.2860608 0.6755687 -0.9632800
H 1.5931410 1.4574615 -1.6503484
C -3.1213017 -0.5241765 1.2869728
O -3.7604705 0.2033589 2.0141946
O -2.9810918 -1.8473485 1.4661011
C -2.9684520 -0.7667346 -1.1986180
O -2.3298760 -1.2974100 -2.0802479
O -4.3079105 -0.6666833 -1.1861355
C -3.6502505 -2.4138633 2.6166332
H -3.4191481 -3.4775467 2.5866711
H -3.2689285 -1.9587201 3.5330889
H -4.7267050 -2.2447103 2.5435204
C -5.0044341 -1.2740157 -2.2996745
H -6.0616683 -1.1015989 -2.1036975
H -4.6995953 -0.8029974 -3.2367047
H -4.7833424 -2.3426025 -2.3404995
H -0.7909897 1.2239683 -1.4723265
H -3.5543168 1.6954179 -0.2683258
Pt 2.6296555 -0.3809735 0.0016372
I 2.3555985 0.8912121 2.3410051
I 3.3491924 -1.9378446 -2.0181322

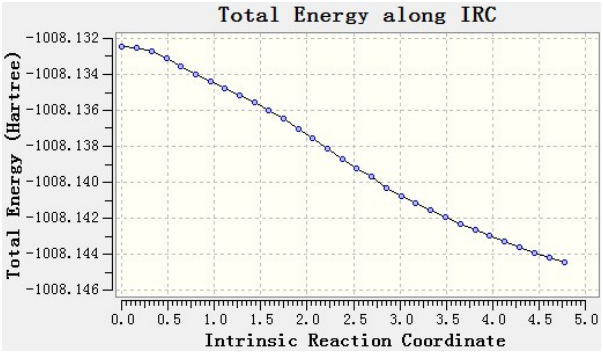


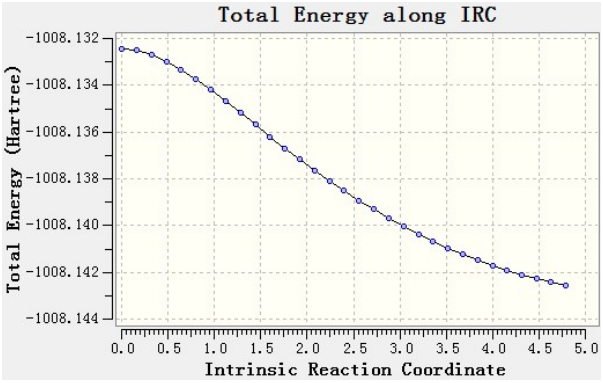


(12). Transition state 1D-a-TS1

38
1D-a-TS1, Free Energies=-1007.933422

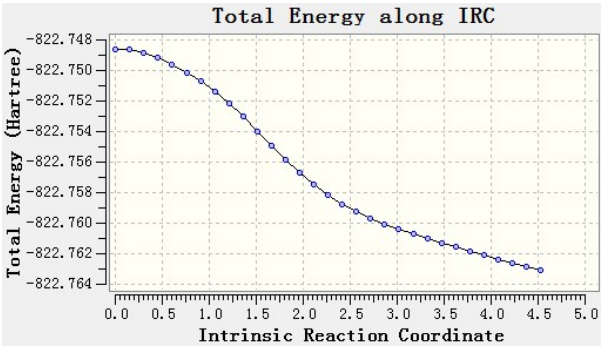
C	3.462772	-2.8153282	-2.2989030
O	3.312342	-1.5970583	-3.0869819
C	3.582348	-0.4978179	-2.3131256
C	4.292147	-0.9306940	-1.0371177
C	3.740927	-2.3656744	-0.8578009
H	2.545618	-3.3986117	-2.4047088
H	4.296313	-3.3726074	-2.7393045
H	4.013251	0.3100389	-2.9123569
H	4.456803	-3.0096690	-0.3467661
H	2.812731	-2.3637132	-0.2791541
C	4.021328	0.0743378	0.1119666
C	2.495420	0.2409698	0.3915718
H	2.332946	1.2107208	0.8706790
H	2.165096	-0.5440855	1.0827726
C	1.621291	0.1509973	-0.7984719
C	0.442989	0.0424018	-1.2893603
H	0.141396	-0.1033571	-2.3182855
C	4.724417	-0.3832860	1.4034590
O	5.413366	-1.3740038	1.5075200
O	4.461191	0.4701579	2.4053669
C	4.610543	1.4419629	-0.3054274
O	3.952347	2.3856508	-0.6836304
O	5.951788	1.4283091	-0.2413074
C	5.055526	0.1592652	3.6872586
H	4.728967	0.9555403	4.3542793
H	4.700884	-0.8119285	4.0384351
H	6.143967	0.1428808	3.6000183
C	6.622745	2.6519544	-0.6248711
H	7.684573	2.4480048	-0.4957804
H	6.395843	2.8955797	-1.6649948
H	6.300654	3.4720699	0.0200697
H	2.558537	-0.0073036	-1.9408476
H	5.373217	-0.9642933	-1.2097949
Pt	-1.168690	0.1780457	0.0960532
I	-3.087675	0.4515915	1.9723288
I	-1.333960	2.7932428	-0.5732102
I	-2.891948	-0.6967358	-1.7621369
I	-0.521424	-2.3062786	1.0277258

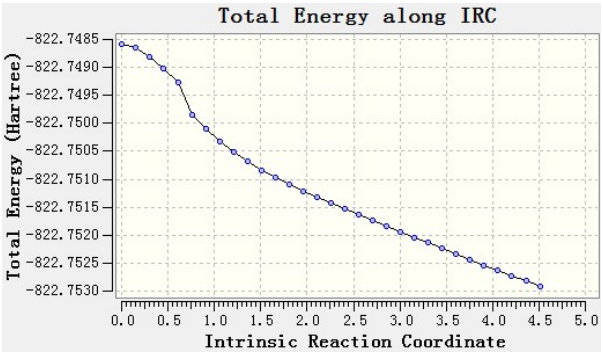




(13). Transition state 2D-b-TS1

39
2D-b-TS1, Free Energies=-822.526514
C 4.8842024 8.0085219 1.17852650
C 5.0721569 7.0219355 2.33742740
C 4.6389102 5.5966248 1.95478219
C 3.3652626 5.6405990 1.02833814
C 2.5411112 6.9478894 1.21088104
C 3.3856285 8.1815110 0.82658351
H 5.3254268 8.9780809 1.43031394
H 6.1199569 6.9683532 2.64723751
H 3.7283361 5.6156699 -0.01307146
H 1.6292638 6.8980626 0.60879820
H 2.9696398 9.0521403 1.34569300
H 4.4968873 7.3528553 3.21113702
H 5.4384247 7.6362044 0.30913446
H 3.2761129 8.3789462 -0.24578353
H 2.2258078 7.0075916 2.25963185
H 4.4004035 5.0219859 2.86332797
O 5.7243782 4.9864803 1.27951312
C 5.6872075 3.5545073 1.19863682
H 5.4851991 3.1476641 2.20237603
C 2.5243764 4.4601806 1.12577367
C 1.7367466 3.5051570 1.28247106
H 1.4650167 4.2765442 2.15090591
H 4.8755452 3.2172377 0.53948423
C 7.0063593 3.0451077 0.66995904
C 7.0292782 2.0397895 -0.30463004
C 8.2201228 3.5372150 1.17123317
C 8.2448324 1.5263223 -0.76750034
H 6.0938468 1.6525042 -0.70110419
C 9.4343606 3.0318562 0.70315118
H 8.2095938 4.3238751 1.91962485
C 9.4502749 2.0226167 -0.26596874
H 8.2473226 0.7450042 -1.52216918
H 10.3687452 3.4232445 1.09595387
H 10.3957321 1.6284467 -0.62764228
Pt 0.7218646 1.8842569 1.22236081
I -0.6737053 2.7251678 3.44544808
I -1.2400981 2.8969413 -0.38135109
I 1.9831417 0.8836595 -0.96977570
I 2.4244560 0.4827776 2.83279214

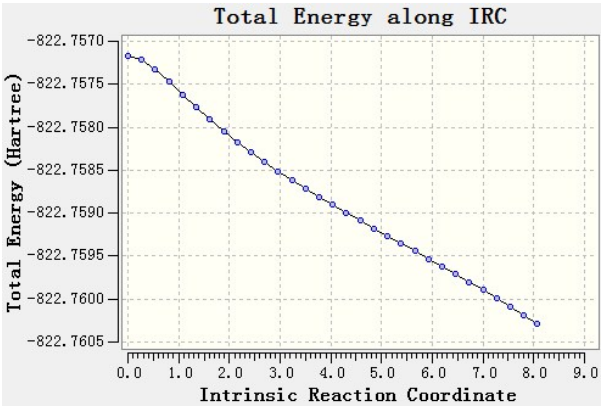


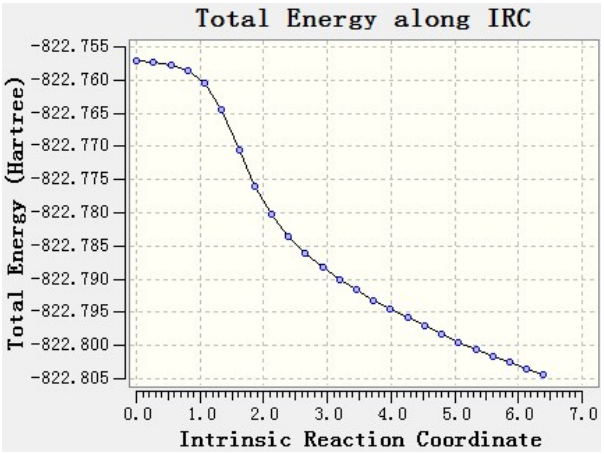


(14). Transition state 2D-b-TS2

39
2D-b-TS2, Free Energies=-822.528533

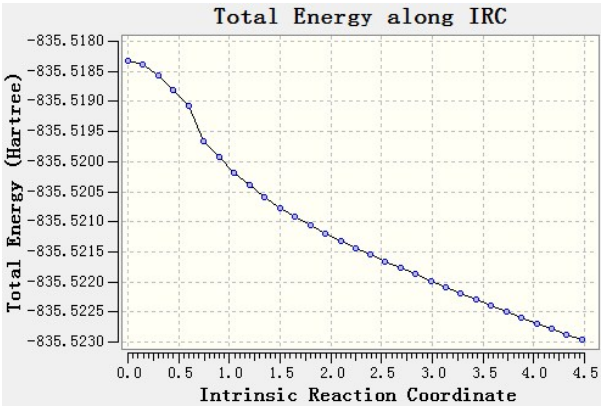
C	4.0492080	4.5988644	-0.9834196
C	3.9102105	3.8597020	0.3527143
C	2.8699695	2.7238133	0.2954347
C	1.7979624	2.9777123	-0.7925977
C	1.4845265	4.4847219	-0.8842226
C	2.7170946	5.2795925	-1.3791801
H	4.8501860	5.3431227	-0.9218984
H	4.8618464	3.4214127	0.6691592
H	2.2354046	2.6603337	-1.7489800
H	0.6330020	4.6472746	-1.5543554
H	2.6758595	6.2926948	-0.9631164
H	3.6125497	4.5710691	1.1332614
H	4.3557150	3.8855802	-1.7583256
H	2.6730334	5.3910033	-2.4688092
H	1.1675032	4.8386281	0.1053333
H	2.3808502	2.6244799	1.2743896
O	3.5702331	1.4979858	0.0094987
C	2.9349423	0.3363763	0.4592694
H	2.7416828	0.3595260	1.5410864
C	0.5234424	2.1766632	-0.5974687
C	0.2569141	0.9573157	-0.2185989
H	-0.4307007	2.6729526	-0.8341447
H	1.8725021	0.2851209	0.0048482
C	3.6821288	-0.8878931	0.0397888
C	3.9013755	-1.9225853	0.9619889
C	4.1719347	-1.0166243	-1.2708913
C	4.6134483	-3.0629421	0.5854307
H	3.5175321	-1.8320396	1.9740219
C	4.8790780	-2.1569233	-1.6459217
H	4.0029332	-0.2176847	-1.9859181
C	5.1015001	-3.1826616	-0.7181674
H	4.7828724	-3.8560520	1.3075261
H	5.2547343	-2.2507892	-2.6605928
H	5.6513073	-4.0717052	-1.0134877
Pt	-0.8372952	-0.5021659	0.2324057
I	-2.9966237	1.1729296	0.3198427
I	-1.3527264	-1.0433199	-2.4031969
I	0.2082997	-2.9865287	0.4921745
I	-0.3804455	-0.0368098	2.9122962

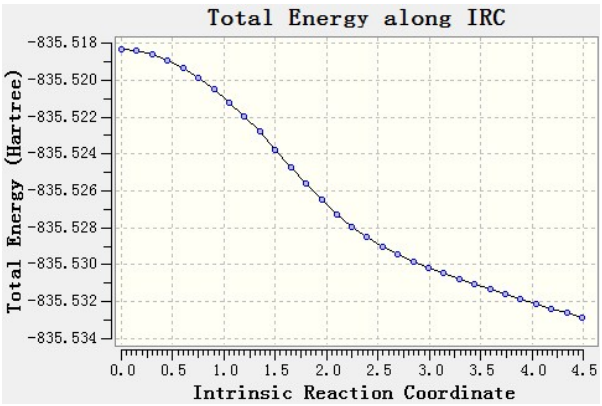




(15). Transition state 3D-b-TS1

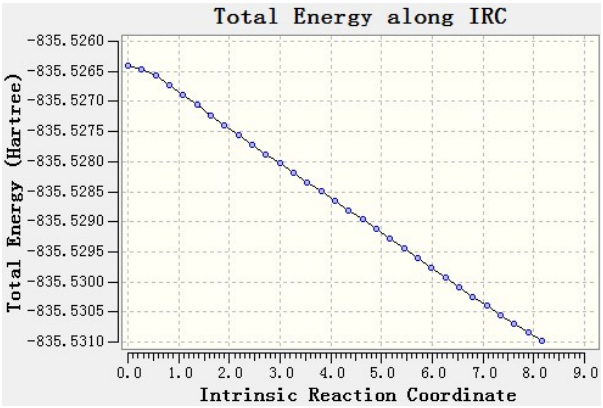
39
3D-b-TS1, Free Energies=-835.309415
C 3.9905246 4.6070092 -0.5669552
C 3.8628596 3.8381045 0.7537200
C 3.1401589 2.4930191 0.5698056
C 1.9962952 2.6255651 -0.5040819
C 1.4726624 4.0857524 -0.6324487
C 2.6010084 5.0267591 -1.1069383
H 4.6234038 5.4898066 -0.4323291
H 4.8445646 3.6219283 1.1853906
H 2.4319744 2.3403646 -1.4762039
H 0.6249442 4.1163667 -1.3229877
H 2.3555924 6.0428663 -0.7787784
H 3.3176593 4.4425122 1.4892748
H 4.5048976 3.9700296 -1.2960633
H 2.6199236 5.0508871 -2.2022940
H 1.0950513 4.3990102 0.3484051
H 2.6973711 2.1720094 1.5252903
O 4.1053519 1.5410628 0.1544638
C 3.7245267 0.1696598 0.2868338
H 3.3134160 0.0051066 1.2959516
C 0.9081976 1.6806666 -0.3181970
C -0.0751592 0.9452230 -0.0977791
H -0.2751806 1.9329959 0.5418944
H 2.9343524 -0.0923586 -0.4311474
C 4.9218039 -0.7227516 0.0540698
C 4.7248538 -2.0261677 -0.4200469
C 6.2232191 -0.2950179 0.3419735
C 5.8029990 -2.8972010 -0.5972522
H 3.7214115 -2.3730083 -0.6547267
C 7.3135503 -1.1510510 0.1618254
H 6.3888747 0.7161242 0.6978631
C 7.0865730 -2.4438821 -0.3031952
H 5.6413806 -3.9046014 -0.9640581
H 8.3200667 -0.8125144 0.3814893
Pt -1.3896235 -0.4395061 0.0186059
I -2.8177869 1.1292968 1.7773830
I -2.9166754 0.4922333 -2.0397592
I -0.1286652 -2.1325128 -1.6974705
I -0.1876909 -1.6941456 2.1277423
Br 8.6036333 -3.6455298 -0.5566392

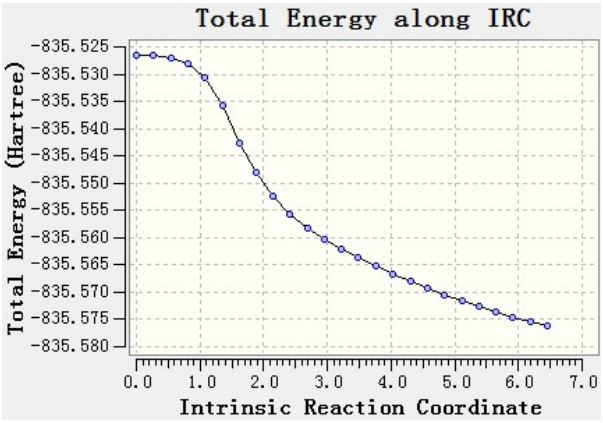




(16). Transition state 3D-b-TS2

39
3D-b-TS2, Free Energies=-835.310950
C -5.3905592 -3.09806574 -0.5138532
C -4.8867111 -2.42540490 0.7686643
C -3.5179462 -1.74204960 0.5813397
C -2.7047986 -2.38290400 -0.5692388
C -2.9530245 -3.90416995 -0.6051997
C -4.4248686 -4.21935938 -0.9658859
H -6.3950227 -3.50487663 -0.3567189
H -5.5897113 -1.66667272 1.1264650
H -3.0846437 -1.95115390 -1.5050445
H -2.2755744 -4.37390677 -1.3268300
H -4.7088220 -5.16913860 -0.4986093
H -4.7988652 -3.17668668 1.5634034
H -5.4890614 -2.34172787 -1.3022222
H -4.5177936 -4.36745068 -2.0479587
H -2.6960159 -4.32516538 0.3755415
H -2.9433899 -1.80755672 1.5157733
O -3.7563561 -0.34992593 0.2937258
C -2.7042038 0.50855594 0.6181216
H -2.3926495 0.41101202 1.6671568
C -1.2177437 -2.08278462 -0.5117870
C -0.5083799 -1.01272766 -0.2773702
H -0.5223392 -2.90523040 -0.7415388
H -1.7536443 0.18864967 0.0357257
C -3.0237297 1.92076104 0.2512758
C -2.6551966 2.96583491 1.1109665
C -3.6918843 2.22171693 -0.9465901
C -2.9593786 4.29079360 0.7951905
H -2.1263277 2.74694691 2.0338928
C -3.9994191 3.53991253 -1.2763650
H -3.9821908 1.41906173 -1.6165116
C -3.6281903 4.55906226 -0.3969180
H -2.6772136 5.09482419 1.4652136
H -4.5170528 3.77122441 -2.2004133
Pt 1.0915039 -0.04460082 -0.1086315
I 2.4800823 -2.36756134 0.2761935
I 1.5952814 -0.19386646 -2.7947171
I 0.8940630 2.65057182 -0.3563457
I 0.7708695 0.17716440 2.6226181
Br -4.0591440 6.40116088 -0.8498023





7. Reference 37

Complete List of Authors for References with more than 10 Authors

(37) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, . Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.