

Electronic Supplementary Information

Alkane C–H Activation and Ligand Exchange

on Silica Supported d^0 Metal Alkylidenes:

Relevance to Alkane Metathesis

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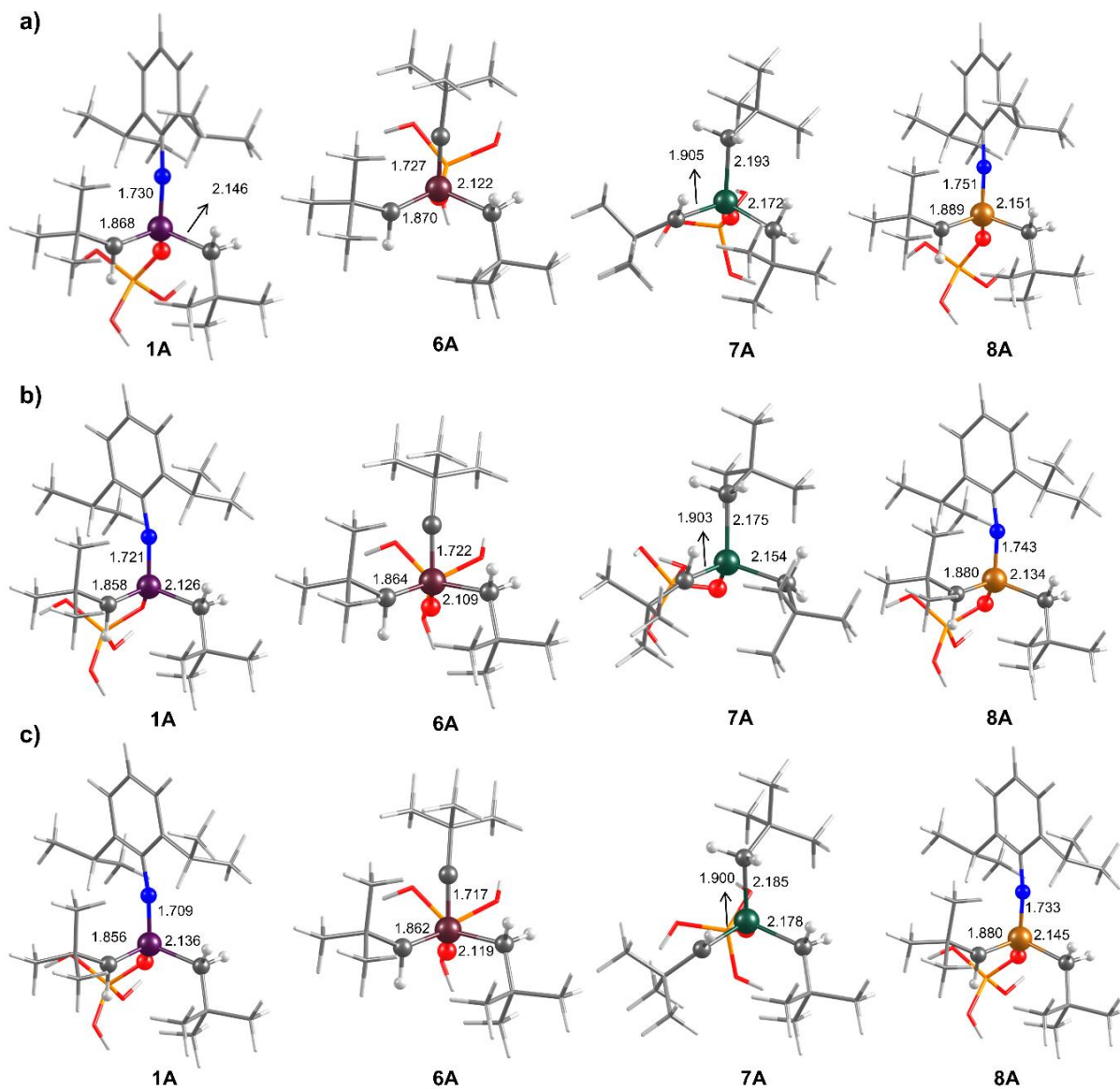


Figure S1. DFT/BS1 optimized structures of catalysts **1A**, **6A-8A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

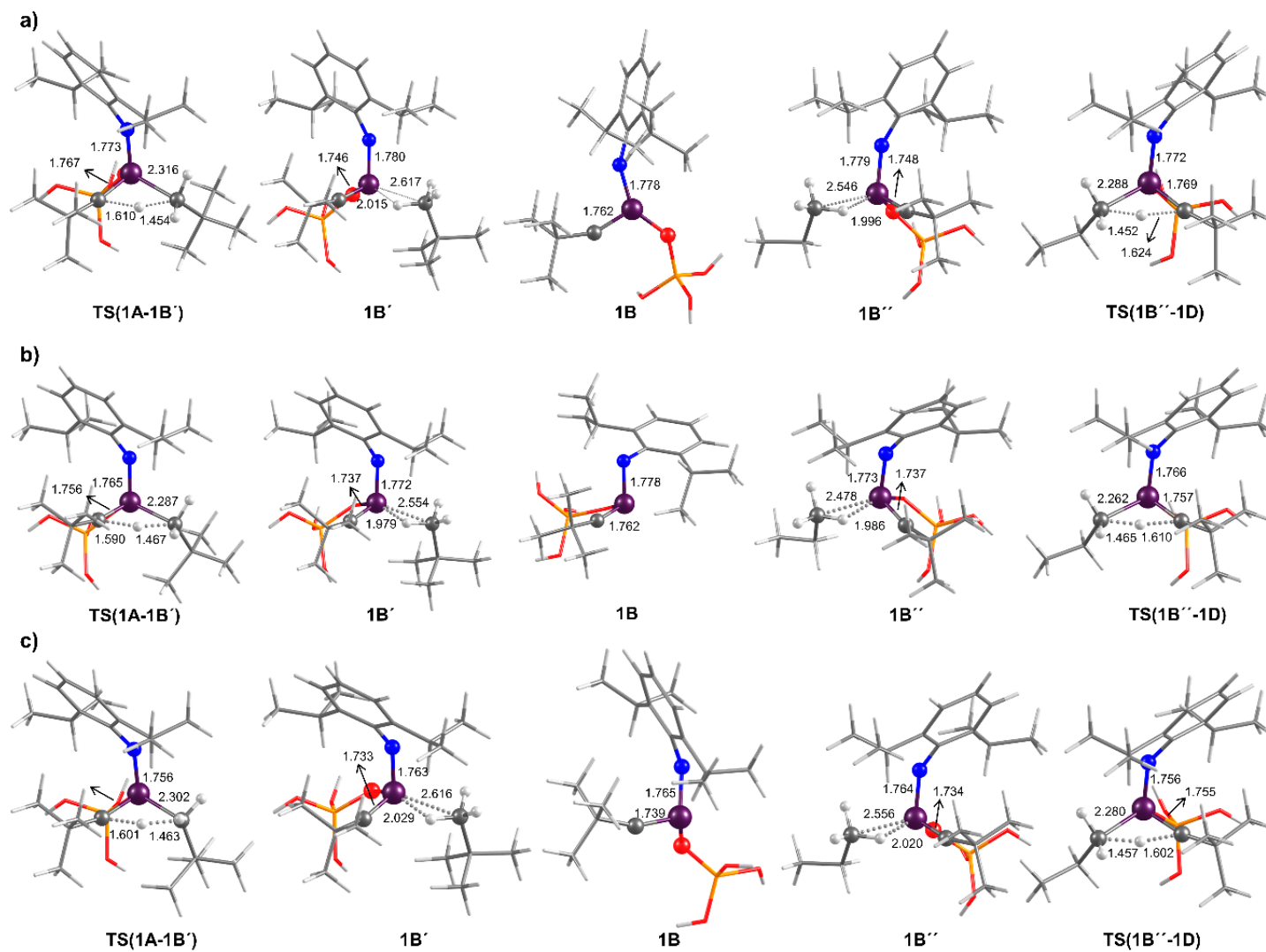


Figure S2. DFT/BS1 optimized structures of the minima and transition states involved in the α -H abstraction mechanism of ligand exchange between propane and catalyst **1A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

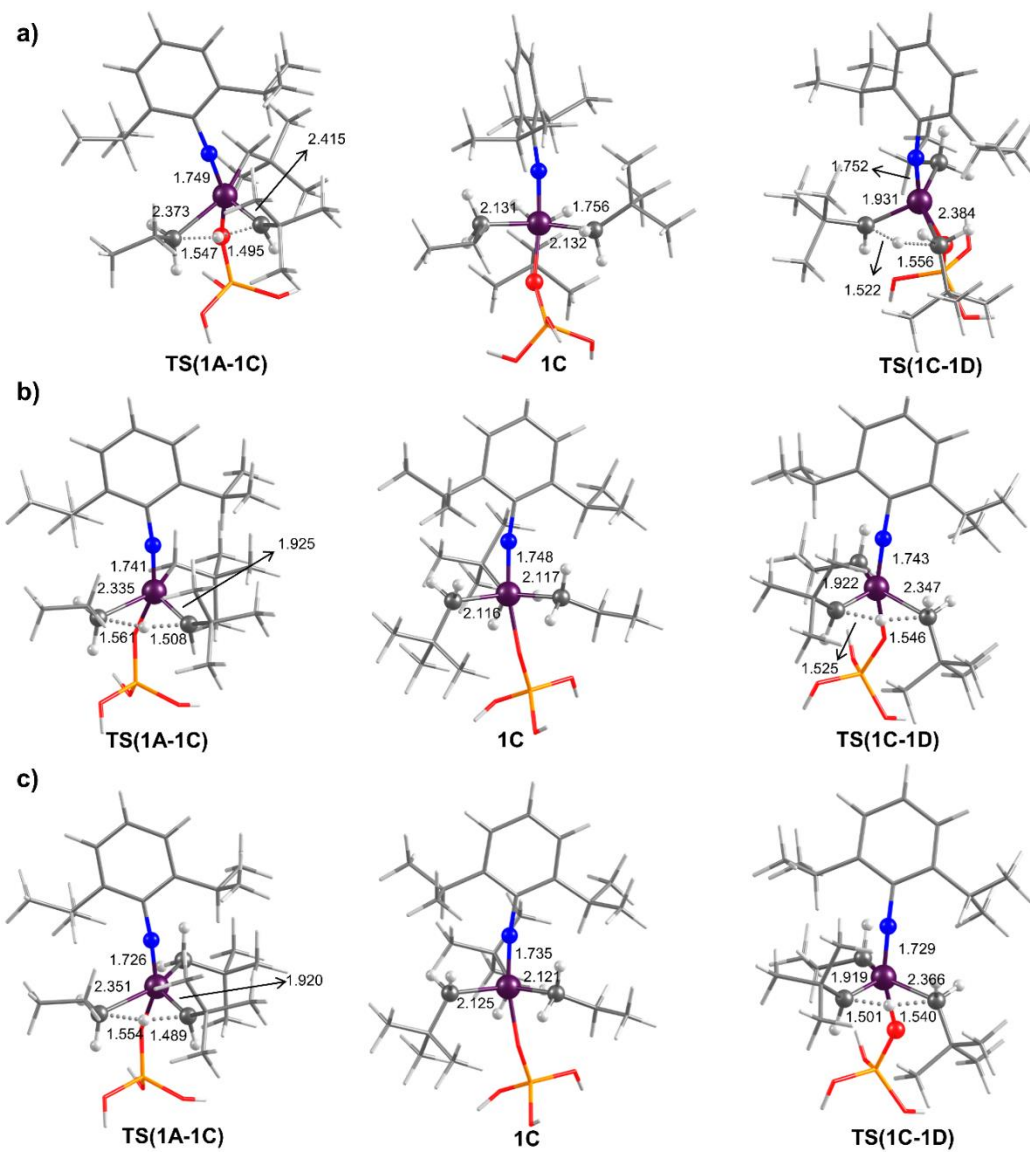


Figure S3. DFT/BS1 optimized structures of the minima and transition states involved in the C-H addition mechanism of ligand exchange between propane and catalyst **1A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

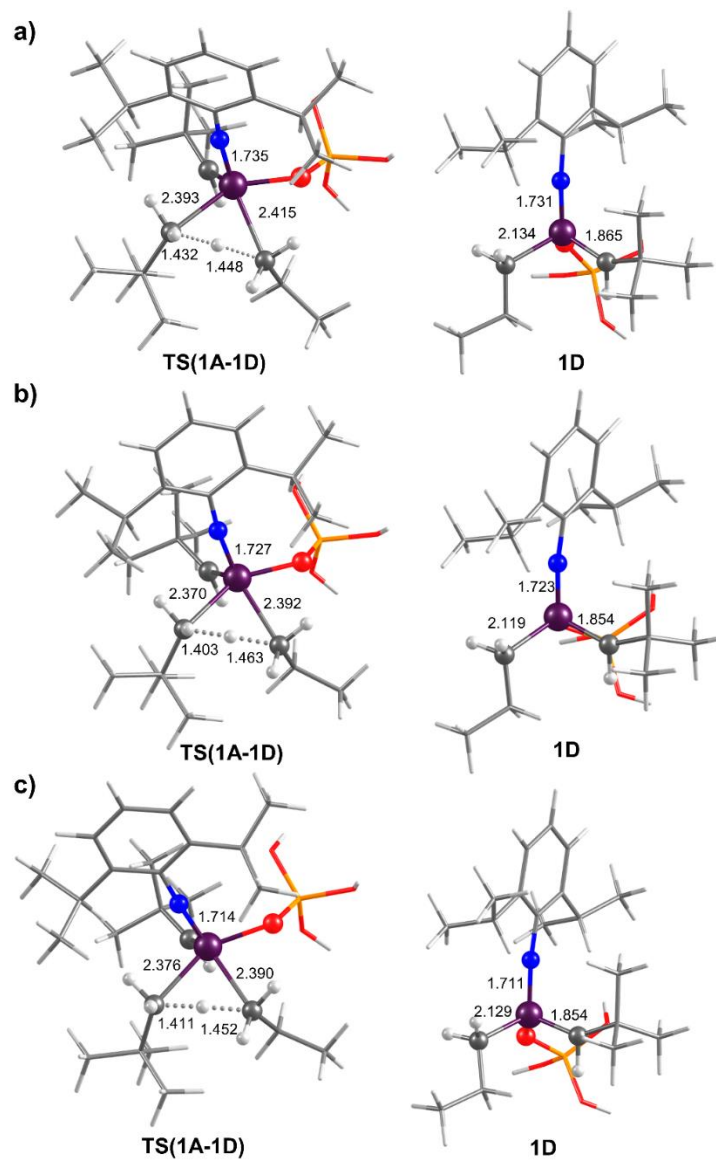


Figure S4. DFT/BS1 optimized structure of the transition state involved in the σ -bond metathesis mechanism of ligand exchange between propane and catalyst **1A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. The optimized structure of the product **1D** is also shown. Distances are given in Å.

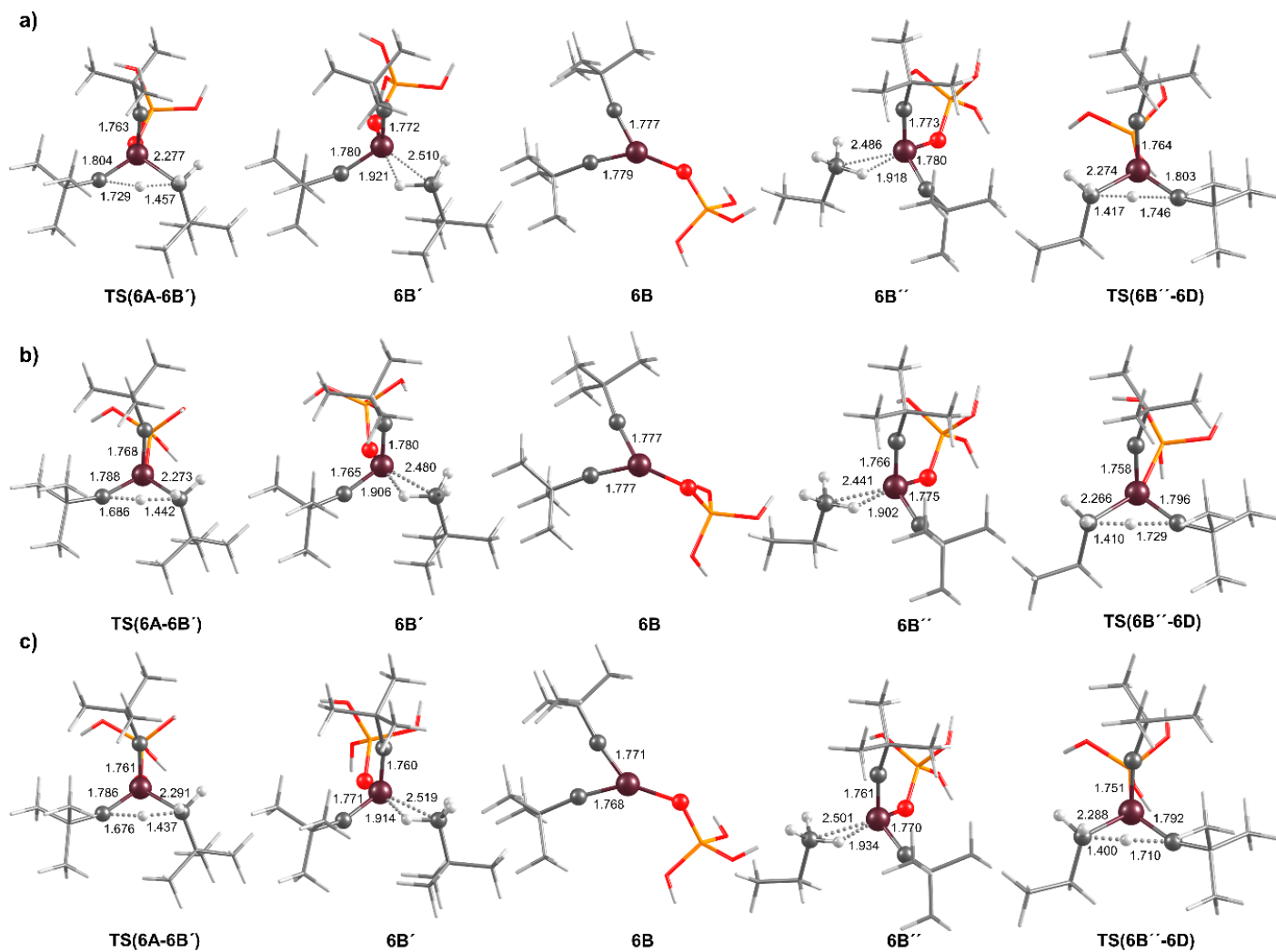


Figure S5. DFT/BS1 optimized structures of the minima and transition states involved in the α -H abstraction mechanism of ligand exchange between propane and catalyst **6A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

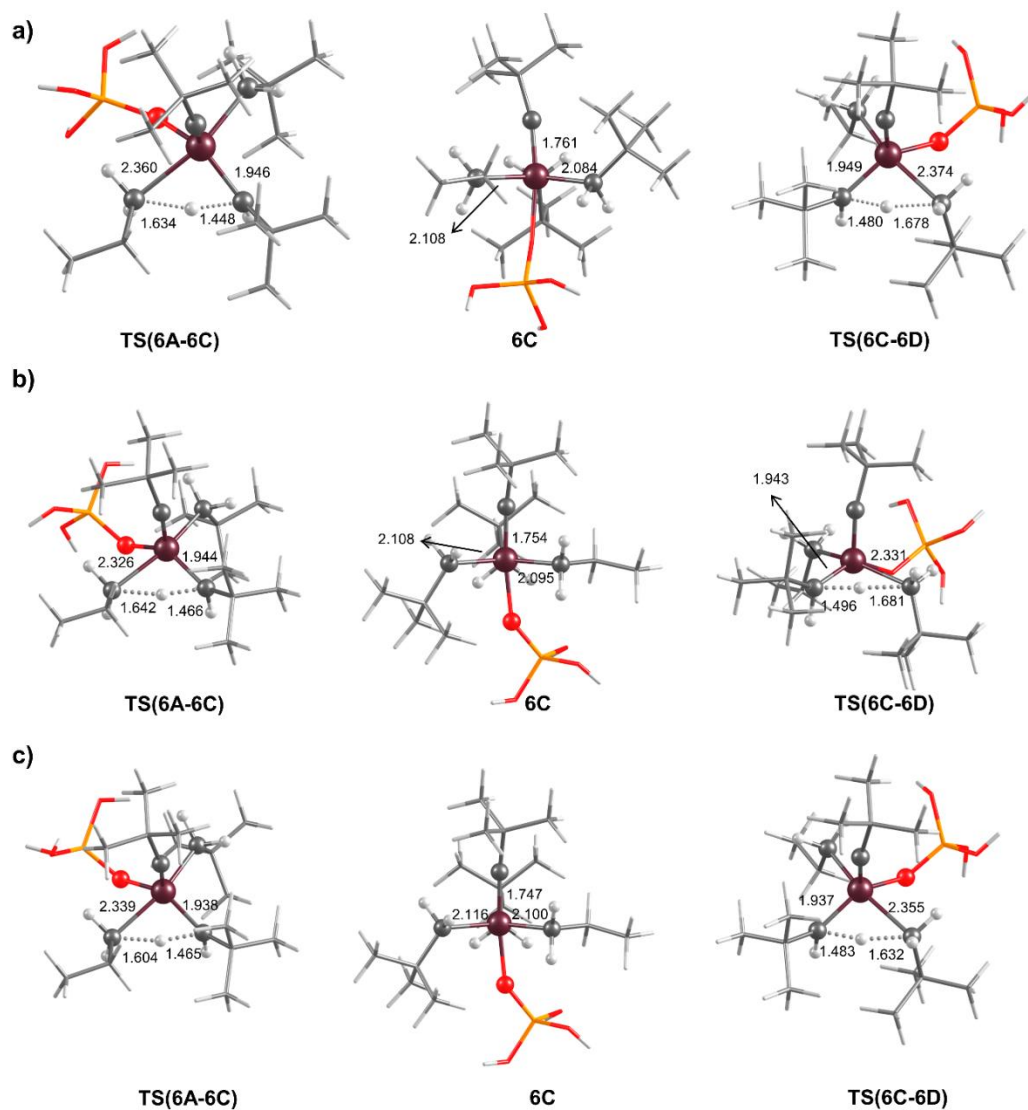


Figure S6. DFT/BS1 optimized structures of the minima and transition states involved in the C-H addition mechanism of ligand exchange between propane and catalyst **6A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

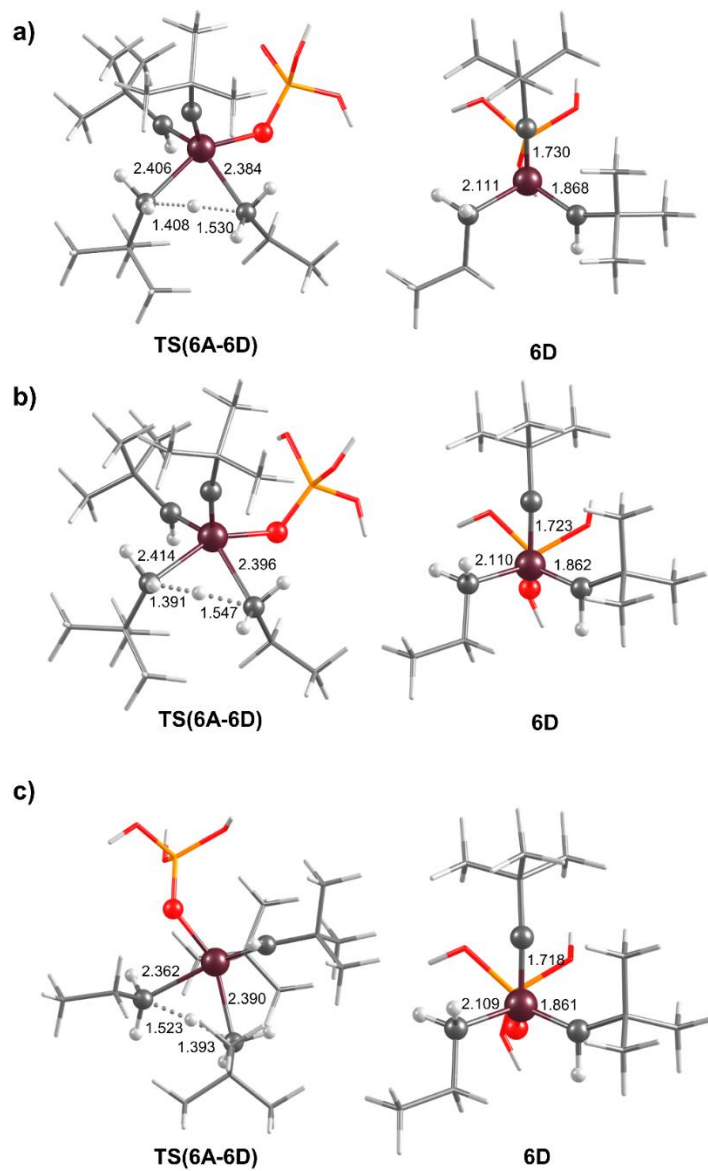


Figure S7. DFT/BS1 optimized structure of the transition state involved in the σ -bond metathesis mechanism of ligand exchange between propane and catalyst **6A** with functionals *a)* B3PW91; *b)* B3PW91-D3; *c)* ω B97xD. The optimized structure of the product **6D** is also shown. Distances are given in Å.

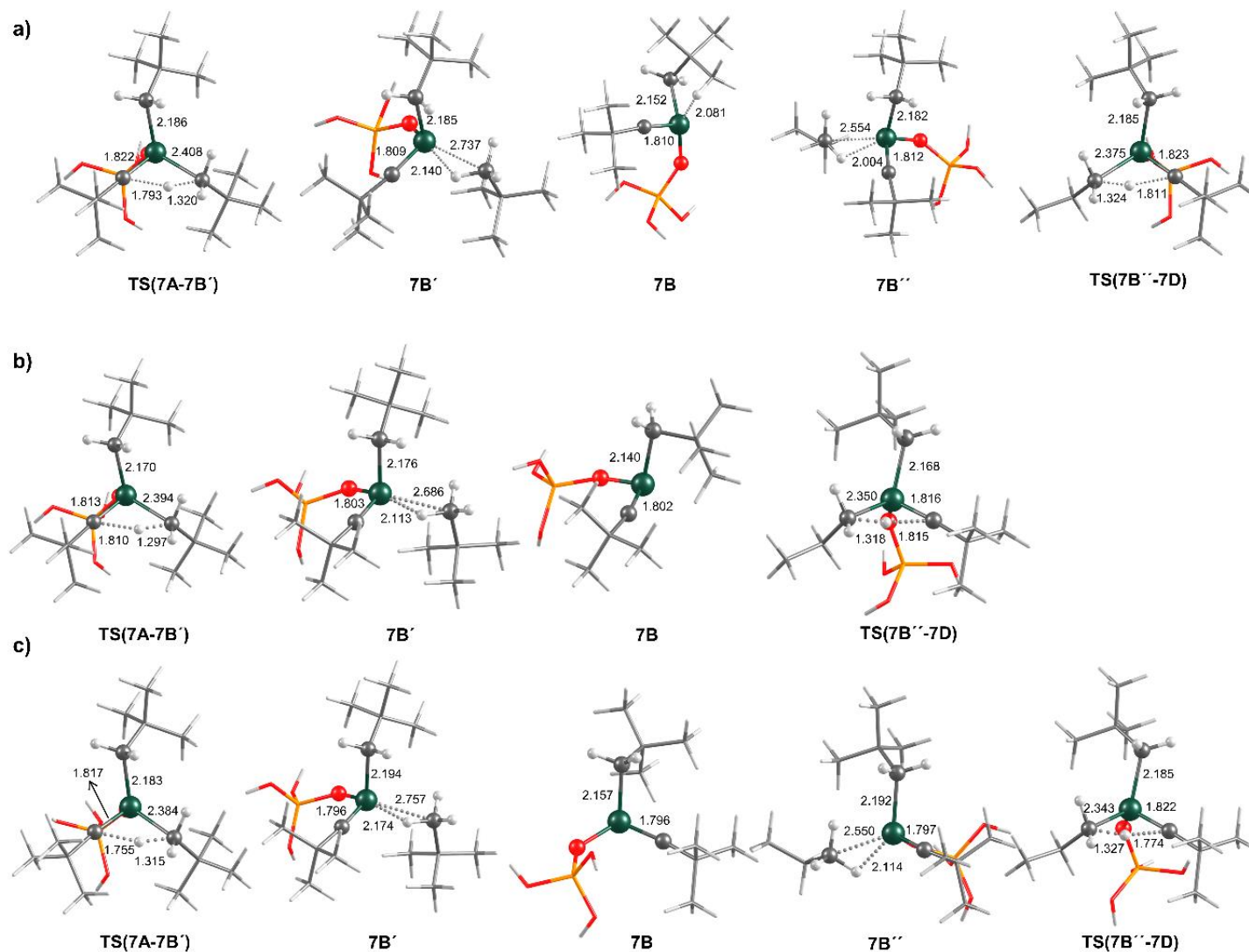


Figure S8. DFT/BS1 optimized structures of the minima and transition states involved in the α -H abstraction mechanism of ligand exchange between propane and catalyst **7A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

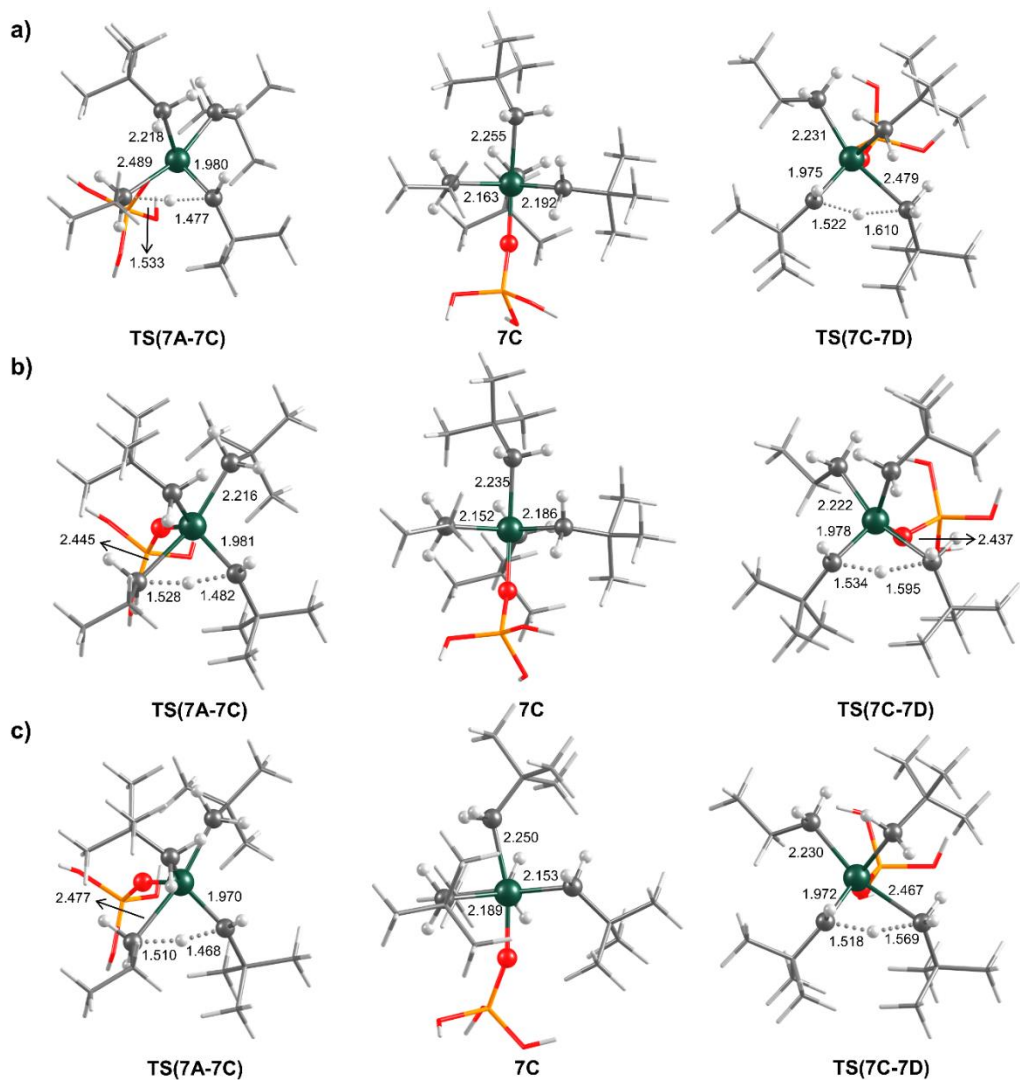


Figure S9. DFT/BS1 optimized structures of the minima and transition states involved in the C-H addition mechanism of ligand exchange between propane and catalyst **7A** with functionals a) B3PW91; b) B3PW91-D3; c) ω B97xD. Distances are given in Å.

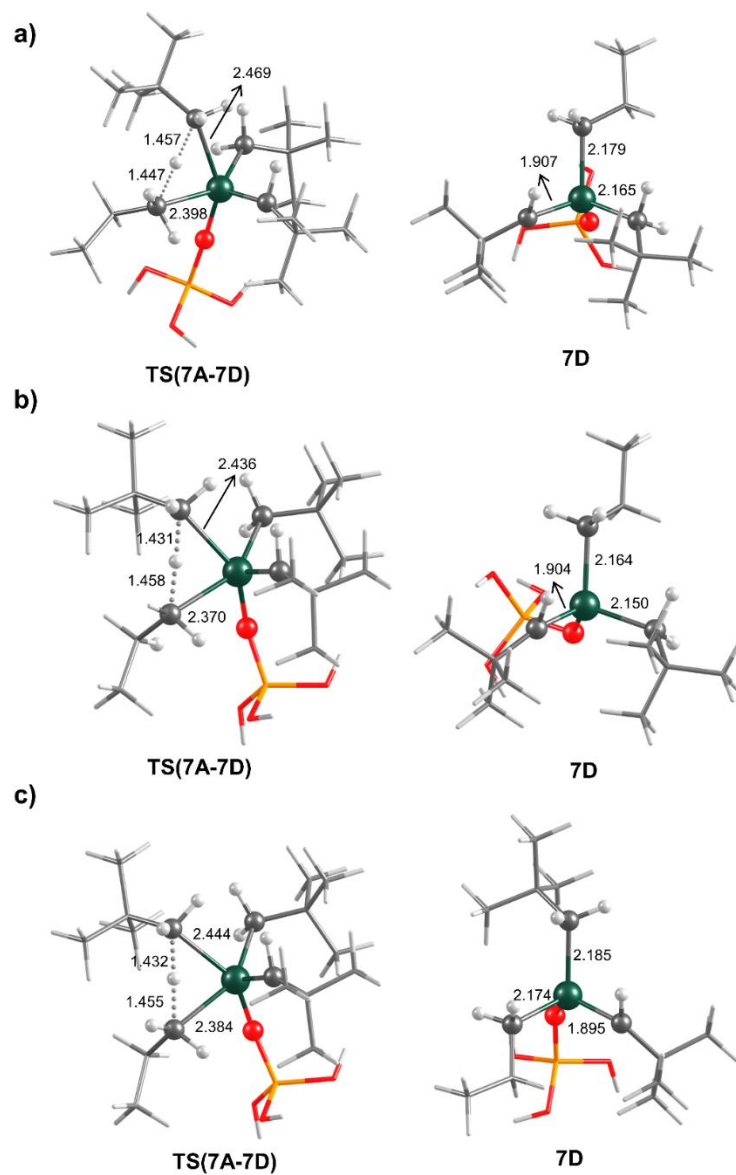


Figure S10. DFT/BS1 optimized structure of the transition state involved in the σ -bond metathesis mechanism of ligand exchange between propane and catalyst **7A** with functionals *a)* B3PW91; *b)* B3PW91-D3; *c)* ω B97xD. The optimized structure of the product **7D** is also shown. Distances are given in Å.

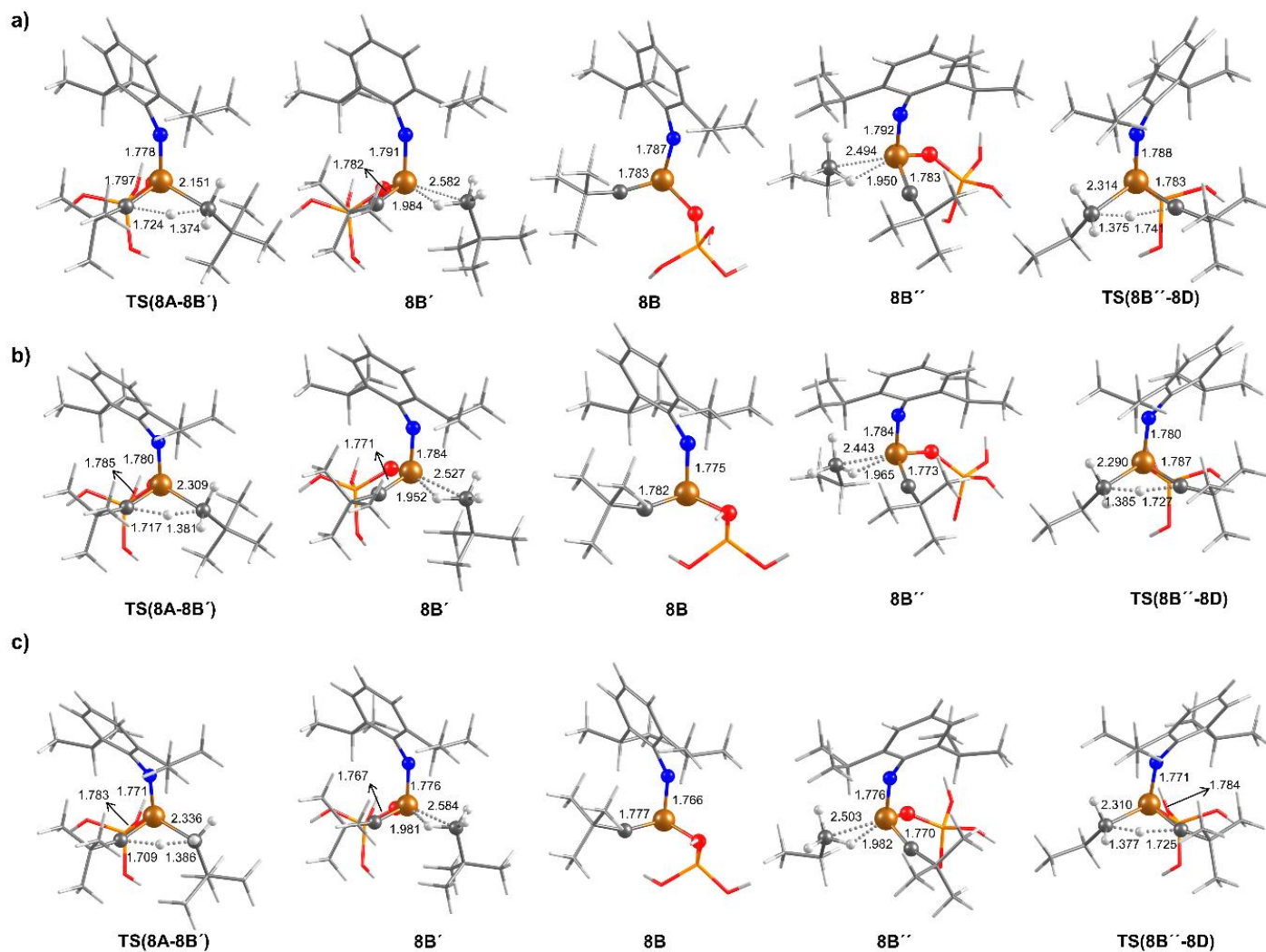


Figure S11. DFT/BS1 optimized structures of the minima and transition states involved in the α -H abstraction mechanism of ligand exchange with catalyst **8A** between propane and functionals *a)* B3PW91; *b)* B3PW91-D3; *c)* ω B97xD. Distances are given in Å.

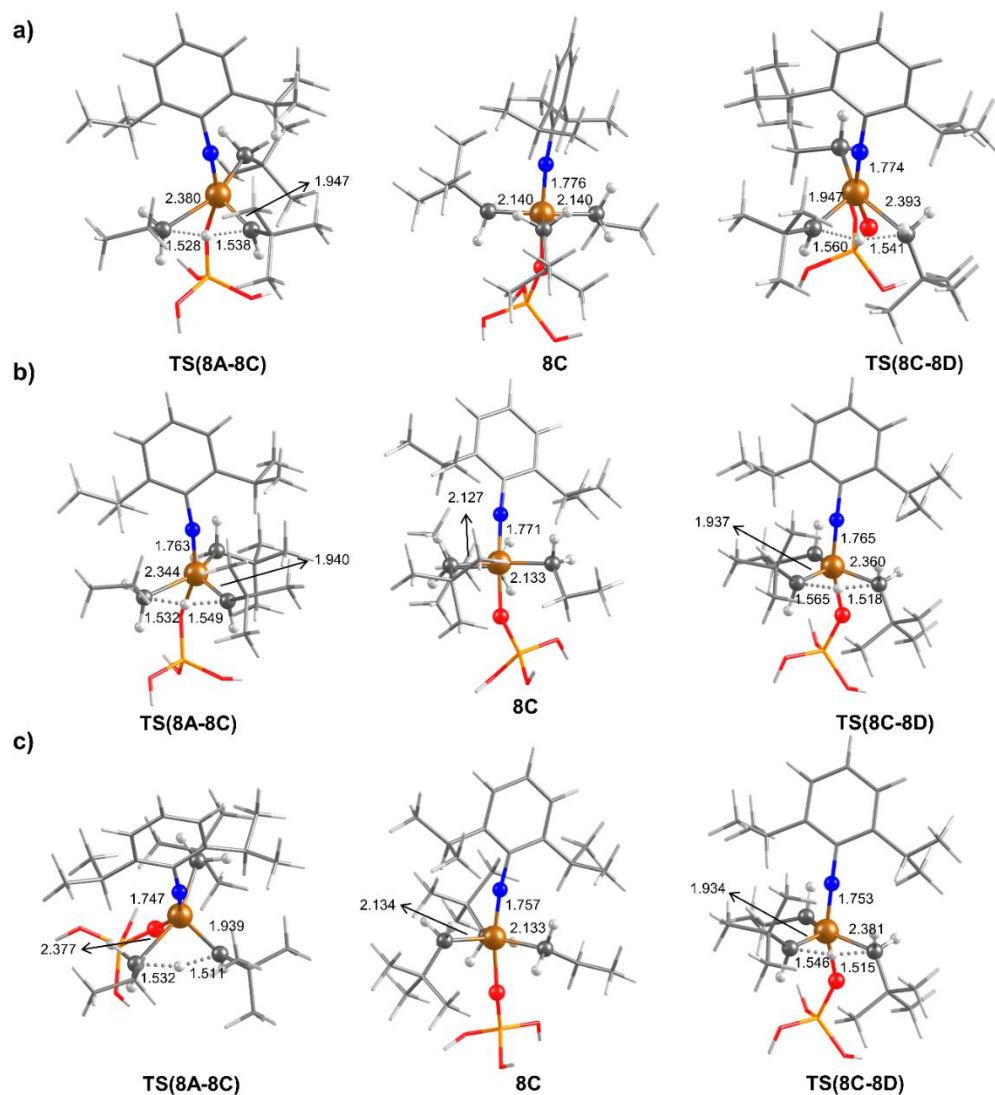


Figure S12. DFT/BS1 optimized structures of the minima and transition states involved in the C-H addition mechanism of ligand exchange with catalyst **8A** between propane and functionals *a)* B3PW91; *b)* B3PW91-D3; *c)* ω B97xD. Distances are given in Å.

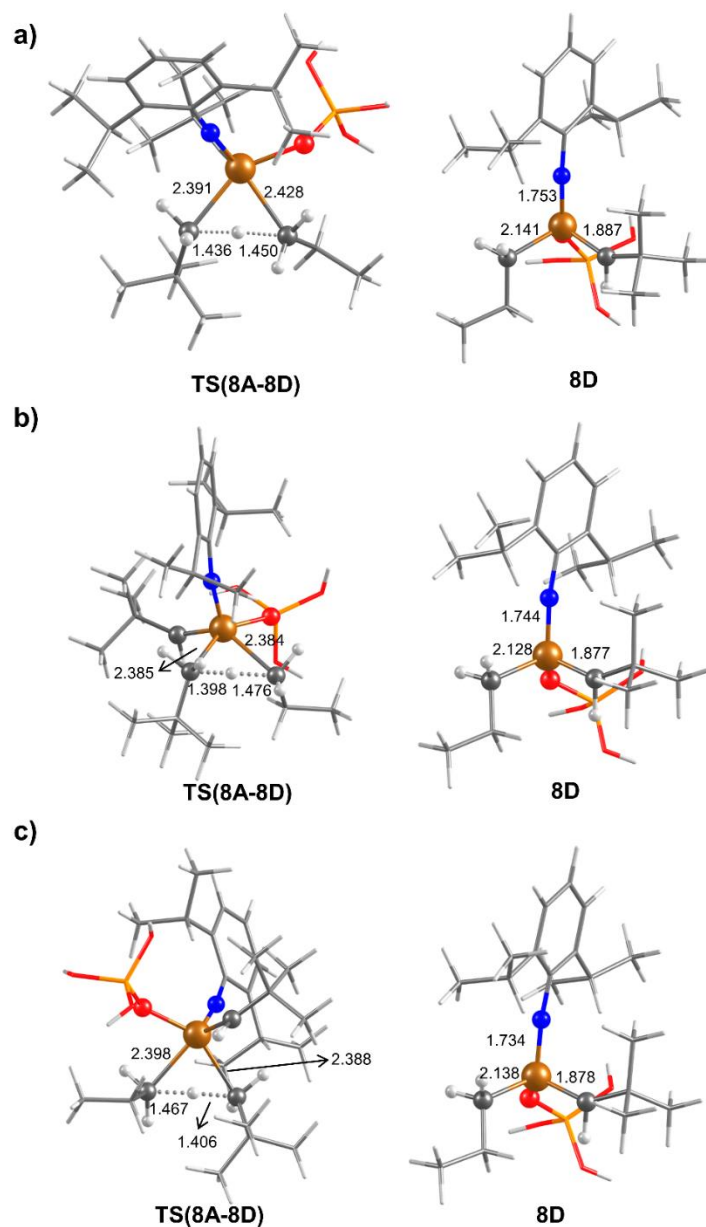


Figure S13. DFT/BS1 optimized structure of the transition state involved in the σ -bond metathesis mechanism of ligand exchange between propane and catalyst **8A** with functionals *a)* B3PW91; *b)* B3PW91-D3; *c)* ω B97xD. The optimized structure of the product **8D** is also shown. Distances are given in Å.

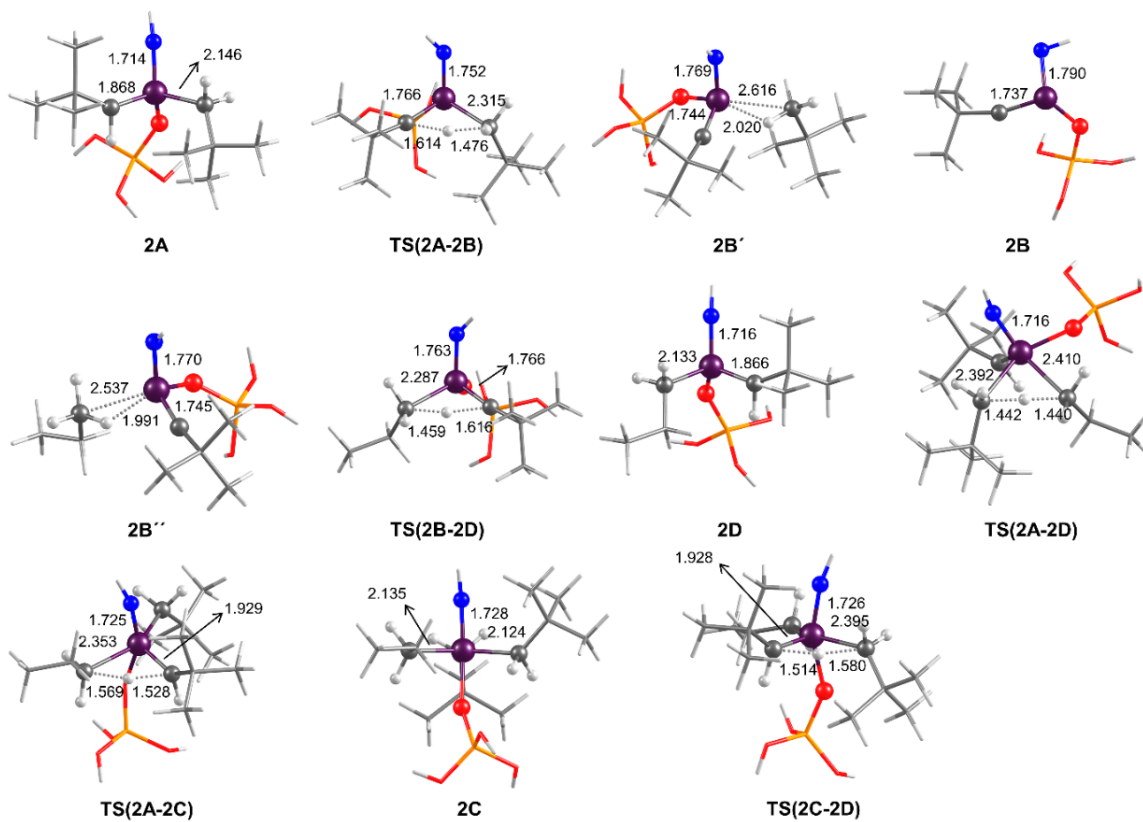


Figure S14. B3PW91/BS1 optimized structures of the minima and transition states involved in the three mechanisms of ligand exchange reaction between **2** and propane. Distances are given in Å.

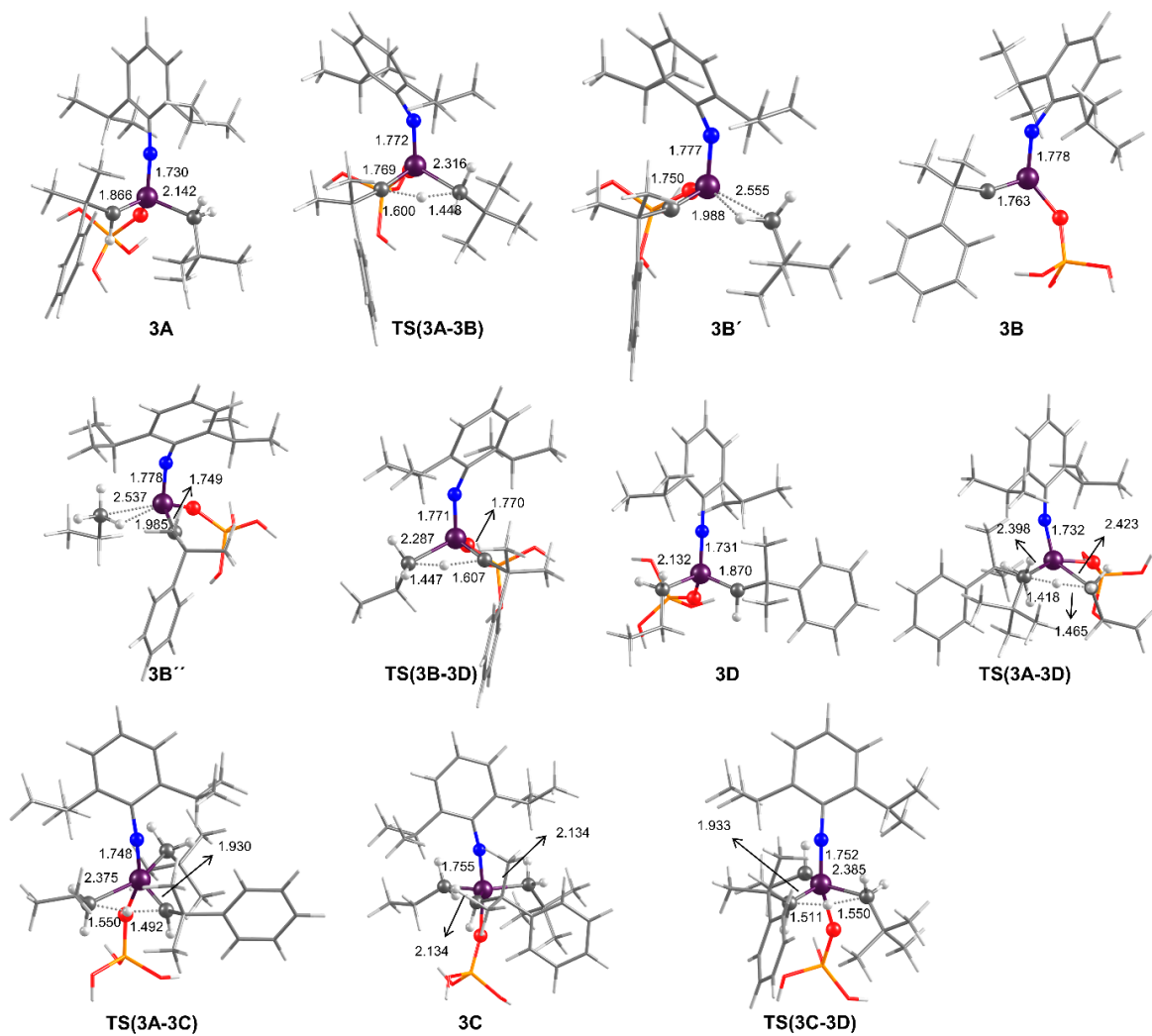


Figure S15. B3PW91/BS1 optimized structures of the minima and transition states involved in the three mechanisms of ligand exchange reaction between **3** and propane. Distances are given in Å.

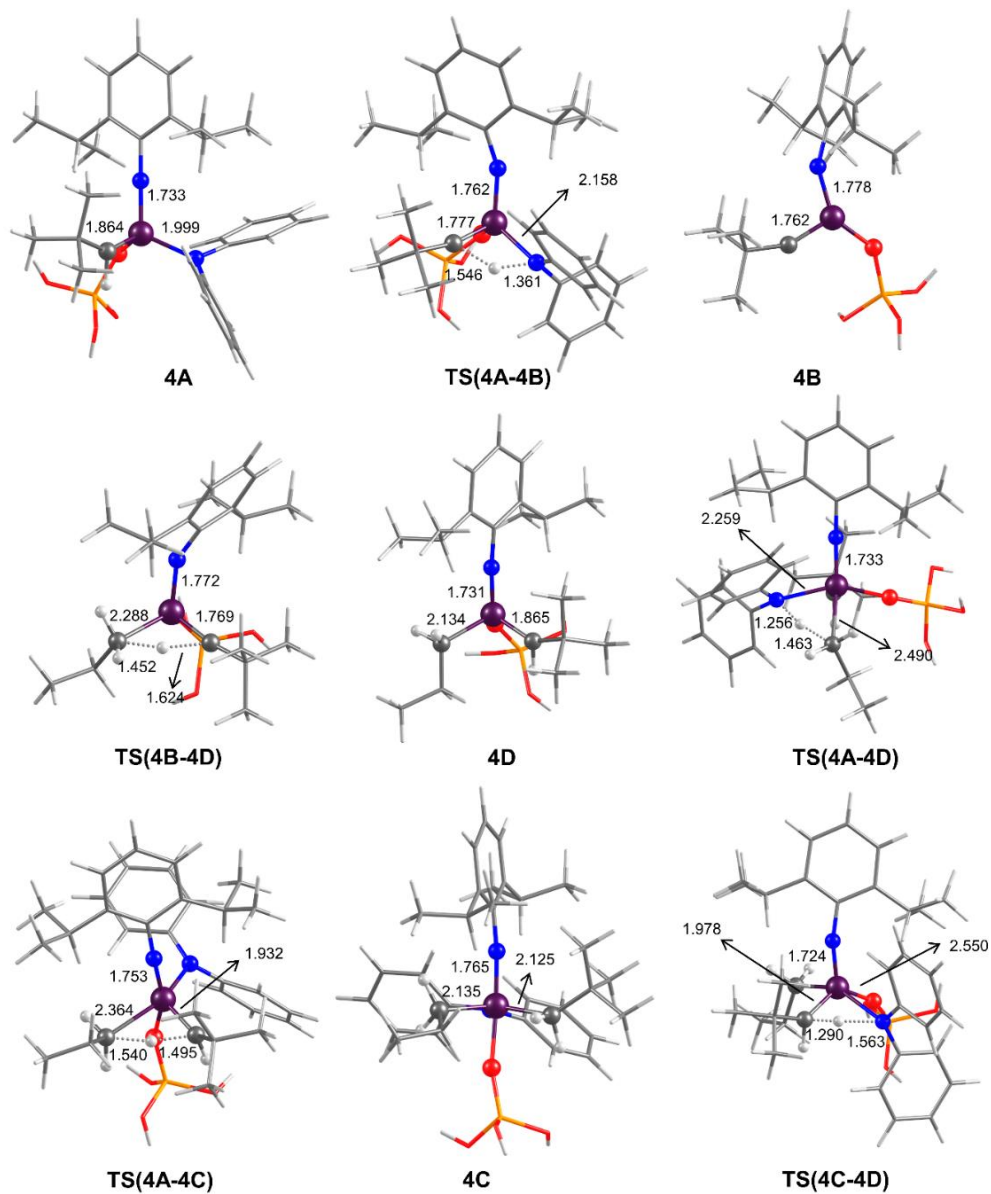


Figure S16. B3PW91/BS1 optimized structures of the minima and transition states involved in the three mechanisms of ligand exchange reaction between **4** and propane. Distances are given in Å.

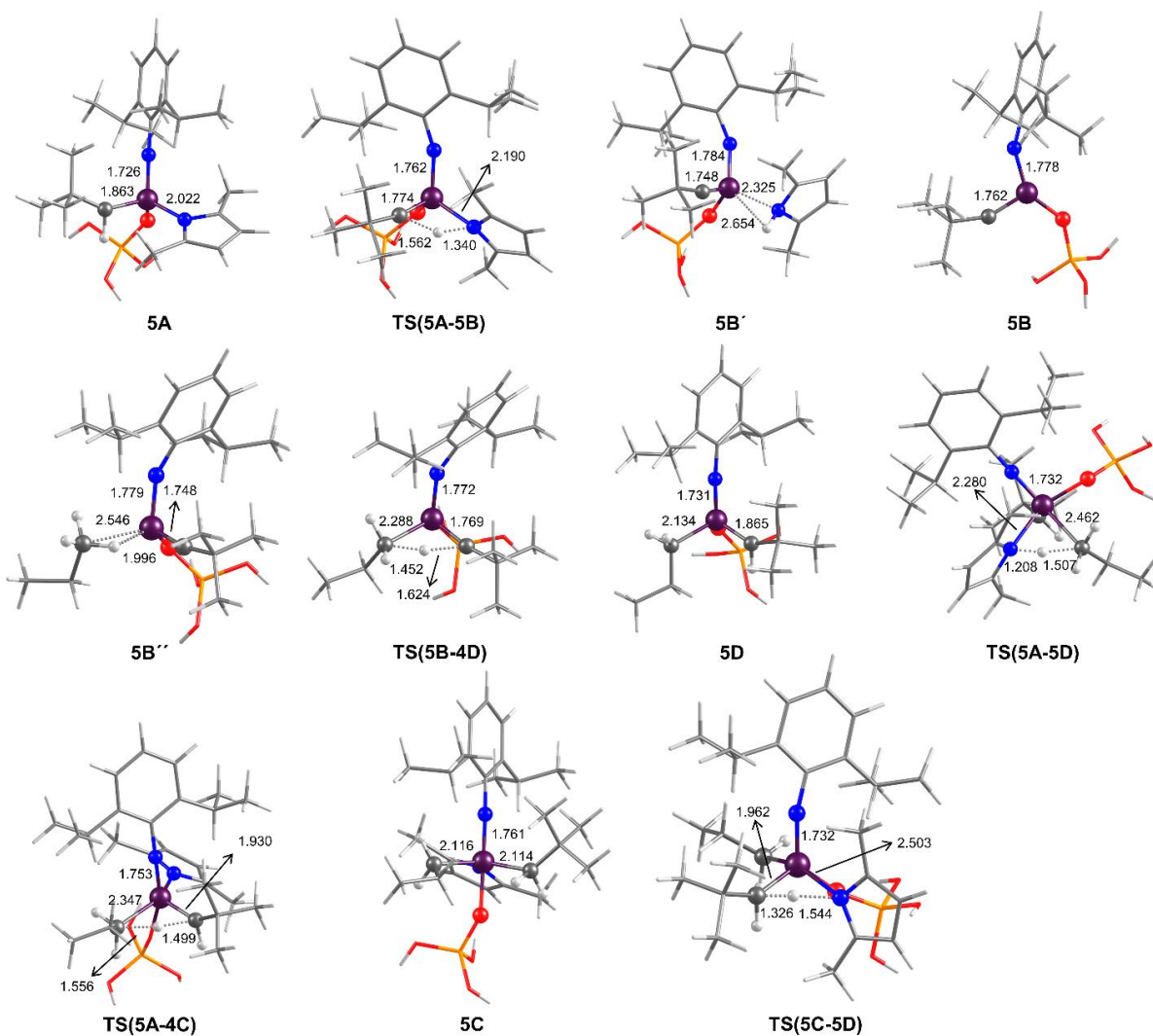


Figure S17. B3PW91/BS1 optimized structures of the minima and transition states involved in the three mechanisms of ligand exchange reaction between **5** and propane. Distances are given in Å.

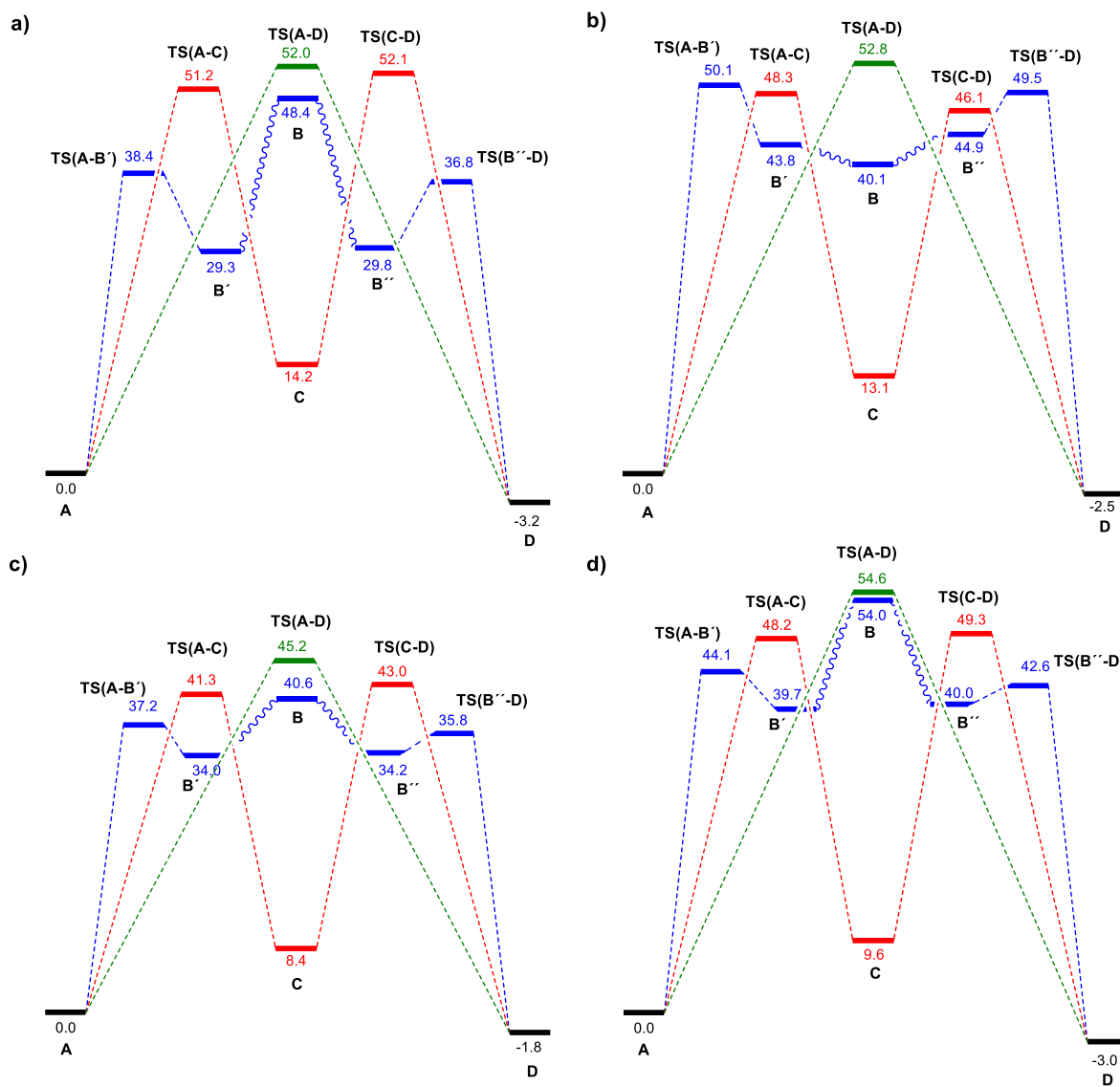


Figure S18. Electronic energy profiles (kcal mol⁻¹) for the ligand exchange between propane and catalysts *a*) **1A**; *b*) **6A**; *c*) **7A**; *d*) **8A** calculated at the B3PW91/BS1 level of theory. The three pathways are color coded: α -H abstraction in blue, σ -bond metathesis in green and C-H addition in red.

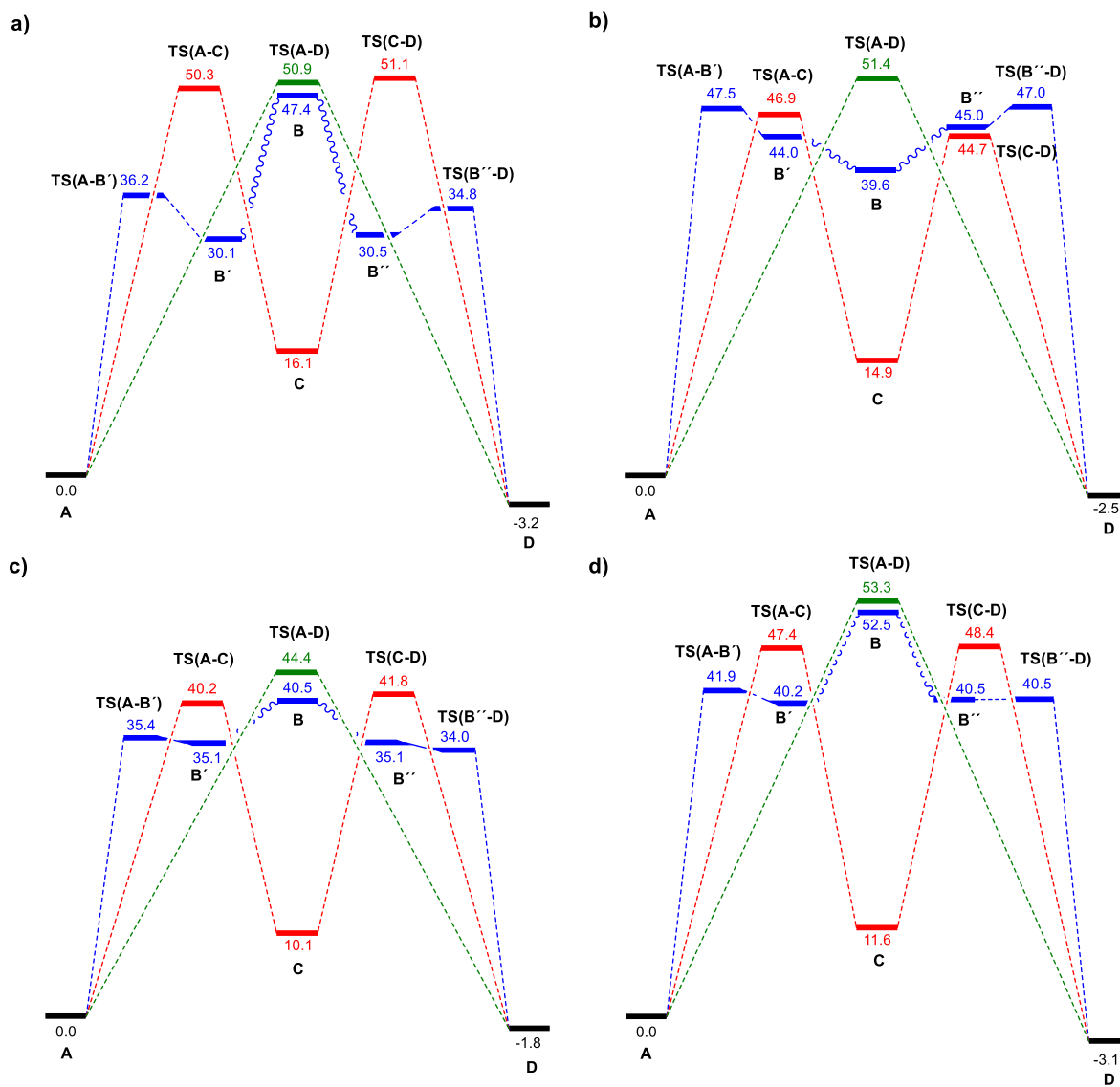


Figure S19. Enthalpic energy profiles at 150°C (kcal mol⁻¹) for the ligand exchange between propane and catalysts *a)* **1A**; *b)* **6A**; *c)* **7A**; *d)* **8A** calculated at the B3PW91/BS1 level of theory. The three pathways are color coded: α -H abstraction in blue, σ -bond metathesis in green and C-H addition in red.

Table S1. Gibbs free energies at 150°C (ΔG_{150}) and their ΔH and $T\Delta S_{\text{tot}}$ components (in kcal mol⁻¹) of the intermediates and transition states involved in the ligand exchange process between propane and catalysts **1A**, **6A-8A** at the B3PW91-D3/BS1 level. The origin of energies is the system **A** + propane.

	1A			6A			7A			8A		
	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$
TS(A-B')	34.4	34.7	0.3	42.9	45.2	2.3	33.1	35.8	2.8	38.9	41.8	2.9
B'	28.1	29.2	1.1	39.4	41.4	2.0	31.2	36.1	4.8	36.1	40.2	4.1
B	33.7	55.2	21.5	30.2	55.1	24.9	32.9	52.5	19.7	43.9	63.4	19.4
B''	28.6	34.7	6.1	43.6	50.2	6.6	-	-	-	38.5	45.0	6.4
TS(B''-D)	33.6	39.1	5.5	44.6	51.7	7.1	32.6	39.0	6.4	41.4	44.5	3.1
TS(A-D)	54.7	36.5	-18.2	56.4	40.7	-15.7	46.0	29.4	-16.6	55.6	38.5	-17.1
TS(A-C)	53.1	35.0	-18.1	54.2	37.3	-16.9	43.8	27.9	-15.9	49.7	31.6	-18.1
C	16.3	0.3	-16.0	17.0	0.6	-16.4	15.6	-3.1	-18.7	12.9	-2.4	-15.3
TS(C-D)	56.1	35.5	-20.5	48.2	35.8	-12.5	45.1	29.2	-15.8	52.4	32.2	-20.2
D	-0.5	2.0	2.5	-1.5	2.8	4.3	-2.3	3.0	5.3	-0.5	2.0	2.5

Table S2. Gibbs free energies at 150°C (ΔG_{150}) and their ΔH and $T\Delta S_{\text{tot}}$ components (in kcal mol⁻¹) of the intermediates and transition states involved in the ligand exchange process between propane and catalysts **1A**, **6A-8A** at the ω B97xD/BS1 level. The origin of energies is the system **A** + propane.

	1A			6A			7A			8A		
	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$	ΔG	ΔH	$T\Delta S_{\text{tot}}$
TS(A-B')	38.3	37.4	-1.0	46.7	48.3	1.6	38.0	35.4	-2.5	49.0	45.1	-3.9
B'	30.1	30.9	0.7	43.8	47.3	3.5	36.2	37.7	1.6	42.7	42.8	0.1
B	26.5	43.9	17.4	26.3	48.1	21.8	35.5	52.4	16.8	46.5	62.5	16.0
B''	29.5	33.4	3.9	46.5	50.6	4.1	39.6	41.1	1.5	47.1	46.5	-0.5
TS(B''-D)	38.2	39.5	1.4	50.3	52.8	2.5	37.2	37.2	0.0	47.4	47.1	-0.3
TS(A-D)	62.9	42.2	-20.7	62.5	43.5	-18.9	55.1	32.5	-22.6	67.5	44.2	-23.3
TS(A-C)	63.0	39.4	-23.6	55.6	37.3	-18.3	50.3	29.5	-20.9	59.0	36.6	-22.4
C	24.4	5.9	-18.5	22.2	3.8	-18.5	16.3	-3.8	-20.1	22.6	0.3	-22.3
TS(C-D)	62.8	41.2	-21.6	52.6	35.3	-17.4	54.2	31.7	-22.5	62.4	38.1	-24.3
D	-0.7	0.8	1.5	-0.8	1.0	1.8	-1.4	1.6	3.0	2.3	1.7	-0.7

**Cartesian coordinates of all reactants, products, intermediates, and
transition states**

1A

E = -1290.6776170

Mo	0.605595000	0.190231000	-0.204474000
C	0.905648000	2.088908000	-1.157828000
H	0.804795000	1.775578000	-2.216024000
H	0.035848000	2.724565000	-0.954353000
C	2.193418000	2.930539000	-1.015285000
N	-1.116418000	0.033100000	-0.248634000
O	1.796254000	-1.120252000	-0.967951000
Si	3.040388000	-2.108744000	-0.517371000
C	0.978063000	0.507470000	1.598019000
H	2.090413000	0.494145000	1.584274000
C	0.407148000	0.599471000	2.994075000
O	4.122028000	-1.416016000	0.544092000
H	4.853690000	-0.981367000	0.094088000
O	3.938596000	-2.498820000	-1.866345000
H	3.403292000	-2.619342000	-2.657041000
O	2.354308000	-3.413505000	0.246736000
H	2.992355000	-3.943837000	0.734452000
C	-2.436495000	-0.364230000	-0.326089000
C	-3.445857000	0.630682000	-0.410246000
C	-2.765223000	-1.746809000	-0.310993000
C	-4.774962000	0.215505000	-0.493318000
C	-4.112284000	-2.099886000	-0.389395000
C	-5.110554000	-1.134405000	-0.483150000
H	-5.562541000	0.959955000	-0.564150000
H	-4.388801000	-3.149921000	-0.377162000
H	-6.152712000	-1.435946000	-0.545554000
C	2.203028000	3.984120000	-2.139337000
H	3.089984000	4.626206000	-2.072049000
H	2.207651000	3.509212000	-3.127338000
H	1.317956000	4.627708000	-2.081920000
C	2.224025000	3.656022000	0.334396000
H	1.355038000	4.315265000	0.443837000
H	2.210663000	2.946711000	1.166167000
H	3.125569000	4.273387000	0.425182000
C	3.449272000	2.057493000	-1.157482000
H	3.526541000	1.328556000	-0.342097000
H	3.444248000	1.505118000	-2.104339000
H	4.357147000	2.672004000	-1.132665000
C	-1.121224000	0.703469000	2.975879000
H	-1.508255000	0.766559000	3.999473000
H	-1.447674000	1.594706000	2.431486000
H	-1.571929000	-0.167032000	2.492045000
C	0.995426000	1.836634000	3.699791000
H	0.627451000	1.895426000	4.730885000
H	2.089758000	1.792138000	3.736627000
H	0.708525000	2.758012000	3.183778000
C	0.827503000	-0.668024000	3.767062000
H	0.424257000	-1.566636000	3.290018000
H	1.917655000	-0.766802000	3.806653000
H	0.453165000	-0.627317000	4.797186000

C	-1.679692000	-2.805265000	-0.255818000
H	-0.816135000	-2.364184000	0.256363000
C	-3.078889000	2.101722000	-0.461743000
H	-2.090220000	2.196354000	0.000945000
C	-2.953547000	2.568621000	-1.921060000
H	-3.914159000	2.480919000	-2.441552000
H	-2.638808000	3.617312000	-1.967869000
H	-2.219564000	1.968487000	-2.467104000
C	-4.045803000	2.999431000	0.317392000
H	-3.660526000	4.024099000	0.350449000
H	-5.035528000	3.045189000	-0.150346000
H	-4.175436000	2.652323000	1.347228000
C	-2.075883000	-4.055357000	0.535751000
H	-2.853049000	-4.636916000	0.027306000
H	-1.205823000	-4.709505000	0.649742000
H	-2.443691000	-3.800259000	1.534664000
C	-1.229336000	-3.181682000	-1.676700000
H	-0.402359000	-3.898170000	-1.637709000
H	-2.055517000	-3.637055000	-2.234742000
H	-0.890970000	-2.302458000	-2.233070000

1B

E = -1092.8841856

Mo	-0.703102000	-0.177728000	-0.241455000
N	1.033010000	-0.352490000	0.101632000
O	-1.944115000	1.238141000	-0.742239000
Si	-3.569339000	1.540964000	-0.769132000
C	-1.412331000	-1.598567000	0.521556000
C	-1.430290000	-2.862297000	1.305368000
O	-4.167411000	0.740221000	-2.096050000
H	-5.127716000	0.679427000	-2.094143000
O	-3.790502000	3.196592000	-0.818420000
H	-3.114867000	3.642446000	-1.338921000
O	-4.439405000	1.028513000	0.551970000
H	-4.431182000	1.665580000	1.272949000
C	2.292331000	0.175144000	0.034427000
C	3.130684000	-0.188077000	-1.063426000
C	2.775359000	1.021429000	1.075710000
C	4.434858000	0.297352000	-1.085163000
C	4.092147000	1.469341000	0.998576000
C	4.917535000	1.118788000	-0.067543000
H	5.091174000	0.031021000	-1.908039000
H	4.484187000	2.107283000	1.785132000
H	5.938830000	1.487155000	-0.106666000
C	-0.564110000	-3.914997000	0.587930000
H	-0.584036000	-4.858985000	1.145010000
H	-0.937412000	-4.106962000	-0.423016000
H	0.473790000	-3.577799000	0.513675000
C	-2.887947000	-3.359159000	1.406089000
H	-2.924445000	-4.288851000	1.986732000
H	-3.521629000	-2.616230000	1.898691000
H	-3.303996000	-3.554470000	0.413421000
C	-0.869499000	-2.586245000	2.713169000
H	0.162257000	-2.227380000	2.654968000
H	-1.468773000	-1.830828000	3.231177000
H	-0.884572000	-3.505197000	3.310678000

C	1.855447000	1.427048000	2.210130000
H	1.125828000	0.613966000	2.330163000
C	2.565822000	-1.058699000	-2.167831000
H	1.896015000	-1.782197000	-1.680888000
C	1.701219000	-0.231827000	-3.135370000
H	2.302439000	0.524718000	-3.652231000
H	1.235767000	-0.875199000	-3.890081000
H	0.899559000	0.302312000	-2.608581000
C	3.623477000	-1.845090000	-2.945535000
H	3.137787000	-2.546884000	-3.631061000
H	4.258038000	-1.190155000	-3.553195000
H	4.271023000	-2.419528000	-2.275990000
C	2.572642000	1.609041000	3.550977000
H	3.235284000	2.481746000	3.548008000
H	1.839999000	1.766846000	4.349220000
H	3.171585000	0.730157000	3.808698000
C	1.065961000	2.695400000	1.843645000
H	0.354907000	2.952629000	2.636857000
H	1.741319000	3.546883000	1.702563000
H	0.500449000	2.567753000	0.914051000

1B'

E = -1290.6308716

Mo	0.663251000	0.214310000	-0.325439000
C	1.363387000	2.725396000	-0.564285000
H	0.952656000	2.409374000	-1.532071000
H	0.792439000	3.616089000	-0.282102000
C	2.876062000	2.989847000	-0.638892000
N	-1.041768000	0.226133000	-0.833605000
O	1.528223000	-1.359987000	-1.092139000
Si	2.419561000	-2.588705000	-0.457243000
C	0.660199000	0.001075000	1.407938000
H	1.151224000	2.055760000	0.332386000
C	0.350177000	-0.240753000	2.846632000
O	3.870971000	-2.138053000	0.233944000
H	4.591497000	-2.163804000	-0.403716000
O	2.856543000	-3.612411000	-1.705732000
H	2.178513000	-3.664238000	-2.387108000
O	1.522771000	-3.342232000	0.726458000
H	2.040588000	-3.982487000	1.224761000
C	-2.370923000	0.090092000	-0.477071000
C	-3.149551000	1.239199000	-0.171289000
C	-2.962710000	-1.204065000	-0.483362000
C	-4.501900000	1.067612000	0.126863000
C	-4.316451000	-1.313386000	-0.164296000
C	-5.086751000	-0.194369000	0.137934000
H	-5.110882000	1.935127000	0.363019000
H	-4.781457000	-2.294430000	-0.150930000
H	-6.139742000	-0.306016000	0.381692000
C	3.127508000	4.089560000	-1.679908000
H	4.198575000	4.301072000	-1.766428000
H	2.764706000	3.792081000	-2.670407000
H	2.624385000	5.022437000	-1.402454000
C	3.380511000	3.443593000	0.737516000
H	2.871538000	4.357098000	1.064827000
H	3.213063000	2.669633000	1.494946000

H	4.454935000	3.652703000	0.706529000
C	3.598578000	1.702289000	-1.057184000
H	3.436598000	0.890366000	-0.333206000
H	3.270895000	1.358227000	-2.045665000
H	4.681210000	1.861965000	-1.109413000
C	-0.706707000	-1.359599000	2.933359000
H	-0.931042000	-1.576513000	3.985045000
H	-1.633066000	-1.061578000	2.434604000
H	-0.336768000	-2.271953000	2.458273000
C	-0.200197000	1.051151000	3.478426000
H	-0.421929000	0.885740000	4.539376000
H	0.527702000	1.867106000	3.410797000
H	-1.121405000	1.365990000	2.979776000
C	1.632968000	-0.680637000	3.578255000
H	2.042207000	-1.586331000	3.123453000
H	2.401085000	0.098174000	3.531862000
H	1.416166000	-0.885031000	4.633864000
C	-2.133562000	-2.418861000	-0.864355000
H	-1.139813000	-2.289285000	-0.420068000
C	-2.522925000	2.621805000	-0.229427000
H	-1.500245000	2.520329000	0.155862000
C	-2.425887000	3.105249000	-1.685907000
H	-3.426443000	3.213681000	-2.119088000
H	-1.926843000	4.080178000	-1.746294000
H	-1.869900000	2.391095000	-2.300602000
C	-3.229560000	3.667184000	0.637290000
H	-2.650493000	4.597002000	0.652082000
H	-4.223075000	3.917120000	0.248702000
H	-3.347756000	3.324888000	1.670317000
C	-2.691469000	-3.743871000	-0.339871000
H	-3.631701000	-4.019127000	-0.831896000
H	-1.976499000	-4.549288000	-0.536593000
H	-2.869943000	-3.709964000	0.739712000
C	-1.946663000	-2.479626000	-2.389604000
H	-1.311466000	-3.329254000	-2.666384000
H	-2.912797000	-2.602720000	-2.892601000
H	-1.477623000	-1.565140000	-2.762612000

1B''

E = -1212.0244913

Mo	-0.671232000	0.701984000	-0.274359000
N	0.908067000	0.118277000	-0.848077000
O	-2.099597000	-0.387485000	-1.043635000
Si	-3.330951000	-1.274859000	-0.406513000
C	-0.683523000	0.462767000	1.456756000
C	-0.425893000	0.111477000	2.882830000
O	-2.671200000	-2.506054000	0.498356000
H	-3.334165000	-2.985465000	1.005245000
O	-4.282330000	-1.819391000	-1.670047000
H	-3.762347000	-2.026493000	-2.453299000
O	-4.389987000	-0.445934000	0.580319000
H	-5.126998000	-0.073970000	0.085816000
C	2.107944000	-0.486713000	-0.519840000
C	2.208848000	-1.904476000	-0.575815000

C	3.240036000	0.307348000	-0.191144000
C	3.439523000	-2.491315000	-0.279911000
C	4.447484000	-0.336417000	0.082450000
C	4.553341000	-1.723063000	0.046301000
H	3.531548000	-3.572896000	-0.305860000
H	5.322284000	0.255190000	0.335271000
H	5.501495000	-2.203933000	0.270956000
C	-0.171052000	-1.407139000	2.959730000
H	-0.030946000	-1.705891000	4.005656000
H	-1.013977000	-1.963295000	2.541695000
H	0.727995000	-1.678152000	2.399108000
C	-1.661256000	0.477757000	3.728319000
H	-1.496322000	0.202558000	4.777041000
H	-1.860495000	1.553803000	3.687157000
H	-2.550864000	-0.044137000	3.365436000
C	0.809433000	0.874922000	3.395129000
H	1.694301000	0.620163000	2.804872000
H	0.655958000	1.958297000	3.339147000
H	1.005696000	0.617304000	4.442875000
C	3.135556000	1.823076000	-0.202037000
H	2.145128000	2.073814000	0.200096000
C	1.006652000	-2.736835000	-0.988217000
H	0.118600000	-2.276606000	-0.539850000
C	0.823667000	-2.686948000	-2.514270000
H	1.686777000	-3.132726000	-3.022221000
H	-0.070937000	-3.245402000	-2.813356000
H	0.715396000	-1.655625000	-2.861115000
C	1.054587000	-4.186746000	-0.501092000
H	0.100886000	-4.679270000	-0.715782000
H	1.838650000	-4.765901000	-1.003056000
H	1.226757000	-4.246932000	0.578465000
C	4.170543000	2.529972000	0.676576000
H	5.186029000	2.423501000	0.279027000
H	3.956285000	3.603382000	0.720073000
H	4.166281000	2.141715000	1.699939000
C	3.199847000	2.353432000	-1.644023000
H	3.061350000	3.441267000	-1.671524000
H	4.175018000	2.128646000	-2.090154000
H	2.431579000	1.887502000	-2.268543000
C	-0.606594000	3.236559000	-0.503900000
H	-0.058262000	4.101757000	-0.114097000
H	-0.044172000	2.919398000	-1.390103000
C	-2.065650000	3.586978000	-0.807217000
H	-0.504967000	2.567075000	0.416311000
C	-2.180157000	4.698895000	-1.847926000
H	-3.227685000	4.942838000	-2.046936000
H	-1.683054000	5.612782000	-1.505064000
H	-1.719754000	4.404138000	-2.797142000
H	-2.608984000	2.701038000	-1.164785000
H	-2.560563000	3.887022000	0.123361000

1C

E = -1409.7656513

Mo	0.494843000	0.053671000	-0.170923000
C	0.676177000	2.127626000	-0.660828000
H	-0.047167000	2.259197000	-1.478384000

H	0.231262000	2.621127000	0.217708000
C	1.984507000	2.862304000	-1.027305000
N	-1.260061000	0.089875000	-0.134427000
O	2.446337000	-0.329314000	-0.308978000
Si	3.860684000	-0.951961000	0.223628000
C	0.735683000	-0.550460000	1.859547000
H	0.721485000	-1.651728000	1.790342000
C	-0.086206000	-0.062468000	3.068142000
O	4.488902000	-0.220055000	1.586620000
H	5.072356000	0.516154000	1.377648000
O	5.056101000	-0.770067000	-0.932398000
H	4.735843000	-0.900814000	-1.830076000
O	3.579264000	-2.543743000	0.631195000
H	4.307081000	-2.932801000	1.126682000
C	-2.630788000	-0.058848000	-0.249246000
C	-3.447282000	1.106421000	-0.332173000
C	-3.233532000	-1.350412000	-0.299905000
C	-4.823583000	0.956829000	-0.494919000
C	-4.617598000	-1.432963000	-0.461571000
C	-5.413803000	-0.299424000	-0.565110000
H	-5.445950000	1.844709000	-0.568540000
H	-5.083100000	-2.414003000	-0.505134000
H	-6.488467000	-0.394734000	-0.693509000
C	1.596178000	4.313132000	-1.382136000
H	2.487973000	4.901883000	-1.629033000
H	0.923722000	4.345573000	-2.246967000
H	1.091485000	4.806563000	-0.543599000
C	2.950933000	2.905313000	0.163180000
H	2.494966000	3.420914000	1.017033000
H	3.227710000	1.899694000	0.485755000
H	3.865828000	3.449429000	-0.100078000
C	2.664761000	2.235541000	-2.251396000
H	3.008312000	1.222871000	-2.030242000
H	1.974098000	2.192329000	-3.102756000
H	3.530858000	2.832901000	-2.559634000
C	-0.252585000	1.463486000	3.038827000
H	-0.731862000	1.819622000	3.958332000
H	0.717978000	1.966561000	2.953031000
H	-0.877622000	1.772613000	2.194998000
C	0.708775000	-0.443427000	4.334555000
H	0.166709000	-0.140643000	5.238810000
H	0.871521000	-1.525815000	4.386507000
H	1.690049000	0.043349000	4.349444000
C	-1.461322000	-0.729675000	3.144126000
H	-2.069464000	-0.501694000	2.266229000
H	-1.358083000	-1.818030000	3.218787000
H	-2.008128000	-0.387463000	4.030806000
C	-2.444993000	-2.642762000	-0.184787000
H	-1.399311000	-2.378001000	-0.000427000
C	-2.859112000	2.503506000	-0.268936000
H	-1.803610000	2.398828000	-0.011022000
C	-2.939372000	3.195972000	-1.637453000
H	-3.980826000	3.338949000	-1.947034000
H	-2.462846000	4.181770000	-1.601202000
H	-2.442483000	2.604410000	-2.413047000
C	-3.515279000	3.362577000	0.820748000

H	-3.011319000	4.332585000	0.892502000
H	-4.571371000	3.559091000	0.606321000
H	-3.458560000	2.876748000	1.799571000
C	-2.923217000	-3.504108000	0.994290000
H	-3.942058000	-3.873117000	0.833340000
H	-2.273558000	-4.378504000	1.110625000
H	-2.915465000	-2.945190000	1.932845000
C	-2.515033000	-3.456342000	-1.486317000
H	-1.908976000	-4.365179000	-1.406420000
H	-3.544308000	-3.764704000	-1.700809000
H	-2.157076000	-2.881494000	-2.344807000
C	0.432312000	-1.235593000	-1.866767000
H	-0.576382000	-1.240716000	-2.290172000
H	1.068761000	-0.607000000	-2.515695000
C	0.997346000	-2.649433000	-1.781723000
H	1.973088000	-2.643914000	-1.290010000
H	0.347147000	-3.268098000	-1.150849000
C	1.120869000	-3.307624000	-3.160330000
H	0.151791000	-3.364387000	-3.668197000
H	1.798606000	-2.739785000	-3.808369000
H	1.515062000	-4.326306000	-3.076538000
H	1.783892000	-0.269212000	2.027589000

1D

E = -1212.0770190

Mo	-0.676113000	0.424108000	-0.260217000
N	1.015878000	0.057617000	-0.249333000
O	-2.021927000	-0.666614000	-1.117804000
Si	-3.489548000	-1.342120000	-0.772712000
C	-1.066396000	0.810546000	1.522649000
H	-2.167707000	0.955520000	1.458372000
C	-0.530557000	0.918272000	2.928764000
O	-3.437129000	-2.748675000	0.109536000
H	-3.319347000	-3.531698000	-0.437187000
O	-4.250784000	-1.730608000	-2.202849000
H	-4.048230000	-1.119413000	-2.918038000
O	-4.301611000	-0.220918000	0.151572000
H	-5.071138000	-0.580944000	0.603411000
C	2.270850000	-0.517005000	-0.291932000
C	3.398543000	0.316462000	-0.509437000
C	2.417505000	-1.917224000	-0.104856000
C	4.659091000	-0.279368000	-0.557556000
C	3.703618000	-2.454896000	-0.155994000
C	4.816466000	-1.650716000	-0.384368000
H	5.534564000	0.340019000	-0.729638000
H	3.840200000	-3.523033000	-0.014880000
H	5.807974000	-2.093640000	-0.422763000
C	0.981863000	0.678806000	2.980344000
H	1.347631000	0.786962000	4.007901000
H	1.236214000	-0.326040000	2.630973000
H	1.514397000	1.394201000	2.347205000
C	-1.248817000	-0.124427000	3.809009000
H	-0.894858000	-0.059341000	4.844845000
H	-2.332414000	0.036256000	3.811456000

H	-1.059301000	-1.139450000	3.445850000
C	-0.845230000	2.332167000	3.458211000
H	-0.345214000	3.096119000	2.854421000
H	-1.921960000	2.533806000	3.439024000
H	-0.501241000	2.436365000	4.494243000
C	1.205912000	-2.806112000	0.107529000
H	0.416747000	-2.179448000	0.542656000
C	3.221575000	1.806425000	-0.734777000
H	2.268921000	2.083399000	-0.269857000
C	4.321582000	2.655362000	-0.089142000
H	5.292907000	2.513372000	-0.575873000
H	4.073140000	3.718483000	-0.175574000
H	4.439771000	2.420010000	0.973223000
C	3.105984000	2.109417000	-2.237391000
H	2.925631000	3.176976000	-2.406139000
H	4.028907000	1.834968000	-2.760942000
H	2.283046000	1.549485000	-2.691706000
C	0.690033000	-3.337039000	-1.239517000
H	1.446691000	-3.967339000	-1.720164000
H	-0.213301000	-3.940451000	-1.096541000
H	0.445514000	-2.520076000	-1.924590000
C	1.453434000	-3.957266000	1.087710000
H	0.511666000	-4.472784000	1.302637000
H	2.143091000	-4.705005000	0.680630000
H	1.867124000	-3.597304000	2.034852000
C	-0.761111000	2.390027000	-1.085887000
H	0.090146000	2.995617000	-0.756055000
H	-0.622861000	2.220703000	-2.169711000
C	-2.074937000	3.133517000	-0.830903000
H	-2.137742000	3.386351000	0.234926000
H	-2.935841000	2.481482000	-1.035377000
C	-2.214346000	4.408235000	-1.668311000
H	-3.155556000	4.927173000	-1.454705000
H	-1.393177000	5.104153000	-1.462498000
H	-2.193873000	4.181784000	-2.740486000

TS(1A-1B)

E = -1290.61642173

Mo	0.615596000	0.317173000	-0.225184000
C	1.003915000	2.600313000	-0.277685000
H	0.121483000	2.830467000	-0.884115000
H	0.949533000	3.299160000	0.568928000
C	2.317839000	2.873085000	-1.046977000
N	-1.059190000	0.086198000	-0.760676000
O	1.806357000	-1.045652000	-0.966100000
Si	2.849663000	-2.128766000	-0.297464000
C	0.639148000	0.250805000	1.540221000
H	0.916717000	1.673507000	0.838673000
C	0.405223000	0.174212000	3.008943000
O	4.086383000	-1.471463000	0.608714000
H	4.872531000	-1.302868000	0.079656000
O	3.624896000	-2.945146000	-1.532790000
H	3.050267000	-3.093354000	-2.290775000
O	1.975535000	-3.125769000	0.708316000
H	2.536886000	-3.709111000	1.228777000
C	-2.371323000	-0.245785000	-0.473881000

C	-3.315325000	0.773813000	-0.172993000
C	-2.773475000	-1.608496000	-0.539669000
C	-4.640444000	0.404626000	0.062219000
C	-4.110142000	-1.917053000	-0.286268000
C	-5.041120000	-0.926604000	0.012216000
H	-5.374344000	1.170358000	0.294539000
H	-4.432538000	-2.953158000	-0.322978000
H	-6.077182000	-1.191720000	0.204798000
C	2.415518000	4.391191000	-1.277326000
H	3.329195000	4.641256000	-1.828415000
H	1.562536000	4.760809000	-1.857226000
H	2.439277000	4.935649000	-0.326648000
C	3.527475000	2.407546000	-0.222648000
H	3.550196000	2.897390000	0.757647000
H	3.517474000	1.324812000	-0.052702000
H	4.461744000	2.654859000	-0.739274000
C	2.311563000	2.167548000	-2.412425000
H	2.309550000	1.074469000	-2.318493000
H	1.439432000	2.462365000	-3.007100000
H	3.208444000	2.432843000	-2.983300000
C	-0.135765000	-1.242327000	3.293976000
H	-0.281455000	-1.369544000	4.373040000
H	-1.094530000	-1.401439000	2.792211000
H	0.564092000	-2.003735000	2.939798000
C	-0.628808000	1.226687000	3.448743000
H	-0.806420000	1.152244000	4.528000000
H	-0.276248000	2.243252000	3.240608000
H	-1.580615000	1.078990000	2.931122000
C	1.732529000	0.387515000	3.762130000
H	2.480983000	-0.344769000	3.447609000
H	2.137511000	1.387386000	3.572549000
H	1.575089000	0.286656000	4.842539000
C	-1.768868000	-2.683696000	-0.917690000
H	-0.813405000	-2.420372000	-0.449813000
C	-2.886307000	2.231046000	-0.164363000
H	-1.889890000	2.264252000	0.294039000
C	-2.753655000	2.759277000	-1.602341000
H	-3.725217000	2.738851000	-2.108678000
H	-2.394194000	3.795537000	-1.608533000
H	-2.059979000	2.145108000	-2.184517000
C	-3.793999000	3.147726000	0.659588000
H	-3.352829000	4.147926000	0.727898000
H	-4.782423000	3.265294000	0.201341000
H	-3.936809000	2.770631000	1.677374000
C	-2.137800000	-4.084345000	-0.422877000
H	-3.014337000	-4.488607000	-0.942516000
H	-1.306794000	-4.772138000	-0.609220000
H	-2.346287000	-4.092702000	0.651887000
C	-1.544748000	-2.690493000	-2.439059000
H	-0.782030000	-3.428460000	-2.713465000
H	-2.471175000	-2.950236000	-2.964243000
H	-1.214174000	-1.709124000	-2.790186000

TS(1A-1C)

E = -1409.7066723

Mo	-0.5111786000	0.021463000	0.016636000
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C	-0.279891000	-1.702305000	-1.334817000
H	0.404768000	-1.351370000	-2.125532000
H	0.344463000	-2.353408000	-0.702382000
C	-1.360885000	-2.584543000	-1.991541000
N	1.234837000	0.120156000	0.030994000
O	-2.336661000	0.291915000	-0.777844000
Si	-3.911623000	0.548566000	-0.449272000
C	-1.034743000	-0.247941000	1.855631000
H	-1.007907000	1.157435000	1.345158000
C	-0.516725000	-0.355726000	3.277689000
O	-4.554864000	-0.483437000	0.701803000
H	-4.867874000	-1.312453000	0.325890000
O	-4.860123000	0.329263000	-1.807311000
H	-4.424147000	0.606715000	-2.618991000
O	-4.083486000	2.079315000	0.200136000
H	-4.967010000	2.228779000	0.552254000
C	2.577029000	0.157580000	-0.298292000
C	3.441778000	-0.862873000	0.190769000
C	3.087378000	1.183666000	-1.147069000
C	4.793446000	-0.810951000	-0.155029000
C	4.445880000	1.178767000	-1.456496000
C	5.300359000	0.197346000	-0.963608000
H	5.461139000	-1.585361000	0.212702000
H	4.846629000	1.956930000	-2.098393000
H	6.356659000	0.216194000	-1.217432000
C	-0.663533000	-3.816369000	-2.604352000
H	-1.386308000	-4.470534000	-3.108683000
H	0.087046000	-3.515175000	-3.344565000
H	-0.155364000	-4.409458000	-1.834961000
C	-2.375829000	-3.082586000	-0.953457000
H	-1.874138000	-3.645557000	-0.156831000
H	-2.902945000	-2.246326000	-0.488699000
H	-3.117897000	-3.747332000	-1.413164000
C	-2.077612000	-1.838721000	-3.125431000
H	-2.589448000	-0.954730000	-2.743909000
H	-1.358310000	-1.517280000	-3.888849000
H	-2.814234000	-2.486786000	-3.616057000
C	-0.492660000	-1.856738000	3.631040000
H	-0.193032000	-1.990407000	4.676937000
H	-1.480018000	-2.312793000	3.502001000
H	0.216466000	-2.397779000	2.998056000
C	-1.502274000	0.363964000	4.220222000
H	-1.169553000	0.272366000	5.260466000
H	-1.570637000	1.431140000	3.982923000
H	-2.508249000	-0.062780000	4.146872000
C	0.880840000	0.242665000	3.453099000
H	1.594395000	-0.204885000	2.760037000
H	0.875886000	1.322010000	3.275317000
H	1.236238000	0.072588000	4.475353000
C	2.169750000	2.228870000	-1.752299000
H	1.340973000	2.364593000	-1.053625000
C	2.946061000	-2.027865000	1.029279000
H	1.889447000	-1.848227000	1.250271000
C	3.038351000	-3.345110000	0.242195000
H	4.079097000	-3.591678000	0.003668000
H	2.627025000	-4.172633000	0.831040000

H	2.484765000	-3.287715000	-0.699032000
C	3.702458000	-2.148473000	2.360271000
H	3.262101000	-2.939136000	2.977374000
H	4.755028000	-2.407322000	2.201996000
H	3.673165000	-1.215889000	2.931096000
C	2.830804000	3.597865000	-1.943497000
H	3.592347000	3.582393000	-2.730796000
H	2.079178000	4.334870000	-2.244601000
H	3.303161000	3.951377000	-1.021788000
C	1.581134000	1.724917000	-3.080958000
H	0.881909000	2.458510000	-3.498080000
H	2.375828000	1.558580000	-3.816681000
H	1.045289000	0.779805000	-2.951737000
C	-0.856959000	2.343315000	0.363611000
H	-0.660310000	2.509249000	-0.702956000
H	-1.912466000	2.589615000	0.504687000
C	0.055904000	3.217191000	1.218387000
H	-0.211322000	3.103402000	2.277936000
H	1.096406000	2.880741000	1.134086000
C	-0.042836000	4.696899000	0.841653000
H	0.260139000	4.861312000	-0.198288000
H	-1.070442000	5.060995000	0.946913000
H	0.600447000	5.313926000	1.478533000
H	-2.116799000	-0.462481000	1.802349000

TS(1A-1D)

E = -1409.70540590

Mo	0.555459000	0.196592000	-0.179259000
C	-0.032404000	2.286042000	-1.186216000
H	-0.653950000	2.074145000	-2.067399000
H	-0.714265000	2.345735000	-0.332858000
C	0.636994000	3.675741000	-1.345074000
N	-1.096512000	-0.317242000	-0.042265000
O	1.567499000	-1.531341000	-0.273468000
Si	2.442117000	-2.367034000	0.823223000
C	1.051894000	0.837320000	1.504635000
H	2.113951000	1.104444000	1.300587000
C	0.650109000	0.988676000	2.954652000
O	3.803332000	-1.585184000	1.405720000
H	4.582002000	-1.786556000	0.876830000
O	3.047820000	-3.751395000	0.099742000
H	2.443889000	-4.111556000	-0.557122000
O	1.489595000	-2.705304000	2.151642000
H	1.988142000	-3.125043000	2.859996000
C	-2.371885000	-0.801214000	-0.292748000
C	-3.502753000	-0.019588000	0.066011000
C	-2.539277000	-2.075758000	-0.899270000
C	-4.774121000	-0.525839000	-0.209549000
C	-3.834930000	-2.525556000	-1.152030000
C	-4.949124000	-1.764078000	-0.815455000
H	-5.646054000	0.066692000	0.055577000
H	-3.974559000	-3.494852000	-1.622868000
H	-5.948973000	-2.136171000	-1.021354000
C	1.420507000	3.795006000	-2.661629000
H	1.753078000	4.828513000	-2.810877000
H	2.314567000	3.165066000	-2.671463000

H	0.799210000	3.520417000	-3.522164000
C	-0.490744000	4.724649000	-1.367593000
H	-1.183850000	4.543447000	-2.196689000
H	-1.068196000	4.706010000	-0.436807000
H	-0.081091000	5.734584000	-1.488579000
C	1.569327000	3.982213000	-0.168401000
H	1.034486000	3.923346000	0.784043000
H	2.408702000	3.279922000	-0.123238000
H	1.986076000	4.991874000	-0.261036000
C	-0.533688000	0.073166000	3.291534000
H	-0.815914000	0.197682000	4.343668000
H	-1.402010000	0.306287000	2.671842000
H	-0.267561000	-0.972618000	3.117517000
C	0.270878000	2.457258000	3.228812000
H	-0.006616000	2.581558000	4.282336000
H	1.107556000	3.133007000	3.022043000
H	-0.581219000	2.766446000	2.615087000
C	1.851675000	0.602836000	3.839300000
H	2.153408000	-0.429919000	3.647980000
H	2.714115000	1.251125000	3.647778000
H	1.586569000	0.697272000	4.898895000
C	-1.347652000	-2.924451000	-1.302986000
H	-0.460515000	-2.503590000	-0.822789000
C	-3.372619000	1.347515000	0.713276000
H	-2.309207000	1.509436000	0.918266000
C	-3.847204000	2.458509000	-0.235399000
H	-4.913767000	2.353144000	-0.463182000
H	-3.701353000	3.444813000	0.219235000
H	-3.301107000	2.435867000	-1.183018000
C	-4.119859000	1.424502000	2.052320000
H	-3.939195000	2.390981000	2.535666000
H	-5.202191000	1.324316000	1.916052000
H	-3.797177000	0.635473000	2.737770000
C	-1.471225000	-4.377056000	-0.826197000
H	-2.301240000	-4.904313000	-1.309482000
H	-0.557110000	-4.932388000	-1.065247000
H	-1.622428000	-4.427440000	0.256155000
C	-1.130014000	-2.859009000	-2.822998000
H	-0.238991000	-3.427570000	-3.112877000
H	-1.986318000	-3.276717000	-3.364973000
H	-0.995878000	-1.826350000	-3.162262000
C	1.975446000	0.457657000	-2.115783000
H	1.740517000	-0.580212000	-2.374701000
H	1.019150000	1.379482000	-1.538831000
C	3.438495000	0.598994000	-1.696782000
H	3.625957000	-0.004040000	-0.801367000
H	3.648484000	1.640979000	-1.418378000
C	4.413277000	0.173165000	-2.797767000
H	5.454864000	0.294577000	-2.479534000
H	4.263926000	-0.878543000	-3.065550000
H	4.270499000	0.769279000	-3.706281000
H	1.785677000	1.045858000	-3.023839000

TS(1B-1D)

E = -1212.01324140

Mo	-0.659629000	0.588239000	-0.357037000
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N	0.942934000	-0.022088000	-0.803890000
O	-2.090913000	-0.518966000	-1.089738000
Si	-3.394846000	-1.314479000	-0.475154000
C	-0.730006000	0.674274000	1.408276000
C	-0.516142000	0.675690000	2.881754000
O	-2.850121000	-2.356635000	0.702380000
H	-3.569570000	-2.757711000	1.200185000
O	-4.181101000	-2.081957000	-1.734341000
H	-3.569713000	-2.401594000	-2.405741000
O	-4.559253000	-0.349326000	0.226431000
H	-5.209663000	-0.042448000	-0.413068000
C	2.158396000	-0.572153000	-0.438351000
C	2.268003000	-1.980938000	-0.279723000
C	3.294662000	0.266731000	-0.279786000
C	3.514759000	-2.513055000	0.050296000
C	4.516699000	-0.324528000	0.042914000
C	4.633160000	-1.700538000	0.211801000
H	3.615820000	-3.585680000	0.184947000
H	5.394639000	0.301446000	0.170556000
H	5.593598000	-2.139183000	0.468429000
C	-0.425267000	-0.802395000	3.314156000
H	-0.318191000	-0.860337000	4.403605000
H	-1.322663000	-1.351779000	3.017802000
H	0.439634000	-1.288605000	2.854040000
C	-1.709748000	1.351672000	3.583787000
H	-1.574817000	1.321840000	4.671450000
H	-1.801389000	2.401745000	3.285336000
H	-2.646375000	0.845483000	3.334197000
C	0.792498000	1.405307000	3.235953000
H	1.646007000	0.933463000	2.741352000
H	0.755338000	2.456875000	2.929509000
H	0.959877000	1.380753000	4.319131000
C	3.173039000	1.763392000	-0.510829000
H	2.206307000	2.070404000	-0.092223000
C	1.057689000	-2.871477000	-0.506784000
H	0.183765000	-2.350170000	-0.097854000
C	0.810869000	-3.062127000	-2.012587000
H	1.656702000	-3.580156000	-2.479165000
H	-0.089551000	-3.663907000	-2.181480000
H	0.679491000	-2.098869000	-2.512977000
C	1.139088000	-4.227388000	0.198400000
H	0.181571000	-4.749526000	0.104424000
H	1.905613000	-4.875647000	-0.241997000
H	1.359572000	-4.118191000	1.265260000
C	4.253564000	2.595046000	0.184645000
H	5.242834000	2.434025000	-0.258287000
H	4.028379000	3.662094000	0.082726000
H	4.320173000	2.363538000	1.252572000
C	3.142236000	2.072460000	-2.016862000
H	2.999094000	3.145163000	-2.194955000
H	4.086716000	1.777317000	-2.487555000
H	2.335029000	1.525683000	-2.513383000
C	-0.593130000	2.858323000	-0.636176000
H	-0.304053000	3.638584000	0.080270000
H	0.194168000	2.866897000	-1.396779000
C	-1.977956000	3.186604000	-1.210445000

H	-0.577769000	2.060711000	0.577070000
C	-2.055630000	4.619672000	-1.743206000
H	-3.049522000	4.835341000	-2.147926000
H	-1.852012000	5.345360000	-0.948249000
H	-1.324826000	4.784353000	-2.542035000
H	-2.230913000	2.489220000	-2.020298000
H	-2.741146000	3.042459000	-0.435212000

TS(1C-1D)

E = -1409.70518416

Mo	0.398150000	-0.088672000	-0.126172000
C	1.016913000	2.151482000	0.406370000
H	0.674417000	2.429308000	-0.597662000
H	0.264690000	2.544509000	1.099390000
C	2.383376000	2.847812000	0.640577000
N	-1.321619000	0.241188000	-0.048865000
O	2.252159000	-0.203653000	-0.849685000
Si	3.602746000	-1.080668000	-1.104842000
C	0.859897000	-0.584331000	1.682530000
H	1.877026000	-1.003595000	1.626321000
C	0.261757000	-0.704455000	3.072955000
O	5.002319000	-0.183732000	-1.240731000
H	5.190599000	0.062320000	-2.151859000
O	3.546554000	-1.952249000	-2.530227000
H	2.670884000	-2.302527000	-2.722397000
O	3.796811000	-2.034454000	0.255961000
H	4.673338000	-2.428751000	0.307645000
C	-2.672023000	0.416336000	-0.289808000
C	-3.144609000	1.640476000	-0.846669000
C	-3.584789000	-0.633668000	0.008393000
C	-4.510454000	1.788144000	-1.074737000
C	-4.942559000	-0.425476000	-0.246289000
C	-5.410323000	0.768360000	-0.777258000
H	-4.882105000	2.718037000	-1.493163000
H	-5.647148000	-1.222307000	-0.023099000
H	-6.472003000	0.906378000	-0.962476000
C	2.068418000	4.301993000	1.043823000
H	2.993699000	4.874329000	1.178619000
H	1.473518000	4.807107000	0.274046000
H	1.508017000	4.345378000	1.985157000
C	3.198023000	2.190629000	1.759867000
H	2.649613000	2.197257000	2.708939000
H	3.451989000	1.156132000	1.510245000
H	4.136296000	2.732882000	1.921710000
C	3.217321000	2.876564000	-0.647733000
H	3.503767000	1.872009000	-0.958678000
H	2.658199000	3.350097000	-1.464081000
H	4.132279000	3.459624000	-0.491000000
C	-0.981806000	0.168140000	3.264425000
H	-1.400733000	0.013619000	4.265000000
H	-0.734816000	1.231061000	3.167713000
H	-1.751980000	-0.061854000	2.526013000
C	1.320117000	-0.314741000	4.123685000
H	0.925158000	-0.474537000	5.133506000
H	2.229471000	-0.915618000	4.016903000
H	1.599577000	0.739525000	4.038606000

C	-0.093262000	-2.192536000	3.270941000
H	-0.859487000	-2.513267000	2.560959000
H	0.786163000	-2.830518000	3.133076000
H	-0.473311000	-2.354409000	4.286340000
C	-3.143546000	-1.974917000	0.566959000
H	-2.062654000	-1.922834000	0.728481000
C	-2.170179000	2.738186000	-1.228276000
H	-1.360419000	2.708237000	-0.494097000
C	-1.561865000	2.453112000	-2.612013000
H	-2.337477000	2.482500000	-3.385411000
H	-0.802899000	3.201371000	-2.867437000
H	-1.094951000	1.463613000	-2.651203000
C	-2.764569000	4.148650000	-1.183717000
H	-1.971536000	4.889886000	-1.326791000
H	-3.500884000	4.312987000	-1.978214000
H	-3.249159000	4.353159000	-0.223781000
C	-3.816809000	-2.283004000	1.912585000
H	-4.901341000	-2.391170000	1.802315000
H	-3.435199000	-3.223925000	2.324087000
H	-3.635714000	-1.493261000	2.647230000
C	-3.410139000	-3.108077000	-0.435578000
H	-3.039497000	-4.061451000	-0.043342000
H	-4.482228000	-3.224022000	-0.630157000
H	-2.916231000	-2.918336000	-1.392517000
C	0.013655000	-1.585989000	-1.680610000
H	-1.037831000	-1.556710000	-1.992527000
H	0.609114000	-1.249605000	-2.544347000
C	0.387104000	-3.027317000	-1.311509000
H	1.415629000	-3.080884000	-0.930356000
H	-0.242946000	-3.364297000	-0.478583000
C	0.230500000	-4.014014000	-2.474063000
H	-0.800311000	-4.023665000	-2.845040000
H	0.871307000	-3.744265000	-3.323483000
H	0.491188000	-5.035853000	-2.175679000
H	1.113875000	0.856145000	1.262517000

2A

E = -823.885848489

Mo	-0.185966000	-0.033922000	-1.015617000
C	-1.206717000	1.847230000	-0.862285000
H	-0.653577000	2.419917000	-1.632396000
H	-2.218944000	1.716029000	-1.262097000
C	-1.265534000	2.690907000	0.429847000
N	-0.869103000	-0.680618000	-2.448385000
O	1.699719000	0.229763000	-0.757667000
Si	2.874485000	-0.259543000	0.299654000
C	-0.939032000	-1.074978000	0.340644000
H	-0.396667000	-0.697184000	1.233695000
C	-1.838293000	-2.250806000	0.641268000
O	2.415415000	-0.199987000	1.900088000
H	2.641588000	0.637060000	2.318426000
O	4.178242000	0.770581000	0.178372000
H	4.358513000	1.051098000	-0.724517000
O	3.210953000	-1.839233000	-0.077227000
H	3.732668000	-2.288298000	0.595218000
C	-1.731672000	4.109836000	0.050960000

H	-1.810676000	4.749480000	0.938662000
H	-1.029105000	4.585501000	-0.643073000
H	-2.714665000	4.084666000	-0.432570000
C	-2.267005000	2.100079000	1.428302000
H	-3.269835000	2.043332000	0.989698000
H	-1.978730000	1.090313000	1.731681000
H	-2.330839000	2.721751000	2.329192000
C	0.117931000	2.795199000	1.089639000
H	0.473321000	1.818619000	1.438652000
H	0.861848000	3.191051000	0.388547000
H	0.087070000	3.462838000	1.958922000
C	-2.566421000	-2.748475000	-0.610736000
H	-3.217475000	-3.593022000	-0.357679000
H	-3.180659000	-1.957046000	-1.050139000
H	-1.854427000	-3.080895000	-1.371907000
C	-2.874400000	-1.825288000	1.700288000
H	-3.512019000	-2.675633000	1.969640000
H	-2.386339000	-1.469951000	2.614778000
H	-3.516372000	-1.023608000	1.322937000
C	-0.967800000	-3.387568000	1.216141000
H	-0.215608000	-3.709026000	0.489047000
H	-0.445630000	-3.067498000	2.124326000
H	-1.591415000	-4.252703000	1.471504000
H	-0.981494000	-1.159960000	-3.334014000

2B

E = -626.091109656

Mo	0.303037000	-1.377253000	0.335640000
N	0.930489000	-2.157686000	-1.147757000
O	-1.562880000	-0.868252000	0.148722000
Si	-2.292947000	0.604467000	-0.031898000
C	1.330582000	0.022818000	0.369021000
C	2.340937000	1.042642000	-0.018629000
O	-2.242206000	1.345838000	1.454849000
H	-2.523210000	2.265742000	1.426311000
O	-3.842363000	0.341725000	-0.597388000
H	-4.222869000	-0.476071000	-0.261732000
O	-1.594309000	1.648557000	-1.121880000
H	-1.819920000	1.441219000	-2.034231000
C	3.743287000	0.507929000	0.333065000
H	4.503443000	1.247121000	0.054905000
H	3.836373000	0.315883000	1.407273000
H	3.952745000	-0.421148000	-0.205207000
C	2.067326000	2.356487000	0.737676000
H	2.801165000	3.116500000	0.443666000
H	1.067035000	2.732991000	0.507651000
H	2.139447000	2.210995000	1.820179000
C	2.226553000	1.268575000	-1.538514000
H	2.361989000	0.328711000	-2.080864000
H	1.242425000	1.673663000	-1.789135000
H	2.992841000	1.981090000	-1.866073000
H	0.210775000	-2.864451000	-1.408909000

2B'

E = -823.842629305

Mo	0.222059000	-0.041595000	-0.961082000
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C	2.826615000	-0.111060000	-0.724496000
H	2.548130000	-0.805272000	-1.528003000
H	3.576344000	0.554195000	-1.165174000
C	3.336544000	-0.847471000	0.523893000
N	0.130749000	0.475091000	-2.650964000
O	-1.133381000	-1.410160000	-0.634975000
Si	-2.448152000	-1.537050000	0.342993000
C	-0.204048000	1.355297000	-0.007562000
H	2.039219000	0.647627000	-0.409313000
C	-0.655669000	2.677821000	0.513742000
O	-2.119351000	-1.766850000	1.963047000
H	-2.009814000	-2.698699000	2.176827000
O	-3.300373000	-2.904254000	-0.108843000
H	-3.247477000	-3.061582000	-1.057226000
O	-3.347751000	-0.139063000	0.228214000
H	-4.068662000	-0.122839000	0.865832000
C	4.530655000	-1.725124000	0.125298000
H	4.920018000	-2.265782000	0.994509000
H	4.246320000	-2.466538000	-0.630005000
H	5.347310000	-1.121506000	-0.286051000
C	3.768490000	0.177680000	1.580830000
H	4.569619000	0.823308000	1.203956000
H	2.929825000	0.816472000	1.879602000
H	4.139975000	-0.325856000	2.479554000
C	2.206494000	-1.722015000	1.083971000
H	1.336719000	-1.113975000	1.376686000
H	1.881335000	-2.477689000	0.358312000
H	2.528072000	-2.254602000	1.985617000
C	-1.704287000	3.246333000	-0.461465000
H	-2.063862000	4.218202000	-0.102337000
H	-1.276545000	3.388561000	-1.459033000
H	-2.555461000	2.565625000	-0.546558000
C	0.552964000	3.628609000	0.600539000
H	0.237843000	4.607214000	0.981444000
H	1.317128000	3.234530000	1.279016000
H	1.010182000	3.774990000	-0.383314000
C	-1.284768000	2.496597000	1.907669000
H	-2.124752000	1.799667000	1.856856000
H	-0.554717000	2.096795000	2.618642000
H	-1.646169000	3.458914000	2.290710000
H	-0.079271000	1.370916000	-3.094314000

2B''

E = -745.236043492

Mo	0.684308000	0.080392000	-0.785669000
N	0.889944000	-0.415835000	-2.471832000
O	-0.770567000	1.376447000	-0.631525000
Si	-2.207618000	1.424808000	0.165213000
C	0.223164000	-1.354299000	0.094267000
C	-0.196374000	-2.704395000	0.567849000
O	-3.026319000	0.003773000	-0.126437000
H	-3.822966000	-0.070640000	0.408595000
O	-3.041051000	2.781870000	-0.347969000
H	-2.875831000	2.974739000	-1.276624000
O	-2.106188000	1.603121000	1.821067000
H	-2.100669000	2.529759000	2.080573000

C	-0.935712000	-3.415907000	-0.581032000
H	-1.265840000	-4.410313000	-0.257359000
H	-1.813105000	-2.840068000	-0.888052000
H	-0.283681000	-3.539669000	-1.451583000
C	-1.133996000	-2.556573000	1.780729000
H	-1.476584000	-3.541850000	2.120284000
H	-0.621879000	-2.063951000	2.613170000
H	-2.004787000	-1.952395000	1.515170000
C	1.056327000	-3.507795000	0.965397000
H	1.732565000	-3.629374000	0.113098000
H	1.604002000	-3.009088000	1.772242000
H	0.768157000	-4.504248000	1.320382000
C	3.049564000	0.510459000	0.025904000
H	4.014497000	0.007284000	0.155049000
H	3.094171000	0.961804000	-0.971964000
C	2.793697000	1.524051000	1.144434000
H	2.386412000	-0.414525000	0.120994000
C	3.868044000	2.608745000	1.188209000
H	3.675927000	3.317955000	1.998398000
H	4.859978000	2.173679000	1.351877000
H	3.901874000	3.174002000	0.250537000
H	1.809246000	1.999104000	1.021906000
H	2.751194000	0.993773000	2.102365000
H	0.808169000	-1.316297000	-2.946764000

2C

E = -942.982931363

Mo	-0.199210000	0.415539000	-0.809358000
C	1.447373000	1.758338000	-1.034553000
H	1.593259000	1.781316000	-2.126468000
H	1.010919000	2.734584000	-0.776802000
C	2.813358000	1.607768000	-0.332514000
N	-1.224375000	1.388283000	-1.804617000
O	0.757219000	-0.959292000	0.256043000
Si	0.839320000	-2.089662000	1.436156000
C	-1.402710000	0.598679000	0.931160000
H	-1.694089000	-0.441802000	1.140306000
C	-2.598556000	1.540175000	1.145980000
O	1.162941000	-1.501462000	2.962044000
H	2.105119000	-1.454134000	3.151527000
O	2.079805000	-3.165518000	1.125048000
H	2.189771000	-3.352447000	0.187837000
O	-0.663484000	-2.809478000	1.521487000
H	-0.788701000	-3.316855000	2.329726000
C	3.657946000	2.834382000	-0.735931000
H	4.652198000	2.787686000	-0.275365000
H	3.794175000	2.883135000	-1.822328000
H	3.183014000	3.768228000	-0.414070000
C	2.660780000	1.607024000	1.194532000
H	2.140078000	2.509562000	1.537233000
H	2.097465000	0.735929000	1.538736000
H	3.643525000	1.591554000	1.680925000
C	3.550007000	0.342746000	-0.793892000
H	3.002184000	-0.557666000	-0.507164000
H	3.677092000	0.339709000	-1.883529000
H	4.549537000	0.293105000	-0.346078000

C	-2.213575000	3.006601000	0.909136000
H	-3.058104000	3.670397000	1.128031000
H	-1.382574000	3.302463000	1.560874000
H	-1.905603000	3.175785000	-0.126638000
C	-3.032496000	1.384301000	2.618844000
H	-3.891100000	2.029314000	2.841473000
H	-3.321594000	0.350684000	2.839001000
H	-2.220793000	1.657542000	3.302328000
C	-3.782911000	1.149003000	0.253378000
H	-3.532580000	1.241572000	-0.806790000
H	-4.085309000	0.111399000	0.436728000
H	-4.649491000	1.789716000	0.453847000
C	-0.420595000	-1.185548000	-2.204421000
H	-0.466445000	-0.767978000	-3.215772000
H	0.500781000	-1.772496000	-2.101167000
C	-1.648234000	-2.047096000	-1.910322000
H	-1.595036000	-2.439140000	-0.887744000
H	-2.554730000	-1.430234000	-1.966122000
C	-1.783391000	-3.218464000	-2.889740000
H	-1.869968000	-2.863854000	-3.922862000
H	-0.910541000	-3.878694000	-2.837593000
H	-2.670734000	-3.820171000	-2.665009000
H	-0.609063000	0.839053000	1.660863000
H	-1.919545000	1.805937000	-2.415672000

2D

E = -745.285648558

Mo	0.228046000	0.310418000	-0.943876000
N	1.102649000	0.089079000	-2.403173000
O	-1.665259000	0.015187000	-0.747272000
Si	-2.701889000	-0.730125000	0.305251000
C	1.254620000	-0.560783000	0.348869000
H	0.599526000	-0.448542000	1.239827000
C	2.508480000	-1.354481000	0.618870000
O	-2.771218000	-2.383383000	0.180688000
H	-3.364426000	-2.690046000	-0.512017000
O	-4.244049000	-0.175680000	0.011771000
H	-4.265833000	0.734641000	-0.299673000
O	-2.124620000	-0.385685000	1.826911000
H	-2.506212000	-0.936022000	2.517871000
C	3.346854000	-1.545997000	-0.648370000
H	4.258845000	-2.108594000	-0.418034000
H	2.786473000	-2.099024000	-1.408348000
H	3.632418000	-0.582752000	-1.080615000
C	2.106005000	-2.731255000	1.184836000
H	2.998373000	-3.323332000	1.420054000
H	1.518241000	-2.626279000	2.103313000
H	1.504672000	-3.290904000	0.461518000
C	3.337036000	-0.594402000	1.674937000
H	3.640724000	0.387947000	1.300094000
H	2.764864000	-0.445109000	2.597271000
H	4.242040000	-1.159536000	1.927851000
C	0.657661000	2.335738000	-0.430649000
H	1.689867000	2.584007000	-0.699257000
H	0.008898000	2.917274000	-1.111257000
C	0.372541000	2.712352000	1.024945000

H	1.091310000	2.194829000	1.672671000
H	-0.619595000	2.353624000	1.332583000
C	0.451157000	4.221091000	1.276000000
H	0.260062000	4.462969000	2.327505000
H	1.442097000	4.610329000	1.016247000
H	-0.284714000	4.761855000	0.669954000
H	1.367357000	-0.193785000	-3.339489000

TS(2A-2B)

E = -823.827213853

Mo	-0.190004000	0.003224000	1.074375000
C	-2.374973000	-0.620076000	0.630969000
H	-2.434003000	-1.132470000	1.599091000
H	-3.199867000	0.102798000	0.657601000
C	-2.581568000	-1.609032000	-0.535501000
N	-0.294493000	0.561097000	2.742546000
O	1.409619000	-1.070255000	0.758465000
Si	2.628321000	-1.028125000	-0.345713000
C	-0.241260000	1.427180000	0.031201000
H	-1.576586000	0.530210000	0.162607000
C	-0.313243000	2.770035000	-0.611026000
O	2.153947000	-1.258179000	-1.929656000
H	2.184908000	-2.185911000	-2.183865000
O	3.671359000	-2.295798000	-0.031477000
H	3.749804000	-2.476400000	0.910936000
O	3.357746000	0.465314000	-0.261637000
H	3.992375000	0.601975000	-0.972168000
C	-3.954479000	-2.275596000	-0.341967000
H	-4.154598000	-2.990479000	-1.148245000
H	-4.002636000	-2.819567000	0.608000000
H	-4.759840000	-1.532579000	-0.345832000
C	-2.562525000	-0.868695000	-1.880090000
H	-3.323625000	-0.079659000	-1.907912000
H	-1.585710000	-0.411135000	-2.069205000
H	-2.772013000	-1.558978000	-2.704448000
C	-1.493933000	-2.693049000	-0.531858000
H	-0.496504000	-2.275755000	-0.714794000
H	-1.466670000	-3.228738000	0.424468000
H	-1.683591000	-3.431176000	-1.319310000
C	0.945620000	3.537456000	-0.156342000
H	0.969536000	4.523084000	-0.635509000
H	0.946912000	3.679973000	0.928299000
H	1.852730000	2.990444000	-0.426241000
C	-1.578129000	3.517652000	-0.151174000
H	-1.607056000	4.521290000	-0.591031000
H	-2.486708000	2.991401000	-0.464555000
H	-1.600712000	3.618979000	0.938045000
C	-0.308180000	2.631666000	-2.144964000
H	0.578461000	2.088126000	-2.482821000
H	-1.192749000	2.090700000	-2.495875000
H	-0.310535000	3.622238000	-2.615236000
H	-0.341571000	1.458384000	3.225353000

TS(2A-2C)

E = -942.921851266

Mo	0.189755000	-0.468576000	-0.736477000
C	-1.691535000	-1.476465000	-1.236047000
H	-1.812989000	-1.296704000	-2.319118000
H	-1.385842000	-2.531611000	-1.161599000
C	-3.064987000	-1.322835000	-0.549286000
N	1.084934000	-1.471138000	-1.817469000
O	-0.859386000	1.150570000	-0.216188000
Si	-1.069030000	2.304681000	0.916712000
C	1.096494000	-0.785857000	0.936082000
H	1.629380000	0.326800000	0.033646000
C	2.197019000	-1.629550000	1.549537000
O	-1.216428000	1.724609000	2.478657000
H	-2.118988000	1.473892000	2.700219000
O	-2.469372000	3.169672000	0.634752000
H	-2.665646000	3.268493000	-0.302150000
O	0.292279000	3.272153000	0.941057000
H	0.309162000	3.864837000	1.699414000
C	-3.950147000	-2.511707000	-0.974654000
H	-4.953615000	-2.436262000	-0.536522000
H	-4.062705000	-2.547477000	-2.064440000
H	-3.514854000	-3.465085000	-0.652565000
C	-2.925467000	-1.353549000	0.979582000
H	-2.428122000	-2.273846000	1.308605000
H	-2.332389000	-0.507040000	1.337623000
H	-3.907872000	-1.315522000	1.466971000
C	-3.766224000	-0.030015000	-0.987785000
H	-3.175552000	0.846507000	-0.718047000
H	-3.914629000	-0.021273000	-2.074709000
H	-4.753808000	0.058932000	-0.518535000
C	1.497727000	-2.647323000	2.474722000
H	2.246684000	-3.258783000	2.990913000
H	0.889569000	-2.145747000	3.235051000
H	0.845842000	-3.313197000	1.901378000
C	3.107025000	-0.719727000	2.398931000
H	3.871824000	-1.316149000	2.909204000
H	3.618896000	0.020863000	1.775199000
H	2.533282000	-0.181228000	3.160699000
C	3.038482000	-2.378629000	0.514503000
H	2.416987000	-3.040245000	-0.094441000
H	3.552162000	-1.685527000	-0.158778000
H	3.798862000	-2.983780000	1.020552000
C	1.708536000	1.260634000	-1.224763000
H	1.124259000	1.449953000	-2.135507000
H	1.574338000	2.139326000	-0.589225000
C	3.169129000	1.020228000	-1.588663000
H	3.763199000	0.869231000	-0.676722000
H	3.264617000	0.092815000	-2.166488000
C	3.765427000	2.182009000	-2.385966000
H	3.226767000	2.331714000	-3.328589000
H	3.708156000	3.118518000	-1.821021000
H	4.818192000	1.999553000	-2.627905000
H	0.551174000	-0.204467000	1.698205000
H	1.620202000	-1.804201000	-2.614357000

TS(2A-2D)**E = -942.917510028**

Mo	0.095123000	-0.005662000	-0.823220000
C	2.478742000	-0.160532000	-0.940582000
H	2.733287000	-0.644217000	-1.893954000
H	2.388778000	0.910174000	-1.149241000
C	3.644994000	-0.350542000	0.062570000
N	-0.007843000	0.860401000	-2.301335000
O	-1.663809000	-0.928979000	-0.712952000
Si	-3.113290000	-0.604758000	-0.037141000
C	-0.004253000	1.300534000	0.516792000
H	-0.020586000	0.706460000	1.455032000
C	-0.205304000	2.781684000	0.744292000
O	-3.136592000	-0.612258000	1.635614000
H	-3.334782000	-1.487857000	1.982487000
O	-4.192652000	-1.810351000	-0.470702000
H	-4.017479000	-2.146027000	-1.355564000
O	-3.621788000	0.909974000	-0.517154000
H	-4.423674000	1.185599000	-0.061502000
C	4.033168000	-1.828309000	0.227064000
H	4.953108000	-1.913901000	0.816426000
H	3.262155000	-2.401795000	0.749694000
H	4.216285000	-2.304940000	-0.743098000
C	4.860772000	0.401131000	-0.512912000
H	5.139711000	0.008056000	-1.497141000
H	4.648254000	1.470095000	-0.626583000
H	5.730865000	0.299847000	0.146773000
C	3.305467000	0.238326000	1.435351000
H	3.046467000	1.297921000	1.359338000
H	2.456995000	-0.278063000	1.896691000
H	4.160369000	0.147261000	2.115527000
C	-0.324529000	3.557105000	-0.570967000
H	-0.473863000	4.623047000	-0.364205000
H	0.578962000	3.447194000	-1.178386000
H	-1.169012000	3.192401000	-1.161102000
C	0.981352000	3.334133000	1.558773000
H	0.804560000	4.386850000	1.808586000
H	1.117335000	2.785393000	2.497094000
H	1.913600000	3.276743000	0.987986000
C	-1.501838000	2.958918000	1.561900000
H	-2.356602000	2.552455000	1.015791000
H	-1.437766000	2.444486000	2.526997000
H	-1.680409000	4.023390000	1.756037000
C	0.659910000	-2.286109000	-0.284542000
H	-0.116030000	-2.612515000	-0.984737000
H	1.526377000	-1.162034000	-0.528887000
C	0.254956000	-2.575576000	1.161296000
H	-0.658187000	-2.021215000	1.407641000
H	1.034886000	-2.214439000	1.845764000
C	0.015601000	-4.064883000	1.422267000
H	-0.264559000	-4.247749000	2.465722000
H	-0.789790000	-4.447433000	0.785874000
H	0.914296000	-4.654944000	1.209643000
H	1.560943000	-2.857636000	-0.544031000
H	-0.074202000	1.016619000	-3.302364000

TS(2B-2D)**E = -745.224124015**

Mo	0.390669000	0.458265000	-0.887382000
N	0.846939000	0.264928000	-2.578952000
O	-1.539716000	0.637757000	-0.649809000
Si	-2.668960000	-0.155264000	0.246970000
C	1.042896000	-0.914249000	0.013353000
C	1.692862000	-2.133381000	0.568319000
O	-2.534687000	-1.783416000	-0.073033000
H	-3.088378000	-2.315236000	0.507423000
O	-4.171804000	0.475266000	-0.123911000
H	-4.237130000	0.735342000	-1.048573000
O	-2.529183000	0.027359000	1.899070000
H	-2.998919000	0.804367000	2.217956000
C	0.955532000	-3.340595000	-0.047386000
H	1.357899000	-4.270978000	0.369829000
H	-0.115599000	-3.290279000	0.163992000
H	1.084487000	-3.364102000	-1.133567000
C	1.542199000	-2.159180000	2.101681000
H	1.983001000	-3.075733000	2.511605000
H	2.050663000	-1.305852000	2.563343000
H	0.487830000	-2.120142000	2.388816000
C	3.182056000	-2.173568000	0.180568000
H	3.304937000	-2.148754000	-0.906269000
H	3.726393000	-1.322471000	0.604963000
H	3.649126000	-3.089888000	0.559759000
C	1.887936000	1.957379000	-0.025421000
H	2.887875000	1.771042000	0.387339000
H	2.066271000	2.489006000	-0.965479000
C	1.066037000	2.777164000	0.977620000
H	1.796506000	0.510267000	0.140053000
C	1.802390000	4.040482000	1.430240000
H	1.201507000	4.611621000	2.145082000
H	2.751853000	3.788753000	1.915342000
H	2.024452000	4.694387000	0.580284000
H	0.100782000	3.063419000	0.538753000
H	0.829349000	2.158428000	1.852491000
H	1.337550000	-0.431163000	-3.140380000

TS(2C-2D)**E = -942.918103453**

Mo	0.168777000	-0.543054000	-0.909815000
C	-2.045595000	0.318595000	-1.212930000
H	-1.736914000	0.614595000	-2.223555000
H	-2.730132000	-0.524553000	-1.355961000
C	-2.778032000	1.506826000	-0.544709000
N	-0.230878000	-1.736631000	-2.090876000
O	0.552511000	1.269852000	-0.201207000
Si	1.331485000	2.138324000	0.941402000
C	-0.428504000	-1.370069000	0.726018000
H	-0.122831000	-0.696488000	1.543052000
C	-1.022958000	-2.670913000	1.234159000
O	0.762828000	3.690558000	1.146948000
H	1.204756000	4.322937000	0.571905000
O	2.953635000	2.333234000	0.594838000

H	3.338822000	1.568669000	0.154641000
O	1.045131000	1.344433000	2.385333000
H	1.267691000	1.877737000	3.154912000
C	-4.227259000	1.480945000	-1.070746000
H	-4.795838000	2.331311000	-0.676309000
H	-4.253693000	1.541117000	-2.164995000
H	-4.746567000	0.563044000	-0.770746000
C	-2.806754000	1.389257000	0.984052000
H	-3.283676000	0.454517000	1.302354000
H	-1.797711000	1.425097000	1.404408000
H	-3.380368000	2.213503000	1.422660000
C	-2.145249000	2.846104000	-0.947631000
H	-1.121064000	2.928486000	-0.583393000
H	-2.137970000	2.960052000	-2.038763000
H	-2.724397000	3.678841000	-0.532001000
C	-1.626515000	-3.540528000	0.128961000
H	-2.016339000	-4.470268000	0.558043000
H	-2.454910000	-3.030502000	-0.373975000
H	-0.879132000	-3.793727000	-0.626766000
C	-2.102171000	-2.360945000	2.289909000
H	-2.476129000	-3.291253000	2.732570000
H	-1.704215000	-1.737665000	3.097660000
H	-2.954241000	-1.836670000	1.845532000
C	0.135390000	-3.432803000	1.911716000
H	0.913692000	-3.683724000	1.185175000
H	0.591706000	-2.838577000	2.710365000
H	-0.238661000	-4.363419000	2.353827000
C	2.292362000	-0.521889000	-1.457492000
H	2.429832000	-1.062734000	-2.401467000
H	2.553533000	0.528950000	-1.652062000
C	3.236547000	-1.120903000	-0.405124000
H	3.103643000	-0.625409000	0.567914000
H	2.969525000	-2.171020000	-0.230397000
C	4.714311000	-1.047811000	-0.805649000
H	4.889594000	-1.581227000	-1.746514000
H	5.038730000	-0.010984000	-0.958626000
H	5.363725000	-1.489756000	-0.041325000
H	-1.422735000	-0.497691000	-0.011344000
H	-0.487298000	-2.234862000	-2.938579000

3A

E = -1482.33410116

Mo	-0.068552000	0.503851000	0.666550000
C	0.477236000	-0.475777000	2.491581000
H	-0.140406000	0.112113000	3.200281000
H	0.049044000	-1.485076000	2.495915000
C	1.924984000	-0.535424000	3.026017000
N	-1.556002000	-0.279550000	0.256140000
O	0.089818000	2.416043000	0.871322000
Si	0.865497000	3.681494000	0.146675000
C	1.150449000	-0.154562000	-0.583980000
H	2.025851000	0.486183000	-0.348137000
C	1.340859000	-1.026542000	-1.810834000
O	2.461687000	3.386803000	-0.230903000

H	3.061052000	3.613677000	0.487515000
O	0.891080000	4.975640000	1.195980000
H	0.093042000	5.048181000	1.729097000
O	0.066813000	3.973723000	-1.279944000
H	0.550112000	4.559179000	-1.871464000
C	-2.805349000	-0.671228000	-0.182468000
C	-3.286844000	-1.954740000	0.187492000
C	-3.578842000	0.198840000	-0.997906000
C	-4.549694000	-2.339406000	-0.263472000
C	-4.831251000	-0.244377000	-1.422949000
C	-5.317788000	-1.497282000	-1.060862000
H	-4.939515000	-3.315265000	0.010560000
H	-5.439687000	0.400497000	-2.049818000
H	-6.297644000	-1.818439000	-1.403863000
C	1.869798000	-0.911902000	4.519174000
H	2.878537000	-0.994779000	4.942153000
H	1.324188000	-0.158079000	5.098851000
H	1.366245000	-1.874435000	4.663125000
C	2.734171000	-1.603952000	2.282223000
H	2.287302000	-2.595554000	2.420025000
H	2.774534000	-1.403472000	1.208177000
H	3.762334000	-1.646892000	2.660093000
C	2.621546000	0.827972000	2.897695000
H	2.749757000	1.119059000	1.848410000
H	2.046594000	1.615319000	3.399403000
H	3.619773000	0.800856000	3.350551000
C	0.349314000	-2.195378000	-1.786747000
H	0.455827000	-2.817245000	-2.682190000
H	0.488980000	-2.822870000	-0.901918000
H	-0.671910000	-1.809386000	-1.759911000
C	1.036630000	-0.167809000	-3.064673000
H	-0.003900000	0.169349000	-3.039423000
H	1.674658000	0.717731000	-3.120036000
H	1.194224000	-0.759402000	-3.973631000
C	-3.070757000	1.582184000	-1.357789000
H	-1.975158000	1.536317000	-1.372811000
C	-2.468517000	-2.851700000	1.096776000
H	-1.419787000	-2.562360000	0.965159000
C	-2.840080000	-2.593024000	2.566250000
H	-3.889282000	-2.849746000	2.751760000
H	-2.220088000	-3.198745000	3.236856000
H	-2.699685000	-1.540693000	2.830629000
C	-2.588976000	-4.340954000	0.758939000
H	-1.880496000	-4.919266000	1.361348000
H	-3.588295000	-4.733837000	0.976745000
H	-2.372871000	-4.533226000	-0.296583000
C	-3.514395000	2.064826000	-2.741774000
H	-4.589680000	2.271989000	-2.782078000
H	-2.996805000	2.997134000	-2.988061000
H	-3.281894000	1.330639000	-3.519714000
C	-3.474268000	2.597000000	-0.275527000
H	-3.048609000	3.580675000	-0.498470000
H	-4.564905000	2.694327000	-0.226748000
H	-3.119110000	2.289331000	0.712549000
C	2.805573000	-1.497622000	-1.868994000
C	3.840021000	-0.553406000	-1.972523000

C	3.164284000	-2.849561000	-1.831695000
C	5.174212000	-0.943291000	-2.038836000
H	3.603426000	0.507513000	-2.003195000
C	4.501483000	-3.244958000	-1.897953000
H	2.398630000	-3.613583000	-1.750764000
C	5.513190000	-2.295741000	-2.002363000
H	5.951119000	-0.187573000	-2.120944000
H	4.747705000	-4.303216000	-1.867030000
H	6.553887000	-2.603551000	-2.054377000

3B

E = -1284.54380307

Mo	0.083594000	0.229055000	0.652478000
N	1.552616000	-0.507444000	-0.025493000
O	-0.512830000	2.015045000	1.097691000
Si	-1.904413000	2.913555000	0.984173000
C	-1.199080000	-0.897278000	0.211502000
C	-1.796525000	-2.115402000	-0.411707000
O	-1.430224000	4.400428000	0.414476000
H	-2.172887000	4.948580000	0.142691000
O	-2.631505000	2.989472000	2.485056000
H	-2.005008000	3.166219000	3.193959000
O	-3.041148000	2.330891000	-0.071502000
H	-3.410088000	1.473033000	0.170466000
C	2.882825000	-0.359962000	-0.309128000
C	3.302288000	0.300393000	-1.500877000
C	3.835927000	-0.929712000	0.589527000
C	4.668741000	0.362741000	-1.767155000
C	5.186296000	-0.825018000	0.271088000
C	5.605619000	-0.185408000	-0.894879000
H	5.011480000	0.855685000	-2.672281000
H	5.928860000	-1.251039000	0.938702000
H	6.665530000	-0.113921000	-1.122382000
C	-1.175175000	-2.339031000	-1.809014000
H	-1.601315000	-3.238102000	-2.266901000
H	-1.369719000	-1.492415000	-2.471894000
H	-0.091812000	-2.461322000	-1.720011000
C	-1.455546000	-3.321030000	0.483224000
H	-0.369324000	-3.427326000	0.546941000
H	-1.845924000	-3.195371000	1.497201000
H	-1.862654000	-4.245921000	0.060046000
C	3.345477000	-1.601671000	1.856859000
H	2.421003000	-2.132568000	1.587043000
C	2.283824000	0.935120000	-2.427255000
H	1.327865000	0.424323000	-2.246283000
C	2.082967000	2.420036000	-2.080322000
H	3.009916000	2.983538000	-2.236114000
H	1.305004000	2.863308000	-2.711480000
H	1.783024000	2.559550000	-1.036692000
C	2.621253000	0.766184000	-3.912209000
H	1.792113000	1.130225000	-4.527806000
H	3.509101000	1.340025000	-4.200151000
H	2.799498000	-0.283064000	-4.167211000
C	4.325109000	-2.622948000	2.438963000
H	5.225189000	-2.144496000	2.841164000
H	3.853797000	-3.165544000	3.264735000

H	4.636408000	-3.354872000	1.687432000
C	2.966227000	-0.563958000	2.928032000
H	2.559231000	-1.054093000	3.819382000
H	3.836272000	0.030236000	3.229304000
H	2.210075000	0.142627000	2.559228000
C	-3.309989000	-1.869377000	-0.542623000
C	-4.266993000	-2.714023000	0.026470000
C	-3.759932000	-0.750158000	-1.260922000
C	-5.631026000	-2.454303000	-0.122418000
H	-3.959795000	-3.585987000	0.593926000
C	-5.119186000	-0.487486000	-1.408311000
H	-3.034538000	-0.070489000	-1.701019000
C	-6.063665000	-1.342090000	-0.837850000
H	-6.355276000	-3.127474000	0.328723000
H	-5.439357000	0.387542000	-1.967500000
H	-7.125121000	-1.139276000	-0.949044000

3B'

E = -1482.28994017

Mo	-0.053954000	0.199247000	0.951950000
C	1.099020000	-1.724356000	2.178108000
H	1.057448000	-0.874335000	2.876899000
H	0.292874000	-2.416108000	2.431901000
C	2.496817000	-2.380276000	2.269256000
N	-1.749966000	-0.286501000	0.737317000
O	0.070546000	2.021983000	1.642018000
Si	0.692890000	3.458927000	1.135429000
C	0.685354000	0.149593000	-0.632991000
H	1.021640000	-1.468497000	1.071045000
C	1.002092000	0.007282000	-2.087678000
O	2.269196000	3.429971000	0.585715000
H	2.907257000	3.520450000	1.300382000
O	0.729654000	4.494567000	2.447083000
H	-0.028499000	4.373720000	3.027946000
O	-0.244420000	4.005516000	-0.123805000
H	0.140427000	4.764452000	-0.573277000
C	-2.776142000	-0.635090000	-0.121822000
C	-3.049817000	-2.005146000	-0.384398000
C	-3.590472000	0.387253000	-0.683818000
C	-4.132158000	-2.321870000	-1.206187000
C	-4.653042000	0.008560000	-1.504627000
C	-4.929428000	-1.329934000	-1.768004000
H	-4.354195000	-3.363456000	-1.417980000
H	-5.280127000	0.776038000	-1.948085000
H	-5.763689000	-1.599112000	-2.410079000
C	2.668609000	-2.939984000	3.688102000
H	3.652606000	-3.408526000	3.796059000
H	2.592394000	-2.148523000	4.442363000
H	1.910732000	-3.698275000	3.914149000
C	2.592609000	-3.515601000	1.241902000
H	1.814376000	-4.269785000	1.404507000
H	2.493280000	-3.135047000	0.219238000
H	3.563408000	-4.016696000	1.314578000
C	3.570797000	-1.323686000	1.984453000
H	3.437725000	-0.872430000	0.995059000
H	3.543262000	-0.521193000	2.731367000

H	4.569043000	-1.772482000	2.016194000
C	0.530882000	1.294571000	-2.807527000
H	0.773925000	1.228350000	-3.873606000
H	-0.550847000	1.412090000	-2.697125000
H	1.014400000	2.181538000	-2.393566000
C	0.222465000	-1.189721000	-2.661724000
H	0.374519000	-1.278326000	-3.743583000
H	0.526084000	-2.129548000	-2.190305000
H	-0.845350000	-1.050380000	-2.477916000
C	-3.319018000	1.845137000	-0.355293000
H	-2.231885000	1.980432000	-0.322733000
C	-2.204888000	-3.087329000	0.265174000
H	-1.170891000	-2.718074000	0.271769000
C	-2.632807000	-3.296650000	1.727159000
H	-3.664757000	-3.661677000	1.774559000
H	-1.993604000	-4.037862000	2.223005000
H	-2.582593000	-2.359185000	2.289077000
C	-2.203429000	-4.418960000	-0.489850000
H	-1.476269000	-5.104506000	-0.041271000
H	-3.179069000	-4.915713000	-0.445295000
H	-1.939605000	-4.286720000	-1.543932000
C	-3.859284000	2.831543000	-1.392947000
H	-4.954959000	2.871454000	-1.394625000
H	-3.497520000	3.838368000	-1.162522000
H	-3.528547000	2.578422000	-2.405748000
C	-3.860349000	2.186432000	1.043049000
H	-3.617929000	3.222337000	1.305472000
H	-4.950379000	2.073244000	1.073228000
H	-3.425589000	1.529857000	1.801768000
C	2.525270000	-0.133636000	-2.246553000
C	3.369745000	0.818797000	-1.654349000
C	3.111245000	-1.166942000	-2.984804000
C	4.751381000	0.741089000	-1.805982000
H	2.938058000	1.622777000	-1.062831000
C	4.497652000	-1.246361000	-3.134604000
H	2.490822000	-1.921534000	-3.457311000
C	5.324084000	-0.293284000	-2.547718000
H	5.384409000	1.493556000	-1.342261000
H	4.927385000	-2.058271000	-3.715863000
H	6.402671000	-0.353548000	-2.665812000

3B''

E = -1403.68316095

Mo	-0.098553000	0.248166000	0.960544000
N	1.657392000	0.092613000	0.731650000
O	-0.598017000	2.127904000	1.142784000
Si	-1.538726000	3.197476000	0.319857000
C	-0.856733000	-0.393152000	-0.479174000
C	-1.222162000	-0.996316000	-1.796606000
O	-0.818254000	3.490199000	-1.149469000
H	-1.386951000	3.979182000	-1.752383000
O	-1.716115000	4.564378000	1.265906000
H	-0.914840000	4.775685000	1.755875000
O	-3.103916000	2.708793000	0.004010000
H	-3.705920000	2.924457000	0.723099000
C	2.703883000	-0.271358000	-0.097231000

C	3.249809000	0.688124000	-0.993848000
C	3.263779000	-1.574422000	-0.001283000
C	4.336117000	0.310128000	-1.783720000
C	4.357146000	-1.889887000	-0.808878000
C	4.891490000	-0.963094000	-1.698217000
H	4.759981000	1.026070000	-2.481692000
H	4.796875000	-2.881053000	-0.749563000
H	5.738453000	-1.232383000	-2.323398000
C	-1.151626000	0.115964000	-2.871213000
H	-1.439392000	-0.296617000	-3.844310000
H	-1.820686000	0.944218000	-2.630546000
H	-0.133396000	0.509552000	-2.939971000
C	-0.203395000	-2.093131000	-2.155659000
H	0.804414000	-1.671755000	-2.145904000
H	-0.231463000	-2.917558000	-1.436797000
H	-0.396264000	-2.497722000	-3.155866000
C	2.704860000	-2.570662000	0.999878000
H	1.615608000	-2.431763000	1.007452000
C	2.679389000	2.095112000	-1.045559000
H	1.592607000	2.017574000	-0.928768000
C	3.204544000	2.925484000	0.137309000
H	4.292971000	3.040909000	0.075356000
H	2.755527000	3.925136000	0.134060000
H	2.964284000	2.444973000	1.089774000
C	2.933171000	2.823738000	-2.366906000
H	2.369008000	3.761358000	-2.381524000
H	3.990867000	3.077864000	-2.503665000
H	2.614897000	2.226068000	-3.227557000
C	2.968210000	-4.035305000	0.642444000
H	4.030023000	-4.292307000	0.726084000
H	2.426313000	-4.693154000	1.330631000
H	2.643184000	-4.267980000	-0.376523000
C	3.223028000	-2.259686000	2.413902000
H	2.775236000	-2.932990000	3.155145000
H	4.310213000	-2.388135000	2.458789000
H	2.997294000	-1.227333000	2.697964000
C	-0.726005000	-1.490161000	2.698483000
H	-0.734721000	-2.576976000	2.840468000
H	0.242623000	-1.158323000	3.089745000
C	-1.920499000	-0.828400000	3.390958000
H	-0.831826000	-1.496547000	1.559172000
C	-1.925981000	-1.096602000	4.894629000
H	-2.788236000	-0.623815000	5.373603000
H	-1.975164000	-2.170894000	5.102819000
H	-1.021681000	-0.704461000	5.372566000
H	-1.914209000	0.257632000	3.220048000
H	-2.845040000	-1.200240000	2.935648000
C	-2.664779000	-1.521710000	-1.699418000
C	-3.679739000	-0.664756000	-1.245235000
C	-3.016133000	-2.824035000	-2.068041000
C	-5.000519000	-1.097684000	-1.171989000
H	-3.428150000	0.347937000	-0.939315000
C	-4.341143000	-3.259192000	-1.992540000
H	-2.258503000	-3.514944000	-2.423239000
C	-5.339266000	-2.399143000	-1.545179000
H	-5.770010000	-0.413977000	-0.822038000

H	-4.588021000	-4.275949000	-2.287383000
H	-6.370523000	-2.736988000	-1.487518000

3C

E = -1601.4249815

Mo	-0.082769000	0.471334000	-0.380107000
C	-0.593408000	-1.096328000	-1.738104000
H	0.313792000	-1.223013000	-2.339266000
H	-0.646426000	-1.963166000	-1.056322000
C	-1.809860000	-1.109639000	-2.692891000
N	1.600843000	-0.013681000	-0.265087000
O	-1.903797000	1.252548000	-0.375755000
Si	-3.241413000	2.060625000	0.108020000
C	-0.306247000	0.269398000	1.742808000
H	0.549324000	0.835232000	2.136436000
C	-0.362308000	-1.095508000	2.470511000
O	-4.654850000	1.179214000	0.139690000
H	-5.088624000	1.130854000	-0.717838000
O	-3.572819000	3.332818000	-0.926362000
H	-2.784621000	3.769528000	-1.262505000
O	-2.976934000	2.537121000	1.685806000
H	-3.779418000	2.848858000	2.116599000
C	2.953909000	-0.220387000	-0.087719000
C	3.553625000	-1.401960000	-0.613031000
C	3.752140000	0.728728000	0.612820000
C	4.921940000	-1.597690000	-0.436521000
C	5.116782000	0.474462000	0.760188000
C	5.706350000	-0.672267000	0.243671000
H	5.384941000	-2.493551000	-0.840200000
H	5.730976000	1.194481000	1.294747000
H	6.771378000	-0.845444000	0.370934000
C	-1.594896000	-2.295268000	-3.657355000
H	-2.441804000	-2.387676000	-4.348074000
H	-0.686359000	-2.164325000	-4.256592000
H	-1.506303000	-3.240025000	-3.109209000
C	-3.124005000	-1.340121000	-1.940882000
H	-3.096572000	-2.282577000	-1.383770000
H	-3.322006000	-0.542496000	-1.224467000
H	-3.962583000	-1.393432000	-2.646648000
C	-1.889299000	0.177927000	-3.525444000
H	-2.111402000	1.041561000	-2.892779000
H	-0.947277000	0.367014000	-4.055422000
H	-2.680400000	0.100009000	-4.280639000
C	-0.545026000	-0.790369000	3.979343000
H	-0.620339000	-1.721265000	4.552382000
H	0.310094000	-0.220781000	4.360761000
H	-1.450763000	-0.205660000	4.163465000
C	0.960719000	-1.853935000	2.315546000
H	1.140954000	-2.167388000	1.284524000
H	1.794734000	-1.209739000	2.609776000
H	0.987094000	-2.741351000	2.957400000
C	3.181204000	2.002627000	1.207578000
H	2.115205000	2.025668000	0.967339000
C	2.739887000	-2.416409000	-1.394317000
H	1.688232000	-2.240962000	-1.152428000
C	2.917228000	-2.192432000	-2.904549000

H	3.958591000	-2.360489000	-3.202324000
H	2.287280000	-2.881937000	-3.477533000
H	2.652761000	-1.169131000	-3.189840000
C	3.056188000	-3.869081000	-1.018586000
H	2.357720000	-4.545693000	-1.522377000
H	4.065762000	-4.166149000	-1.322527000
H	2.969344000	-4.031912000	0.060093000
C	3.316305000	2.026106000	2.737063000
H	4.367518000	2.034348000	3.045710000
H	2.842437000	2.923223000	3.150546000
H	2.844752000	1.151440000	3.195331000
C	3.822014000	3.252820000	0.587679000
H	3.356343000	4.161042000	0.985550000
H	4.892875000	3.307467000	0.811803000
H	3.710791000	3.260132000	-0.500827000
C	0.487315000	2.326332000	-1.267136000
H	1.538367000	2.283103000	-1.567850000
H	-0.124489000	2.265869000	-2.183584000
C	0.199555000	3.629213000	-0.523652000
H	-0.848483000	3.666782000	-0.209305000
H	0.781239000	3.667614000	0.405645000
C	0.528022000	4.868103000	-1.363465000
H	1.585354000	4.883788000	-1.648304000
H	-0.059242000	4.887940000	-2.289052000
H	0.316252000	5.790125000	-0.811042000
H	-1.208430000	0.848943000	1.958044000
C	-1.569037000	-1.930544000	2.019314000
C	-2.856778000	-1.372763000	2.045705000
C	-1.455293000	-3.274168000	1.639308000
C	-3.980544000	-2.123217000	1.713725000
H	-2.990085000	-0.333161000	2.330482000
C	-2.580174000	-4.032475000	1.307951000
H	-0.481231000	-3.751215000	1.608962000
C	-3.849244000	-3.462275000	1.346382000
H	-4.958761000	-1.651743000	1.733547000
H	-2.457758000	-5.074956000	1.024670000
H	-4.725754000	-4.051687000	1.091146000

3D

E = -1403.73223872

Mo	0.095699000	-0.911835000	-0.347784000
N	1.025763000	0.534055000	-0.145119000
O	-0.302126000	-2.301274000	0.932333000
Si	0.468752000	-3.236566000	2.056188000
C	-1.475798000	-0.341133000	-1.186686000
H	-2.074653000	-1.275425000	-1.187389000
C	-2.221648000	0.843839000	-1.766882000
O	0.839286000	-4.768297000	1.534364000
H	0.111459000	-5.389872000	1.633049000
O	-0.519500000	-3.425543000	3.383033000
H	-1.107859000	-2.677562000	3.526149000
O	1.913321000	-2.473441000	2.368214000
H	2.545782000	-3.011639000	2.854147000
C	1.756718000	1.618106000	0.303659000
C	2.824960000	2.100090000	-0.497187000
C	1.430885000	2.237602000	1.538967000

C	3.570563000	3.179744000	-0.024562000
C	2.210580000	3.317012000	1.956953000
C	3.274276000	3.785137000	1.192489000
H	4.398316000	3.554968000	-0.619606000
H	1.981359000	3.800974000	2.902378000
H	3.868273000	4.624883000	1.542718000
C	-1.312105000	2.073715000	-1.843796000
H	-1.846825000	2.927652000	-2.273423000
H	-0.921557000	2.357842000	-0.864009000
H	-0.452291000	1.852208000	-2.481476000
C	-2.658416000	0.484471000	-3.207175000
H	-1.777081000	0.300487000	-3.829850000
H	-3.284624000	-0.411606000	-3.237159000
H	-3.229285000	1.309562000	-3.646876000
C	0.285611000	1.741011000	2.403168000
H	-0.341572000	1.096550000	1.774877000
C	3.177510000	1.421188000	-1.807243000
H	2.290119000	0.860957000	-2.119833000
C	3.522162000	2.409879000	-2.926614000
H	4.457647000	2.945709000	-2.731562000
H	3.651338000	1.874772000	-3.873532000
H	2.731139000	3.154145000	-3.062540000
C	4.313897000	0.408121000	-1.597415000
H	4.537040000	-0.124370000	-2.528678000
H	5.229417000	0.913230000	-1.268752000
H	4.047866000	-0.331774000	-0.836512000
C	0.811066000	0.892757000	3.571541000
H	1.459655000	1.490135000	4.222494000
H	-0.021128000	0.522667000	4.182263000
H	1.387003000	0.032570000	3.218392000
C	-0.610724000	2.877641000	2.910373000
H	-1.486313000	2.465966000	3.423176000
H	-0.088663000	3.522380000	3.625819000
H	-0.964489000	3.506629000	2.087927000
C	1.048762000	-1.863163000	-2.000838000
H	1.366083000	-1.134399000	-2.754353000
H	1.969586000	-2.282385000	-1.557388000
C	0.223315000	-2.974712000	-2.655161000
H	-0.637085000	-2.525118000	-3.167367000
H	-0.192187000	-3.646607000	-1.891154000
C	1.033653000	-3.808449000	-3.651841000
H	0.416200000	-4.582089000	-4.121935000
H	1.444315000	-3.176879000	-4.447715000
H	1.874383000	-4.306781000	-3.156673000
C	-3.469235000	1.086779000	-0.895021000
C	-4.462599000	0.099979000	-0.792736000
C	-3.660935000	2.273077000	-0.177510000
C	-5.598255000	0.290159000	-0.011293000
H	-4.352168000	-0.837183000	-1.332230000
C	-4.798891000	2.469111000	0.606556000
H	-2.920694000	3.063986000	-0.227716000
C	-5.773628000	1.480013000	0.694914000
H	-6.349357000	-0.493526000	0.044163000
H	-4.919697000	3.403785000	1.148118000
H	-6.659859000	1.632375000	1.304660000

TS(3A-3B)**E = -1482.27558317**

Mo	0.023488000	0.323538000	0.689955000
C	0.991636000	-1.330041000	1.985769000
H	0.053953000	-1.713886000	2.400947000
H	1.528628000	-2.219683000	1.627451000
C	1.864387000	-0.646252000	3.065241000
N	-1.710322000	-0.037651000	0.646418000
O	0.361486000	2.239320000	0.885644000
Si	1.183974000	3.372991000	0.023036000
C	0.756154000	-0.297664000	-0.795468000
H	1.091476000	-1.056959000	0.567240000
C	1.131317000	-0.963778000	-2.078435000
O	2.781606000	3.013195000	-0.304974000
H	3.375542000	3.337937000	0.379235000
O	1.252096000	4.776508000	0.926996000
H	0.450201000	4.921764000	1.439469000
O	0.412640000	3.553638000	-1.438613000
H	0.912054000	4.090316000	-2.061977000
C	-2.837106000	-0.455581000	-0.038847000
C	-3.286377000	-1.797954000	0.087270000
C	-3.566144000	0.483299000	-0.819860000
C	-4.453365000	-2.173813000	-0.578829000
C	-4.720217000	0.046240000	-1.470181000
C	-5.167094000	-1.266937000	-1.355753000
H	-4.809623000	-3.196022000	-0.494690000
H	-5.283052000	0.746623000	-2.079513000
H	-6.070261000	-1.582644000	-1.870917000
C	2.349403000	-1.740587000	4.032249000
H	2.966415000	-1.306889000	4.827573000
H	1.506046000	-2.255359000	4.505776000
H	2.954611000	-2.490312000	3.510553000
C	3.082477000	0.033041000	2.420730000
H	3.670689000	-0.678913000	1.831831000
H	2.788078000	0.850453000	1.751972000
H	3.736354000	0.455425000	3.192132000
C	1.049117000	0.386220000	3.860221000
H	0.734800000	1.237730000	3.243742000
H	0.154013000	-0.067802000	4.300032000
H	1.651174000	0.796594000	4.678525000
C	0.991597000	0.092508000	-3.201950000
H	1.283473000	-0.353115000	-4.158672000
H	-0.045330000	0.433733000	-3.271974000
H	1.624324000	0.961545000	-3.011667000
C	0.156585000	-2.120226000	-2.366366000
H	0.353106000	-2.567279000	-3.347442000
H	0.226792000	-2.905453000	-1.607503000
H	-0.868043000	-1.741343000	-2.361600000
C	-3.107750000	1.929348000	-0.900417000
H	-2.012299000	1.927404000	-0.943124000
C	-2.527046000	-2.772003000	0.970971000
H	-1.460033000	-2.559640000	0.827557000
C	-2.853472000	-2.518060000	2.452187000
H	-3.914865000	-2.706879000	2.648316000
H	-2.269219000	-3.180445000	3.102549000
H	-2.640707000	-1.481115000	2.729201000

C	-2.748733000	-4.244449000	0.617676000
H	-2.073314000	-4.876030000	1.204720000
H	-3.769574000	-4.571592000	0.845206000
H	-2.559859000	-4.439925000	-0.442761000
C	-3.599248000	2.673095000	-2.144628000
H	-4.681309000	2.847525000	-2.121439000
H	-3.113960000	3.652400000	-2.201792000
H	-3.363692000	2.126761000	-3.063899000
C	-3.512135000	2.687282000	0.375083000
H	-3.138659000	3.717200000	0.345133000
H	-4.603415000	2.724573000	0.472120000
H	-3.104767000	2.200354000	1.265408000
C	2.597518000	-1.418518000	-1.980181000
C	3.583358000	-0.491295000	-1.606698000
C	2.996937000	-2.728072000	-2.266481000
C	4.922601000	-0.863046000	-1.531990000
H	3.294812000	0.528025000	-1.362636000
C	4.340409000	-3.101656000	-2.189474000
H	2.263583000	-3.472703000	-2.558025000
C	5.308858000	-2.172226000	-1.822968000
H	5.668099000	-0.126056000	-1.244636000
H	4.624982000	-4.125131000	-2.419540000
H	6.354281000	-2.462620000	-1.764042000

TS(3A-3C)

E = -1601.36229395

Mo	-0.092946000	-0.659385000	0.012216000
C	0.012307000	-0.271500000	2.178315000
H	1.045882000	-0.526124000	2.465818000
H	-0.005551000	0.830902000	2.157264000
C	-0.928162000	-0.738483000	3.305863000
N	1.449598000	0.156437000	-0.101472000
O	-1.270273000	-2.234132000	0.430387000
Si	-2.681164000	-2.955096000	0.053175000
C	-1.330959000	0.345631000	-1.074775000
H	-0.633926000	-0.806444000	-1.716277000
C	-1.484625000	1.516929000	-2.034790000
O	-3.960681000	-1.887466000	-0.142043000
H	-4.401658000	-1.691380000	0.691240000
O	-3.181929000	-4.005740000	1.251109000
H	-2.452507000	-4.437771000	1.706178000
O	-2.517452000	-3.718541000	-1.423658000
H	-3.353649000	-4.065707000	-1.751086000
C	2.751210000	0.579207000	0.096356000
C	2.993993000	1.933137000	0.464618000
C	3.837314000	-0.337149000	-0.024983000
C	4.313767000	2.337877000	0.674142000
C	5.131514000	0.129988000	0.195000000
C	5.377216000	1.456086000	0.537011000
H	4.509397000	3.367895000	0.959840000
H	5.966989000	-0.556724000	0.101790000
H	6.395411000	1.796787000	0.703740000
C	-0.539801000	0.012558000	4.596091000
H	-1.166440000	-0.301794000	5.440669000
H	0.505216000	-0.180882000	4.865172000
H	-0.660028000	1.095581000	4.475521000

C	-2.389723000	-0.397424000	2.985774000
H	-2.509242000	0.680249000	2.821928000
H	-2.721001000	-0.910747000	2.080685000
H	-3.053964000	-0.687152000	3.809282000
C	-0.767568000	-2.242244000	3.568300000
H	-0.990402000	-2.813520000	2.666115000
H	0.261266000	-2.471548000	3.872542000
H	-1.433166000	-2.575180000	4.374256000
C	-2.336595000	1.058631000	-3.243457000
H	-2.505936000	1.899763000	-3.923934000
H	-1.820977000	0.267399000	-3.798794000
H	-3.310687000	0.671224000	-2.933742000
C	-0.130715000	1.995370000	-2.561838000
H	0.539055000	2.295283000	-1.755252000
H	0.360358000	1.187271000	-3.109802000
H	-0.256521000	2.836037000	-3.251757000
C	3.598069000	-1.804735000	-0.323782000
H	2.668148000	-1.865902000	-0.893776000
C	1.878633000	2.939373000	0.684805000
H	0.935766000	2.462627000	0.400495000
C	1.771072000	3.323158000	2.169285000
H	2.678203000	3.832306000	2.514234000
H	0.925699000	4.002044000	2.326329000
H	1.621568000	2.441702000	2.798725000
C	2.059565000	4.196221000	-0.178392000
H	1.205676000	4.869189000	-0.048223000
H	2.958716000	4.754888000	0.103565000
H	2.145338000	3.950663000	-1.241560000
C	4.695473000	-2.448732000	-1.177510000
H	5.640540000	-2.544485000	-0.631994000
H	4.394701000	-3.460281000	-1.469222000
H	4.887402000	-1.875025000	-2.089488000
C	3.396542000	-2.593248000	0.981280000
H	3.170668000	-3.644103000	0.767732000
H	4.302650000	-2.559904000	1.596502000
H	2.575662000	-2.182954000	1.577134000
C	0.259999000	-2.063197000	-1.870661000
H	0.866932000	-2.722097000	-1.237969000
H	-0.625186000	-2.651685000	-2.126973000
C	1.044513000	-1.636394000	-3.107839000
H	0.399000000	-1.042251000	-3.769295000
H	1.873654000	-0.975542000	-2.826659000
C	1.581309000	-2.834568000	-3.893519000
H	2.268552000	-3.431994000	-3.284366000
H	0.765555000	-3.493158000	-4.210595000
H	2.122790000	-2.512824000	-4.789858000
H	-2.302717000	-0.123625000	-0.842663000
C	-2.252289000	2.613707000	-1.272476000
C	-1.736567000	3.903187000	-1.104775000
C	-3.521575000	2.342925000	-0.737003000
C	-2.459156000	4.887475000	-0.428604000
H	-0.762394000	4.156462000	-1.507499000
C	-4.242878000	3.321391000	-0.059165000
H	-3.959643000	1.354505000	-0.847211000
C	-3.714379000	4.602178000	0.099411000
H	-2.034435000	5.881987000	-0.319113000

H	-5.223214000	3.081881000	0.344110000
H	-4.277033000	5.367535000	0.626580000

TS(3A-3D)

E = -1601.36260725

Mo	0.127922000	-0.440697000	0.541799000
C	-1.534799000	0.773628000	1.771874000
H	-1.032585000	1.451840000	2.473108000
H	-1.634196000	1.302687000	0.819080000
C	-2.964546000	0.463804000	2.286701000
N	1.116920000	0.919719000	0.125967000
O	1.352528000	-2.013874000	0.430755000
Si	1.503263000	-3.299769000	-0.562198000
C	-0.977149000	-0.716175000	-0.956032000
H	-1.551901000	-1.633551000	-0.711314000
C	-1.302210000	-0.169121000	-2.335707000
O	0.138721000	-4.258822000	-0.712031000
H	0.129903000	-4.972714000	-0.066503000
O	2.673299000	-4.329376000	0.049472000
H	3.359757000	-3.851513000	0.525806000
O	1.871595000	-2.770962000	-2.102497000
H	1.834963000	-3.484249000	-2.747982000
C	2.135614000	1.856525000	0.010751000
C	1.915681000	3.194344000	0.433235000
C	3.384865000	1.473803000	-0.549973000
C	2.962930000	4.109430000	0.322319000
C	4.392613000	2.435365000	-0.636021000
C	4.196815000	3.741030000	-0.200885000
H	2.806697000	5.132862000	0.653018000
H	5.354203000	2.151147000	-1.054721000
H	4.999487000	4.469538000	-0.275700000
C	-2.951191000	0.052684000	3.767311000
H	-3.976601000	-0.047015000	4.140940000
H	-2.453970000	-0.908174000	3.927247000
H	-2.445541000	0.804252000	4.384963000
C	-3.786961000	1.759320000	2.156906000
H	-3.328977000	2.577812000	2.724242000
H	-3.866582000	2.071373000	1.110057000
H	-4.803459000	1.614155000	2.542193000
C	-3.636538000	-0.632716000	1.454114000
H	-3.682566000	-0.358600000	0.396635000
H	-3.099766000	-1.584686000	1.534695000
H	-4.662061000	-0.803421000	1.801989000
C	-0.393172000	1.011570000	-2.694600000
H	-0.671120000	1.427616000	-3.668925000
H	-0.427944000	1.806961000	-1.946476000
H	0.643104000	0.669226000	-2.745340000
C	-1.043269000	-1.287653000	-3.371904000
H	0.014172000	-1.561314000	-3.351412000
H	-1.618461000	-2.193254000	-3.162766000
H	-1.307628000	-0.938004000	-4.376075000
C	3.652512000	0.060305000	-1.029355000
H	2.696559000	-0.464353000	-1.076983000
C	0.589571000	3.643269000	1.017162000
H	-0.118980000	2.823677000	0.877453000
C	0.713942000	3.902256000	2.526125000

H	1.413068000	4.721229000	2.729521000
H	-0.255877000	4.177207000	2.955968000
H	1.083208000	3.015739000	3.052036000
C	0.017486000	4.869482000	0.293334000
H	-0.976541000	5.112334000	0.684742000
H	0.647233000	5.755331000	0.429480000
H	-0.074105000	4.689452000	-0.782353000
C	4.262792000	0.019883000	-2.436037000
H	5.282534000	0.420460000	-2.458279000
H	4.304030000	-1.015458000	-2.787739000
H	3.661585000	0.594393000	-3.147655000
C	4.539556000	-0.694017000	-0.027351000
H	4.716077000	-1.718733000	-0.374402000
H	5.515537000	-0.207238000	0.083482000
H	4.070066000	-0.740878000	0.959757000
C	0.021417000	-1.433351000	2.749738000
H	1.115646000	-1.466312000	2.688066000
H	-0.807659000	-0.381969000	2.154968000
C	-0.562195000	-2.843751000	2.784457000
H	-0.370574000	-3.346434000	1.830258000
H	-1.653966000	-2.792226000	2.890581000
C	0.005099000	-3.695275000	3.923023000
H	-0.442795000	-4.695446000	3.937009000
H	1.089069000	-3.814387000	3.819361000
H	-0.185390000	-3.231193000	4.897447000
H	-0.210747000	-0.905683000	3.685600000
C	-2.791869000	0.227281000	-2.330378000
C	-3.202187000	1.565856000	-2.273661000
C	-3.794138000	-0.755171000	-2.359162000
C	-4.554562000	1.909737000	-2.255416000
H	-2.463602000	2.359806000	-2.256699000
C	-5.144878000	-0.416458000	-2.341539000
H	-3.521338000	-1.805672000	-2.396186000
C	-5.534060000	0.921057000	-2.289863000
H	-4.838959000	2.958307000	-2.220353000
H	-5.894965000	-1.202461000	-2.370017000
H	-6.587087000	1.188142000	-2.278941000

TS(3B-3D)

E = -1403.67256078

Mo	-0.076265000	0.326876000	0.855311000
N	1.656129000	-0.016895000	0.721223000
O	-0.441605000	2.225380000	1.134561000
Si	-1.314322000	3.370139000	0.336391000
C	-0.883265000	-0.291199000	-0.593367000
C	-1.335733000	-0.961489000	-1.848064000
O	-0.606597000	3.597686000	-1.151136000
H	-1.140684000	4.141061000	-1.739019000
O	-1.360924000	4.749219000	1.278206000
H	-0.539690000	4.892013000	1.759844000
O	-2.918303000	2.997054000	0.060928000
H	-3.485057000	3.265733000	0.790899000
C	2.751394000	-0.435331000	-0.012716000
C	3.415102000	0.489213000	-0.864919000
C	3.234844000	-1.763117000	0.135568000
C	4.544854000	0.053711000	-1.557735000

C	4.374992000	-2.137692000	-0.576250000
C	5.028040000	-1.244216000	-1.419331000
H	5.059206000	0.742900000	-2.220528000
H	4.757950000	-3.148769000	-0.475843000
H	5.911251000	-1.558931000	-1.968553000
C	-1.313313000	0.098698000	-2.975957000
H	-1.656704000	-0.356849000	-3.910630000
H	-1.961834000	0.944627000	-2.739964000
H	-0.296854000	0.476528000	-3.119953000
C	-0.358642000	-2.093256000	-2.214418000
H	0.652981000	-1.688282000	-2.293131000
H	-0.346474000	-2.877743000	-1.451603000
H	-0.622712000	-2.547807000	-3.175935000
C	2.541114000	-2.721080000	1.088492000
H	1.464215000	-2.529568000	0.998932000
C	2.916232000	1.919564000	-0.975471000
H	1.820636000	1.890249000	-0.943793000
C	3.384249000	2.742911000	0.236012000
H	4.478039000	2.812580000	0.255066000
H	2.979027000	3.759983000	0.188896000
H	3.053962000	2.285537000	1.172773000
C	3.304873000	2.618151000	-2.280813000
H	2.788419000	3.580666000	-2.349187000
H	4.380537000	2.822238000	-2.335606000
H	3.028018000	2.023494000	-3.157684000
C	2.768242000	-4.199741000	0.765425000
H	3.805190000	-4.504411000	0.946626000
H	2.136217000	-4.824595000	1.405636000
H	2.526345000	-4.428760000	-0.277432000
C	2.943461000	-2.418823000	2.541606000
H	2.404177000	-3.068397000	3.241681000
H	4.016467000	-2.588560000	2.684740000
H	2.731557000	-1.376858000	2.799646000
C	-0.965052000	-1.288041000	2.209144000
H	-1.360108000	-2.275950000	1.937863000
H	-0.051527000	-1.491047000	2.777085000
C	-2.019730000	-0.529385000	3.025784000
H	-1.051436000	-1.118379000	0.774154000
C	-2.530393000	-1.352861000	4.210861000
H	-3.278889000	-0.795517000	4.783017000
H	-2.994164000	-2.284367000	3.869108000
H	-1.713712000	-1.614576000	4.892027000
H	-1.608267000	0.418430000	3.398295000
H	-2.862222000	-0.264621000	2.374860000
C	-2.777990000	-1.451174000	-1.630680000
C	-3.746662000	-0.550072000	-1.159690000
C	-3.172335000	-2.766189000	-1.897685000
C	-5.065874000	-0.952506000	-0.972924000
H	-3.458009000	0.472769000	-0.929276000
C	-4.495690000	-3.170289000	-1.707935000
H	-2.451253000	-3.490618000	-2.262021000
C	-5.447735000	-2.266870000	-1.245986000
H	-5.799316000	-0.235888000	-0.612197000
H	-4.777693000	-4.197343000	-1.924877000
H	-6.477331000	-2.581641000	-1.099189000

TS(3C-3D)**E = -1601.36197425**

Mo	-0.142470000	0.645851000	0.081140000
C	0.724953000	-0.252593000	2.113701000
H	0.015382000	0.393316000	2.644653000
H	0.336977000	-1.272447000	2.212845000
C	2.102832000	-0.124288000	2.816327000
N	-1.669236000	-0.204764000	0.209849000
O	1.249046000	2.045602000	0.352820000
Si	2.329307000	3.101816000	-0.260784000
C	1.007438000	-0.589050000	-0.862118000
H	1.894099000	-0.005389000	-1.148318000
C	1.036880000	-2.013523000	-1.402563000
O	3.606483000	3.464646000	0.747736000
H	3.422337000	4.219909000	1.314901000
O	1.646568000	4.589948000	-0.599031000
H	0.745704000	4.520592000	-0.931041000
O	3.002092000	2.356744000	-1.599616000
H	3.800023000	2.802219000	-1.902114000
C	-2.996257000	-0.578314000	0.314268000
C	-3.612209000	-0.661926000	1.596775000
C	-3.745974000	-0.862371000	-0.861544000
C	-4.952035000	-1.034417000	1.671502000
C	-5.086929000	-1.228050000	-0.720090000
C	-5.690857000	-1.318382000	0.526262000
H	-5.431059000	-1.105846000	2.642803000
H	-5.670168000	-1.444354000	-1.611293000
H	-6.734902000	-1.607727000	0.608505000
C	2.072162000	-1.085982000	4.020305000
H	2.997354000	-1.002381000	4.602282000
H	1.234675000	-0.858201000	4.690102000
H	1.973359000	-2.128685000	3.696731000
C	3.272476000	-0.509253000	1.903436000
H	3.164845000	-1.526168000	1.510170000
H	3.355622000	0.181718000	1.059805000
H	4.217494000	-0.468210000	2.456745000
C	2.313273000	1.302284000	3.341607000
H	2.357179000	2.019421000	2.521648000
H	1.502601000	1.593287000	4.021245000
H	3.253923000	1.364797000	3.900931000
C	-0.074945000	-2.871033000	-0.794802000
H	-0.076184000	-3.873715000	-1.234318000
H	0.028599000	-2.969778000	0.289893000
H	-1.043818000	-2.408940000	-0.984844000
C	0.804669000	-1.918605000	-2.930118000
H	-0.191408000	-1.517704000	-3.136666000
H	1.537806000	-1.268709000	-3.414969000
H	0.883497000	-2.913985000	-3.380180000
C	-3.159442000	-0.760479000	-2.258715000
H	-2.101121000	-0.502284000	-2.153799000
C	-2.834046000	-0.305743000	2.848970000
H	-1.799374000	-0.614825000	2.675717000
C	-2.839885000	1.216814000	3.066927000
H	-3.859098000	1.574652000	3.250514000
H	-2.225716000	1.490296000	3.932472000
H	-2.455752000	1.751282000	2.192086000

C	-3.313129000	-1.030055000	4.110283000
H	-2.619060000	-0.837259000	4.934812000
H	-4.299835000	-0.683808000	4.437337000
H	-3.366202000	-2.112859000	3.959147000
C	-3.256247000	-2.091859000	-3.019083000
H	-4.298925000	-2.371744000	-3.204844000
H	-2.761953000	-2.011463000	-3.993501000
H	-2.787131000	-2.911228000	-2.466898000
C	-3.834202000	0.360761000	-3.063690000
H	-3.368629000	0.457030000	-4.050667000
H	-4.898957000	0.153401000	-3.218394000
H	-3.752617000	1.324049000	-2.553011000
C	-1.180163000	2.296077000	-0.920873000
H	-2.265721000	2.138891000	-0.902413000
H	-0.978167000	3.174366000	-0.286828000
C	-0.734596000	2.571490000	-2.362378000
H	0.358402000	2.654421000	-2.426051000
H	-0.994208000	1.711245000	-2.992723000
C	-1.369575000	3.829064000	-2.966279000
H	-2.462942000	3.758127000	-2.964468000
H	-1.107982000	4.728982000	-2.394812000
H	-1.043596000	3.989994000	-4.000169000
H	1.115718000	-0.553594000	0.644189000
C	2.436426000	-2.610886000	-1.150444000
C	3.574479000	-1.987988000	-1.686806000
C	2.628643000	-3.779322000	-0.404014000
C	4.848789000	-2.508342000	-1.484039000
H	3.471877000	-1.076117000	-2.269408000
C	3.905901000	-4.304521000	-0.198273000
H	1.779393000	-4.298548000	0.026658000
C	5.022323000	-3.672204000	-0.735597000
H	5.709461000	-2.000418000	-1.910847000
H	4.021648000	-5.213568000	0.386120000
H	6.016619000	-4.079179000	-0.574482000

4A

E = -1611.45813148

Mo	-0.210036000	0.568043000	0.005981000
N	1.309403000	-0.257453000	0.126766000
O	-0.178343000	2.090809000	-1.201328000
Si	-0.965801000	3.531106000	-1.345124000
C	-0.523904000	1.197043000	1.732509000
H	-1.435643000	1.806038000	1.544064000
C	0.031994000	1.355505000	3.127927000
O	-1.682422000	3.766157000	-2.824640000
H	-1.083561000	4.135639000	-3.480839000
O	0.108642000	4.792444000	-1.159967000
H	0.795311000	4.614105000	-0.510215000
O	-2.188854000	3.509791000	-0.213947000
H	-2.883962000	4.153962000	-0.379510000
C	2.539885000	-0.880364000	0.118302000
C	2.637690000	-2.273326000	0.372316000
C	3.704682000	-0.099223000	-0.129111000
C	3.907055000	-2.854643000	0.379709000
C	4.943518000	-0.737509000	-0.111311000
C	5.051079000	-2.102579000	0.141894000

H	3.999353000	-3.920142000	0.573980000
H	5.843973000	-0.160051000	-0.297450000
H	6.028107000	-2.578137000	0.152156000
C	1.048027000	0.257585000	3.458914000
H	1.459600000	0.408260000	4.463571000
H	0.576753000	-0.729817000	3.429142000
H	1.874614000	0.254768000	2.743863000
C	-1.129359000	1.311314000	4.139446000
H	-0.748914000	1.433532000	5.160166000
H	-1.851458000	2.112768000	3.949017000
H	-1.664851000	0.358923000	4.086336000
C	0.718282000	2.735199000	3.213432000
H	1.566284000	2.790079000	2.523009000
H	0.019773000	3.541788000	2.965816000
H	1.093075000	2.911739000	4.228965000
C	3.591547000	1.379052000	-0.451531000
H	2.685563000	1.745740000	0.045880000
C	1.414741000	-3.134723000	0.625456000
H	0.536315000	-2.485777000	0.556120000
C	1.270006000	-4.227147000	-0.443202000
H	2.115850000	-4.923695000	-0.421655000
H	0.357519000	-4.807769000	-0.271868000
H	1.210366000	-3.796726000	-1.446671000
C	1.438380000	-3.745263000	2.034174000
H	0.520099000	-4.313331000	2.220130000
H	2.282628000	-4.432512000	2.159823000
H	1.523966000	-2.971600000	2.803149000
C	4.769640000	2.213348000	0.061060000
H	5.696867000	1.993685000	-0.479649000
H	4.563736000	3.279293000	-0.083962000
H	4.952497000	2.044278000	1.127009000
C	3.397633000	1.579702000	-1.963546000
H	3.266841000	2.641391000	-2.200860000
H	4.270543000	1.212737000	-2.515397000
H	2.515916000	1.043160000	-2.323691000
N	-1.743525000	-0.654957000	-0.381298000
C	-1.635063000	-1.393726000	-1.590232000
C	-2.018447000	-2.744745000	-1.660328000
C	-1.100886000	-0.785893000	-2.738806000
C	-1.853267000	-3.462580000	-2.839290000
H	-2.446721000	-3.221519000	-0.784407000
C	-0.917462000	-1.521670000	-3.908736000
H	-0.863364000	0.275199000	-2.725335000
C	-1.292547000	-2.861595000	-3.968060000
H	-2.157725000	-4.505404000	-2.873922000
H	-0.503008000	-1.030895000	-4.785273000
H	-1.162979000	-3.429074000	-4.884948000
C	-2.871394000	-0.950317000	0.434908000
C	-2.722676000	-1.362620000	1.763816000
C	-4.163973000	-0.829224000	-0.097202000
C	-3.842446000	-1.630035000	2.549245000
H	-1.720961000	-1.466983000	2.168696000
C	-5.278288000	-1.099293000	0.691551000
H	-4.282032000	-0.514005000	-1.129872000
C	-5.125055000	-1.498896000	2.019558000
H	-3.708529000	-1.952239000	3.578670000

H	-6.272507000	-0.989655000	0.266491000
H	-5.996296000	-1.708067000	2.633599000

4B

E = -1092.88418562

Mo	-0.703102000	-0.177728000	-0.241455000
N	1.033010000	-0.352490000	0.101632000
O	-1.944115000	1.238141000	-0.742239000
Si	-3.569339000	1.540964000	-0.769132000
C	-1.412331000	-1.598567000	0.521556000
C	-1.430290000	-2.862297000	1.305368000
O	-4.167411000	0.740221000	-2.096050000
H	-5.127716000	0.679427000	-2.094143000
O	-3.790502000	3.196592000	-0.818420000
H	-3.114867000	3.642446000	-1.338921000
O	-4.439405000	1.028513000	0.551970000
H	-4.431182000	1.665580000	1.272949000
C	2.292331000	0.175144000	0.034427000
C	3.130684000	-0.188077000	-1.063426000
C	2.775359000	1.021429000	1.075710000
C	4.434858000	0.297352000	-1.085163000
C	4.092147000	1.469341000	0.998576000
C	4.917535000	1.118788000	-0.067543000
H	5.091174000	0.031021000	-1.908039000
H	4.484187000	2.107283000	1.785132000
H	5.938830000	1.487155000	-0.106666000
C	-0.564110000	-3.914997000	0.587930000
H	-0.584036000	-4.858985000	1.145010000
H	-0.937412000	-4.106962000	-0.423016000
H	0.473790000	-3.577799000	0.513675000
C	-2.887947000	-3.359159000	1.406089000
H	-2.924445000	-4.288851000	1.986732000
H	-3.521629000	-2.616230000	1.898691000
H	-3.303996000	-3.554470000	0.413421000
C	-0.869499000	-2.586245000	2.713169000
H	0.162257000	-2.227380000	2.654968000
H	-1.468773000	-1.830828000	3.231177000
H	-0.884572000	-3.505197000	3.310678000
C	1.855447000	1.427048000	2.210130000
H	1.125828000	0.613966000	2.330163000
C	2.565822000	-1.058699000	-2.167831000
H	1.896015000	-1.782197000	-1.680888000
C	1.701219000	-0.231827000	-3.135370000
H	2.302439000	0.524718000	-3.652231000
H	1.235767000	-0.875199000	-3.890081000
H	0.899559000	0.302312000	-2.608581000
C	3.623477000	-1.845090000	-2.945535000
H	3.137787000	-2.546884000	-3.631061000
H	4.258038000	-1.190155000	-3.553195000
H	4.271023000	-2.419528000	-2.275990000
C	2.572642000	1.609041000	3.550977000
H	3.235284000	2.481746000	3.548008000
H	1.839999000	1.766846000	4.349220000
H	3.171585000	0.730157000	3.808698000
C	1.065961000	2.695400000	1.843645000
H	0.354907000	2.952629000	2.636857000

H	1.741319000	3.546883000	1.702563000
H	0.500449000	2.567753000	0.914051000

4C

E = -1730.53836586

Mo	0.302117000	-0.528375000	-0.059795000
N	-1.400903000	-0.084942000	0.070659000
O	2.113972000	-1.353971000	-0.277810000
Si	3.535733000	-2.107447000	-0.038502000
C	0.370092000	-1.476659000	1.840548000
H	0.057522000	-2.474026000	1.470402000
C	-0.347143000	-1.134920000	3.156304000
O	4.303476000	-1.712851000	1.396380000
H	4.950959000	-1.011608000	1.269467000
O	4.637494000	-1.688631000	-1.226021000
H	4.210451000	-1.462315000	-2.058149000
O	3.226456000	-3.744540000	0.021854000
H	3.981856000	-4.258346000	0.323962000
C	-2.739247000	0.254620000	0.045015000
C	-3.116360000	1.612375000	0.275563000
C	-3.746305000	-0.722009000	-0.219613000
C	-4.467573000	1.953334000	0.216805000
C	-5.078607000	-0.313370000	-0.278387000
C	-5.447202000	1.009331000	-0.065277000
H	-4.757739000	2.985226000	0.396051000
H	-5.846747000	-1.051993000	-0.491719000
H	-6.492712000	1.301340000	-0.112961000
C	-0.079022000	0.321719000	3.552982000
H	-0.555293000	0.554121000	4.512796000
H	0.993021000	0.517791000	3.654552000
H	-0.473354000	1.013048000	2.802634000
C	0.248929000	-2.059475000	4.239035000
H	-0.223062000	-1.868021000	5.210174000
H	0.089916000	-3.115213000	3.991182000
H	1.326908000	-1.899598000	4.350533000
C	-1.854180000	-1.389441000	3.087145000
H	-2.342631000	-0.741590000	2.357527000
H	-2.058884000	-2.430680000	2.813184000
H	-2.317922000	-1.206684000	4.063515000
C	-3.427516000	-2.186543000	-0.451985000
H	-2.355925000	-2.315279000	-0.279997000
C	-2.106385000	2.695767000	0.609555000
H	-1.111312000	2.243991000	0.582688000
C	-2.131393000	3.833696000	-0.421550000
H	-3.109097000	4.327293000	-0.453168000
H	-1.390174000	4.596449000	-0.160337000
H	-1.903914000	3.471115000	-1.427862000
C	-2.338951000	3.251654000	2.023065000
H	-1.547200000	3.961300000	2.285771000
H	-3.297060000	3.779167000	2.091222000
H	-2.344551000	2.456287000	2.773663000
C	-4.172672000	-3.103997000	0.528994000
H	-5.254827000	-3.079007000	0.360622000
H	-3.846794000	-4.141852000	0.398163000
H	-3.990552000	-2.816888000	1.567534000
C	-3.737928000	-2.602633000	-1.898155000

H	-3.431354000	-3.639158000	-2.075016000
H	-4.812322000	-2.535024000	-2.102939000
H	-3.225018000	-1.965979000	-2.624989000
C	-0.108727000	-1.791087000	-1.731344000
H	-1.077628000	-1.534278000	-2.164263000
H	0.680539000	-1.442963000	-2.412337000
C	0.020705000	-3.295980000	-1.497627000
H	0.964642000	-3.521227000	-0.994008000
H	-0.782749000	-3.646023000	-0.836196000
C	-0.046662000	-4.079044000	-2.813767000
H	-0.984359000	-3.891237000	-3.348121000
H	0.777042000	-3.796857000	-3.478676000
H	0.027863000	-5.156323000	-2.630625000
H	1.446560000	-1.548339000	2.029782000
N	1.078832000	1.251475000	-0.514322000
C	1.029796000	1.664382000	-1.862591000
C	1.763579000	2.043314000	0.428163000
C	2.175808000	2.200293000	-2.482204000
C	-0.135366000	1.508047000	-2.632336000
C	1.613176000	3.444157000	0.425020000
C	2.589508000	1.460569000	1.403368000
C	2.146023000	2.572850000	-3.820467000
H	3.083111000	2.322506000	-1.898722000
C	-0.147051000	1.868067000	-3.979534000
H	-1.033395000	1.116478000	-2.166205000
C	2.261749000	4.226701000	1.371710000
H	0.990337000	3.905728000	-0.334541000
C	3.217384000	2.254868000	2.362797000
H	2.763877000	0.390404000	1.386164000
C	0.987732000	2.404250000	-4.582660000
H	3.041166000	2.988688000	-4.275872000
H	-1.061159000	1.740356000	-4.553435000
C	3.060500000	3.638033000	2.355256000
H	2.134945000	5.305965000	1.347737000
H	3.849603000	1.782563000	3.110357000
H	0.971940000	2.690655000	-5.630061000
H	3.559462000	4.253054000	3.098408000

4D

E = -1212.07701855

Mo	-0.676113000	0.424108000	-0.260217000
N	1.015878000	0.057617000	-0.249333000
O	-2.021927000	-0.666614000	-1.117804000
Si	-3.489548000	-1.342120000	-0.772712000
C	-1.066396000	0.810546000	1.522649000
H	-2.167707000	0.955520000	1.458372000
C	-0.530557000	0.918272000	2.928764000
O	-3.437129000	-2.748675000	0.109536000
H	-3.319347000	-3.531698000	-0.437187000
O	-4.250784000	-1.730608000	-2.202849000
H	-4.048230000	-1.119413000	-2.918038000
O	-4.301611000	-0.220918000	0.151572000
H	-5.071138000	-0.580944000	0.603411000
C	2.270850000	-0.517005000	-0.291932000
C	3.398543000	0.316462000	-0.509437000
C	2.417505000	-1.917224000	-0.104856000

C	4.659091000	-0.279368000	-0.557556000
C	3.703618000	-2.454896000	-0.155994000
C	4.816466000	-1.650716000	-0.384368000
H	5.534564000	0.340019000	-0.729638000
H	3.840200000	-3.523033000	-0.014880000
H	5.807974000	-2.093640000	-0.422763000
C	0.981863000	0.678806000	2.980344000
H	1.347631000	0.786962000	4.007901000
H	1.236214000	-0.326040000	2.630973000
H	1.514397000	1.394201000	2.347205000
C	-1.248817000	-0.124427000	3.809009000
H	-0.894858000	-0.059341000	4.844845000
H	-2.332414000	0.036256000	3.811456000
H	-1.059301000	-1.139450000	3.445850000
C	-0.845230000	2.332167000	3.458211000
H	-0.345214000	3.096119000	2.854421000
H	-1.921960000	2.533806000	3.439024000
H	-0.501241000	2.436365000	4.494243000
C	1.205912000	-2.806112000	0.107529000
H	0.416747000	-2.179448000	0.542656000
C	3.221575000	1.806425000	-0.734777000
H	2.268921000	2.083399000	-0.269857000
C	4.321582000	2.655362000	-0.089142000
H	5.292907000	2.513372000	-0.575873000
H	4.073140000	3.718483000	-0.175574000
H	4.439771000	2.420010000	0.973223000
C	3.105984000	2.109417000	-2.237391000
H	2.925631000	3.176976000	-2.406139000
H	4.028907000	1.834968000	-2.760942000
H	2.283046000	1.549485000	-2.691706000
C	0.690033000	-3.337039000	-1.239517000
H	1.446691000	-3.967339000	-1.720164000
H	-0.213301000	-3.940451000	-1.096541000
H	0.445514000	-2.520076000	-1.924590000
C	1.453434000	-3.957266000	1.087710000
H	0.511666000	-4.472784000	1.302637000
H	2.143091000	-4.705005000	0.680630000
H	1.867124000	-3.597304000	2.034852000
C	-0.761111000	2.390027000	-1.085887000
H	0.090146000	2.995617000	-0.756055000
H	-0.622861000	2.220703000	-2.169711000
C	-2.074937000	3.133517000	-0.830903000
H	-2.137742000	3.386351000	0.234926000
H	-2.935841000	2.481482000	-1.035377000
C	-2.214346000	4.408235000	-1.668311000
H	-3.155556000	4.927173000	-1.454705000
H	-1.393177000	5.104153000	-1.462498000
H	-2.193873000	4.181784000	-2.740486000

TS(4A-4B)

E = -1611.37833692

Mo	0.232014000	-0.401845000	-0.133072000
N	-1.257457000	0.305660000	-0.753935000
O	0.468769000	-2.174605000	-0.910711000
Si	0.711208000	-3.701210000	-0.346074000
C	0.125231000	-0.571805000	1.632611000

H	1.448257000	0.082875000	1.173335000
C	-0.262977000	-0.637934000	3.074197000
O	1.970410000	-3.892838000	0.732719000
H	2.808375000	-4.027114000	0.278600000
O	1.115239000	-4.670640000	-1.645708000
H	0.681142000	-4.390705000	-2.458053000
O	-0.671305000	-4.188019000	0.442359000
H	-0.540875000	-4.998742000	0.944403000
C	-2.571286000	0.733507000	-0.726293000
C	-2.853791000	2.085571000	-1.061944000
C	-3.620873000	-0.176956000	-0.424875000
C	-4.183537000	2.506764000	-1.052676000
C	-4.930421000	0.305103000	-0.428895000
C	-5.217195000	1.632562000	-0.731360000
H	-4.416643000	3.537679000	-1.301455000
H	-5.744921000	-0.372772000	-0.192308000
H	-6.245692000	1.983253000	-0.724170000
C	-0.426131000	-2.120081000	3.465560000
H	-0.717498000	-2.195892000	4.520112000
H	-1.192993000	-2.603309000	2.854966000
H	0.510405000	-2.666638000	3.322613000
C	-1.590332000	0.110371000	3.295174000
H	-1.902243000	0.025919000	4.342993000
H	-1.489442000	1.173086000	3.055153000
H	-2.381820000	-0.303504000	2.664765000
C	0.847064000	-0.000853000	3.933133000
H	1.798060000	-0.527694000	3.800415000
H	0.996055000	1.052780000	3.676534000
H	0.575598000	-0.057578000	4.993525000
C	-3.323001000	-1.644720000	-0.179910000
H	-2.359467000	-1.708221000	0.339629000
C	-1.732383000	3.017404000	-1.488173000
H	-0.843055000	2.739872000	-0.911772000
C	-1.397408000	2.797514000	-2.973100000
H	-2.256448000	3.049996000	-3.605054000
H	-0.555521000	3.429588000	-3.279746000
H	-1.132904000	1.753429000	-3.164912000
C	-2.010765000	4.496900000	-1.211652000
H	-1.109431000	5.088139000	-1.403459000
H	-2.800602000	4.895410000	-1.858508000
H	-2.309679000	4.664963000	-0.171986000
C	-4.353570000	-2.355744000	0.700957000
H	-5.320893000	-2.466753000	0.197546000
H	-3.997238000	-3.362725000	0.939579000
H	-4.523685000	-1.822429000	1.642258000
C	-3.163759000	-2.380127000	-1.521010000
H	-2.887239000	-3.425267000	-1.349438000
H	-4.102645000	-2.355317000	-2.086476000
H	-2.384384000	-1.915953000	-2.131804000
N	1.932523000	0.887356000	0.187723000
C	2.034494000	2.207434000	0.686711000
C	3.243776000	2.916028000	0.617002000
C	0.928314000	2.812548000	1.302770000
C	3.335754000	4.197379000	1.153467000
H	4.109751000	2.461090000	0.147326000
C	1.039231000	4.088861000	1.848318000

H	-0.018044000	2.280248000	1.335304000
C	2.240185000	4.792862000	1.776406000
H	4.280509000	4.730472000	1.086614000
H	0.170104000	4.539286000	2.320016000
H	2.319119000	5.792220000	2.193505000
C	2.940785000	0.382615000	-0.690373000
C	3.842375000	-0.589425000	-0.241906000
C	2.994335000	0.820215000	-2.022309000
C	4.782491000	-1.124973000	-1.121429000
H	3.799768000	-0.912637000	0.794294000
C	3.939010000	0.284643000	-2.891946000
H	2.291742000	1.577728000	-2.358835000
C	4.832057000	-0.691314000	-2.445048000
H	5.483500000	-1.876142000	-0.768029000
H	3.976683000	0.626852000	-3.922234000
H	5.566370000	-1.109436000	-3.127424000

TS(4A-4C)

E = -1730.48920145

Mo	0.315817000	-0.520538000	-0.151420000
N	-1.378068000	-0.244387000	0.207825000
O	1.984347000	-0.678226000	-1.243497000
Si	3.504636000	-1.266348000	-1.310522000
C	0.860197000	-1.674798000	1.299682000
H	0.390330000	-2.306501000	0.029180000
C	0.346241000	-2.414203000	2.520885000
O	4.383567000	-1.070875000	0.090643000
H	4.566221000	-0.146017000	0.302405000
O	4.364158000	-0.545606000	-2.548840000
H	3.788646000	-0.282869000	-3.274168000
O	3.383056000	-2.923308000	-1.517931000
H	4.235796000	-3.367747000	-1.479942000
C	-2.679930000	0.164852000	0.421351000
C	-2.963328000	0.922498000	1.598484000
C	-3.722420000	-0.138189000	-0.498992000
C	-4.275280000	1.339140000	1.821033000
C	-5.012413000	0.312312000	-0.219299000
C	-5.297806000	1.041612000	0.928206000
H	-4.498237000	1.921256000	2.710779000
H	-5.811751000	0.089369000	-0.920745000
H	-6.311099000	1.381843000	1.122898000
C	0.834572000	-1.626903000	3.754308000
H	0.566289000	-2.167702000	4.668949000
H	1.922249000	-1.500203000	3.743665000
H	0.372666000	-0.636724000	3.797784000
C	0.986150000	-3.817942000	2.549232000
H	0.669178000	-4.358802000	3.448155000
H	0.687571000	-4.411253000	1.678734000
H	2.079440000	-3.757409000	2.556515000
C	-1.177595000	-2.546140000	2.557573000
H	-1.666901000	-1.571535000	2.515394000
H	-1.545013000	-3.140195000	1.715554000
H	-1.486517000	-3.047672000	3.481468000
C	-3.483097000	-0.905637000	-1.785625000
H	-2.442526000	-1.240226000	-1.780297000
C	-1.884433000	1.336864000	2.584141000

H	-0.975439000	0.785058000	2.326006000
C	-1.570161000	2.833125000	2.436682000
H	-2.444997000	3.444509000	2.686483000
H	-0.755849000	3.121365000	3.110852000
H	-1.268554000	3.073315000	1.414630000
C	-2.251615000	1.003893000	4.036939000
H	-1.413189000	1.241765000	4.700834000
H	-3.110409000	1.588400000	4.384190000
H	-2.496561000	-0.054754000	4.165874000
C	-4.381098000	-2.146918000	-1.887047000
H	-5.438148000	-1.870110000	-1.961511000
H	-4.133169000	-2.728111000	-2.781398000
H	-4.272078000	-2.798975000	-1.015092000
C	-3.675301000	-0.001133000	-3.012468000
H	-3.423280000	-0.541301000	-3.932171000
H	-4.715435000	0.332220000	-3.098198000
H	-3.045883000	0.890079000	-2.949223000
C	-0.068976000	-2.471218000	-1.431394000
H	-0.451420000	-1.854991000	-2.255105000
H	0.905599000	-2.850133000	-1.747907000
C	-1.043935000	-3.604619000	-1.127462000
H	-0.627274000	-4.249207000	-0.341244000
H	-1.981054000	-3.204810000	-0.725528000
C	-1.330760000	-4.458882000	-2.363289000
H	-1.777388000	-3.859255000	-3.164147000
H	-0.408915000	-4.900346000	-2.756726000
H	-2.022780000	-5.275390000	-2.130607000
H	1.954964000	-1.769437000	1.208318000
N	0.831240000	1.495250000	-0.130064000
C	2.089678000	1.809068000	0.420276000
C	3.123207000	2.362006000	-0.360590000
C	2.363904000	1.515962000	1.766641000
C	4.382512000	2.591157000	0.185528000
H	2.930521000	2.592730000	-1.403136000
C	3.628559000	1.737063000	2.306609000
H	1.568071000	1.110495000	2.383262000
C	4.649741000	2.272426000	1.520401000
H	5.167098000	3.006718000	-0.441383000
H	3.813875000	1.498720000	3.350759000
H	5.635117000	2.449223000	1.941620000
C	0.266630000	2.419925000	-1.016351000
C	0.317971000	3.806386000	-0.758546000
C	-0.393173000	2.000546000	-2.186137000
C	-0.276185000	4.717071000	-1.623591000
H	0.828374000	4.156691000	0.133469000
C	-0.995503000	2.919687000	-3.043616000
H	-0.400557000	0.944997000	-2.451155000
C	-0.943930000	4.284483000	-2.770913000
H	-0.223431000	5.778276000	-1.393380000
H	-1.485671000	2.563389000	-3.946051000
H	-1.405438000	4.999871000	-3.444938000

TS(4A-4D)

E = -1730.48326492

Mo	0.317024000	-0.593786000	0.223233000
N	0.585908000	1.043112000	-0.279425000

O	2.126372000	-1.131026000	0.847276000
Si	3.387485000	-1.918310000	0.164823000
C	0.168077000	-1.522830000	-1.378973000
H	0.033480000	-2.555249000	-0.980562000
C	0.279391000	-1.459358000	-2.882135000
O	3.124311000	-3.515273000	-0.254841000
H	3.322811000	-4.115385000	0.471262000
O	4.641408000	-1.975380000	1.271659000
H	4.621781000	-1.226926000	1.876308000
O	3.799072000	-1.135695000	-1.249798000
H	4.474046000	-1.607084000	-1.748467000
C	0.829780000	2.401824000	-0.416835000
C	-0.143337000	3.241776000	-1.023193000
C	2.064417000	2.941067000	0.039061000
C	0.145417000	4.601259000	-1.154482000
C	2.288461000	4.309045000	-0.112032000
C	1.344298000	5.140120000	-0.704577000
H	-0.590940000	5.252237000	-1.618310000
H	3.225874000	4.730839000	0.240203000
H	1.542733000	6.202588000	-0.815959000
C	0.950270000	-0.155992000	-3.328891000
H	1.008992000	-0.122110000	-4.423047000
H	0.385611000	0.713859000	-2.987219000
H	1.960987000	-0.084332000	-2.918613000
C	-1.133485000	-1.564452000	-3.488985000
H	-1.064095000	-1.575041000	-4.583269000
H	-1.640690000	-2.480815000	-3.171271000
H	-1.755945000	-0.717302000	-3.190442000
C	1.126746000	-2.656043000	-3.357965000
H	2.126175000	-2.623219000	-2.917353000
H	0.662498000	-3.609365000	-3.082034000
H	1.226624000	-2.632648000	-4.449422000
C	3.118003000	2.075536000	0.705103000
H	2.823145000	1.033013000	0.569335000
C	-1.479287000	2.723124000	-1.523375000
H	-1.499304000	1.643049000	-1.344795000
C	-2.642554000	3.360085000	-0.747408000
H	-2.657106000	4.447543000	-0.880176000
H	-3.604578000	2.979233000	-1.109628000
H	-2.573269000	3.152369000	0.323623000
C	-1.652694000	2.957673000	-3.031740000
H	-2.586723000	2.505079000	-3.382607000
H	-1.696845000	4.026742000	-3.267713000
H	-0.829417000	2.525366000	-3.607124000
C	4.501879000	2.244985000	0.065015000
H	4.897298000	3.258404000	0.196550000
H	5.216911000	1.554007000	0.524602000
H	4.469552000	2.025644000	-1.005468000
C	3.171452000	2.353623000	2.215586000
H	3.906204000	1.703167000	2.704092000
H	3.459572000	3.391227000	2.419835000
H	2.200803000	2.178110000	2.690702000
C	-0.166776000	-1.965776000	2.244004000
H	0.648206000	-1.440824000	2.755951000
H	-1.189097000	-1.338171000	1.407128000
C	0.206404000	-3.431642000	2.012275000

H	1.050869000	-3.497422000	1.317234000
H	-0.625787000	-3.960902000	1.525833000
C	0.565797000	-4.173111000	3.302681000
H	0.814688000	-5.223354000	3.109999000
H	1.428458000	-3.707299000	3.792281000
H	-0.266887000	-4.152545000	4.014929000
H	-1.011952000	-1.913159000	2.952677000
N	-1.883032000	-0.536937000	0.733799000
C	-2.385016000	0.372386000	1.712529000
C	-3.709498000	0.295437000	2.177833000
C	-1.524233000	1.302144000	2.313241000
C	-4.150457000	1.133681000	3.196439000
H	-4.392799000	-0.423835000	1.739336000
C	-1.969404000	2.124792000	3.347221000
H	-0.505710000	1.407037000	1.952671000
C	-3.286131000	2.051974000	3.792969000
H	-5.181014000	1.057917000	3.533392000
H	-1.279654000	2.837579000	3.790833000
H	-3.635827000	2.701666000	4.589685000
C	-2.845507000	-1.163480000	-0.118952000
C	-2.971455000	-2.557121000	-0.143425000
C	-3.690352000	-0.395942000	-0.930797000
C	-3.897995000	-3.170287000	-0.985164000
H	-2.345995000	-3.163656000	0.504549000
C	-4.623974000	-1.011739000	-1.759618000
H	-3.616127000	0.685530000	-0.896132000
C	-4.728642000	-2.402239000	-1.798660000
H	-3.978361000	-4.254019000	-0.990785000
H	-5.271052000	-0.399314000	-2.382007000
H	-5.454961000	-2.880257000	-2.449403000

TS(4B-4D)

E = -1212.01324140

Mo	-0.659629000	0.588239000	-0.357037000
N	0.942934000	-0.022088000	-0.803890000
O	-2.090913000	-0.518966000	-1.089738000
Si	-3.394846000	-1.314479000	-0.475154000
C	-0.730006000	0.674274000	1.408276000
C	-0.516142000	0.675690000	2.881754000
O	-2.850121000	-2.356635000	0.702380000
H	-3.569570000	-2.757711000	1.200185000
O	-4.181101000	-2.081957000	-1.734341000
H	-3.569713000	-2.401594000	-2.405741000
O	-4.559253000	-0.349326000	0.226431000
H	-5.209663000	-0.042448000	-0.413068000
C	2.158396000	-0.572153000	-0.438351000
C	2.268003000	-1.980938000	-0.279723000
C	3.294662000	0.266731000	-0.279786000
C	3.514759000	-2.513055000	0.050296000
C	4.516699000	-0.324528000	0.042914000
C	4.633160000	-1.700538000	0.211801000
H	3.615820000	-3.585680000	0.184947000
H	5.394639000	0.301446000	0.170556000
H	5.593598000	-2.139183000	0.468429000
C	-0.425267000	-0.802395000	3.314156000
H	-0.318191000	-0.860337000	4.403605000

H	-1.322663000	-1.351779000	3.017802000
H	0.439634000	-1.288605000	2.854040000
C	-1.709748000	1.351672000	3.583787000
H	-1.574817000	1.321840000	4.671450000
H	-1.801389000	2.401745000	3.285336000
H	-2.646375000	0.845483000	3.334197000
C	0.792498000	1.405307000	3.235953000
H	1.646007000	0.933463000	2.741352000
H	0.755338000	2.456875000	2.929509000
H	0.959877000	1.380753000	4.319131000
C	3.173039000	1.763392000	-0.510829000
H	2.206307000	2.070404000	-0.092223000
C	1.057689000	-2.871477000	-0.506784000
H	0.183765000	-2.350170000	-0.097854000
C	0.810869000	-3.062127000	-2.012587000
H	1.656702000	-3.580156000	-2.479165000
H	-0.089551000	-3.663907000	-2.181480000
H	0.679491000	-2.098869000	-2.512977000
C	1.139088000	-4.227388000	0.198400000
H	0.181571000	-4.749526000	0.104424000
H	1.905613000	-4.875647000	-0.241997000
H	1.359572000	-4.118191000	1.265260000
C	4.253564000	2.595046000	0.184645000
H	5.242834000	2.434025000	-0.258287000
H	4.028379000	3.662094000	0.082726000
H	4.320173000	2.363538000	1.252572000
C	3.142236000	2.072460000	-2.016862000
H	2.999094000	3.145163000	-2.194955000
H	4.086716000	1.777317000	-2.487555000
H	2.335029000	1.525683000	-2.513383000
C	-0.593130000	2.858323000	-0.636176000
H	-0.304053000	3.638584000	0.080270000
H	0.194168000	2.866897000	-1.396779000
C	-1.977956000	3.186604000	-1.210445000
H	-0.577769000	2.060711000	0.577070000
C	-2.055630000	4.619672000	-1.743206000
H	-3.049522000	4.835341000	-2.147926000
H	-1.852012000	5.345360000	-0.948249000
H	-1.324826000	4.784353000	-2.542035000
H	-2.230913000	2.489220000	-2.020298000
H	-2.741146000	3.042459000	-0.435212000

TS(4C-4D)

E = -1730.48225876

Mo	-0.032706000	-0.669583000	0.238674000
N	-1.607273000	-0.110160000	-0.185298000
O	1.238438000	-1.021116000	-1.129016000
Si	2.389732000	-1.857033000	-1.991709000
C	0.158383000	-0.676799000	2.207311000
H	1.066165000	-1.275553000	2.407894000
C	-0.654700000	-0.458769000	3.480155000
O	3.720369000	-2.279580000	-1.112725000
H	4.256606000	-1.530837000	-0.811533000
O	2.887447000	-0.922923000	-3.276573000
H	2.152758000	-0.523362000	-3.753182000
O	1.639928000	-3.260129000	-2.479628000

H	2.253747000	-3.907026000	-2.841864000
C	-2.703552000	0.302435000	-0.925263000
C	-2.521357000	1.129836000	-2.068023000
C	-3.998159000	-0.114898000	-0.516918000
C	-3.660246000	1.544542000	-2.758379000
C	-5.094991000	0.326327000	-1.257283000
C	-4.935366000	1.154107000	-2.362329000
H	-3.546626000	2.180734000	-3.630806000
H	-6.092494000	0.010854000	-0.964190000
H	-5.804236000	1.489339000	-2.921950000
C	-1.711596000	0.634700000	3.293439000
H	-2.304073000	0.748661000	4.207912000
H	-1.246502000	1.599861000	3.068684000
H	-2.390962000	0.392082000	2.472931000
C	0.303782000	-0.037774000	4.612103000
H	-0.250155000	0.115418000	5.545486000
H	1.063431000	-0.806063000	4.796944000
H	0.816131000	0.899069000	4.369037000
C	-1.329594000	-1.787520000	3.861591000
H	-2.023495000	-2.114935000	3.082031000
H	-0.590479000	-2.582095000	4.011097000
H	-1.891973000	-1.672893000	4.795654000
C	-4.205836000	-1.065083000	0.647622000
H	-3.240957000	-1.176366000	1.151911000
C	-1.144666000	1.514263000	-2.579841000
H	-0.427494000	1.383152000	-1.762224000
C	-0.730305000	0.570722000	-3.720948000
H	-1.429870000	0.642013000	-4.561059000
H	0.262632000	0.848299000	-4.094943000
H	-0.703217000	-0.472200000	-3.391311000
C	-1.047060000	2.979267000	-3.019584000
H	-0.011681000	3.217494000	-3.283325000
H	-1.661740000	3.188764000	-3.901817000
H	-1.349182000	3.656663000	-2.216862000
C	-5.214094000	-0.525940000	1.670307000
H	-6.221427000	-0.449430000	1.246899000
H	-5.274097000	-1.198357000	2.532628000
H	-4.927787000	0.465984000	2.032552000
C	-4.623931000	-2.455356000	0.142944000
H	-4.721183000	-3.154072000	0.981190000
H	-5.590087000	-2.415136000	-0.372400000
H	-3.888018000	-2.862495000	-0.556771000
C	-0.524968000	-2.759207000	0.191487000
H	-1.489494000	-2.911443000	0.688128000
H	-0.662938000	-2.981914000	-0.876251000
C	0.533069000	-3.689087000	0.787065000
H	1.535767000	-3.417456000	0.433848000
H	0.547730000	-3.568122000	1.878335000
C	0.279894000	-5.159326000	0.444738000
H	-0.708762000	-5.482368000	0.790673000
H	0.324697000	-5.312887000	-0.638032000
H	1.028080000	-5.810822000	0.910080000
H	0.711918000	0.399650000	1.761431000
N	1.494368000	1.306220000	0.756925000
C	2.856064000	1.000110000	0.584504000
C	3.563302000	0.297461000	1.576055000

C	3.538629000	1.326440000	-0.603403000
C	4.887128000	-0.092759000	1.376949000
H	3.068140000	0.074173000	2.516498000
C	4.865218000	0.952440000	-0.794151000
H	3.006658000	1.872619000	-1.375930000
C	5.548241000	0.229507000	0.190696000
H	5.408225000	-0.639569000	2.158496000
H	5.364298000	1.208191000	-1.724827000
H	6.582932000	-0.064251000	0.039032000
C	1.109244000	2.646374000	0.786952000
C	-0.253167000	3.004167000	0.685246000
C	2.032468000	3.696761000	0.997283000
C	-0.664966000	4.328496000	0.802324000
H	-0.993578000	2.229730000	0.511350000
C	1.610272000	5.017941000	1.094358000
H	3.088177000	3.464758000	1.094236000
C	0.259408000	5.353129000	1.002179000
H	-1.725204000	4.558807000	0.725063000
H	2.353002000	5.796268000	1.254303000
H	-0.064390000	6.386561000	1.081590000

5A

E = -1381.70247139

Mo	-0.677467000	-0.347998000	-0.124748000
N	0.942297000	0.247770000	-0.106326000
O	-1.950097000	0.706151000	-1.125268000
Si	-3.374023000	1.466973000	-0.775063000
C	-1.160341000	-0.292503000	1.674010000
H	-2.228058000	-0.598865000	1.613461000
C	-0.756562000	0.179920000	3.051275000
O	-4.384098000	0.596662000	0.225397000
H	-4.982064000	0.020669000	-0.262361000
O	-4.230611000	1.688033000	-2.186741000
H	-3.669937000	1.879474000	-2.945255000
O	-2.983512000	2.877689000	0.010480000
H	-3.746125000	3.312657000	0.404980000
C	2.218728000	0.762509000	-0.185683000
C	3.335690000	-0.099454000	-0.026084000
C	2.387828000	2.156032000	-0.417650000
C	4.611567000	0.461505000	-0.106730000
C	3.687394000	2.654626000	-0.489760000
C	4.792254000	1.820557000	-0.336661000
H	5.480233000	-0.181026000	0.011618000
H	3.841957000	3.714691000	-0.666706000
H	5.795735000	2.233329000	-0.396300000
C	0.666382000	0.745045000	3.062257000
H	0.939591000	1.059910000	4.075772000
H	1.389872000	-0.002999000	2.727398000
H	0.752770000	1.611074000	2.399875000
C	-0.848217000	-1.000812000	4.037823000
H	-0.636640000	-0.654674000	5.056215000
H	-1.847595000	-1.448720000	4.035684000
H	-0.122537000	-1.780883000	3.788101000
C	-1.750856000	1.276896000	3.485755000
H	-1.739113000	2.115656000	2.783403000
H	-2.774242000	0.889123000	3.531261000

H	-1.486628000	1.653661000	4.480984000
C	1.186673000	3.059614000	-0.625104000
H	0.341361000	2.604995000	-0.096296000
C	3.175855000	-1.589498000	0.215964000
H	2.103930000	-1.805406000	0.252675000
C	3.773328000	-2.411427000	-0.935506000
H	4.857738000	-2.270645000	-1.008128000
H	3.584009000	-3.478436000	-0.778898000
H	3.334850000	-2.130003000	-1.897277000
C	3.784756000	-2.015312000	1.559666000
H	3.602267000	-3.080503000	1.738182000
H	4.868943000	-1.857575000	1.578796000
H	3.353423000	-1.452433000	2.393005000
C	1.373473000	4.469993000	-0.057143000
H	2.115483000	5.048028000	-0.619305000
H	0.427771000	5.018210000	-0.114074000
H	1.688775000	4.444273000	0.990735000
C	0.813894000	3.117724000	-2.115581000
H	-0.081858000	3.730724000	-2.262029000
H	1.628872000	3.557111000	-2.702206000
H	0.610313000	2.119252000	-2.512992000
N	-0.715830000	-2.291754000	-0.679238000
C	-1.149511000	-3.482613000	-0.089580000
C	-0.312339000	-2.597036000	-1.992041000
C	-1.028426000	-4.495122000	-1.008791000
C	-0.501220000	-3.936062000	-2.210830000
H	-1.294844000	-5.530478000	-0.836622000
H	-0.289358000	-4.458128000	-3.135441000
C	0.197985000	-1.558885000	-2.940266000
H	-0.548520000	-0.784490000	-3.164778000
H	1.097916000	-1.052466000	-2.569146000
H	0.458354000	-2.035218000	-3.889228000
C	-1.656702000	-3.578826000	1.308814000
H	-0.921223000	-3.234762000	2.042867000
H	-2.571984000	-2.995439000	1.469174000
H	-1.892021000	-4.623012000	1.532246000

5B'

E = -1381.64322468

Mo	0.555140000	0.569486000	-0.118594000
N	-0.942775000	-0.176924000	-0.736437000
O	2.115477000	0.001330000	-1.165909000
Si	3.559027000	-0.681929000	-0.780857000
C	0.783338000	0.008779000	1.521678000
H	1.176960000	2.853799000	1.080631000
C	0.760722000	-0.665478000	2.857616000
O	4.434504000	0.098555000	0.410852000
H	5.129788000	0.644790000	0.030256000
O	4.562612000	-0.585962000	-2.118576000
H	4.101772000	-0.786079000	-2.939653000
O	3.280642000	-2.244780000	-0.284176000
H	4.033306000	-2.623662000	0.180219000
C	-1.965086000	-1.089097000	-0.539090000
C	-3.300352000	-0.623765000	-0.394350000
C	-1.694244000	-2.487787000	-0.560813000
C	-4.324310000	-1.556898000	-0.227001000

C	-2.758596000	-3.372985000	-0.385729000
C	-4.063738000	-2.922679000	-0.209229000
H	-5.347153000	-1.209916000	-0.109668000
H	-2.564020000	-4.441323000	-0.388529000
H	-4.873689000	-3.633517000	-0.069307000
C	1.812484000	-1.790886000	2.869405000
H	1.809304000	-2.294341000	3.844185000
H	1.601954000	-2.531831000	2.094294000
H	2.812810000	-1.387712000	2.688628000
C	-0.633343000	-1.253372000	3.145079000
H	-0.640374000	-1.758683000	4.118952000
H	-1.397450000	-0.469601000	3.165669000
H	-0.920461000	-1.975445000	2.376327000
C	1.123190000	0.369872000	3.940880000
H	2.111377000	0.802192000	3.753604000
H	0.389763000	1.182303000	3.977093000
H	1.140770000	-0.108503000	4.927452000
C	-0.289458000	-2.994554000	-0.837609000
H	0.412093000	-2.328238000	-0.323502000
C	-3.605020000	0.859058000	-0.511607000
H	-2.719881000	1.398655000	-0.159133000
C	-3.799744000	1.238439000	-1.988687000
H	-4.664800000	0.714526000	-2.411156000
H	-3.969493000	2.316268000	-2.100183000
H	-2.918193000	0.967608000	-2.576839000
C	-4.799323000	1.319720000	0.329105000
H	-4.884255000	2.412121000	0.299346000
H	-5.747570000	0.920552000	-0.047875000
H	-4.700845000	1.012764000	1.375591000
C	-0.015396000	-4.409027000	-0.321897000
H	-0.571139000	-5.169455000	-0.883175000
H	1.049314000	-4.636612000	-0.433664000
H	-0.275740000	-4.514897000	0.736728000
C	0.019613000	-2.902837000	-2.340756000
H	1.051149000	-3.214857000	-2.537530000
H	-0.652044000	-3.554147000	-2.912399000
H	-0.104883000	-1.878426000	-2.702453000
N	0.487534000	2.849452000	0.329698000
C	-0.835196000	3.262800000	0.690724000
C	0.839650000	3.522314000	-0.884537000
C	-1.307413000	4.028291000	-0.327784000
C	-0.268214000	4.184390000	-1.310192000
H	-2.303236000	4.447413000	-0.379409000
H	-0.342636000	4.741474000	-2.234855000
C	-1.437970000	2.881616000	1.997337000
H	-1.463886000	1.796668000	2.133520000
H	-0.878730000	3.310756000	2.838508000
H	-2.460281000	3.261748000	2.048696000
C	2.216074000	3.433488000	-1.449861000
H	2.259482000	4.006249000	-2.378736000
H	2.960981000	3.856447000	-0.763403000
H	2.512504000	2.402215000	-1.671730000

5C

E = -1500.79008346

Mo	0.577802000	-0.282848000	0.154346000
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N	-1.146110000	-0.046013000	-0.115274000
O	2.511154000	-0.593037000	0.446151000
Si	4.027846000	-0.451887000	-0.174382000
C	0.446335000	-0.865792000	2.182709000
H	0.797210000	-1.898967000	1.991113000
C	-0.729770000	-0.885952000	3.166687000
O	5.169531000	-1.344474000	0.649038000
H	5.610568000	-0.828448000	1.330860000
O	4.579782000	1.113776000	-0.122292000
H	3.901219000	1.782086000	-0.318121000
O	3.942502000	-1.088152000	-1.718115000
H	4.803764000	-1.156312000	-2.141676000
C	-2.474955000	0.216057000	-0.389406000
C	-2.979189000	1.543745000	-0.247799000
C	-3.341367000	-0.837168000	-0.808335000
C	-4.327308000	1.773718000	-0.524188000
C	-4.677870000	-0.538309000	-1.070246000
C	-5.176007000	0.751706000	-0.931056000
H	-4.717794000	2.782495000	-0.424357000
H	-5.342293000	-1.334131000	-1.394880000
H	-6.221055000	0.960100000	-1.143129000
C	-1.275508000	0.526449000	3.399175000
H	-2.086566000	0.512720000	4.136404000
H	-0.495750000	1.197124000	3.777964000
H	-1.668832000	0.946670000	2.470496000
C	-0.186362000	-1.435881000	4.502087000
H	-0.984029000	-1.478800000	5.253073000
H	0.216370000	-2.447909000	4.381576000
H	0.613922000	-0.800794000	4.898146000
C	-1.855704000	-1.804403000	2.682558000
H	-2.301470000	-1.428344000	1.759700000
H	-1.485241000	-2.819833000	2.497882000
H	-2.649037000	-1.872294000	3.435827000
C	-2.848272000	-2.256877000	-1.023214000
H	-1.843589000	-2.322267000	-0.595948000
C	-2.105476000	2.720836000	0.149827000
H	-1.122478000	2.332621000	0.429680000
C	-1.899283000	3.670393000	-1.040924000
H	-2.848703000	4.120575000	-1.353578000
H	-1.213003000	4.477889000	-0.767527000
H	-1.470167000	3.149015000	-1.899401000
C	-2.675124000	3.495486000	1.347717000
H	-1.971979000	4.276573000	1.655847000
H	-3.619896000	3.990533000	1.097909000
H	-2.858746000	2.845533000	2.207818000
C	-3.718234000	-3.305843000	-0.317043000
H	-4.725681000	-3.355716000	-0.743740000
H	-3.271267000	-4.299625000	-0.428029000
H	-3.817224000	-3.095505000	0.751429000
C	-2.749830000	-2.567613000	-2.525539000
H	-2.325564000	-3.564452000	-2.688487000
H	-3.740280000	-2.545204000	-2.993921000
H	-2.123198000	-1.838814000	-3.048881000
C	0.741906000	-1.869832000	-1.236736000
H	-0.117646000	-1.887128000	-1.908986000
H	1.642435000	-1.576967000	-1.792440000

C	0.967776000	-3.236950000	-0.581979000
H	1.826101000	-3.182821000	0.096157000
H	0.096591000	-3.525327000	0.022051000
C	1.227181000	-4.321623000	-1.633257000
H	0.383532000	-4.415436000	-2.325490000
H	2.119694000	-4.083027000	-2.219984000
H	1.384197000	-5.296185000	-1.158592000
H	1.307735000	-0.349072000	2.626930000
N	1.108050000	1.560848000	-0.516465000
C	1.792682000	2.520038000	0.217464000
C	1.124366000	1.936640000	-1.856495000
C	2.242479000	3.491726000	-0.657882000
C	1.823223000	3.119694000	-1.964046000
H	2.779571000	4.387820000	-0.372477000
H	1.995878000	3.661727000	-2.884887000
C	1.939828000	2.464930000	1.703581000
H	0.970044000	2.406909000	2.212860000
H	2.543540000	1.609645000	2.027607000
H	2.438350000	3.372982000	2.052472000
C	0.485609000	1.139648000	-2.947567000
H	1.052380000	0.235958000	-3.202141000
H	-0.533818000	0.832324000	-2.688192000
H	0.430588000	1.750417000	-3.852746000

TS(5A-5B)

E = -1381.61880838

Mo	0.567549000	0.409826000	-0.295177000
N	-1.056316000	-0.188042000	-0.630121000
O	1.841099000	-0.508649000	-1.440617000
Si	3.221306000	-1.378775000	-1.197888000
C	1.002514000	0.094708000	1.395992000
H	1.133921000	1.599203000	0.996713000
C	1.129092000	-0.325987000	2.824842000
O	4.388799000	-0.638595000	-0.264526000
H	5.032486000	-0.162889000	-0.799257000
O	3.957767000	-1.608208000	-2.678782000
H	3.327150000	-1.749245000	-3.392257000
O	2.792994000	-2.791429000	-0.432995000
H	3.553584000	-3.271192000	-0.090084000
C	-2.243823000	-0.842849000	-0.357691000
C	-3.457253000	-0.114540000	-0.494708000
C	-2.255668000	-2.221775000	-0.012924000
C	-4.657094000	-0.771348000	-0.219525000
C	-3.487476000	-2.822522000	0.249094000
C	-4.678939000	-2.108907000	0.161647000
H	-5.593539000	-0.228935000	-0.308412000
H	-3.517556000	-3.872100000	0.525014000
H	-5.624456000	-2.599031000	0.377336000
C	2.015071000	-1.586466000	2.877528000
H	2.129982000	-1.912344000	3.918139000
H	1.569464000	-2.404074000	2.305345000
H	3.006058000	-1.383012000	2.462974000
C	-0.256862000	-0.637545000	3.418901000
H	-0.155481000	-0.987229000	4.453231000
H	-0.896440000	0.249700000	3.420646000
H	-0.763137000	-1.414225000	2.839408000

C	1.809847000	0.801254000	3.626229000
H	2.801096000	1.027823000	3.221294000
H	1.215756000	1.721146000	3.615188000
H	1.929289000	0.494200000	4.671380000
C	-0.969716000	-3.027536000	-0.016018000
H	-0.169115000	-2.375877000	0.352733000
C	-3.440957000	1.313290000	-1.014423000
H	-2.514927000	1.781545000	-0.663910000
C	-3.383745000	1.311463000	-2.551619000
H	-4.282203000	0.845418000	-2.971826000
H	-3.318490000	2.334869000	-2.938324000
H	-2.513212000	0.754429000	-2.910115000
C	-4.607862000	2.171217000	-0.518354000
H	-4.457932000	3.213425000	-0.818907000
H	-5.564907000	1.850502000	-0.944904000
H	-4.698841000	2.141704000	0.572313000
C	-0.998437000	-4.262004000	0.888471000
H	-1.682371000	-5.031682000	0.513065000
H	-0.001266000	-4.711850000	0.927816000
H	-1.300099000	-4.013539000	1.911533000
C	-0.604418000	-3.424708000	-1.456418000
H	0.362060000	-3.937824000	-1.476058000
H	-1.366017000	-4.093022000	-1.874878000
H	-0.533291000	-2.543482000	-2.100373000
N	0.693551000	2.548725000	0.159170000
C	-0.273563000	3.369451000	0.765160000
C	1.518643000	3.358775000	-0.639091000
C	-0.063017000	4.652440000	0.333175000
C	1.062357000	4.646589000	-0.543988000
H	-0.642344000	5.514664000	0.637392000
H	1.496637000	5.501211000	-1.046954000
C	-1.252681000	2.857492000	1.767483000
H	-1.766596000	1.950047000	1.437025000
H	-0.773284000	2.628295000	2.728115000
H	-2.008536000	3.623479000	1.958157000
C	2.663550000	2.803161000	-1.419504000
H	3.227953000	3.625854000	-1.865600000
H	3.353883000	2.227759000	-0.790096000
H	2.346071000	2.144769000	-2.238560000

TS(5A-5C)

E = -1500.74138510

Mo	-0.581689000	0.378061000	0.252490000
N	1.121738000	0.060439000	-0.014115000
O	-2.456927000	0.823226000	-0.113523000
Si	-3.887973000	0.523086000	-0.884102000
C	-0.624850000	0.704702000	2.154029000
H	-0.470546000	1.874107000	1.228456000
C	0.270904000	0.822003000	3.373093000
O	-3.799992000	-0.451394000	-2.210444000
H	-3.222343000	-1.230329000	-2.126346000
O	-4.526404000	1.936938000	-1.503262000
H	-4.801892000	2.540710000	-0.807358000
O	-4.887430000	-0.080979000	0.320099000
H	-5.653362000	-0.534607000	-0.046590000
C	2.359107000	-0.404201000	-0.416412000

C	2.791980000	-1.683157000	0.046851000
C	3.185208000	0.363461000	-1.284928000
C	4.034979000	-2.151622000	-0.380079000
C	4.417306000	-0.162410000	-1.671360000
C	4.845895000	-1.408477000	-1.229424000
H	4.371204000	-3.128597000	-0.044007000
H	5.053933000	0.416473000	-2.335049000
H	5.808220000	-1.800121000	-1.547252000
C	0.054484000	-0.458973000	4.204970000
H	0.616557000	-0.388824000	5.143076000
H	-1.001839000	-0.602902000	4.455479000
H	0.402057000	-1.342850000	3.663639000
C	-0.188423000	2.036060000	4.206717000
H	0.409251000	2.112501000	5.121718000
H	-0.067113000	2.971790000	3.650797000
H	-1.240763000	1.947400000	4.497415000
C	1.753210000	0.972398000	3.026098000
H	2.112997000	0.129584000	2.433484000
H	1.934397000	1.886566000	2.452453000
H	2.347337000	1.028653000	3.944719000
C	2.779338000	1.732290000	-1.798543000
H	1.799170000	1.962516000	-1.374269000
C	1.947550000	-2.566854000	0.948981000
H	1.066380000	-1.993500000	1.249686000
C	1.446159000	-3.805894000	0.192316000
H	2.283644000	-4.426618000	-0.147191000
H	0.817574000	-4.419511000	0.845855000
H	0.847025000	-3.525013000	-0.677666000
C	2.704318000	-2.975955000	2.221498000
H	2.043412000	-3.543859000	2.885345000
H	3.563526000	-3.617256000	1.996394000
H	3.076027000	-2.106848000	2.773470000
C	3.763413000	2.814599000	-1.329190000
H	4.758707000	2.660208000	-1.759505000
H	3.421499000	3.807788000	-1.639320000
H	3.872878000	2.814077000	-0.240087000
C	2.641316000	1.752901000	-3.328033000
H	2.303608000	2.738019000	-3.668222000
H	3.598525000	1.545265000	-3.818411000
H	1.920686000	1.008007000	-3.676441000
C	-0.467278000	2.696494000	-0.092764000
H	-0.309859000	2.536077000	-1.166947000
H	-1.490723000	3.061205000	0.019228000
C	0.555252000	3.698143000	0.440384000
H	0.348601000	3.913331000	1.498000000
H	1.561186000	3.266257000	0.411903000
C	0.535262000	5.008644000	-0.347549000
H	0.778601000	4.839420000	-1.402224000
H	-0.454021000	5.477142000	-0.309452000
H	1.261193000	5.723490000	0.054064000
H	-1.688200000	0.808908000	2.421444000
N	-1.136066000	-1.495036000	-0.530867000
C	-1.976585000	-2.415719000	0.074567000
C	-1.010696000	-1.846378000	-1.864520000
C	-2.364538000	-3.351640000	-0.864875000
C	-1.763198000	-2.985679000	-2.099904000

H	-3.001918000	-4.206142000	-0.675752000
H	-1.843223000	-3.501378000	-3.048887000
C	-0.207448000	-1.055173000	-2.846409000
H	-0.315253000	-1.494803000	-3.841673000
H	-0.543267000	-0.011512000	-2.926713000
H	0.860363000	-1.046350000	-2.601404000
C	-2.373541000	-2.346944000	1.513952000
H	-1.507200000	-2.257216000	2.179716000
H	-3.047879000	-1.505831000	1.715407000
H	-2.905039000	-3.263053000	1.786973000

TS(5A-5D)

E = -1500.72683739

Mo	-0.598929000	-0.432064000	-0.230971000
N	0.831568000	0.505082000	0.044401000
O	-1.947552000	0.976207000	-0.576825000
Si	-3.072780000	1.782465000	0.294934000
C	-1.052309000	-1.020737000	1.477611000
H	-1.985075000	-1.580719000	1.242007000
C	-0.798361000	-0.838626000	2.960450000
O	-4.236852000	0.845827000	1.045729000
H	-5.000312000	0.692461000	0.479820000
O	-3.936538000	2.777787000	-0.735246000
H	-3.400244000	3.095129000	-1.468565000
O	-2.297520000	2.613833000	1.513846000
H	-2.912399000	3.023707000	2.130600000
C	1.993276000	1.256661000	-0.028664000
C	3.213453000	0.729756000	0.477947000
C	1.945590000	2.560350000	-0.595482000
C	4.358841000	1.523021000	0.390551000
C	3.126870000	3.299636000	-0.656238000
C	4.327601000	2.793567000	-0.171788000
H	5.298396000	1.132739000	0.772597000
H	3.102970000	4.296984000	-1.087724000
H	5.234740000	3.389049000	-0.227830000
C	-0.017256000	0.456563000	3.219228000
H	0.147357000	0.580911000	4.296103000
H	0.954454000	0.437770000	2.722331000
H	-0.569845000	1.321263000	2.842580000
C	-0.010511000	-2.038511000	3.520687000
H	0.180495000	-1.887055000	4.589532000
H	-0.571134000	-2.973602000	3.415648000
H	0.953575000	-2.152123000	3.016490000
C	-2.161230000	-0.759076000	3.677058000
H	-2.764704000	0.064841000	3.287449000
H	-2.731677000	-1.686204000	3.548492000
H	-2.012890000	-0.602536000	4.751835000
C	0.657096000	3.168138000	-1.121843000
H	-0.145046000	2.442144000	-0.967721000
C	3.319201000	-0.650266000	1.103470000
H	2.322864000	-1.103013000	1.080676000
C	4.260803000	-1.560223000	0.301646000
H	5.285607000	-1.171620000	0.301734000
H	4.284586000	-2.562502000	0.742374000
H	3.929085000	-1.659967000	-0.734385000
C	3.779445000	-0.569541000	2.567359000

H	3.784344000	-1.567231000	3.020035000
H	4.797380000	-0.171098000	2.641499000
H	3.128428000	0.072791000	3.166983000
C	0.278000000	4.433807000	-0.339368000
H	1.043335000	5.212183000	-0.434636000
H	-0.663090000	4.848247000	-0.717879000
H	0.140818000	4.213060000	0.722102000
C	0.745968000	3.458255000	-2.627657000
H	-0.209460000	3.845467000	-2.999560000
H	1.512779000	4.208366000	-2.851546000
H	0.989029000	2.556012000	-3.197845000
C	-2.019841000	-1.483085000	-1.946203000
H	-2.144863000	-0.538234000	-2.487624000
H	-0.678027000	-2.026916000	-1.527422000
C	-3.334059000	-1.905035000	-1.281899000
H	-3.624652000	-1.166477000	-0.525460000
H	-3.192787000	-2.854318000	-0.745880000
C	-4.485610000	-2.068652000	-2.278355000
H	-5.411633000	-2.376311000	-1.778621000
H	-4.683035000	-1.127674000	-2.804182000
H	-4.247822000	-2.824723000	-3.035142000
H	-1.771045000	-2.225599000	-2.725224000
N	0.454798000	-2.228867000	-1.157830000
C	0.707103000	-3.517726000	-0.644683000
C	1.369390000	-2.012766000	-2.213438000
C	1.757904000	-4.057813000	-1.332952000
C	2.172984000	-3.112739000	-2.321992000
H	2.170558000	-5.045101000	-1.168208000
H	2.970150000	-3.237705000	-3.043900000
C	1.352489000	-0.771849000	-3.042681000
H	0.345395000	-0.532349000	-3.408361000
H	1.728135000	0.104883000	-2.503002000
H	1.988976000	-0.915297000	-3.919821000
C	-0.144889000	-4.149321000	0.399784000
H	-0.125622000	-3.595294000	1.341113000
H	-1.194341000	-4.223237000	0.085849000
H	0.211639000	-5.164399000	0.593059000

TS(5C-5D)

E = -1500.72838008

Mo	0.293867000	0.535034000	0.548163000
N	-1.104553000	-0.306639000	-0.031757000
O	1.928358000	-0.236934000	1.153255000
Si	3.332131000	-1.125648000	1.085366000
C	0.096602000	2.465714000	0.258480000
H	0.960731000	2.862165000	0.825448000
C	-0.781843000	3.590639000	-0.286893000
O	3.759093000	-1.598106000	-0.431017000
H	3.716417000	-0.883062000	-1.095620000
O	3.169521000	-2.565214000	1.910770000
H	2.995378000	-2.432063000	2.847588000
O	4.450302000	-0.139529000	1.841505000
H	5.351779000	-0.460327000	1.734610000
C	-1.979664000	-1.326406000	-0.369611000
C	-1.505110000	-2.665129000	-0.497049000
C	-3.352135000	-1.018633000	-0.582676000

C	-2.418826000	-3.652611000	-0.864326000
C	-4.214044000	-2.053487000	-0.945369000
C	-3.758341000	-3.357725000	-1.093300000
H	-2.073110000	-4.676766000	-0.966855000
H	-5.264347000	-1.832202000	-1.113862000
H	-4.448033000	-4.147080000	-1.379463000
C	-1.449824000	3.165899000	-1.600602000
H	-2.117663000	3.955840000	-1.960889000
H	-0.701143000	2.977630000	-2.377428000
H	-2.037795000	2.255257000	-1.471421000
C	0.103286000	4.822630000	-0.558186000
H	-0.497847000	5.641436000	-0.969408000
H	0.576151000	5.183645000	0.362080000
H	0.892999000	4.591573000	-1.280834000
C	-1.850854000	3.962874000	0.754385000
H	-2.531660000	3.127398000	0.937506000
H	-1.394594000	4.245448000	1.709086000
H	-2.440051000	4.816107000	0.397998000
C	-3.909970000	0.382172000	-0.420192000
H	-3.082601000	1.026403000	-0.108850000
C	-0.077344000	-3.059242000	-0.177099000
H	0.539091000	-2.154690000	-0.176905000
C	-0.009780000	-3.667255000	1.233991000
H	-0.578389000	-4.603132000	1.277538000
H	1.029785000	-3.870356000	1.504062000
H	-0.432324000	-2.986195000	1.980150000
C	0.545424000	-4.008646000	-1.207804000
H	1.609279000	-4.134906000	-0.988459000
H	0.082499000	-5.001387000	-1.184656000
H	0.455533000	-3.615576000	-2.224761000
C	-4.468420000	0.918352000	-1.746703000
H	-5.330477000	0.330493000	-2.080231000
H	-4.800617000	1.955701000	-1.631935000
H	-3.718565000	0.886148000	-2.542879000
C	-4.980551000	0.440388000	0.679565000
H	-5.320261000	1.471649000	0.824917000
H	-5.857871000	-0.161309000	0.418682000
H	-4.596350000	0.071712000	1.635094000
C	-0.261722000	0.438742000	2.617077000
H	-0.122715000	-0.624578000	2.866833000
H	0.539380000	0.976993000	3.146017000
C	-1.633595000	0.909248000	3.086084000
H	-1.755714000	1.974985000	2.861419000
H	-2.412986000	0.387956000	2.517276000
C	-1.859184000	0.682163000	4.583412000
H	-1.784989000	-0.381330000	4.838034000
H	-1.111574000	1.216501000	5.180718000
H	-2.849036000	1.032169000	4.897669000
H	0.714027000	1.876680000	-0.756031000
N	1.659940000	0.920172000	-1.513491000
C	1.481580000	0.200682000	-2.685346000
C	2.988652000	1.312025000	-1.457188000
C	2.689562000	0.107783000	-3.346214000
C	3.651710000	0.806463000	-2.564107000
H	2.858792000	-0.402378000	-4.286471000
H	4.691349000	0.985554000	-2.812035000

C	0.160241000	-0.348965000	-3.113311000
H	-0.638674000	0.397436000	-3.034223000
H	0.216894000	-0.663432000	-4.159269000
H	-0.156217000	-1.218926000	-2.528240000
C	3.529251000	2.251259000	-0.423098000
H	4.609970000	2.351706000	-0.554600000
H	3.100987000	3.257826000	-0.522855000
H	3.365791000	1.910861000	0.604599000

6A

E = -974.531420492

C	-1.162084000	-1.346400000	1.372517000
H	-0.290842000	-1.705934000	1.956709000
H	-1.763800000	-0.762596000	2.075512000
C	-1.974488000	-2.574693000	0.896033000
O	1.341534000	-0.979515000	-1.003736000
Si	2.988597000	-0.861644000	-0.942867000
C	-1.485289000	0.543220000	-1.148318000
H	-1.670953000	-0.288894000	-1.867011000
C	-2.248353000	1.784724000	-1.550894000
O	3.611450000	0.655254000	-1.220697000
H	3.645078000	0.886574000	-2.154213000
O	3.626742000	-1.843422000	-2.129644000
H	3.089958000	-2.625163000	-2.294462000
O	3.445603000	-1.288159000	0.598998000
H	4.384279000	-1.156774000	0.766283000
C	-2.116864000	-3.541645000	2.085405000
H	-2.724209000	-4.414311000	1.815261000
H	-1.138287000	-3.904971000	2.420132000
H	-2.599603000	-3.047441000	2.936036000
C	-3.374528000	-2.151604000	0.436740000
H	-3.927803000	-1.681760000	1.257989000
H	-3.322071000	-1.429972000	-0.383040000
H	-3.953370000	-3.017956000	0.095581000
C	-1.255896000	-3.309378000	-0.246574000
H	-1.192987000	-2.694223000	-1.154200000
H	-0.235935000	-3.591768000	0.039172000
H	-1.791632000	-4.225123000	-0.523160000
C	-2.103649000	2.913718000	-0.530836000
H	-2.679533000	3.791285000	-0.846727000
H	-2.463596000	2.596469000	0.452138000
H	-1.056677000	3.212348000	-0.427071000
C	-3.738459000	1.414409000	-1.688929000
H	-4.316993000	2.280295000	-2.031818000
H	-3.883008000	0.607139000	-2.416114000
H	-4.151703000	1.085911000	-0.730263000
C	-1.719840000	2.256202000	-2.921293000
H	-0.661774000	2.529762000	-2.856364000
H	-1.819085000	1.469121000	-3.677239000
H	-2.281028000	3.131137000	-3.271074000
C	0.257780000	1.158693000	0.993918000
C	0.854211000	2.177694000	1.900672000
C	-0.236783000	2.917109000	2.696180000
H	-0.855800000	2.214226000	3.261779000
H	0.230448000	3.609414000	3.405758000
H	-0.889634000	3.494371000	2.037099000

C	1.690245000	3.176297000	1.077927000
H	2.164785000	3.900532000	1.750324000
H	2.469799000	2.659197000	0.511905000
H	1.063648000	3.730070000	0.372509000
C	1.777199000	1.416606000	2.877947000
H	2.544863000	0.858008000	2.335887000
H	2.266819000	2.129787000	3.551519000
H	1.205782000	0.708937000	3.486503000
Re	-0.138898000	-0.155302000	-0.055434000

6B

E = -776.751289790

O	1.981776000	-0.718715000	-0.210636000
Si	3.498581000	-0.128654000	0.068105000
C	-1.483558000	-0.982924000	-0.021590000
C	-2.716024000	-1.789599000	0.054208000
O	4.562119000	-0.328383000	-1.190804000
H	4.939765000	-1.212205000	-1.231700000
O	4.163540000	-0.935642000	1.366186000
H	3.503118000	-1.179047000	2.022991000
O	3.331687000	1.510881000	0.293648000
H	4.160727000	1.992106000	0.210556000
C	-3.586756000	-1.348954000	1.244424000
H	-4.448587000	-2.018702000	1.339429000
H	-3.017691000	-1.374996000	2.177634000
H	-3.965260000	-0.332748000	1.100501000
C	-2.225604000	-3.240343000	0.280910000
H	-3.093682000	-3.906319000	0.335460000
H	-1.586998000	-3.574892000	-0.541969000
H	-1.662349000	-3.324408000	1.214541000
C	-3.507859000	-1.710516000	-1.263918000
H	-3.847940000	-0.690107000	-1.460775000
H	-2.889733000	-2.028498000	-2.107812000
H	-4.388785000	-2.360100000	-1.210044000
C	-1.030885000	1.117862000	-0.033029000
C	-1.825302000	2.356031000	0.056234000
C	-2.373127000	2.557767000	1.480869000
H	-1.560558000	2.557678000	2.212307000
H	-2.903300000	3.514692000	1.545029000
H	-3.072117000	1.761996000	1.753033000
C	-2.966937000	2.353595000	-0.976121000
H	-3.479878000	3.321618000	-0.962022000
H	-2.583434000	2.174999000	-1.984289000
H	-3.705003000	1.579434000	-0.745927000
C	-0.823441000	3.487643000	-0.282411000
H	-0.424819000	3.370672000	-1.293849000
H	-1.341508000	4.450838000	-0.218745000
H	0.014533000	3.498253000	0.420398000
Re	0.123965000	-0.232635000	-0.117771000

6B'

E = -974.461562876

C	-1.844239000	-1.188132000	1.310366000
H	-0.912420000	-1.752662000	1.456133000
H	-2.111234000	-0.801919000	2.298345000
C	-2.950628000	-2.062538000	0.693258000

O	1.267110000	-0.766517000	-1.389671000
Si	2.697603000	-1.446255000	-0.934903000
C	-0.993045000	1.105730000	-1.064231000
H	-1.820866000	-0.204516000	0.701385000
C	-1.475692000	2.451032000	-1.492833000
O	3.431642000	-2.006362000	-2.327896000
H	2.789930000	-2.161179000	-3.028667000
O	2.353658000	-2.657356000	0.161604000
H	3.104271000	-2.880270000	0.720751000
O	3.827971000	-0.458597000	-0.208138000
H	4.377722000	-0.008944000	-0.857879000
C	-3.257093000	-3.199420000	1.678935000
H	-4.037769000	-3.854978000	1.278312000
H	-2.369431000	-3.813941000	1.866687000
H	-3.609249000	-2.809778000	2.640695000
C	-4.207712000	-1.213149000	0.465398000
H	-4.568473000	-0.775529000	1.403303000
H	-4.008510000	-0.396897000	-0.238150000
H	-5.016619000	-1.821807000	0.047920000
C	-2.465126000	-2.645028000	-0.640047000
H	-2.210070000	-1.848388000	-1.351423000
H	-1.581229000	-3.278568000	-0.500013000
H	-3.245279000	-3.260431000	-1.101297000
C	-0.334190000	3.125287000	-2.281142000
H	-0.665327000	4.099450000	-2.660413000
H	0.543200000	3.279425000	-1.646642000
H	-0.030735000	2.507959000	-3.131951000
C	-1.886333000	3.330091000	-0.299784000
H	-2.264455000	4.299050000	-0.647590000
H	-2.676369000	2.849598000	0.287032000
H	-1.036139000	3.512828000	0.362101000
C	-2.688315000	2.254339000	-2.426460000
H	-2.424994000	1.621829000	-3.279127000
H	-3.520177000	1.779328000	-1.895938000
H	-3.037082000	3.222714000	-2.805226000
C	0.787289000	0.608144000	1.218503000
C	1.350778000	1.620501000	2.156047000
C	1.967281000	2.776229000	1.346087000
H	1.209366000	3.285983000	0.745296000
H	2.421686000	3.508734000	2.024101000
H	2.743415000	2.401469000	0.672913000
C	2.453178000	0.947056000	2.999386000
H	2.896512000	1.671167000	3.694201000
H	2.043447000	0.117544000	3.584651000
H	3.240672000	0.550944000	2.352821000
C	0.239594000	2.149937000	3.081633000
H	-0.208002000	1.335414000	3.661303000
H	0.651764000	2.878061000	3.790289000
H	-0.554166000	2.636022000	2.507588000
Re	-0.094632000	-0.118533000	-0.136277000

6B''

E = -895.854248185

O	-1.280548000	-0.678504000	-1.271326000
Si	-2.891962000	-0.519155000	-0.975210000
C	1.472310000	0.404450000	-1.050618000

H	1.849884000	-0.913101000	0.840631000
C	2.372902000	1.485496000	-1.544078000
O	-3.513256000	-1.434495000	0.275330000
H	-3.794779000	-2.303656000	-0.027748000
O	-3.694914000	-1.072658000	-2.334621000
H	-3.191161000	-0.905657000	-3.137957000
O	-3.219224000	1.074578000	-0.619354000
H	-4.112188000	1.190886000	-0.279760000
C	3.063224000	2.233484000	-0.391199000
H	3.733668000	3.008958000	-0.781065000
H	2.326917000	2.712637000	0.258667000
H	3.660139000	1.547384000	0.219492000
C	1.518700000	2.463393000	-2.375820000
H	2.154763000	3.251603000	-2.796079000
H	1.023015000	1.942827000	-3.200541000
H	0.745822000	2.930341000	-1.759199000
C	3.441999000	0.842047000	-2.451965000
H	4.058996000	0.132629000	-1.890553000
H	2.975020000	0.301330000	-3.280275000
H	4.102216000	1.613299000	-2.866750000
C	1.605655000	-1.915439000	1.363625000
H	2.014175000	-1.696400000	2.355355000
H	0.553953000	-2.176917000	1.550609000
C	2.368925000	-3.023846000	0.643406000
H	3.405762000	-2.701589000	0.488357000
H	1.943612000	-3.170255000	-0.356485000
C	2.339532000	-4.337968000	1.420789000
H	2.899022000	-5.116600000	0.894022000
H	2.784581000	-4.222662000	2.415225000
H	1.313506000	-4.698324000	1.555119000
Re	0.234575000	-0.411904000	-0.064913000
C	-0.355125000	0.628701000	1.243972000
C	-0.558674000	1.816270000	2.120182000
C	-1.834166000	1.590199000	2.958061000
H	-2.019924000	2.453285000	3.609043000
H	-2.698686000	1.451207000	2.304071000
H	-1.739232000	0.698630000	3.585679000
C	-0.742243000	3.071592000	1.246367000
H	-0.943285000	3.941461000	1.883456000
H	0.156751000	3.277485000	0.659246000
H	-1.580169000	2.938753000	0.556952000
C	0.652507000	1.986151000	3.056061000
H	0.499387000	2.846516000	3.718171000
H	0.791212000	1.099900000	3.684768000
H	1.571646000	2.148482000	2.486032000

6C

E = -1093.62118202

C	-0.169433000	2.281282000	-0.134087000
H	-0.598746000	2.575447000	-1.104021000
H	-0.933376000	2.553034000	0.609538000
C	1.096186000	3.132079000	0.122192000
O	1.825670000	-0.004394000	-0.002366000
Si	3.141985000	-0.953100000	-0.002014000
C	-0.239142000	-0.832583000	1.678695000
H	0.378208000	-1.720093000	1.458705000

C	-1.413384000	-1.215400000	2.589180000
O	2.976118000	-2.402627000	0.822717000
H	3.259279000	-2.327998000	1.739522000
O	4.426675000	-0.200054000	0.767344000
H	4.463112000	0.742896000	0.578676000
O	3.494632000	-1.351970000	-1.586608000
H	4.198860000	-2.005117000	-1.649800000
C	0.626483000	4.601898000	0.151433000
H	1.477766000	5.273715000	0.314078000
H	0.151292000	4.888699000	-0.793932000
H	-0.095032000	4.775759000	0.958263000
C	1.738585000	2.808314000	1.477730000
H	1.014353000	2.927245000	2.293447000
H	2.115517000	1.783110000	1.495377000
H	2.572993000	3.490174000	1.681950000
C	2.120140000	2.979522000	-1.010252000
H	2.475028000	1.949290000	-1.077726000
H	1.678334000	3.253484000	-1.976248000
H	2.980063000	3.640087000	-0.845150000
C	-2.193100000	0.030006000	3.027333000
H	-3.018890000	-0.238823000	3.696266000
H	-1.542190000	0.727505000	3.568335000
H	-2.608490000	0.558730000	2.165605000
C	-0.815522000	-1.883934000	3.844313000
H	-1.607923000	-2.171581000	4.545431000
H	-0.254466000	-2.788649000	3.584063000
H	-0.135164000	-1.204486000	4.370561000
C	-2.342243000	-2.220046000	1.901416000
H	-2.773433000	-1.793322000	0.992470000
H	-1.797033000	-3.128198000	1.618443000
H	-3.162558000	-2.515039000	2.566063000
C	0.104148000	-0.908666000	-1.950404000
H	-0.617716000	-0.636045000	-2.726885000
H	1.112413000	-0.628047000	-2.277116000
C	0.050528000	-2.418927000	-1.688683000
H	-0.954572000	-2.706510000	-1.355548000
H	0.741740000	-2.689781000	-0.881576000
C	0.427648000	-3.218968000	-2.939831000
H	0.373756000	-4.295989000	-2.747686000
H	-0.244659000	-2.991250000	-3.774702000
H	1.448566000	-2.979047000	-3.251482000
H	0.435948000	-0.147077000	2.225946000
Re	-0.215109000	0.154183000	-0.157478000
C	-1.937879000	0.213085000	-0.517956000
C	-3.298224000	0.299164000	-1.116048000
C	-3.258104000	1.399323000	-2.200240000
H	-4.238845000	1.480664000	-2.683037000
H	-3.012077000	2.372970000	-1.766022000
H	-2.516006000	1.170658000	-2.971199000
C	-4.351150000	0.677838000	-0.056916000
H	-5.329978000	0.792475000	-0.536575000
H	-4.440906000	-0.091359000	0.714596000
H	-4.100239000	1.625068000	0.430316000
C	-3.677419000	-1.045345000	-1.769127000
H	-4.663257000	-0.960662000	-2.240748000
H	-2.955927000	-1.331102000	-2.539734000

H -3.723847000 -1.850639000 -1.030645000

6D

E = -1182.27221308

O -1.616334000 1.454186000 0.281957000
Si -1.887705000 2.614833000 -0.846830000
C -0.690216000 -1.591248000 0.698904000
H -1.684328000 -1.583975000 1.208640000
C -0.372393000 -2.964923000 0.157976000
O -0.659766000 3.700752000 -1.035402000
H -0.705681000 4.451865000 -0.436588000
O -3.189439000 3.511135000 -0.361258000
H -3.884218000 3.003450000 0.068124000
O -2.090794000 1.837958000 -2.282577000
H -2.097560000 2.415650000 -3.051257000
C 1.008732000 -3.027057000 -0.493991000
H 1.210558000 -4.037657000 -0.867562000
H 1.072029000 -2.332939000 -1.336764000
H 1.788867000 -2.760574000 0.224577000
C -1.450031000 -3.347217000 -0.876678000
H -1.277170000 -4.361048000 -1.257542000
H -2.451927000 -3.321537000 -0.433715000
H -1.439070000 -2.654897000 -1.724351000
C -0.425715000 -3.960696000 1.334264000
H 0.325981000 -3.713637000 2.090707000
H -1.409163000 -3.953252000 1.817733000
H -0.233968000 -4.980763000 0.981088000
C 0.477682000 0.393504000 2.716393000
H 1.364523000 -0.207354000 2.934599000
H 0.802814000 1.448828000 2.781368000
C -0.616402000 0.122395000 3.758091000
H -0.858092000 -0.947847000 3.752086000
H -1.547218000 0.646516000 3.491344000
C -0.208648000 0.547601000 5.171396000
H -0.997064000 0.329167000 5.900121000
H 0.698196000 0.021609000 5.489694000
H -0.000050000 1.622455000 5.216142000
Re -0.233929000 0.209242000 0.748662000
C 1.252632000 0.298990000 -0.114136000
C 2.445558000 0.619437000 -0.946453000
C 2.800988000 2.098975000 -0.684382000
H 3.671281000 2.382277000 -1.288155000
H 1.964121000 2.752340000 -0.946195000
H 3.050790000 2.259994000 0.369107000
C 2.098911000 0.434163000 -2.436010000
H 2.958132000 0.717670000 -3.054916000
H 1.848825000 -0.606801000 -2.659893000
H 1.245984000 1.057960000 -2.717448000
C 3.637654000 -0.273849000 -0.559202000
H 4.521543000 0.012745000 -1.140699000
H 3.878102000 -0.167600000 0.502900000
H 3.425916000 -1.327376000 -0.757580000

6D_2

E = -895.929525777

O -1.535237000 -0.949813000 -0.702795000

Si	-3.046879000	-0.320489000	-0.926938000
C	1.646643000	-0.441122000	-1.015703000
H	1.523423000	-1.435624000	-1.507850000
C	2.815016000	0.312757000	-1.603875000
O	-3.804759000	0.202544000	0.459525000
H	-4.256308000	-0.504395000	0.931171000
O	-4.030049000	-1.519681000	-1.540962000
H	-3.574302000	-2.093532000	-2.165070000
O	-2.879646000	0.999272000	-1.921237000
H	-3.690388000	1.510623000	-2.007677000
C	3.065152000	1.642375000	-0.893078000
H	3.925637000	2.157010000	-1.336032000
H	2.193970000	2.297688000	-0.978771000
H	3.265745000	1.480888000	0.169783000
C	2.530724000	0.570282000	-3.097654000
H	3.381799000	1.075346000	-3.570205000
H	2.355829000	-0.367939000	-3.636035000
H	1.644381000	1.200426000	-3.221939000
C	4.067629000	-0.577432000	-1.474073000
H	4.295793000	-0.782760000	-0.423283000
H	3.929277000	-1.536774000	-1.985519000
H	4.936533000	-0.081150000	-1.922145000
C	0.798559000	-1.555924000	1.713725000
H	1.649914000	-1.141651000	2.260362000
H	-0.058623000	-1.528346000	2.412217000
C	1.086478000	-3.003834000	1.297242000
H	2.003269000	-3.025474000	0.694384000
H	0.285689000	-3.388803000	0.646687000
C	1.236847000	-3.948664000	2.492630000
H	1.461150000	-4.971437000	2.170375000
H	2.048334000	-3.618252000	3.150611000
H	0.318707000	-3.979992000	3.090159000
Re	0.142069000	-0.377657000	0.089240000
C	0.221182000	1.187631000	0.820586000
C	0.009680000	2.527622000	1.434955000
C	-1.147418000	2.389315000	2.448305000
H	-1.342449000	3.360459000	2.918308000
H	-2.062667000	2.048968000	1.956099000
H	-0.893668000	1.674059000	3.236976000
C	-0.387038000	3.536960000	0.340599000
H	-0.593932000	4.512894000	0.795016000
H	0.415996000	3.666748000	-0.390655000
H	-1.281419000	3.201726000	-0.191359000
C	1.279020000	3.000959000	2.165443000
H	1.088573000	3.964191000	2.652650000
H	1.580534000	2.282657000	2.933810000
H	2.113001000	3.129480000	1.471192000

TS(6A-6B)

E = -974.451566984

C	-1.450367000	-1.143532000	1.405693000
H	-0.555174000	-1.513302000	1.925242000
H	-1.967976000	-0.528652000	2.149057000
C	-2.331242000	-2.331984000	0.962254000
O	1.363032000	-0.883565000	-1.228113000
Si	2.951868000	-1.111002000	-0.858193000

C	-1.330549000	0.652221000	-1.106390000
H	-1.735026000	-0.169415000	0.359763000
C	-2.174854000	1.788945000	-1.581538000
O	3.677932000	-1.810828000	-2.190821000
H	3.044618000	-2.298885000	-2.726954000
O	3.011566000	-2.063715000	0.507683000
H	3.871783000	-2.048393000	0.938386000
O	3.858172000	0.249641000	-0.530320000
H	4.197952000	0.657297000	-1.333323000
C	-2.597698000	-3.191926000	2.208301000
H	-3.229310000	-4.051477000	1.956876000
H	-1.663816000	-3.575783000	2.633916000
H	-3.111493000	-2.615552000	2.986131000
C	-3.666917000	-1.836569000	0.393219000
H	-4.207615000	-1.224801000	1.125103000
H	-3.514238000	-1.239628000	-0.512104000
H	-4.310487000	-2.681248000	0.125148000
C	-1.597493000	-3.171430000	-0.092763000
H	-1.401044000	-2.587393000	-1.001310000
H	-0.640629000	-3.545249000	0.289693000
H	-2.200565000	-4.037598000	-0.387832000
C	-1.251511000	2.677435000	-2.442382000
H	-1.824880000	3.515364000	-2.855629000
H	-0.426127000	3.077351000	-1.847448000
H	-0.826733000	2.107269000	-3.274089000
C	-2.761939000	2.606993000	-0.419296000
H	-3.359957000	3.442845000	-0.801534000
H	-3.414704000	1.987770000	0.205937000
H	-1.969239000	3.011486000	0.215275000
C	-3.318645000	1.251495000	-2.465433000
H	-2.923326000	0.650664000	-3.289444000
H	-4.005864000	0.625551000	-1.887365000
H	-3.895958000	2.083486000	-2.886185000
C	0.664400000	0.975213000	1.043379000
C	1.060186000	2.188530000	1.811929000
C	1.213977000	3.390444000	0.862287000
H	0.263879000	3.638248000	0.381137000
H	1.553768000	4.269777000	1.422273000
H	1.949220000	3.176996000	0.080823000
C	2.409563000	1.908232000	2.505340000
H	2.730839000	2.786928000	3.077987000
H	2.323622000	1.061851000	3.193948000
H	3.178751000	1.666853000	1.766937000
C	-0.016978000	2.484648000	2.872465000
H	-0.140882000	1.635833000	3.552951000
H	0.273127000	3.356727000	3.470089000
H	-0.984686000	2.692950000	2.406535000
Re	-0.063856000	-0.149312000	-0.102068000

TS(6A-6C)

E = -1093.56499357

C	-0.479323000	2.052042000	0.789143000
H	-1.145390000	1.837674000	1.636196000
H	0.443244000	2.447352000	1.239047000
C	-1.121108000	3.184451000	-0.061534000
O	-1.796027000	-0.000179000	-0.487502000

Si	-3.083699000	-0.991564000	-0.378679000
C	1.801557000	0.614358000	-1.062035000
H	1.214393000	-0.696309000	-1.246132000
C	3.319153000	0.595605000	-0.980619000
O	-3.560405000	-1.748841000	-1.790918000
H	-4.226474000	-1.238937000	-2.262409000
O	-4.429900000	-0.114157000	0.090200000
H	-4.186866000	0.683896000	0.570431000
O	-2.713345000	-2.227306000	0.690019000
H	-3.347103000	-2.949860000	0.636856000
C	-0.834880000	4.526159000	0.638843000
H	-1.311658000	5.361452000	0.110061000
H	-1.216321000	4.518875000	1.666410000
H	0.241729000	4.728553000	0.684351000
C	-0.537961000	3.249035000	-1.481711000
H	0.550970000	3.369279000	-1.459828000
H	-0.777593000	2.342135000	-2.052035000
H	-0.954433000	4.097073000	-2.039129000
C	-2.644079000	3.017894000	-0.162799000
H	-2.901031000	2.083659000	-0.665064000
H	-3.097656000	3.016106000	0.837338000
H	-3.091493000	3.848295000	-0.723114000
C	3.733564000	2.052330000	-0.683045000
H	4.826463000	2.129958000	-0.654518000
H	3.370056000	2.739853000	-1.454660000
H	3.337050000	2.380992000	0.281854000
C	3.916741000	0.172636000	-2.336149000
H	5.010704000	0.227172000	-2.307273000
H	3.641842000	-0.856709000	-2.589653000
H	3.570057000	0.825138000	-3.145400000
C	3.849906000	-0.320622000	0.120716000
H	3.449735000	-0.027895000	1.093606000
H	3.569975000	-1.363007000	-0.062003000
H	4.943260000	-0.265667000	0.163189000
C	0.060730000	-1.851149000	-1.313128000
H	-0.658403000	-2.300702000	-0.624184000
H	-0.480204000	-1.581259000	-2.227551000
C	1.171151000	-2.866138000	-1.603039000
H	1.733137000	-3.068210000	-0.681793000
H	1.900156000	-2.455553000	-2.317467000
C	0.622785000	-4.181670000	-2.158950000
H	1.427551000	-4.896988000	-2.363247000
H	-0.070223000	-4.646942000	-1.449647000
H	0.074346000	-4.015588000	-3.092455000
H	1.493057000	1.077231000	-2.020661000
Re	0.174184000	0.165838000	-0.092740000
C	0.758714000	-0.471415000	1.400381000
C	0.906140000	-1.082014000	2.749537000
C	-0.494095000	-1.193574000	3.386690000
H	-0.413233000	-1.671660000	4.370051000
H	-0.936514000	-0.202398000	3.525159000
H	-1.167678000	-1.781884000	2.758183000
C	1.807638000	-0.194017000	3.628464000
H	1.874502000	-0.623883000	4.634201000
H	2.821082000	-0.121624000	3.223659000
H	1.399268000	0.816950000	3.715919000

C	1.524175000	-2.485159000	2.599255000
H	1.629032000	-2.945357000	3.588137000
H	0.886052000	-3.128674000	1.987300000
H	2.515137000	-2.437114000	2.138794000

TS(6A-6D)

E = -1093.55782774

C	2.415759000	-0.195361000	0.707844000
H	2.566266000	-0.018569000	1.779668000
H	2.200288000	-1.259652000	0.606133000
C	3.720019000	0.128030000	-0.064425000
O	-1.345374000	1.285687000	-0.654959000
Si	-2.950603000	1.049694000	-0.844846000
C	0.166301000	-1.215372000	-1.308645000
H	0.476165000	-0.671647000	-2.231710000
C	-0.001411000	-2.684136000	-1.619720000
O	-3.439518000	-0.241723000	-1.783946000
H	-3.399514000	-0.039078000	-2.723916000
O	-3.579144000	2.392713000	-1.623431000
H	-3.106750000	3.196935000	-1.385902000
O	-3.636601000	0.800850000	0.659030000
H	-4.570128000	0.574770000	0.592735000
C	4.315075000	1.470943000	0.386863000
H	5.280740000	1.644789000	-0.101563000
H	3.666728000	2.315393000	0.137017000
H	4.484844000	1.483754000	1.469863000
C	4.735294000	-0.981128000	0.266517000
H	4.912473000	-1.045535000	1.346107000
H	4.378613000	-1.959538000	-0.074746000
H	5.699044000	-0.787269000	-0.219255000
C	3.490139000	0.153197000	-1.579845000
H	3.082016000	-0.797795000	-1.933509000
H	2.792260000	0.947748000	-1.868943000
H	4.432337000	0.335182000	-2.109730000
C	-0.451885000	-3.493156000	-0.403662000
H	-0.533436000	-4.556282000	-0.658381000
H	0.259398000	-3.391710000	0.422419000
H	-1.427877000	-3.146332000	-0.056421000
C	1.338418000	-3.244073000	-2.140220000
H	1.223223000	-4.294542000	-2.432629000
H	1.688373000	-2.689749000	-3.018287000
H	2.116768000	-3.194015000	-1.371274000
C	-1.061644000	-2.808830000	-2.734272000
H	-2.014819000	-2.383381000	-2.408401000
H	-0.742547000	-2.284392000	-3.642711000
H	-1.216801000	-3.862968000	-2.993734000
C	0.901972000	2.311868000	0.615469000
H	-0.056708000	2.473169000	1.123668000
H	1.647669000	0.976746000	0.574739000
C	1.041849000	3.250617000	-0.582717000
H	0.253011000	3.027437000	-1.309701000
H	1.997366000	3.073661000	-1.096133000
C	0.962682000	4.729276000	-0.194336000
H	1.068532000	5.381378000	-1.068957000
H	0.002035000	4.958081000	0.280831000

H	1.752127000	4.995154000	0.518160000
H	1.672563000	2.539465000	1.365782000
Re	0.132656000	0.134598000	0.022836000
C	-0.470901000	-0.677517000	1.422479000
C	-1.038137000	-1.115283000	2.728727000
C	-2.327241000	-1.927807000	2.509658000
H	-2.122377000	-2.869443000	1.994582000
H	-2.776843000	-2.162723000	3.481474000
H	-3.043446000	-1.350703000	1.920149000
C	-1.367588000	0.149885000	3.547923000
H	-1.781137000	-0.137913000	4.521816000
H	-0.469605000	0.751123000	3.721054000
H	-2.104243000	0.763366000	3.022769000
C	0.010224000	-1.965521000	3.471172000
H	-0.390501000	-2.276257000	4.442711000
H	0.265919000	-2.865623000	2.904402000
H	0.928797000	-1.397630000	3.648540000

TS(6B-6D)

E = -1182.18995298

O	-1.376391000	-1.086905000	-1.008003000
Si	-2.944278000	-0.635666000	-1.103948000
C	1.608598000	-0.295425000	-1.046203000
H	1.747552000	-0.806432000	0.627791000
C	2.769734000	0.384945000	-1.688359000
O	-3.853349000	-0.909493000	0.248172000
H	-4.267164000	-1.777521000	0.254998000
O	-3.650994000	-1.555598000	-2.287674000
H	-3.040188000	-1.802013000	-2.988727000
O	-2.998928000	0.986309000	-1.406424000
H	-3.874719000	1.367083000	-1.293575000
C	3.451497000	1.394635000	-0.750230000
H	4.291394000	1.886925000	-1.254918000
H	2.745076000	2.163272000	-0.427412000
H	3.843418000	0.897486000	0.144017000
C	2.220748000	1.110904000	-2.934354000
H	3.044376000	1.587071000	-3.478840000
H	1.721859000	0.408488000	-3.608539000
H	1.498461000	1.882281000	-2.652732000
C	3.790575000	-0.683814000	-2.129833000
H	4.190160000	-1.227565000	-1.267022000
H	3.326542000	-1.411387000	-2.801738000
H	4.632870000	-0.213887000	-2.651622000
C	1.230894000	-1.517177000	1.717413000
H	2.004153000	-1.047405000	2.336923000
H	0.322210000	-1.437565000	2.326927000
C	1.591783000	-2.970607000	1.404057000
H	2.489387000	-2.996349000	0.773330000
H	0.794923000	-3.433011000	0.807381000
C	1.819910000	-3.792088000	2.672978000
H	2.082559000	-4.826255000	2.429162000
H	2.634366000	-3.372931000	3.274084000
H	0.921717000	-3.814458000	3.299731000
Re	0.165238000	-0.494406000	-0.000653000
C	-0.265429000	0.994826000	0.820753000
C	-0.359897000	2.422399000	1.233345000

C	-1.727261000	2.641702000	1.912735000
H	-1.838459000	3.689990000	2.215595000
H	-2.538476000	2.385999000	1.226148000
H	-1.827712000	2.013238000	2.802982000
C	-0.263135000	3.319237000	-0.015163000
H	-0.390741000	4.371022000	0.267864000
H	0.709203000	3.211636000	-0.504271000
H	-1.040505000	3.053158000	-0.736847000
C	0.771375000	2.751964000	2.224234000
H	0.696022000	3.796190000	2.549422000
H	0.710802000	2.117079000	3.114361000
H	1.753266000	2.604043000	1.765689000

TS(6B-6D_2)

E = -895.846824201

O	-1.394327000	-0.974949000	-0.988072000
Si	-2.995794000	-0.610555000	-0.866306000
C	1.564154000	-0.017676000	-1.042474000
H	1.800824000	-0.667920000	0.560908000
C	2.651064000	0.794552000	-1.660024000
O	-3.729124000	-0.996815000	0.580811000
H	-4.045783000	-1.905549000	0.593026000
O	-3.804735000	-1.523795000	-2.009901000
H	-3.266510000	-1.674242000	-2.793825000
O	-3.179249000	1.030417000	-1.077745000
H	-4.070616000	1.326152000	-0.867487000
C	3.315975000	1.755488000	-0.660810000
H	4.103039000	2.339069000	-1.153136000
H	2.584442000	2.450391000	-0.241141000
H	3.775345000	1.205326000	0.167867000
C	1.994514000	1.594808000	-2.805034000
H	2.756156000	2.183708000	-3.329072000
H	1.518172000	0.925268000	-3.527361000
H	1.230953000	2.276535000	-2.419776000
C	3.713123000	-0.157736000	-2.247127000
H	4.190849000	-0.748796000	-1.458322000
H	3.261605000	-0.850618000	-2.962621000
H	4.495260000	0.415016000	-2.759412000
C	1.368663000	-1.516596000	1.610209000
H	2.088608000	-1.031702000	2.278893000
H	0.458980000	-1.610622000	2.218367000
C	1.879960000	-2.879230000	1.139233000
H	2.794955000	-2.743022000	0.548661000
H	1.151143000	-3.334445000	0.456106000
C	2.147789000	-3.827877000	2.307666000
H	2.521838000	-4.793017000	1.952010000
H	2.894716000	-3.411296000	2.992478000
H	1.235509000	-4.015161000	2.884493000
Re	0.169795000	-0.397437000	0.035545000
C	-0.298534000	0.986849000	1.022981000
C	-0.419686000	2.357706000	1.591950000
C	-1.741290000	2.441551000	2.383175000
H	-1.865693000	3.445107000	2.807854000
H	-2.591873000	2.228811000	1.730419000
H	-1.755260000	1.716025000	3.202273000
C	-0.446966000	3.387128000	0.446619000

H	-0.582104000	4.396236000	0.854013000
H	0.486537000	3.369546000	-0.122517000
H	-1.270303000	3.174258000	-0.240601000
C	0.767257000	2.631020000	2.534352000
H	0.672832000	3.628940000	2.978330000
H	0.797691000	1.900957000	3.350107000
H	1.718560000	2.581797000	1.996857000

TS(6C-6D)

E = -1093.56852404

C	-0.181310000	1.781120000	-1.179097000
H	0.855493000	1.569056000	-1.450749000
H	-0.773003000	1.670178000	-2.096682000
C	-0.301749000	3.234360000	-0.667145000
O	1.640666000	0.534822000	0.589248000
Si	3.144493000	0.233674000	0.048561000
C	-2.095391000	0.202242000	0.674954000
H	-2.107961000	0.952894000	1.492216000
C	-3.522696000	-0.218599000	0.374744000
O	3.650316000	-1.361922000	0.036521000
H	3.933710000	-1.664016000	0.905115000
O	4.253655000	1.028133000	1.019128000
H	3.879144000	1.820668000	1.415979000
O	3.229568000	0.715438000	-1.551763000
H	4.066597000	0.477055000	-1.963010000
C	-1.767633000	3.688002000	-0.639331000
H	-1.845961000	4.740491000	-0.343092000
H	-2.233564000	3.585543000	-1.626620000
H	-2.360262000	3.107150000	0.076127000
C	0.299176000	3.403660000	0.734816000
H	-0.244641000	2.810989000	1.482004000
H	1.340984000	3.077100000	0.760422000
H	0.249640000	4.452072000	1.052184000
C	0.469333000	4.138484000	-1.647254000
H	1.528368000	3.862289000	-1.681937000
H	0.067195000	4.049081000	-2.662864000
H	0.400331000	5.192559000	-1.350677000
C	-3.633014000	-1.120296000	-0.852053000
H	-4.676960000	-1.409089000	-1.017152000
H	-3.274998000	-0.610051000	-1.752113000
H	-3.038662000	-2.026169000	-0.720686000
C	-4.426963000	1.014615000	0.191020000
H	-5.470915000	0.703900000	0.071058000
H	-4.376371000	1.683907000	1.057372000
H	-4.146150000	1.587863000	-0.698310000
C	-3.983750000	-0.994929000	1.627358000
H	-3.361139000	-1.879232000	1.791063000
H	-3.937195000	-0.371778000	2.527231000
H	-5.021870000	-1.321348000	1.498872000
C	0.351428000	-1.470495000	1.820943000
H	-0.362780000	-2.302188000	1.882188000
H	1.328763000	-1.904044000	1.577827000
C	0.426019000	-0.747183000	3.169646000
H	-0.559439000	-0.331782000	3.430386000
H	1.111270000	0.106406000	3.089178000
C	0.888939000	-1.653153000	4.314684000

H	0.927213000	-1.113902000	5.268371000
H	0.213761000	-2.507455000	4.439423000
H	1.890248000	-2.052519000	4.116515000
H	-1.441030000	1.031934000	-0.361284000
Re	-0.232532000	-0.139913000	0.215206000
C	-0.303130000	-1.342600000	-1.018428000
C	0.038811000	-2.328381000	-2.083322000
C	1.032251000	-3.340647000	-1.475694000
H	1.320685000	-4.066958000	-2.244414000
H	1.931793000	-2.840761000	-1.107395000
H	0.574895000	-3.886475000	-0.644711000
C	0.707451000	-1.565401000	-3.244806000
H	1.012049000	-2.277103000	-4.020846000
H	0.014614000	-0.847155000	-3.694354000
H	1.589764000	-1.020398000	-2.899672000
C	-1.205751000	-3.072748000	-2.595381000
H	-0.903284000	-3.784779000	-3.371361000
H	-1.692516000	-3.635684000	-1.793496000
H	-1.936561000	-2.386279000	-3.031372000

7A

E = -954.476939854

C	1.331571000	-1.374061000	1.280800000
H	0.757434000	-1.268260000	2.223013000
H	1.125613000	-2.419252000	0.967802000
C	2.832622000	-1.240901000	1.609608000
O	-1.135024000	0.787158000	0.874283000
Si	-2.177271000	2.010442000	1.292682000
C	1.192892000	0.722328000	-1.260141000
H	1.500797000	-0.255804000	-1.732156000
C	1.751534000	1.942380000	-1.946722000
O	-2.413239000	3.141306000	0.105186000
H	-1.803790000	3.884475000	0.157550000
O	-1.561393000	2.839692000	2.595465000
H	-1.166928000	2.278827000	3.270484000
O	-3.616375000	1.241193000	1.575998000
H	-4.372777000	1.835275000	1.606073000
C	3.192488000	-2.222425000	2.740032000
H	4.253451000	-2.149060000	3.008313000
H	2.605200000	-2.017498000	3.643035000
H	2.994600000	-3.258682000	2.441591000
C	3.686610000	-1.571725000	0.379619000
H	3.489896000	-2.591623000	0.026330000
H	3.476495000	-0.877965000	-0.439762000
H	4.754893000	-1.503593000	0.616222000
C	3.136851000	0.189171000	2.076594000
H	2.903086000	0.909849000	1.285986000
H	2.542465000	0.449019000	2.961598000
H	4.194536000	0.300291000	2.343830000
C	1.324416000	3.195794000	-1.166704000
H	1.696310000	4.103699000	-1.655658000
H	0.232458000	3.258073000	-1.113582000
H	1.716819000	3.173206000	-0.144389000
C	1.198112000	2.027006000	-3.382895000
H	1.590465000	2.911457000	-3.900338000
H	1.481710000	1.143667000	-3.965862000

H	0.105281000	2.088846000	-3.374666000
C	3.288931000	1.877610000	-2.003311000
H	3.717965000	1.823869000	-0.998067000
H	3.625454000	0.996443000	-2.561284000
H	3.696307000	2.765152000	-2.502715000
C	-0.772922000	-1.840400000	-1.441232000
C	-2.077467000	-2.564749000	-1.028506000
C	-2.315635000	-3.761687000	-1.964712000
H	-1.495121000	-4.485633000	-1.896697000
H	-3.246617000	-4.285443000	-1.714432000
H	-2.385311000	-3.434173000	-3.008198000
C	-3.266260000	-1.598953000	-1.145163000
H	-4.206068000	-2.102590000	-0.889862000
H	-3.161916000	-0.740802000	-0.472155000
H	-3.359514000	-1.217128000	-2.168570000
C	-1.981251000	-3.078789000	0.416697000
H	-1.872624000	-2.255107000	1.135512000
H	-2.886934000	-3.626813000	0.701716000
H	-1.128637000	-3.756351000	0.543711000
Ta	0.063412000	-0.302511000	-0.119083000
H	0.041812000	-2.585400000	-1.534427000
H	-0.890814000	-1.432243000	-2.455676000

7B

E = -756.695932977

O	1.385897000	-1.294467000	-0.192659000
Si	2.943698000	-0.920329000	0.213679000
C	-0.251425000	1.359658000	-0.193772000
C	0.072173000	2.799260000	0.058795000
O	3.654935000	0.297127000	-0.667757000
H	4.057126000	-0.017053000	-1.483221000
O	3.892111000	-2.265640000	-0.078238000
H	3.447929000	-3.088418000	0.149300000
O	2.929068000	-0.443182000	1.804213000
H	3.750957000	-0.021285000	2.073721000
C	-1.189740000	3.665090000	-0.118131000
H	-0.958298000	4.725478000	0.043981000
H	-1.599044000	3.558367000	-1.128695000
H	-1.967376000	3.376337000	0.596710000
C	1.154781000	3.273309000	-0.930785000
H	1.411595000	4.325656000	-0.751835000
H	2.061088000	2.669820000	-0.828420000
H	0.800679000	3.181598000	-1.963677000
C	0.597090000	2.950989000	1.499777000
H	-0.161060000	2.636264000	2.224172000
H	1.484520000	2.330242000	1.653239000
H	0.859947000	3.996251000	1.707423000
C	-1.685101000	-1.027741000	1.216560000
C	-2.984212000	-0.908665000	0.349609000
C	-3.854121000	-2.163620000	0.522444000
H	-4.134003000	-2.280255000	1.574059000
H	-4.775449000	-2.099344000	-0.070503000
H	-3.315984000	-3.068730000	0.218361000
C	-2.682982000	-0.788738000	-1.189983000
H	-3.593387000	-0.495342000	-1.722901000
H	-2.050744000	0.127991000	-1.447799000

H	-2.358782000	-1.733188000	-1.649285000
C	-3.771561000	0.339918000	0.769335000
H	-3.151390000	1.233773000	0.663107000
H	-4.677984000	0.463331000	0.164210000
H	-4.076100000	0.254876000	1.817290000
Ta	-0.360652000	-0.438269000	-0.373568000
H	-1.772096000	-0.462158000	2.144860000
H	-1.491850000	-2.083429000	1.467330000

7B'

E = -954.422798652

C	-2.942241000	-0.457796000	0.015886000
H	-2.576929000	-1.436269000	-0.322131000
H	-3.751817000	-0.668620000	0.722942000
C	-3.396388000	0.421996000	-1.159277000
O	1.245544000	-0.152315000	-1.227398000
Si	2.530032000	0.831515000	-1.563262000
C	-0.097309000	1.156206000	1.221279000
H	-2.233014000	0.134807000	0.675504000
C	0.206049000	2.305077000	2.130358000
O	2.150191000	2.421157000	-1.877411000
H	2.000054000	2.583536000	-2.813868000
O	3.247085000	0.293381000	-2.974760000
H	3.294980000	-0.666136000	-3.029682000
O	3.544410000	0.791531000	-0.248633000
H	4.226129000	1.469993000	-0.282485000
C	-4.419518000	-0.334592000	-2.013743000
H	-4.749518000	0.277690000	-2.860061000
H	-3.997027000	-1.262510000	-2.416391000
H	-5.306246000	-0.596534000	-1.426211000
C	-4.014499000	1.715657000	-0.612232000
H	-4.896961000	1.501245000	0.000503000
H	-3.296403000	2.264179000	0.006778000
H	-4.327929000	2.373375000	-1.430174000
C	-2.157239000	0.765373000	-1.998648000
H	-1.416189000	1.320848000	-1.384797000
H	-1.705353000	-0.127331000	-2.450700000
H	-2.394209000	1.447212000	-2.822859000
C	-0.843054000	2.367688000	3.257631000
H	-0.630196000	3.200037000	3.940576000
H	-1.848788000	2.514774000	2.848295000
H	-0.846475000	1.439385000	3.838048000
C	0.185127000	3.627592000	1.339854000
H	0.417858000	4.477095000	1.995131000
H	0.915160000	3.603429000	0.525799000
H	-0.803997000	3.800996000	0.901003000
C	1.603458000	2.101048000	2.747329000
H	1.635383000	1.179140000	3.336859000
H	2.361561000	2.022326000	1.963424000
H	1.860573000	2.940152000	3.406738000
C	0.211404000	-1.884880000	1.430944000
C	0.526673000	-3.284471000	0.850666000
C	0.359173000	-4.353284000	1.944649000
H	-0.671905000	-4.378456000	2.317119000
H	0.606326000	-5.355381000	1.570920000
H	1.015062000	-4.141158000	2.796129000

C	1.974537000	-3.320133000	0.340656000
H	2.225232000	-4.305369000	-0.071550000
H	2.136132000	-2.568687000	-0.438853000
H	2.676998000	-3.107142000	1.154012000
C	-0.423394000	-3.621982000	-0.310615000
H	-0.296325000	-2.925906000	-1.153455000
H	-0.234676000	-4.627651000	-0.705812000
H	-1.472616000	-3.590641000	0.011140000
Ta	-0.214583000	-0.231983000	0.066006000
H	-0.753518000	-1.924413000	1.981614000
H	0.948247000	-1.625484000	2.200892000

7B''

E = -875.816802025

O	-0.267992000	1.421092000	0.619221000
Si	-1.629571000	2.357878000	0.657331000
C	-1.074826000	-1.287952000	-0.663436000
C	-2.303252000	-1.872985000	-1.283006000
O	-2.158357000	2.533668000	-0.906635000
H	-3.053512000	2.882760000	-0.960869000
O	-1.248820000	3.805875000	1.400658000
H	-0.396001000	4.158540000	1.128352000
O	-2.882344000	1.747154000	1.565297000
H	-2.863804000	2.060989000	2.474663000
C	-3.429931000	-1.975115000	-0.236555000
H	-4.339495000	-2.397594000	-0.682969000
H	-3.129839000	-2.623002000	0.594933000
H	-3.668545000	-0.989593000	0.173885000
C	-1.992373000	-3.277092000	-1.837190000
H	-2.883015000	-3.718076000	-2.303012000
H	-1.198460000	-3.230682000	-2.589475000
H	-1.661013000	-3.948599000	-1.037252000
C	-2.759421000	-0.959090000	-2.437210000
H	-2.957474000	0.052293000	-2.071780000
H	-1.983877000	-0.891573000	-3.206796000
H	-3.672237000	-1.353280000	-2.902119000
C	1.094211000	-2.106458000	1.771504000
H	1.094484000	-3.191277000	1.933398000
H	2.055764000	-1.892645000	1.281618000
C	0.931601000	-1.369982000	3.105791000
H	0.170758000	-2.103121000	1.072603000
C	1.997251000	-1.775270000	4.122481000
H	1.857752000	-1.246882000	5.070219000
H	1.954717000	-2.850209000	4.328843000
H	3.003824000	-1.544903000	3.756864000
H	0.969366000	-0.280992000	2.960192000
H	-0.066597000	-1.583826000	3.504741000
C	1.661108000	-0.261617000	-1.619441000
H	2.032094000	-1.310953000	-1.583221000
H	1.170252000	-0.183991000	-2.596386000
Ta	0.296711000	-0.365951000	0.080658000
C	2.861125000	0.710388000	-1.545390000
C	2.382805000	2.143019000	-1.823620000
H	1.926481000	2.212561000	-2.817251000
H	1.630042000	2.457460000	-1.092879000
H	3.216848000	2.854457000	-1.786138000

C	3.515130000	0.657160000	-0.154267000
H	2.820376000	0.984245000	0.633987000
H	3.857971000	-0.358210000	0.085349000
H	4.388518000	1.317742000	-0.093609000
C	3.914910000	0.323801000	-2.597408000
H	3.481922000	0.342084000	-3.603524000
H	4.768817000	1.013339000	-2.585673000
H	4.298042000	-0.688103000	-2.419201000

7C

E = -1073.57410872

C	-0.734231000	1.896638000	-0.552865000
H	-1.624258000	1.721268000	-1.185978000
H	-1.136138000	2.342209000	0.375062000
C	0.168626000	2.927989000	-1.271208000
O	1.646207000	-0.054868000	-0.339526000
Si	3.223754000	-0.516298000	-0.539436000
C	0.149126000	-0.888032000	1.976486000
H	1.043352000	-1.511071000	1.810610000
C	0.406091000	0.011060000	3.209003000
O	3.815394000	-1.442399000	0.705560000
H	4.297017000	-0.932117000	1.364116000
O	4.217552000	0.819024000	-0.600469000
H	3.903207000	1.521379000	-1.178391000
O	3.232981000	-1.433790000	-1.922704000
H	4.047500000	-1.931483000	-2.045768000
C	-0.669785000	4.181369000	-1.583219000
H	-0.064114000	4.942752000	-2.089843000
H	-1.516672000	3.939630000	-2.235361000
H	-1.069716000	4.627696000	-0.665815000
C	1.345315000	3.339648000	-0.377465000
H	0.990822000	3.773679000	0.564770000
H	1.980436000	2.483355000	-0.134592000
H	1.962079000	4.098051000	-0.874968000
C	0.695825000	2.350635000	-2.593288000
H	1.318203000	1.466698000	-2.422583000
H	-0.128832000	2.057191000	-3.253736000
H	1.297268000	3.093919000	-3.130228000
C	-0.824054000	0.870464000	3.534833000
H	-0.646412000	1.479160000	4.429391000
H	-1.071721000	1.554298000	2.714786000
H	-1.704390000	0.246539000	3.725594000
C	1.615714000	0.926811000	2.973641000
H	1.849491000	1.502920000	3.876771000
H	2.501657000	0.340032000	2.708950000
H	1.437292000	1.640345000	2.162577000
C	0.704934000	-0.890984000	4.420563000
H	-0.137841000	-1.558737000	4.631841000
H	1.587360000	-1.514564000	4.238107000
H	0.894251000	-0.293283000	5.320966000
C	-2.418896000	-0.636056000	0.462583000
C	-3.797464000	-0.283980000	-0.168455000
C	-4.868041000	-1.231201000	0.407650000
H	-4.903060000	-1.162058000	1.500973000
H	-5.867918000	-0.991199000	0.023637000
H	-4.650748000	-2.273737000	0.146705000

C	-3.809450000	-0.432662000	-1.696183000
H	-4.800846000	-0.195306000	-2.101344000
H	-3.088787000	0.237664000	-2.178863000
H	-3.571055000	-1.458816000	-1.998296000
C	-4.200305000	1.152950000	0.199054000
H	-3.503263000	1.893511000	-0.203250000
H	-5.196432000	1.388813000	-0.194413000
H	-4.233729000	1.282527000	1.287279000
Ta	-0.275650000	-0.152431000	-0.044536000
H	-2.501266000	-0.372247000	1.532148000
H	-2.346212000	-1.743014000	0.491076000
C	-0.387425000	-1.613803000	-1.634883000
H	0.342076000	-1.303007000	-2.397301000
H	-1.384456000	-1.550671000	-2.089013000
C	-0.094505000	-3.057150000	-1.201518000
H	0.909858000	-3.117676000	-0.763484000
H	-0.795811000	-3.364520000	-0.413404000
C	-0.185903000	-4.055925000	-2.358898000
H	0.028704000	-5.076897000	-2.023674000
H	-1.187447000	-4.051720000	-2.803364000
H	0.529819000	-3.802623000	-3.148336000
H	-0.669865000	-1.583642000	2.212021000

7D

E = -875.874131564

C	-1.658801000	-1.354496000	-0.858641000
H	-1.093989000	-1.816932000	-1.693172000
H	-1.818954000	-2.197676000	-0.150348000
C	-3.025266000	-0.883343000	-1.394558000
O	1.394209000	-0.034410000	-0.945685000
Si	2.988051000	0.349743000	-1.209799000
C	-0.794686000	1.291679000	0.938963000
H	-1.434390000	0.664948000	1.623417000
C	-0.883822000	2.776735000	1.182543000
O	3.464995000	1.791356000	-0.546573000
H	3.302471000	2.550248000	-1.115743000
O	3.241278000	0.487139000	-2.846857000
H	2.756000000	-0.155980000	-3.373121000
O	3.845592000	-0.859701000	-0.468224000
H	4.784572000	-0.668993000	-0.377984000
C	-3.697667000	-2.035760000	-2.162480000
H	-4.671576000	-1.730436000	-2.563912000
H	-3.077848000	-2.364770000	-3.005023000
H	-3.861585000	-2.901732000	-1.510330000
C	-3.940128000	-0.458976000	-0.239895000
H	-4.109436000	-1.290526000	0.455388000
H	-3.499733000	0.371733000	0.318678000
H	-4.918245000	-0.136277000	-0.615135000
C	-2.819397000	0.301699000	-2.348263000
H	-2.361603000	1.144133000	-1.818939000
H	-2.162529000	0.026933000	-3.182851000
H	-3.773155000	0.637514000	-2.772591000
C	-0.061945000	3.510473000	0.110635000
H	-0.082813000	4.593571000	0.279199000
H	0.981520000	3.179645000	0.132550000
H	-0.462885000	3.313558000	-0.889582000

C	-0.310598000	3.107906000	2.574599000
H	-0.367833000	4.185486000	2.773602000
H	-0.868699000	2.590305000	3.362727000
H	0.737372000	2.799933000	2.645598000
C	-2.347467000	3.249177000	1.113946000
H	-2.783611000	3.032866000	0.133659000
H	-2.958836000	2.749541000	1.874001000
H	-2.415412000	4.330086000	1.287829000
C	0.319579000	-1.597267000	1.942062000
C	0.801232000	-3.010258000	1.568836000
C	1.231533000	-3.842687000	2.779432000
H	0.404027000	-3.958730000	3.488496000
H	1.564136000	-4.844139000	2.483811000
H	2.057418000	-3.357542000	3.311605000
Ta	-0.087317000	-0.326371000	0.219237000
H	-0.529266000	-1.657495000	2.640405000
H	1.111303000	-1.068941000	2.502146000
H	0.004800000	-3.549055000	1.035573000
H	1.646231000	-2.946983000	0.868573000

TS(7A-7B)

E = -954.417905616

C	0.039710000	2.552081000	-0.383848000
H	1.117287000	2.640967000	-0.600524000
H	-0.433569000	3.173425000	-1.158017000
C	-0.320474000	3.161952000	0.992697000
O	-0.007357000	-0.932343000	1.356165000
Si	-1.200335000	-1.917366000	1.936072000
C	-0.998116000	-0.095855000	-1.492912000
H	-0.652386000	1.574092000	-0.939265000
C	-2.130080000	-0.383468000	-2.424863000
O	-2.696886000	-1.197488000	2.062350000
H	-2.862916000	-0.857141000	2.947160000
O	-0.823056000	-2.351885000	3.505043000
H	0.106233000	-2.570337000	3.626078000
O	-1.320237000	-3.211027000	0.901682000
H	-2.110188000	-3.739453000	1.052904000
C	-0.094231000	4.681376000	0.921787000
H	-0.351846000	5.159328000	1.873687000
H	0.953060000	4.917194000	0.700974000
H	-0.713530000	5.137114000	0.141111000
C	-1.798879000	2.880168000	1.302317000
H	-2.450718000	3.284125000	0.519519000
H	-2.000102000	1.805171000	1.379356000
H	-2.089526000	3.345664000	2.250864000
C	0.560059000	2.586365000	2.111644000
H	0.378264000	1.517077000	2.280718000
H	1.625116000	2.723577000	1.891025000
H	0.352062000	3.092965000	3.060658000
C	-1.934632000	0.378096000	-3.750243000
H	-2.747604000	0.152765000	-4.451906000
H	-1.926137000	1.461381000	-3.584308000
H	-0.986176000	0.100675000	-4.220625000
C	-3.471737000	0.027057000	-1.787814000
H	-4.308760000	-0.207025000	-2.457961000
H	-3.626112000	-0.495620000	-0.839499000

H	-3.495158000	1.104042000	-1.586010000
C	-2.139935000	-1.899520000	-2.703610000
H	-1.205030000	-2.212429000	-3.179118000
H	-2.247351000	-2.462067000	-1.771990000
H	-2.970574000	-2.158720000	-3.372031000
C	2.074382000	-0.457407000	-1.344421000
C	3.362049000	-0.796052000	-0.557868000
C	4.575533000	-0.768034000	-1.502895000
H	4.715877000	0.229613000	-1.935679000
H	5.500425000	-1.040053000	-0.978276000
H	4.438661000	-1.473116000	-2.330160000
C	3.238361000	-2.201289000	0.050140000
H	4.141430000	-2.470461000	0.611439000
H	2.381796000	-2.265754000	0.729899000
H	3.094511000	-2.952501000	-0.734471000
C	3.591144000	0.223755000	0.569670000
H	2.787004000	0.187154000	1.318483000
H	4.526711000	0.025971000	1.106736000
H	3.650312000	1.246585000	0.175329000
Ta	0.295214000	0.161850000	-0.235619000
H	2.234173000	0.480708000	-1.921935000
H	1.890211000	-1.220221000	-2.109593000

TS(7A-7C)

E = -1073.52171782

C	0.720066000	-2.001949000	-1.127752000
H	0.126242000	-2.882648000	-0.852407000
H	0.536731000	-1.874809000	-2.211881000
C	2.218605000	-2.371407000	-0.950971000
O	0.755247000	-0.029350000	1.335966000
Si	1.573872000	0.560646000	2.652365000
C	0.114560000	1.322729000	-1.661856000
H	-0.881413000	1.604229000	-0.608468000
C	0.883852000	2.575899000	-2.047781000
O	3.209166000	0.317930000	2.574058000
H	3.490667000	-0.569218000	2.818659000
O	1.049580000	-0.213509000	4.026680000
H	0.094524000	-0.316527000	4.082601000
O	1.309152000	2.198627000	2.644570000
H	1.902552000	2.684498000	3.226295000
C	2.587477000	-3.467962000	-1.966676000
H	3.629527000	-3.791624000	-1.846689000
H	1.945967000	-4.348154000	-1.843916000
H	2.465653000	-3.107035000	-2.994660000
C	3.134452000	-1.161449000	-1.188503000
H	2.934446000	-0.703091000	-2.163595000
H	2.997718000	-0.395684000	-0.416911000
H	4.190871000	-1.457685000	-1.168544000
C	2.461361000	-2.919481000	0.462365000
H	2.198696000	-2.175290000	1.220022000
H	1.854508000	-3.813709000	0.646679000
H	3.514032000	-3.195893000	0.601155000
C	1.598445000	2.308866000	-3.384548000
H	2.181238000	3.186267000	-3.688302000
H	2.281275000	1.458154000	-3.301101000
H	0.879494000	2.090885000	-4.182638000

C	1.926333000	2.912962000	-0.971143000
H	2.464486000	3.831510000	-1.232809000
H	1.462124000	3.061961000	0.009147000
H	2.662125000	2.108012000	-0.875630000
C	-0.073875000	3.769577000	-2.222154000
H	-0.853336000	3.550729000	-2.960431000
H	-0.562432000	4.024822000	-1.275949000
H	0.474074000	4.655570000	-2.564286000
C	-1.681571000	1.568174000	0.699007000
H	-1.987430000	0.840286000	1.459584000
H	-1.023398000	2.281935000	1.214767000
C	-2.925557000	2.278439000	0.165181000
H	-2.639818000	3.018721000	-0.595472000
H	-3.570258000	1.557566000	-0.355583000
C	-3.742054000	2.976774000	1.254374000
H	-4.093331000	2.259837000	2.005430000
H	-3.139056000	3.728859000	1.775548000
H	-4.621157000	3.481892000	0.837959000
Ta	-0.165233000	-0.116048000	-0.330723000
C	-2.089945000	-1.069098000	-0.887309000
H	-1.848015000	-1.566107000	-1.843880000
H	-2.740477000	-0.224004000	-1.168458000
C	-2.959459000	-2.053992000	-0.059030000
C	-2.227014000	-3.372369000	0.226255000
H	-1.911433000	-3.864047000	-0.700378000
H	-1.337264000	-3.217180000	0.845853000
H	-2.886651000	-4.065895000	0.761684000
C	-4.230565000	-2.376581000	-0.868233000
H	-3.976942000	-2.832386000	-1.832134000
H	-4.879571000	-3.076134000	-0.326880000
H	-4.810699000	-1.468760000	-1.069830000
C	-3.387161000	-1.441654000	1.282162000
H	-2.522751000	-1.263766000	1.932686000
H	-3.911180000	-0.490364000	1.142331000
H	-4.064051000	-2.119216000	1.816403000
H	-0.551299000	0.961537000	-2.476813000

TS(7A-7D)

E = -1073.51922047

C	0.625572000	-1.540785000	-1.510344000
H	0.624003000	-0.838283000	-2.367843000
H	1.657861000	-1.916143000	-1.470042000
C	-0.272026000	-2.745373000	-1.896544000
O	-1.288212000	0.803413000	-0.624335000
Si	-2.538212000	1.702301000	-1.236718000
C	-0.376219000	-1.076052000	1.722780000
H	0.486479000	-1.785684000	1.588407000
C	-1.270816000	-1.401317000	2.892761000
O	-3.172820000	2.801117000	-0.168128000
H	-3.882939000	2.436502000	0.369604000
O	-3.785409000	0.682387000	-1.643333000
H	-3.488709000	-0.178564000	-1.957944000
O	-1.878616000	2.548069000	-2.500753000
H	-2.439029000	3.261362000	-2.821944000
C	0.169526000	-3.274217000	-3.274195000
H	-0.427246000	-4.143016000	-3.579558000

H	0.060359000	-2.503797000	-4.046534000
H	1.221591000	-3.581051000	-3.256709000
C	-0.122206000	-3.876413000	-0.870562000
H	0.921983000	-4.204712000	-0.802242000
H	-0.440599000	-3.550426000	0.123846000
H	-0.725693000	-4.747211000	-1.153683000
C	-1.751232000	-2.340314000	-1.988661000
H	-2.134100000	-2.019904000	-1.012529000
H	-1.876069000	-1.519204000	-2.707256000
H	-2.367484000	-3.179871000	-2.332228000
C	-2.421543000	-0.384572000	2.954430000
H	-3.080861000	-0.598532000	3.803591000
H	-2.037275000	0.634364000	3.072458000
H	-3.022229000	-0.420392000	2.039413000
C	-0.453098000	-1.319542000	4.196665000
H	-1.085144000	-1.541034000	5.065488000
H	0.372476000	-2.039948000	4.189722000
H	-0.027871000	-0.319404000	4.327303000
C	-1.855922000	-2.818830000	2.753201000
H	-2.449579000	-2.909189000	1.837926000
H	-1.061504000	-3.572603000	2.716947000
H	-2.504112000	-3.056428000	3.605648000
C	2.608694000	-0.228314000	0.578706000
C	3.796378000	0.353746000	-0.228997000
C	4.902812000	-0.711886000	-0.319342000
H	4.554791000	-1.596600000	-0.864851000
H	5.784540000	-0.321893000	-0.842437000
H	5.220993000	-1.035838000	0.678087000
C	4.373271000	1.581214000	0.494293000
H	5.226390000	1.990817000	-0.058530000
H	3.635680000	2.382387000	0.600160000
H	4.723471000	1.314686000	1.498283000
C	3.374299000	0.750321000	-1.651184000
H	2.590864000	1.517220000	-1.641504000
H	4.225285000	1.160645000	-2.207462000
H	2.996874000	-0.110695000	-2.211038000
Ta	0.177019000	-0.124716000	0.162909000
H	2.491478000	-1.287352000	0.320037000
H	2.867345000	-0.228073000	1.646454000
C	0.806553000	1.971550000	1.143664000
H	-0.192163000	1.898300000	1.602139000
H	1.674725000	0.872082000	0.780249000
C	0.870997000	3.163058000	0.184179000
H	0.222398000	2.992496000	-0.682945000
H	1.887613000	3.263639000	-0.216440000
C	0.468538000	4.478934000	0.853419000
H	0.550242000	5.320426000	0.156641000
H	-0.568018000	4.436630000	1.204340000
H	1.107240000	4.695944000	1.717485000
H	1.477482000	2.133278000	1.997934000

TS(7B-7D)

E = -875.814289757

O	-0.159462000	1.509502000	0.551113000
Si	-1.430181000	2.557797000	0.419697000
C	-1.060586000	-1.186790000	-0.793585000

C	-2.257829000	-1.757343000	-1.480969000
O	-1.774737000	2.715826000	-1.197063000
H	-2.612879000	3.160053000	-1.359237000
O	-1.010843000	3.996123000	1.159327000
H	-0.103047000	4.261977000	0.982806000
O	-2.818637000	2.077876000	1.200847000
H	-2.864276000	2.407164000	2.103863000
C	-3.460391000	-1.800082000	-0.517939000
H	-4.349515000	-2.198161000	-1.023402000
H	-3.249009000	-2.444279000	0.343569000
H	-3.691522000	-0.798755000	-0.142831000
C	-1.955740000	-3.179635000	-1.991153000
H	-2.822738000	-3.595407000	-2.519913000
H	-1.104048000	-3.172343000	-2.678429000
H	-1.714729000	-3.852543000	-1.160437000
C	-2.595203000	-0.845806000	-2.677571000
H	-2.780511000	0.178273000	-2.341896000
H	-1.765907000	-0.820393000	-3.391431000
H	-3.487647000	-1.215314000	-3.197897000
C	0.457931000	-2.060822000	1.724221000
H	0.042897000	-3.073857000	1.820444000
H	1.528733000	-2.221920000	1.525586000
C	0.218864000	-1.309342000	3.044133000
H	-0.372189000	-1.946681000	0.698728000
C	0.609974000	-2.133889000	4.272223000
H	0.429104000	-1.576547000	5.196880000
H	0.029689000	-3.061714000	4.320847000
H	1.671116000	-2.404224000	4.245448000
H	0.777852000	-0.363062000	3.056107000
H	-0.841448000	-1.035004000	3.114681000
C	1.915755000	-0.485961000	-1.348893000
H	2.167640000	-1.559922000	-1.208484000
H	1.605271000	-0.415216000	-2.398114000
Ta	0.284886000	-0.338045000	0.097764000
C	3.179853000	0.370905000	-1.104458000
C	2.910897000	1.822374000	-1.527979000
H	2.649007000	1.874392000	-2.590602000
H	2.077887000	2.252199000	-0.960827000
H	3.794523000	2.452133000	-1.367745000
C	3.569412000	0.344054000	0.383886000
H	2.792177000	0.798243000	1.017336000
H	3.743064000	-0.682232000	0.732688000
H	4.489292000	0.911741000	0.568897000
C	4.355556000	-0.180095000	-1.929235000
H	4.110806000	-0.186210000	-2.997087000
H	5.261008000	0.425484000	-1.794843000
H	4.593719000	-1.209751000	-1.637088000

TS(7C-7D)

E = -1073.51908709

C	1.185136000	-1.920271000	-0.129205000
H	0.231424000	-2.332051000	0.228636000
H	1.366705000	-2.418440000	-1.089774000
C	2.271060000	-2.367938000	0.880003000
O	-0.396591000	0.319775000	1.419654000
Si	-1.401822000	0.279812000	2.744665000

C	1.652924000	0.949134000	-1.127824000
H	1.495316000	0.690862000	-2.201861000
C	2.864957000	1.844945000	-0.939145000
O	-1.421227000	-1.178514000	3.535278000
H	-2.160616000	-1.738593000	3.277762000
O	-2.973537000	0.531945000	2.258478000
H	-3.071639000	1.218561000	1.589710000
O	-0.780398000	1.428272000	3.760337000
H	-1.123683000	1.375023000	4.657669000
C	2.131237000	-3.888275000	1.085496000
H	2.894192000	-4.264848000	1.778110000
H	1.149153000	-4.139954000	1.501743000
H	2.242540000	-4.427797000	0.137810000
C	3.674908000	-2.086556000	0.330849000
H	3.821078000	-2.555495000	-0.649690000
H	3.853163000	-1.012858000	0.221238000
H	4.444819000	-2.477362000	1.006124000
C	2.103184000	-1.675981000	2.238810000
H	2.219585000	-0.590768000	2.158737000
H	1.114081000	-1.869622000	2.665427000
H	2.853955000	-2.040314000	2.950303000
C	4.093069000	1.290375000	-1.684070000
H	4.950390000	1.962637000	-1.563516000
H	4.384893000	0.304600000	-1.312369000
H	3.889928000	1.197379000	-2.757065000
C	3.184644000	2.025898000	0.551092000
H	4.014008000	2.730086000	0.681347000
H	2.318636000	2.417695000	1.094920000
H	3.475762000	1.080191000	1.018203000
C	2.514454000	3.218910000	-1.546042000
H	2.250025000	3.129891000	-2.605568000
H	1.669472000	3.675743000	-1.023251000
H	3.373012000	3.896853000	-1.469722000
C	-1.655908000	1.679266000	-0.913392000
H	-1.595193000	1.899745000	-1.991331000
H	-2.668551000	1.271970000	-0.772671000
C	-1.530469000	3.009154000	-0.146417000
H	-1.635781000	2.842269000	0.935831000
H	-0.518489000	3.419128000	-0.265774000
C	-2.543808000	4.070280000	-0.584741000
H	-2.421492000	4.310199000	-1.646995000
H	-3.572351000	3.715026000	-0.448523000
H	-2.432053000	5.000369000	-0.015192000
H	1.720815000	-0.479341000	-0.607740000
Ta	-0.045534000	0.208650000	-0.441956000
C	-0.925213000	-0.979135000	-2.101837000
H	-1.111062000	-0.199110000	-2.861935000
H	-0.082597000	-1.566036000	-2.504411000
C	-2.163153000	-1.915626000	-2.090719000
C	-3.438606000	-1.178862000	-1.660541000
H	-3.379728000	-0.848582000	-0.618006000
H	-3.624121000	-0.298879000	-2.285577000
H	-4.309163000	-1.840131000	-1.747641000
C	-2.373960000	-2.455219000	-3.518404000
H	-3.237669000	-3.130071000	-3.564577000
H	-2.550184000	-1.636463000	-4.225389000

H	-1.495062000	-3.011788000	-3.863826000
C	-1.958005000	-3.112102000	-1.150876000
H	-1.050165000	-3.672275000	-1.398562000
H	-1.882089000	-2.792334000	-0.104958000
H	-2.806415000	-3.803747000	-1.218391000

8A

E = -1289.6040940

C	-0.890639000	-2.041177000	-1.139684000
H	-0.790364000	-1.738705000	-2.202028000
H	-0.029967000	-2.694023000	-0.947915000
C	-2.190134000	-2.869622000	-0.994304000
N	1.198990000	-0.008350000	-0.232365000
O	-1.723992000	1.157846000	-0.928610000
Si	-2.971912000	2.170767000	-0.518869000
C	-0.932222000	-0.472292000	1.657312000
H	-2.045123000	-0.438513000	1.653387000
C	-0.360249000	-0.580599000	3.054410000
O	-4.080821000	1.493342000	0.518557000
H	-4.807300000	1.058928000	0.060015000
O	-3.822831000	2.552235000	-1.896974000
H	-3.266649000	2.699724000	-2.668412000
O	-2.275939000	3.464918000	0.247807000
H	-2.903746000	3.998930000	0.744625000
C	2.530391000	0.350293000	-0.317526000
C	3.512508000	-0.669091000	-0.416486000
C	2.899105000	1.721807000	-0.291596000
C	4.852477000	-0.289883000	-0.505315000
C	4.254682000	2.039974000	-0.377001000
C	5.226234000	1.049554000	-0.486749000
H	5.618425000	-1.055626000	-0.586642000
H	4.559480000	3.082047000	-0.356655000
H	6.275814000	1.322952000	-0.553917000
C	-2.223054000	-3.914725000	-2.124623000
H	-3.117568000	-4.545631000	-2.054064000
H	-2.229754000	-3.433667000	-3.109738000
H	-1.346171000	-4.570270000	-2.078669000
C	-2.220264000	-3.601915000	0.351563000
H	-1.364326000	-4.280117000	0.446542000
H	-2.180820000	-2.897411000	1.186525000
H	-3.133478000	-4.200853000	0.448762000
C	-3.433124000	-1.976307000	-1.120773000
H	-3.491032000	-1.251656000	-0.299595000
H	-3.427793000	-1.418923000	-2.064901000
H	-4.350767000	-2.575775000	-1.090916000
C	1.166855000	-0.705252000	3.027206000
H	1.560408000	-0.777303000	4.047817000
H	1.478112000	-1.598742000	2.477308000
H	1.625921000	0.160813000	2.542701000
C	-0.959566000	-1.814573000	3.755311000
H	-0.588959000	-1.886547000	4.784736000
H	-2.053310000	-1.756946000	3.796640000
H	-0.686710000	-2.735668000	3.231029000
C	-0.756534000	0.685494000	3.840829000
H	-0.341288000	1.581478000	3.368816000
H	-1.845115000	0.800998000	3.884838000

H	-0.380215000	0.632469000	4.869784000
C	1.842039000	2.807777000	-0.216302000
H	0.983692000	2.390886000	0.325163000
C	3.105517000	-2.129521000	-0.474280000
H	2.125845000	-2.202577000	0.011206000
C	2.933922000	-2.577791000	-1.934681000
H	3.884664000	-2.509816000	-2.475764000
H	2.590146000	-3.617267000	-1.985841000
H	2.204835000	-1.951639000	-2.457668000
C	4.064395000	-3.062282000	0.272785000
H	3.649415000	-4.075272000	0.308313000
H	5.039996000	-3.134006000	-0.220758000
H	4.230758000	-2.727544000	1.301429000
C	2.287663000	4.055010000	0.552821000
H	3.063668000	4.614543000	0.018394000
H	1.436883000	4.731000000	0.684902000
H	2.676864000	3.799961000	1.543617000
C	1.361309000	3.183978000	-1.627239000
H	0.550292000	3.917964000	-1.574043000
H	2.182067000	3.618331000	-2.209438000
H	0.992748000	2.307625000	-2.169102000
W	-0.545067000	-0.154815000	-0.164596000

8B

E = -1091.8018100

N	-0.809582000	0.412678000	-0.725466000
O	2.157995000	0.402868000	-1.010070000
Si	3.446708000	0.842493000	-0.059963000
C	0.695303000	-1.768135000	0.433349000
C	0.512779000	-2.420860000	1.760758000
O	2.999822000	2.210307000	0.764484000
H	3.578873000	2.412776000	1.505928000
O	4.741616000	1.070966000	-1.083468000
H	4.515104000	1.574590000	-1.871895000
O	3.924097000	-0.267708000	1.073739000
H	4.172840000	-1.122484000	0.709195000
C	-1.936100000	0.842787000	-0.061606000
C	-1.919847000	2.103565000	0.593004000
C	-3.116593000	0.050307000	-0.092880000
C	-3.088537000	2.534995000	1.218624000
C	-4.261501000	0.542214000	0.534603000
C	-4.252081000	1.769575000	1.190469000
H	-3.094042000	3.489137000	1.736794000
H	-5.175307000	-0.044081000	0.518637000
H	-5.152404000	2.130556000	1.680232000
C	-0.147967000	-1.430091000	2.738010000
H	-0.296953000	-1.904704000	3.715578000
H	0.482520000	-0.547371000	2.879591000
H	-1.118753000	-1.096775000	2.361312000
C	1.873073000	-2.874788000	2.324302000
H	1.739325000	-3.361824000	3.297915000
H	2.353716000	-3.591566000	1.649633000
H	2.540887000	-2.018919000	2.453142000
C	-0.398497000	-3.650992000	1.573381000
H	-1.385397000	-3.357644000	1.203118000
H	0.038060000	-4.362161000	0.863987000

H	-0.532403000	-4.167698000	2.531205000
C	-3.127709000	-1.263530000	-0.853298000
H	-2.132697000	-1.717157000	-0.707107000
C	-0.658600000	2.948430000	0.567391000
H	0.196597000	2.265839000	0.617572000
C	-0.553812000	3.703286000	-0.768557000
H	-1.383306000	4.411077000	-0.881806000
H	0.384918000	4.265895000	-0.817289000
H	-0.578461000	3.007779000	-1.612180000
C	-0.535929000	3.918379000	1.744767000
H	0.452408000	4.388441000	1.730996000
H	-1.278233000	4.723620000	1.696116000
H	-0.653517000	3.406572000	2.705657000
C	-4.157831000	-2.273404000	-0.342502000
H	-5.183215000	-1.949962000	-0.553659000
H	-4.018449000	-3.238710000	-0.840460000
H	-4.069449000	-2.430612000	0.736922000
C	-3.314394000	-1.020653000	-2.360975000
H	-3.245391000	-1.960617000	-2.921717000
H	-4.299755000	-0.584328000	-2.558290000
H	-2.562108000	-0.326533000	-2.749040000
W	0.579175000	-0.683443000	-0.977201000

8B'

E = -1289.5408379

C	1.132865000	2.746848000	-0.476132000
H	0.687389000	2.472754000	-1.440493000
H	0.550438000	3.606190000	-0.126409000
C	2.634596000	3.056188000	-0.592294000
N	-1.137840000	0.192010000	-0.683486000
O	1.449302000	-1.294020000	-1.109020000
Si	2.367045000	-2.575066000	-0.614214000
C	0.739637000	0.017347000	1.510669000
H	0.971602000	2.054221000	0.430629000
C	0.496983000	-0.239816000	2.958667000
O	3.840521000	-2.176441000	0.053392000
H	4.542393000	-2.161615000	-0.605037000
O	2.748934000	-3.477178000	-1.966388000
H	2.031121000	-3.506921000	-2.607070000
O	1.500776000	-3.414868000	0.528111000
H	2.038683000	-4.052945000	1.007298000
C	-2.474433000	0.000477000	-0.391182000
C	-3.321451000	1.122241000	-0.183918000
C	-3.004055000	-1.319179000	-0.355892000
C	-4.677910000	0.900227000	0.056221000
C	-4.366152000	-1.479148000	-0.099456000
C	-5.203637000	-0.386621000	0.104312000
H	-5.336728000	1.748442000	0.217392000
H	-4.783318000	-2.480775000	-0.057542000
H	-6.261488000	-0.538049000	0.300975000
C	2.825468000	4.179058000	-1.620592000
H	3.887297000	4.423101000	-1.731844000
H	2.444442000	3.887591000	-2.606012000
H	2.303537000	5.091989000	-1.313546000
C	3.169661000	3.496710000	0.776805000
H	2.652061000	4.393933000	1.134042000

H	3.039521000	2.706423000	1.524437000
H	4.238146000	3.728739000	0.717901000
C	3.373005000	1.792703000	-1.053182000
H	3.251780000	0.969854000	-0.330321000
H	3.026608000	1.456111000	-2.037950000
H	4.450895000	1.972702000	-1.131165000
C	-0.556512000	-1.357841000	3.087670000
H	-0.739141000	-1.581529000	4.146101000
H	-1.502296000	-1.057252000	2.627821000
H	-0.210438000	-2.269712000	2.593192000
C	-0.026868000	1.044833000	3.628197000
H	-0.204909000	0.872093000	4.696408000
H	0.697560000	1.861880000	3.536986000
H	-0.967366000	1.365248000	3.169910000
C	1.806893000	-0.684536000	3.637457000
H	2.196302000	-1.590879000	3.165793000
H	2.574709000	0.092060000	3.557922000
H	1.637187000	-0.890161000	4.701613000
C	-2.102553000	-2.510825000	-0.629399000
H	-1.134633000	-2.305350000	-0.157622000
C	-2.755508000	2.528280000	-0.278473000
H	-1.743767000	2.486445000	0.144404000
C	-2.626195000	2.957883000	-1.749259000
H	-3.614068000	3.009672000	-2.220442000
H	-2.162637000	3.948622000	-1.833169000
H	-2.022869000	2.242047000	-2.315662000
C	-3.538180000	3.574056000	0.519782000
H	-2.999917000	4.528291000	0.520160000
H	-4.525399000	3.766166000	0.085040000
H	-3.681710000	3.264699000	1.559900000
C	-2.613303000	-3.829196000	-0.043583000
H	-3.513972000	-4.187327000	-0.555815000
H	-1.847074000	-4.602945000	-0.155839000
H	-2.843375000	-3.736234000	1.022707000
C	-1.853314000	-2.654757000	-2.139878000
H	-1.166708000	-3.486124000	-2.339208000
H	-2.791718000	-2.859367000	-2.668225000
H	-1.417736000	-1.741097000	-2.553680000
W	0.600072000	0.229410000	-0.253219000

8B''

E = -1210.9346485

N	1.030754000	0.035694000	-0.705970000
O	-1.938695000	-0.520910000	-1.049246000
Si	-3.230531000	-1.410419000	-0.528654000
C	-0.742520000	0.442794000	1.551248000
C	-0.580756000	0.120506000	2.996553000
O	-2.689938000	-2.458158000	0.641523000
H	-3.407862000	-2.882716000	1.121529000
O	-3.892968000	-2.169779000	-1.860126000
H	-3.227833000	-2.455849000	-2.494393000
O	-4.484919000	-0.523748000	0.114202000
H	-5.140014000	-0.289560000	-0.550841000
C	2.253531000	-0.549442000	-0.439506000
C	2.377602000	-1.965237000	-0.480581000
C	3.387752000	0.266297000	-0.179592000

C	3.634758000	-2.527212000	-0.256538000
C	4.621785000	-0.352005000	0.025384000
C	4.752741000	-1.736347000	-0.008825000
H	3.744688000	-3.607350000	-0.274425000
H	5.497933000	0.258230000	0.223784000
H	5.721793000	-2.197792000	0.160562000
C	0.221949000	-1.189560000	3.120935000
H	0.353825000	-1.452516000	4.177774000
H	-0.304006000	-2.009432000	2.623663000
H	1.209041000	-1.088479000	2.661040000
C	-1.965291000	-0.055092000	3.649193000
H	-1.860799000	-0.317433000	4.709298000
H	-2.551311000	0.866912000	3.578992000
H	-2.525121000	-0.848029000	3.146316000
C	0.181245000	1.265176000	3.691192000
H	1.179434000	1.388546000	3.260182000
H	-0.357784000	2.214188000	3.593497000
H	0.292683000	1.051751000	4.760952000
C	3.251335000	1.779084000	-0.178205000
H	2.273118000	2.004589000	0.267044000
C	1.165842000	-2.827170000	-0.791446000
H	0.302429000	-2.364856000	-0.298012000
C	0.882510000	-2.826089000	-2.302722000
H	1.719980000	-3.270615000	-2.852764000
H	-0.016805000	-3.411652000	-2.528177000
H	0.731165000	-1.807776000	-2.671341000
C	1.268974000	-4.260383000	-0.265093000
H	0.311367000	-4.774026000	-0.398958000
H	2.026256000	-4.843922000	-0.801665000
H	1.516604000	-4.282228000	0.801024000
C	4.306810000	2.502564000	0.661967000
H	5.307521000	2.419775000	0.223358000
H	4.072521000	3.571068000	0.721988000
H	4.351898000	2.106999000	1.681588000
C	3.243789000	2.319735000	-1.617487000
H	3.079338000	3.404385000	-1.632259000
H	4.204336000	2.121007000	-2.105934000
H	2.462283000	1.838693000	-2.213899000
C	-0.517594000	3.090713000	-0.467029000
H	-0.079990000	3.970341000	0.021049000
H	0.163396000	2.859311000	-1.292850000
C	-1.956215000	3.376926000	-0.911474000
H	-0.453577000	2.424656000	0.482804000
C	-2.023352000	4.542753000	-1.896522000
H	-3.056011000	4.741116000	-2.197412000
H	-1.622663000	5.458765000	-1.449195000
H	-1.445306000	4.331867000	-2.802539000
H	-2.406377000	2.488723000	-1.378910000
H	-2.566134000	3.590446000	-0.026829000
W	-0.594934000	0.610291000	-0.217333000

8C

E = -1408.6994646

C	0.646158000	2.117444000	-0.648665000
H	-0.078561000	2.261823000	-1.464228000
H	0.195306000	2.617503000	0.224967000

C	1.950352000	2.866531000	-1.012037000
N	-1.322726000	0.081991000	-0.135180000
O	2.408398000	-0.318080000	-0.266406000
Si	3.829979000	-0.931489000	0.269513000
C	0.694637000	-0.558758000	1.883066000
H	0.734507000	-1.661487000	1.821352000
C	-0.162798000	-0.121354000	3.089972000
O	4.460323000	-0.173039000	1.614003000
H	5.040409000	0.562414000	1.393247000
O	5.011626000	-0.766411000	-0.899850000
H	4.692847000	-0.934408000	-1.791832000
O	3.542851000	-2.512983000	0.705420000
H	4.261951000	-2.894452000	1.219223000
C	-2.697073000	-0.045661000	-0.242653000
C	-3.504302000	1.126406000	-0.300684000
C	-3.314396000	-1.329071000	-0.308050000
C	-4.884396000	0.992687000	-0.448663000
C	-4.701269000	-1.397380000	-0.453938000
C	-5.488844000	-0.255857000	-0.529418000
H	-5.498250000	1.887899000	-0.503101000
H	-5.175524000	-2.373750000	-0.509061000
H	-6.565879000	-0.338938000	-0.645867000
C	1.554375000	4.312512000	-1.374020000
H	2.442700000	4.908072000	-1.616631000
H	0.887341000	4.337142000	-2.243326000
H	1.039691000	4.804341000	-0.540606000
C	2.909232000	2.920690000	0.184117000
H	2.443412000	3.434143000	1.033909000
H	3.193611000	1.919059000	0.512581000
H	3.820904000	3.472363000	-0.074548000
C	2.641980000	2.239688000	-2.229787000
H	2.991970000	1.229935000	-2.004805000
H	1.956612000	2.188711000	-3.084955000
H	3.505934000	2.841267000	-2.535761000
C	-0.377450000	1.398712000	3.080498000
H	-0.890484000	1.726013000	3.992434000
H	0.578981000	1.933036000	3.028000000
H	-0.990256000	1.701587000	2.225475000
C	0.617913000	-0.498159000	4.365096000
H	0.050534000	-0.226608000	5.263621000
H	0.812346000	-1.575979000	4.403395000
H	1.583800000	0.017416000	4.406991000
C	-1.516340000	-0.834547000	3.124599000
H	-2.114796000	-0.606156000	2.240333000
H	-1.379109000	-1.920685000	3.176496000
H	-2.090779000	-0.531271000	4.008024000
C	-2.534950000	-2.630294000	-0.233442000
H	-1.488062000	-2.377938000	-0.037860000
C	-2.901826000	2.517362000	-0.233545000
H	-1.847989000	2.400199000	0.026405000
C	-2.970892000	3.210994000	-1.602213000
H	-4.010347000	3.364056000	-1.913812000
H	-2.484414000	4.192084000	-1.565938000
H	-2.479225000	2.613631000	-2.376751000
C	-3.549149000	3.385657000	0.853918000
H	-3.030582000	4.347774000	0.929133000

H	-4.600951000	3.599555000	0.635014000
H	-3.505000000	2.898189000	1.832574000
C	-3.018697000	-3.530143000	0.913782000
H	-4.038849000	-3.889293000	0.739443000
H	-2.373585000	-4.411420000	1.001234000
H	-3.009766000	-3.003892000	1.871156000
C	-2.605600000	-3.396389000	-1.563460000
H	-1.998591000	-4.307196000	-1.519300000
H	-3.635430000	-3.696473000	-1.787288000
H	-2.250745000	-2.789078000	-2.400732000
C	0.433814000	-1.273014000	-1.848939000
H	-0.563134000	-1.285641000	-2.300279000
H	1.084876000	-0.670530000	-2.510565000
C	0.987764000	-2.693924000	-1.739483000
H	1.955696000	-2.690607000	-1.231130000
H	0.322092000	-3.297692000	-1.109791000
C	1.128056000	-3.372921000	-3.105096000
H	0.166055000	-3.428997000	-3.626199000
H	1.819605000	-2.819329000	-3.751083000
H	1.513008000	-4.393366000	-3.001989000
H	1.729714000	-0.244470000	2.082375000
W	0.452870000	0.038313000	-0.158080000

8D

E = -1211.0031792

N	-1.100310000	-0.003486000	-0.226290000
O	1.947284000	0.736597000	-1.059386000
Si	3.409235000	1.463225000	-0.764685000
C	1.019065000	-0.753938000	1.592620000
H	2.123954000	-0.880374000	1.534710000
C	0.485927000	-0.867380000	3.001803000
O	3.326218000	2.881836000	0.088845000
H	3.178279000	3.653975000	-0.466045000
O	4.114364000	1.841286000	-2.222713000
H	3.947825000	1.193196000	-2.914197000
O	4.261872000	0.374988000	0.156774000
H	5.021996000	0.757187000	0.606272000
C	-2.373034000	0.531112000	-0.277523000
C	-3.474428000	-0.333467000	-0.504230000
C	-2.565654000	1.924968000	-0.087422000
C	-4.752494000	0.223842000	-0.559261000
C	-3.866904000	2.424738000	-0.146265000
C	-4.953825000	1.588998000	-0.384418000
H	-5.607074000	-0.422321000	-0.737833000
H	-4.035857000	3.487812000	-0.002334000
H	-5.958061000	2.001680000	-0.428331000
C	-1.032936000	-0.667040000	3.043621000
H	-1.402419000	-0.770058000	4.070449000
H	-1.311226000	0.325420000	2.677190000
H	-1.543071000	-1.405060000	2.417757000
C	1.169097000	0.199563000	3.879885000
H	0.814651000	0.131108000	4.915493000
H	2.257119000	0.070697000	3.886644000
H	0.951660000	1.206513000	3.509738000
C	0.832804000	-2.267402000	3.545583000
H	0.355171000	-3.048703000	2.945792000

H	1.914517000	-2.442051000	3.531395000
H	0.488403000	-2.373347000	4.581408000
C	-1.382067000	2.848115000	0.137110000
H	-0.591628000	2.249535000	0.608610000
C	-3.251891000	-1.817594000	-0.728923000
H	-2.306511000	-2.071037000	-0.236145000
C	-4.346074000	-2.699744000	-0.119137000
H	-5.305439000	-2.585501000	-0.636016000
H	-4.064092000	-3.755043000	-0.199031000
H	-4.504238000	-2.470034000	0.939253000
C	-3.083742000	-2.112282000	-2.228123000
H	-2.870062000	-3.174051000	-2.395381000
H	-3.997927000	-1.860379000	-2.777741000
H	-2.263205000	-1.528522000	-2.656129000
C	-0.842066000	3.362031000	-1.207260000
H	-1.598453000	3.968460000	-1.718047000
H	0.046393000	3.985621000	-1.056085000
H	-0.568247000	2.536856000	-1.871381000
C	-1.679955000	4.015528000	1.083145000
H	-0.755045000	4.554759000	1.313028000
H	-2.371848000	4.740254000	0.639671000
H	-2.113768000	3.668502000	2.026085000
C	0.742704000	-2.321257000	-1.069264000
H	-0.113320000	-2.933629000	-0.762521000
H	0.618968000	-2.154601000	-2.156150000
C	2.048729000	-3.081733000	-0.806429000
H	2.103742000	-3.328124000	0.260997000
H	2.918113000	-2.441219000	-1.011575000
C	2.172739000	-4.361710000	-1.636655000
H	3.106210000	-4.892392000	-1.418515000
H	1.341872000	-5.045277000	-1.428390000
H	2.157164000	-4.141404000	-2.710255000
W	0.615060000	-0.364310000	-0.209109000

TS(8A-8B')

E = -1289.5338305

C	0.896781000	2.607212000	-0.165235000
H	0.013549000	2.803876000	-0.782551000
H	0.800164000	3.314980000	0.671399000
C	2.214049000	2.928136000	-0.912886000
N	-1.157034000	0.061576000	-0.633690000
O	1.677157000	-1.046793000	-0.988873000
Si	2.789418000	-2.182502000	-0.540835000
C	0.671684000	0.187278000	1.650356000
H	0.865601000	1.718409000	0.882307000
C	0.472093000	0.065374000	3.120905000
O	4.202367000	-1.564842000	0.087523000
H	4.872324000	-1.424325000	-0.589079000
O	3.258219000	-3.013595000	-1.909404000
H	2.532770000	-3.158454000	-2.525321000
O	2.089982000	-3.138889000	0.622697000
H	2.725814000	-3.701419000	1.075863000
C	-2.481072000	-0.272861000	-0.423330000
C	-3.449541000	0.751199000	-0.242995000
C	-2.871990000	-1.639825000	-0.441331000
C	-4.787939000	0.385554000	-0.093449000

C	-4.223521000	-1.945376000	-0.278248000
C	-5.179989000	-0.948896000	-0.108868000
H	-5.539550000	1.157197000	0.043787000
H	-4.537812000	-2.984740000	-0.282994000
H	-6.227079000	-1.211989000	0.013997000
C	2.273812000	4.451410000	-1.116543000
H	3.186937000	4.734299000	-1.651994000
H	1.418405000	4.808792000	-1.700567000
H	2.272555000	4.980076000	-0.156773000
C	3.422100000	2.478411000	-0.077811000
H	3.418898000	2.952261000	0.910441000
H	3.435808000	1.392877000	0.075549000
H	4.357732000	2.755219000	-0.576336000
C	2.245715000	2.246998000	-2.290170000
H	2.274250000	1.152462000	-2.217075000
H	1.372653000	2.526085000	-2.891048000
H	3.141518000	2.548847000	-2.844019000
C	-0.107910000	-1.340053000	3.381793000
H	-0.240218000	-1.492355000	4.459542000
H	-1.079329000	-1.456553000	2.892864000
H	0.562160000	-2.114315000	2.998342000
C	-0.517495000	1.134065000	3.621570000
H	-0.674906000	1.031867000	4.701915000
H	-0.136404000	2.145171000	3.437320000
H	-1.484467000	1.034919000	3.120183000
C	1.818990000	0.212698000	3.854843000
H	2.534710000	-0.536909000	3.505813000
H	2.255986000	1.202088000	3.682277000
H	1.682210000	0.087850000	4.935829000
C	-1.835748000	-2.726965000	-0.668718000
H	-0.923513000	-2.423576000	-0.140739000
C	-3.024861000	2.209160000	-0.263044000
H	-2.051727000	2.258376000	0.242013000
C	-2.822179000	2.691570000	-1.708943000
H	-3.768497000	2.656959000	-2.260263000
H	-2.459546000	3.726723000	-1.731918000
H	-2.104131000	2.057552000	-2.237983000
C	-3.972418000	3.148605000	0.487304000
H	-3.536901000	4.152010000	0.546345000
H	-4.937944000	3.249347000	-0.021002000
H	-4.163009000	2.801274000	1.507785000
C	-2.236114000	-4.096864000	-0.115577000
H	-3.065611000	-4.542360000	-0.676989000
H	-1.389669000	-4.787416000	-0.188609000
H	-2.532617000	-4.038059000	0.936695000
C	-1.487887000	-2.830404000	-2.162815000
H	-0.704970000	-3.580742000	-2.325737000
H	-2.367991000	-3.130856000	-2.742979000
H	-1.133035000	-1.871388000	-2.550275000
W	0.546772000	0.287356000	-0.139390000

TS(8A-8C)

E = -1408.6378443

C	-0.299066000	-1.703237000	-1.357650000
H	0.370602000	-1.363245000	-2.167964000
H	0.341976000	-2.371448000	-0.758782000

C	-1.402660000	-2.575602000	-1.995596000
N	1.299348000	0.108561000	0.001535000
O	-2.304311000	0.323380000	-0.736257000
Si	-3.881239000	0.603849000	-0.409333000
C	-0.968419000	-0.263010000	1.862212000
H	-0.928429000	1.184308000	1.342589000
C	-0.421496000	-0.398373000	3.272312000
O	-4.534184000	-0.428759000	0.730950000
H	-4.857818000	-1.252581000	0.352543000
O	-4.822267000	0.409934000	-1.773204000
H	-4.388454000	0.699795000	-2.581652000
O	-4.014274000	2.131510000	0.249324000
H	-4.889704000	2.302254000	0.611737000
C	2.646591000	0.139487000	-0.310721000
C	3.499853000	-0.894849000	0.166925000
C	3.176071000	1.175933000	-1.133722000
C	4.857121000	-0.844205000	-0.158441000
C	4.539019000	1.170731000	-1.424596000
C	5.382426000	0.176630000	-0.938658000
H	5.514543000	-1.630664000	0.202455000
H	4.952070000	1.958728000	-2.046493000
H	6.442441000	0.194834000	-1.176523000
C	-0.736957000	-3.815275000	-2.625176000
H	-1.478216000	-4.458149000	-3.116730000
H	0.003553000	-3.522449000	-3.378754000
H	-0.221877000	-4.417267000	-1.867448000
C	-2.403156000	-3.059823000	-0.937237000
H	-1.893299000	-3.629742000	-0.150933000
H	-2.909023000	-2.216699000	-0.460619000
H	-3.164253000	-3.713756000	-1.381196000
C	-2.132172000	-1.816464000	-3.112305000
H	-2.621269000	-0.923981000	-2.720339000
H	-1.425224000	-1.506353000	-3.891691000
H	-2.891549000	-2.450159000	-3.586662000
C	-0.402931000	-1.903707000	3.605558000
H	-0.082695000	-2.054620000	4.642964000
H	-1.396813000	-2.349605000	3.491099000
H	0.288028000	-2.442262000	2.950870000
C	-1.380220000	0.316336000	4.245212000
H	-1.025449000	0.209860000	5.276625000
H	-1.445944000	1.386853000	4.022240000
H	-2.390933000	-0.102287000	4.189642000
C	0.984341000	0.187079000	3.427696000
H	1.679211000	-0.248092000	2.708246000
H	0.982175000	1.270207000	3.273766000
H	1.361955000	-0.007274000	4.437621000
C	2.270068000	2.233237000	-1.736315000
H	1.443254000	2.376703000	-1.036494000
C	2.985541000	-2.078232000	0.968374000
H	1.931113000	-1.889890000	1.193000000
C	3.059633000	-3.370483000	0.139188000
H	4.097306000	-3.623015000	-0.106478000
H	2.635905000	-4.211649000	0.699444000
H	2.508820000	-3.273721000	-0.800519000
C	3.735114000	-2.255129000	2.296817000
H	3.278770000	-3.057271000	2.887083000

H	4.783396000	-2.527961000	2.133729000
H	3.720954000	-1.341068000	2.897403000
C	2.943905000	3.595841000	-1.926833000
H	3.704821000	3.573508000	-2.714625000
H	2.199615000	4.340919000	-2.226707000
H	3.420605000	3.943609000	-1.005155000
C	1.674961000	1.737918000	-3.065387000
H	0.978918000	2.476309000	-3.479865000
H	2.467233000	1.569169000	-3.803180000
H	1.135626000	0.794156000	-2.938626000
C	-0.772002000	2.354222000	0.372643000
H	-0.569526000	2.540707000	-0.691225000
H	-1.821691000	2.626729000	0.512303000
C	0.153386000	3.210342000	1.235685000
H	-0.116730000	3.088643000	2.293877000
H	1.188190000	2.857632000	1.149173000
C	0.078011000	4.694592000	0.874923000
H	0.386254000	4.865419000	-0.162509000
H	-0.944198000	5.073454000	0.981609000
H	0.728963000	5.295349000	1.519410000
H	-2.056089000	-0.455216000	1.840783000
W	-0.470091000	0.021962000	0.001688000

TS(8A-8D)

E = -1408.6276461

C	0.102591000	2.317234000	-1.109272000
H	-0.486909000	2.183503000	-2.027299000
H	-0.616530000	2.385044000	-0.286817000
C	0.856401000	3.672804000	-1.175472000
N	-1.181835000	-0.271034000	-0.128481000
O	1.441102000	-1.598344000	-0.281801000
Si	2.247656000	-2.535640000	0.793430000
C	0.958534000	0.719218000	1.583727000
H	2.051409000	0.906525000	1.455765000
C	0.491789000	0.850079000	3.018125000
O	3.617223000	-1.841755000	1.453090000
H	4.408303000	-2.059634000	0.949676000
O	2.815502000	-3.894559000	0.000812000
H	2.208619000	-4.208526000	-0.676633000
O	1.226733000	-2.900801000	2.058237000
H	1.676348000	-3.355186000	2.777796000
C	-2.482192000	-0.701840000	-0.340088000
C	-3.572660000	0.152174000	-0.031147000
C	-2.714518000	-2.005716000	-0.857576000
C	-4.869025000	-0.312443000	-0.264598000
C	-4.030500000	-2.415153000	-1.066642000
C	-5.106233000	-1.580938000	-0.777666000
H	-5.710432000	0.337391000	-0.038383000
H	-4.219923000	-3.408717000	-1.462079000
H	-6.123833000	-1.921225000	-0.948765000
C	1.692333000	3.805564000	-2.458210000
H	2.091079000	4.822616000	-2.544469000
H	2.547264000	3.123283000	-2.469622000
H	1.087087000	3.611066000	-3.351496000
C	-0.206122000	4.787635000	-1.185430000
H	-0.882268000	4.684870000	-2.041579000

H	-0.812914000	4.764890000	-0.273535000
H	0.266361000	5.775137000	-1.249035000
C	1.762917000	3.867477000	0.043717000
H	1.193346000	3.802524000	0.975203000
H	2.551536000	3.108681000	0.082718000
H	2.247044000	4.850377000	0.009068000
C	-0.786717000	0.032771000	3.244605000
H	-1.121081000	0.135673000	4.283831000
H	-1.592840000	0.369453000	2.588871000
H	-0.605304000	-1.024938000	3.035526000
C	0.227110000	2.332156000	3.344989000
H	-0.100067000	2.437028000	4.386427000
H	1.130866000	2.937543000	3.216546000
H	-0.556206000	2.743967000	2.700562000
C	1.597286000	0.318455000	3.950218000
H	1.814796000	-0.729315000	3.727616000
H	2.524967000	0.890582000	3.835863000
H	1.281557000	0.393086000	4.997566000
C	-1.551645000	-2.911461000	-1.217996000
H	-0.703699000	-2.612534000	-0.595486000
C	-3.373813000	1.555395000	0.513161000
H	-2.311249000	1.660230000	0.756562000
C	-3.725983000	2.609783000	-0.547090000
H	-4.784919000	2.549266000	-0.822281000
H	-3.537083000	3.620899000	-0.169350000
H	-3.137774000	2.470830000	-1.459019000
C	-4.167215000	1.801377000	1.804089000
H	-3.928823000	2.788838000	2.214462000
H	-5.247917000	1.775120000	1.627273000
H	-3.935929000	1.051238000	2.565869000
C	-1.821032000	-4.394323000	-0.942774000
H	-2.582763000	-4.811486000	-1.611030000
H	-0.907120000	-4.977445000	-1.101599000
H	-2.147753000	-4.556593000	0.088816000
C	-1.147117000	-2.694745000	-2.685535000
H	-0.268975000	-3.297606000	-2.943922000
H	-1.962856000	-2.977719000	-3.360622000
H	-0.903773000	-1.645345000	-2.881430000
C	2.055172000	0.416879000	-2.028866000
H	1.773513000	-0.588447000	-2.363362000
H	1.128047000	1.374401000	-1.456842000
C	3.510310000	0.447686000	-1.556939000
H	3.631544000	-0.201132000	-0.682312000
H	3.771522000	1.462067000	-1.225432000
C	4.495695000	0.010073000	-2.643260000
H	5.531073000	0.055103000	-2.287212000
H	4.294288000	-1.018606000	-2.961857000
H	4.419276000	0.651104000	-3.528832000
H	1.939820000	1.059762000	-2.912295000
W	0.519571000	0.159613000	-0.165935000

TS(8B''-8D)

E = -1210.9305481

N	-1.040667000	0.067901000	-0.686801000
O	1.963703000	0.631340000	-1.040649000
Si	3.272517000	1.489881000	-0.511315000

C	0.751669000	-0.642394000	1.512665000
C	0.586728000	-0.642856000	2.991877000
O	2.745963000	2.499430000	0.697937000
H	3.468601000	2.903966000	1.188056000
O	3.930753000	2.284794000	-1.822440000
H	3.263868000	2.605354000	-2.438144000
O	4.518816000	0.572978000	0.101589000
H	5.153505000	0.317900000	-0.575381000
C	-2.279452000	0.598695000	-0.380321000
C	-2.424520000	2.005903000	-0.241638000
C	-3.404404000	-0.259616000	-0.252292000
C	-3.693230000	2.517268000	0.033091000
C	-4.650213000	0.309913000	0.013905000
C	-4.801409000	1.685036000	0.160089000
H	-3.820146000	3.589196000	0.151496000
H	-5.519316000	-0.332946000	0.116682000
H	-5.779617000	2.107138000	0.373773000
C	0.385471000	0.826216000	3.418236000
H	0.298437000	0.887081000	4.509486000
H	1.229513000	1.443482000	3.098711000
H	-0.525174000	1.237759000	2.973469000
C	1.850535000	-1.209622000	3.667125000
H	1.746956000	-1.181930000	4.758548000
H	2.021770000	-2.250538000	3.371598000
H	2.734192000	-0.629845000	3.385984000
C	-0.645162000	-1.472403000	3.398856000
H	-1.550944000	-1.076064000	2.931227000
H	-0.533634000	-2.520454000	3.097816000
H	-0.778026000	-1.452366000	4.487096000
C	-3.243121000	-1.756718000	-0.452011000
H	-2.277838000	-2.030551000	-0.007234000
C	-1.223689000	2.917521000	-0.429185000
H	-0.355889000	2.410154000	0.009582000
C	-0.929877000	3.111638000	-1.925885000
H	-1.768413000	3.614544000	-2.421179000
H	-0.034991000	3.729301000	-2.066325000
H	-0.766712000	2.150067000	-2.420446000
C	-1.350258000	4.271879000	0.272471000
H	-0.399634000	4.811032000	0.208102000
H	-2.114076000	4.906990000	-0.191157000
H	-1.601995000	4.157852000	1.331854000
C	-4.316754000	-2.601231000	0.238675000
H	-5.300925000	-2.473634000	-0.225979000
H	-4.064038000	-3.664437000	0.163354000
H	-4.409465000	-2.349349000	1.299982000
C	-3.173345000	-2.093760000	-1.950580000
H	-3.000225000	-3.165836000	-2.106041000
H	-4.114751000	-1.831669000	-2.446307000
H	-2.370544000	-1.535135000	-2.441470000
C	0.563761000	-2.810372000	-0.605426000
H	0.358400000	-3.637046000	0.089375000
H	-0.277959000	-2.823720000	-1.305034000
C	1.916093000	-3.065843000	-1.290013000
H	0.566323000	-2.092371000	0.566986000
C	2.018832000	-4.486332000	-1.850267000
H	2.984296000	-4.645453000	-2.340396000

H	1.920505000	-5.230706000	-1.052765000
H	1.232315000	-4.678386000	-2.587608000
H	2.072031000	-2.347572000	-2.106365000
H	2.728334000	-2.895575000	-0.571895000
W	0.596688000	-0.520077000	-0.274475000

TS(8C-8D)

E = -1408.6360630

C	0.962278000	2.162255000	0.430785000
H	0.632871000	2.455487000	-0.574705000
H	0.196577000	2.553288000	1.110560000
C	2.318908000	2.873122000	0.692443000
N	-1.371956000	0.245048000	-0.059207000
O	2.229104000	-0.160029000	-0.809688000
Si	3.591705000	-1.018034000	-1.100121000
C	0.809185000	-0.595574000	1.713480000
H	1.835865000	-0.995974000	1.685056000
C	0.186306000	-0.735046000	3.092534000
O	4.968581000	-0.093994000	-1.252127000
H	5.139488000	0.165775000	-2.162909000
O	3.512331000	-1.871207000	-2.532239000
H	2.642819000	-2.248268000	-2.701482000
O	3.813307000	-1.975439000	0.250774000
H	4.693819000	-2.361966000	0.292949000
C	-2.722724000	0.427034000	-0.298375000
C	-3.195491000	1.655803000	-0.842939000
C	-3.639063000	-0.622688000	-0.012306000
C	-4.561514000	1.809803000	-1.068387000
C	-4.997185000	-0.409362000	-0.262633000
C	-5.464377000	0.790406000	-0.780158000
H	-4.930568000	2.744831000	-1.477875000
H	-5.702549000	-1.207910000	-0.047538000
H	-6.525990000	0.932733000	-0.962481000
C	1.986639000	4.315529000	1.120604000
H	2.904439000	4.894990000	1.274695000
H	1.392931000	4.829118000	0.355499000
H	1.417322000	4.335123000	2.057395000
C	3.129937000	2.201645000	1.806333000
H	2.571524000	2.180509000	2.749475000
H	3.399518000	1.175743000	1.538073000
H	4.059508000	2.751730000	1.990478000
C	3.165124000	2.935678000	-0.586749000
H	3.465366000	1.940923000	-0.915949000
H	2.609930000	3.421058000	-1.398813000
H	4.073373000	3.523404000	-0.409719000
C	-1.065625000	0.129236000	3.267975000
H	-1.504801000	-0.038769000	4.257665000
H	-0.821798000	1.194384000	3.188651000
H	-1.818493000	-0.095060000	2.510295000
C	1.222757000	-0.347017000	4.164831000
H	0.809434000	-0.511589000	5.166400000
H	2.135808000	-0.945100000	4.073426000
H	1.500988000	0.708537000	4.089029000
C	-0.164325000	-2.226167000	3.271364000
H	-0.914288000	-2.544664000	2.543056000
H	0.721128000	-2.858550000	3.145954000

H	-0.564002000	-2.399413000	4.277295000
C	-3.200937000	-1.973685000	0.525548000
H	-2.121093000	-1.923750000	0.694804000
C	-2.219470000	2.754782000	-1.217530000
H	-1.408390000	2.716287000	-0.485393000
C	-1.614243000	2.480194000	-2.604628000
H	-2.390740000	2.519949000	-3.376683000
H	-0.851656000	3.226599000	-2.855404000
H	-1.153336000	1.488106000	-2.653400000
C	-2.809255000	4.166709000	-1.160059000
H	-2.014821000	4.907385000	-1.299087000
H	-3.547488000	4.339577000	-1.950989000
H	-3.291029000	4.364247000	-0.197252000
C	-3.881057000	-2.308478000	1.861116000
H	-4.964811000	-2.416202000	1.742960000
H	-3.500574000	-3.256414000	2.257599000
H	-3.705641000	-1.532027000	2.611187000
C	-3.459680000	-3.088742000	-0.499262000
H	-3.087682000	-4.048852000	-0.124807000
H	-4.530738000	-3.203584000	-0.700343000
H	-2.963547000	-2.878767000	-1.450962000
C	0.040474000	-1.630580000	-1.647985000
H	-1.008168000	-1.631187000	-1.971566000
H	0.627417000	-1.314602000	-2.527092000
C	0.430627000	-3.066198000	-1.257674000
H	1.459966000	-3.104781000	-0.875515000
H	-0.195960000	-3.394709000	-0.418668000
C	0.282853000	-4.072375000	-2.403206000
H	-0.747839000	-4.096320000	-2.773627000
H	0.921910000	-3.811621000	-3.256866000
H	0.551944000	-5.087105000	-2.088696000
H	1.059095000	0.883554000	1.285854000
W	0.369396000	-0.091370000	-0.114985000