Supplementary Information

Simple s-block metal hydrides for selective hydrogenation of quinoline compounds

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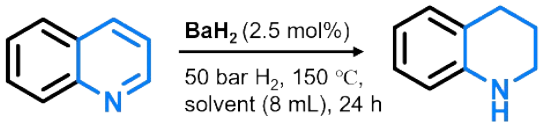
Table S1. Screening of solvents.



Entry [a]	Solvent	Yield (%) [b]
1	Tetrahydrofuran (THF)	>99
2[c]	1,4-dioxane	11
3	2-Methyltetrahydrofuran	0
4	Benzene	18
5	Toluene	12
6	Cyclohexane	3
7	Methylcyclohexane	<1
8	n-hexane	1
9	THF: Toluene=1:1	>99
10	THF: n-hexane=1:1	>99

[a] Reaction conditions: quinoline (4 mmol), BaH_2 (2.5 mol%), solvent (8 mL), 150 °C, 50 bar H_2, 24 h. [b] Yield of 1,2,3,4-tetrahydroquinoline were calculated by GC using dodecane as the internal standard.

Table S2. Screening of reaction pressure, temperature, and BaH_2 concentration.

Entry[a]	BaH_2 concentration (mol%)	P_{H2} (bar)	T (°C)	t (h)	Yield (%)[c]
1	20	30	100	48	99
2	20	50	100	12	>99
3	20	30	150	16	99
4	20	50	150	9	99
5	2.5	50	150	24	>99
6	2.5	40	150	24	92
7	2.5	30	150	24	77
8	2.5	50	100	24	57
9[b]	2.5	--	150	24	<1

[a] Reaction conditions: quinoline (4 mmol), THF (8 mL). [b] quinoline (0.0525 mmol), THF (3 mL), 50 bar Ar. [c]Yield of 1,2,3,4-tetrahydroquinoline was calculated by GC using dodecane as the internal standard.

Table S3. Selective hydrogenation of quinoline over recently developed transition metal based catalysts.

Catalyst	Solvent	P_{H2} (bar)	T (℃)	t (h)	Yield (%)	TON	Ref
BaH_2	THF	50	150	24	>99	40	This work
Fe-N-C	$^{i}PrOH/H_2O$	40	130	56	87	7	[1]
Ni-phen@SiO_2-1000	H_2O/MeOH	50	120	20	87	19	[2]
Co@NGS	isopropanol	40	140	24	84	8	[3]
Co_3O_4-Co/NGr@Al_2O_3	Toluene	20	120	48	98	25	[4]
Co-Mo-S-0.83	Toluene	12	150	10	98	---	[5]
Co-^{iPr}[PN(H)P]	THF	10	120	48	99	20	[6]
Fe-PNP ($KO^{t}Bu$)	THF	50	80	24	77	26	[7]
$Mn(CO)_5Br$	THF	15	45	18	>99	50	[8]
CoW@C-0.05	Toluene	8	100	6	99	---	[9]
$2Ir_n$/SC	EtOH	20	100	3	99	---	[10]
$Au_{0.9}Pd_{0.1}$/CNR	Toluene	20	100	10	92.6	---	[11]
Ru/HT-C12A7	---	10	80	12	98.3	---	[12]
Ru SAs/N-C	THF	35	100	4	>99	100	[13]
Rh NP/Lewic acidic IL	---	30	80	15-48	95	95	[14]
Pt_{AD}/C-Al_2O_3	Toluene	20	120	2.5	98.9	---	[15]
5wt% Ru/MgO	THF	50	150	0.7	92	3680	[16]
0.5wt% Au/HSA-TiO2	Toluene	20	140	48	100	5000	[17]

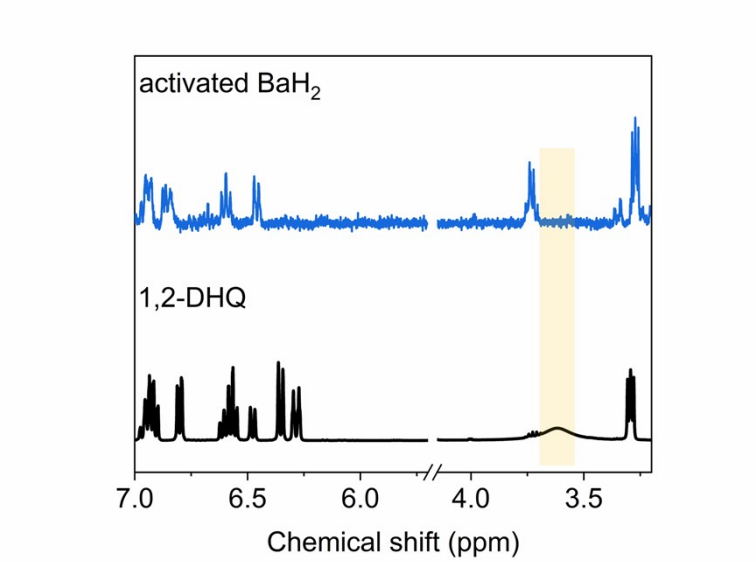


Figure S1. ^{1}H NMR spectra of the quinoline-activated BaH_2 sample (blue line, in $CDCl_3$) and the reference 1,2-dihydroquinoline (1,2-DHQ) sample (black line, in $CDCl_3$). The broad resonance at 3.62 ppm is ascribed to an N-H proton, and the multiplet at 3.72 ppm arises from THF.

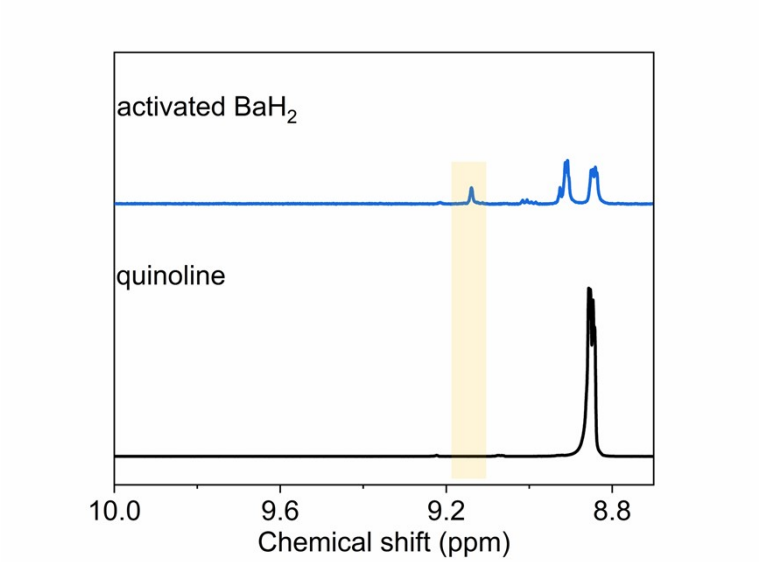


Figure S2. ^{1}H NMR spectra of the quinoline-activated BaH_2 sample and the reference quinoline sample. The signal at 9.14 ppm is characteristic of a hydride ligand coordinated to the Ba center.

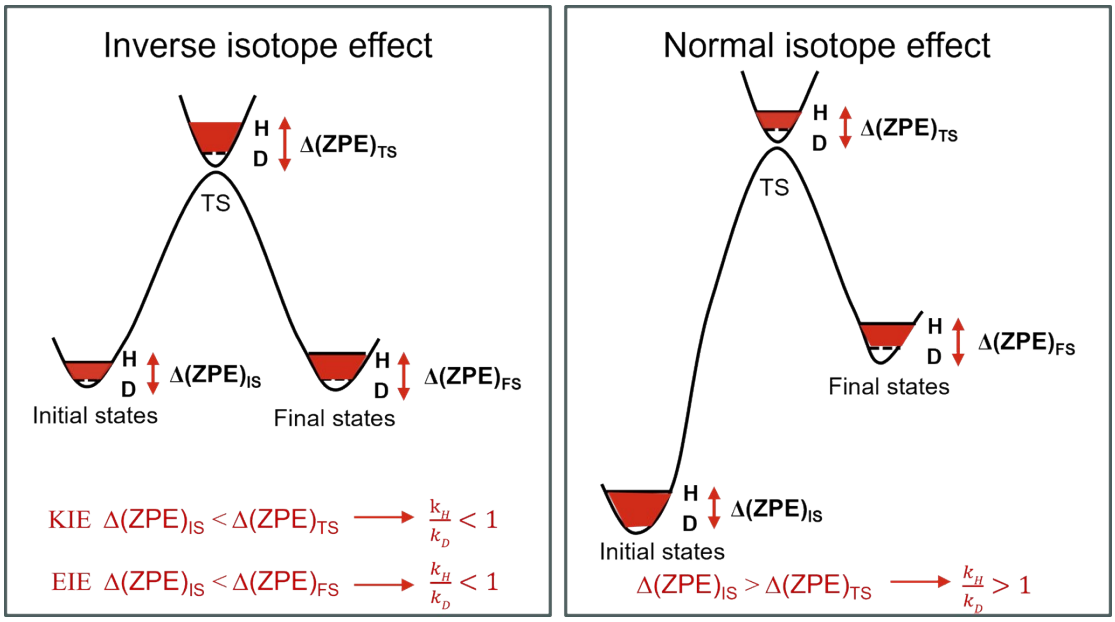


Figure S3. The schematic diagram of inverse and normal isotopic effect. Adapted with permission from refs[18]. Copyright 2020 Springer Nature, 2011 American Chemical Society and 2019 American Chemical Society.

Based on the Arrhenius equation, the isotopic effect (k_H/k_D) is calculated by using the equation[16a]:

$$\frac{kH}{kD} = \exp\left[\frac{\Delta\Delta ZPE}{RT}\right] = \exp\left[\frac{\Delta(ZPE)_{TS} - \Delta(ZPE)_{IS}}{RT}\right]$$

(R is the universal gas constant, 8.314 J mol^{-1} K^{-1}; T=423 K, and Δ(ZPE) is the zero-point vibrational energy between deuterium- and hydrogen-substituted moieties.)

As for the inverse isotopic effect, the inverse kinetic isotopic effect (iKIE) is expected when $\Delta(ZPE)_{TS}$ is bigger than $\Delta(ZPE)_{IS}$. In addition, the inverse equilibrium isotope effect (iEIE) is also present when $\Delta(ZPE)_{FS}$ is bigger than $\Delta(ZPE)_{IS}$.

Table S4. The differences in zero-point vibrational energy (ZPE) between deuterium- and hydrogen-substituted moieties for the simulated intermediates and transition states shown in Fig. 3b.

	Intermediate/Transition state	ZPE (kJ/mol)
TS_{1-2}	1	1677.43
	TS_{1-2}	1673.88
	2	1688.30
	1 (D)	1674.44
	TS_{1-2} (D)	1671.05
	2 (D)	1679.86
	ΔΔZPE	0.16
TS_{2-3}	2	1688.30
	H_2	26.03
	TS_{2-3}	1726.80
	3	1739.45
	2 (D)	1679.86
	D_2	18.42
	TS_{2-3} (D)	1708.98
	3 (D)	1718.90
	ΔΔZPE	-1.77

Here, both the kinetic and equilibrium isotopic effects were considered. In the simulated reaction pathway, the dissociation of H_2 (**2**→**TS_{2-3}**→**3**) was predicted to be the rate-determining step. As shown in Table S4, the ΔZPE of **TS_{2-3}** and **3** were calculated to be larger than that in **2**, resulting in both an inverse kinetic isotope effect (iKIE, k_H/k_D=0.61) and inverse equilibrium isotopic effect (iEIE, k_H/K_D=0.28). By contrast, a normal isotope effect was predicted for the hydride transfer step such as **1**→**TS_{1-2}**→**2**, where the Δ(ZPE) of **TS_{1-2}** was smaller than that of **1** (k_H/k_D=1.05). These computational results are consistent our experimental findings (Figure 4): an inverse isotope effect (k_{H2}/k_{D2}≈0.68) was identified when H_2 was replaced by D_2 in the reactant stream; a normal isotope effect (k_{Ba-H}/k_{Ba-D}≈1.03) was observed when BaD_2 instead of BaH_2 was used as the catalyst precursor.

Table S5. EDA-NOCV results for intermediates **1** and **4**

Energy term	Energy value (kcal/mol)		Description
	1	**4**	
ΔE_{int}	-21.7	-31.1	Total interaction energy
ΔE_{Pauli}	46.5	67.6	Pauli repulsion
ΔE_{disp}	-10.4	-17.8	Dispersion interaction
ΔE_{elstat}	-23.9	-32.7	Electrostatic interaction
ΔE_{orb}	-12.7	-18.6	Total orbital interaction
$\Delta E_{orb(1)}$	-5.3 (41.7%)	-9.0 (48.4%)	σ-Donation from ligand lone pair (N:sp² or C=C π) → Ba 6s/5d hybrid orbital
$\Delta E_{orb(2)}$	-3.5 (27.6%)	-3.8 (20.4%)	π-Backdonation from Ba 5d → ligand π* (C=N or C=C) orbital
$\Delta E_{orb(rest)}$	-3.9 (30.7%)	-5.8 (31.2%)	Sum of minor orbital polarization and higher-order interactions

Note: EDA–NOCV analysis reveals that the orbital term is dominated by two major components: σ-donation from the ligand to Ba ($\Delta E_{orb(1)}$) and a smaller π-backdonation from Ba to the ligand ($\Delta E_{orb(2)}$), while other minor polarization effects are collectively included in $\Delta E_{orb(rest)}$.

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The atomic coordinates of the states in Figure 3b.

Structure **0**

Charge = 0 Multiplicity = 1

Free Energy: -1357.239028 hartree

Ba	-5.922146000	-0.248902000	2.151334000
C	-8.334816000	-3.907213000	0.075581000
C	-8.248963000	-2.581444000	0.491450000
C	-7.843145000	-1.532105000	-0.398138000
C	-7.504291000	-1.939890000	-1.747926000
C	-7.601562000	-3.282563000	-2.132102000
C	-8.018546000	-4.280021000	-1.242540000
H	-8.664824000	-4.668997000	0.789235000
H	-8.525013000	-2.308795000	1.515205000
C	-6.902356000	-0.923361000	-2.598373000
H	-7.317537000	-3.550678000	-3.155841000
H	-8.097528000	-5.320815000	-1.564639000
C	-6.862308000	0.365600000	-2.205938000
H	-6.440942000	-1.240843000	-3.539904000
H	-6.372846000	1.128397000	-2.821684000
N	-7.699408000	-0.271427000	0.052843000
C	-7.563838000	0.789070000	-0.938143000
H	-7.030574000	1.641083000	-0.480970000
H	-8.566172000	1.212386000	-1.210651000
C	-4.276456000	2.587404000	0.120593000
O	-4.093123000	1.614596000	1.167927000
C	-2.967806000	1.967767000	1.994553000
C	-2.664662000	3.422862000	1.658366000
C	-3.039665000	3.481196000	0.173203000
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O	-6.982674000	2.400313000	2.037238000
C	-8.389760000	2.626046000	1.913090000
C	-8.851606000	2.969655000	3.331860000
C	-7.598768000	3.614417000	3.977352000
H	-5.544519000	3.048023000	3.354532000
H	-6.298304000	4.333581000	2.357131000
H	-8.565396000	3.467857000	1.216480000
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H	-9.725227000	3.637479000	3.327017000
H	-9.132248000	2.050950000	3.869001000
H	-7.741441000	4.683459000	4.192465000
H	-7.338408000	3.109103000	4.917907000
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C	-3.936829000	-4.817440000	3.096093000
C	-5.398639000	-5.191438000	2.767553000
H	-6.356482000	-4.047771000	4.367553000
H	-7.132028000	-3.813336000	2.765216000
H	-3.305362000	-2.731752000	2.621272000
H	-3.737120000	-3.007723000	4.335525000
H	-3.250194000	-5.109150000	2.288669000
H	-3.596312000	-5.312673000	4.017176000
H	-5.545393000	-5.289893000	1.681131000
H	-5.720102000	-6.128927000	3.243751000

Structure **1**

Charge = 0 Multiplicity = 1

Free Energy: -1526.617792 hartree

C	0.168247000	-1.253909000	2.686258000
C	0.430080000	-0.359310000	1.672302000
C	-0.101552000	0.956120000	1.744481000
C	-0.895058000	1.291755000	2.890054000
C	-0.609034000	-0.823009000	3.790573000
H	0.728516000	1.676843000	-0.128027000
H	0.553706000	-2.274737000	2.662619000
H	1.037926000	-0.644362000	0.809471000
C	0.118088000	1.938392000	0.740091000

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C	-0.436369000	3.195233000	0.861700000
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C	-2.558194000	2.721412000	9.896273000
C	-1.283554000	3.310122000	9.597259000
C	-1.158218000	4.724462000	9.893310000
C	-2.231195000	5.438557000	10.438295000
C	-3.461823000	4.830735000	10.720976000
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H	2.606129000	-2.235377000	8.389982000
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O	-3.197224000	3.271219000	6.051722000
C	-4.467997000	2.671333000	5.751027000
C	-5.385660000	3.145349000	6.867910000
C	-4.913349000	4.592836000	7.058756000
H	-2.803181000	4.486679000	7.678551000
H	-3.059268000	5.350810000	6.135556000
H	-4.820846000	3.014485000	4.760598000
H	-4.333880000	1.578600000	5.707201000
H	-6.450738000	3.063259000	6.606937000
H	-5.202228000	2.554563000	7.779535000
H	-5.416398000	5.253875000	6.335569000
H	-5.107168000	4.977601000	8.069270000
C	-0.113357000	4.545869000	5.620001000
O	0.225683000	3.147498000	5.545419000
C	1.507234000	2.974268000	4.915798000
C	1.833151000	4.320419000	4.278209000
C	1.161460000	5.296111000	5.250090000

H	-0.926708000	4.752038000	4.904805000
H	-0.465609000	4.765715000	6.636972000
H	2.247668000	2.697835000	5.685005000
H	1.435070000	2.151645000	4.190263000
H	2.916000000	4.480955000	4.172470000
H	1.372373000	4.392283000	3.280402000
H	1.787778000	5.440938000	6.144673000
H	0.952839000	6.282799000	4.811657000
H	-0.808427000	-1.508895000	4.622345000

Structure **2**

Charge = 0 Multiplicity = 1

Free Energy: -1526.630131 hartree

C	-1.953885000	-1.881556000	4.891514000
C	-1.063378000	-1.978610000	3.882954000
C	-0.823950000	-0.851539000	2.992907000
C	-1.388087000	0.419257000	3.401991000
C	-2.806954000	-0.641172000	5.015952000
H	0.455000000	-1.903415000	1.624297000
H	-2.110042000	-2.710180000	5.590924000
H	-0.469766000	-2.888203000	3.740017000
C	0.038748000	-0.926050000	1.892150000
C	-0.969367000	1.566168000	2.649955000
C	-0.113938000	1.454653000	1.556882000
C	0.395563000	0.208216000	1.153975000
H	-1.372272000	2.544302000	2.931429000
H	0.156304000	2.357148000	0.999204000
H	1.059892000	0.127417000	0.290657000
N	-2.179930000	0.561685000	4.484484000
Ba	-0.730044000	2.079128000	6.245217000

C	-4.325842000	2.310996000	10.052430000
C	-3.122222000	1.951679000	9.454095000
C	-1.948465000	2.762775000	9.568712000
C	-2.102910000	4.005837000	10.295642000
C	-3.330492000	4.340663000	10.882336000
C	-4.447689000	3.504404000	10.786498000
H	-5.190118000	1.646966000	9.950066000
H	-3.045808000	1.012336000	8.896577000
C	-0.978868000	4.928878000	10.246176000
H	-3.408145000	5.295820000	11.413530000
H	-5.394098000	3.777135000	11.258846000
C	0.207414000	4.547992000	9.730260000
H	-1.134918000	5.954629000	10.598155000
H	1.044292000	5.250884000	9.658730000
N	-0.805662000	2.409374000	8.946544000
C	0.418147000	3.113646000	9.308637000
H	1.117497000	3.077155000	8.444711000
H	0.972948000	2.575123000	10.119465000
C	2.482557000	0.440105000	6.729852000
O	1.892859000	1.215942000	5.664076000
C	2.281350000	0.674651000	4.385579000
C	2.636283000	-0.775322000	4.676665000
C	3.307873000	-0.656600000	6.050263000
H	3.086148000	1.103289000	7.369832000
H	1.668164000	0.017604000	7.345410000
H	1.443805000	0.802671000	3.688399000
H	3.152689000	1.235106000	4.000514000
H	1.716310000	-1.378190000	4.741018000
H	3.285253000	-1.215895000	3.906365000

H	3.303996000	-1.594403000	6.624141000
H	4.354176000	-0.331608000	5.934866000
C	-2.913925000	5.013698000	6.805414000
O	-2.590733000	4.146284000	5.697620000
C	-3.811726000	3.709080000	5.077365000
C	-4.791925000	3.599844000	6.236154000
C	-4.414690000	4.818773000	7.093477000
H	-2.279389000	4.724547000	7.655638000
H	-2.675328000	6.056059000	6.536792000
H	-4.143195000	4.457585000	4.332792000
H	-3.601252000	2.755915000	4.569599000
H	-5.842462000	3.606233000	5.910753000
H	-4.608131000	2.665279000	6.790822000
H	-4.984005000	5.703812000	6.769984000
H	-4.608417000	4.659422000	8.162834000
C	0.503427000	5.600478000	6.033656000
O	0.759225000	4.289922000	5.494120000
C	1.996648000	4.285868000	4.748555000
C	2.451651000	5.743184000	4.698119000
C	1.847882000	6.313959000	5.986346000
H	-0.248960000	6.111958000	5.408187000
H	0.096732000	5.488858000	7.049745000
H	2.718044000	3.643842000	5.277906000
H	1.810225000	3.849358000	3.754737000
H	3.546178000	5.835385000	4.646689000
H	2.022512000	6.252405000	3.820084000
H	2.459980000	6.031042000	6.858907000
H	1.744435000	7.408595000	5.976762000
H	-3.793022000	-0.832445000	4.518841000

H	-3.073448000	-0.472312000	6.078254000

Structure **3**

Charge = 0 Multiplicity = 1

Free Energy: -1527.786175 hartree

C	-1.789474000	-0.275074000	3.835407000
C	-0.902207000	0.046774000	2.876730000
C	-0.732121000	-0.787684000	1.687907000
C	-1.677701000	-1.831037000	1.474511000
C	-2.599757000	-1.539215000	3.747697000
H	0.997353000	0.231973000	0.913672000
H	-1.896605000	0.339162000	4.733579000
H	-0.283790000	0.944575000	2.966681000
C	0.280589000	-0.576285000	0.741923000
C	-1.575784000	-2.624589000	0.317331000
H	-3.609391000	-1.384523000	4.159093000
C	-0.553170000	-2.396381000	-0.605955000
C	0.382126000	-1.374558000	-0.401843000
H	-2.304665000	-3.421798000	0.153679000
H	-0.486924000	-3.028775000	-1.494942000
H	1.179646000	-1.200896000	-1.127499000
N	-2.728729000	-1.970215000	2.362229000
Ba	-5.160623000	-0.952364000	0.578340000
C	-10.013283000	-0.525373000	0.675023000
C	-8.711743000	-0.096940000	0.432207000
C	-8.182826000	-0.004948000	-0.897108000
C	-9.063097000	-0.430281000	-1.967377000
C	-10.367770000	-0.858121000	-1.685684000
C	-10.865601000	-0.901231000	-0.378942000
H	-10.379945000	-0.554993000	1.706343000

H	-8.075159000	0.221898000	1.263635000
C	-8.461068000	-0.543056000	-3.288309000
H	-11.000386000	-1.182092000	-2.519720000
H	-11.889878000	-1.225689000	-0.181065000
C	-7.238054000	-0.025994000	-3.528584000
H	-9.001062000	-1.101381000	-4.061155000
H	-6.751569000	-0.148573000	-4.502512000
N	-6.906127000	0.379816000	-1.103862000
C	-6.562007000	0.795985000	-2.456835000
H	-5.466694000	0.753005000	-2.575873000
H	-6.821233000	1.875847000	-2.619055000
H	-4.928913000	-3.711671000	1.852067000
C	-5.032008000	2.758026000	0.283794000
O	-4.175956000	1.670476000	0.659127000
C	-2.869823000	2.226237000	0.842175000
C	-2.747150000	3.368154000	-0.188663000
C	-4.192815000	3.560815000	-0.707628000
H	-5.951920000	2.318992000	-0.126418000
H	-5.274234000	3.360402000	1.180297000
H	-2.780123000	2.609236000	1.874190000
H	-2.136337000	1.420788000	0.709815000
H	-2.358035000	4.279332000	0.288373000
H	-2.060017000	3.102227000	-1.004479000
H	-4.497385000	4.616430000	-0.748401000
H	-4.305333000	3.137275000	-1.717217000
C	-6.789948000	-0.464328000	3.894104000
O	-5.942795000	0.266986000	2.986974000
C	-5.269578000	1.338184000	3.681141000
C	-5.800880000	1.306677000	5.115912000

C	-6.244611000	-0.151741000	5.281022000
H	-7.833257000	-0.117701000	3.782926000
H	-6.745212000	-1.531237000	3.625877000
H	-4.184425000	1.152461000	3.634126000
H	-5.480230000	2.287148000	3.167309000
H	-5.040799000	1.618150000	5.847107000
H	-6.667409000	1.979541000	5.217891000
H	-5.381845000	-0.799461000	5.506056000
H	-6.996506000	-0.293397000	6.070623000
C	-3.861640000	-1.677466000	-2.813412000
O	-3.614378000	-0.773237000	-1.720418000
C	-2.594854000	0.181999000	-2.073882000
C	-2.026390000	-0.296818000	-3.406744000
C	-3.226518000	-1.017594000	-4.031521000
H	-3.391525000	-2.651615000	-2.589560000
H	-4.949135000	-1.822537000	-2.907710000
H	-3.063443000	1.174948000	-2.165487000
H	-1.845905000	0.212930000	-1.270364000
H	-1.646818000	0.533841000	-4.019114000
H	-1.200119000	-1.004688000	-3.236447000
H	-3.923696000	-0.290238000	-4.478041000
H	-2.946736000	-1.747442000	-4.804806000
H	-2.129394000	-2.324392000	4.382967000
H	-3.352271000	-2.781172000	2.221119000

Structure **4**

Charge = 0 Multiplicity = 1

Free Energy: -1527.787394 hartree

C	-3.262996000	2.219564000	2.355500000
C	-5.192599000	0.977716000	3.254955000

C	-4.351417000	-0.085848000	3.687108000
C	-2.452073000	0.968811000	2.560581000
H	-7.175147000	1.831609000	3.357259000
H	-3.008464000	2.691497000	1.394592000
C	-6.529553000	1.012830000	3.685512000
C	-4.879338000	-1.087107000	4.513654000
C	-6.210764000	-1.047126000	4.937813000
C	-7.027938000	0.010786000	4.521552000
H	-4.225631000	-1.906373000	4.825484000
H	-6.606780000	-1.831012000	5.586882000
H	-8.069464000	0.058953000	4.849614000
Ba	-3.610766000	-1.456631000	-0.091554000
C	-6.730537000	-0.913666000	-4.226935000
C	-6.053379000	-0.720209000	-3.027153000
C	-5.245458000	0.440940000	-2.791539000
C	-5.146906000	1.378810000	-3.891744000
C	-5.835724000	1.147955000	-5.089973000
C	-6.640713000	0.018994000	-5.275995000
H	-7.350828000	-1.807747000	-4.349044000
H	-6.154163000	-1.452716000	-2.221440000
C	-4.186993000	2.461761000	-3.734921000
H	-5.720400000	1.874470000	-5.902331000
H	-7.181093000	-0.136307000	-6.212666000
C	-3.609113000	2.698748000	-2.540694000
H	-3.916197000	3.048864000	-4.619662000
H	-2.855100000	3.484560000	-2.421930000
N	-4.572108000	0.589424000	-1.635336000
C	-4.047104000	1.912209000	-1.329350000
H	-3.197846000	1.811528000	-0.627975000

H	-4.798714000	2.518388000	-0.756878000
C	-0.778316000	0.589721000	-1.628468000
O	-1.199438000	-0.049883000	-0.419064000
C	-0.011477000	-0.523355000	0.221510000
C	0.859647000	-1.064396000	-0.917017000
C	0.404754000	-0.242955000	-2.149828000
H	-1.639787000	0.630210000	-2.306601000
H	-0.466399000	1.624631000	-1.397414000
H	0.485210000	0.315647000	0.744313000
H	-0.299679000	-1.281021000	0.964408000
H	1.930510000	-0.950727000	-0.696351000
H	0.660962000	-2.135144000	-1.068378000
H	1.201751000	0.407771000	-2.537214000
H	0.089092000	-0.906646000	-2.966227000
C	-7.214831000	-0.288804000	0.329081000
O	-6.398820000	-1.477479000	0.414590000
C	-7.133538000	-2.554427000	1.025580000
C	-8.378296000	-1.911050000	1.628258000
C	-8.630580000	-0.744304000	0.666944000
H	-6.838206000	0.447803000	1.056256000
H	-7.109564000	0.132342000	-0.678712000
H	-7.395609000	-3.296116000	0.249251000
H	-6.488389000	-3.043644000	1.772488000
H	-9.220721000	-2.614594000	1.697387000
H	-8.155055000	-1.533064000	2.637020000
H	-9.145744000	-1.096537000	-0.241684000
H	-9.230887000	0.063433000	1.110985000
C	-1.754900000	-3.460662000	-2.674483000
O	-2.489047000	-2.223046000	-2.585018000

C	-2.673972000	-1.651753000	-3.898618000
C	-2.279114000	-2.752172000	-4.876761000
C	-1.196607000	-3.503032000	-4.093299000
H	-0.981188000	-3.470912000	-1.891804000
H	-2.444303000	-4.303508000	-2.487144000
H	-3.717373000	-1.326098000	-3.995607000
H	-2.023161000	-0.766729000	-3.999462000
H	-3.137805000	-3.414432000	-5.075220000
H	-1.927660000	-2.349840000	-5.837940000
H	-1.027676000	-4.530836000	-4.445632000
H	-0.239139000	-2.959187000	-4.144517000
H	-2.458505000	-3.652281000	1.565791000
H	-3.001419000	2.962121000	3.144539000
H	-1.413935000	0.973020000	2.223309000
N	-4.685362000	1.899311000	2.355444000
H	-5.297515000	2.683113000	2.151543000
C	-2.969625000	-0.092012000	3.208870000
H	-2.365588000	-0.985439000	3.392742000

Structure **5**

Charge = 0 Multiplicity = 1

Free Energy: -1527.795414 hartree

C	-2.109877000	2.024361000	3.347871000
C	-4.345511000	1.067811000	3.268685000
C	-3.769675000	-0.240757000	3.528005000
C	-1.429683000	0.678340000	3.083889000
H	-6.072469000	2.332730000	3.199087000
H	-1.530578000	2.853546000	2.913992000
C	-5.705545000	1.321929000	3.412378000
C	-4.723835000	-1.244339000	3.921389000

C	-6.085453000	-0.974008000	4.046489000
C	-6.605838000	0.308156000	3.800859000
H	-4.354015000	-2.255294000	4.123868000
H	-6.760066000	-1.782349000	4.348000000
H	-7.671169000	0.520837000	3.910868000
Ba	-3.795182000	0.063547000	0.409508000
C	-4.288568000	0.074253000	-4.510574000
C	-4.472515000	0.463364000	-3.188022000
C	-4.013830000	1.731197000	-2.700614000
C	-3.317521000	2.567407000	-3.656645000
C	-3.154635000	2.146515000	-4.983525000
C	-3.636217000	0.912273000	-5.433389000
H	-4.669530000	-0.899379000	-4.836245000
H	-5.003205000	-0.194671000	-2.494297000
C	-2.670422000	3.757206000	-3.123064000
H	-2.610427000	2.801777000	-5.672806000
H	-3.503854000	0.604922000	-6.473316000
C	-2.908906000	4.161906000	-1.859190000
H	-1.947187000	4.282765000	-3.756498000
H	-2.391386000	5.029396000	-1.435199000
N	-4.158452000	2.059962000	-1.400656000
C	-3.958643000	3.455771000	-1.033979000
H	-3.695598000	3.513367000	0.040304000
H	-4.918574000	4.031365000	-1.110355000
C	-0.759425000	0.678295000	-1.667038000
O	-1.367498000	-0.365832000	-0.891502000
C	-0.818795000	-1.594681000	-1.374323000
C	-0.779697000	-1.424823000	-2.893769000
C	-0.590973000	0.100855000	-3.083942000

H	-1.415642000	1.557398000	-1.617580000
H	0.216533000	0.935811000	-1.216917000
H	0.196267000	-1.732956000	-0.956074000
H	-1.462341000	-2.411432000	-1.024558000
H	0.023871000	-2.019899000	-3.351224000
H	-1.735316000	-1.747972000	-3.332762000
H	0.400084000	0.350099000	-3.489975000
H	-1.348163000	0.507017000	-3.766402000
C	-7.377387000	0.365946000	-0.472175000
O	-6.400621000	-0.668085000	-0.224502000
C	-7.034286000	-1.840276000	0.325468000
C	-8.443598000	-1.399253000	0.705381000
C	-8.733073000	-0.320855000	-0.344445000
H	-7.254183000	1.161598000	0.283788000
H	-7.185338000	0.796483000	-1.465443000
H	-7.047108000	-2.632990000	-0.442492000
H	-6.444828000	-2.194298000	1.184420000
H	-9.161580000	-2.232178000	0.691757000
H	-8.438003000	-0.958492000	1.714635000
H	-9.019680000	-0.783043000	-1.303295000
H	-9.528707000	0.377758000	-0.047873000
C	-3.667903000	-3.643402000	0.427619000
O	-3.907125000	-2.572834000	-0.506394000
C	-4.375095000	-3.094891000	-1.767013000
C	-4.599191000	-4.588519000	-1.535258000
C	-3.589508000	-4.902944000	-0.425046000
H	-2.745173000	-3.419859000	0.985202000
H	-4.503762000	-3.692194000	1.148664000
H	-5.287987000	-2.554302000	-2.056981000

H	-3.601600000	-2.907137000	-2.530371000
H	-5.625514000	-4.772653000	-1.178805000
H	-4.443479000	-5.179351000	-2.449279000
H	-3.830899000	-5.811540000	0.145147000
H	-2.577039000	-5.016871000	-0.845646000
H	-2.179441000	2.200420000	4.439869000
H	-0.554291000	0.596756000	3.758792000
N	-3.444170000	2.025686000	2.732527000
H	-3.852721000	2.957820000	2.703600000
C	-2.402944000	-0.463863000	3.288690000
H	-1.994577000	-1.456302000	3.511218000
H	-0.993308000	0.702818000	2.060540000

Structure H_2

Charge = 0 Multiplicity = 1

Free Energy: -1.181666 hartree

H	-1.023917000	-0.099432000	0.000000000
H	-1.785174000	-0.099432000	0.000000000

Structure quinoline

Charge = 0 Multiplicity = 1

Free Energy: -401.600474 hartree

C	-11.417495000	-3.140929000	5.079375000
C	-10.038582000	-3.117797000	5.079185000
C	-9.337432000	-1.880378000	5.079287000
C	-10.088395000	-0.658168000	5.079579000
C	-11.508843000	-0.715023000	5.079776000
C	-12.159307000	-1.931198000	5.079675000
H	-11.947942000	-4.096510000	5.079293000
H	-9.448632000	-4.036933000	5.078951000
C	-9.359003000	0.560529000	5.079676000

H	-12.073742000	0.221006000	5.080010000
H	-13.251462000	-1.968748000	5.079825000
C	-7.982873000	0.521396000	5.079479000
C	-7.336316000	-0.742400000	5.079189000
H	-9.899893000	1.510806000	5.079908000
H	-7.386317000	1.436174000	5.079545000
H	-6.239736000	-0.782320000	5.079025000
N	-7.973391000	-1.894423000	5.079094000

Structure THF

Charge = 0 Multiplicity = 1

Free Energy: -232.22731 hartree

C	-4.590282000	-3.004232000	-0.612512000
O	-4.316578000	-1.687652000	-0.131481000
C	-3.553483000	-0.961597000	-1.094883000
C	-3.049750000	-1.994624000	-2.103079000
C	-4.196500000	-3.010467000	-2.090422000
H	-3.993964000	-3.742175000	-0.040244000
H	-5.656284000	-3.237334000	-0.448464000
H	-4.194199000	-0.205318000	-1.590868000
H	-2.738680000	-0.423626000	-0.581247000
H	-2.850605000	-1.562316000	-3.094861000
H	-2.120042000	-2.463136000	-1.739432000
H	-5.032271000	-2.649312000	-2.712459000
H	-3.908050000	-4.009121000	-2.450616000

Structure 1,2,3,4-tetrahydroquinoline

Charge = 0 Multiplicity = 1

Free Energy: -403.975205 hartree

C	-0.702181000	-2.760763000	2.224535000
C	-0.735709000	-0.895507000	0.609156000

C	0.082632000	-0.104698000	1.459576000
C	0.641075000	-2.224554000	2.711113000
H	-1.875845000	-0.931814000	-1.229088000
H	-1.489536000	-2.501198000	2.963363000
C	-1.246408000	-0.320662000	-0.575472000
C	0.365407000	1.213720000	1.088803000
C	-0.141788000	1.780298000	-0.085121000
C	-0.954158000	0.998831000	-0.914823000
H	1.002859000	1.812362000	1.747354000
H	0.094455000	2.813868000	-0.348429000
H	-1.363533000	1.418546000	-1.837987000
H	0.868960000	-2.634722000	3.706869000
H	-0.679595000	-3.859193000	2.151182000
H	1.431238000	-2.569368000	2.022417000
C	0.614342000	-0.694704000	2.750140000
N	-0.995339000	-2.217028000	0.912179000
H	-1.747026000	-2.655761000	0.392498000
H	1.619584000	-0.293985000	2.957764000
H	-0.022774000	-0.367766000	3.592674000

Structure **TS0-1**

Charge = 0 Multiplicity = 1

Free Energy: -1758.835871 hartree

Ba	-5.572489000	-0.430132000	2.121286000
C	-7.929274000	-4.106077000	-0.061248000
C	-7.884426000	-2.830676000	0.493257000
C	-7.714773000	-1.658312000	-0.313845000
C	-7.537553000	-1.885377000	-1.734963000
C	-7.579483000	-3.184449000	-2.258696000
C	-7.785506000	-4.304779000	-1.446043000

H	-8.083052000	-4.966572000	0.597892000
H	-8.002304000	-2.703595000	1.570688000
C	-7.142100000	-0.729847000	-2.527106000
H	-7.422638000	-3.315123000	-3.335209000
H	-7.827676000	-5.308290000	-1.875672000
C	-7.196453000	0.510870000	-2.000642000
H	-6.755146000	-0.899888000	-3.537981000
H	-6.860661000	1.384090000	-2.570574000
N	-7.634379000	-0.437241000	0.254315000
C	-7.799983000	0.708110000	-0.630293000
H	-7.364116000	1.600846000	-0.149920000
H	-8.886202000	0.962716000	-0.752505000
C	-4.618151000	2.593664000	-0.006759000
O	-4.037537000	1.595396000	0.856542000
C	-2.767864000	2.048088000	1.359568000
C	-2.796328000	3.560883000	1.190193000
C	-3.573462000	3.704522000	-0.123637000
H	-4.868520000	2.128591000	-0.973002000
H	-5.548450000	2.949700000	0.463401000
H	-2.670484000	1.707466000	2.401047000
H	-1.954348000	1.595381000	0.762603000
H	-3.350455000	4.025736000	2.021849000
H	-1.789226000	4.001198000	1.155560000
H	-4.033049000	4.694618000	-0.257646000
H	-2.906008000	3.518289000	-0.980709000
C	-6.045935000	2.932864000	3.543636000
O	-6.710406000	2.119701000	2.570387000
C	-8.101238000	2.431242000	2.684411000
C	-8.359857000	2.593754000	4.191259000

C	-6.954036000	2.884122000	4.778387000
H	-5.043063000	2.517164000	3.713200000
H	-5.949770000	3.962999000	3.152023000
H	-8.304718000	3.372505000	2.140495000
H	-8.669626000	1.622799000	2.208636000
H	-9.074984000	3.406505000	4.384095000
H	-8.778395000	1.671198000	4.616594000
H	-6.913285000	3.824334000	5.346912000
H	-6.635031000	2.071316000	5.447143000
C	-4.304907000	-3.017275000	-0.343290000
O	-3.969216000	-1.721886000	0.199856000
C	-3.093383000	-1.015531000	-0.704492000
C	-2.675418000	-2.039457000	-1.755864000
C	-3.904418000	-2.951786000	-1.810816000
H	-3.728001000	-3.791143000	0.192406000
H	-5.374595000	-3.197970000	-0.183081000
H	-3.649689000	-0.176587000	-1.153448000
H	-2.249625000	-0.605179000	-0.130039000
H	-2.431323000	-1.569091000	-2.719673000
H	-1.792553000	-2.604915000	-1.414786000
H	-4.707475000	-2.481578000	-2.398511000
H	-3.701298000	-3.946269000	-2.233906000
H	-3.653245000	0.269650000	4.457122000
C	-5.908455000	-4.116547000	3.414605000
O	-5.059183000	-3.037116000	3.023163000
C	-3.702976000	-3.497332000	3.133010000
C	-3.749605000	-5.026382000	2.915075000
C	-5.255528000	-5.338580000	2.778821000
H	-5.930342000	-4.195743000	4.518312000

H	-6.923326000	-3.902365000	3.057026000
H	-3.112000000	-2.956929000	2.380582000
H	-3.313155000	-3.241036000	4.133096000
H	-3.187369000	-5.330475000	2.020721000
H	-3.310630000	-5.548825000	3.777788000
H	-5.547815000	-5.399261000	1.719250000
H	-5.547735000	-6.277258000	3.271508000
C	-6.458015000	-1.639529000	7.167217000
C	-6.566941000	-1.446612000	5.805537000
C	-7.843653000	-1.262600000	5.208370000
C	-9.011608000	-1.283049000	6.040282000
C	-8.864126000	-1.485215000	7.439678000
C	-7.612280000	-1.659723000	7.991475000
H	-5.471096000	-1.774284000	7.616253000
H	-5.679135000	-1.425366000	5.171744000
C	-10.271862000	-1.094949000	5.413396000
H	-9.759723000	-1.498146000	8.066216000
H	-7.503663000	-1.813362000	9.067746000
C	-10.329234000	-0.904993000	4.050435000
C	-9.121476000	-0.896539000	3.309994000
H	-11.179412000	-1.103707000	6.022963000
H	-11.279162000	-0.757530000	3.533245000
H	-9.126352000	-0.733199000	2.225803000
N	-7.930841000	-1.063595000	3.858378000

Structure **TS1-2**

Charge = 0 Multiplicity = 1

Free Energy: -1526.593475 hartree

C	-2.504145000	-1.740907000	3.466072000
C	-1.565068000	-1.643498000	2.488700000

C	-0.826227000	-0.418015000	2.327963000
C	-1.202175000	0.686418000	3.162948000
C	-2.731727000	-0.617730000	4.355964000
H	0.478552000	-1.117791000	0.755373000
H	-3.072450000	-2.660609000	3.625196000
H	-1.358187000	-2.480603000	1.815572000
C	0.206102000	-0.261290000	1.379347000
C	-0.523984000	1.920665000	2.975873000
H	-2.001841000	-1.299352000	5.885552000
C	0.488607000	2.047346000	2.035796000
C	0.867453000	0.952208000	1.232640000
H	-0.802453000	2.763961000	3.609308000
H	1.000218000	3.006845000	1.920264000
H	1.667614000	1.060312000	0.496649000
N	-2.193059000	0.594246000	4.103663000
Ba	-1.176482000	1.286455000	6.805152000
C	-3.762350000	2.172698000	10.862780000
C	-2.616326000	1.905588000	10.119679000
C	-1.595905000	2.892119000	9.914472000
C	-1.838316000	4.188450000	10.515727000
C	-3.003225000	4.424179000	11.256093000
C	-3.973199000	3.433191000	11.449062000
H	-4.503978000	1.379095000	11.001192000
H	-2.463982000	0.906339000	9.696580000
C	-0.904964000	5.248089000	10.163238000
H	-3.156393000	5.424171000	11.677566000
H	-4.869929000	3.633648000	12.039886000
C	0.229355000	4.970206000	9.489933000
H	-1.169687000	6.280011000	10.419622000

H	0.917215000	5.768440000	9.190352000
N	-0.533857000	2.627140000	9.129814000
C	0.601610000	3.536160000	9.197076000
H	1.158950000	3.484510000	8.244116000
H	1.342569000	3.196697000	9.967855000
C	2.606388000	0.446569000	7.001015000
O	1.439782000	0.403629000	6.161126000
C	1.723036000	-0.309970000	4.937135000
C	3.109960000	-0.917343000	5.128974000
C	3.769937000	0.081973000	6.086198000
H	2.683514000	1.450858000	7.444414000
H	2.492773000	-0.285467000	7.821079000
H	0.932546000	-1.056682000	4.773483000
H	1.701706000	0.404835000	4.098906000
H	3.035721000	-1.908769000	5.604331000
H	3.646282000	-1.033135000	4.176042000
H	4.624320000	-0.335371000	6.638420000
H	4.115359000	0.972125000	5.535187000
C	-3.504463000	4.238824000	7.417320000
O	-2.988213000	3.377023000	6.377905000
C	-3.532362000	3.753614000	5.098006000
C	-4.157487000	5.126957000	5.314625000
C	-4.635693000	5.027559000	6.766836000
H	-3.825879000	3.617929000	8.264372000
H	-2.694128000	4.899066000	7.766291000
H	-2.724627000	3.747907000	4.352125000
H	-4.283883000	3.005966000	4.790377000
H	-3.391847000	5.914407000	5.218041000
H	-4.962760000	5.338048000	4.596132000

H	-4.792273000	6.003648000	7.248406000
H	-5.580588000	4.462349000	6.820646000
C	-0.195694000	4.850506000	5.888500000
O	0.300560000	3.498911000	5.799409000
C	1.654554000	3.496551000	5.310845000
C	1.873336000	4.885701000	4.724249000
C	1.013285000	5.749800000	5.652175000
H	-0.963161000	4.998510000	5.111031000
H	-0.659795000	4.990841000	6.874216000
H	2.342480000	3.310134000	6.153683000
H	1.761731000	2.682295000	4.582781000
H	2.934702000	5.173204000	4.710398000
H	1.489779000	4.931101000	3.691422000
H	1.543521000	5.937327000	6.599833000
H	0.732509000	6.720653000	5.218812000
H	-3.663410000	-0.614812000	4.925672000

Structure **TS2-3**

Charge = 0 Multiplicity = 1

Free Energy: -1527.781245 hartree

C	-0.557060000	-0.213113000	2.437875000
C	0.253212000	-0.567300000	1.422681000
C	-0.109414000	-1.661693000	0.527901000
C	-1.449287000	-2.162884000	0.623107000
C	-1.802761000	-1.007839000	2.725543000
H	1.772111000	-1.750757000	-0.510081000
H	-0.295619000	0.610678000	3.109333000
H	1.190050000	-0.032485000	1.236128000
C	0.758259000	-2.159588000	-0.453353000
C	-1.852318000	-3.139325000	-0.322770000

H	-2.580284000	-0.351196000	3.155609000
C	-0.964541000	-3.626813000	-1.281572000
C	0.351372000	-3.147932000	-1.355321000
H	-2.874032000	-3.524069000	-0.281607000
H	-1.305801000	-4.392929000	-1.984014000
H	1.042559000	-3.531107000	-2.109340000
N	-2.338226000	-1.677101000	1.544608000
Ba	-5.043355000	-0.887322000	0.741543000
C	-9.883355000	-1.425643000	1.079730000
C	-8.692893000	-0.742048000	0.848503000
C	-8.277838000	-0.364485000	-0.472363000
C	-9.146218000	-0.788823000	-1.553878000
C	-10.335511000	-1.478689000	-1.284831000
C	-10.730439000	-1.794644000	0.020105000
H	-10.165837000	-1.666279000	2.109963000
H	-8.063681000	-0.443934000	1.691053000
C	-8.634406000	-0.601340000	-2.903630000
H	-10.957285000	-1.789816000	-2.131894000
H	-11.668154000	-2.322225000	0.209382000
C	-7.533211000	0.145938000	-3.120442000
H	-9.137652000	-1.120166000	-3.727172000
H	-7.114137000	0.258087000	-4.126543000
N	-7.105135000	0.272834000	-0.671982000
C	-6.905064000	0.900176000	-1.972816000
H	-5.822100000	1.015162000	-2.152010000
H	-7.300144000	1.949934000	-1.974285000
H	-3.881352000	-3.256351000	2.358650000
C	-4.574116000	2.795601000	0.010027000
O	-4.167715000	1.733712000	0.892288000

C	-3.268732000	2.232003000	1.901696000
C	-3.285790000	3.751930000	1.756471000
C	-3.583412000	3.925507000	0.263274000
H	-4.562197000	2.414811000	-1.019307000
H	-5.606951000	3.095743000	0.256448000
H	-3.615599000	1.879155000	2.884750000
H	-2.264368000	1.817410000	1.713828000
H	-4.097659000	4.188702000	2.360099000
H	-2.338051000	4.211084000	2.072727000
H	-3.997154000	4.911846000	0.008382000
H	-2.667337000	3.770652000	-0.329722000
C	-6.443936000	-0.042148000	4.251225000
O	-6.044171000	0.530734000	2.990169000
C	-6.693697000	1.804547000	2.787679000
C	-7.815419000	1.849484000	3.818162000
C	-7.204220000	1.061642000	4.982274000
H	-7.089178000	-0.918118000	4.058669000
H	-5.543820000	-0.385314000	4.784509000
H	-5.960794000	2.611782000	2.955706000
H	-7.040871000	1.853353000	1.745939000
H	-8.097299000	2.878477000	4.084682000
H	-8.709864000	1.335897000	3.430335000
H	-6.504736000	1.697879000	5.548971000
H	-7.950190000	0.661905000	5.684087000
C	-3.668903000	-0.982330000	-2.691201000
O	-3.559865000	-0.188788000	-1.492460000
C	-2.321811000	0.552481000	-1.489519000
C	-1.489264000	-0.047164000	-2.616371000
C	-2.567587000	-0.476802000	-3.617081000

H	-3.514399000	-2.043758000	-2.431760000
H	-4.683904000	-0.862963000	-3.100067000
H	-2.546391000	1.616522000	-1.675524000
H	-1.856129000	0.457832000	-0.499205000
H	-0.768911000	0.672961000	-3.031265000
H	-0.933788000	-0.923218000	-2.252717000
H	-2.923995000	0.388734000	-4.199227000
H	-2.228189000	-1.250915000	-4.320487000
H	-1.579404000	-1.747768000	3.535157000
H	-3.201200000	-2.600933000	1.981343000

Structure **TS4-5**

Charge = 0 Multiplicity = 1

Free Energy: -1527.762225 hartree

C	-2.174594000	0.755470000	3.690085000
C	-4.537282000	1.283214000	3.295564000
C	-4.907375000	-0.005799000	3.796941000
C	-2.533389000	-0.710396000	3.796933000
H	-5.185575000	3.247890000	2.705623000
H	-1.203654000	0.893555000	3.194755000
C	-5.498904000	2.277673000	3.103289000
C	-6.271889000	-0.214981000	4.093612000
C	-7.229760000	0.789247000	3.908885000
C	-6.848572000	2.038749000	3.411654000
H	-6.576143000	-1.191278000	4.482776000
H	-8.276297000	0.590431000	4.154160000
H	-7.588827000	2.827696000	3.259428000
Ba	-3.680091000	-0.385794000	0.356352000
C	-5.157106000	0.414620000	-4.372632000
C	-5.040972000	0.659723000	-3.008042000

C	-4.152124000	1.660369000	-2.493350000
C	-3.355614000	2.370193000	-3.473290000
C	-3.493515000	2.091378000	-4.839863000
C	-4.392194000	1.129048000	-5.312414000
H	-5.863954000	-0.348045000	-4.716072000
H	-5.647748000	0.093657000	-2.297323000
C	-2.308473000	3.236089000	-2.951590000
H	-2.858619000	2.637090000	-5.546848000
H	-4.494376000	0.935205000	-6.382693000
C	-2.243230000	3.521136000	-1.635345000
H	-1.547961000	3.607897000	-3.647138000
H	-1.431926000	4.134594000	-1.228439000
N	-4.021548000	1.843162000	-1.164404000
C	-3.343945000	3.051688000	-0.714150000
H	-2.935875000	2.881540000	0.302092000
H	-4.073704000	3.891335000	-0.570978000
C	-1.698752000	-0.901390000	-2.947730000
O	-1.628238000	-0.789352000	-1.507299000
C	-0.426033000	-0.092237000	-1.124028000
C	0.491588000	-0.183953000	-2.335763000
C	-0.516566000	-0.099700000	-3.487298000
H	-1.623281000	-1.968224000	-3.214618000
H	-2.670329000	-0.518039000	-3.287415000
H	-0.672268000	0.962147000	-0.898513000
H	-0.030692000	-0.567869000	-0.214015000
H	1.243332000	0.618589000	-2.352586000
H	1.016801000	-1.153246000	-2.345873000
H	-0.815390000	0.945440000	-3.655481000
H	-0.137494000	-0.507287000	-4.435720000

C	-7.255621000	0.293200000	0.121833000
O	-6.397598000	-0.826842000	-0.207010000
C	-7.105942000	-2.061919000	-0.007361000
C	-8.172281000	-1.729050000	1.025689000
C	-8.578732000	-0.312493000	0.601159000
H	-6.765183000	0.883393000	0.911866000
H	-7.366973000	0.931718000	-0.767874000
H	-7.558567000	-2.386038000	-0.962714000
H	-6.376913000	-2.820448000	0.309144000
H	-9.007504000	-2.444545000	1.021617000
H	-7.727153000	-1.714241000	2.033344000
H	-9.305126000	-0.356498000	-0.225947000
H	-9.023616000	0.273588000	1.417453000
C	-3.073601000	-3.971688000	-0.168878000
O	-4.002717000	-2.985748000	-0.644010000
C	-4.315301000	-3.250165000	-2.026069000
C	-3.294212000	-4.296776000	-2.510042000
C	-2.239451000	-4.320160000	-1.392080000
H	-2.499872000	-3.526287000	0.658817000
H	-3.625140000	-4.850885000	0.214245000
H	-5.352522000	-3.615718000	-2.101610000
H	-4.249568000	-2.298301000	-2.573987000
H	-3.773740000	-5.283212000	-2.602772000
H	-2.871548000	-4.036053000	-3.490840000
H	-1.730774000	-5.290385000	-1.297414000
H	-1.480088000	-3.539003000	-1.548773000
H	-1.753262000	-1.253399000	2.235023000
H	-2.089654000	1.178924000	4.715815000
H	-1.782678000	-1.348861000	4.262598000

N	-3.195986000	1.454378000	2.905650000
H	-2.958548000	2.426653000	2.723671000
C	-3.877506000	-1.005831000	3.982296000
H	-4.183992000	-2.006506000	4.302453000

Structure **TS5-6**

Charge = 0 Multiplicity = 1

Free Energy: -1528.951072 hartree

C	-1.563933000	-3.533197000	2.233505000
C	-0.667102000	-1.580701000	1.035275000
C	-0.611615000	-0.846858000	2.284733000
C	-0.946291000	-3.017326000	3.534876000
H	-0.545173000	-1.508647000	-1.106871000
H	-2.646109000	-3.283893000	2.230892000
C	-0.489983000	-0.920759000	-0.184494000
C	-0.345626000	0.551159000	2.178113000
C	-0.160206000	1.194013000	0.946494000
C	-0.237252000	0.467361000	-0.249921000
H	-0.271442000	1.130680000	3.104722000
H	0.058203000	2.266218000	0.925113000
H	-0.080564000	0.953598000	-1.216351000
Ba	-3.719494000	0.372459000	0.839483000
C	-7.922237000	-2.284745000	0.510339000
C	-7.022950000	-1.224683000	0.475238000
C	-6.817938000	-0.440751000	-0.707156000
C	-7.557838000	-0.858903000	-1.878770000
C	-8.454425000	-1.934195000	-1.811510000
C	-8.663928000	-2.649622000	-0.627907000
H	-8.055170000	-2.837471000	1.445954000
H	-6.466453000	-0.958867000	1.378928000

C	-7.218205000	-0.195995000	-3.130094000
H	-8.988554000	-2.221456000	-2.724062000
H	-9.375327000	-3.477698000	-0.591527000
C	-6.416755000	0.887330000	-3.139389000
H	-7.593205000	-0.627771000	-4.064614000
H	-6.124094000	1.365900000	-4.080389000
N	-5.932305000	0.576243000	-0.713918000
C	-5.968266000	1.504189000	-1.836630000
H	-4.968222000	1.962384000	-1.964429000
H	-6.631931000	2.380211000	-1.611413000
C	-4.798572000	3.993130000	0.508987000
O	-3.661908000	3.127907000	0.300810000
C	-2.708616000	3.751980000	-0.581661000
C	-3.123970000	5.217123000	-0.653931000
C	-4.646129000	5.117166000	-0.510895000
H	-5.716712000	3.406225000	0.376391000
H	-4.768878000	4.371393000	1.544822000
H	-1.698749000	3.596945000	-0.174170000
H	-2.762614000	3.266897000	-1.573766000
H	-2.693799000	5.776796000	0.192685000
H	-2.799186000	5.699552000	-1.587042000
H	-5.118795000	6.051506000	-0.175383000
H	-5.102268000	4.826247000	-1.470969000
C	-5.371958000	1.609800000	4.073487000
O	-5.513314000	1.614622000	2.650341000
C	-6.905393000	1.845316000	2.393546000
C	-7.657799000	1.069248000	3.489391000
C	-6.580968000	0.816884000	4.576445000
H	-4.401296000	1.156945000	4.321700000

H	-5.386356000	2.651625000	4.445868000
H	-7.107680000	2.929569000	2.465726000
H	-7.107443000	1.510406000	1.368476000
H	-8.507256000	1.654191000	3.870296000
H	-8.053741000	0.122427000	3.096504000
H	-6.895056000	1.143176000	5.578357000
H	-6.326736000	-0.252518000	4.633286000
C	-4.250567000	-3.369396000	-0.222931000
O	-3.761696000	-2.069713000	-0.589851000
C	-3.813202000	-1.905550000	-2.023426000
C	-4.281548000	-3.247762000	-2.586654000
C	-5.074835000	-3.836150000	-1.414524000
H	-3.394609000	-4.043031000	-0.037987000
H	-4.829900000	-3.273037000	0.706379000
H	-4.525508000	-1.096509000	-2.248697000
H	-2.813669000	-1.611906000	-2.383589000
H	-4.882980000	-3.122105000	-3.498496000
H	-3.418353000	-3.889471000	-2.828225000
H	-6.083096000	-3.399439000	-1.371722000
H	-5.168704000	-4.931243000	-1.456213000
H	-1.562911000	-3.384380000	4.378060000
H	-1.490456000	-4.630499000	2.166010000
H	0.053213000	-3.484979000	3.663841000
H	-3.486107000	-1.189694000	3.715665000
H	-2.574582000	-1.246554000	3.649766000
C	-0.918181000	-1.507217000	3.510855000
N	-0.873559000	-2.960715000	1.087443000
H	-1.149535000	-3.362706000	0.196887000
H	-0.613830000	-0.996879000	4.434450000