

Thermodynamic, Electronic and Strain Effects in the Competition Between 5-Exo-dig and 6-Endo-Dig Cyclizations of Vinyl and Aryl Radicals

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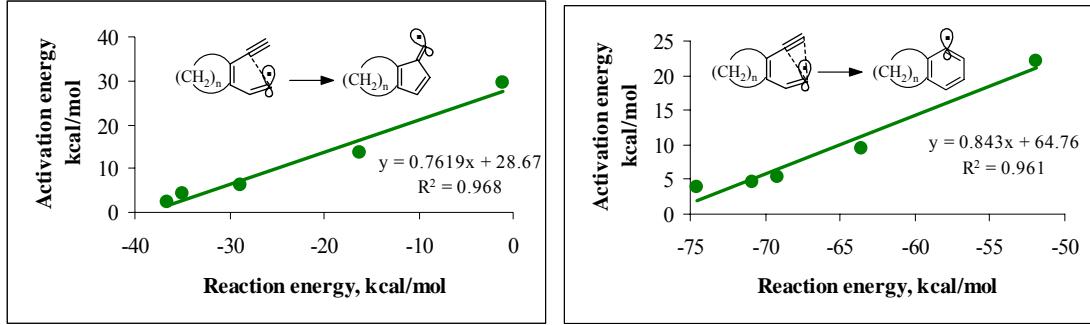


Figure S1. Correlation of reaction energy with activation barrier for 5-exo and 6-endo cyclizations of cyclic hexa-1,3-diene-5-yne-1-yl derivatives (**21**, **24-26**).

Table S1. Computed activation as well as reaction energies (kcal/mol) and the zero-point energy correction (kcal/mol), enthalpy (kcal/mol), free energy (kcal/mol) and entropy (cal/Mol/K) of barriers for 5-endo-dig, 5-exo-dig and 6-endo-dig radical cyclizations involving benzannelated enediyne upon addition of H as well as SnH_3 radicals and 1,4-didehydronaphthalene (DDN).

Energy (kcal/mol)	X =	H ^a	H ^b	DDN ^a	H ^c
$\Delta E(\alpha-\beta)$		-11.3	-11.7	-15.0	-10.7
$\Delta E^\ddagger(5\text{-exo})$		2.4	3.3	1.0	3.0
$\Delta E^\ddagger(6\text{-endo})$		4.2	4.8	4.6	4.7
$\Delta E_r(5\text{-exo})^d$		-37.9	-33.3	-41.5	-36.6
$\Delta E_r(6\text{-endo})$		-62.2	-57.7	-62.6	-60.4
$\Delta E_0(5\text{-exo})$		15.6	15.5	14.1	16.1
$\Delta E_0(6\text{-endo})$		26.0	25.5	26.7	26.2
$\Delta E_{ZPE}^\ddagger(5\text{-exo})$		2.0	2.8	0.7	2.4
$\Delta E_{ZPE}^\ddagger(6\text{-endo})$		4.2	4.7	4.6	4.5
$\Delta H^\ddagger(5\text{-exo})$		1.6	2.2	0.4	2.1
$\Delta H^\ddagger(6\text{-endo})$		3.6	3.9	3.7	3.8
$\Delta G^\ddagger(5\text{-exo})$		2.7	3.8	1.5	3.4
$\Delta G^\ddagger(6\text{-endo})$		5.1	5.6	5.3	5.2
$\Delta S^\ddagger(5\text{-exo})$		-3.7	-4.1	-3.9	-3.8
$\Delta S^\ddagger(6\text{-endo})$		-4.8	-5.2	-5.0	-5.0

^aComputed at the UB3LYP/6-31G** level. ^bUB3LYP/6-311++G** level. ^c UB3LYP/LANL2DZ level. ^dThe more stable E-isomer is considered for 5-exo (by 0.05-0.1 kcal/mol) products. The reaction barriers and energies at the UB3LYP/6-31G** level are comparable with the UB3LYP/LANL2DZ results ($E_a(5\text{-exo}) = 2.4$ vs 3.0; $\Delta E_r(5\text{-exo}) = -37.9$ vs -36.6 and $E_a(6\text{-endo}) = 4.2$ vs 4.7; $\Delta E_r(5\text{-exo}) = -62.2$ vs -60.4).

Table S2. The incipient C...C distances in the reactant and transition state geometries of 5-endo, 5-exo and 6-endo cyclizations of benzannelated enediyne upon addition of H as well as SnH_3 radicals and 1,4-didehydronaphthalene (DDN) at the UB3LYP level with both 6-31G** and LANL2DZ basis sets.

C-C distance (Å)	UB3LYP/ 6-31G** X = H	UB3LYP/ 6-311++G** X = H	UB3LYP/ 6-31G** X = DDN	UB3LYP/ LANL2DZ X = H	UB3LYP/ LANL2DZ X = SnH_3
$d(CC)_R(5\text{-exo})$	2.832	2.851	2.714	2.873	2.767
$d(CC)_{TS}(5\text{-exo})$	2.327	2.290	2.358	2.325	2.340
$d(CC)_R(6\text{-endo})$	3.263	3.270	3.189	3.301	3.243
$d(CC)_{TS}(6\text{-endo})$	2.463	2.420	2.451	2.442	2.430

Table S3. The activation and reaction energies for 5-exo and 6-endo cyclizations of tin-substituted radical arising from the benzannelated enediyne with the activataion parameters (all in kcal/mol and entropy in cal/M/K) calculated at the UB3LYP/LANL2DZ level.

System	R	E _a	ΔE _r	ΔE _o	ΔE [‡] _{ZPE}	ΔH [‡]	ΔG [‡]	ΔS [‡]	E _a ^{solv}	ΔE _r ^{solv}
	H	1.6	-36.6	13.9	1.1	0.7	2.0	-4.4	1.5	-37.0
	Me	14.0	-36.5	14.0	1.0	0.7	1.5	-2.8	-	-
	H	6.5	-16.0	13.3	6.0	5.4	7.1	-5.6	5.9	-17.3
	Me	9.1	-12.7	14.8	5.8	5.3	7.1	-6.1	-	-
	H	5.2	-57.2	25.9	5.1	4.6	6.3	-5.9	4.7	-58.0
	Me	5.5	-56.8	25.8	5.4	4.2	7.9	-12.2	-	-
	H	8.1	-37.8	23.1	7.9	7.8	7.7	0.4	7.2	-39.1
	Me	11.0	-34.4	25.3	8.0	7.3	9.9	-8.5	-	-

Table S4. The activation and reaction energies for 5-exo and 6-endo cyclizations of tin-substituted radical arising from the benzannelated enediyne calculated at the UBLYP, UB3PW91 and QCISD levels with the LANL2DZ basis set.

System	BLYP			B3PW91			BP86			QCISD	
	E _a	ΔE _r	ΔE _o	E _a	ΔE _r	ΔE _o	E _a	ΔE _r	ΔE _o	E _a	
	0.6	-33.4	10.9	1.1	-40.6	14.1	0.2	-37.7	10.9	4.1	
	2.8	-15.3	8.8	8.1	-18.0	15.8	6.9	-14.9	13.3	6.4	
	4.1	-53.1	23.0	4.8	-61.5	26.7	3.4	-58.2	23.5	9.1	
	4.4	-36.5	18.0	10.1	-39.8	26.2	8.9	-36.5	23.6	10.9	

Table S5. The Incipient C...C distances (Å) Involved in the 5-Exo and 6-Endo Cyclizations of radicals 11-13 calculated at the UB3LYP/6-31G** (UB3LYP/LANL2DZ for tin-substituted cases) Level.

	5-exo				6-endo	
	r'(R)	r'(TS)	R''(R)	r''(TS)		
11	2.806	2.348	3.289	2.436		
12	2.886	2.274	3.390	2.425		
13	2.993	2.257	3.510	2.419		

Table S6. The Activation Barriers, Reaction Energies and Intrinsic Barriers (all in kcal/mol) 5-Exo-Dig and 6-Endo-Dig Cyclizations of the Parent Radical 4 at the UB3LYP/6-31G** and UB3LYP/cc-PVDZ//6-31G** Levels.

	5-exo				6-endo		
	Method	ΔE [‡]	ΔE _r	ΔE _o	ΔE [‡]	ΔE _r	ΔE _o
4^a	I ^b	4.1	-35.0	17.1	4.7	-70.8	29.5
	II ^c	4.1	-34.8	17.1	4.6	-70.1	29.1
	III ^d	4.1	-34.8	17.1	4.5	-70.2	29.1

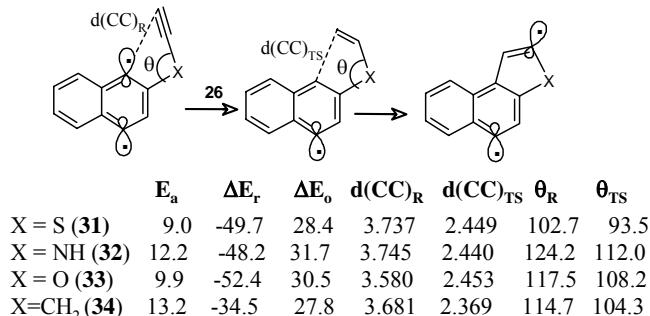
^aThe activation barriers at the BD(T)/3-21G*/B3LYP/6-31G** level for 5-exo and 6-endo cyclizations are 5.9 and 9.4 kcal/mol, respectively. ^bCalculated at the UB3LYP/6-31G** level. ^c Calculated at the UB3LYP/cc-PVDZ level. ^d Single-point calculations at the UB3LYP/cc-PVDZ on UB3LYP/6-31G** geometries.

Table S7. The Activation Barriers, Reaction Energies and Intrinsic Barriers (all in kcal/mol) 5-Exo-Dig and 6-Endo-Dig Cyclizations of Radicals (36-39) at the UB3LYP/6-31G** and UB3LYP/cc-PVDZ//6-31G** Levels.

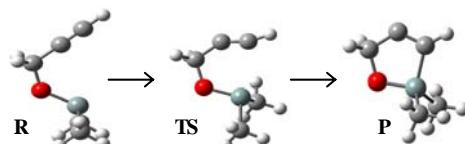
		5-exo			6-endo		
	Method	ΔE^\ddagger	ΔE_r	ΔE_o	ΔE^\ddagger	ΔE_r	ΔE_o
33^a	I ^b	4.1	-34.4	16.9	21.8 ^c	-58.7	46.5
	II ^c	4.2	-34.2	17.0	9.9	-58.1	32.5
34	I ^d	NA	NA	NA	NA	NA	NA
	II	1.6	-35.8	13.6	4.7	-53.3	23.9
35	I	1.0	-39.8	13.6	5.9	-55.6	26.4
	II	1.1	-37.2	13.1	5.6	-55.4	25.9
36	I	1.3	-38.7	13.9	19.8 ^e	-54.5	42.7
	II	1.3	-36.0	13.1	10.2	-54.2	31.5

^a The activation barriers at the BD(T)/cc-pVDZ//B3LYP/6-31G** level for 5-exo and 6-endo cyclizations are respectively 5.8 and 10.2. ^b Calculated at the UB3LYP/6-31G** level. ^c Single-point calculations at the UB3LYP/cc-PVDZ on UB3LYP/6-31G** geometries. ^d The 6-31G** geometries of reactant and product show unusual energies by different Lewis structures instead of diradicals, but the 5-exo and 6-endo TSs exhibit proper saddle point geometries in which the former is more stable than the latter by 1.8 kcal/mol as expected. ^eThe barriers for 6-endo cyclizations of both **33** and **36** are unexpectedly much higher than the 5-endo case and this indicates the problem of 6-31G** on absolute energies and not on the geometries, since the same structures provide a better trend through the single-point calculations at UB3LYP/cc-PVDZ and BD(T) levels (see above).

Scheme S1. UB3LYP/6-31G** analysis of 5-endo-dig step in cycloaromatization/radical cyclizations cascades of X-ethynyl substituted naphthalenes.



Scheme S2. Geometries of stationary points for the 5-endo cyclization of Si-radical **45**



Reference #25

Gaussian 98, Revision A.9. Gaussian, Inc. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A., Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. Pittsburgh, PA, 1998.

Gaussian 03, revision C.01; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian, Inc.: Wallingford CT, 2004.

Table S8. The Total Energies (a.u.) of the Reactant and TS for 5-Exo-Dig and 6-Endo-Dig Cyclizations of Selected Radicals (**1**, **4**, **5** and **33**) Calculated at the BD(T)/6-31G** Level on B3LYP/6-31G** Geometry.

Radical system	Reactant	TS (5-exo-dig)	TS (6-endo-dig)
	-232.00444	-231.99496	-231.98928
	-230.79052	-230.78210	-230.78081
	-384.01548	-384.00989	-384.00721
	-383.33850	-383.32906	-383.32220

**Computed Geometries at the
UB3LYP/6-31G** Level**

1-R

Total energy = -232.67999
 6 -0.091451 0.952406 -0.934598
 6 0.023210 1.033918 0.600572
 1 0.912706 0.967656 -1.377969
 1 -0.591775 1.862066 -1.294341
 1 0.423998 2.019121 0.870321
 1 -0.981517 0.974097 1.037440
 6 0.871176 -0.000837 1.193323
 6 1.585972 -0.838289 1.690231
 1 2.210602 -1.585209 2.121958
 6 -0.843119 -0.250435 -1.457104
 6 -1.396246 -1.200496 -0.740341
 1 -0.922658 -0.302236 -2.551509
 1 -1.948605 -2.113095 -0.918399

1 (5-exo TS)

Total energy = -232.67291
 6 -0.136223 1.052622 -1.063833
 6 -0.013858 1.142538 0.468880
 1 0.845606 1.196709 -1.536217
 1 -0.778139 1.860855 -1.433964
 1 0.631856 1.978056 0.760995
 1 -1.007566 1.338334 0.890237
 6 0.501532 -0.102817 1.074714
 6 1.124209 -0.834101 1.835926
 1 1.561259 -1.642070 2.376839
 6 -0.682115 -0.306654 -1.439346
 6 -0.671626 -1.277615 -0.552325
 1 -1.047445 -0.449218 -2.461418
 1 -0.937077 -2.326502 -0.540569

1 (5-exo P)

Total energy = -232.74081
 6 -0.313293 1.139050 -1.082259
 6 0.192440 1.138013 0.388130
 1 0.404026 1.612107 -1.765753
 1 -1.251977 1.697128 -1.196039
 1 1.178209 1.603259 0.479408
 1 -0.481258 1.689548 1.050289
 6 0.255978 -0.341858 0.796209
 6 0.634181 -0.815755 1.968410
 1 0.746502 -1.781966 2.440894
 6 -0.499810 -0.322265 -1.405944
 6 -0.186800 -1.121755 -0.375146
 1 -0.850235 -0.667888 -2.373705
 1 -0.241435 -2.204773 -0.371504

1 (6-endo TS)

Total energy = -232.66582
 6 0.060416 1.180102 -0.721862
 6 0.049298 1.187751 0.832430
 1 1.105129 1.221623 -1.055651
 1 -0.416975 2.099342 -1.077928
 1 0.682988 2.004159 1.198293
 1 -0.965170 1.384856 1.202788
 6 0.491782 -0.115654 1.328984
 6 0.620074 -1.326586 1.188833
 1 0.863831 -2.350352 1.365773
 6 -0.617558 -0.030432 -1.345419
 6 -0.455653 -1.284327 -0.966113
 1 -1.269146 0.183317 -2.200834
 1 -0.890814 -2.208073 -1.333565

1 (6-endo P)

Total energy = -232.74514
 6 0.031587 1.202640 -0.699649
 6 0.106363 1.199795 0.853441
 1 1.044373 1.348065 -1.107837
 1 -0.557729 2.064467 -1.023269
 1 0.779930 1.994100 1.193320
 1 -0.881894 1.421033 1.285570
 6 0.537835 -0.144831 1.316845
 6 0.330732 -1.299933 0.698590
 1 0.620477 -2.259914 1.118554
 6 -0.528461 -0.089060 -1.255782
 6 -0.357025 -1.254848 -0.612067
 1 -1.015718 -0.061657 -2.226957
 1 -0.715625 -2.188671 -1.038549

2-R

Total energy = -272.00309
 6 1.285569 .473794 -.641094
 6 1.345622 .695884 .885899
 1 2.312847 .505381 -1.022496
 1 .742792 1.301849 -1.108859
 1 1.846964 -.161786 1.355558
 1 1.984450 1.565664 1.087315
 6 .050645 .911796 1.532398
 6 -.998982 1.127742 2.090462
 1 -1.936592 1.298314 2.566149
 6 .655105 -.866350 -1.071533
 1 .825699 -1.002256 -2.154516
 1 1.192968 -1.687095 -.574713
 6 -.789478 -.986603 -.799121
 6 -1.909532 -1.218802 -1.443829
 1 -1.927231 -1.401782 -2.524647
 1 -2.875593 -1.243057 -.942884

2 (5-exo TS)

Total energy = -271.99595
 6 1.352314 0.512424 -0.910432
 6 1.398082 0.620947 0.622969
 1 2.366578 0.445989 -1.317745
 1 0.887408 1.414262 -1.324034
 1 1.980447 -0.218112 1.028354
 1 1.910124 1.538865 0.932856
 6 0.047603 0.594904 1.228311
 6 -.827850 0.851873 2.048956
 1 -1.735500 0.926528 2.603666
 6 0.514254 -0.720050 -1.296405
 1 0.332641 -0.748298 -2.381588
 1 1.077251 -1.630318 -1.042992
 6 -.753432 -0.697795 -0.535785
 6 -2.012191 -1.049342 -0.666741
 1 -2.738744 -0.864852 0.122884
 1 -2.392888 -1.541835 -1.566636

2 (5-exo P)

Total energy = -272.05460
 6 1.356631 0.585915 -1.023108
 6 1.279533 0.796105 0.501235
 1 2.382484 0.476891 -1.386683
 1 0.909739 1.444262 -1.537971
 1 2.004415 0.144497 1.007951
 1 1.487736 1.821027 0.817680
 6 -.139100 0.347721 0.862391
 6 -.794514 0.717553 1.943471
 1 -1.758376 0.548264 2.404049
 6 0.494667 -.668484 -1.258680
 1 0.120751 -.759980 -2.282699
 1 1.088017 -1.569682 -1.047866
 6 -.625921 -0.549324 -0.236804
 6 -1.829928 -1.123940 -0.327898
 1 -2.586043 -.995012 0.440482

1 -2.096935 -1.743537 -1.178577

2 (6-endo TS)

Total energy = -271.99159
 6 1.296754 0.714982 -0.519143
 6 1.357137 0.926857 1.015653
 1 2.316663 0.770524 -0.917255
 1 0.726606 1.533917 -0.970327
 1 2.110112 0.260835 1.458108
 1 1.681963 1.950387 1.238840
 6 0.045589 0.636337 1.600321
 6 -.1071961 0.136433 1.537232
 1 -2.062720 -0.167813 1.793242
 6 0.661152 -0.630619 -0.935524
 1 0.862206 -0.798991 -2.006845
 1 1.168402 -1.444458 -0.396857
 6 -.803092 -.721058 -0.701339
 6 -1.850039 -1.025895 -1.439810
 1 -2.865404 -1.023913 -1.047497
 1 -1.751072 -1.302710 -2.495754

2 (6-endo P)

Total energy = -272.06929
 6 1.289858 0.800388 -0.579329
 6 1.324495 1.027501 0.956705
 1 2.309270 0.828418 -0.980427
 1 0.733903 1.623575 -1.042379
 1 2.106849 0.410403 1.421574
 1 1.583267 2.070389 1.178981
 6 -.002348 0.671178 1.508610
 6 -.985806 -0.029610 0.960179
 1 -1.942740 -0.176839 1.458661
 6 0.611138 -.534621 -0.931957
 1 0.597661 -.680960 -2.016996
 1 1.212428 -1.354290 -.511500
 6 -.798059 -.635306 -0.375174
 6 -1.798540 -1.249211 -1.024361
 1 -2.788380 -1.339397 -0.586209
 1 -1.656686 -1.683220 -2.009744

3-R

Total energy = -386.34242
 6 -.448801 -.108809 -1.756338
 6 -.390455 -.465573 -0.395346
 6 0.877528 -.734992 0.086161
 6 2.052847 -.684507 -0.627783
 6 1.957757 -.324626 -1.981713
 6 0.708205 -.039776 -2.535884
 1 -1.416380 0.109814 -2.204564
 1 3.013857 -.911846 -0.175012
 1 2.854921 -.270910 -2.592760
 1 0.632124 0.234922 -3.583819
 6 -.631147 -.519376 0.468076
 1 -.590518 -.1391997 1.127491
 6 -1.838867 0.749378 1.338183
 6 -.817193 0.936387 2.366806
 6 0.020916 1.081359 3.224554
 1 0.765449 1.210749 3.975217
 1 -2.823993 0.686068 1.818525
 1 -1.867310 1.631678 0.686177
 1 -2.512887 -.635275 -0.171552

3 (5-exo TS)

Total energy = -386.33583
 6 -.577666 .076287 -1.931479
 6 -.614012 .080557 -.528655
 6 .592875 -.064055 .130092
 6 1.820682 -.196111 -.483007
 6 1.836752 -.197879 -1.886266
 6 .641947 -.062471 -2.599595

1 -1.500336 .180333 -2.499198
 1 2.740552 -.301599 .086247
 1 2.778759 -.308121 -2.417563
 1 .660409 -.067986 -3.685609
 6 -1.858994 .250118 .311165
 1 -2.728869 -.230085 -.149893
 6 -1.604340 -.347333 1.709071
 6 -.301786 .067462 2.272458
 6 .526515 .423354 3.102283
 1 1.393398 .733634 3.639826
 1 -1.615476 -1.442065 1.636716
 1 -2.400152 -.060882 2.405309
 1 -2.100111 1.317183 .407758

3 (5-exo P)

Total energy = -386.40301
 6 -.768819 -.000959 -1.861555
 6 -.776070 .023945 -.468120
 6 .432882 -.000141 .244627
 6 1.657311 -.042722 -.429771
 6 1.659413 -.067769 -1.823176
 6 .453763 -.049222 -2.536000
 1 -1.701230 .016256 -2.420149
 1 2.587604 -.062523 .130022
 1 2.602209 -.106528 -2.361182
 1 .469877 -.073822 -3.621849
 6 -1.959475 .114269 .471299
 1 -2.747816 -.605507 .225522
 6 -1.352391 -.138435 1.877631
 6 .172250 .025803 1.698806
 6 1.056815 .158505 2.666361
 1 1.063800 .209824 3.746255
 1 -1.562536 -1.162824 2.205371
 1 -1.750295 .534401 2.641217
 1 -2.415688 1.111071 .414172

3 (6-endo TS)

Total energy = -386.32407
 6 -.549553 .000000 -1.810564
 6 -.504654 .000000 -.400802
 6 .763911 .000000 .156325
 6 1.943876 .000000 -.563977
 6 1.867983 .000000 -1.961889
 6 .614157 .000000 -2.578241
 1 -1.518103 .000000 -2.308845
 1 2.910684 .000000 -.065518
 1 2.775816 .000000 -2.559934
 1 .541292 .000000 -3.661973
 6 -1.840018 .000000 .342830
 1 -2.408381 -.871015 -.002771
 6 -1.871220 .000000 1.912181
 6 -.548250 .000000 2.525148
 6 .670697 .000000 2.576426
 1 1.690558 .000000 2.888614
 1 -2.432525 -.873498 2.264293
 1 -2.432525 .873498 2.264293
 1 -2.408381 .871015 -.002771

3 (6-endo P)

Total energy = -386.40741
 6 -.543584 .000000 -1.749461
 6 -.547613 .000000 -.353137
 6 .687835 .000000 .327791
 6 1.882975 .000000 -.403967
 6 1.869616 .000000 -1.797553
 6 .650498 .000000 -2.474248
 1 -1.492425 .000000 -2.281901
 1 2.828939 .000000 .131759
 1 2.804755 .000000 -2.349983
 1 .624960 .000000 -3.559979

6 -1.883435 .000000 .383606
 1 -2.457886 -.872819 .052475
 6 -.1833555 .000000 1.956494
 6 -.446036 .000000 2.462162
 6 .700685 .000000 1.806865
 1 1.665086 .000000 2.311195
 1 -2.369932 -.874219 2.346327
 1 -2.369932 .874219 2.346327
 1 -2.457886 .872819 .052475

4-R

Total energy = -231.45636
 1 0.097661 -.0000054 -2.355912
 6 0.074596 0.000042 -1.268276
 6 1.250478 0.000010 -.596518
 1 2.161658 -.0000047 -1.189012
 6 1.429835 0.000004 0.853283
 6 0.473700 0.000065 1.769226
 1 0.437526 0.000073 2.850610
 6 -1.207738 -.0000020 -.667624
 6 -2.331579 -.0000069 -0.210181
 1 -3.305304 -.0000110 0.221586
 1 2.472708 -.0000051 1.193271

4-R (5-exo TS)

Total energy = -231.44983
 6 -.655373 -.002204 -2.165987
 6 -.6465165 0.000564 -.932734
 6 1.498559 -.001865 -.105293
 6 1.122164 -.001225 1.165613
 6 -.313282 0.002093 1.448726
 6 -1.164118 0.002765 0.399511
 1 -0.404867 -.002961 -3.202540
 1 2.435271 -.005354 -.645540
 1 -2.242338 0.005319 0.521688
 1 -0.676970 0.004869 2.471288
 1 1.832204 -.002637 1.996080

4-R (5-exo P)

Total energy = -231.51220
 6 -.1356838 0.000000 -.690550
 6 -.1327448 0.000000 0.780824
 6 -.041194 0.000000 1.201741
 6 0.826804 0.000000 0.004677
 6 2.150949 0.000000 -.025411
 6 -.089855 0.000000 -1.165540
 1 2.926819 0.000000 -.780762
 1 0.238806 0.000000 -2.195817
 1 -2.208258 0.000000 1.411945
 1 0.329983 0.000000 2.217263
 1 -2.261865 0.000000 -1.287075

4 (6-endo TS)

Total energy = -231.44888
 6 -1.203520 0.000000 -.684866
 6 -1.221837 0.000000 0.727237
 6 -.029621 0.000000 1.382827
 6 1.274676 0.000000 0.735569
 6 1.510954 0.000000 -.578560
 6 -.657436 0.000000 -1.783518
 1 -2.161168 0.000000 1.271466
 1 -.038330 0.000000 2.470069
 1 2.447263 0.000000 -1.127615
 1 -.419728 0.000000 -2.822937
 1 2.132663 0.000000 1.416876

4 (6-endo P)

Total energy = -231.56922
 6 -1.213890 -.0000137 -.632598
 6 -1.226356 -.0000181 0.771573

6 -.0000102 -.0000035 1.399785
 6 1.226251 0.000139 0.771739
 6 1.213984 0.000168 -.632416
 6 0.000090 0.000035 -.1324436
 1 -2.153717 -.0000240 -1.178899
 1 -2.162269 -.0000310 1.322823
 1 2.162074 0.000246 1.323143
 1 2.153876 0.000303 -.1178607
 1 0.000180 0.000065 -.2.410332

5-R

Total energy = -385.11704
 6 -.548356 0.000017 -.1.682493
 6 -.564893 0.000003 -.2.76045
 6 0.664287 -.000013 0.437064
 6 1.859127 -.000011 -.2.299120
 6 1.861536 0.000002 -.1.691012
 6 0.651385 0.000016 -.2.387223
 1 -1.495684 0.000027 -.2.211520
 1 2.802447 -.000022 0.240450
 1 2.803878 0.000001 -.2.230582
 1 0.641183 0.000026 -.3.472805
 6 0.737387 -.0000033 1.905021
 6 -.270768 -.0000020 2.757539
 1 -.366704 0.000042 3.835083
 6 -1.826871 0.000003 0.391479
 6 -2.937438 0.000004 0.876824
 1 -3.896345 0.000005 1.340738
 1 1.758844 0.000108 2.306433

5 (5-exo TS)

Total energy = -385.11317
 6 0.044491 -.005711 -.063939
 6 -.117616 -.003972 1.154152
 6 1.924241 -.003001 2.270446
 6 1.390500 -.000771 3.479576
 6 -.069777 0.000079 3.613784
 6 -.817232 -.001687 2.412228
 1 0.407736 -.006659 -.1.066330
 1 2.922867 -.004148 1.856070
 6 -.2127879 -.0000892 2.462732
 6 -.2874112 0.001605 3.692927
 6 -2.136879 0.003405 4.879843
 6 -.742644 0.002662 4.839142
 1 -2.780685 -.002256 1.535031
 1 -3.959353 0.002206 3.724524
 1 -2.649286 0.005407 5.837369
 1 -.169053 0.004058 5.762078
 1 1.993194 0.000110 4.392508

5 (5-exo P)

Total energy = -385.17736
 6 -.854081 0.000000 -.1.801612
 6 -.865044 0.000000 -.0.334948
 6 0.477706 0.000000 0.112495
 6 1.350536 0.000000 -.1.089579
 6 2.673461 0.000000 -.1.129986
 6 0.422767 0.000000 -.2.249459
 1 3.449678 0.000000 -.1.883515
 1 0.754153 0.000000 -.3.279678
 6 -1.911387 0.000000 0.584719
 6 -.1.604931 0.000000 1.950837
 6 -.276993 0.000000 2.388336
 6 0.779014 0.000000 1.467778
 1 -2.945835 0.000000 0.252294
 1 -2.409494 0.000000 2.680562
 1 -.061626 0.000000 3.452729
 1 1.810780 0.000000 1.807029
 1 -1.743944 0.000000 -.2.420898

5 (6-endo TS)

Total energy = -385.11030
 6 -0.601635 .000032 -1.763871
 6 -0.631809 .000301 -0.342096
 6 0.624000 -0.000298 0.331501
 6 1.906150 -0.000791 -0.383978
 6 2.108614 -0.000559 -1.696867
 6 -0.060767 0.002004 -2.862315
 1 3.028946 -0.000987 -2.271176
 1 0.169244 0.000773 -3.903586
 1 2.783187 -0.001339 0.274400
 6 -1.827556 0.000466 0.392701
 6 -1.803022 0.000384 1.783392
 1 -2.771358 0.001316 -0.143097
 1 -2.733643 0.000019 2.342349
 6 -0.576735 -0.000472 2.455127
 6 0.614480 -0.000732 1.735721
 1 -0.550992 -0.000473 3.540809
 1 1.564293 -0.001323 2.264414

5 (6-endo P)

Total energy = -385.21615
 6 -1.868966 0.000000 -1.712372
 6 -1.877399 0.000000 -0.336236
 6 -0.655802 0.000000 0.389559
 6 0.595384 0.000000 -0.327109
 6 0.556553 0.000000 -1.747418
 6 -0.642991 0.000000 -2.422636
 1 -2.805933 0.000000 -2.261301
 1 -2.811644 0.000000 0.216253
 6 -0.554008 0.000000 1.788060
 6 1.812638 0.000000 0.409356
 1 1.495895 0.000000 -2.294589
 1 -0.653954 0.000000 -3.508610
 6 1.819276 0.000000 1.786261
 6 0.593343 0.000000 2.515361
 1 2.750278 0.000000 -0.139700
 1 2.760487 0.000000 2.329496
 1 0.596700 0.000000 3.601499

6-R

Total energy = -385.12090
 6 -.460986 .000000 -1.900583
 6 -.476339 .000000 -.485907
 6 .776000 .000000 .118765
 6 1.986842 .000000 -.528710
 6 1.963382 .000000 -1.934281
 6 .739397 .000000 -2.608702
 1 -1.407923 .000000 -2.436342
 1 2.928661 .000000 .012969
 1 2.896508 .000000 -2.491379
 6 -1.741223 .000000 .240068
 6 -1.911254 .000000 1.582374
 1 -2.637427 .000000 -.376023
 1 -2.926896 .000000 1.972600
 6 -.875506 .000000 2.550534
 6 -.047024 .000000 3.436872
 1 .706244 .000000 4.189966
 1 .721090 .000000 -3.694369

6 (5-exo TS)

Total energy = -385.11512
 6 -.660575 .000000 -1.887735
 6 -.671311 .000000 -.481760
 6 .560389 .000000 .165314
 6 1.779263 .000000 -.467950
 6 1.769250 .000000 -1.875318
 6 .557231 .000000 -2.571690
 1 -1.599123 .000000 -2.437629
 1 2.716794 .000000 .081817

1 2.709129 .000000 -2.421281
 6 -1.853843 .000000 .367577
 6 -1.678245 .000000 1.706795
 1 -2.847182 .000000 -.070696
 1 -2.517103 .000000 2.395891
 6 -.365209 .000000 2.278481
 6 .493476 .000000 3.162067
 1 1.392884 .000000 3.734844
 1 .562044 .000000 -3.657621

6 (5-exo P)

Total energy = -385.17736
 6 -.810341 .000000 -1.827248
 6 -.819964 .000000 -.434169
 6 .397782 .000000 .286930
 6 1.619317 .000000 -.372947
 6 1.623076 .000000 -1.773833
 6 .422589 .000000 -2.490641
 1 -1.739033 .000000 -2.391333
 1 2.551265 .000000 .184746
 1 2.568303 .000000 -2.308542
 6 -1.920616 .000000 .535117
 6 -1.422333 .000000 1.793230
 1 -2.971624 .000000 .268930
 1 -1.983418 .000000 2.718611
 6 .061505 .000000 1.734130
 6 .897715 .000000 2.760097
 1 .835273 .000000 3.840156
 1 .446860 .000000 -3.576568

6 (6-endo TS)

Total energy = -385.11179
 6 -.566285 .000000 -1.778041
 6 -.555200 .000000 -.362495
 6 .709558 .000000 .242417
 6 1.901727 .000000 -.452272
 6 1.854411 .000000 -1.853325
 6 .617879 .000000 -2.507964
 1 -1.522806 .000000 -2.296400
 1 2.858439 .000000 .064484
 1 2.777050 .000000 -2.427950
 6 -.1818269 .000000 .369400
 6 -1.936078 .000000 1.721804
 1 -2.725346 .000000 -.231019
 1 -2.908703 .000000 2.207833
 6 -.754055 .000000 2.496199
 6 .461819 .000000 2.659403
 1 1.448064 .000000 3.065729
 1 .580256 .000000 -3.593436

6 (6-endo P)

Total energy = -385.21618
 6 -.623758 .000000 -1.708963
 6 -.630988 .000000 -.287511
 6 .625571 .000000 .406682
 6 1.829141 .000000 -.347195
 6 1.797374 .000000 -1.723589
 6 .559708 .000000 -2.411584
 1 -1.574764 .000000 -2.235329
 1 2.777913 .000000 .182693
 1 2.725245 .000000 -2.288214
 6 -.1843844 .000000 .456119
 6 -.1834267 .000000 1.838889
 1 -2.788721 .000000 -.082546
 1 -2.759633 .000000 2.406974
 6 -.583416 .000000 2.462117
 6 .622168 .000000 1.837638
 1 1.565274 .000000 2.378256
 1 .548550 .000000 -3.497454

7-R

Total energy = -538.77556
 6 -1.681030 0.000000 -2.922263
 6 -1.680493 0.000000 -1.528491
 6 -.469539 0.000000 -0.798046
 6 0.677586 0.000000 -1.578418
 6 0.736230 0.000000 -2.951861
 6 -.483750 0.000000 -3.643575
 1 -2.629066 0.000000 -3.451854
 1 -2.634158 0.000000 -1.009840
 1 1.683251 0.000000 -3.484897
 1 -.496398 0.000000 -4.730287
 6 -.397667 0.000000 0.681058
 6 -.1555177 0.000000 1.476396
 6 -.1494017 0.000000 2.865971
 6 -.256700 0.000000 3.512734
 6 0.906726 0.000000 2.754092
 6 0.858558 0.000000 1.346779
 1 -.2530134 0.000000 1.002761
 1 -.2413649 0.000000 3.443458
 1 -.199717 0.000000 4.596749
 6 2.109284 0.000000 0.650680
 6 3.250025 0.000000 0.235065
 1 4.221078 0.000000 -0.202983
 1 1.878569 0.000000 3.236162

7 (5-exo TS)

Total energy = -538.77472
 6 -.1771530 0.000000 -2.861390
 6 -.1781061 0.000000 -.1466266
 6 -.569004 0.000000 -.0747687
 6 0.591309 0.000000 -1.507264
 6 0.653093 0.000000 -2.880731
 6 -.0568063 0.000000 -.3573495
 1 -.2714490 0.000000 -3.400045
 1 -.2732548 0.000000 -.941547
 1 1.599651 0.000000 -3.414664
 1 -.0576666 0.000000 -4.660362
 6 -.432961 0.000000 0.719112
 6 -.1515464 0.000000 1.608217
 6 -.1313154 0.000000 2.985938
 6 -.016135 0.000000 3.505878
 6 1.074035 0.000000 2.641717
 6 0.880991 0.000000 1.250131
 1 -.2529029 0.000000 1.220934
 1 -.2168204 0.000000 3.655390
 1 0.144685 0.000000 4.579525
 6 2.029807 0.000000 0.383597
 6 3.196590 0.000000 0.011885
 1 4.138706 0.000000 -0.486536
 1 2.087184 0.000000 3.029447

7 (5-exo P)

Total energy = -538.84013
 6 -.2003378 0.000000 -2.647635
 6 -.2005116 0.000000 -1.250102
 6 -.785863 0.000000 -.573905
 6 0.428451 0.000000 -1.299262
 6 0.426187 0.000000 -2.690451
 6 -.800018 0.000000 -3.361932
 1 -.2946698 0.000000 -3.185842
 1 -.2943830 0.000000 -.703349
 1 1.358171 0.000000 -3.248555
 1 -.818551 0.000000 -4.447694
 6 -.473459 0.000000 0.862487
 6 -.1300492 0.000000 1.984980
 6 -.715137 0.000000 3.253979
 6 0.677086 0.000000 3.401063
 6 1.511450 0.000000 2.279879
 6 0.931701 0.000000 1.014727

1 -2.381837 0.000000 1.880637
 1 -1.347848 0.000000 4.136746
 1 1.112277 0.000000 4.395990
 6 1.564020 0.000000 -0.329614
 6 2.857421 0.000000 -0.601985
 1 3.499448 0.000000 -1.471797
 1 2.591749 0.000000 2.390492

7 (6-endo TS)

Total energy = -538.76712
 6 -1.554466 0.000000 -2.912547
 6 -1.557205 0.000000 -1.520726
 6 -0.353486 0.000000 -0.773361
 6 0.809620 0.000000 -1.546136
 6 0.856488 0.000000 -2.924920
 6 -0.353519 0.000000 -3.627412
 1 -2.501212 0.000000 -3.444547
 1 -2.516415 0.000000 -1.014190
 1 1.804397 0.000000 -3.458026
 1 -0.358859 0.000000 -4.714337
 6 -0.353930 0.000000 0.716194
 6 -1.554034 0.000000 1.449554
 6 -1.573453 0.000000 2.840733
 6 -0.379831 0.000000 3.565501
 6 0.826375 0.000000 2.878175
 6 0.855747 0.000000 1.473603
 1 -2.503928 0.000000 0.928861
 1 -2.527179 0.000000 3.360178
 1 -0.391960 0.000000 4.650865
 6 2.097005 0.000000 0.776786
 6 2.830788 0.000000 -0.201800
 1 3.649115 0.000000 -0.885853
 1 1.769435 0.000000 3.415182

7 (6-endo P)

Total energy = -538.86529
 6 -1.557872 0.000000 -2.834235
 6 -1.559178 0.000000 -1.451133
 6 -0.355305 0.000000 -0.708440
 6 0.873657 0.000000 -1.437662
 6 0.851482 0.000000 -2.850716
 6 -0.343378 0.000000 -3.543412
 1 -2.500578 0.000000 -3.373213
 1 -2.511858 0.000000 -0.933543
 1 1.797382 0.000000 -3.385743
 1 -0.345949 0.000000 -4.629360
 6 -0.332594 0.000000 0.751728
 6 -1.499619 0.000000 1.549495
 6 -1.430967 0.000000 2.931630
 6 -0.186351 0.000000 3.587489
 6 0.978084 0.000000 2.845319
 6 0.929681 0.000000 1.432754
 1 -2.475942 0.000000 1.077795
 1 -2.347986 0.000000 3.513384
 1 -0.142268 0.000000 4.672471
 6 2.087578 0.000000 0.618321
 6 2.131010 0.000000 -0.722541
 1 3.061191 0.000000 -1.284986
 1 1.948646 0.000000 3.331610

8-R

Total energy = -616.19100
 6 1.488333 -0.000233 -2.486844
 6 1.517931 0.002107 -1.080260
 6 2.771460 0.008331 -0.410611
 6 3.942151 0.012281 -1.183495
 6 3.897883 0.010144 -2.574890
 6 2.664852 0.003784 -3.230141
 1 0.524381 -0.004954 -2.985106
 1 4.902475 0.017077 -0.674607

1 4.821498 0.013354 -3.145968
 1 2.618744 0.002064 -4.314867
 6 2.874962 0.010402 1.054405
 6 1.869091 0.006343 1.909751
 6 0.283377 -0.001385 -0.363898
 6 -0.832984 -0.004279 0.124846
 1 3.901330 0.015579 1.442539
 1 1.772057 0.006755 2.987194
 6 -2.120507 -0.006316 0.739115
 6 -2.757501 1.205837 1.071050
 6 -4.015324 1.198993 1.667554
 6 -4.658613 -0.009851 1.942833
 6 -4.035508 -1.216933 1.617910
 6 -2.777874 -1.220259 1.020963
 1 -2.254071 2.142711 0.856359
 1 -4.495341 2.140266 1.918837
 1 -5.639852 -0.011214 2.408040
 1 -4.531301 -2.159591 1.830376
 1 -2.290314 -2.155835 0.767467

8 (5-exo TS)

Total energy = -616.19004
 6 -0.010368 0.008229 -0.812811
 6 -0.057415 -0.001367 0.414289
 6 2.231426 -0.112013 1.278893
 6 1.809402 -0.105612 2.530705
 6 0.377992 -0.044677 2.843716
 6 -0.539701 0.006919 1.764989
 6 -1.916944 0.065949 2.029712
 6 -2.384183 0.073983 3.342538
 6 -1.479931 0.023122 4.406240
 6 -0.110055 -0.035690 4.155145
 1 -2.611833 0.105186 1.197129
 1 -3.451933 0.119853 3.534096
 1 -1.842467 0.029323 5.429921
 1 0.594098 -0.075267 4.981981
 1 2.504894 -0.145145 3.375712
 1 3.189043 -0.149940 0.777766
 6 0.167199 0.014113 -2.222255
 6 0.199130 -1.196175 -2.947401
 6 0.366808 -1.184104 -4.328538
 6 0.504681 0.026416 -5.012672
 6 0.474217 1.230799 -4.304899
 6 0.307064 1.230726 -2.923647
 1 0.092134 -2.134210 -2.412729
 1 0.390385 -2.122787 -4.874307
 1 0.634963 0.031174 -6.090683
 1 0.581489 2.174165 -4.832249
 1 0.283281 2.163930 -2.370659

8 (5-exo P)

Total energy = -616.26063
 6 -2.724442 -0.046222 -1.778123
 6 -2.932688 -0.038245 -0.327147
 6 -1.663894 -0.018230 0.299733
 6 -0.634254 -0.013462 -0.778349
 6 0.674205 0.003604 -0.638276
 6 -1.398603 -0.031982 -2.049043
 6 -4.093632 -0.046841 0.444077
 6 -3.975272 -0.035300 1.838601
 6 -2.718704 -0.015517 2.452166
 6 -1.548206 -0.006804 1.682780
 1 -5.073454 -0.062208 -0.025499
 1 -4.871253 -0.041797 2.452642
 1 -2.649311 -0.006816 3.535923
 1 -0.571451 0.008571 2.158273
 1 -3.523005 -0.061276 -2.511094
 6 2.030872 0.021654 -0.439298
 6 2.780794 -1.196960 -0.327190
 6 4.150158 -1.162978 -0.132825

6 4.834140 0.058897 -0.042220
 6 4.120416 1.262204 -0.150290
 6 2.750668 1.259788 -0.344884
 1 2.253136 -2.142202 -0.396922
 1 4.699415 -2.096486 -0.049547
 1 5.908556 0.073172 0.110311
 1 4.646604 2.210002 -0.080563
 1 2.19994 2.190699 -0.428129
 1 -0.928581 -0.033296 -3.023676

8 (6-endo TS)

Total energy = -616.18372
 6 1.348122 -0.257601 -2.921310
 6 1.244707 -0.074978 -1.531719
 6 2.418536 .152015 -.754465
 6 3.654234 .187349 -1.419725
 6 3.743496 .006664 -2.796482
 6 2.586959 -.217683 -3.550854
 1 .442456 -.428689 -3.494339
 1 4.556192 .358291 -.837373
 1 4.713450 .039400 -3.283748
 1 2.653695 -.359990 -4.625089
 6 2.365630 .330785 .699367
 6 1.284018 .317809 1.471328
 6 .001895 -.102575 -.847397
 6 -.704495 -.020065 .163418
 1 3.343556 .478832 1.172436
 1 1.188800 .413625 2.547721
 6 -1.847504 -.035553 1.027506
 6 -2.907299 -.925766 .761529
 6 -4.032610 -.943889 1.580190
 6 -4.121321 -.081982 2.675907
 6 -3.076459 .804173 2.946340
 6 -1.948354 .831790 2.130870
 1 -2.831754 -.1595755 -.088432
 1 -4.841839 -.1635157 1.363971
 1 -4.999959 -.099856 3.313725
 1 -3.142138 1.480252 3.793715
 1 -1.139800 1.526092 2.330401

8 (6-endo P)

Total energy = -616.28084
 6 1.093510 -0.051191 -2.981487
 6 1.057988 -0.025284 -1.560444
 6 2.295999 0.017635 -0.823262
 6 3.515246 0.026960 -1.549014
 6 3.517711 0.000285 -2.926045
 6 2.298339 -.038149 -3.646473
 1 0.155536 -.081402 -3.526771
 1 4.451366 0.055910 -.997099
 1 4.459134 0.008920 -3.467264
 1 2.318470 -0.058266 -4.732027
 6 2.237007 0.043326 0.597660
 6 1.039193 0.034835 1.271865
 6 -0.108182 -0.035449 -0.789671
 6 -0.214344 0.003364 0.573585
 1 3.169490 0.060877 1.155286
 1 1.035514 0.028191 2.357896
 6 -1.518845 0.005282 1.276866
 6 -2.654905 -.540233 0.653812
 6 -3.890480 -.543308 1.294940
 6 -4.019366 -.002996 2.576521
 6 -2.901026 0.545480 3.205393
 6 -1.664051 0.551825 2.562280
 1 -2.552800 -0.972573 -0.337191
 1 -4.753878 -.974575 0.796412
 1 -4.982270 -.007852 3.078602
 1 -2.991698 0.977976 4.197679
 1 -0.811633 1.008499 3.055338

9-R

Total energy = -616.19864
 6 -.036852 -.061083 -3.672086
 6 -.012748 -.037367 -2.265363
 6 1.235586 .028601 -1.590460
 6 2.406480 .067783 -2.363937
 6 2.368250 .043673 -3.754733
 6 1.139189 -.021164 -4.413952
 1 -.999261 -.111561 -4.170661
 1 3.364302 .118286 -1.852960
 1 3.293701 .075361 -4.321984
 1 1.096361 -.040529 -5.498555
 6 1.372328 .058333 -.123750
 6 .425709 .031318 .786820
 6 -.1256423 -.080927 -1.564840
 6 -.2355137 -.121312 -1.056002
 1 -.3297913 -.155135 -.561201
 1 2.413094 .109766 .221367
 6 -.202569 .023783 2.020638
 6 -.615917 1.240864 2.645183
 6 -.1274111 1.219383 3.864424
 6 -.1555640 .004695 4.505088
 6 -.1167636 -1.200760 3.903828
 6 -.508358 -1.203963 2.684990
 1 -.401309 2.181248 2.148399
 1 -.1573496 2.156126 4.326147
 1 -.0272820 -.002514 5.459466
 1 -.1384275 -.2144675 4.396170
 1 -.211300 -2.137511 2.218707

9 (5-exo TS)

Total energy = -616.19067
 6 .530762 .141120 -3.490074
 6 .420133 .043244 -2.097317
 6 1.584111 -.081111 -1.304215
 6 2.838166 -.107493 -1.921330
 6 2.939565 -.007811 -3.308994
 6 1.788451 .115892 -4.092380
 1 -.369559 .234753 -4.088527
 1 3.732919 -.204584 -1.312460
 1 3.917278 -.027398 -.3781444
 1 1.869987 .191601 -5.172422
 6 1.362550 -.183321 .138250
 6 .123575 -.113633 .604614
 6 -.854293 .061812 -1.423804
 6 -.2086796 .115995 -1.365894
 1 -.3092287 .155283 -1.010834
 1 2.220794 -.347466 .794833
 6 -.643356 -.069207 1.803380
 6 -.1647221 -1.032442 2.058488
 6 -.2411738 -.967423 3.218169
 6 -.2207682 .060609 4.143979
 6 -.1229687 1.029081 3.898991
 6 -.459419 .973967 2.742210
 1 -.1805836 -.1827675 1.337301
 1 -.3171918 -.1721056 3.403296
 1 -.2809064 .108875 5.046831
 1 -.1069111 1.831845 4.613056
 1 .294072 1.730145 2.545925

9 (5-exo P)

Total energy = -616.24309
 6 .574602 -.095471 -3.354178
 6 .513982 -.039002 -1.968244
 6 1.691506 .059716 -1.190905
 6 2.940412 .099084 -1.809571
 6 2.999070 .040213 -3.206414
 6 1.831731 -.055950 -3.970926
 1 -.332425 -.170995 -3.946735
 1 3.851164 .175017 -1.222088

1 3.964134 .069712 -3.703988
 1 1.900393 -.101693 -5.053709
 6 1.303479 .092785 .215534
 6 -.050666 .017043 .343693
 6 -.641073 -.049691 -1.036380
 6 -.1919704 -.042643 -1.374082
 1 -.2884680 .006446 -.890604
 1 2.003453 .135452 1.042536
 6 -.816887 .010043 1.598306
 6 -.1951817 -.804578 1.763347
 6 -.2653108 -.817864 2.967903
 6 -.2236213 -.020645 4.034986
 6 -.1109090 .790414 3.887439
 6 -.409931 .808294 2.682912
 1 -.2262441 -.1454974 .952203
 1 -.3522343 -.1460395 3.075771
 1 -.2784357 -.030562 4.972374
 1 -.779708 1.419656 4.709349
 1 .449049 1.461844 2.564368

9 (6-endo TS)

Total energy = -616.18866
 6 -.520957 -.274643 -3.813118
 6 -.442561 -.204655 -2.415548
 6 .798302 .154119 -.1807519
 6 1.891425 .422124 -2.649431
 6 1.793236 .347200 -.0434565
 6 .577139 -.004061 -.4622155
 1 -.1470933 -.548748 -4.262043
 1 2.839326 .695864 -2.193235
 1 2.660628 .561679 -4.651653
 1 .483269 -.067172 -.5701765
 6 1.027062 .266796 -.359144
 6 .203482 .079272 .655431
 6 -.1565776 -.480794 -.1568786
 6 -.2079564 -.582249 -.465092
 1 -.2712873 -.724180 .381084
 1 2.055981 .554768 -.108382
 6 -.032229 .062761 2.036318
 6 -.511456 1.221153 2.712912
 6 -.787545 1.182410 4.072171
 6 -.611338 .000514 4.802861
 6 -.152060 -.1151936 4.152669
 6 .129363 -.1132643 2.794084
 1 -.650554 2.136705 2.147071
 1 -.142709 2.079554 4.571470
 1 -.831469 -.022765 5.865655
 1 -.012712 -2.071238 4.714610
 1 .482917 -.2026683 2.290646

9 (6-endo P)

Total energy = -616.28014
 6 -.354062 .116667 -.3858646
 6 -.392653 .091842 -.2440051
 6 .830855 -.072700 -.1696395
 6 2.045359 -.199740 -2.423465
 6 .2052081 -.172180 -.3799864
 6 .844555 -.013572 -.4523465
 1 -.1284380 .239925 -.4404057
 1 2.973734 -.320878 -.1871129
 1 2.989512 -.272265 -.4338988
 1 .868661 .006416 -.5608868
 6 .784848 -.092699 -.277049
 6 -.398972 .036882 .431227
 6 -.1550148 .217603 -.1659212
 6 -.1621916 .197996 -.306127
 1 -.2567352 .268529 .223402
 1 1.722444 -.186782 .263317
 6 -.422718 .011324 1.915287
 6 -.1286426 .852107 2.637549

6 -.1303136 .834204 4.031127
 6 -.458154 -.026327 4.733655
 6 .402728 -.870071 4.029613
 6 .418652 -.853231 2.636259
 1 -.1930172 1.543776 2.102376
 1 -.1972538 1.499410 4.568969
 1 -.472208 -.041354 5.819408
 1 1.056619 -.1551652 4.566123
 1 1.070319 -.1533752 2.096795

10-R

Total energy = -847.274158
 6 1.023181 -.0066660 -3.789482
 6 1.157687 0.007281 -2.386159
 6 2.460759 0.042952 -1.817532
 6 3.565626 0.062196 -2.683229
 6 3.415927 0.047628 -4.066432
 6 2.135438 0.013092 -4.623097
 1 0.023243 -.003766 -4.209959
 1 4.562428 0.089485 -2.250845
 1 4.292821 0.063315 -4.706656
 1 2.003949 0.001540 -5.700770
 6 2.718261 0.062049 -0.368649
 6 1.851283 0.049525 0.618770
 6 -.026886 -.014810 -.1597508
 6 -.1110549 -.036842 -1.041131
 1 3.784328 0.091195 -0.108902
 6 1.367090 0.048591 1.917813
 6 1.114065 -.1176181 2.609718
 6 0.591417 -.1166225 3.893587
 6 0.292993 0.043787 4.535902
 6 0.526062 1.255982 3.871097
 6 1.047842 1.270377 2.587092
 1 1.341235 -.2113062 2.111950
 1 0.413176 -.2108071 4.404824
 1 -.0117083 0.042025 5.540982
 1 0.296450 2.196100 4.364672
 1 1.223596 2.208753 2.071688
 6 -.2369157 -.060557 -.0373667
 6 -.3566654 -.038946 -1.117870
 6 -.4798696 -.061255 -.471308
 6 -.4860818 -.105560 0.923580
 6 -.3680121 -.127651 1.669692
 6 -.2442187 -.105570 1.033547
 1 -.3514255 -.004334 -2.201251
 1 -.5713191 -.044040 -1.056994
 1 -.5823635 -.122954 1.425691
 1 -.3722418 -.162133 2.754397
 1 -.1526049 -.123275 1.612767

10 (5-exo TS)

Total energy = -847.26841
 6 -.070443 -.1367345 .042560
 6 1.036838 -.822689 .017577
 6 .860838 1.512047 -.146713
 6 2.171690 1.685244 -.190563
 6 3.074475 .537983 -.081723
 6 2.471953 -.737541 .025644
 6 3.278370 -.1880040 .130147
 6 4.667382 -.1760300 .129287
 6 5.262266 -.500107 .022232
 6 4.469083 .641885 -.083965
 1 2.807430 -.2854444 .210791
 1 5.284675 -.2649862 .210806
 1 6.344454 -.408542 .020912
 1 4.930398 1.622248 -.168093
 1 2.612158 2.676814 -.329280
 6 -.400490 2.156019 -.120139
 6 -.1297964 2.051081 -.1211667
 6 -.2545639 2.660642 -.1162425

6 -2.941358 3.376182 -0.027408
 6 -2.073964 3.476287 1.065414
 6 -.823177 2.871766 1.028776
 1 -.992617 1.490548 -2.089174
 1 -3.217483 2.576841 -2.011889
 1 -3.918913 3.847617 .006902
 1 -2.376875 4.029584 1.949935
 1 -.150477 2.944652 1.877410
 6 -1.403263 -1.845362 .064990
 6 -2.024534 -2.302118 -1.119480
 6 -3.328744 -2.783274 -1.089399
 6 -4.040285 -2.823310 .113129
 6 -3.436164 -2.376096 1.291538
 6 -2.132658 -1.892051 1.274472
 1 -1.468918 -2.272307 -2.051037
 1 -3.793816 -3.130042 -2.007655
 1 -5.058288 -3.200623 .131632
 1 -3.985388 -2.403903 2.228116
 1 -1.661620 -1.541989 2.186909

10 (5-exo P)

Total energy = -847.32653
 6 -2.589256 0.272915 -0.708920
 6 -2.819611 0.248512 0.729846
 6 -1.570368 0.089249 1.373609
 6 -.0527911 0.016676 0.311893
 6 0.770328 -0.086479 0.509875
 6 -1.261166 0.137117 -0.988193
 6 -3.988632 0.344541 1.485138
 6 -3.894927 0.283297 2.879536
 6 -2.655883 0.127970 3.510074
 6 -1.478640 0.029126 2.757102
 1 -4.954416 0.465943 1.002231
 1 -4.796274 0.357543 3.481150
 1 -2.605695 0.082314 4.593908
 1 -0.516070 -0.093024 3.245801
 1 -3.376731 0.356226 -1.449014
 6 2.015930 -0.210434 1.091281
 6 2.577919 -1.498738 1.365475
 6 3.844576 -1.610301 1.913860
 6 4.602516 -0.467359 2.206485
 6 4.072156 0.803473 1.940758
 6 2.808776 0.943226 1.391705
 1 1.991276 -2.383595 1.141550
 1 4.251570 -2.596091 2.120079
 1 5.594740 -0.565808 2.635220
 1 4.656432 1.690877 2.166570
 1 2.400129 1.926178 1.182985
 6 -.643753 0.122666 -2.321615
 6 0.531589 -.602963 -2.586393
 6 1.088981 -.621344 -3.863723
 6 0.485856 0.081125 -4.907680
 6 -.680760 0.808346 -4.660718
 6 -1.235026 0.832780 -3.384013
 1 0.999497 -1.169832 -1.789159
 1 1.994969 -1.192865 -4.044264
 1 0.921883 0.066245 -5.902203
 1 -1.153878 1.368199 -.5462494
 1 -2.123605 1.427281 -3.194648

10 (6-endo TS)

Total energy = -847.25836
 6 0.868293 -0.017487 -4.200431
 6 0.851469 -0.015986 -2.795525
 6 2.075669 -0.013292 -2.067843
 6 3.277200 -0.017100 -2.796052
 6 3.281637 -0.023114 -4.186839
 6 2.073421 -0.021936 -4.893179
 1 -.076933 -0.018379 -4.733811
 1 4.218282 -0.014025 -2.251677

1 4.225694 -0.026778 -4.723626
 1 2.074909 -.025173 -5.978866
 6 2.113310 0.011070 -0.606811
 6 1.094481 0.011722 0.252475
 6 -.349636 -0.014743 -2.038110
 6 -.921511 -0.015388 -0.934440
 1 3.122487 0.056613 -0.182725
 6 0.954778 -0.015456 1.675422
 6 1.262632 -1.187875 2.408211
 6 1.111628 -1.220902 3.790804
 6 0.642714 -0.097353 4.478048
 6 0.324183 1.064719 3.767446
 6 0.469485 1.108015 2.385852
 1 1.628087 -2.059294 1.873497
 1 1.363869 -2.125688 4.336926
 1 0.524189 -0.127362 5.557014
 1 -.040856 1.940687 4.296068
 1 0.215471 2.007693 1.834633
 6 -2.044869 0.028750 -0.037257
 6 -.3019466 1.033119 -0.198828
 6 -4.133650 1.073466 0.634686
 6 -4.292074 0.120187 1.643327
 6 -3.328966 -0.876227 1.813197
 6 -2.212663 -.925096 0.982063
 1 -2.890797 1.769869 -.984919
 1 -4.879493 1.850889 0.497082
 1 -5.161411 0.154314 2.293347
 1 -3.447462 -1.620098 2.595361
 1 -1.464428 -1.697825 1.114416

10 (6-endo P)

Total energy = -847.33819
 6 -1.810051 .040949 .703092
 6 -1.825842 .027012 2.100691
 6 -.528857 -.018545 2.721070
 6 .621678 -.066002 1.890767
 6 .562285 -.054557 .506901
 6 -.734496 .035354 -.137018
 6 -2.991416 .061070 2.911478
 6 -2.880078 .048988 4.283648
 6 -1.605755 -.000961 4.901233
 6 -.459082 -.035816 4.139218
 1 -3.963200 .098713 2.429627
 1 -3.773232 .075991 4.900648
 1 -1.536848 -.012783 5.984951
 1 .517619 -.077856 4.614495
 6 1.834426 -.180314 -.259998
 6 2.925839 .651736 .037983
 6 4.140303 .506944 -.633038
 6 4.286458 -.475217 -1.612974
 6 3.209060 -.310168 -.1917478
 6 1.994518 -.163316 -1.250691
 1 2.812247 1.425033 .792179
 1 4.970366 1.164734 -.391561
 1 5.231162 -.589369 -2.136401
 1 3.315266 -.2081201 -2.675107
 1 1.163733 -.1819040 -.149856
 6 -.952474 .169414 -1.604910
 6 -.193357 1.049966 -2.392572
 6 -.463809 1.199571 -3.751599
 6 -1.495430 .474035 -4.350691
 6 -2.260325 -.400347 -3.577467
 6 -1.992408 -.549185 -2.217583
 1 .604147 1.625966 -1.936151
 1 .131211 1.889363 -4.343196
 1 -1.701790 .590883 -5.410569
 1 -3.065600 -.969687 -4.032863
 1 -2.585267 -1.231385 -1.615760
 1 1.593073 -.153017 2.369186

18-R

Total energy = -401.17301
 6 -.545822 0.000003 -1.662629
 6 -.581579 -.000012 -0.255386
 6 0.650792 -0.000018 0.452431
 6 1.854688 -0.000005 -0.261763
 6 1.866817 0.000003 -1.653322
 6 0.660315 0.000008 -2.356101
 1 -1.487780 0.000010 -2.200952
 1 2.777512 -.000002 0.308325
 1 2.812558 0.000009 -2.186234
 1 0.657122 0.000018 -3.441688
 7 0.765209 -.000019 1.854433
 6 -.130519 0.000049 2.716238
 1 0.074370 0.000091 3.795374
 6 -1.849257 -.000013 0.397770
 6 -2.968117 -.000012 0.861663
 1 -3.934149 -.000013 1.310735

18 (5-exo TS)

Total energy = -401.16633
 6 -.598615 0.000000 -2.979818
 6 -.227680 0.000000 -1.803030
 6 2.014646 0.000000 -1.427522
 7 2.009294 0.000000 -0.178697
 6 0.740566 0.000000 0.448360
 6 -.409039 0.000000 -0.375626
 1 -.632879 0.000000 -4.046085
 1 2.893795 0.000000 -2.076312
 6 -1.674408 0.000000 0.226291
 6 -1.787945 0.000000 1.616520
 6 -.644217 0.000000 2.419524
 6 0.623315 0.000000 1.835759
 1 -.2559003 0.000000 -0.401875
 1 -2.772728 0.000000 2.073650
 1 -.739699 0.000000 3.500998
 1 1.525709 0.000000 2.437751

12 (5-exo P)

Total energy = -401.21687
 7 -.886873 0.000000 -1.763173
 6 -.823929 0.000000 -0.343932
 6 0.507569 0.000000 0.126236
 6 1.348505 0.000000 -1.086482
 6 2.661538 0.000000 -1.227975
 6 0.331810 0.000000 -2.188656
 1 3.370610 0.000000 -2.045321
 1 0.582491 0.000000 -3.245008
 6 -1.898358 0.000000 0.536336
 6 -1.619416 0.000000 1.908692
 6 -.301254 0.000000 2.378284
 6 0.780592 0.000000 1.488521
 1 -2.916354 0.000000 0.161213
 1 -2.439306 0.000000 2.620807
 1 -.113778 0.000000 3.447807
 1 1.802108 0.000000 1.856576

12 (6-endo TS)

Total energy = -401.16224
 6 -.822784 .000000 -1.709975
 6 -.795236 .000000 -.318692
 6 -.578764 .000000 .375734
 6 .641150 .000000 -.361844
 6 .592155 .000000 -1.764943
 6 -.627063 .000000 -2.434889
 1 -.2775646 .000000 -2.230327
 1 -.2710821 .000000 .263520
 7 -.650211 .000000 1.778752
 6 1.855785 .000000 .379585

1 1.526384 .000000 -2.317216
 1 -.646751 .000000 -3.520329
 6 2.427495 .000000 1.467722
 6 .286004 .000000 2.605949
 1 3.174580 .000000 2.229891
 1 .111283 .000000 3.691310

12 (6-endo P)

Total energy = -401.25377
 6 -1.800131 .000000 -1.697963
 6 -1.780120 .000000 -3.20947
 6 -.548955 .000000 .384576
 6 .679381 .000000 -.378007
 6 .622943 .000000 -1.795997
 6 -.593815 .000000 -2.440136
 1 -2.750181 .000000 -2.223973
 1 -2.693704 .000000 .264372
 7 -.566126 .000000 1.747641
 6 1.842804 .000000 .399341
 1 1.552528 .000000 -2.356182
 1 -.632026 .000000 -3.525207
 6 1.861943 .000000 1.755059
 6 .579907 .000000 2.390338
 1 2.769496 .000000 2.350483
 1 .533026 .000000 3.479439

14-R

Total energy = -348.20415
 6 -0.090722 0.039342 -0.601443
 6 -.072393 0.008740 0.758361
 6 1.095108 -0.062834 1.632124
 6 2.364678 -0.110490 1.260805
 1 3.317690 -0.170293 1.769737
 6 1.038585 0.010875 -1.452387
 6 1.972512 -0.011264 -2.226623
 1 2.809303 -0.036532 -2.885027
 1 0.872185 -0.081518 2.706962
 6 -.1478770 0.111378 1.315029
 1 -1.654800 -0.587157 2.141889
 1 -1.648909 1.119763 1.721687
 6 -2.381076 -0.171332 0.092394
 1 -2.637778 -1.235735 0.070459
 1 -3.318972 0.390342 0.116005
 6 -1.508291 0.168990 -1.137778
 1 -1.694282 -0.493406 -1.989823
 1 -1.682226 1.194102 -1.494784

14 (5-exo TS)

Total energy = -348.19443
 6 0.131889 -0.140917 -2.889093
 6 0.152107 -0.074674 -1.653549
 6 2.249442 -0.032266 -0.798135
 6 1.881770 0.039695 0.475125
 6 0.443266 0.059039 0.731323
 6 -.388295 -0.000969 -0.335040
 1 0.412924 -0.195363 -3.916761
 1 3.186637 -.075672 -1.336642
 1 2.592518 0.076460 1.304207
 6 -.1843761 0.081886 0.067866
 1 -2.258912 1.068499 -0.181828
 1 -2.470812 -0.658387 -0.440723
 6 -1.775503 -0.148467 1.603939
 1 -2.517444 0.439965 2.150837
 1 -1.976385 -1.203305 1.817696
 6 -.316561 0.186560 2.025686
 1 -.230603 1.209088 2.422309
 1 0.055954 -.480611 2.812176

14 (5-exo P)

Total energy = -348.25001

6 -.920732 -0.069910 -1.654635
 6 -.886399 -.082021 -.185600
 6 0.391964 0.019602 0.242949
 6 1.273871 0.099985 -.935283
 6 2.593044 0.198035 -.977030
 6 0.350082 0.041014 -2.113211
 1 3.358998 0.260253 -1.739813
 1 0.683100 0.092776 -3.141461
 1 -1.813049 -.131694 -2.267282
 6 -.1858649 -.0230201 0.950440
 1 -2.730573 0.430739 0.876416
 1 -2.252320 -.1255825 1.002310
 6 -.9666534 0.111070 2.188013
 1 -1.141937 1.152693 2.475688
 1 -1.206747 -.0507230 3.057652
 6 0.522151 -.047935 1.736565
 1 1.165577 0.730648 2.162701
 1 0.944161 -1.010198 2.060533

14 (6-endo TS)

Total energy = -348.19558
 6 -.140144 0.026882 -.701529
 6 -.152417 0.026336 0.663764
 6 1.027359 0.047917 1.513185
 6 2.294457 0.062111 1.093779
 1 3.225282 0.070681 1.651635
 6 1.100742 0.054600 -1.370062
 6 2.329231 0.061182 -1.388693
 1 3.358084 0.069171 -1.668765
 1 0.834169 0.046098 2.592646
 6 -.1576576 0.046084 1.178977
 1 -1.734199 -.644283 2.016029
 1 -1.827822 1.049736 1.553176
 6 -.2418677 -.324970 -.067298
 1 -2.603052 -.1404465 -.0687788
 1 -3.392499 0.171869 -.084868
 6 -.1535536 0.042529 -1.287184
 1 -1.654666 -.656333 -2.122210
 1 -1.775922 1.041501 -1.678500

14 (6-endo P)

Total energy = -348.31439
 6 -.156939 0.040393 -.751356
 6 -.131316 0.036349 0.659499
 6 1.079297 0.099160 1.348508
 6 2.281801 0.163967 0.636628
 1 3.227604 0.203539 1.170890
 6 1.053355 0.112409 -1.397984
 6 2.280171 0.171219 -.768816
 1 3.212774 0.216871 -1.323931
 1 1.093395 0.091062 2.435175
 6 -.1546296 -.018394 1.200435
 1 -1.650264 -.680843 2.066378
 1 -1.863262 0.982386 1.526896
 6 -.2376212 -.490266 -.019970
 1 -2.425028 -.1584809 -.020073
 1 -3.403761 -.116466 -.005867
 6 -.1581271 -.016965 -.1263543
 1 -1.700629 -.681243 -2.124893
 1 -1.906362 0.982261 -1.584988

15-R

Total energy = -348.20378
 6 -.2166960 0.209571 -1.202031
 6 -.128225 0.354590 0.331963
 6 -.625171 0.319142 0.660155
 6 0.066729 -.327682 -.475210
 6 -.971595 -.712508 -1.512482
 1 -3.119314 -.184408 -1.568556
 1 -2.008513 1.188383 -1.668805

1 -2.623065 -.502831 0.807431
 1 -.2618314 1.260092 0.698707
 1 -.601197 -.622033 -2.538089
 1 -.1264967 -.1762608 -1.367449
 6 -.063027 0.797940 1.755761
 6 1.396796 -.539399 -0.607656
 1 -.398745 1.300549 2.653248
 1 1.761131 -.1012593 -1.518297
 6 2.376533 -.190034 0.352923
 6 3.258528 0.087221 1.138934
 1 4.011327 0.342399 1.847664

15 (5-exo TS)

Total energy = -348.19515
 6 -.2123075 0.092424 -1.322494
 6 -.2108236 0.264187 0.217201
 6 -.6020230 0.251820 0.555390
 6 0.105374 -.365062 -.569659
 6 -.873313 -.767723 -1.642691
 1 -.3050954 -.354215 -.1690968
 1 -.2017739 1.073958 -1.798111
 1 -.2604339 -.0587081 0.702450
 1 -.2618151 1.171182 0.553003
 1 -.494475 -.618541 -2.658466
 1 -.1115165 -.1835839 -.1544350
 6 0.090005 0.675871 1.586560
 6 1.448481 -.454586 -.485098
 1 -.086871 1.161364 2.536175
 1 2.072965 -.876581 -1.266321
 6 2.089510 0.041608 0.696936
 6 3.037329 0.301901 1.447179
 1 3.639665 0.623112 2.266640

15 (5-exo P)

Total energy = -348.25301
 6 -.2133426 0.098043 -.1269606
 6 -.2012955 0.301080 0.270665
 6 -.528065 0.229643 0.498924
 6 0.123207 -.407462 -.658437
 6 -.9111731 -.775437 -.1685051
 1 -.309136 -.345387 -.1563351
 1 -.2059561 1.072790 -.764386
 1 -.2518702 -.515948 0.804450
 1 -.2472059 1.234524 0.611111
 1 -.597543 -.597704 -.2718349
 1 -.1161669 -.1843055 -.1607477
 6 0.399906 0.575326 1.417772
 6 1.459099 -.459368 -.461729
 1 0.272797 1.065948 2.373604
 1 2.234112 -.850516 -.1107074
 6 1.722022 0.153479 0.865403
 6 2.900774 0.297844 1.453241
 1 3.278783 0.700460 2.384383

15 (6-endo TS)

Total energy = -348.19619
 6 -.2025808 0.127523 -1.327250
 6 -.2018946 0.286112 0.207186
 6 -.525861 0.262373 0.570078
 6 0.193294 -.375126 -.545388
 6 -.805725 -.772291 -.1613178
 1 -.2962585 -.287914 -.1709811
 1 -.1878165 1.105852 -.1798617
 1 -.2523930 -.567509 0.679362
 1 -.522838 1.193103 0.551676
 1 -.410026 -.666506 -2.627973
 1 -.1081209 -.1829316 -.1484431
 6 0.015254 0.742841 1.688011
 6 1.539574 -.554852 -.603139
 1 -.427071 1.237157 2.547031

1 2.011279 -1.013809 -1.467746
 6 2.311345 -0.115006 0.494977
 6 2.473056 0.402974 1.595980
 1 2.857452 0.801655 2.506853

15 (6-endo P)

Total energy = -348.31383
 6 -2.032819 0.119584 -1.237360
 6 -1.883205 0.352538 0.287304
 6 -0.386624 0.253343 0.505414
 6 0.223533 -0.374494 -0.592193
 6 -0.811099 -0.746502 -1.635058
 1 -2.987293 -0.340770 -1.507528
 1 -1.974072 1.082926 -1.756109
 1 -2.403432 -0.432106 0.855124
 1 -2.305766 1.309070 0.612625
 1 -0.475462 -0.563950 -2.661321
 1 -1.049251 -1.817547 -1.565489
 6 0.366130 0.670985 1.602638
 6 1.607487 -0.596291 -0.608572
 1 -0.109806 1.160681 2.449366
 1 2.097730 -1.077724 -1.450841
 6 2.300081 -0.160076 0.501908
 6 1.756741 0.462862 1.605890
 1 2.366001 0.787723 2.444342

16-R

Total energy = -348.20084
 6 -0.747705 -0.590274 -2.080794
 6 -0.593078 -0.065035 -0.693533
 6 0.579605 -0.281766 -0.086831
 6 1.477076 -1.049068 -1.068042
 6 0.738832 -0.924914 -2.429711
 1 -1.387946 -1.483787 -2.092344
 1 -1.192974 0.127531 -2.778059
 1 2.493977 -0.641454 -1.110895
 1 1.567453 -2.097330 -0.750712
 1 1.163114 -0.091900 -2.998511
 1 0.829569 -1.824813 -3.044504
 6 1.006700 0.061014 1.256277
 6 0.278577 0.706766 2.200224
 1 2.020031 -0.229130 1.525849
 1 0.735399 0.904034 3.167589
 6 -1.052751 1.157391 2.026969
 6 -2.192962 1.558407 1.921554
 1 -3.194383 1.901723 1.804904

16 (5-exo TS)

Total energy = -348.19052
 6 -0.420101 -0.262762 -1.949459
 6 -0.400752 -0.007724 -0.477340
 6 0.799979 -0.088992 0.105801
 6 1.864686 -0.411723 -0.929240
 6 1.111246 -0.202924 -2.278910
 1 -0.851561 -1.248300 -2.175614
 1 -0.996303 0.472039 -2.522716
 1 2.751734 0.228427 -0.851968
 1 2.213461 -1.447871 -0.815931
 1 1.347397 0.789861 -2.674149
 1 1.400042 -0.934952 -3.038716
 6 0.896687 0.076739 1.544464
 6 -0.265543 0.295974 2.202057
 1 1.847242 0.033140 2.067069
 1 -0.320759 0.449230 3.274737
 6 -1.490284 0.340716 1.456591
 6 -2.712768 0.452307 1.302491
 1 -3.690157 0.508756 0.878558

16 (5-exo P)

Total energy = -348.25004

6 -0.407568 -0.264358 -1.726431
 6 -0.374553 0.000434 -0.249684
 6 0.868028 -0.069226 0.278920
 6 1.908598 -0.387160 -0.757712
 6 1.112296 -0.195721 -2.088866
 1 -0.832603 -1.253651 -1.950543
 1 -0.995971 0.462676 -2.299182
 1 2.792627 0.259954 -0.710738
 1 2.273960 -1.418466 -0.645962
 1 1.335634 0.795229 -2.496989
 1 1.391815 -0.928331 -2.851342
 6 0.805928 0.134391 1.732890
 6 -0.489808 0.328351 2.081466
 1 1.654157 0.136062 2.407524
 1 -0.889681 0.520675 3.068136
 6 -1.330588 0.251951 0.854092
 6 -2.646262 0.379715 0.785964
 1 -3.406358 0.355593 0.015263

16 (6-endo TS)

Total energy = -348.19398
 6 -0.469565 0.053049 -2.085264
 6 -0.559293 -0.006426 -0.591496
 6 0.623161 -0.009518 0.056207
 6 1.749827 0.057211 -0.979858
 6 1.022883 0.461175 -2.290419
 1 -0.690616 -0.930521 -2.524626
 1 -1.167221 0.764537 -2.540629
 1 2.535403 0.771007 -0.704997
 1 2.233941 -0.925040 -1.074964
 1 1.077919 1.547234 -2.415894
 1 1.464734 0.003814 -3.180503
 6 0.862775 -0.101145 1.479562
 6 -0.121251 -0.191411 2.417723
 1 1.898165 -0.090313 1.814447
 1 0.111280 -0.247257 3.476453
 6 -1.459620 -0.204298 1.967103
 6 -2.347582 -0.178441 1.120153
 1 -3.271618 -0.174633 0.588445

17-R

Total energy = -269.49739
 6 -0.433569 -0.000110 -0.582284
 6 -0.420755 0.000023 0.733008
 6 0.297822 0.002280 1.981759
 6 1.617319 0.006982 2.100761
 1 2.331845 0.009097 2.913007
 6 0.215688 0.002182 -1.810711
 6 0.761010 -0.005875 -2.894415
 1 1.245439 -0.007657 -3.843100
 1 -0.318435 -0.000234 2.888010
 6 -1.785648 -0.003845 0.109699
 1 -2.387583 0.909291 0.107834
 1 -2.382462 -0.920325 0.107354

17 (5-exo TS)

Total energy = -269.45029
 6 -0.765184 0.363495 -0.381568
 6 -0.727379 0.264768 0.936129
 6 0.541242 -0.056007 1.581548
 6 1.536936 -0.162898 0.698345
 1 2.604957 -0.327060 0.788040
 6 0.385848 0.097373 -1.154308
 6 1.046838 -0.098461 -2.197223
 1 1.926717 -0.339462 -2.755405
 1 0.661477 -0.164297 2.658757
 6 -2.021292 -0.152759 0.301475
 1 -2.884591 0.511223 0.352408
 1 -2.290614 -1.213473 0.249821

17 (5-exo P)

Total energy = -269.49893
 6 -0.754407 0.461217 -0.341751
 6 -0.772283 0.306674 0.985334
 6 0.545242 -0.098726 1.484272
 6 1.381551 -0.168706 0.412623
 1 2.452722 -0.340618 0.429277
 6 0.593175 0.082293 -0.833422
 6 0.989391 -0.097738 -2.083365
 1 1.876946 -0.445565 -2.596853
 1 0.824404 -0.262494 2.519110
 6 -1.993297 -0.173602 0.246259
 1 -2.900869 0.427154 0.287252
 1 -2.189432 -1.246944 0.141514

17 (6-endo TS)

Total energy = -269.46223
 6 -0.793049 0.210564 -0.708305
 6 -0.789787 0.221427 0.617023
 6 0.286186 0.003558 1.543211
 6 1.542962 -0.035906 1.076702
 1 2.488041 -0.182993 1.588547
 6 0.338357 -0.010750 -1.484533
 6 1.569441 -0.145577 -1.402271
 1 2.586872 -0.208965 -1.721559
 1 0.073344 -0.161273 2.604026
 6 -2.111901 -0.081819 -0.039675
 1 -2.888450 0.685182 -0.062509
 1 -2.513054 -1.100932 -0.021423

17 (6-endo P)

Total energy = -269.58003
 6 -0.807816 -0.000044 -0.766762
 6 -0.806736 -0.000104 0.606105
 6 0.324099 -0.000115 1.389885
 6 1.536669 -0.000129 0.664551
 1 2.479370 -0.000210 1.205550
 6 0.357526 0.000047 -1.454432
 6 1.560521 -0.000030 -0.741424
 1 2.515597 -0.000069 -1.258986
 1 0.317893 -0.000109 2.475837
 6 -2.136743 0.000290 -0.074963
 1 -2.738748 0.912431 -0.080026
 1 -2.739230 -0.911530 -0.080142

18-R

Total energy = -308.85284
 6 -0.331437 -0.015469 -0.599934
 6 -0.318046 0.009184 0.763255
 6 0.721330 0.041783 1.777399
 6 2.025671 0.056101 1.553455
 1 2.925240 0.079239 2.153785
 6 0.671482 -0.019179 -1.588489
 6 1.513052 -0.022709 -2.462186
 1 2.261945 -0.025625 -3.219645
 1 0.367438 0.055030 2.816404
 6 -1.832172 -0.009712 0.881838
 1 -2.259249 -0.896628 1.364197
 1 -2.283847 0.881843 1.332191
 6 -1.852806 -0.038125 -0.685411
 1 -2.284589 -0.942587 -1.127226
 1 -2.309387 0.837477 -1.159260

18 (5-exo TS)

Total energy = -308.83153
 6 -0.103098 -0.123318 -2.689951
 6 -0.070429 -0.066067 -1.447399
 6 1.972100 -0.038011 -0.560512
 6 1.655060 0.023217 0.730627
 6 0.211559 0.041748 0.945603

6 -0.599329 -0.002040 -0.129617
 1 0.221329 -0.171006 -3.706004
 1 2.889026 -0.069730 -1.133625
 1 2.382137 0.056240 1.542929
 6 -1.882636 0.043743 0.690617
 1 -2.507048 0.933003 0.553501
 1 -2.518466 -0.846252 0.634860
 6 -0.925739 0.095337 1.950501
 1 -1.000030 1.013581 2.543692
 1 -1.011876 -0.763496 2.625440

18 (5-exo TS)

Total energy = -308.87884
 6 -1.051317 -0.110088 -1.379743
 6 -1.011075 -0.052500 0.085972
 6 0.256045 0.031322 0.527022
 6 1.172907 0.037604 -0.623392
 6 2.492407 0.107429 -0.677301
 6 0.238665 -0.057272 -1.806270
 1 3.255776 0.120989 -1.44973
 1 0.589582 -0.078210 -2.829918
 1 -1.925145 -0.180985 -2.016582
 6 -1.619781 -0.027473 1.479998
 1 -2.242722 0.841331 1.720770
 1 -2.149939 -0.933654 1.793953
 6 -0.119418 0.072436 1.998852
 1 0.114374 0.998321 2.536193
 1 0.207480 -0.776538 2.609731

18 (6-endo TS)

Total energy = -308.83774
 6 -0.444036 -0.002830 -0.716125
 6 -0.452583 -0.000536 0.646890
 6 0.681478 -0.001082 1.542312
 6 1.941694 0.000232 1.096376
 1 2.889979 -0.000666 1.623221
 6 0.753153 -0.002405 -1.453980
 6 1.985974 0.001292 -1.392285
 1 3.022219 0.004448 -1.646314
 1 0.484688 -0.002963 2.620361
 6 -1.970557 0.004014 0.731886
 1 -2.426776 -0.881872 1.187886
 1 -2.419630 0.897122 1.180957
 6 -1.955046 -0.000730 -0.846453
 1 -2.396487 -0.891924 -1.305758
 1 -2.394451 0.888127 -1.312083

18 (6-endo P)

Total energy = -308.95419
 6 -0.451027 0.121530 -0.754369
 6 -0.440536 -0.007371 0.646638
 6 0.726475 -0.210641 1.369063
 6 1.920992 -0.284047 0.634823
 1 2.862093 -0.442602 1.155297
 6 0.735144 0.043184 -1.432184
 6 1.935165 -0.158404 -0.768114
 1 2.877557 -0.220977 -1.305299
 1 0.735928 -0.310543 2.450760
 6 -1.949274 0.161713 0.755988
 1 -2.496152 -0.707013 1.137096
 1 -2.287859 1.051403 1.297140
 6 -1.958210 0.305850 -0.818603
 1 -2.506513 -0.480230 -1.347296
 1 -2.297431 1.279079 -1.187142

19-R

Total energy = -387.52351
 6 -0.589506 0.010711 -1.702946
 6 -0.601134 -0.011287 -0.179326
 6 0.537392 0.001163 0.568816

6 1.908472 0.025540 -0.080306
 6 1.897420 -0.326994 -1.571142
 6 0.767276 0.416291 -2.286774
 1 -1.376600 0.689150 -2.051648
 1 2.570668 -0.659886 0.464783
 1 1.750668 -1.408690 -1.690177
 1 0.910704 1.498121 -2.165180
 6 0.539712 0.010038 2.039127
 6 -0.502782 -0.008957 2.852910
 1 0.635300 -0.008129 3.927029
 6 -1.893416 -0.055629 0.414375
 6 -3.039754 -0.091731 0.812483
 1 -4.027169 -0.125929 1.210228
 1 1.540183 0.035733 2.491383
 1 2.345267 1.026394 0.061825
 1 2.869246 -0.089002 -2.017649
 1 0.784446 0.213408 -3.363372
 1 -0.874197 -0.986044 -2.070526

19 (5-exo TS)

Total energy = -387.51972
 6 -0.721051 0.097100 -1.979955
 6 -0.669457 0.013842 -0.513897
 6 0.557321 0.011379 0.069500
 6 1.723518 0.066248 -0.763418
 6 2.921002 0.094885 -1.049944
 6 0.407685 0.150473 -2.668233
 1 0.686938 0.208463 -3.711329
 6 -1.948366 -0.058690 0.282822
 6 -1.716397 -0.499085 1.734979
 6 -0.523458 0.245634 2.344943
 6 0.767019 -0.056922 1.570261
 1 -2.649694 -0.740613 -0.216074
 1 -1.518402 -1.578820 1.759615
 1 -0.396045 -0.024561 3.399201
 1 1.561358 0.641623 1.857682
 1 -1.703480 0.109335 -2.462382
 1 1.140854 -1.056888 1.835056
 1 -0.720225 1.325572 2.316567
 1 -2.623100 -0.330647 2.326567
 1 -2.436737 0.928079 0.264161
 1 3.871641 0.129268 -1.531405

19 (5-exo P)

Total energy = -387.58190
 6 -0.774555 0.102534 -1.923150
 6 -0.777291 0.014462 -0.450175
 6 0.505152 0.000534 -0.003781
 6 1.396622 0.074625 -1.185713
 6 2.719988 0.090415 -1.199050
 6 0.499321 0.135250 -2.373397
 1 0.847284 0.195344 -3.395757
 6 -1.976294 -0.048520 0.451612
 6 -1.569048 -0.478956 1.874114
 6 -0.296816 0.244780 2.345461
 6 0.907623 -0.075819 1.439856
 1 -2.726856 -0.739544 0.045049
 1 -1.387209 -1.561872 1.882302
 1 -0.068641 -0.027032 3.382260
 1 1.735687 0.613689 1.646875
 1 -1.669440 0.132242 -2.535743
 1 1.292814 -1.080159 1.672826
 1 -0.476308 1.328106 2.335397
 1 -2.393680 -0.293295 2.571494
 1 -2.467973 0.936096 0.482392
 1 3.506105 0.140596 -1.941760

19 (6-endo TS)

Total energy = -387.51723
 6 -0.699055 -0.009940 -1.762177

6 -0.654018 0.014957 -0.245327
 6 0.506783 -0.000932 0.479806
 6 1.857256 -0.038389 -0.210695
 6 1.796414 0.316451 -1.700937
 6 0.640247 -0.419848 -2.384726
 1 -0.991571 0.986133 -2.126069
 1 2.287368 -1.044202 -0.086021
 1 2.751644 0.074888 -2.180292
 1 0.629345 -0.215562 -3.461099
 6 0.533182 -0.004064 1.945561
 6 -0.496078 0.028735 2.791414
 1 -0.512435 0.027999 3.876881
 6 -1.864406 0.062201 0.488906
 6 -2.586874 0.090073 1.477861
 1 -3.388236 0.125230 2.179957
 1 1.542168 -0.037723 2.375162
 1 2.544365 0.639564 0.312032
 1 1.651870 1.399255 -1.813270
 1 0.782120 -1.502646 -2.269477
 1 -1.497348 -0.688404 -2.085921

19 (6-endo P)

Total energy = -387.63593
 6 -0.716298 -0.058638 -1.786485
 6 -0.709481 0.021356 -0.268619
 6 0.488525 0.001931 0.483392
 6 1.835029 -0.165537 -0.201032
 6 1.794941 0.143321 -1.702868
 6 0.609758 -0.568829 -2.364546
 1 -0.922462 0.944177 -2.187108
 1 2.173965 -1.202552 -0.060011
 1 2.739791 -0.158024 -2.168813
 1 0.621640 -0.419583 -3.449995
 6 0.421686 0.111631 1.881151
 6 -0.791659 0.234686 2.554407
 1 -0.809982 0.319287 3.637990
 6 -1.875490 0.146610 0.462985
 6 -1.993976 0.253099 1.827465
 1 -2.954363 0.347819 2.325840
 1 1.348222 0.099419 2.450323
 1 2.580025 0.463874 0.300341
 1 1.698356 1.226683 -1.855951
 1 0.697275 -1.650327 -2.193757
 1 -1.550676 -0.688552 -2.113966

20-R

Total energy = -476.40285
 6 -.308474 .000239 -2.052958
 6 -.220431 .000075 -.647728
 6 1.055358 -.000244 -.109418
 6 2.220035 -.000409 -.837447
 6 2.114650 -.000240 -2.238154
 6 .849909 .000078 -2.829584
 1 -1.286743 .000488 -2.529268
 1 3.192001 -.000659 -.351651
 1 3.010803 -.000361 -2.851416
 1 .758901 .000209 -3.911431
 7 -1.391073 .000235 .124760
 1 -2.276986 .000493 -.364594
 6 -1.546381 .000120 1.493309
 8 -2.658324 .000434 2.005465
 6 -.338367 -.000104 2.305226
 6 .549216 -.000314 3.127330
 1 1.353031 -.000490 3.827864

20 (5-exo TS)

Total energy = -476.40101
 6 -0.212017 0.000742 -2.114411
 6 -0.286331 -0.000019 -0.714373
 6 0.899002 0.002492 0.000308

6 2.147332 0.005660 -0.572188
 6 2.217964 0.006256 -1.976899
 6 1.042438 0.003845 -2.729999
 1 -1.120931 -0.001121 -2.711523
 1 3.051589 0.007560 0.030434
 1 3.185288 0.008663 -2.470628
 1 1.097355 0.004339 -3.814311
 7 -1.496025 -0.002961 -0.010740
 1 -2.380503 -0.006130 -0.499661
 6 -1.576440 -0.004592 1.360636
 8 -2.638965 -0.008170 1.962390
 6 -0.282275 -0.001442 2.064787
 6 0.469128 -0.000934 3.027951
 1 1.238286 0.000723 3.766882

20 (5-exo P)

Total energy = -476.47487
 6 -.624998 -.000053 -2.069229
 6 -.578604 .000003 -.681102
 6 .645531 -.000046 .019241
 6 1.846620 -.000151 -.682043
 6 1.814395 -.000203 -2.080730
 6 .593135 -.000153 -2.760498
 1 -1.570471 -.000020 -2.602604
 1 2.791141 -.000190 -.146853
 1 2.743632 -.000283 -2.641317
 1 .583383 -.000195 -3.846311
 7 -1.634080 .000086 .237203
 1 -2.616035 .000268 .005894
 6 -1.196480 .000170 1.554722
 8 -1.899916 .000278 2.543766
 6 .334818 .000027 1.456747
 6 1.120283 -.000005 2.515139
 1 .978037 .000044 3.587157

20 (6-endo TS)

Total energy = -476.39464
 6 -.315747 .000935 -1.958810
 6 -.231156 -.000071 -.552747
 6 1.046215 -.001331 -.002287
 6 2.206338 -.001552 -.745210
 6 2.104381 -.000277 -2.144018
 6 .839878 .000767 -2.736865
 1 -1.293924 .001866 -2.435590
 1 3.181558 -.002596 -.264756
 1 3.001150 -.000370 -2.756587
 1 .748081 .001673 -3.818635
 7 -1.423568 -.000564 .194452
 1 -2.292390 .000027 -.326004
 6 -.1628687 -.000139 1.562748
 8 -2.749578 .000560 2.048843
 6 -.386118 -.000026 2.315838
 6 .829082 .000819 2.435814
 1 1.832018 .004121 2.802889

20 (6-endo P)

Total energy = -476.49052
 6 -.320090 -.000081 -1.925613
 6 -.300912 -.000036 -.520818
 6 .938666 -.000247 .168405
 6 2.132775 -.000505 -.574555
 6 2.106685 -.000573 -1.960993
 6 .874035 -.000355 -2.632530
 1 -1.272084 .000092 -2.449082
 1 3.079280 -.000647 -.041230
 1 3.033919 -.000783 -2.524491
 1 .849471 -.000395 -3.717922
 7 -1.475705 .000210 .210933
 1 -2.363460 .000539 -.278522
 6 -1.597190 .000301 1.612394

8 -2.692851 .001060 2.153218
 6 -.284686 .000171 2.236343
 6 .901465 -.000111 1.620557
 1 1.841140 -.000138 2.169841

21-R

Total energy = -441.68054
 6 -1.768449 .465428 -2.067936
 6 -.1586226 .355528 -.686765
 6 -.451428 -.299190 -.155647
 6 .439076 -.779691 -1.114467
 6 .312069 -.681551 -2.474370
 6 -.838771 -.043784 -2.972988
 1 -2.655895 .972094 -2.436381
 1 -2.323915 .790149 -.020840
 1 1.065759 -1.082980 -3.146711
 1 -.991772 .051480 -4.043730
 7 -.242725 -.495483 1.212117
 6 1.127699 -.763922 1.644000
 1 1.580213 -1.446500 .915622
 1 1.086700 -1.298204 2.601008
 6 1.972482 .433287 1.790704
 6 2.640497 1.430345 1.928274
 1 3.235127 2.308303 2.032920
 6 -.1078536 .217139 2.163739
 1 -.823774 -.117402 3.172206
 1 -.951442 1.309601 2.121040
 1 -2.132395 -.019705 1.992790

21 (5-exo TS)

Total energy = -441.67448
 6 -1.999536 .004613 -1.850014
 6 -1.830249 .015831 -.461577
 6 -.531912 .027385 .085537
 6 .520018 -.005192 -.822685
 6 .392959 -.013305 -2.188254
 6 -.909660 -.009441 -2.720348
 1 -3.008503 -.000092 -2.252684
 1 -2.703663 .013056 .182674
 1 1.262510 -.028837 -2.840575
 1 -1.061106 -.020421 -.3795863
 7 -.234516 .091427 1.452082
 6 1.109844 -.374566 1.789918
 1 1.175132 -1.477950 1.758429
 1 1.331028 -.064768 2.817392
 6 2.149607 .172988 .899425
 6 3.223403 .597682 .506049
 1 4.081974 .967136 -.006248
 6 -.1262450 -.254646 2.415400
 1 -.881340 -.074934 3.424241
 1 -2.137625 .385323 2.277693
 1 -1.588942 -1.306599 2.349659

21 (5-exo P)

Total energy = -441.74554
 6 -1.832125 .006710 -1.878345
 6 -1.825811 -.024770 -.480807
 6 -.594123 .038115 .178694
 6 .607978 .102104 -.560317
 6 .584020 .137808 -1.950831
 6 -.645609 .090948 -2.614288
 1 -2.783560 -.040465 -2.400770
 1 -2.757568 -.094421 .070495
 1 1.513148 .186268 -2.511660
 1 -.679271 .110903 -3.698861
 7 -.343183 .080136 1.545927
 6 1.094245 -.115414 1.773389
 1 1.298878 -.144370 2.114739
 1 1.471653 .571471 2.538092
 6 1.732734 .119591 .400606

6 3.019794 .300593 .179894
 1 3.677417 .468443 -.660937
 6 -1.270284 -.461985 2.514724
 1 -.966391 -.152152 3.518849
 1 -2.273233 -.064896 2.338443
 1 -1.323709 -.1563937 2.493805

21 (6-endo TS)

Total energy = -441.66375
 6 -1.689149 -.074902 -2.060217
 6 -.1635409 -.031854 -.663783
 6 -.401377 .077248 .016107
 6 .729942 .122587 -.806431
 6 .710401 .056800 -2.178722
 6 -.530932 -.033542 -2.831454
 1 -2.659162 -.155729 -2.542691
 1 -2.563358 -.094719 -.106481
 1 1.633141 .086351 -2.754219
 1 -.581576 -.072082 -3.915902
 7 -.331000 .191330 1.421866
 6 .784732 -.444913 2.135129
 1 .678842 -.1544961 2.179643
 1 .758622 -.088368 3.171558
 6 2.066489 -.117386 1.508091
 6 2.744515 .193104 .540811
 1 3.534809 .468057 -.121286
 6 -.1574459 .171927 2.171565
 1 -1.362114 .420438 3.215003
 1 -2.259007 .930338 1.783127
 1 -2.091724 -.803045 2.151611

21 (6-endo P)

Total energy = -441.75028
 6 -.1576615 -.065430 -2.049090
 6 -.1579243 -.049824 -.652542
 6 -.375007 .032942 .065979
 6 .846700 .091976 -.665259
 6 .821574 .068048 -2.061050
 6 -.381846 -.006879 -2.763312
 1 -.2524026 -.133823 -2.576234
 1 -.2524646 -.116553 -.127642
 1 1.765477 .117227 -2.598120
 1 -.384031 -.018024 -3.848530
 7 -.338717 .120809 1.460452
 6 .838523 -.387685 2.175227
 1 .783616 -.1480725 2.352599
 1 .861154 .083831 3.166434
 6 2.053851 -.048566 1.392313
 6 2.103499 .199545 .094409
 1 3.018766 .458230 -.433061
 6 -.1572737 .132358 2.219878
 1 -1.350557 .424998 3.249819
 1 -2.268594 .867760 1.806348
 1 -2.078339 -.847493 2.245908

22-R

Total energy = -402.36948
 6 -.513030 .360067 -1.849754
 6 -.442677 .044545 -.474908
 6 .776744 -.461977 -.043294
 6 1.889329 -.661334 -.823802
 6 1.792454 -.342299 -2.188081
 6 .587696 .164953 -2.682138
 1 -1.439130 .764770 -2.254141
 1 2.811710 -.1056424 -.406442
 1 2.643909 -.489002 -2.845776
 1 .500689 .415682 -.3735402
 7 -.1520148 .263843 .380148
 1 -2.418866 .290217 -.079404
 6 -.1539709 -.376647 1.691726

6 -.658041 .275759 2.667698
 6 .054715 .788852 3.495929
 1 .691845 1.252964 4.212655
 1 -1.263865 -1.442049 1.625836
 1 -2.570149 -.334580 2.061385

22 (5-exo TS)

Total energy = -402.36395
 6 -.775368 .157350 -1.829501
 6 -.648813 .078119 -.431630
 6 .624051 -.129923 .078882
 6 1.764836 -.240165 -.679265
 6 1.627862 -.159681 -2.076387
 6 .361443 .037509 -2.632416
 1 -1.753134 .315378 -2.280077
 1 2.739842 -.392496 -.223308
 1 2.501439 -.249738 -2.715586
 1 .252334 .099275 -3.711449
 7 -1.708746 .240328 .466415
 1 -2.619466 -.004822 .099100
 6 -1.456752 -.302350 1.800131
 6 -.113817 .069097 2.292394
 6 .768504 .365178 3.085499
 1 1.664990 .610619 3.607600
 1 -1.526630 -1.403855 1.822170
 1 -2.209823 .092542 2.490400

22 (5-exo P)

Total energy = -402.43375
 6 -.814332 .004484 -1.829610
 6 -.776734 .030435 -.433862
 6 .452257 .010888 .254044
 6 1.654770 -.010146 -.449698
 6 1.625201 -.032057 -.845850
 6 .398817 -.029746 -2.521872
 1 -1.760200 .016355 -2.363312
 1 2.597838 -.023557 .088555
 1 2.553229 -.055939 -2.408173
 1 .386114 -.052846 -3.607953
 7 -1.849339 .121178 .454104
 1 -2.701952 -.357490 1.96131
 6 -1.361464 -.097941 1.825728
 6 .174189 .015009 1.700838
 6 1.026264 .099494 2.703323
 1 1.005096 .129346 3.783125
 1 -1.638029 -1.094171 2.199728
 1 -1.770539 .647543 2.514923

22 (6-endo TS)

Total energy = -402.35346
 6 -.583952 .000000 -1.778366
 6 -.510034 .000000 -.365700
 6 .780696 .000000 .166238
 6 1.935885 .000000 -.580841
 6 1.837977 .000000 -1.981673
 6 .568750 .000000 -2.561686
 1 -1.562470 .000000 -2.256756
 1 2.911473 .000000 -.099189
 1 2.732796 .000000 -2.596983
 1 .466844 .000000 -3.643338
 7 -1.688891 .000000 .368527
 1 -2.539894 .000000 -.171007
 6 -.1874327 .000000 1.815945
 6 -.594546 .000000 2.519583
 6 .622027 .000000 2.601364
 1 1.637782 .000000 2.927293
 1 -2.459577 -.880785 2.125551
 1 -2.459577 .880785 2.125551

22 (6-endo P)

Total energy = -402.43946
 6 -.585804 .000000 -1.724097
 6 -.561078 .000000 -.320510
 6 .694761 .000000 .341883
 6 1.870976 .000000 -.410625
 6 1.838866 .000000 -1.805816
 6 .602614 .000000 -2.453343
 1 -1.542761 .000000 -2.240660
 1 2.823419 .000000 .113853
 1 2.761964 .000000 -2.376086
 1 .556174 .000000 -3.538702
 7 -1.735860 .000000 .406432
 1 -2.598720 .000000 -.115596
 6 -1.846113 .000000 1.870716
 6 -.477171 .000000 2.442378
 6 .685612 .000000 1.815102
 1 1.637054 .000000 2.343145
 1 -2.411044 -.881984 2.217445
 1 -2.411044 .881984 2.217445

23-R

Total energy = -1045.73729
 6 1.630353 -.009730 -4.049160
 6 1.654625 -.006445 -2.639656
 6 2.909387 -.002930 -.1970184
 6 4.079185 -.003673 -2.745930
 6 4.038427 -.007306 -4.136697
 6 2.805193 -.010191 -4.792315
 1 0.666510 -.012312 -4.547549
 1 5.039157 -.001017 -2.236318
 1 4.962956 -.007704 -4.706081
 1 2.758774 -.012924 -5.877014
 6 3.050685 0.002629 -.505571
 6 2.104285 .005006 0.406952
 6 0.412088 -.006563 -1.945586
 6 -.710756 -.007637 -1.472798
 6 4.092820 0.005834 -0.160660
 6 1.550031 0.008876 1.680072
 6 1.228421 -.1212364 2.349160
 6 0.633200 -1.205747 3.600916
 6 0.338879 0.016092 4.206886
 6 0.624928 1.234359 3.589847
 6 1.219804 1.233758 2.338154
 1 1.461511 -.2.152958 1.862109
 1 0.393777 -.2.128502 4.118478
 1 0.378467 2.160069 4.098718
 1 1.445507 2.171474 1.842208
 6 -2.013303 -.008001 -.897443
 6 -.3156387 0.044580 -.1722131
 6 -.4433687 0.045341 -.1711951
 6 -.4566007 -.007090 0.211762
 6 -.3463087 -.060204 1.057605
 6 -.2188294 -.060564 0.501241
 1 -.3030731 0.085137 -.2.798824
 1 -.5320847 0.085687 -.1.794234
 1 -.3.612469 -.1.00229 2.130949
 1 -.1.317116 -.1.02267 1.144581
 9 -.0242309 0.019546 5.424329
 9 -.5.802818 -.006596 0.749516

23 (5-exo TS)

Total energy = -1045.73184
 6 -.1.431700 -.041260 -.0252041
 6 -.1.415863 -.063266 0.982363
 6 0.761101 -.074802 1.841063
 6 0.351035 -.1.13453 3.097954
 6 -.1.079745 -.1.09712 3.409933
 6 -.1.968478 -.084172 2.309883
 6 -.3.352493 -.082210 2.534850
 6 -.3.850732 -.104211 3.836811

6 -.2.972129 -.0129307 4.923449
 6 -.1.593957 -.0132740 4.709952
 1 -.026973 -.063271 1.684879
 1 -.4.923743 -.1.02169 4.002932
 1 -.3.362019 -.1.46694 5.936913
 1 -.0909821 -.1.52913 5.554048
 1 1.060094 -.1.62316 3.929321
 6 1.888486 -.013346 0.985820
 6 2.343043 -.1.163599 0.292365
 6 3.424919 -.1.095801 -.575858
 6 4.054744 0.130596 -.772599
 6 3.632777 1.289269 -.1.255057
 6 2.551550 1.216868 0.743448
 1 1.836606 -.2.109185 0.454376
 1 3.786345 -.1.972180 -.1.102853
 1 4.152564 2.223373 -.3.09257
 1 2.206514 2.109280 1.254940
 6 -.1.280916 -.0.007336 -.1.658737
 6 -.1.295495 -.1.200727 -.2.417029
 6 -.1.161441 -.1.167968 -.3.799740
 6 -.1.013952 0.063355 -.4.431739
 6 -.0996341 1.260495 -.3.722094
 6 -.1.130179 1.222867 -.2.339464
 1 -.1.413467 -.2.149957 -.1.905676
 1 -.1.169741 -.2.075865 -.4.392780
 1 -.0.877891 2.197100 -.4.255702
 1 -.1.117793 2.144167 -.1.767393
 9 5.104297 0.198657 -.1.617895
 9 -.0.884973 0.097276 -.5.773465

23 (5-exo P)

Total energy = -1045.78950
 6 -.2.983054 -.021999 -.0170862
 6 -.3.016201 -.027266 1.286664
 6 -.1.682826 -.045966 1.757657
 6 -.0.788579 -.0.044794 0.565713
 6 0.528701 -.014357 0.585047
 6 -.1.697078 -.034064 -.624322
 6 -.4.077752 -.023683 2.191464
 6 -.3.793177 -.035917 3.561298
 6 -.2.472080 -.052767 4.020500
 6 -.1.401762 -.058476 3.116449
 1 -.5.106546 -.0.010200 1.842230
 1 -.4.609156 -.032196 4.278178
 1 -.2.273546 -.062519 5.088059
 1 -.0.375424 -.0.073052 3.472304
 1 -.3.866556 -.036515 -.798720
 6 1.837260 0.012386 1.029636
 6 2.567167 -.1.197985 1.258760
 6 3.889757 -.1.164488 1.666585
 6 4.514871 0.070022 1.848463
 6 3.847360 1.276640 1.631475
 6 2.525280 1.253182 1.222370
 1 2.064998 -.2.148624 1.115601
 1 4.448192 -.2.076200 1.849227
 1 4.374458 2.211878 1.786107
 1 1.991859 2.180622 1.045865
 6 -.1.261340 -.0.018076 -.2.027065
 6 -.0.071105 -.6.433630 -.2.441728
 6 0.322958 -.6.36705 -.3.777919
 6 -.0.484670 0.000121 -.4.711825
 6 -.1.668537 0.631255 -.4.346280
 6 -.2.045027 0.621757 -.3.006651
 1 0.545482 -.1.155060 -.1.711563
 1 1.237008 -.1.122203 -.4.102021
 1 -.2.266666 1.129202 -.5.101618
 1 -.2.951054 1.139066 -.2.707584
 9 5.802369 0.097965 2.245147
 9 -.0.108374 0.011262 -.6.008329

24-R

Total energy = -1076.32546

6	2.018184	0.121798	-4.321484
6	2.030600	0.101448	-2.911588
6	3.280749	0.085090	-2.232659
6	4.456089	0.092286	-3.000360
6	4.426760	0.113150	-4.391239
6	3.198289	0.127443	-5.055992
1	1.057985	0.133966	-4.826925
1	5.411779	0.080239	-2.482664
1	5.355753	0.117848	-4.953535
1	3.159899	0.143524	-6.141052
6	3.410781	0.057316	-0.767115
6	2.453693	0.039627	0.135153
6	0.782411	0.099044	-2.228279
6	-0.346265	0.103258	-1.768318
1	4.451194	0.048227	-0.415750
6	1.899463	0.008187	1.407448
6	1.568478	-1.223220	2.043425
6	0.966733	-1.256502	3.294544
6	0.661312	-0.058749	3.960094
6	0.968884	1.172906	3.349363
6	1.566869	1.211820	2.106458
1	1.796496	-2.152348	1.531843
1	0.738458	-2.215710	3.744107
1	0.724502	2.086119	3.882318
1	1.796341	2.165594	1.643111
6	-1.651850	0.108933	-1.202508
6	-2.790253	0.029904	-2.024229
6	-4.075412	0.035775	-1.486108
6	-4.245208	0.122642	-0.098398
6	-3.118578	0.203036	0.735666
6	-1.843719	0.196147	0.195135
1	-2.661473	-0.037105	-3.099706
1	-4.928429	-0.026991	-2.150966
1	-3.272356	0.271849	1.807427
1	-0.979558	0.261062	0.846588
8	0.070569	0.022446	5.186673
8	-5.452340	0.136512	0.535920
6	-0.266553	-1.184601	5.853333
1	-0.988410	-1.777153	5.277091
1	0.621265	-1.797466	6.054400
1	-0.719946	-0.888664	6.800271
6	-6.628975	0.059187	-0.254168
1	-6.708934	0.907476	-0.945717
1	-6.670944	-0.875702	-0.827340
1	-7.464349	0.088025	0.446713

24 (5-exo TS)

Total energy = -1076.31978

6	-1.684790	-0.141093	0.120387
6	-1.667760	-0.123716	1.354938
6	0.517014	-0.038409	2.224620
6	0.099981	-0.058398	3.480923
6	-1.331855	-0.080191	3.785176
6	-2.218955	-0.115749	2.683056
6	-3.603028	-0.146428	2.907841
6	-4.104434	-0.139218	4.208740
6	-3.227888	-0.102998	5.296753
6	-1.850006	-0.075051	5.084455
1	-4.275472	-0.175243	2.056395
1	-5.177625	-0.162297	4.372896
1	-3.619100	-0.097759	6.310000
1	-1.167244	-0.048596	5.929698
1	0.803241	-0.083266	4.318878
6	1.654531	0.060960	1.387822
6	2.070277	-1.027001	0.575281
6	3.160723	-0.914895	-0.266991
6	3.874515	0.293335	-0.350492
6	3.474492	1.389108	0.426934

6	2.378456	1.270915	1.276549
1	1.519589	-1.960468	0.627329
1	3.485258	-1.748560	-0.881092
1	4.007059	2.331582	0.378052
1	2.070100	2.122858	1.874162
6	-1.530182	-0.139274	-1.285866
6	-1.574532	-1.337799	-2.026503
6	-1.430356	-1.340004	-3.411287
6	-1.240118	-0.130682	-4.093259
6	-1.197691	1.074237	-3.372152
6	-1.340042	1.071416	-1.960902
1	-1.722782	-2.276055	-1.501960
1	-1.467295	-2.281690	-3.945687
1	-1.049043	1.998858	-3.919955
1	-1.303016	2.004998	-1.444837
8	4.930625	0.296946	-1.214330
8	-1.087820	-0.016305	-5.443239
6	-1.113074	-1.199669	-6.226883
1	-0.305815	-1.887882	-5.946121
1	-2.074915	-1.721111	-6.141974
1	-0.968842	-0.879498	-7.259599
6	5.685924	1.490786	-1.347826
1	5.069486	2.321046	-1.715338
1	6.151640	1.783789	-0.398213
1	6.466749	1.273190	-2.077903

1	6.351892	1.797983	1.858781
1	5.790579	1.797079	3.556511
1	7.270586	0.910603	3.103841

25-R

Total energy = -1673.17848

6	1.716281	-0.019655	-4.129950
6	1.788448	-0.010734	-2.722466
6	3.060241	-0.002518	-2.089826
6	4.206497	-0.004537	-2.898027
6	4.120584	-0.014564	4.287183
6	2.869123	-0.021962	-4.906731
1	0.736800	-0.024764	-4.596149
1	5.181681	0.001920	-2.419469
1	5.027141	-0.016160	-4.884235
1	2.791161	-0.029195	-5.989158
6	3.244208	0.010061	-0.631699
6	2.331394	0.007617	0.309374
6	0.559988	-0.009103	-2.005367
6	-0.568316	-0.009073	-1.549115
1	4.292626	0.023908	-0.311381
6	1.788132	0.008310	1.580139
6	1.471075	-1.192591	2.271721
6	0.862537	-1.124760	3.514614
7	0.544330	0.005931	4.116519
6	0.818670	1.137635	3.495113
6	1.425001	1.207724	2.251331
6	-1.901418	-0.004649	-1.077048
6	-2.984012	0.048541	-1.974361
6	-4.282058	0.050433	-1.475284
7	-4.567570	0.004381	-0.190928
6	-3.570213	-0.046288	0.666654
6	-2.231962	-0.053503	0.287429
9	0.491728	2.274729	4.114915
9	0.580118	-2.262875	4.153961
9	1.765482	-2.373138	1.717496
9	1.674073	2.389192	1.676896
9	-1.267975	-0.107210	1.215542
9	-3.869443	-0.093225	1.964548
9	-5.300217	0.101486	-2.335263
9	-2.763981	0.097018	-3.291944

25 (5-exo TS)

Total energy = -1673.17316

6	-1.519339	-0.01920	-0.066779
6	-1.565380	-0.005628	1.166553
6	.553944	-.004127	2.067383
6	.127101	-.077508	3.313547
6	-1.308744	-.077867	3.595661
6	-2.163764	-.035868	2.471044
6	-3.553880	-.020783	2.648932
6	-4.087380	-.057381	3.936388
6	-3.241861	-.105963	5.048208
6	-1.857137	-.116349	4.879372
1	-4.203268	.015644	1.780786
1	-5.164268	-.048527	4.071597
1	-3.663100	-.133610	6.048362
1	-1.199897	-.150456	5.743442
1	.827538	-.145750	4.148694
6	1.667573	.024889	1.201511
6	2.147777	-.1141024	.564682
6	3.192936	-.1040913	-.345308
7	3.774065	.097582	-.667725
6	3.338931	1.201467	-.093383
6	2.300863	1.231336	.829080
6	-1.279085	-.003072	-1.453560
6	-.621912	-1.070693	-2.097572
6	-.439792	-1.024460	-3.475209
7	-.855995	-.029304	-4.231174
6	-1.473906	.978823	-3.651065

6 -1.711856 1.050465 -2.283204
 9 -1.889210 1.980677 -4.427206
 9 -2.348717 2.100213 -1.757334
 9 1.605926 -2.328633 .846629
 9 3.644588 -2.151979 -.930151
 9 3.937223 2.347778 -.425733
 9 1.908023 2.389222 1.370468
 9 -.162354 -2.104158 -1.385033
 9 .187407 -2.037097 -4.073673

25 (5-exo P)

Total energy = -1673.23071

6 -2.412542 2.041810 -0.288788
 6 -1.590788 3.242726 -0.346058
 6 -0.234405 2.854455 -0.272030
 6 -0.198134 1.370224 -0.166178
 6 0.870374 0.628629 -0.005760
 6 -1.629499 0.929732 -0.204269
 6 -1.933576 4.589974 -0.450985
 6 -0.906730 5.539081 -0.480016
 6 0.434401 5.148402 -0.404811
 6 0.783974 3.796090 -0.298785
 1 -2.973599 4.897478 -0.507423
 1 -1.153225 6.593245 -0.561467
 1 1.215210 5.902144 -0.430494
 1 1.826055 3.496319 -0.241737
 1 -3.494536 2.038333 -0.318297
 6 0.206693 -0.120163 0.138681
 6 2.570739 -0.421228 1.414729
 6 3.717328 -1.193593 1.487173
 7 4.341509 -1.686293 0.432193
 6 3.842379 -1.428787 -0.763592
 6 2.704057 -0.669879 -0.979146
 6 -2.103568 -0.455070 -0.119568
 6 -3.252729 -0.792647 0.615338
 6 -3.675287 -2.116379 0.680337
 7 -3.056116 -3.109612 0.078608
 6 -1.982795 -2.819943 -0.624474
 6 -1.472734 -1.531735 -0.762058
 9 4.484718 -1.934352 -1.818415
 9 2.251338 -0.443287 -2.213773
 9 4.234141 -1.463395 2.687929
 9 1.984855 0.048904 2.520165
 9 -0.394091 -1.340005 -1.538764
 9 -1.360204 -3.822238 -1.247038
 9 -4.764337 -2.406420 1.394387
 9 -3.952495 0.149527 1.266633

26-R

Total energy = -946.50519

6 1.237063 0.007153 -3.373652
 6 1.249604 0.003143 -1.964990
 6 2.495750 -0.001866 -1.277594
 6 3.675254 -0.002594 -2.039192
 6 3.663102 0.001358 -3.430107
 6 2.431086 0.006200 -0.474562
 1 0.296601 0.010991 -3.911661
 1 4.628969 -0.006396 -1.519062
 1 4.578507 0.000743 -4.011024
 6 2.619149 -0.006280 0.188766
 6 1.664914 -0.007270 1.091895
 6 -0.003035 0.004283 -1.290413
 6 -1.133608 0.005765 -0.837134
 1 3.657372 -0.009292 0.545066
 6 1.053184 -0.009425 2.335646
 6 0.696530 -1.234198 2.980355
 6 0.047201 -1.224032 4.204987
 6 -0.280078 -0.013441 4.832058
 6 0.052859 1.199171 4.211907
 6 0.702246 1.213302 2.987349

1 0.945560 -2.171475 2.493943
 1 -0.208785 -2.166223 4.681312
 1 -0.788814 -0.014992 5.790972
 1 -0.198722 2.139809 4.693617
 1 0.955657 2.152161 2.506283
 6 -2.451544 0.006829 -0.295762
 6 -3.568586 0.011703 -1.156163
 6 -4.858621 0.012736 -0.634605
 6 -5.058307 0.008970 0.748051
 6 -3.957879 0.004144 1.608428
 6 -2.662884 0.003063 1.097970
 1 -3.408692 0.014627 -2.229470
 1 -5.710619 0.016492 -1.308054
 1 -6.066241 0.009794 1.152355
 1 -4.107921 0.001204 2.684009
 1 -1.808725 -0.000685 1.765364
 9 2.395050 0.010105 -5.423675

26 (5-exo TS)

Total energy = -946.49941

6 -0.939408 -0.044289 -0.850308
 6 -0.933842 -0.049870 0.383959
 6 1.241026 -0.042231 1.262655
 6 0.817592 -0.076051 2.515077
 6 -0.615288 -0.068487 2.814586
 6 -1.495969 -0.055413 1.706924
 6 -2.882388 -0.052191 1.912766
 6 -3.363921 -0.061096 3.215029
 6 -2.520303 -0.074133 4.321434
 6 -1.142356 -0.078716 4.110134
 1 -3.572846 -0.043248 1.077583
 1 -2.945871 -0.081496 5.318744
 1 -0.467891 -0.089801 4.961600
 1 1.518621 -0.129097 3.352905
 6 2.369502 0.028173 0.410076
 6 2.784693 -1.097197 -0.344762
 6 3.872299 -1.009937 -1.204885
 6 4.566420 0.195880 -1.350326
 6 4.160616 1.320556 -0.624293
 6 3.074886 1.246562 0.239847
 1 2.242439 -0.2030789 -0.235360
 1 4.182050 -1.885232 -1.768674
 1 5.413656 0.259567 -2.026433
 1 4.695904 2.259500 -0.734160
 1 2.756493 2.119297 0.801058
 6 -0.776769 -0.027591 -2.256695
 6 -0.823482 -1.227559 -3.001712
 6 -0.674419 -1.203024 -4.383897
 6 -0.479150 0.008918 -5.052489
 6 -0.433179 1.202460 -4.326547
 6 -0.580478 1.191500 -2.943924
 1 -0.976817 -2.166420 -2.479848
 1 -0.711173 -2.132860 -4.943903
 1 -0.363990 0.023200 -6.132076
 1 -0.280680 2.146235 -4.841863
 1 -0.543463 2.115833 -2.377208
 9 -4.700325 -0.058030 3.412416

26 (5-exo P)

Total energy = -946.55790

6 -2.592243 -0.034046 -0.559421
 6 -2.607247 -0.033599 0.897827
 6 -1.267091 -0.038392 1.350872
 6 -0.388266 -0.035575 0.148041
 6 0.927463 0.006485 0.158467
 6 -1.312720 -0.038049 -1.030645
 6 -3.655268 -0.035736 1.819000
 6 -3.359861 -0.039431 3.185661
 6 -2.029327 -0.042028 3.597325
 6 -0.958655 -0.041867 2.703838

1 -4.689462 -0.033199 1.487242

1 -4.142777 -0.040325 3.936025

1 0.061675 -0.045567 3.072278

1 -3.483429 -0.058438 -1.175746

6 2.264058 0.046580 0.489092

6 3.019131 -1.158210 0.666583

6 4.368911 -1.102126 0.969388

6 5.023417 0.130871 1.104318

6 4.302953 1.321712 0.930138

6 2.952927 1.295339 0.625535

1 2.512867 -2.112578 0.566154

1 4.923449 -2.026119 1.105532

1 6.081970 0.163454 1.341530

1 4.807042 2.278164 1.034322

1 2.396840 2.216358 0.487380

6 -0.896520 -0.029712 -2.439727

6 0.289447 -0.654510 -2.865166

6 0.656230 -0.652537 -4.209830

6 -0.152373 -0.029877 -5.161476

6 -1.332682 0.596296 -4.754655

6 -1.697224 0.600637 -3.411149

1 0.917057 -1.159303 -2.138995

1 1.574890 -1.145439 -4.514936

1 0.135483 -0.028441 -6.208614

1 -1.965170 1.093615 -5.484519

1 -2.599617 1.117990 -3.099801

9 -1.762352 -0.045946 4.923115

27-R

Total energy = -946.50574

6 1.127433 -0.000558 -3.447231
 6 1.123171 -0.001303 -2.037126
 6 2.366222 -0.002276 -1.344067
 6 3.553585 -0.003101 -2.091011
 6 3.511198 -0.002661 -3.476053
 6 2.310165 -0.001283 -4.176681
 1 0.174518 0.000295 -3.965383
 1 4.517417 -0.003823 -1.592588
 1 2.313554 -0.000882 -5.260724
 6 2.481961 -0.001570 0.122807
 6 1.516676 -0.000419 1.014956
 6 -0.132453 -0.000642 -1.368268
 6 -1.265066 -0.000517 -0.919330
 1 3.516729 -0.001489 0.487868
 6 0.921021 0.000300 2.267975
 6 0.578389 -1.223286 2.921056
 6 -0.054039 -1.210602 4.154653
 6 -0.377294 0.001368 4.780695
 6 -0.057364 1.212718 4.151785
 6 0.574840 1.224320 2.918227
 1 0.825024 -2.161464 2.435190
 1 -0.299401 -2.151664 4.638646
 1 -0.873593 0.001808 5.746094
 1 -0.305838 2.154191 4.633340
 1 0.818153 2.1162044 2.429861
 6 -2.582622 0.000404 -0.376956
 6 -3.701800 0.050891 -1.233200
 6 -4.990732 0.052503 -0.708684
 6 -5.188425 0.003968 0.673351
 6 -4.086092 -0.046503 1.529816
 6 -2.792311 -0.048615 1.016323
 1 -3.544487 0.088739 -2.306267
 1 -5.843689 0.091778 -1.379877
 1 -6.195401 0.005316 1.079999
 1 -4.233826 -0.084407 2.605122
 1 -1.937122 -0.088385 1.681329
 9 4.672131 -0.003430 -4.163426

27 (5-exo TS)

Total energy = -946.50025

6 -0.383305 -1.360744 0.043424
 6 0.712758 -0.794385 0.017120
 6 0.487007 1.538748 -0.147296
 6 1.793678 1.742164 -0.195409
 6 2.719025 0.613673 -0.086566
 6 2.144447 -0.675705 0.023352
 6 2.978385 -1.798755 0.127689
 6 4.364495 -1.657573 0.125138
 6 4.902407 -0.378746 0.014816
 6 4.109608 0.756292 -0.092056
 1 2.532286 -2.784203 0.210266
 1 5.024937 -2.513563 0.205045
 1 4.576696 1.731924 -0.176254
 1 2.213249 2.741978 -0.337490
 6 -0.785553 2.160163 -0.119189
 6 -1.687164 2.027548 -1.204087
 6 -2.944915 2.615837 -1.153349
 6 -3.346186 3.335763 -0.023099
 6 -2.474365 3.462401 1.063382
 6 -1.213172 2.880016 1.025171
 1 -1.377320 1.463347 -2.077611
 1 -3.620270 2.511583 -1.997676
 1 -4.331628 3.790307 0.012462
 1 -2.781725 4.019291 1.944034
 1 -0.536771 2.973691 1.868776
 6 -1.706732 -1.865137 0.066185
 6 -2.321526 -2.326039 -1.119947
 6 -3.615869 -2.833192 -1.090270
 6 -4.323319 -2.895282 0.113732
 6 -3.725497 -2.444190 1.293858
 6 -2.431800 -1.934377 1.277056
 1 -1.768726 -2.279027 -2.052474
 1 -4.076295 -3.182983 -2.009676
 1 -5.333583 -3.292834 0.132085
 1 -4.271846 -2.489358 2.231405
 1 -1.965411 -1.581467 2.190791
 9 6.244663 -0.235508 0.010933

27 (5-exo P)

Total energy = -946.55842

6 -2.459138 -0.036374 -0.509293
 6 -2.486318 -0.036380 0.947344
 6 -1.150816 -0.041906 1.414496
 6 -0.260917 -0.038468 0.221889
 6 1.054594 0.005726 0.235306
 6 -1.174174 -0.040833 -0.966145
 6 -3.551037 -0.038170 1.848432
 6 -3.237371 -0.042521 3.205543
 6 -1.929593 -0.046239 3.686094
 6 -0.868159 -0.046228 2.773612
 1 -4.588479 -0.034679 1.531506
 1 -1.760111 -0.050179 4.756925
 1 0.158176 -0.050460 3.128742
 1 -3.344314 -0.060667 -1.133945
 6 2.398613 0.047891 0.528599
 6 3.160147 -1.156014 0.687853
 6 4.517802 -1.098064 0.951931
 6 5.174990 0.135785 1.065797
 6 4.448417 1.325715 0.910608
 6 3.090409 1.297679 0.644861
 1 2.652303 -2.111079 0.603058
 1 5.077049 -2.021307 1.073443
 1 6.239925 0.169677 1.272261
 1 4.954453 2.282811 0.998489
 1 2.529841 2.217967 0.520616
 6 -0.745185 -0.031268 -2.371459
 6 0.438359 -0.666080 -2.788629
 6 0.817044 -0.661505 -4.129959
 6 0.022980 -0.026100 -5.085467
 6 -1.155024 0.609493 -4.686707

6 -1.531949 0.610644 -3.346575
 1 1.053820 -1.180969 -2.059341
 1 1.733306 -1.162143 -4.429450
 1 0.320261 -0.022504 -6.129972
 1 -1.775975 1.116022 -5.420071
 1 -2.432569 1.134312 -3.040741
 9 -4.251082 -0.043057 4.099965

28-R

Total energy = -614.91781

6 -1.947889 0.000000 -3.393333
 6 -1.970470 0.000000 -1.999916
 6 -0.771108 0.000000 -1.250430
 6 0.389215 0.000000 -2.010383
 6 0.469528 0.000000 -3.383067
 6 -0.738592 0.000000 -4.094659
 1 -2.886995 0.000000 -3.938465
 1 -2.933165 0.000000 -1.498412
 1 1.425110 0.000000 -3.900593
 1 -0.733557 0.000000 -5.181423
 6 -0.724765 0.000000 0.230494
 6 -1.899944 0.000000 0.997053
 6 -1.867296 0.000000 2.387803
 6 -0.650261 0.000000 3.059685
 6 0.551466 0.000000 2.336584
 6 0.522206 0.000000 0.913019
 1 -2.863671 0.000000 0.502023
 1 -2.796534 0.000000 2.949095
 1 -0.611046 0.000000 4.143309
 6 1.770149 0.000000 0.217942
 6 2.905633 0.000000 -0.210893
 1 3.877360 0.000000 -0.647279
 6 1.787619 0.000000 3.051861
 6 2.808749 0.000000 3.700661
 1 3.717055 0.000000 4.257213

28 → 29 (6-endo TS)

Total energy = -614.91044

6 -1.965357 0.000000 -3.320692
 6 -1.926726 0.000000 -1.929561
 6 -0.700887 0.000000 -1.219083
 6 0.438651 0.000000 -2.025637
 6 0.444140 0.000000 -3.405260
 6 -0.786194 0.000000 -4.071139
 1 -2.927589 0.000000 -3.824046
 1 -2.871049 0.000000 -1.395927
 1 1.375770 0.000000 -3.966252
 1 -0.824199 0.000000 -5.157379
 6 -0.658191 0.000000 0.270565
 6 -1.839999 0.000000 1.032208
 6 -1.822946 0.000000 2.423564
 6 -0.617577 0.000000 3.118627
 6 0.589533 0.000000 2.408771
 6 0.572094 0.000000 0.989782
 1 -2.802356 0.000000 0.535792
 1 -2.761357 0.000000 2.969559
 1 -0.596473 0.000000 4.202724
 6 1.790058 0.000000 0.257272
 6 2.498282 0.000000 -0.739156
 1 3.297592 0.000000 -1.445364
 6 1.833198 0.000000 3.111894
 6 2.871552 0.000000 3.733052
 1 3.791885 0.000000 4.269651

29 (6-endo P)

Total energy = -615.00939

6 -1.846841 0.000000 -3.309219
 6 -1.869417 0.000000 -1.926396
 6 -0.676677 0.000000 -1.165803
 6 0.562891 0.000000 -1.876667

6 0.562365 0.000000 -3.290035
 6 -0.621827 0.000000 -4.000301
 1 -2.781294 0.000000 -3.862270
 1 -2.830366 0.000000 -1.424539
 1 1.516309 0.000000 -3.810411
 1 -0.608327 0.000000 -5.086112
 6 -0.676039 0.000000 0.294733
 6 -1.857444 0.000000 1.070209
 6 -1.811586 0.000000 2.453652
 6 -0.585339 0.000000 3.132591
 6 0.610182 0.000000 2.417996
 6 0.575149 0.000000 0.991135
 1 -2.825331 0.000000 0.582190
 1 -2.736952 0.000000 3.021415
 1 -0.555770 0.000000 4.216805
 6 1.745322 0.000000 0.198703
 6 1.807397 0.000000 -1.141989
 1 2.746891 0.000000 -1.688768
 6 1.865140 0.000000 3.099660
 6 2.920430 0.000000 3.692358
 1 3.852612 0.000000 4.207935

28 → 30 (5-exo TS)

Total energy = -614.91732

6 -2.436757 0.000000 -3.045910
 6 -2.299379 0.000000 -1.658053
 6 -1.018298 0.000000 -1.069554
 6 0.055373 0.000000 -1.946603
 6 -0.028500 0.000000 -3.319369
 6 -1.314659 0.000000 -3.880652
 1 -3.431186 0.000000 -3.482177
 1 -3.191544 0.000000 -1.038221
 1 0.857026 0.000000 -3.949471
 1 -1.437299 0.000000 -4.960585
 6 -0.741268 0.000000 0.378636
 6 -1.746561 0.000000 1.353088
 6 -1.430585 0.000000 2.709133
 6 -0.101582 0.000000 3.120474
 6 0.935862 0.000000 2.173758
 6 0.615636 0.000000 0.788896
 1 -2.788490 0.000000 1.052181
 1 -2.224684 0.000000 3.449448
 1 0.153008 0.000000 4.174555
 6 1.674020 0.000000 -0.179641
 6 2.788288 0.000000 -0.682608
 1 3.684826 0.000000 -1.258552
 6 2.289102 0.000000 2.628432
 6 3.419018 0.000000 3.061202
 1 4.420092 0.000000 3.425450

30 (5-exo P)

Total energy = -614.98484

6 -2.424266 0.000000 -2.947520
 6 -2.428988 0.000000 -1.550382
 6 -1.210312 0.000000 -0.872969
 6 0.005682 0.000000 -1.593710
 6 0.006092 0.000000 -2.985211
 6 -1.218693 0.000000 -3.658734
 1 -3.366175 0.000000 -3.488041
 1 -3.368935 0.000000 -1.005684
 1 0.939301 0.000000 -3.541146
 1 -1.234993 0.000000 -4.744525
 6 -0.901084 0.000000 0.563831
 6 -1.736316 0.000000 1.678712
 6 -1.158484 0.000000 2.952265
 6 0.226501 0.000000 3.111336
 6 1.087401 0.000000 1.993637
 6 0.503467 0.000000 0.716333
 1 -2.816544 0.000000 1.566530
 1 -1.794310 0.000000 3.832418

1 0.662288 0.000000 4.104715
 6 1.138266 0.000000 -0.621740
 6 2.434336 0.000000 -0.889834
 6 2.503240 0.000000 2.172906
 6 3.700308 0.000000 2.355684
 1 4.755784 0.000000 2.499607
 1 3.060688 0.000000 -1.771502

31 (6-endo P)

Total energy = -615.07612
 6 -2.417551 0.000000 -2.833160
 6 -2.438644 0.000000 -1.433029
 6 -1.232466 0.000000 -0.740517
 6 0.005881 0.000000 -1.450587
 6 0.014668 0.000000 -2.841380
 6 -1.205600 0.000000 -3.528501
 1 -3.353666 0.000000 -3.383786
 1 -3.385991 0.000000 -0.900859
 1 0.951335 0.000000 -3.392109
 1 -1.209001 0.000000 -4.614585
 6 -0.932590 0.000000 0.704711
 6 -1.679458 0.000000 1.865344
 6 -1.004253 0.000000 3.118048
 6 0.375905 0.000000 3.222584
 6 1.172707 0.000000 2.043069
 6 0.481477 0.000000 0.812946
 1 -2.765801 0.000000 1.845633
 1 -1.600240 0.000000 4.026114
 1 0.853927 0.000000 4.197025
 6 1.103576 0.000000 -0.462915
 6 2.482241 0.000000 -0.533344
 6 2.570945 0.000000 1.880757
 6 3.232992 0.000000 0.686289
 1 4.318802 0.000000 0.643277
 1 3.011646 0.000000 -1.482599

30 → 31 (6-endo TS)

Total energy = -614.97625
 6 -2.502335 0.000000 -2.805139
 6 -2.473389 0.000000 -1.407767
 6 -1.239741 0.000000 -0.759207
 6 -0.037336 0.000000 -1.509953
 6 -0.073313 0.000000 -2.900697
 6 -1.314442 0.000000 -3.544630
 1 -3.457090 0.000000 -3.322734
 1 -3.400265 0.000000 -0.840932
 1 0.846109 0.000000 -3.479384
 1 -1.356811 0.000000 -4.629803
 6 -0.894932 0.000000 0.671505
 6 -1.671053 0.000000 1.828926
 6 -1.030044 0.000000 3.076061
 6 0.361788 0.000000 3.180006
 6 1.155828 0.000000 2.019255
 6 0.510388 0.000000 0.773122
 1 -2.755943 0.000000 1.776115
 1 -1.628392 0.000000 3.982145
 1 0.839200 0.000000 4.154368
 6 1.119005 0.000000 -0.567508
 6 2.425061 0.000000 -0.827039
 6 2.579971 0.000000 1.962534
 6 3.628032 0.000000 1.321465
 1 4.658383 0.000000 1.044778
 1 2.993882 0.000000 -1.750161

32 (5-exo P)

Total energy = -615.01550
 6 -2.518984 0.000000 -2.882919
 6 -2.524933 0.000000 -1.482483
 6 -1.315388 0.000000 -0.795855
 6 -0.073203 0.000000 -1.534916

6 -0.089852 0.000000 -2.926917
 6 -1.317875 0.000000 -3.597237
 1 -3.462360 0.000000 -3.421207
 1 -3.466716 0.000000 -0.941178
 1 0.840564 0.000000 -3.487317
 1 -1.337524 0.000000 -4.682889
 6 -1.015094 0.000000 0.661383
 6 -1.651438 0.000000 1.910480
 6 -0.845172 0.000000 3.069020
 6 0.567701 0.000000 3.052655
 6 1.203038 0.000000 1.807421
 6 0.364889 0.000000 0.715926
 1 -2.732669 0.000000 2.015697
 1 -1.341945 0.000000 4.035182
 1 1.114193 0.000000 3.991298
 6 1.028990 0.000000 -0.561251
 6 2.368616 0.000000 -0.305523
 6 2.579113 0.000000 1.183370
 6 3.750743 0.000000 1.799290
 1 3.199294 0.000000 -1.000055
 1 4.120257 0.000000 2.815802

30 → 32 (5-exo TS)

Total energy = -614.96884
 6 -2.558886 0.000000 -2.856786
 6 -2.530755 0.000000 -1.458246
 6 -1.300691 0.000000 -0.805104
 6 -0.089924 0.000000 -1.566253
 6 -0.130749 0.000000 -2.956413
 6 -1.373415 0.000000 -3.598633
 1 -3.514323 0.000000 -3.373238
 1 -3.458303 0.000000 -0.892737
 1 0.788446 0.000000 -3.535110
 1 -1.417950 0.000000 -4.683626
 6 -0.962102 0.000000 0.635224
 6 -1.656374 0.000000 1.847913
 6 -0.914610 0.000000 3.042999
 6 0.488241 0.000000 3.067585
 6 1.192360 0.000000 1.851367
 6 0.429901 0.000000 0.696917
 1 -2.741926 0.000000 1.887357
 1 -1.448842 0.000000 3.988619
 1 1.019366 0.000000 4.013699
 6 1.053245 0.000000 -0.619348
 6 2.381515 0.000000 -0.596945
 6 2.622091 0.000000 1.620691
 6 3.801339 0.000000 2.010782
 1 3.197336 0.000000 -1.307150
 1 4.869094 0.000000 2.007696

28-R (Ph-substituted)

Total energy = -1077.06944
 6 -3.207035 2.313061 -4.413157
 6 -3.266621 2.353211 -3.020581
 6 -2.138555 2.031418 -2.232345
 6 -1.008274 1.666166 -2.948636
 6 -0.894539 1.606185 -4.318241
 6 -2.029576 1.946679 -5.070175
 1 -4.092642 2.560498 -4.990805
 1 -4.204376 2.610496 -2.536130
 1 0.033561 1.317160 -4.803882
 1 -1.991782 1.919942 -6.155981
 6 -2.161314 2.082950 -0.751984
 6 -3.043396 2.945219 -0.086760
 6 -3.088502 3.010366 1.304168
 6 -2.247601 2.210353 2.068377
 6 -1.341373 1.335699 1.445958
 6 -1.286870 1.271682 0.021264
 1 -3.683747 3.598812 -0.669106
 1 -3.776924 3.694061 1.791265

1 -2.275387 2.250224 3.151847
 6 -0.352836 0.391360 -0.589044
 6 0.470224 -0.397466 -1.018561
 6 -0.499697 0.513540 2.245556
 6 0.197301 -0.184918 2.956764
 6 1.425177 -1.295847 -1.571486
 6 1.248139 -1.816296 -2.869741
 6 2.185053 -2.693996 -3.407205
 6 3.309025 -3.067623 -2.666177
 6 3.493672 -2.556272 -1.379284
 6 2.563251 -1.677477 -0.832036
 1 0.372760 -1.522593 -3.439532
 1 2.037990 -3.089253 -4.408097
 1 4.037156 -3.753038 -3.089547
 1 4.367560 -2.841380 -0.800854
 1 2.705700 -1.272512 0.164557
 6 1.018538 -1.021449 3.766518
 6 1.638141 -2.161661 3.215280
 6 2.440059 -2.977933 4.007637
 6 2.639140 -2.675763 5.357002
 6 2.028595 -1.549137 5.913015
 6 1.224062 -0.727032 5.129246
 1 1.477142 -2.395512 2.168001
 1 2.910154 -3.854446 3.571404
 1 3.265692 -3.314945 5.971883
 1 2.179801 -1.310472 6.961672
 1 0.748709 0.149155 5.557908

38→29 (6-endo TS, Ph-substituted)

Total energy = -1077.05928
 6 -3.998703 1.031141 -3.915802
 6 -3.995327 .974610 -2.525498
 6 -2.830666 .626281 -1.798689
 6 -1.701595 .373365 -2.581630
 6 -1.668664 .409793 -3.961487
 6 -2.842456 .742888 -4.646009
 1 -4.913706 1.302958 -4.433791
 1 -4.915392 1.214257 -2.003002
 1 -7.54970 .184801 -4.505467
 1 -2.853034 .780109 -5.732285
 6 -2.834189 .531838 -.314120
 6 -4.022125 .668112 .424602
 6 -4.040947 .577892 1.813731
 6 -2.869253 .342275 2.525465
 6 -1.656982 .190144 1.837720
 6 -1.637884 .281748 .417990
 1 -4.961254 .833948 -.088915
 1 -4.982036 .688109 2.343917
 1 -2.877815 .269867 3.607460
 6 -4.17962 .116568 -.287448
 6 .271354 .044204 -1.309578
 6 -4.49869 -.056042 2.549493
 6 .579497 -.264991 3.163116
 6 1.397848 -.139172 -2.176694
 6 2.234457 -1.260100 -2.007131
 6 3.345454 -1.437130 -2.826800
 6 3.637724 -.507803 -3.828120
 6 2.813309 .605535 -4.004001
 6 1.701630 .793413 -3.186084
 1 1.999638 -1.980166 -1.230296
 1 3.983464 -2.304613 -2.686009
 1 4.504096 -.650273 -4.467097
 1 3.039499 1.333449 -4.777525
 1 1.062726 1.660430 -3.313084
 6 1.799817 -.509286 3.855493
 6 3.015926 -.584440 3.146321
 6 4.209024 -.822759 3.821792
 6 4.213152 -.989925 5.208886
 6 3.013308 -.917407 5.920594
 6 1.814753 -.679196 5.254355

1	3.006029	-452727	2.069322	6	-1.266042	.515076	1.926304	6	5.682823	-2.008397	.145649								
1	5.139682	-.877706	3.264667	6	-1.697290	.529491	.567040	6	6.108953	-.678407	.112635								
1	5.146314	-1.175573	5.732312	1	-4.941328	1.457667	1.082314	6	5.165727	.351503	.082746								
1	3.011860	-1.046776	6.998911	1	-4.191237	1.419249	3.423588	6	3.804302	.061582	.085494								
1	.880730	-.621905	5.803686	1	-1.841211	.821324	3.974555	1	3.988956	-3.341537	.174340								
29 (6-endo P, Ph-substituted)																			
Total energy = -1077.14460																			
6	-4.141563	-.075860	-3.756286	6	1.200467	-.124993	2.609948	6	7.169891	-.446416	.110210								
6	-4.110725	.072763	-2.382588	6	1.262105	-.483436	-2.013347	1	5.491377	1.387272	.056985								
6	-2.895998	.066204	-1.657811	6	1.040597	-1.418938	-3.045292	1	3.071707	.860583	.062676								
6	-1.675581	-.080874	-2.393902	6	2.078808	-1.782267	-3.897854	31 (6-endo P, Ph-substituted)											
6	-1.737913	-.257492	-3.796413	6	3.350397	-1.225257	-3.739787	Total energy = -1077.19484	6	-4.728390	.145523	-2.143884							
6	-2.944832	-.253167	-4.469172	6	3.580055	-.297131	-2.721159	6	-4.675293	.093113	-.747234								
1	-5.093099	-.068658	-4.279361	6	2.548728	.074772	-1.863205	6	-3.434576	.058457	-.119306								
1	-5.049934	.186734	-1.853937	1	.051857	-1.850005	-3.162187	6	-2.226417	.086497	-.881124								
1	-.817022	-4.12835	-4.345653	1	1.895951	-2.503951	-4.688594	6	-2.296393	.127794	-2.273019								
1	-2.965601	-.394554	-5.545728	1	4.157473	-.1512397	-4.407077	6	-3.550783	.157344	-2.894637								
6	-2.875823	.182271	-2.01607	1	4.565888	.141159	-2.596488	1	-5.690679	.171714	-2.646628								
6	-4.035914	.345372	.588181	1	2.720576	.799717	-1.074308	1	-5.591530	.073413	-.163492								
6	-3.959377	.431655	1.968761	6	2.527889	-.478089	2.987805	1	-1.396464	.135974	-2.875675								
6	-2.725944	.360550	2.629420	6	2.936699	-.392525	4.333978	1	-3.605432	.189323	-3.978945								
6	-1.547791	.203542	1.899988	6	4.234748	-.737628	4.698641	6	-3.081325	-.032315	1.306344								
6	-1.618853	.114068	.474392	6	5.145486	-1.173337	3.733222	6	-3.790522	-.114060	2.488224								
1	-5.010582	.405746	.118193	6	4.749794	-1.263196	2.396376	6	-3.077271	-.224393	3.713331								
1	-4.868861	.556555	2.548492	6	3.454171	-.920206	2.021227	6	-1.694881	-.261261	3.767067								
1	-2.675758	.429707	3.710737	1	2.226302	-.053627	5.080947	6	-9.42048	-.177963	2.562746								
6	-.475925	-.025593	-.334908	1	4.537154	-.666859	5.739337	6	-1.665842	-.053268	1.360394								
6	-.398891	-.082633	-1.681175	1	6.157533	-1.441941	4.021129	1	-4.876733	-.100793	2.502273								
6	-.282109	.139816	2.544407	1	5.453898	-1.603365	1.642641	1	-3.642393	-.288017	4.638639								
6	.809268	.089185	3.079988	1	3.143686	-.990543	.983940	1	-1.181518	-.354459	4.718651								
6	.929641	-.139590	-2.352449	30 (5-exo P, Ph-substituted)															
6	1.891677	-.061692	-1.908631	Total energy = -1077.14336	6	.303148	.019373	-.065745	6	.442468	-.210311	2.346259							
6	3.161800	-.1099487	-2.482063	6	-5.782099	.900629	-.106587	6	1.100075	-.105773	1.148593								
6	3.495775	-.213433	-3.507598	6	-5.229596	-.380338	-.028483	6	.961784	.105082	-1.402412								
6	2.551588	.714152	-3.951163	6	-3.841689	-.514090	-.003350	6	1.676358	-.984334	-1.922213								
6	1.280370	.752681	-3.379148	6	-3.016964	.630876	-.056446	6	2.279302	-.904773	-3.176975								
1	1.628171	-.1753098	-1.114236	6	-3.568658	1.905535	-.133607	6	2.186006	.267876	-3.928689								
1	3.889765	-.1824720	-2.129748	6	-4.960304	2.032987	-.158549	6	1.482570	1.360831	-3.419249								
1	4.484475	-.243333	-3.956014	1	-6.861436	1.019584	-.127006	6	.873211	1.279266	-2.166724								
1	2.806790	1.416436	-4.739578	1	-5.874653	-.1253643	.011564	1	1.755897	-.1895897	-1.338116								
1	.560377	1.492695	-.7314247	1	-2.929391	2.782789	-.173551	1	2.823884	-.1759688	-3.567018								
6	2.100343	.032879	3.677914	1	-5.408704	3.020263	-.218823	1	2.659389	.330087	-4.904131								
6	3.252832	-.044627	2.869347	6	-2.982744	-.1703770	.072789	1	1.407087	2.278120	-3.996114								
6	4.515926	-.096811	3.450984	6	-3.308026	-.056499	.142068	1	.322418	2.128223	-1.772412								
6	4.654194	-.073368	4.841095	6	-2.272577	-.3994617	.205056	6	2.593516	-.115360	1.165103								
6	3.518349	.002868	5.650690	6	-9.39690	-.3590624	.198913	6	3.359142	.847894	.489144								
6	2.250500	.055884	5.078941	6	-.587389	-.223297	.129222	6	4.750197	.840310	.577765								
1	3.138725	-.061608	1.790343	6	-1.632740	-.1284458	.066246	6	5.404337	-.126897	1.342878								
1	5.396423	-.155160	2.817862	1	-4.344444	-.338019	.146937	6	4.654674	-.1086247	2.024648								
1	5.641712	-.114039	5.290971	1	-2.506984	-.5053524	.259485	6	3.263366	-.1078627	1.937703								
1	3.621182	.021438	6.731714	1	-.145521	-.4328041	.247922	1	2.864395	1.611618	-.100031								
1	1.365842	.115741	5.704444	6	-1.590098	.196863	-.015347	1	5.324097	1.597086	.050674								
28→30 (5-exo TS, ph-substituted)																			
Total energy = -1077.06920																			
6	-5.153822	.958202	-2.926412	6	.783946	-.1844519	.123680	1	6.488462	-.131443	1.408023								
6	-4.825230	.946832	-.1571507	6	1.973778	-.1587276	.121836	1	5.152219	-1.843676	2.623611								
6	-3.477761	.870694	-1.155679	6	.338008	2.048055	-.097470	1	2.679767	-1.827032	2.465244								
6	-2.542549	.797548	-2.177594	6	.841217	2.533078	-.1348201	30→31 (6-endo TS, Ph-substituted)											
6	-2.813758	.799249	-3.526254	6	1.745990	3.580970	-.1383508	Total energy = -1077.12405	6	-4.539751	-.034969	-2.779153							
6	-4.160846	.888385	-3.908175	6	2.192420	4.184530	-.198503	6	-4.664328	-.012056	-1.387199								
1	-6.197902	1.015211	-3.219557	6	1.716909	3.720670	1.037042	6	-3.509813	.001959	-.607005								
1	-5.624006	.979447	-.836215	6	.811548	2.674519	1.100927	6	-2.229981	-.004962	-1.219917								
1	-2.023236	.740412	-4.269732	1	.500587	2.063452	-.2264755	6	-2.113262	-.029612	-2.606841								
1	4.429587	.899549	4.961259	1	2.112364	3.936544	-.2342327	6	-3.277437	-.044552	-3.382051								
6	-3.043657	.859106	.257058	1	2.902059	5.004899	-.237272	1	-5.431782	-.046175	-3.398681								
6	-3.918052	1.176572	1.304848	1	2.060408	4.185002	1.957059	1	-5.647614	-.006451	-.924900								
6	-3.493872	1.164635	2.631377	6	.447708	2.313714	2.057032	1	-1.136918	-.037107	-3.080395								
6	-2.180391	.834853	2.944547	6	3.364573	-.1277351	.118758	1	-3.199534	-.064235	-4.465172								

6	-3.326707	.018085	.852599	1	2.224858	1.615995	-4.444352	1	-1.575145	0.000000	-2.392212
6	-4.221550	.017094	1.920156	1	.328531	1.494547	-2.861939	1	2.937095	0.000000	-0.265352
6	-3.715178	.017622	3.229035	6	2.361910	-.092786	2.550837	1	2.736271	0.000000	-2.757159
6	-2.342827	.017195	3.481018	6	2.892646	1.126886	3.083076	6	-1.710391	0.000000	0.298286
6	-1.428298	.020536	2.410990	6	3.905202	1.098690	4.026435	6	-1.793770	0.000000	1.649049
6	-1.940872	.024353	1.106324	6	4.435063	-.120087	4.475326	1	-2.643347	0.000000	-0.259968
1	-5.294814	.013098	1.752884	6	3.932188	-1.325303	3.963927	1	-2.783124	0.000000	2.101878
1	-4.406712	.016436	4.066345	6	2.918956	-1.326482	3.020477	6	-0.699314	0.000000	2.549279
1	-1.971367	.015099	4.500616	1	2.485310	2.069559	2.733725	6	0.184823	0.000000	3.379973
6	-1.188904	.016694	-.151118	1	4.291978	2.033819	4.421158	1	0.984880	0.000000	4.083271
6	.142813	.017558	-.267678	1	5.230090	-.130328	5.214093	Total energy = -384.44911 (cc-PVDZ)			
6	-.006958	.014104	2.503959	1	4.338407	-2.270997	4.311154	6	-.590844	0.000000	-1.936685
6	1.064517	.010837	1.860939	1	2.527577	-2.259655	2.628921	6	-.492632	0.000000	-0.503888
6	1.115927	.055693	-1.310980	30→32 (5-exo TS, Ph-substituted)				6	0.799807	0.000000	0.006120
6	1.847427	-1.102234	-1.670124	Total energy = -1077.12489				6	1.957435	0.000000	-0.729964
6	2.813883	-1.047478	-2.667493	6	-4.846499	-.020772	-3.193548	6	1.843498	0.000000	-2.151436
6	3.089232	.156808	-3.323388	6	-4.893298	.014485	-1.796112	6	0.568564	0.000000	-2.671599
6	2.384163	1.312719	-2.973171	6	-3.700365	.022576	-1.077075	1	-1.583307	0.000000	-2.396204
6	1.414100	1.270749	-1.977817	6	-2.449152	-.001760	-1.771078	1	2.948868	0.000000	-0.269992
1	1.638556	-0.305461	-1.157403	6	-2.415648	-.036994	-3.162238	1	2.744585	0.000000	-2.769053
1	3.358617	-1.948072	-2.935809	6	-3.622214	-.047777	-3.869515	6	-1.7111692	0.000000	0.298723
1	3.847725	.194395	-4.099412	1	-5.772734	-.027428	-3.760781	6	-1.796120	0.000000	1.651926
1	2.591518	2.250462	-3.480933	1	-5.850016	.033642	-1.281586	1	-2.650029	0.000000	-0.262840
1	.864066	2.166640	-1.706873	1	-1.466636	-.058624	-3.689636	1	-2.792168	0.000000	2.106053
6	2.500357	-.047722	1.751895	1	-3.608001	-.077348	-4.955044	6	-0.702334	0.000000	2.557194
6	3.230987	.989886	1.146906	6	-3.439331	.044976	.377721	6	0.182449	0.000000	3.393851
6	4.620333	.924478	1.077617	6	-4.199050	.058107	1.550266	1	0.983277	0.000000	4.106579
6	5.301120	-1.73635	1.606755	6	-3.524248	.053543	2.784237				
6	4.584302	-1.210881	2.207648	6	-2.124786	.031250	2.884939	33 (5-exo TS)			
6	3.194883	-1.153457	2.278642	6	-1.352961	.019891	1.710050	Total energy = -384.42693 (6-31G**)			
1	2.700860	1.842248	.737671	6	-2.051075	.034552	.514479	6	-.596186	0.000000	-1.976058
1	5.172948	1.734089	.610331	1	-5.285122	.067896	1.529608	6	-.643087	0.000000	-0.555948
1	6.384683	-.221260	1.551406	1	-4.109305	.063113	3.699370	6	0.564279	0.000000	0.131628
1	5.108520	-2.067127	2.621963	1	-1.647401	.021353	3.859514	6	1.800201	0.000000	-0.462539
1	2.632175	-1.955437	2.745058	6	-1.362166	.017249	-.762599	6	1.849210	0.000000	-1.884764
32 (5-exo P, Ph-substituted)			6	-.028530	-.004506	-.696991	6	0.649570	0.000000	-2.558579	
Total energy = -1077.16532			6	.085011	-.017332	1.557190	1	-1.517848	0.000000	-2.552669	
6	-4.670139	.065574	-3.394469	6	1.239223	-.034543	2.023157	1	2.725641	0.000000	0.107209
6	-4.727235	.030526	-1.996208	6	1.138355	.092804	-1.515170	1	2.808890	0.000000	-2.393640
6	-3.544658	.025340	-1.263954	6	2.229898	-.784915	-1.332370	6	-1.856478	0.000000	0.247786
6	-2.271652	.063851	-1.950766	6	3.367245	-.673318	-2.125254	6	-1.722151	0.000000	1.592045
6	-2.240007	.091271	-3.344233	6	3.451580	.320041	-3.104903	1	-2.833684	0.000000	-0.224595
6	-3.441810	.090646	-4.060129	6	2.387112	1.208062	-3.286216	1	-2.580702	0.000000	2.256417
1	-5.592358	.069879	-3.968281	6	1.244439	1.104124	-2.500131	6	-0.424712	0.000000	2.198579
1	-5.687982	.003139	-1.489837	1	2.165039	-1.550336	-.566755	6	0.399009	0.000000	3.116147
1	-1.291719	.104678	-3.871458	1	4.194839	-1.360845	-1.976936	1	1.279773	0.000000	3.717505
1	-3.418284	.109935	-5.145657	1	4.343262	.406051	-3.718684				
6	-3.305095	-.034431	.199886	1	2.450560	1.986151	-4.041622	Total energy = -384.44241 (cc-PVDZ)			
6	-3.994182	-.112668	1.417610	1	.420951	1.799068	-2.631139	6	-.598040	0.000000	-1.979024
6	-3.239577	-.180470	2.608759	6	2.583220	-.130505	2.436610	6	-.645710	0.000000	-0.556640
6	-1.827659	-.180811	2.652301	6	3.371874	1.030874	2.621338	6	.563795	0.000000	.131921
6	-1.141265	-.101956	1.437533	6	4.691607	.924828	3.043112	6	1.802628	0.000000	-.462541
6	-1.927197	-.026302	.311415	6	5.257860	-.329804	3.290529	6	1.852462	0.000000	-1.887065
1	-5.079053	-.126280	1.474296	6	4.490041	-1.485349	3.113234	6	.650445	0.000000	-2.561894
1	-3.777987	-.241676	3.550429	6	3.168644	-1.394881	2.693035	1	-1.525410	0.000000	-2.558558
1	-1.316579	-.244499	3.608462	1	2.930642	2.002466	2.425789	1	2.733656	0.000000	.110446
6	-1.210267	.041403	-.929304	1	5.284720	1.824361	3.179295	1	2.818338	0.000000	-2.398287
6	.132609	.010129	-.629540	1	6.289548	-.406637	3.620025	6	-.1860861	0.000000	.247565
6	.259414	-.075069	.891660	1	4.925640	-2.461468	3.305917	6	-1.724290	0.000000	1.594314
6	1.372468	-.076924	1.593512	1	2.568682	-2.289206	2.559827	1	-2.844450	0.000000	-2.25991
6	1.280403	.084084	-1.539707					6	-2.586304	0.000000	2.264668
6	2.461719	-.643031	-1.304595					6	-.423913	0.000000	2.199479
6	3.535036	-.564585	-2.189841					6	.403861	0.000000	3.119069
6	3.456016	.242304	-3.326126					1	1.281909	0.000000	3.736616
6	2.292246	.974963	-3.569992								
6	1.218358	.898430	-2.686790					33 (5-exo P)			
1	2.527253	-.1288519	-.435875					Total energy = -384.48827 (6-31G**)			
1	4.434590	-1.140910	-1.993622					6	-.854883	0.000000	-1.876803
1	4.294397	.302155	-4.013806					6	-.828590	0.000000	-0.476071

6 0.407433 0.000000 0.217555
 6 1.621684 0.000000 -0.459359
 6 1.612674 0.000000 -1.867377
 6 0.381955 0.000000 -2.491503
 1 -1.787599 0.000000 -2.434057
 1 2.562021 0.000000 0.085527
 1 2.542528 0.000000 -2.428213
 6 -1.909045 0.000000 0.516385
 6 -1.381211 0.000000 1.762337
 1 -2.965215 0.000000 0.272393
 1 -1.921583 0.000000 2.700034
 6 0.100568 0.000000 1.670147
 6 0.958140 0.000000 2.678772
 1 0.917503 0.000000 3.759815

 Total energy = -384.50362 (cc-PVDZ)
 6 -0.857038 0.000000 -1.879891
 6 -0.829628 0.000000 -0.476704
 6 0.408360 0.000000 0.217548
 6 1.624337 0.000000 -0.460732
 6 1.615649 0.000000 -1.871277
 6 0.382338 0.000000 -2.496112
 1 -1.796008 0.000000 -2.438690
 1 2.570240 0.000000 0.086666
 1 2.551252 0.000000 -2.434808
 6 -1.911865 0.000000 0.516746
 6 -1.382427 0.000000 1.765440
 1 -2.974547 0.000000 0.272360
 1 -1.925692 0.000000 2.708891
 6 0.101440 0.000000 1.671548
 6 0.958216 0.000000 2.685351
 1 0.918452 0.000000 3.774078

33 (6-endo TS)

Total energy = -384.39871 (6-31G**)
 6 -0.577452 0.000000 -1.859550
 6 -0.544988 0.000000 -0.379613
 6 0.705228 0.000000 0.173464
 6 1.869638 0.000000 -0.499611
 6 1.780767 0.000000 -1.967308
 6 0.568916 0.000000 -2.585166
 1 -1.580990 0.000000 -2.277693
 1 2.865365 0.000000 -0.073932
 1 2.745328 0.000000 -2.467640
 6 -1.794974 0.000000 0.346328
 6 -1.873966 0.000000 1.708142
 1 -2.715371 0.000000 -0.230002
 1 -2.839915 0.000000 2.201399
 6 -0.678070 0.000000 2.454150
 6 0.542584 0.000000 2.589068
 1 1.539494 0.000000 2.968435

 Total energy = -384.44009 (cc-PVDZ)
 6 -0.607377 0.000000 -1.838354
 6 -0.553108 0.000000 -.403338
 6 0.723532 0.000000 1.68277
 6 1.898938 0.000000 -.551381
 6 1.831029 0.000000 -1.971045
 6 .573002 0.000000 -2.536778
 1 -1.583926 0.000000 -2.330845
 1 2.879031 0.000000 -.066468
 1 2.750707 0.000000 -2.561184
 6 -1.800660 0.000000 .352453
 6 -1.891914 0.000000 1.710461
 1 -2.725810 0.000000 -.230825
 1 -2.867127 0.000000 2.201572
 6 -.698954 0.000000 2.476433
 6 .527443 0.000000 2.596960
 1 1.535544 0.000000 2.965622

33 (6-endo P)

Total energy = -384.52690 (6-31G**)
 6 -0.602053 0.000000 -1.785413
 6 -0.625649 0.000000 -0.354543
 6 0.625587 0.000000 0.354623
 6 1.847077 0.000000 -0.372867
 6 1.852851 0.000000 -1.756281
 6 0.611025 0.000000 -2.395684
 1 -1.537878 0.000000 -2.338318
 1 2.785122 0.000000 0.177044
 1 2.785688 0.000000 -2.311961
 6 -1.847195 0.000000 0.372830
 6 -1.852869 0.000000 1.756258
 1 -2.785205 0.000000 -0.177098
 1 -2.785482 0.000000 2.312287
 6 -0.610939 0.000000 2.395667
 6 0.602123 0.000000 1.785393
 1 1.537998 0.000000 2.338149

Total energy = -384.54166 (cc-PVDZ)

6 -0.603476 0.000000 -1.787738
 6 -.626189 0.000000 -.354594
 6 .626188 0.000000 .354598
 6 1.849842 0.000000 -.373515
 6 1.856363 0.000000 -1.759343
 6 .612002 0.000000 -.2399592
 1 -1.545023 0.000000 -2.343417
 1 2.793495 0.000000 .179171
 1 2.795002 0.000000 -2.318050
 6 -1.849849 0.000000 .373511
 6 -1.856364 0.000000 1.759334
 1 -2.793498 0.000000 -.179179
 1 -2.794977 0.000000 2.318087
 6 -.612002 0.000000 2.399590
 6 .603480 0.000000 1.787743
 1 1.545030 0.000000 2.343415

34-R

Total energy = -423.75757 (6-31G**)

6 -.856440 0.000000 -1.633686
 6 -.780474 0.000000 -.193440
 6 .497504 0.000000 .405376
 6 1.637312 0.000000 -.329959
 6 1.588112 0.000000 -1.790610
 6 .272929 0.000000 -2.398111
 1 -1.836126 0.000000 -2.108444
 1 2.626065 0.000000 .130731
 1 .205334 0.000000 -3.482500
 6 -1.994364 0.000000 .573146
 6 -2.094581 0.000000 1.935658
 1 -2.927563 0.000000 .013857
 1 -3.094053 0.000000 2.367268
 6 -1.038361 0.000000 2.870576

6 -.267023 0.000000 3.811717
 1 .480422 0.000000 4.570586
 6 2.726785 0.000000 -2.546490
 1 3.709002 0.000000 -2.085036
 1 2.688520 0.000000 -3.631520

Total energy = -423.77221 (cc-PVDZ)

6 -1.918866 0.000201 -1.475342
 6 -1.840832 0.000704 -.111346
 6 -.564118 0.000443 .563466
 6 .609181 -.000343 -.226806
 6 .558412 -.000848 -1.586440
 6 -.721618 -.000594 -2.293123
 1 -2.890751 .000400 -1.975009
 1 -2.756331 .001322 .489482
 1 1.466491 -.001487 -2.202340
 6 -.787254 -.001118 -3.661359
 1 .120187 -.001772 -4.268903

1 -1.746587 -.000981 -4.184205
 6 -.534612 .001021 2.001505
 6 .577914 .000895 2.798643
 1 -1.502539 .001615 2.511943
 1 .422001 .001364 3.882857
 6 1.931040 .000155 2.391147
 6 3.140737 -.000430 2.224943
 1 4.187630 -.000973 1.994442

34 (5-exo TS)

Total energy = -423.78775 (6-31G**)

6 -.889977 .000024 -1.684397
 6 -.976020 -.002691 -.269149
 6 .236255 .003793 .437033
 6 1.473141 .011903 -.122568
 6 1.572414 .014447 -1.565202
 6 .341593 .008333 -2.307106
 1 -1.801602 -.004663 -2.277820
 1 2.383626 .016691 .472171
 1 .397733 .010224 -.3392005
 6 -2.180787 -.011855 .518864
 6 -2.059914 -.014636 1.872708
 1 -3.156433 -.015990 .042490
 1 -2.926492 -.021769 2.526189
 6 -.772150 -.012047 2.494648
 6 .043039 -.022046 3.420394
 1 .917503 -.025275 4.030573
 6 2.807772 .022785 -2.206797
 1 3.734185 .027892 -1.642985
 1 2.879284 .024828 -3.289183

Total energy = -423.77030 (cc-PVDZ)

6 -.874193 .000068 -1.694174
 6 -.908856 -.010630 -.257271
 6 .318508 .001177 .443447
 6 1.522270 .022326 -.179756
 6 1.586870 .033473 -.1642847
 6 .322402 .021238 -.2356841
 1 -1.815424 -.009052 -2.253116
 1 2.471326 .031539 .369394
 1 .347811 .029294 -.3449277
 6 -.2114532 -.032569 .509472
 6 -.2054718 -.041659 1.879092
 1 -.3085370 -.042032 .008235
 1 -2.974891 -.058318 2.469293
 6 -.840412 -.030367 2.613047
 6 -.110653 -.027510 3.612035
 1 .710251 -.020345 4.303088
 6 2.784508 .054703 -2.307196
 1 3.731065 .064107 -1.763058
 1 2.828067 .063306 -3.398611

34 (5-exo P)

Total energy = -423.84753 (6-31G**)

6 -1.064636 .002724 -1.613734
 6 -1.112195 -.004220 -.213178
 6 .100187 -.002091 .537528
 6 1.327193 .006697 -.081741
 6 1.400561 .013876 -1.515228
 6 .167409 .011602 -2.247643
 1 -1.980744 .001266 -2.198085
 1 2.246149 .008240 .497742
 1 .215979 .017091 -.3332954
 6 -2.224685 -.013828 .723018
 6 -1.756637 -.018031 1.997933
 1 -3.269835 -.017220 .434505
 1 -2.342239 -.025209 2.907766
 6 -.272348 -.011032 1.977645
 6 .539360 -.011925 3.022772
 1 .453563 -.017997 4.101008

6	-0.150232	-0.000098	0.528346	6	-1.312844	-0.000154	2.569709	6	2.329319	0.000000	-3.669857
6	-0.125196	-0.001040	-0.843036	1	-4.665377	-0.000261	0.586914	6	3.588784	0.000000	-3.061547
6	-1.393949	-0.003849	-1.507720	1	-4.688992	-0.000460	3.069073	6	3.667339	0.000000	-1.672983
1	-1.438827	-0.004875	-2.598962	1	-2.529696	-0.000344	4.333413	6	2.502370	0.000000	-0.884377
6	-3.757952	-0.005871	1.413806	1	-0.384515	-0.000080	3.138267	1	0.212441	0.000000	-3.414627
6	-3.712528	-0.004775	2.793022	6	1.277626	0.000234	-1.547626	1	2.245717	0.000000	-4.758858
6	-2.466122	-0.002089	3.470802	6	1.762497	0.000172	-2.857429	1	4.498303	0.000000	-3.665297
6	-1.284388	-0.000515	2.760651	6	3.147886	-0.000065	-3.061922	1	4.635702	0.000000	-1.169638
1	-4.718996	-0.007939	0.892428	6	4.033136	-0.000257	-1.975001	6	2.585656	0.000000	0.537352
1	-4.640082	-0.005990	3.369948	6	3.549844	-0.000224	-0.660030	6	2.141227	0.000000	1.682733
1	-2.446946	0.001261	4.562972	6	2.171922	0.000033	-0.455283	1	2.016552	0.000000	2.748065
1	-0.321520	0.001561	3.273693	1	1.079596	0.000252	-3.709950	1	-3.462987	0.000000	-1.120198
6	1.186893	0.000874	-1.511763	1	3.543324	-0.000118	-4.080159				
6	1.368104	-0.000353	-2.902998	1	5.110366	-0.000394	-2.155257				
6	2.647763	0.001498	-3.459669	1	4.236839	-0.000263	0.188759				
6	3.776214	0.004599	-2.632049	6	1.383617	0.000483	0.811454				
6	3.618434	0.005909	-1.246694	6	1.932736	0.000430	2.018681				
6	2.333361	0.004113	-0.676276	1	1.682898	0.000334	3.075013				
1	0.499284	-0.002705	-3.562863	1	-3.458375	0.000017	-1.524896				
1	2.764943	0.000508	-4.545521								
1	4.778339	0.005993	-3.065492								
1	4.488018	0.008358	-0.587739								
6	2.192949	0.005590	0.758838								
6	2.514290	0.008066	1.946849								
1	2.618486	0.009639	3.014573								
1	-3.525041	-0.007637	-1.301880								
35 (5-exo P)											
Total energy = -692.48678 (6-31G**)											
6	-2.554474	.000134	-8.783777								
6	-2.487867	.000265	.543850								
6	-1.207932	.000208	1.199853								
6	-0.049643	.000009	.375756								
6	-1.155190	-0.000117	-1.017922								
6	-1.416118	-0.000051	-1.652069								
1	-1.486858	-0.000130	-2.735847								
6	-3.664842	0.000447	1.337892								
6	-3.594224	0.000562	2.712720								
6	-2.334151	0.000489	3.356649								
6	-1.171103	0.000311	2.618885								
1	-4.629771	0.000491	.837310								
1	-4.503562	0.000698	3.306315								
1	-2.285840	0.000573	4.441716								
1	-.205094	0.00253	3.115318								
6	1.191309	-0.000250	-1.603305								
6	1.620982	-0.000351	-2.929012								
6	2.994329	-0.000432	-3.192972								
6	3.923807	-0.000406	-2.148019								
6	3.497450	-0.000297	-8.15199								
6	2.133160	-0.000227	-.550447								
1	.906124	-0.000358	-3.747005								
1	3.343124	-0.000513	-4.221487								
1	4.986281	-0.000482	-2.372262								
1	4.223183	-0.000303	-.006860								
6	1.388787	-0.000184	.746513								
6	1.929488	-0.000148	1.953958								
1	2.923876	-0.000181	2.379366								
1	-3.534084	0.000189	-1.349093								
Total energy = -692.50863 (cc-PVDZ)											
6	-2.498688	0.000057	-1.002154								
6	-2.504054	-0.000113	0.423061								
6	-1.257918	-0.000118	1.147777								
6	-0.052382	0.000088	0.385617								
6	-0.091977	0.000275	-1.016300								
6	-1.320307	0.000239	-1.715703								
1	-1.332308	0.000297	-2.807627								
6	-3.727475	-0.000254	1.148357								
6	-3.741074	-0.000362	2.526779								
6	-2.518173	-0.000294	3.241089								
35 (6-endo P)											
Total energy = -692.51195 (6-31G**)											
6	-2.459972	.000000	-.515643								
6	-2.392830	.000000	.909058								
6	-1.113592	.000000	1.543679								
6	.083463	.000000	.723346								
6	-.022748	0.000000	-.692203								
6	-1.328893	0.000000	-1.277417								
1	-1.430923	0.000000	-2.355856								
6	-3.569303	0.000000	1.697488								
6	-3.501651	0.000000	3.074094								
6	-2.242718	0.000000	3.708311								
6	-1.081523	0.000000	2.961348								
1	-4.531973	0.000000	1.192895								
1	-4.410360	0.000000	3.668489								
1	-2.183709	0.000000	4.792672								
1	-1.31972	0.000000	3.483669								
6	1.171484	0.000000	-1.523763								
6	1.140094	0.000000	-2.940805								
6	2.300888	0.000000	-3.689962								
6	3.563601	0.000000	-3.063942								
6	3.642365	0.000000	-1.687662								
6	2.465350	0.000000	-.901615								
1	.190120	0.000000	-3.462487								
1	2.237243	0.000000	-4.774082								
1	4.468049	0.000000	-3.664566								
1	4.602805	0.000000	-1.182132								
6	2.468385	0.000000	.506061								
6	1.396722	0.000000	1.318777								
1	1.513496	0.000000	2.396404								
1	-3.437515	0.000000	-.989913								
Total energy = -692.53620 (cc-PVDZ)											
6	-2.436237	0.000000	-.632758								
6	-2.437048	0.000000	0.795805								
6	-1.187570	0.000000	1.490745								
6	0.048565	0.000000	0.727207								
6	0.010857	0.000000	-.693184								
6	-1.267783	0.000000	-1.341162								
1	-1.317814	0.000000	-2.429234								
6	-3.650966	0.000000	1.529947								
6	-3.647772	0.000000	2.910700								
6	-2.417926	0.000000	3.604245								
6	-1.221261	0.000000	2.910640								
1	-4.594543	0.000000	0.978196								
1	-4.588682	0.000000	3.465257								
1	-2.409306	0.000000	4.696411								
1	-0.291439	0.000000	3.478921								
6	1.244722	0.000000	-1.467841								
6	1.278991	0.000000	-2.887079								
6	2.475204	0.000000	-3.583160								
6	3.709313	0.000000	-2.897853								
6	3.723818	0.000000	-1.516896								
6	2.509614	0.000000	-0.785286								
1	0.348436	0.000000	-3.454299								
1											

1 4.664894 0.000000 -0.963896
 6 2.444945 0.000000 0.623782
 6 1.333454 0.000000 1.386349
 1 1.398322 0.000000 2.474475
 1 -3.395077 0.000000 -1.156906

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Total energy = -691.73611 (6-31G**)
 6 1.578873 -2.011043 0.447516
 6 2.510316 -1.004811 0.165286
 6 1.942090 0.292086 -0.201053
 6 0.549529 0.377620 -0.239245
 6 -0.347758 -0.612771 0.026159
 6 0.234268 -1.896365 0.406479
 1 -0.426376 -2.712712 0.681474
 6 3.920588 -1.141006 0.212577
 6 4.742504 -0.074512 -0.080698
 6 4.195050 1.180691 -0.436339
 6 2.830932 1.359883 -0.496334
 1 4.338615 -2.104349 0.486498
 1 5.820655 -0.196806 -0.039893
 1 4.858856 2.009091 -0.664920
 1 2.407084 2.320307 -0.771052
 6 -1.814066 -0.433419 -0.047284
 6 -2.658620 -1.526114 -0.297486
 6 -4.041807 -1.383788 -0.362656
 6 -4.623569 -0.128442 -0.179845
 6 -3.810852 0.974015 0.058415
 6 -2.411071 0.845566 0.126239
 1 -2.221160 -2.503180 -0.472476
 1 -4.662611 -2.251459 -0.564577
 1 -5.701248 -0.007574 -0.228788
 1 -4.246478 1.957553 0.199378
 6 -1.643157 2.024140 0.380778
 6 -1.087137 3.076050 0.611477
 1 -0.564017 3.982452 0.810429

Total energy = -691.76302 (cc-PVDZ)

6 -2.549981 -.113486 -.485057
 6 -2.551909 -.115579 .917537
 6 -1.230140 -.119193 1.546359
 6 -.126473 -.128404 .687416
 6 -.135964 -.137886 -.677725
 6 -1.463256 -.121307 -1.290517
 1 -1.543857 -.080266 -2.378682
 6 -3.702927 -.109374 1.748670
 6 -3.581680 -.107496 3.123733
 6 -2.303350 -.112496 3.734867
 6 -1.157208 -.119378 2.967065
 1 -4.686211 -.105179 1.274981
 1 -4.477949 -.103195 3.747770
 1 -2.226749 -.112257 4.824343
 1 -.170630 -.126360 3.433559
 6 1.088363 -.158709 -1.510713
 6 1.062917 -.695870 -2.809883
 6 2.200003 -.723364 -3.616209
 6 3.408292 -.208294 -.3137830
 6 3.465128 .322792 -.1851887
 6 2.324177 .355311 -1.024871
 1 .135589 -.1127073 -.3189391
 1 2.142494 -1.155692 -4.617395
 1 4.304240 -.224576 -.3761545
 1 4.400319 .727454 -1.461903
 6 2.460230 .925426 .281961
 6 2.675785 1.438117 1.363922
 1 2.830717 1.882277 2.327232

36 (5-exo TS)

Total energy = -691.73410 (6-31G**)
 6 -2.528907 -.001062 -.832937

6 -2.621760 -.001304 .565429
 6 -1.350388 -.000923 1.287815
 6 -.189222 -.000353 .510757
 6 -.130129 -.000102 -.852841
 6 -.1392491 -.000499 -1.565984
 1 -1.403773 -.000315 -2.651805
 6 -3.828733 -.001905 1.309698
 6 -3.808172 -.002102 2.687422
 6 -2.579102 -.001710 3.388844
 6 -1.382655 -.001140 2.707567
 1 -4.769998 -.002200 .769318
 1 -4.741824 -.002555 3.241801
 1 -2.582560 -.001871 4.474813
 1 -.437971 -.000845 3.241568
 6 1.192701 .000675 -1.493967
 6 1.408913 .000766 -2.877111
 6 2.701038 .001539 -3.398428
 6 3.805487 .002230 -2.542999
 6 3.612636 .002112 -1.164278
 6 2.315546 .001328 -.628825
 1 .562841 .000205 -.3556446
 1 2.846161 .001589 -4.474555
 1 4.812616 .002836 -2.948089
 1 4.460149 .002625 -.487048
 6 2.134423 .001182 .799604
 6 2.432300 .001189 1.989772
 1 2.505456 .001008 3.053217

Total energy = -691.76087 (cc-PVDZ)

6 -2.580817 -.010421 -.664111
 6 -2.580629 -.008354 .740172
 6 -1.262662 -.002596 1.376460
 6 -.153103 .000134 .522017
 6 -.185401 -.002051 -.845191
 6 -1.494094 -.007690 -1.473437
 1 -.1577772 -.009489 -2.562318
 6 -3.737435 -.011314 1.564097
 6 -3.625716 -.008805 2.939865
 6 -2.350723 -.003243 3.558682
 6 -1.200506 -.000243 2.797490
 1 -4.717627 -.015628 1.083915
 1 -4.525836 -.011135 3.558347
 1 -2.280920 -.001332 4.648694
 1 -.216820 .003975 3.269941
 6 1.092859 .001699 -1.573652
 6 1.217165 .000157 -2.970466
 6 2.474261 .004077 -3.576635
 6 3.634251 .009641 -2.793882
 6 3.532336 .011163 -1.403005
 6 2.271139 .007168 -.782660
 1 .322885 -.004269 -.3595465
 1 2.548823 .002775 -4.666153
 1 4.618308 .012772 -3.266821
 1 4.427706 .015462 -.779681
 6 2.179476 .008601 .656716
 6 2.553009 .011109 1.830300
 1 2.700800 .012679 2.892978

36 (5-exo P)

Total energy = -691.79776 (6-31G**)
 6 0.158185 0.000970 0.065390
 6 0.059533 0.000277 1.466419
 6 1.304216 -.0000412 2.203142
 6 2.515198 -.000288 1.455053
 6 2.512785 0.000520 0.055654
 6 1.295755 0.001108 -.677674
 1 1.289872 0.001680 -1.763831
 6 -1.171017 0.000200 2.173866
 6 -1.186795 -.000517 3.550524
 6 0.028375 -.001182 4.275810

6 1.240171 -.0001130 3.620322

6 -2.095914 0.000716 1.605785

6 -2.132343 -.0000570 4.084239

6 0.003586 -.0001740 5.361612

6 2.170632 -.0001642 4.181474

6 3.897406 0.000040 -.431596

6 4.421428 0.000223 -.1722678

6 5.810304 -.0000443 -.1886006

6 6.660911 -.001315 -.775951

6 6.139115 -.001535 0.522574

6 4.759319 -.0000849 0.688065

1 3.767742 0.000868 -.2590307

1 6.233000 -.0000295 -.2886340

1 7.736852 -.0001813 -.922288

1 6.804423 -.0002181 1.381235

6 3.922711 -.0000755 1.927174

6 4.375594 -.001478 3.170755

1 5.336670 -.002067 3.66595

Total energy = -691.82171 (cc-PVDZ)

6 -2.520234 .000129 -.867903

6 -2.525638 .000252 .538569

6 -1.233318 .000205 1.195811

6 -.067873 .000035 .370685

6 -.167782 -.000098 -.1029698

6 -1.431891 -.000044 -.1683754

1 -.1505436 -.000127 -.2773452

6 -3.715043 .000420 1.316895

6 -3.654581 .000526 2.694310

6 -2.396913 .000462 3.345217

6 -1.223895 .000305 2.617721

1 -4.675078 .000460 .797465

1 -4.572930 .000652 3.284995

1 -2.354417 .000537 4.436730

1 -2.69150 .000248 3.141481

6 1.175586 -.000233 -.1622850

6 1.600523 -.000361 -.2953078

6 2.975337 -.000486 -.3219083

6 3.907813 -.000475 -.2172405

6 3.484119 -.000344 -.836988

6 2.116875 -.000225 -.570283

1 .880022 -.000372 -.3774058

1 3.325023 -.000591 -.4253842

1 4.975915 -.000571 -.2400464

1 4.208684 -.000336 -.020121

6 1.385576 -.000072 .730075

6 1.990633 -.000006 1.910673

1 1.791602 .000151 2.977768

36 (6-endo TS)

Total energy = -691.704587 (6-31G**)

6 0.047778 0.000000 0.004263

6 -.030761 0.000000 1.388055

6 1.276253 0.000000 2.183724

6 2.414612 0.000000 1.420705

6 2.542331 0.000000 0.086166

6 1.209551 0.000000 -.646727

1 1.303942 0.000000 -.1726664

6 -1.222818 0.000000 2.151904

6 -1.236509 0.000000 3.531439

6 -0.029720 0.000000 4.255706

6 1.179976 0.000000 3.595715

1 -2.153320 0.000000 1.595898

1 -2.184748 0.000000 4.060224

1 -0.047495 0.000000 5.341308

1 2.102553 0.000000 4.166025

6 3.802230 0.000000 -.672313

6 3.857174 0.000000 -.2074642

6 5.063836 0.000000 -.2767705

6 6.277825 0.000000 -.2078818

6 6.269678 0.000000 -0.689784
 6 5.060237 0.000000 0.022821
 1 2.938087 0.000000 -2.648301
 1 5.052620 0.000000 -3.853318
 1 7.219228 0.000000 -2.618548
 1 7.200183 0.000000 -0.132444
 6 5.032929 0.000000 1.437232
 6 4.527676 0.000000 2.552519
 1 4.349690 0.000000 3.604132

Total energy = -691.75408 (cc-PVDZ)
 6 -2.493476 .000000 -.580414
 6 -2.551865 .000000 .820639
 6 -1.256176 .000000 1.495831
 6 -.101255 .000000 .694133
 6 -.065280 .000000 -.681804
 6 -.1374325 .000000 -1.336165
 1 -.1435603 .000000 -2.424696
 6 -.3738969 .000000 1.598514
 6 -.3680049 .000000 2.977619
 6 -.2428661 .000000 3.640100
 6 -.1252262 .000000 2.918842
 1 -.4699466 .000000 1.080139
 1 -.4602135 .000000 3.562820
 1 -.2395431 .000000 4.731758
 1 -.292964 .000000 3.438378
 6 1.176022 .000000 -1.498676
 6 1.135929 .000000 -2.906864
 6 2.293434 .000000 -3.683059
 6 3.553869 .000000 -3.077069
 6 3.636133 .000000 -1.688599
 6 2.473912 .000000 -.896101
 1 .176843 .000000 -3.422840
 1 2.207385 .000000 -.4717165
 1 4.462075 .000000 -3.682708
 1 4.605988 .000000 -1.188370
 6 2.559210 .000000 .524548
 6 2.111473 .000000 1.668980
 1 1.987322 .000000 2.734559

36 (6-endo P)

Total energy = -691.82293 (6-31G**)
 6 0.151967 0.000000 0.072635
 6 0.051136 0.000000 1.476174
 6 1.295737 0.000000 2.193372
 6 2.546398 0.000000 1.453070
 6 2.548754 0.000000 0.031888
 6 1.282027 0.000000 -0.657250
 1 1.245910 0.000000 -1.740634
 6 -.179666 0.000000 2.175383
 6 -.201060 0.000000 3.553737
 6 0.012194 0.000000 4.271183
 6 1.224358 0.000000 3.608785
 1 -.2100879 0.000000 1.601607
 1 -.2147045 0.000000 4.086519
 1 -.003899 0.000000 5.356968
 1 2.134431 0.000000 4.197551
 6 3.799058 0.000000 -0.708550
 6 3.870151 0.000000 -2.123835
 6 5.082205 0.000000 -2.786542
 6 6.295538 0.000000 -2.069365
 6 6.274482 0.000000 -0.690958
 6 5.044015 0.000000 0.008612
 1 2.959896 0.000000 -2.712376
 1 5.097907 0.000000 -3.872329
 1 7.241491 0.000000 -2.602195
 1 7.195924 0.000000 -0.117520
 6 4.943120 0.000000 1.412051
 6 3.813235 0.000000 2.142188
 1 3.849102 0.000000 3.225511

Total energy = -691.84935 (cc-PVDZ)
 6 -2.440409 .000000 -.498216
 6 -2.441765 .000000 .911744
 6 -.1.147197 .000000 1.538134
 6 .048720 .000000 .709515
 6 -.048666 .000000 -.709469
 6 -.1.362891 .000000 -1.308476
 1 -.1.475637 .000000 -2.392729
 6 -.3.620654 .000000 1.699255
 6 -.3.542492 .000000 3.078036
 6 -.2.278643 .000000 3.707202
 6 -.1.115760 .000000 2.957250
 1 -.4.586312 .000000 1.190463
 1 -.4.452919 .000000 3.681035
 1 -.2.215497 .000000 4.797522
 1 -.159442 .000000 3.480256
 6 1.147200 .000000 -1.538112
 6 1.115708 .000000 -2.957195
 6 2.278568 .000000 -3.707212
 6 3.542424 .000000 -3.078101
 6 3.620645 .000000 -1.699306
 6 2.441821 .000000 -.911737
 1 .159357 .000000 -3.480158
 1 2.215337 .000000 -4.797526
 1 4.452852 .000000 -3.681098
 1 4.586344 .000000 -.1.190589
 6 2.440456 .000000 .498202
 6 1.362969 .000000 1.308500
 1 1.475714 .000000 2.392743

6 -.1.443430 -.0000040 1.475260
 1 -.1.630053 -.0000080 2.551562
 6 -.3.054375 -.000144 -.761131
 6 -.4.198102 -.000168 -.0.284416
 1 -.5.156235 -.000184 0.199027
 50 1.566983 0.000126 1.620276
 1 2.492351 -.1.399676 1.216869
 1 2.492407 1.399809 1.216590
 1 1.244312 0.000303 3.309966

Total energy = -389.45677 (B3PW91)
 6 -.1.865859 -.000203 -.2.903201
 6 -.1.797298 -.000130 -.1.491110
 6 -.0.522677 -.000048 -.0.844426
 6 0.628397 -.000040 -.1.660188
 6 0.550232 -.0000112 -.3.058608
 6 -.0.705918 -.000195 -.3.686291
 1 -.2.844106 -.000266 -.3.375126
 1 1.613388 0.000026 -.1.196954
 1 1.460013 -.0000104 -.3.652285
 1 -.0.779547 -.0000252 -.4.770009
 6 -.0.396432 0.000028 0.633759
 6 -.1.431930 0.000060 1.470728
 1 -.1.608248 0.000107 2.540997
 6 -.3.032574 -.000143 -.0.764285
 6 -.4.150010 -.000162 -.2.61404
 1 -.5.102090 -.000175 0.219502
 50 1.548702 0.000118 1.599381
 1 2.466277 -.1.396947 1.182895
 1 2.466146 1.397255 1.182846
 1 1.237452 0.000132 3.289276

Computed Geometries at the DFT/LANL2DZ Level**11 (R = SnH₃)**

Total energy = -389.59568 (B3LYP)
 6 -.1.871029 -.000170 -.2.910960
 6 -.1.802751 -.000120 -.1.495225
 6 -.0.524491 -.000023 -.0.846081
 6 0.628541 0.000010 -.1.665500
 6 0.549860 -.000033 -.3.067016
 6 -.0.708961 -.000124 -.3.696318
 1 -.2.849607 -.000241 -.3.383144
 1 1.614491 0.000064 -.1.205261
 1 1.460055 0.000000 -.3.661008
 1 -.0.782595 -.000163 -.4.780563
 6 -.0.394310 0.000034 0.637798
 6 -.1.429115 0.000092 1.477477
 1 -.1.603340 0.000120 2.548318
 6 -.3.042678 -.000167 -.0.770147
 6 -.4.161603 -.000214 -.0.268902
 1 -.5.113496 -.0000251 0.211333
 50 1.552752 0.000087 1.604684
 1 2.466691 -.1.392100 1.188589
 1 2.466766 1.392051 1.188024
 1 1.242680 0.000450 3.288774

Total energy = -389.40775 (BLYP)
 6 -.1.892912 -.000217 -.2.929035
 6 -.1.817112 -.000132 -.1.501325
 6 -.0.521869 -.000010 -.0.854542
 6 0.635738 -.000021 -.1.686152
 6 0.547592 -.000106 -.3.098000
 6 -.0.724938 -.000201 -.3.724932
 1 -.2.880866 -.000294 -.3.400264
 1 1.630602 0.000044 -.1.225859
 1 1.460756 -.000101 -.3.702374
 1 -.0.804519 -.000270 -.4.817010
 6 -.0.396908 0.000068 0.637218

11 (R = SnH₃, 5-exo TS)

Total energy = -389.59315 (B3LYP)
 6 -.1.296442 0.015906 -.3.890739
 6 -.1.320115 0.011948 -.2.649269
 6 0.844718 0.002708 -.1.760289
 6 0.472300 0.000069 -.0.477251
 6 -.0.985561 0.003534 -.0.188034
 6 -.1.866958 0.009583 -.1.310167
 1 -.1.086653 0.018505 -.4.937237
 1 1.761864 0.001734 -.2.339434
 6 -.3.265203 0.013125 -.1.108749
 6 -.3.794750 0.010750 0.193361
 6 -.2.927761 0.004798 1.303778
 6 -.1.534732 0.001213 1.109870
 1 -.3.925343 0.017679 -.1.971621

1 -4.871541 0.013484 0.341626
 1 -3.334784 0.002980 2.311776
 1 -0.878972 -0.003421 1.978457
 50 1.983477 -0.009156 1.058251
 1 1.859839 1.379257 2.059308
 1 1.851377 -1.402951 2.050711
 1 3.497400 -0.011271 0.258821

Total energy = -389.40680 (BLYP)

6 -1.334188 0.013570 -3.938026
 6 -1.358097 0.011165 -2.686918
 6 0.892821 0.004574 -1.773198
 6 0.483229 0.000838 -0.493639
 6 -0.984044 0.002632 -0.208096
 6 -1.883330 0.007839 -1.335424
 1 -1.107452 0.016318 -4.988109
 1 1.827239 0.004954 -2.338508
 6 -3.292540 0.010009 -1.117281
 6 -3.816046 0.006885 1.981117
 6 -2.933814 0.001384 1.310438
 6 -1.532328 -0.000689 1.103266
 1 -3.964200 0.014135 -1.981421
 1 -4.899863 0.008600 0.355384
 1 -3.335507 -0.001227 2.329347
 1 -0.865494 -0.004993 1.973507
 50 1.992863 -0.007184 1.077081
 1 1.868965 1.388346 2.083620
 1 1.864876 -1.409373 2.073817
 1 3.518336 -0.006772 0.282887

Total energy = -389.45498 (B3PW91)

6 -1.285734 0.015809 -3.889627
 6 -1.333630 0.012436 -2.652002
 6 0.857928 0.002904 -1.761069
 6 0.471595 -0.000723 -0.484220
 6 -0.980727 0.002857 -0.196651
 6 -1.865382 0.009652 -1.311189
 1 -1.079140 0.018524 -4.936996
 1 1.780157 0.002396 -2.331688
 6 -3.259612 0.013845 -1.102878
 6 -3.781819 0.011266 0.198502
 6 -2.911456 0.004509 1.302071
 6 -1.522988 0.000366 1.100799
 1 -3.923555 0.019132 -1.962312
 1 -4.857413 0.014544 0.351382
 1 -3.312699 0.002371 2.311799
 1 -0.861600 -0.005228 1.965160
 50 1.974793 -0.009105 1.059984
 1 1.848404 1.385336 2.062574
 1 1.839371 -1.406784 2.056924
 1 3.497769 -0.012544 0.265304

Total energy = -389.61955 (BP86)

6 -1.390582 0.000398 -3.917961
 6 -1.437390 -0.000514 -2.671757
 6 0.894439 -0.002942 -1.791827
 6 0.477618 -0.001800 -0.516903
 6 -0.977841 -0.000125 -0.208731
 6 -1.907487 0.000520 -1.306765
 1 -1.186942 -0.000053 -4.974111
 1 1.832209 -0.005021 -2.353794
 6 -3.306714 0.002060 -1.046374
 6 -3.791588 0.002959 0.279916
 6 -2.879516 0.002208 1.363675
 6 -1.488632 0.000703 1.114533
 1 -4.002950 0.002575 -1.892089
 1 -4.871115 0.004191 0.467821
 1 -3.250607 0.002810 2.394764
 1 -0.793603 0.000062 1.964779
 50 1.996708 -0.000503 1.045347

1 1.879832 1.404391 2.052755
 1 1.882954 -1.405730 2.052653
 1 3.520996 0.001112 0.233035

11 (R = SnH₃, 5-exo P)

Total energy = -389.65401 (B3LYP)

6 0.256728 0.008736 -0.465799
 6 0.293307 -0.009077 1.021650
 6 1.653210 0.001903 1.451238
 6 2.510185 0.027202 0.233358
 6 3.846777 0.044108 0.163894
 6 1.554290 0.029904 -0.919845
 1 4.628331 0.062751 -0.587205
 1 1.883582 0.046529 -1.952633
 6 -0.742576 -0.033139 1.968065
 6 -0.411441 -0.046097 3.341209
 6 0.935749 -0.035113 3.759224
 6 1.982924 -0.010899 2.810859
 1 -1.786801 -0.041907 1.661494
 1 -1.203296 -0.064771 4.086356
 1 1.168664 -0.045401 4.821276
 1 3.021048 -0.002427 3.133281
 50 -1.463958 0.003470 -1.704002
 1 -2.440900 1.376598 -1.389162
 1 -0.938643 0.028722 -3.334571
 1 -2.408984 -1.398791 -1.421855

Total energy = -389.46102 (BLYP)

6 0.256974 0.008813 -0.469021
 6 0.293097 -0.009127 1.026708
 6 1.665486 0.001940 1.460243
 6 2.528937 0.027381 0.233869
 6 3.875160 0.044369 0.163373
 6 1.566512 0.030144 -0.928535
 1 4.665211 0.063100 -0.589825
 1 1.900005 0.046902 -1.967919
 6 -0.749904 -0.033356 1.982298
 6 -0.415245 -0.046390 3.366003
 6 0.942666 -0.035332 3.786669
 6 1.997837 -0.010953 2.830540
 1 -1.802044 -0.042164 1.674180
 1 -1.212705 -0.065175 4.117171
 1 1.177867 -0.045686 4.856628
 1 3.043812 -0.002428 3.154695
 50 -1.474222 0.003480 -1.715376
 1 -2.457217 1.382243 -1.401105
 1 -0.948245 0.029182 -3.353538
 1 -2.424720 -1.404928 -1.434364

Total energy = -389.52145 (B3PW91)

6 0.258342 0.008727 -0.462415
 6 0.293465 -0.009001 1.020084
 6 1.650340 0.001898 1.448371
 6 2.503883 0.026925 0.233723
 6 3.840228 0.043649 0.166644
 6 1.553949 0.029702 -0.916026
 1 4.618243 0.062147 -0.587890
 1 1.881728 0.046247 -1.949000
 6 -0.740356 -0.032854 1.964113
 6 -0.409923 -0.045690 3.333863
 6 0.934131 -0.034810 3.750990
 6 1.979025 -0.010802 2.805303
 1 -1.783961 -0.041509 1.656878
 1 -1.201526 -0.064222 4.078526
 1 1.167074 -0.045034 4.812501
 1 3.016694 -0.002408 3.127912
 50 -1.461758 0.003439 -1.701288
 1 -2.443000 1.380227 -1.384738
 1 -0.936779 0.030543 -3.337721
 1 -2.409080 -1.404401 -1.419952

Total energy = -389.67991 (BP86)

6 0.270053 -0.000007 -0.459774
 6 0.268179 -0.000005 1.030082
 6 1.626368 -0.000054 1.495805
 6 2.515574 -0.000066 0.294332
 6 3.862691 -0.000100 0.261309
 6 1.588633 -0.000103 -0.887834
 1 4.672257 -0.000138 -0.472949
 1 1.946120 -0.000152 -1.920463
 6 -0.796200 0.000034 1.957047
 6 -0.496183 0.000027 3.345145
 6 0.847930 -0.000022 3.797999
 6 1.924326 -0.000064 2.870714
 1 -1.841014 0.000075 1.621259
 1 -1.312454 0.000061 4.077055
 1 1.056705 -0.000024 4.874129
 1 2.963266 -0.000095 3.219966
 50 -1.429547 0.000045 -1.746170
 1 -2.407033 1.399804 -1.470464
 1 -0.861932 0.000349 -3.378089
 1 -2.406791 -1.399965 -1.470885

11 (R = SnH₃, 6-endo TS)

Total energy = -389.58734 (B3LYP)

6 -2.282734 -0.003349 -2.106340
 6 -2.305512 -0.002751 -0.676908
 6 -1.046506 -0.001003 0.021191
 6 0.257568 0.000187 -0.697219
 6 0.403923 0.000118 -2.031937
 6 -1.721231 -0.002984 -3.210363
 1 1.270145 0.000791 -2.690454
 1 -1.465491 -0.003041 -4.247520
 6 -3.523838 -0.003903 0.039787
 6 -3.533614 -0.003328 1.441249
 1 -4.455996 -0.005239 -0.518735
 1 -4.475297 -0.004185 1.983347
 6 -2.309787 -0.001675 2.140652
 6 -1.095944 -0.000579 1.436452
 1 -2.302814 -0.001247 3.227612
 1 -0.169531 0.000608 2.007974
 50 2.131726 0.002378 0.401777
 1 2.294229 1.395242 1.393010
 1 2.294559 -1.386371 1.398734
 1 3.369958 0.000146 -0.782211

Total energy = -389.40119 (BLYP)

6 -2.309121 -0.004172 -2.129565
 6 -2.321747 -0.003620 -0.694570
 6 -1.050793 -0.001824 0.014137
 6 0.261830 -0.000190 -0.705251
 6 0.422346 -0.000290 -2.045684
 6 -1.772820 -0.003429 -3.257496
 1 1.294759 0.000733 -2.708081
 1 -1.539112 -0.003828 -4.306837
 6 -3.550217 -0.004923 0.029418
 6 -3.561948 -0.004524 1.441529
 1 -4.488906 -0.006267 -0.533984
 1 -4.511709 -0.005487 1.985981
 6 -2.330174 -0.002862 2.148371
 6 -1.106096 -0.001560 1.440243
 1 -2.324626 -0.002614 3.243502
 1 -0.172875 -0.000398 2.016296
 50 2.152100 0.003382 0.416085
 1 2.325842 1.404065 1.410729
 1 2.328732 -1.393556 1.415515
 1 3.395316 0.002639 -0.774148

Total energy = -389.44907 (B3PW91)

6 -2.269494 -0.004204 -2.103131

6	-2.298052	-0.003130	-0.677424		6	-1.165678	0.000000	-1.501801		1	2.820808	-0.000182	-1.772329
6	-1.043109	-0.001055	0.018554		6	-2.407255	0.000000	-2.152824		1	2.951326	-0.000432	-4.278727
6	0.254949	-0.000130	-0.698653		1	-4.589997	0.000000	-1.921800		1	.836357	-0.000351	-5.620535
6	0.406503	-0.000984	-2.030900		1	-4.508292	0.000000	0.592570		7	.739926	.000182	-0.289625
6	-1.729820	-0.004342	-3.215314		6	-2.205233	0.000000	2.112606		6	-.134592	.000184	.612552
1	1.273477	-0.000624	-2.688070		6	0.206046	0.000000	0.648636		6	-1.832217	.000267	-1.856479
1	-1.476740	-0.005098	-4.253399		1	-0.249444	0.000000	-2.105308		6	-2.975029	.000458	-1.417437
6	-3.513542	-0.004040	0.037473		1	-2.449650	0.000000	-3.247364		1	-3.956203	.000622	-1.000140
6	-3.522175	-0.002837	1.435946		6	0.206198	0.000000	2.059279		50	-.058132	-0.00029	2.753451
1	-4.445598	-0.005701	-0.520351		6	-1.024574	0.000000	2.828180		1	.913033	1.395192	3.253359
1	-4.463345	-0.003502	1.977928		1	1.149114	0.000000	2.619957		1	.910154	-1.397129	3.253116
6	-2.301024	-0.000638	2.136363		1	-0.989064	0.000000	3.922655		1	1.518191	.001586	3.447091
6	-1.090404	0.000254	1.430139		50	2.113370	0.000000	-0.348859					
1	-2.293574	0.000396	3.220055		1	2.314763	-1.392012	-1.344251	Total energy = -405.481301 (BLYP)				
1	-0.161869	0.001935	1.998952		1	2.314763	1.392012	-1.344251	6	-0.414564	0.404251	-3.917113	
50	2.125138	0.002588	0.405142		1	3.314526	0.000000	0.884492	6	-0.660854	0.140974	-2.5337523	
1	2.287572	1.399346	1.401326	Total energy = -389.55477 (B3PW91)		6	0.453244	-0.309276	-1.714301				
1	2.289540	-1.391897	1.404196	6	-3.588502	0.000000	-1.383756	6	1.755598	-0.472877	-2.302331		
1	3.370655	0.002388	-0.779701	1	-3.549027	0.000000	0.001162	6	1.952686	-0.199578	-3.667672		
Total energy = -389.61432 (BP86)				6	-2.300451	0.000000	0.688826	6	0.869179	0.240217	-4.485274		
6	-2.323707	-0.001446	-2.091069		6	-1.057525	0.000000	-0.057037	1	-1.251646	0.741344	-4.534402	
6	-2.320468	-0.001686	-0.660087		6	-1.150451	0.000000	-1.482135	1	2.579416	-0.815230	-1.672507	
6	-1.043888	-0.001130	0.026938		6	-2.376787	0.000000	-2.129832	1	2.948045	-0.329386	-4.101676	
6	0.250227	-0.000402	-0.710825		1	-4.541645	0.000000	-1.905018	1	1.030093	0.449007	-5.545509	
6	0.395533	-0.000787	-2.051030		1	-4.464978	0.000000	0.585236	7	0.267963	-0.583226	-0.391318	
6	-1.843980	-0.001838	-3.241442		6	-2.182642	0.000000	2.094934	6	0.071904	-0.871547	0.784871	
1	1.258683	-0.000181	-2.727325		6	0.200394	0.000000	0.648945	6	-1.969569	0.315240	-1.977594	
1	-1.631811	-0.001463	-4.296747		1	-0.238431	0.000000	-2.077281	6	-3.099695	0.477613	-1.500276	
6	-3.534923	-0.002251	0.080349		1	-2.415978	0.000000	-3.215769	1	-4.082193	0.610523	-1.089681	
6	-3.523834	-0.002388	1.489612		6	0.204042	0.000000	2.044819	50	0.061047	0.087032	2.753955	
1	-4.482893	-0.002565	-0.469006		6	-1.013391	0.000000	2.805186	1	-1.525655	-0.217779	3.334229	
1	-4.465648	-0.002847	2.048994		6	1.142333	0.000000	2.596622	1	1.196492	-0.836044	3.652922	
6	-2.284059	-0.001915	2.176025		1	-0.983802	0.000000	3.891026	1	0.429799	1.778448	2.901356	
6	-1.074280	-0.001283	1.449727		50	2.090494	0.000000	-0.349041	Total energy = -405.51257 (B3PW91)				
1	-2.261341	-0.002033	3.271560		1	2.284378	-1.390855	-1.344009	6	-0.384778	0.441884	-3.867675	
1	-0.127964	-0.000959	2.008184		1	2.284378	1.390855	-1.344009	6	-0.638137	0.160064	-2.508744	
50	2.149397	0.001865	0.388092		1	3.295105	0.000000	0.878559	6	0.445101	-0.320998	-1.696123	
1	2.338510	1.407719	1.385843	Total energy = -389.71247 (BP86)		6	1.733660	-0.496667	-2.273374				
1	2.340825	-1.401846	1.388434	6	1.944634	-0.204886	-3.619964						
1	3.382076	0.001697	-0.823717	6	0.886533	0.265774	-4.428091						
11 (R = SnH₃, 6-endo P)				1	-1.207017	0.804299	-4.477859						
Total energy = -389.68676 (B3LYP)				1	2.542268	-0.864403	-1.649123						
6	-3.599587	0.000000	-1.386823		1	2.934130	-0.344447	-4.046627					
6	-3.558097	0.000000	0.000977		1	1.056223	0.489946	-5.476599					
6	-2.305860	0.000000	0.688910		7	0.246247	-0.609917	-0.391181					
6	-1.058831	0.000000	-0.060200		6	0.042009	-0.907041	0.769910					
6	-1.155457	0.000000	-1.488725		6	-1.939561	0.350867	-1.953978					
6	-2.385603	0.000000	-2.135788		6	-3.056543	0.515879	-1.479806					
1	-4.553502	0.000000	-1.907672		1	-4.031705	0.656184	-1.071310					
1	-4.473497	0.000000	0.586589		50	0.053553	0.078923	2.721109					
6	-2.187573	0.000000	2.097894		1	-1.531691	-0.177935	3.321438					
6	0.203960	0.000000	0.646463		1	1.185204	-0.831840	3.634078					
1	-0.245861	0.000000	-2.087471		1	0.453721	1.762228	2.795897					
1	-2.426177	0.000000	-3.222186	Total energy = -405.69195 (BP86)									
6	0.204295	0.000000	2.045299	6	-0.658207	0.448041	-3.869319						
6	-1.016208	0.000000	2.808715	6	-0.822372	0.167812	-2.484179						
1	1.141406	0.000000	2.599850	6	0.332351	-0.300319	-1.737402						
1	-0.984058	0.000000	3.894933	6	1.593154	-0.463192	-2.402794						
50	2.096367	0.000000	-0.347315	6	1.710837	-0.172163	-3.771292						
1	2.291297	-1.386005	-1.338573	6	0.585817	0.284455	-4.515077						
1	2.291297	1.386005	-1.338573	1	-1.531087	0.799791	-4.430174						
1	3.294530	0.000000	0.878558	1	2.452697	-0.820628	-1.826148						
Total energy = -389.49230 (BLYP)				1	2.680028	-0.301500	-4.266200						
6	-3.628567	0.000000	-1.397540	1	0.684180	0.507960	-5.582355						
6	-3.586508	0.000000	0.002094	7	0.223429	-0.588406	-0.412939						
6	-2.325823	0.000000	0.696075	6	0.106492	-0.901741	0.767071						
6	-1.064478	0.000000	-0.063669	6	-2.090041	0.344013	-1.843021						
				6	-3.185932	0.494652	-1.288266						
				1	-4.140719	0.624250	-0.812220						

50 0.241794 0.064739 2.736628
 1 -1.299908 -0.248779 3.442043
 1 1.454334 -0.854252 3.550660
 1 0.614189 1.765694 2.849255

13 (R = SnH₃, 5exo TS)

Total energy = -405.64660 (B3LYP)
 7 -1.181848 .000000 .223641
 6 -1.051019 .000000 1.649487
 6 .276075 .000000 2.160470
 6 1.363352 .000000 1.200223
 6 2.589731 .000000 .933303
 6 -.123494 .000000 -.473995
 1 3.520304 .000000 .406939
 6 -2.164217 .000000 2.499873
 6 -1.959450 .000000 3.892626
 6 -.649531 .000000 4.416816
 6 .466130 .000000 3.558321
 1 -3.161331 .000000 2.070495
 1 -2.812952 .000000 4.565436
 1 -.499091 .000000 5.493472
 1 1.474834 .000000 3.961237
 50 .317177 .000000 -2.556655
 1 1.253125 1.397081 -2.865836
 1 1.253125 -1.397081 -2.865836
 1 -1.099387 .000000 -3.521415

Total energy = -405.47683 (BLYP)
 7 -1.165047 0.000000 0.228812
 6 -1.035473 0.000000 1.664464
 6 0.301588 0.000000 2.190031
 6 1.405313 0.000000 1.241178
 6 2.650045 0.000000 1.003139
 6 -0.105814 0.000000 -0.487271
 1 3.573472 0.000000 0.449055
 6 -2.164707 0.000000 2.513300
 6 -1.970851 0.000000 3.918126
 6 -.655015 0.000000 4.457246
 6 0.476766 0.000000 3.602846
 1 -3.165597 0.000000 2.072351
 1 -2.836599 0.000000 4.588511
 1 -0.512680 0.000000 5.543333
 1 1.489351 0.000000 4.017703
 50 0.297210 0.000000 -2.590149
 1 1.234529 1.402387 -2.915301
 1 1.234529 -1.402387 -2.915301
 1 -1.133294 0.000000 -3.552929

Total energy = -405.49970 (B3PW91)
 7 -1.163075 0.000000 0.230175
 6 -1.032801 0.000000 1.650392
 6 0.287686 0.000000 2.169429
 6 1.386073 0.000000 1.229513
 6 2.603534 0.000000 0.944260
 6 -.111012 0.000000 -0.472977
 1 3.545097 0.000000 0.438202
 6 -2.148336 0.000000 2.493483
 6 -1.953845 0.000000 3.884000
 6 -.650604 0.000000 4.415478
 6 0.467293 0.000000 3.565782
 1 -3.142025 0.000000 2.057257
 1 -2.811718 0.000000 4.550338
 1 -.506468 0.000000 5.492424
 1 1.473131 0.000000 3.974725
 50 0.302900 0.000000 -2.562338
 1 1.238853 1.401698 -2.882523
 1 1.238853 -1.401698 -2.882523
 1 -1.127108 0.000000 -3.518402

Total energy = -405.68091 (BP86)

7 -1.156742 0.000000 0.134048
 6 -1.156372 0.000000 1.568394
 6 0.117695 0.000000 2.224914
 6 1.317184 0.000000 1.411840
 6 2.569092 0.000000 1.258568
 6 -.047601 0.000000 -0.497545

6 3.552412 0.000000 0.817809
 6 -2.361483 0.000000 2.300712
 6 -2.311011 0.000000 3.714183
 6 -.1059065 0.000000 4.381163
 6 0.148904 0.000000 3.645403
 1 -.312941 0.000000 1.759525
 1 -.3240690 0.000000 4.293795
 1 -.1025324 0.000000 5.476585
 1 1.116278 0.000000 4.158922
 50 0.511693 0.000000 -2.564336
 1 1.478171 1.407472 -2.811344
 1 1.478171 -1.407472 -2.811344
 1 -.837605 0.000000 -3.651294

13 (R = SnH₃, 5exo P)

Total energy = -405.68256 (B3LYP)
 7 -1.221286 .000000 .073876
 6 -.1245644 .000000 1.513911
 6 .072405 .000000 2.046751
 6 .987116 .000000 .877115
 6 2.320921 .000000 .848327
 6 .039058 .000000 -.323366
 1 3.129957 .000000 .126275
 6 -.2372501 .000000 2.340651
 6 -.2161101 .000000 3.737224
 6 -.854638 .000000 4.274077
 6 .279754 .000000 3.431250
 1 -.371259 .000000 1.914728
 1 -.3015366 .000000 4.409755
 1 -.721068 .000000 5.353135
 1 1.281336 .000000 3.852530
 50 .535960 .000000 -2.396910
 1 1.479481 1.388140 -2.747389
 1 1.479481 -1.388140 -2.747389
 1 -.903795 .000000 -3.308914

Total energy = -405.50566 (BLYP)
 7 -1.236027 0.000000 0.074432
 6 -.1258765 0.000000 1.524057
 6 .073015 0.000000 2.060294
 6 0.996393 0.000000 0.885384
 6 2.339498 0.000000 0.858540
 6 0.035593 0.000000 -.331190
 1 3.143868 0.000000 0.119024
 6 -.2393891 0.000000 2.359054
 6 -.2179234 0.000000 3.766101
 6 -.862108 0.000000 4.305715
 6 0.281089 0.000000 3.456163
 1 -.3400762 0.000000 1.931606
 1 -.3039466 0.000000 4.444279
 1 -.726618 0.000000 5.392823
 1 1.290151 0.000000 3.879906
 50 0.542430 0.000000 -2.414563
 1 1.488584 1.395134 -2.766535
 1 1.488584 -1.395134 -2.766535
 1 -.903208 0.000000 -3.332135

Total energy = -405.54120 (B3PW91)
 7 -1.222830 0.000000 0.074377
 6 -.1244631 0.000000 1.510452
 6 0.070608 0.000000 2.041780
 6 0.980123 0.000000 0.874230
 6 2.313555 0.000000 0.842927
 6 0.036795 0.000000 -.318232

1 3.117625 0.000000 0.115557
 6 -.2368632 0.000000 2.336201
 6 -.2156637 0.000000 3.729191
 6 -.0853014 0.000000 4.264224
 6 0.278337 0.000000 3.423142
 1 -.3367171 0.000000 1.910908
 1 -.3010260 0.000000 4.401681
 1 -.0718793 0.000000 5.342658
 1 1.279705 0.000000 3.843914
 50 0.537116 0.000000 -2.391307
 1 1.484605 1.392596 -2.742053
 1 1.484605 -1.392596 -2.742053
 1 -.905346 0.000000 -3.309389

Total energy = -405.71575 (BP86)
 7 -.1238705 0.000000 0.095061
 6 -.1233147 0.000000 1.540349
 6 0.104834 0.000000 2.051944
 6 1.001301 0.000000 0.863103
 6 2.342912 0.000000 0.809141
 6 0.025946 0.000000 -.327134
 1 3.135374 0.000000 0.055224
 6 -.2350319 0.000000 2.394258
 6 -.2109889 0.000000 3.793661
 6 -.0786274 0.000000 4.308154
 6 0.338682 0.000000 3.440254
 1 -.3365410 0.000000 1.984583
 1 -.2958105 0.000000 4.487791
 1 -.630933 0.000000 5.393203
 1 1.356426 0.000000 3.845196
 50 0.503789 0.000000 -2.415854
 1 1.449939 1.400623 -2.781812
 1 1.449939 -1.400623 -2.781812
 1 -.960031 0.000000 -3.317486

13 (R = SnH₃, 6-endo TS)

Total energy = -405.64405 (B3LYP)
 6 -.1925368 .000000 -3.847295
 6 -.1896171 .000000 -2.444259
 6 -.664677 .000000 -1.756897
 6 .562297 .000000 -2.498208
 6 .512969 .000000 -3.910244
 6 -.719002 .000000 -4.581549
 1 -.2879086 .000000 -4.368420
 1 -.2811400 .000000 -1.859468
 7 -.704015 .000000 -.339314
 6 1.782777 .000000 -1.747318
 1 1.447568 .000000 -4.464469
 1 -.745106 .000000 -5.668035
 6 2.307993 .000000 -.615791
 6 .210165 .000000 .532945
 1 3.044931 .000000 .159794
 50 .107983 .000000 2.681147
 1 .962535 -1.392155 3.193979
 1 .962535 1.392155 3.193979
 1 -.1478906 .000000 3.342167

Total energy = -405.47427 (BLYP)
 6 -.1929423 0.000000 -3.877891
 6 -.1896602 0.000000 -2.464038
 6 -.653983 0.000000 -1.772569
 6 0.584513 0.000000 -2.523380
 6 0.527653 0.000000 -3.947435
 6 -.0715673 0.000000 -4.620372
 1 -.2891702 0.000000 -4.400319
 1 -.2817807 0.000000 -1.873443
 7 -.0694460 0.000000 -0.345870
 6 1.817987 0.000000 -1.782611
 1 1.467571 0.000000 -4.508767
 1 -.0744602 0.000000 -5.714964

6	2.379074	0.000000	-0.657494	1	-1.426168	.000000	3.003313	6	.315977	-.255477	-2.006718
6	0.214436	0.000000	0.546613		Total energy = -405.53942 (BLYP)			6	.293615	-.185906	-3.408449
1	3.137116	0.000000	0.107205	50	-1.984196	0.000000	-3.798585	6	-.925889	.025068	-4.078742
50	0.086711	0.000000	2.710879	1	-1.985568	0.000000	-2.395988	1	-3.055018	.320259	-3.835237
1	0.951812	-1.395980	3.224395	1	-0.748186	0.000000	-1.667479	1	1.268008	-.430697	-1.511852
1	0.951812	1.395980	3.224395	1	0.520369	0.000000	-2.421472	1	1.217147	-.294900	-3.971515
1	-1.496421	0.000000	3.413727	6	0.480393	0.000000	-3.858039	1	-.955879	.085332	-5.163487
	Total energy = -405.49648 (B3PW91)			6	-0.748723	0.000000	-4.532312	6	-.774518	-.200191	.263380
6	-1.918827	0.000000	-3.837023	1	-2.933978	0.000000	-4.344313	6	-1.838128	-.344645	1.054391
6	-1.885785	0.000000	-2.437255	1	-2.915938	0.000000	-1.820549	1	-2.037462	-.398254	2.120635
6	-0.655174	0.000000	-1.754813	7	-0.763455	0.000000	-0.275687	6	-3.352903	.226575	-1.237228
6	0.566050	0.000000	-2.498225	6	1.697997	0.000000	-1.625124	6	-4.478569	.366673	-7.727116
6	0.513687	0.000000	-3.906724	1	1.425647	0.000000	-4.409845	1	-5.439402	.482658	-3.25762
6	-0.717517	0.000000	-4.572901	1	-0.772642	0.000000	-5.627222	50	1.130677	-.001207	1.325255
1	-2.873663	0.000000	-4.354952	6	1.699537	0.000000	-0.243807	6	.660933	-.002749	3.413795
1	-2.798694	0.000000	-1.849574	6	0.390218	0.000000	0.423494	1	-.016998	.822337	3.665812
7	-0.689193	0.000000	-0.342566	1	2.614149	0.000000	0.357306	1	.186869	-.946249	3.712635
6	1.781335	0.000000	-1.747148	50	0.227420	0.000000	2.580949	1	1.578941	.118470	4.003515
1	1.446278	0.000000	-4.463437	1	1.024953	-1.395079	3.204286	6	2.432530	-1.656261	.891602
1	-0.746495	0.000000	-5.658771	1	1.024953	1.395079	3.204286	1	3.198930	-1.744338	1.673091
6	2.335064	0.000000	-0.633651	1	-1.425018	0.000000	3.034308	1	1.862301	-2.592870	.859898
6	0.222416	0.000000	0.529583		Total energy = -405.57605 (B3PW91)			1	2.940923	-1.528920	-.072297
1	3.072048	0.000000	0.141797	50	0.097419	0.000000	2.679842	6	2.062965	1.852356	.776824
50	0.097419	0.000000	2.679842	1	-1.963992	0.000000	-3.757063	1	1.435831	2.698274	1.084531
1	0.951954	-1.396470	3.200964	6	-1.959137	0.000000	-2.369960	1	3.041457	1.949533	1.265320
1	0.951954	1.396470	3.200964	6	-0.728524	0.000000	-1.655128	1	2.208738	1.911388	-.308545
1	-1.497490	0.000000	3.337820		Total energy = -405.67783 (BP86)			11 (R = SnMe₃, 5-exo TS)			
	Total energy = -405.67783 (BP86)			6	0.513086	0.000000	-2.402544	Total energy = -507.56484			
6	-1.839391	0.000000	-3.906880	6	0.476029	0.000000	-3.825625	6	-1.808005	-.019294	-4.133808
6	-1.832336	0.000000	-2.495787	1	-2.907944	0.000000	-4.295282	6	-1.805778	-.023877	-2.892075
6	-0.605642	0.000000	-1.783185	1	-2.878066	0.000000	-1.792289	6	.374988	.012375	-2.023386
6	0.642140	0.000000	-2.509692	7	-0.747210	0.000000	-0.275556	6	.024685	.003043	-.732351
6	0.612889	0.000000	-3.930965	6	1.678798	0.000000	-1.608610	6	-1.433011	-.023295	-4.33419
6	-0.615146	0.000000	-4.625212	1	1.412541	0.000000	-4.375765	6	-2.330218	-.037873	-1.543796
1	-2.792613	0.000000	-4.446940	1	-0.768900	0.000000	-5.575062	1	-1.613157	-.011608	-5.183055
1	-2.763924	0.000000	-1.919913	6	1.689088	0.000000	-0.240493	1	1.287283	.027933	-2.611258
7	-0.672696	0.000000	-0.363659	6	0.396943	0.000000	0.415688	6	-3.726039	-.066079	-1.325399
6	1.853784	0.000000	-1.743203	1	2.602794	0.000000	0.346063	6	-4.241172	-.079524	-.017762
1	1.564105	0.000000	-4.474717	50	0.220213	0.000000	2.556942	6	-3.360518	-.064060	1.081666
1	-0.623496	0.000000	-5.720792	1	1.014106	-1.392778	3.185484	6	-1.970448	-.036117	.870485
6	2.436179	0.000000	-0.634187	1	1.014106	1.392778	3.185484	1	-4.395565	-.077415	-2.181058
6	0.212887	0.000000	0.549974	1	-1.432822	0.000000	2.999366	1	-5.316050	-.101891	.142865
1	3.177007	0.000000	0.148470		Total energy = -405.75013 (BP86)			1	-3.754997	-.074296	2.094811
50	0.015959	0.000000	2.711060	6	-1.969017	0.000000	-3.793970	1	-1.305004	-.025838	1.730594
1	0.873693	-1.400838	3.249023	6	-1.972735	0.000000	-2.394498	50	1.583843	.026808	.775842
1	0.873693	1.400838	3.249023	6	-0.739351	0.000000	-1.666186	6	3.449524	-.048224	-.270494
1	-1.589734	0.000000	3.383297	6	0.525502	0.000000	-2.415084	1	4.283706	-.055825	.442969
13 (R = SnH₃, 6-endo P)				6	0.490008	0.000000	-3.848065	1	3.517305	-.954665	-.885109
	Total energy = -405.71722 (B3LYP)			6	-0.735026	0.000000	-4.523428	1	3.568657	.824477	-.925006
6	-1.968512	.000000	-3.764924	1	-2.918385	0.000000	-4.341646	6	1.459739	1.836494	1.922598
6	-1.964707	.000000	-2.374749	1	-2.903733	0.000000	-1.818282	1	.497060	1.912504	2.442763
6	-0.731893	.000000	-1.657011	7	-0.761327	0.000000	-0.277840	1	2.261175	1.869821	2.672349
6	.514645	.000000	-2.406317	6	1.698194	0.000000	-1.617376	1	1.562906	2.709651	1.266328
6	.477326	.000000	-3.832917	1	1.437680	0.000000	-4.397495	6	1.389787	-1.686047	2.056235
6	-.742717	.000000	-4.498175	1	-0.756306	0.000000	-5.619045	1	2.190293	-1.694100	2.807648
1	-2.912455	.000000	-4.304271	6	1.697874	0.000000	-0.238306	1	.425507	-1.684334	2.579146
1	-2.884761	.000000	-1.798119	6	0.390544	0.000000	0.419919	1	1.457537	-2.609937	1.468361
7	-.748589	.000000	-2.274385	50	0.218977	0.000000	2.575715		11 (R = SnMe₃, 5-exo P)		
6	1.682871	.000000	-1.610809	1	1.017713	-1.400646	3.205370	Total energy = -507.62562			
1	1.414401	.000000	-4.382883	1	1.017713	1.400646	3.205370	6	.613372	-.000190	-.083860
1	-.770057	.000000	-5.584799	1	-1.442624	0.000000	3.022218	6	.604160	.000016	1.406631
6	1.692351	.000000	-2.40369		11 (R = SnMe₃)			6	1.948097	-.000341	1.884845
6	.396395	.000000	.420472	Total energy = -507.56747				6	2.846727	-.000833	.696590
1	2.605795	.000000	.347346	6	-2.105743	.156851	-3.332247	6	4.185014	-.001287	.675187
50	.221065	.000000	2.561115	6	-2.094933	.081387	-1.916154	6	1.928367	-.000694	-.487670
1	1.012781	-1.388139	3.186569	6	-.856712	-.128961	-1.224323	1	4.991661	-.001665	-.049255
1	1.012781	1.388139	3.186569					1	2.295799	-.000971	-1.508125
								6	-.462476	.000506	2.319453

6 -1.179491 .000632 3.703403
 6 1.152414 .000268 4.167710
 6 2.231297 -.000220 3.255029
 1 -1.495452 .000824 1.977348
 1 -.996886 .001019 4.420949
 1 1.348851 .000365 5.237260
 1 3.257962 -.000505 3.612539
 50 -1.078975 .000134 -1.386221
 6 -2.257991 -1.753258 -1.016995
 1 -1.663217 -2.659555 -1.186578
 1 -2.619394 -1.771730 .019031
 1 -3.128403 -1.780256 -1.685438
 6 -.347897 .000019 -3.399089
 1 .263395 .890273 -3.594483
 1 .263444 -.890214 -3.594416
 1 -1.185701 -.000033 -4.108285
 6 -2.257351 1.754000 -1.017188
 1 -2.621806 1.770967 .017795
 1 -1.661210 2.660019 -1.183413
 1 -3.125769 1.783028 -1.688139

11 (R = SnMe₃, 6-endo TS)

Total energy = -507.55868

6 -2.794039 -.053978 -2.212805
 6 -2.802394 -.033733 -.782859
 6 -1.537247 -.018317 -.095164
 6 -2.31387 -.020071 -.815004
 6 -.099394 -.041587 -2.151965
 6 -2.236886 -.067380 -3.319077
 1 .766540 -.045114 -2.811729
 1 -1.986515 -.082284 -4.357349
 6 -4.016265 -.029237 -.057719
 6 -4.018053 -.010531 1.343531
 1 -4.951784 -.040892 -.610706
 1 -4.956356 -.007275 1.891652
 6 -2.789144 .003622 2.033870
 6 -1.580706 -.000232 1.320962
 1 -2.774604 .017588 3.120901
 1 -.649952 .010210 1.882679
 50 1.673734 .018422 .263753
 6 1.841137 1.808362 1.440964
 1 1.075522 1.845700 2.225461
 1 2.828654 1.856594 1.918810
 1 1.721202 2.693938 .804385
 6 1.876983 -1.717728 1.514035
 1 2.880689 -1.748039 1.958507
 1 1.139908 -1.716941 2.326307
 1 1.732850 -2.630617 .922679
 6 3.217148 .002135 -1.220370
 1 4.200770 .019501 -.733053
 1 3.161099 -.901088 -1.841065
 1 3.146757 .879648 -1.875512

11 (R = SnMe₃, 6-endo P)

Total energy = -507.65801

6 -.324926 .014816 -3.499730
 6 -.375558 .013115 -2.110989
 6 .813720 -.015462 -1.312531
 6 2.083993 -.042998 -2.022957
 6 2.110758 -.040609 -3.451997
 6 .928766 -.012247 -4.179594
 1 -1.246573 .036948 -4.076251
 1 -1.345245 .034492 -1.618586
 6 .791513 -.018054 .136106
 6 3.247609 -.071285 -1.220257
 1 3.074344 -.061493 -3.954199
 1 .952603 -.010514 -5.266360
 6 3.278905 -.075043 .149527
 6 2.008310 -.047317 .826449
 1 4.204650 -.097394 .718775

1 2.026372 -.050023 1.915152
 50 -1.019439 .020522 1.306838
 6 -2.148240 1.797231 .888602
 1 -3.068503 1.814468 1.487222
 1 -1.560632 2.690803 1.134340
 1 -2.426108 1.854263 -.171173
 6 -.427291 .013522 3.365811
 1 -1.315805 .040180 4.009969
 1 .142544 -.891479 3.612353
 1 .190164 .888892 3.604823
 6 -2.215028 -.1.713826 .895905
 1 -1.685812 -2.624626 1.203465
 1 -3.163506 -1.663776 1.446705
 1 -2.441757 -1.797912 -.174195

13 (R = SnMe₃, 5-exo radical)

Total energy = -523.63561

6 -.056991 -.957807 -4.408143
 6 -.410585 -.778936 -3.050353
 6 .187109 .317153 -2.321621
 6 1.112765 1.180214 -2.988850
 6 1.434307 .967175 -4.329530
 6 .851836 -.104537 -.5052795
 1 -.511061 -1.783143 -4.950387
 1 1.552823 2.003555 -2.433262
 1 2.138176 1.634486 -4.821281
 1 1.106304 -.263715 -6.096592
 7 -.115493 .527196 -1.022902
 6 -.466297 .755439 .122987
 6 -1.336573 -1.664221 -2.415560
 6 -2.130186 -2.426087 -1.873008
 1 -2.828118 -.3.086952 -1.412404
 50 .022004 .224901 2.172749
 6 .417284 2.107180 3.103532
 1 -.401043 2.807168 2.899163
 1 .508045 1.987529 4.192377
 1 1.349977 2.543333 2.727616
 6 -.1779752 -.660492 2.902819
 1 -.1984481 -1.603825 2.382741
 1 -1.702319 -.865880 3.977938
 1 -2.625506 .016797 2.735945
 6 1.697202 -.1.13267 2.341753
 1 1.867253 -.3.74346 3.395075
 1 1.509911 -.2.035855 1.779625
 1 2.607576 -.645427 1.948021

13 (R = SnMe₃, in-plane radical)

Total energy = -523.63122

6 -2.733923 0.000000 -3.963067
 6 -2.435726 0.000000 -2.592230
 6 -.1.100617 0.000000 -2.135919
 6 -.031426 0.000000 -3.084995
 6 -.353495 0.000000 -4.466879
 6 -.1.685941 0.000000 -4.905449
 1 -.3.769066 0.000000 -4.294078
 1 -3.222781 0.000000 -1.844324
 7 -.0930322 0.000000 -.722105
 6 1.352621 0.000000 -2.707606
 1 .0459819 0.000000 -5.187482
 1 -.1.906441 0.000000 -5.969723
 6 2.558235 0.000000 -2.492986
 6 .096803 0.000000 0.009422
 1 3.599548 0.000000 -2.264652
 50 .0424728 0.000000 2.135725
 6 1.580103 -.1.758754 2.524395
 1 1.907168 -.1.782658 3.571842
 1 .993417 -.2.663557 2.324169
 1 2.468242 -.1.775012 1.881164
 6 1.580103 1.758754 2.524395
 1 0.993417 2.663557 2.324169

1 1.907168 1.782658 3.571842
 1 2.468242 1.775012 1.881164
 6 -.1.401102 0.000000 3.268159
 1 -.1.998186 0.889418 3.033495
 1 -.1.998186 -.0.889418 3.033495
 1 -.1.180340 0.000000 4.343953

13 (R = SnMe₃, 5-exo TS)

Total energy = -523.62106

7 -.1.269518 .000000 .780194
 6 -.1.127916 .000000 2.205616
 6 .201498 .000000 2.709974
 6 1.287437 .000000 1.747142
 6 2.517842 .000000 1.494278
 6 -.220517 .000000 .067265
 1 3.446573 .000000 .964664
 6 -.2.235824 .000000 3.063504
 6 -.2.024471 .000000 4.455275
 6 -.711790 .000000 4.972747
 6 .398339 .000000 4.107344
 1 -.3.235347 .000000 2.639556
 1 -.2.874758 .000000 5.132377
 1 -.555187 .000000 6.048627
 1 1.409763 .000000 4.503749
 50 .225607 .000000 -2.029927
 6 1.386504 -.1.762919 -2.371431
 1 2.249541 -.1.786891 -1.695354
 1 .784603 -.2.661984 -2.191772
 1 1.751450 -.1.790829 -3.406159
 6 -.1.591981 .000000 -3.171951
 1 -.1.646627 .890886 -3.809815
 1 -.1.646627 -.890886 -3.809815
 1 -.2.456447 .000000 -2.497789
 6 1.386504 1.762919 -2.371431
 1 .784603 2.661984 -2.191772
 1 2.249541 1.786891 -1.695354
 1 1.751450 1.790829 -3.406159

13 (R = SnMe₃, 5-exo P)

Total energy = -523.65582

7 -.1.311904 .000000 .623731
 6 -.1.320907 .000000 2.063988
 6 .003029 .000000 2.581963
 6 .903285 .000000 1.401378
 6 2.236541 .000000 1.358571
 6 -.056804 .000000 .204356
 1 3.031970 .000000 .621687
 6 -.2.436824 .000000 2.905788
 6 -.2.208543 .000000 4.299913
 6 -.895923 .000000 4.821450
 6 .227432 .000000 3.964024
 1 -.3.441297 .000000 2.493235
 1 -.3.054937 .000000 4.982607
 1 -.749255 .000000 5.898866
 1 1.234509 .000000 4.372255
 50 .382965 .000000 -1.900605
 6 1.534453 -.1.754259 -2.344365
 1 2.485909 -.1.755778 -1.797468
 1 .977902 -.2.658093 -2.067021
 1 1.756620 -.1.802673 -3.418365
 6 1.534453 1.754259 -2.344365
 1 .977902 2.658093 -2.067021
 1 2.485909 1.755778 -1.797468
 1 1.756620 1.802673 -3.418365
 6 -.1.503047 .000000 -2.901281
 1 -.1.616970 .890235 -3.531676
 1 -.1.616970 -.890235 -3.531676
 1 -.2.295720 .000000 -2.143970

13 (R = SnMe₃, 6-endo TS)

Total energy = -523.61806
 6 -1.984032 .000000 -4.400980
 6 -1.933495 .000000 -2.998553
 6 -.692715 .000000 -2.326954
 6 .521847 .000000 -3.086856
 6 .452061 .000000 -4.498459
 6 -.788675 .000000 -5.153132
 1 -2.945592 .000000 -4.907874
 1 -2.840056 .000000 -2.400136
 7 -.720300 .000000 -9.06540
 6 1.757468 .000000 -2.358932
 1 1.379391 .000000 -5.065106
 1 -.830297 .000000 -6.239230
 6 2.301956 .000000 -1.236662
 6 .201225 .000000 -.037562
 1 3.053156 .000000 -.475446
 50 .097936 .000000 2.120353
 6 1.146067 -1.756666 2.751827
 1 1.211386 -1.791082 3.847026
 1 .630327 -2.661487 2.407998
 1 2.164349 -1.766242 2.343940
 6 1.146067 1.756666 2.751827
 1 .630327 2.661487 2.407998
 1 1.211386 1.791082 3.847026
 1 2.164349 1.766242 2.343940
 6 -1.929594 .000000 2.823627
 1 -2.458815 .889150 2.460728
 1 -2.458815 -.889150 2.460728
 1 -1.954883 .000000 3.921403

13 (R = SnMe₃, 6-endo P)
 Total energy = -523.69041
 6 -1.938752 .000000 -4.346184
 6 -1.948187 .000000 -2.955944
 6 -.722996 .000000 -2.224711
 6 .530903 .000000 -2.961835
 6 .507159 .000000 -4.388903
 6 -.705837 .000000 -.5067185
 1 -2.877480 .000000 -4.894789
 1 -2.874479 .000000 -2.389135
 7 -.752622 .000000 -.842341
 6 1.692559 .000000 -2.155608
 1 1.450002 .000000 -4.929127
 1 -.721895 .000000 -6.154135
 6 1.686581 .000000 -.785398
 6 .384570 .000000 -.130289
 1 2.594613 .000000 -.188625
 50 .158053 .000000 2.021290
 6 1.128830 1.751938 2.791484
 1 1.003295 1.812005 3.880561
 1 2.204025 1.735428 2.571610
 1 .700430 2.658006 2.345153
 6 -1.928503 .000000 2.463932
 1 -2.405781 .886365 2.029980
 1 -2.405781 -.886365 2.029980
 1 -2.099964 .000000 3.548010
 6 1.128830 -1.751938 2.791484
 1 2.204025 -1.735428 2.571610
 1 1.003295 -1.812005 3.880561
 1 .700430 -2.658006 2.345153

13 (R=Me, out-of-plane radical)
 Total energy = -562.95369
 6 -.784484 .663857 -4.287928
 6 -.782197 .668665 -2.873993
 6 .492893 .659847 -2.193265
 6 1.700473 .646735 -2.958675
 6 1.651182 .642106 -4.353826
 6 .407086 .650423 -5.031464
 1 -1.745043 .671095 -4.796821

1	2.652002	.645726	-2.434144
1	2.579334	.634209	-4.920561
1	.374467	.647220	-6.117295
7	.550438	.657313	-.843011
6	.583619	.743721	.374160
6	-2.009143	.681105	-2.137670
6	-3.063371	.693872	-1.510262
50	.563348	-.533652	2.133999
6	2.323675	.035735	3.205683
1	2.363577	1.126810	3.306735
1	2.324828	-.407920	4.209439
1	3.227554	-.296549	2.680866
6	-1.208886	.068179	3.167575
1	-2.102839	-.201716	2.592416
1	-1.268462	-.417939	4.149626
1	-1.206494	1.154639	3.314899
6	.547492	-2.642198	1.702501
1	.493823	-3.218407	2.636222
1	-.319266	-2.900220	1.082358
1	1.457778	-.2934150	1.165037
6	-4.330702	.720021	-.764921
1	-4.230382	1.297918	.163255
1	-5.127951	1.181637	-1.361928
1	-4.659213	-.293340	-.496492

13 (R=Me, in-plane radical)

Total energy = -562.95065				
6	-2.087425	0.000000	-4.373838	
6	-2.067237	0.000000	-2.971259	
6	-0.848908	0.000000	-2.258989	
6	0.390465	0.000000	-2.973355	
6	0.346744	0.000000	-4.392043	
6	-0.871624	0.000000	-5.087213	
1	-3.035753	0.000000	-4.904796	
1	-2.987534	0.000000	-2.394810	
7	-0.962074	0.000000	-0.840259	
6	1.664323	0.000000	-2.317191	
1	1.287061	0.000000	-4.936930	
1	-0.875612	0.000000	-6.174324	
6	2.778852	0.000000	-1.830838	
6	-0.111369	0.000000	0.090224	
50	-0.276213	0.000000	2.235835	
6	0.757950	-1.757600	2.887410	
1	0.869046	-1.757469	3.979410	
1	0.210267	-2.661948	2.595310	
1	1.756447	-1.799369	2.435380	
6	0.757950	1.757600	2.887410	
1	0.210267	2.661948	2.595310	
1	0.869046	1.757469	3.979410	
1	1.756447	1.799369	2.435380	
6	-2.311209	0.000000	2.927641	
1	-2.839343	0.889317	2.563092	
1	-2.839343	-0.889317	2.563092	
1	-2.340606	0.000000	4.025490	
6	4.110181	0.000000	-1.190810	
1	4.690438	-0.886957	-1.478429	
1	4.690438	0.886957	-1.478429	
1	4.011771	0.000000	-0.096996	

13 (R=Me, 5-exo TS)

```
Total energy = -562.93949
7  -1.499993   .000000   .616700
6  -1.494475   .000000  2.047963
6  -.217159   .000000  2.674613
6  .947529   .000000  1.811588
6  2.196410   .000000  1.668815
6  -.382479   .000000  .009375
6  -2.678886   .000000  2.797763
6  -2.600967   .000000  4.203021
6  -1.342300   .000000  4.841445
```

6	-1.55478	.000000	4.084930
1	-3.633846	.000000	2.280795
1	-3.511272	.000000	4.797174
1	-1.288108	.000000	5.927519
1	.813354	.000000	4.576856
50	.175806	.000000	-2.061004
6	1.359446	-1.758575	-2.356104
1	2.173617	-1.801368	-1.622383
1	.745851	-2.660106	-2.239039
1	1.796266	-1.765085	-3.363039
6	-1.574459	.000000	-3.304448
1	-1.595638	.891074	-3.944088
1	-1.595638	.891074	-3.944088
1	-2.472789	.000000	-2.675951
6	1.359446	1.758575	-2.356104
1	.745851	2.660106	-2.239039
1	2.173617	1.801368	-1.622383
1	1.796266	1.765085	-3.363039
6	3.550085	.000000	1.098089
1	4.114721	.885248	1.421123
1	4.114721	-.885248	1.421123
1	3.532381	.000000	-.003902

13 (R=Me, 5-exo P)

Total energy = -562.97591				
7	-1.443784	.000000	.607263	
6	-1.460915	.000000	2.043208	
6	-.139340	.000000	2.565575	
6	.768013	.000000	1.389070	
6	2.106124	.000000	1.403751	
6	-.181727	.000000	.193865	
6	-2.582168	.000000	2.880682	
6	-2.361680	.000000	4.274621	
6	-1.049976	.000000	4.801620	
6	.076682	.000000	3.950053	
1	-3.584440	.000000	2.462291	
1	-3.210813	.000000	4.954033	
1	-.908327	.000000	5.879968	
1	1.081879	.000000	4.363685	
50	.156236	.000000	-1.930065	
6	1.266740	-1.758306	-2.464375	
1	2.236788	-1.801826	-1.953722	
1	.699065	-2.658175	-2.196065	
1	1.448000	-1.776656	-3.547091	
6	1.266740	1.758306	-2.464375	
1	.699065	2.658175	-2.196065	
1	2.236788	1.801826	-1.953722	
1	1.448000	1.776656	-3.547091	
6	-1.778073	.000000	-2.832669	
1	-1.924903	.890454	-3.456135	
1	-1.924903	-.890454	-3.456135	
1	-2.526047	.000000	-2.031491	
6	3.325573	.000000	.569965	
1	3.941065	.884303	.786973	
1	3.941065	-.884303	.786973	
1	3.106424	.000000	5.09968	

13 (R=Me, 6-endo TS)

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15 (K=MC, 6- $\alpha$ CD)          Total energy = -562.93628
   6  -2.002127   .128937  -4.448872
   6  -1.992760   .079196  -3.046651
   6  -.772109   .069971  -2.339792
   6  .468694   .111758  -3.055820
   6  .437383   .161300  -4.468908
   6  -.783077   .169953  -5.160981
   1  -2.947436   .135777  -4.985466
   1  -2.916239   .046754  -2.475424
   7  -.833686   .018208  -923.159
   6  1.684070   .100979  -2.294293
   1  1.380355   .192688  -5.008377

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1	-.790373	.208327	-6.247411	6	-1.204696	-.675410	.321540	6	-2.759980	0.000000	4.446318
6	2.171934	.066505	-1.139603	50	-.516424	.186424	2.196115	6	-1.466459	0.000000	5.010112
6	.081995	-.000184	-.045217	6	-.199697	2.309399	2.076148	6	-.326478	0.000000	4.185117
50	-.172835	-.075339	2.105064	1	.170720	2.690980	3.037310	1	-.3902848	0.000000	2.587646
6	.678800	1.727857	2.888713	1	.542269	2.535473	1.301418	1	-.3634164	0.000000	5.092362
1	.589933	1.746180	3.982727	1	-1.133044	2.830433	1.831008	1	-1.348496	0.000000	6.091066
1	1.741777	1.804185	2.628688	6	-2.068301	-.299746	3.585504	1	0.669296	0.000000	4.620025
1	.161941	2.607425	2.485945	1	-2.984565	.260449	3.362462	50	-.353639	0.000000	-1.990862
6	-2.246754	-.242541	2.627659	1	-2.295645	-1.371211	3.532216	6	0.781383	-1.770620	-2.352665
1	-2.670464	-1.164873	2.212644	1	-1.758180	-.059912	4.610598	1	1.685444	-1.723300	-1.735734
1	-2.368204	-.260140	3.718893	6	1.290387	-.877861	2.590029	1	0.208435	-2.667731	-2.088943
1	-2.811016	.607071	2.225144	1	2.005145	-.707212	1.775592	1	1.068427	-1.838745	-3.410083
6	.929929	-1.774453	2.803349	1	1.736410	-.541983	3.535140	6	0.781383	1.770620	-2.352665
1	2.007662	-1.628068	2.661284	1	1.085623	-1.952884	2.662683	1	0.208435	2.667731	-2.088943
1	.743020	-1.932517	3.873498	6	3.318636	-1.115423	-1.423912	1	1.685444	1.723300	-1.735734
1	.629952	-2.681432	2.264389	1	3.339191	-2.195962	-1.197545	1	1.068427	1.838745	-3.410083
6	3.216794	.042342	-.096023	1	4.122765	-.903833	-2.149833	6	-2.215836	0.000000	-3.067672
1	3.156042	-.874307	.503655	8	3.565600	-.360692	-.185247	1	-2.296166	0.891234	-3.702845
1	4.213562	.082680	-.554065	6	4.881150	-.644805	.375390	1	-2.296166	0.891234	-3.702845
1	3.120393	.900039	.581414	1	5.682953	-.358079	-.323909	1	-3.053086	0.000000	-2.359427
13 (R=Me, 6-endo P)				1	4.962350	-.044696	1.285041	6	3.210619	0.000000	1.027217
Total energy = -563.00074				1	4.990599	-1.711581	.629789	1	3.770206	0.892402	1.355770
6	-2.185028	.000000	-4.270582	13 (R=OCH ₂ Me, in-plane radical)				1	3.770206	-0.892402	1.355770
6	-2.143770	.000000	-2.881160	Total energy = -677.43724				8	3.128128	0.000000	-0.452420
6	-.891491	.000000	-2.197235	6	-2.520787	0.000000	-4.562933	6	4.435300	0.000000	-1.119093
6	.334608	.000000	-2.975373	6	-2.589555	0.000000	-3.161234	1	4.509931	-0.895419	-1.747917
6	.259209	.000000	-4.401534	6	-1.418934	0.000000	-2.376093	1	4.509931	0.895419	-1.747917
6	-.977639	.000000	-5.034794	6	-0.138033	0.000000	-3.013567	1	5.265753	0.000000	-0.398518
1	-3.142624	.000000	-4.785606	6	-0.089607	0.000000	-4.430990	13 (R=OCH ₂ Me, 5-exo P)			
1	-3.048452	.000000	-2.280266	6	-1.263380	0.000000	-5.199788	Total energy = -677.46741			
7	-.860222	.000000	-.817774	1	-3.433827	0.000000	-5.152595	7	-1.766453	0.000000	0.771791
6	1.519068	.000000	-2.209361	1	-3.543601	0.000000	-2.642646	6	-1.758700	0.000000	2.206638
1	1.181296	.000000	-4.976567	7	-1.605449	0.000000	-0.960365	6	-0.428634	0.000000	2.704900
1	-1.032841	.000000	-6.120549	6	1.089459	0.000000	-2.272414	6	0.458253	0.000000	1.509889
6	1.595517	.000000	-.836822	1	0.882078	0.000000	-4.918164	6	1.789564	0.000000	1.518904
6	.303716	.000000	-.146949	1	-1.200331	0.000000	-6.285015	6	-0.519032	0.000000	0.323424
50	.011552	.000000	2.005457	6	2.177806	0.000000	-1.710125	6	-2.863389	0.000000	3.064986
6	.908891	1.757272	2.855156	6	-0.737482	0.000000	-0.044649	6	-2.617090	0.000000	4.455079
1	.715290	1.794681	3.935389	50	-.597951	0.000000	2.086511	6	-1.296502	0.000000	4.957819
1	1.995023	1.771175	2.700763	6	0.486910	1.777533	2.585737	6	-0.186110	0.000000	4.084612
1	.485147	2.661221	2.399649	1	-0.070819	2.390381	3.304461	1	-3.873186	0.000000	2.665280
6	-2.094365	.000000	2.342908	1	1.459079	1.515091	3.019877	1	-3.453834	0.000000	5.149678
1	-2.548315	.885748	1.883811	1	0.668654	2.367439	1.680204	1	-1.134270	0.000000	6.033210
1	-2.548315	-.885748	1.883811	6	-2.530363	0.000000	3.033251	1	0.826279	0.000000	4.480532
1	-2.319710	.000000	3.417308	1	-3.101354	0.889470	2.739965	50	-0.253693	0.000000	-1.822507
6	.908891	-1.757272	2.855156	1	-3.101354	-.889470	2.739965	6	0.715638	-1.801847	-2.459324
1	1.995023	-1.771175	2.700763	1	-2.418628	0.000000	4.126170	1	1.612460	-1.976811	-1.857179
1	.715290	-1.794681	3.935389	6	0.486910	-1.777533	2.585737	1	0.032756	-2.653418	-2.345867
1	.485147	-2.661221	2.399649	1	1.459079	-1.515091	3.019877	1	1.001775	-1.730396	-3.517404
6	2.915237	.000000	-.089481	1	-0.070819	-2.390381	3.304461	6	0.715638	1.801847	-2.459324
1	3.511960	-.883667	-.348655	1	0.668654	-2.367439	1.680204	1	0.032756	2.653418	-2.345867
1	3.511960	.883667	-.348655	6	3.452107	0.000000	-0.990996	1	1.612460	1.976811	-1.857179
1	2.771007	.000000	.995766	1	4.039511	-.891971	-1.269689	1	1.001775	1.730396	-3.517404
13 (R=OCH ₂ Me, out-of-plane radical)				1	4.039511	0.891971	-1.269689	6	-2.262910	0.000000	-2.569647
Total energy = -677.44856				8	3.206093	0.000000	0.456967	1	-2.458537	0.890449	-3.180972
6	-2.884727	.640571	-4.050032	6	4.429710	0.000000	1.263033	1	-2.458537	-0.890449	-3.180972
6	-2.768454	.315627	-2.698371	1	4.432294	0.895909	1.895649	1	-2.948722	0.000000	-1.714347
6	-1.499409	-.052634	-2.151384	1	4.432294	-0.895909	1.895649	6	3.051077	0.000000	0.766327
6	-.335612	-.079708	-3.012308	1	5.337953	0.000000	0.642770	1	3.642378	0.891394	1.040260
6	-.499952	.257555	-4.375673	13 (R=OCH ₂ Me, 5-exo TS)				1	3.642378	-0.891394	1.040260
6	-1.751426	.612513	-4.902670	Total energy = -677.43377				8	2.790988	0.000000	-0.681722
1	-3.857652	.916286	-4.450256	7	-1.876523	0.000000	0.801943	6	3.996871	0.000000	-1.520358
1	-3.635469	.331052	-2.043777	6	-1.781769	0.000000	2.229266	1	3.980873	-0.895543	-2.151732
7	-1.382206	-.368830	-.845205	6	-0.470323	0.000000	2.780363	1	3.980873	0.895543	-2.151732
6	.943046	-.433830	-2.483306	6	0.650997	0.000000	1.864198	1	4.914199	0.000000	-0.915538
1	.377091	.238274	-5.017860	6	1.879403	0.000000	1.620644	13 (R=OCH ₂ Me, 6-endo TS)			
1	-1.851253	.866054	-5.954159	6	-0.814810	0.000000	0.109919	Total energy = -677.43195			
6	2.024479	-.735500	-1.989829	6	-2.919498	0.000000	3.048139	6	1.549311	.072921	-3.662905

6	1.554141	.011225	-2.253022		1	3.641869	-0.895112	2.531220
6	2.798348	.085285	-1.543121		1	4.532397	0.000000	1.265205
6	3.995317	.260149	-2.275310					
6	3.976580	.321156	-3.676622					
6	2.751128	.216482	-4.372133					
1	.593542	.015383	-4.176121					
1	4.933010	.330466	-1.730132					
1	4.904880	.447221	-4.227879					
1	2.736941	.257469	-5.458353					
7	.306625	-.046244	-1.587386					
6	-.013189	-.242379	-3.78683					
6	2.757126	-.045963	-.116425					
6	2.040040	-.231860	.889647					
50	-1.957822	-.051958	.556298					
6	-2.079991	1.868122	1.485114					
1	-2.940575	1.917808	2.165097					
1	-1.158613	2.036914	2.051766					
1	-2.186923	2.656732	.730532					
6	-3.452187	-.268530	-.973012					
1	-3.302577	.484206	-1.756592					
1	-3.390236	-1.262108	-1.434043					
1	-4.458466	-.141147	-.551432					
6	-2.139876	-1.660750	1.954620					
1	-1.384018	-1.565546	2.741471					
1	-3.133992	-1.651449	2.420555					
1	-2.006666	-2.626788	1.451718					
6	1.704169	-.557398	2.283046					
1	1.319197	-1.588294	2.353842					
1	2.617255	-.484665	2.898215					
8	.689632	.370270	2.798581					
6	.512049	.246260	4.240753					
1	.197470	-.770938	4.525544					
1	1.440378	.498306	4.776692					
1	-.270745	.957574	4.515591					

13 (R=OCH₂Me, 6-endo P)

Total energy = -677.49649

6	-2.537805	0.000000	-4.421518	
6	-2.476538	0.000000	-3.032979	
6	-1.214809	0.000000	-2.366183	
6	0.000427	0.000000	-3.163693	
6	-0.095923	0.000000	-4.588376	
6	-1.341891	0.000000	-5.203465	
1	-3.502832	0.000000	-4.922417	
1	-3.371908	0.000000	-2.418461	
7	-1.165607	0.000000	-0.988669	
6	1.192617	0.000000	-2.412190	
1	0.817457	0.000000	-5.177141	
1	-1.413011	0.000000	-6.288305	
6	1.273632	0.000000	-1.042589	
6	-0.000450	0.000000	-0.322185	
50	-0.265862	0.000000	1.841747	
6	0.401281	1.805327	2.790583	
1	0.120247	1.795179	3.852583	
1	1.485846	1.926007	2.708845	
1	-0.084097	2.671111	2.321150	
6	-2.404548	0.000000	2.053616	
1	-2.837651	0.885403	1.572393	
1	-2.837651	-0.885403	1.572393	
1	-2.686292	0.000000	3.116160	
6	0.401281	-1.805327	2.790583	
1	1.485846	-1.926007	2.708845	
1	0.120247	-1.795179	3.852583	
1	-0.084097	-2.671111	2.321150	
6	2.618488	0.000000	-0.344258	
1	3.195226	-0.890829	-0.641240	
1	3.195226	0.890829	-0.641240	
8	2.415642	0.000000	1.094049	
6	3.635659	0.000000	1.898650	
1	3.641869	0.895112	2.531220	