Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.


# Supplementary Material

## A New Approach for Homogeneous $CO_2$ Reduction by Ni(cyclam): Substituents with Intra-Molecular Hydrogen-Transfer

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## Caption of Content

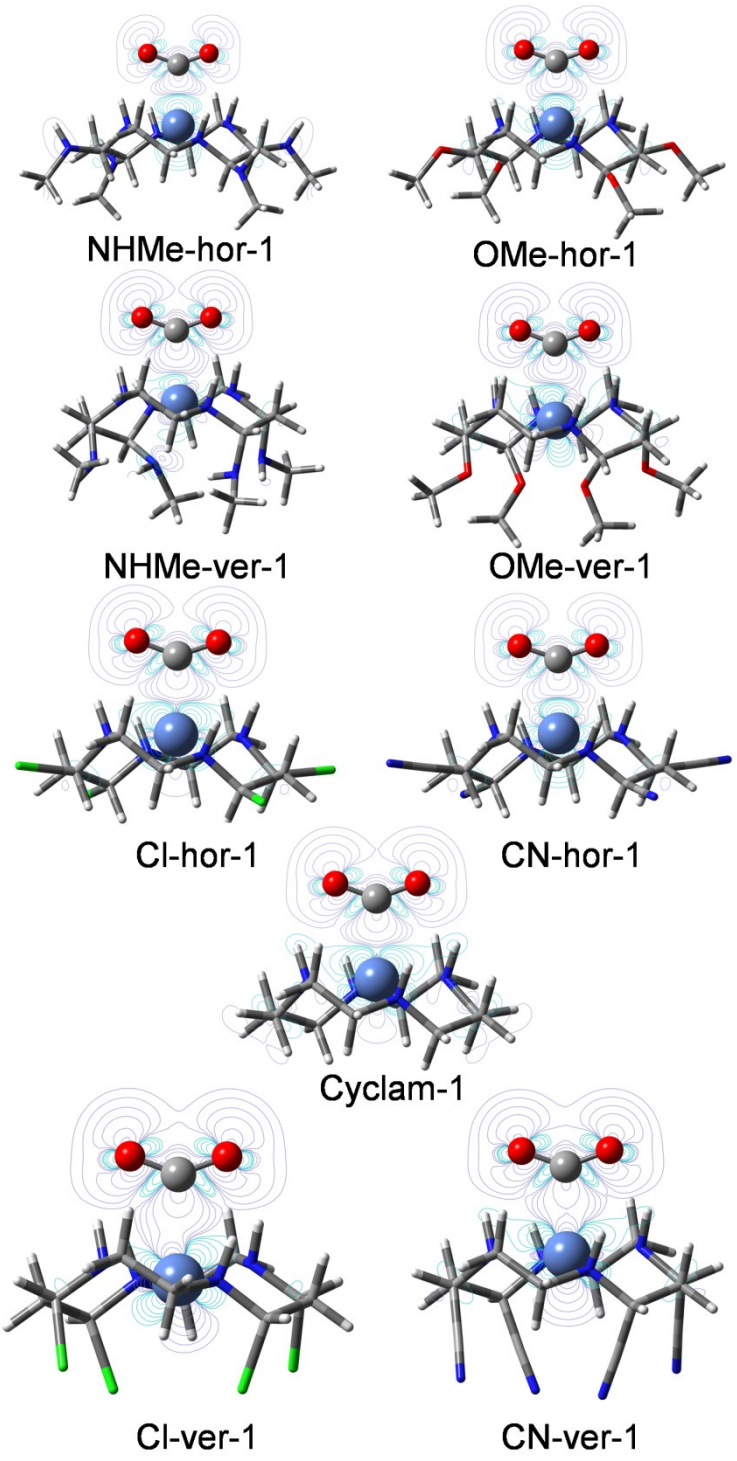


Figure S1. Fukui index of the initial compound of each series. The positive region and negative region of $f^-$ is shown by purple and blue, respectively.

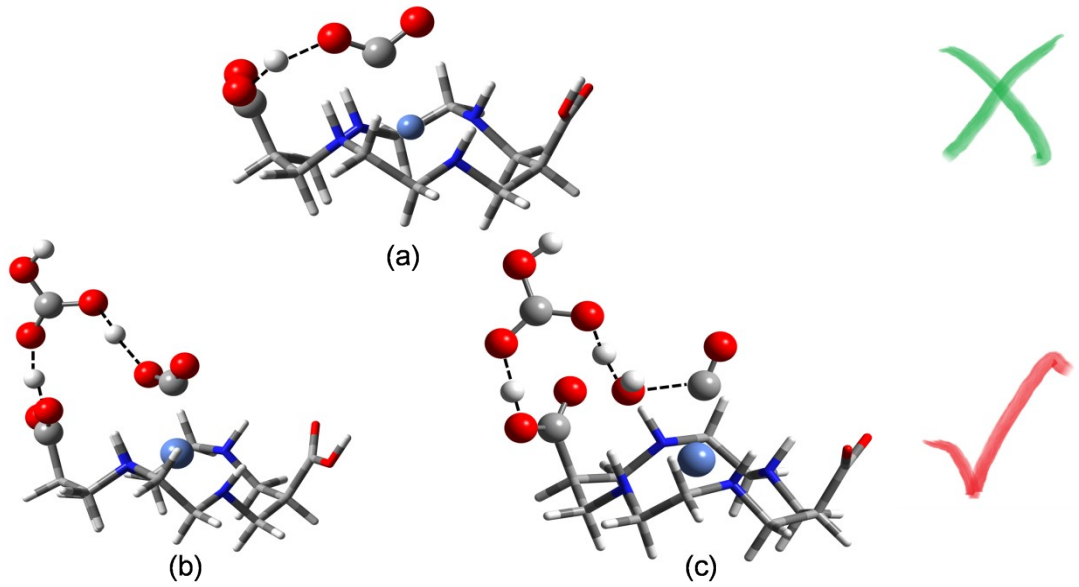


Figure S2. Geometric structures of transition state **meso-COOH-TS2'** (a), **meso-COOH-TS2** (b) and **meso-COOH-TS4** (c). The **meso-COOH-TS2'** represents the directed H-transfer from -COOH group to $CO_2$ without H-transfer shuttle. Note that the transition state **meso-COOH-TS2'** is failed to be localized due probably to the unfavourable reaction direction.

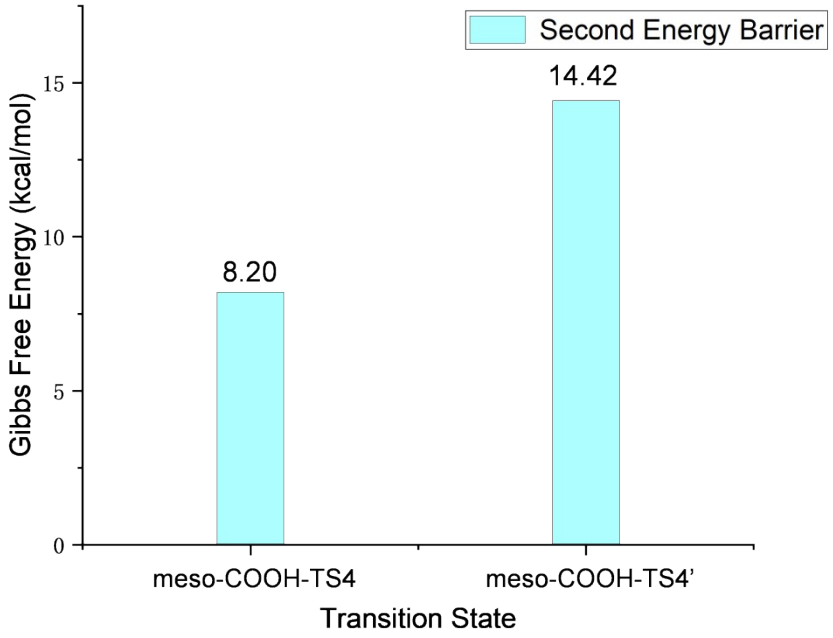


Figure S3. Calculated energy barriers for the second energy barrier of $CO_2$ reduction by **meso-COOH** catalyst**.** The **meso-COOH-TS4** produces CO and $H_2O$ while the **meso-COOH-TS4'** produces C(OH)2 moiety.

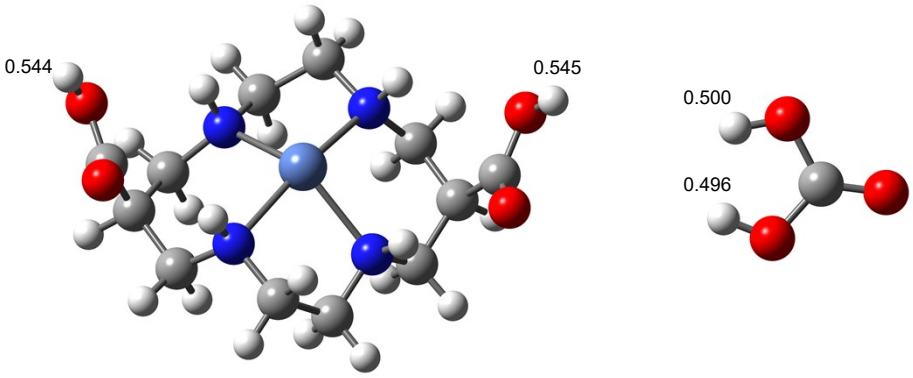


Figure S4. Natural population analysis (NPA) of the selected H atom in meso-COOH compounds and $H_2CO_3$. The hydrogen atoms in **meso-COOH** concentrate more positive charge than that in $H_2CO_3$.

**Table S1.** Cartesian coordinates (Å) SCF energies and Gibbs free energies, at 298.15 K and 1 atm for the optimized structures.

All energies are given in Hartree and on the basis of ωb97XD/BSII.

**cyclam-1**

SCF Energy: -972.2848219
Gibbs Energy: -971.9524809

| | | | |
|---|---|---|---|
| Ni | -1.86471657 | 0.13711152 | 0.00000000 |
| N | -0.01374857 | 1.08984352 | -0.00697800 |
| N | -2.65302557 | 2.02690352 | -0.42965700 |
| H | -2.99552757 | 2.37658752 | 0.46596900 |
| N | -3.71542357 | -0.81573548 | -0.00792600 |
| H | -4.04128257 | -0.54286248 | 0.92462100 |
| N | -1.07606557 | -1.75237448 | -0.42980700 |
| C | 0.95708943 | 0.64922652 | -1.02320200 |
| H | 1.90716843 | 1.18124452 | -0.88762100 |
| H | 0.57268143 | 0.91989552 | -2.01436700 |
| C | 1.21013743 | -0.85771748 | -0.95055300 |
| H | 1.52927043 | -1.12874148 | 0.06446600 |
| H | 2.06003343 | -1.08300148 | -1.60181100 |
| C | 0.04981743 | -1.75123448 | -1.39049600 |
| H | -0.34213657 | -1.40702748 | -2.35543100 |
| H | 0.41299143 | -2.77589848 | -1.53785900 |
| C | -2.22260157 | -2.58375548 | -0.85854600 |
| H | -2.43419457 | -2.33853148 | -1.90555100 |
| H | -1.98580257 | -3.65295748 | -0.81445500 |
| C | -3.43179457 | -2.26587448 | 0.01579000 |
| H | -3.22185557 | -2.53913048 | 1.05451200 |
| H | -4.29965257 | -2.84925448 | -0.31190700 |
| C | -4.68558557 | -0.37478848 | -1.02472600 |
| H | -5.63564957 | -0.90709348 | -0.89018400 |

| | | | |
|---|---|---|---|
| H | -4.30036657 | -0.64482848 | -2.01575400 |
| C | -4.93893857 | 1.13206052 | -0.95143700 |
| H | -5.78868357 | 1.35753452 | -1.60283300 |
| H | -5.25847157 | 1.40252152 | 0.06361200 |
| C | -3.77870357 | 2.02608452 | -1.39056400 |
| H | -3.38648357 | 1.68259352 | -2.35563600 |
| H | -4.14214157 | 3.05073552 | -1.53738800 |
| C | -1.50622957 | 2.85813952 | -0.85789200 |
| H | -1.29429157 | 2.61296652 | -1.90483600 |
| H | -1.74281457 | 3.92738952 | -0.81375100 |
| C | -0.29738657 | 2.53997952 | 0.01685000 |
| H | 0.57061743 | 3.12336152 | -0.31047800 |
| H | -0.50763957 | 2.81322952 | 1.05551100 |
| H | -0.73368557 | -2.10229348 | 0.46577700 |
| H | 0.31138443 | 0.81673352 | 0.92575400 |
| C | -1.86590357 | 0.13673152 | 2.28898800 |
| O | -0.72092457 | 0.30298852 | 2.71250500 |
| O | -3.01069857 | -0.02997748 | 2.71252200 |

**Cyclam-TS2**

SCF Energy: -1237.296919
Gibbs Energy: -1236.936326

| | | | |
|---|---|---|---|
| Ni | -4.20475305 | -0.59414990 | 0.00000000 |
| N | -3.91243505 | 1.24405910 | -0.98827500 |
| N | -3.13293705 | -1.42989090 | -1.58541300 |
| H | -3.86312005 | -1.79737090 | -2.19584200 |
| N | -4.53467005 | -2.41939890 | 0.97553600 |
| H | -5.29931205 | -2.75507690 | 0.38728000 |
| N | -4.56176105 | 0.28658510 | 1.86125400 |
| C | -3.27159305 | 2.38335110 | -0.30598800 |
| C | -3.81055905 | 2.57235310 | 1.12525200 |
| H | -4.87760105 | 2.81654410 | 1.05436200 |

| | | | |
|---|---|---|---|
| H | -3.32041705 | 3.45400410 | 1.54713800 |
| C | -3.64936005 | 1.42239010 | 2.13807300 |
| C | -4.50336205 | -0.80071890 | 2.86752500 |
| H | -3.45206105 | -0.96838590 | 3.11699500 |
| H | -5.02593305 | -0.52051990 | 3.78886400 |
| C | -5.11486905 | -2.08187290 | 2.29817900 |
| H | -6.19028505 | -1.94839390 | 2.14858700 |
| H | -4.98101805 | -2.89778090 | 3.01693900 |
| C | -3.47362505 | -3.44422590 | 0.94429000 |
| C | -2.96452005 | -3.69588190 | -0.48818100 |
| H | -2.27736705 | -4.54584090 | -0.44575800 |
| H | -3.81878305 | -4.02407890 | -1.09381200 |
| C | -2.24203605 | -2.56772590 | -1.25005200 |
| C | -2.46485805 | -0.30079390 | -2.27858700 |
| H | -1.57129605 | -0.03749190 | -1.70546000 |
| H | -2.14601405 | -0.58216290 | -3.28893200 |
| C | -3.41097505 | 0.89855810 | -2.33940100 |
| H | -2.89622305 | 1.74294010 | -2.80994200 |
| H | -4.28293205 | 0.66312210 | -2.95734600 |
| H | -5.51108905 | 0.65636510 | 1.81585000 |
| H | -4.91179305 | 1.45985910 | -1.06887700 |
| C | -6.13931505 | -0.56437290 | -0.70898500 |
| O | -6.70845705 | 0.47785010 | -1.00457100 |
| O | -6.77952505 | -1.74794790 | -0.73963600 |
| C | -10.12483905 | -0.70148090 | -0.32785100 |
| O | -9.40016205 | -1.27560590 | -1.18949600 |
| H | -7.97817205 | -1.58695790 | -1.00766900 |
| O | -11.33573205 | -0.31785990 | -0.67045700 |
| H | -11.77534005 | 0.09982410 | 0.08344100 |
| O | -9.62471905 | -0.53841690 | 0.80095200 |
| H | -3.45867905 | 3.28219010 | -0.86941600 |
| H | -1.83502605 | -2.97277790 | -2.16145500 |
| H | -3.86165805 | -4.36640690 | 1.34346700 |
| H | -3.84889405 | 1.79964210 | 3.12714200 |

| | | | |
|---|---|---|---|
| H | -2.63416205 | 1.06318110 | 2.10456500 |
| H | -2.20881605 | 2.21287310 | -0.26590800 |
| H | -1.42983105 | -2.19915890 | -0.64619600 |
| H | -2.65386905 | -3.11600490 | 1.56116400 |

**Cyclam-3**

With$HCO_3$

SCF Energy: -1237.329867
Gibbs Energy: -1236.96562

| | | | |
|---|---|---|---|
| Ni | -0.40219377 | 0.17367459 | 0.00000000 |
| N | 0.75637623 | 1.85206559 | -0.56803000 |
| N | -1.99930677 | 1.55742459 | 0.07061100 |
| H | -2.17289077 | 1.66946259 | 1.06937800 |
| N | -1.66984477 | -1.49981341 | 0.28443000 |
| H | -1.85683077 | -1.48958141 | 1.28590800 |
| N | 0.73682523 | -1.17233141 | -1.17186700 |
| C | 1.12604223 | 1.87231059 | -1.99864900 |
| H | 1.68142623 | 2.79195859 | -2.22409100 |
| H | 0.20608623 | 1.89695959 | -2.59505600 |
| C | 1.96419423 | 0.65815859 | -2.39544500 |
| H | 2.83340323 | 0.56422359 | -1.73417600 |
| H | 2.37897123 | 0.85387059 | -3.38916500 |
| C | 1.20811023 | -0.66599741 | -2.47972800 |
| H | 0.32785323 | -0.54109541 | -3.12264200 |
| H | 1.85056423 | -1.41705341 | -2.95651400 |
| C | -0.04129677 | -2.42060241 | -1.30757900 |
| H | -0.72184277 | -2.30422341 | -2.15811900 |
| H | 0.60716323 | -3.27622941 | -1.52799200 |
| C | -0.83488877 | -2.67508341 | -0.03220400 |
| H | -0.14398077 | -2.82578441 | 0.80324300 |
| H | -1.43814077 | -3.58533441 | -0.13643800 |

| | | | |
|---|---|---|---|
| C | -2.96164477 | -1.44692841 | -0.42277200 |
| H | -3.54184877 | -2.35447041 | -0.20967200 |
| H | -2.77086577 | -1.43455241 | -1.50222900 |
| C | -3.77639677 | -0.21507641 | -0.02748400 |
| H | -4.79112377 | -0.34979741 | -0.41431700 |
| H | -3.87365377 | -0.16642041 | 1.06505900 |
| C | -3.25884477 | 1.11726159 | -0.56702700 |
| H | -3.06945477 | 1.02962559 | -1.64369700 |
| H | -4.03035677 | 1.88773159 | -0.43939000 |
| C | -1.50003877 | 2.83740759 | -0.47505300 |
| H | -1.62799777 | 2.80297659 | -1.56178000 |
| H | -2.08556577 | 3.68930659 | -0.11091000 |
| C | -0.02685977 | 3.02237359 | -0.12609200 |
| H | 0.34765723 | 3.95057459 | -0.57523700 |
| H | 0.09308023 | 3.10886159 | 0.95827200 |
| H | 1.56048923 | -1.37157041 | -0.59486500 |
| H | 1.62202223 | 1.82551459 | -0.02862500 |
| C | 0.06818223 | 0.23399959 | 1.99992100 |
| O | 1.10486223 | 0.51059959 | 2.61521300 |
| O | -1.01611477 | -0.02937241 | 2.77435700 |
| C | 3.60516623 | -0.17939741 | 0.67531000 |
| O | 4.66793223 | -0.12354741 | -0.02418100 |
| H | -0.75521677 | 0.03062159 | 3.71102900 |
| O | 3.15961423 | 0.88200459 | 1.26782700 |
| H | 2.32298823 | 0.68566759 | 1.86061200 |
| O | 3.05925823 | -1.30246941 | 0.65107600 |

Without$HCO_3$

SCF Energy: -972.9673737
Gibbs Energy: -972.6239437

| | | | |
|---|---|---|---|
| Ni | -1.82815350 | 0.11882998 | 0.00000000 |
| N | 0.11221250 | 0.94670798 | -0.06625800 |

| | | | |
|---|---|---|---|
| N | -2.46688650 | 2.07723498 | -0.47296100 |
| H | -2.78805450 | 2.46773898 | 0.41233400 |
| N | -3.77018450 | -0.71024302 | -0.09563400 |
| H | -2.67479250 | -0.22941902 | 3.65242100 |
| N | -1.18874650 | -1.81025502 | -0.57678000 |
| C | 1.01853650 | 0.46100398 | -1.11724500 |
| H | 2.01220250 | 0.91345798 | -0.99818600 |
| H | 0.63088950 | 0.78827998 | -2.08999500 |
| C | 1.15112350 | -1.06235002 | -1.09858300 |
| H | 1.45623350 | -1.39470402 | -0.09735800 |
| H | 1.97409150 | -1.33245202 | -1.76744800 |
| C | -0.08177450 | -1.84254602 | -1.55596200 |
| H | -0.46117250 | -1.41810702 | -2.49349100 |
| H | 0.20016050 | -2.88257902 | -1.76602800 |
| C | -2.39487250 | -2.52607402 | -1.03703400 |
| H | -2.59366750 | -2.20806402 | -2.06656300 |
| H | -2.24288150 | -3.61201402 | -1.05820700 |
| C | -3.57670250 | -2.17251302 | -0.13960900 |
| H | -3.37656250 | -2.50683002 | 0.88292400 |
| H | -4.47956050 | -2.68915102 | -0.48755700 |
| C | -4.65752750 | -0.17035602 | -1.13964900 |
| H | -5.64876150 | -0.63791002 | -1.07034300 |
| H | -4.24341950 | -0.43812402 | -2.11914700 |
| C | -4.80346150 | 1.34878698 | -1.03802800 |
| H | -5.62580650 | 1.64747898 | -1.69541400 |
| H | -5.11692350 | 1.62402898 | -0.02204800 |
| C | -3.57497250 | 2.16234098 | -1.44708600 |
| H | -3.19472650 | 1.79529798 | -2.40816500 |
| H | -3.86313750 | 3.21093398 | -1.59707100 |
| C | -1.25906750 | 2.81352598 | -0.90070600 |
| H | -1.06580950 | 2.54913498 | -1.94640100 |
| H | -1.41052050 | 3.89906798 | -0.86333600 |
| C | -0.07434250 | 2.40870398 | -0.02911300 |
| H | 0.82845850 | 2.94057098 | -0.35324500 |

| | | | |
|---|---|---|---|
| H | -0.26588850 | 2.68793198 | 1.01150300 |
| H | -0.86208550 | -2.24125102 | 0.28766800 |
| H | 0.45195150 | 0.64802198 | 0.85110300 |
| C | -1.70744750 | 0.05697098 | 2.02260800 |
| O | -0.68192550 | 0.23189198 | 2.66304800 |
| O | -2.86726150 | -0.21906802 | 2.69858300 |
| H | -4.14817950 | -0.46941902 | 0.82024900 |

**Cyclam-TS4**

SCF Energy: -1237.990073
Gibbs Energy: -1237.618958

| | | | |
|---|---|---|---|
| Ni | -3.25383438 | -1.78244970 | -0.04259499 |
| N | -2.47705538 | 0.13660930 | 0.41057001 |
| N | -4.65503738 | -0.72065470 | -1.14047699 |
| H | -5.46546838 | -0.77939470 | -0.49687599 |
| N | -3.97937938 | -3.65117470 | -0.64206699 |
| H | -5.70431438 | -3.37602270 | 2.69778301 |
| N | -1.37508138 | -2.74384770 | 0.03925501 |
| C | -1.20021338 | 0.42883330 | -0.27212599 |
| C | -0.10640838 | -0.57642170 | 0.08902201 |
| H | -0.01591438 | -0.66021570 | 1.18056901 |
| H | 0.84725062 | -0.16623070 | -0.25692899 |
| C | -0.25650338 | -1.96298170 | -0.53567799 |
| C | -1.55475638 | -4.06034870 | -0.61588499 |
| H | -1.46699538 | -3.90364570 | -1.69587799 |
| H | -0.76773838 | -4.76500870 | -0.32508699 |
| C | -2.93160338 | -4.62224970 | -0.27817099 |
| H | -3.00881938 | -4.80505370 | 0.79874401 |
| H | -3.07778438 | -5.58376870 | -0.78472999 |
| C | -4.43992938 | -3.73752070 | -2.04314099 |
| C | -5.54070438 | -2.72376970 | -2.34837299 |
| H | -5.98313838 | -2.99160770 | -3.31241599 |

| | | | |
|---|---|---|---|
| H | -6.34780038 | -2.81182270 | -1.61232399 |
| C | -5.09084238 | -1.26822370 | -2.44114599 |
| C | -4.23819338 | 0.68775530 | -1.22488599 |
| H | -3.54200438 | 0.79789630 | -2.06459399 |
| H | -5.09462538 | 1.34277130 | -1.42139899 |
| C | -3.57140538 | 1.08449230 | 0.08590301 |
| H | -3.20011738 | 2.11483430 | 0.03544301 |
| H | -4.30682038 | 1.02749330 | 0.89397301 |
| H | -1.16784438 | -2.90440570 | 1.02468901 |
| H | -2.30568438 | 0.18705430 | 1.41299101 |
| C | -3.78100338 | -2.12401970 | 1.95339701 |
| O | -3.45106138 | -2.01592570 | 3.05604101 |
| O | -5.39127938 | -3.09606370 | 1.82799101 |
| C | -7.72506238 | -1.28830070 | 0.21609201 |
| O | -8.63471138 | -2.04998970 | 0.86098601 |
| H | -9.47115738 | -1.95705170 | 0.38768901 |
| O | -6.55237238 | -1.31788270 | 0.77316801 |
| H | -6.09877438 | -2.28626770 | 1.38860901 |
| O | -7.99743238 | -0.66113070 | -0.79675199 |
| H | -4.80743338 | -4.75218370 | -2.24292299 |
| H | 0.68223062 | -2.51989370 | -0.42438499 |
| H | -0.86768538 | 1.44320530 | -0.01737399 |
| H | -5.92396538 | -0.66559870 | -2.82032899 |
| H | -1.37651938 | 0.41229930 | -1.35351699 |
| H | -4.25789538 | -1.17802670 | -3.15109599 |
| H | -0.44466138 | -1.86271470 | -1.61103999 |
| H | -3.58081238 | -3.56899270 | -2.70412099 |
| H | -4.77689038 | -3.79390670 | -0.01694299 |

**Cyclam-TS4’**

SCF Energy: -1237.977964
Gibbs Energy: -1237.599015

| | | | |
|---|---|---|---|
| Ni | -2.55941490 | -1.28884824 | 0.00000000 |
| N | -1.62164590 | -3.18967324 | 0.03972300 |
| N | -3.51999490 | -1.95575224 | 1.73315700 |
| H | -4.47361990 | -2.06403124 | 1.35287900 |
| N | -3.36088090 | 0.63457976 | 0.19939200 |
| H | -4.34523790 | 0.47257376 | -0.04136100 |
| N | -0.93051690 | -0.30243124 | -0.91243800 |
| C | -0.19752490 | -3.13531624 | 0.42035300 |
| H | 0.23095510 | -4.14594424 | 0.41909200 |
| H | -0.13012890 | -2.76168424 | 1.44872500 |
| C | 0.62168710 | -2.23662324 | -0.50911800 |
| H | 0.47836010 | -2.54620724 | -1.55340200 |
| H | 1.67902810 | -2.41516524 | -0.29106800 |
| C | 0.37785810 | -0.73343224 | -0.36864400 |
| H | 0.39841510 | -0.45649024 | 0.69251300 |
| H | 1.18814910 | -0.18046624 | -0.86057800 |
| C | -1.16421490 | 1.15355676 | -0.77475300 |
| H | -0.74111690 | 1.46344976 | 0.18565100 |
| H | -0.64375490 | 1.72271276 | -1.55280300 |
| C | -2.66231890 | 1.45925176 | -0.79603000 |
| H | -3.06339990 | 1.23282276 | -1.79083000 |
| H | -2.82494490 | 2.53192976 | -0.63212300 |
| C | -3.33757590 | 1.19540576 | 1.56626700 |
| H | -3.74396890 | 2.21528176 | 1.54381000 |
| H | -2.29673790 | 1.26894176 | 1.90630200 |
| C | -4.16005990 | 0.35569476 | 2.54016800 |
| H | -4.21607090 | 0.91189376 | 3.48141600 |
| H | -5.18116190 | 0.24877176 | 2.15950100 |
| C | -3.58633790 | -1.01751624 | 2.87467000 |
| H | -2.56922690 | -0.90518424 | 3.27343600 |
| H | -4.19276190 | -1.46352624 | 3.67385700 |
| C | -2.91931290 | -3.23871124 | 2.13823400 |
| H | -2.05771690 | -3.00875824 | 2.77603100 |
| H | -3.60847990 | -3.84129124 | 2.74131200 |

| | | | |
|---|---|---|---|
| C | -2.46560090 | -4.03284624 | 0.92095000 |
| H | -1.92902190 | -4.93486124 | 1.23987800 |
| H | -3.33368190 | -4.33751924 | 0.33483900 |
| H | -0.95656790 | -0.55149824 | -1.89989800 |
| H | -1.68330090 | -3.57349724 | -0.90091700 |
| C | -3.86471390 | -1.86433124 | -1.50471100 |
| O | -4.52529490 | -1.18771624 | -2.41803900 |
| O | -4.32311290 | -3.04872124 | -1.34987800 |
| C | -6.81592290 | -1.66846124 | -0.25751400 |
| O | -6.81015590 | -2.68731124 | -0.99715900 |
| H | -5.35085890 | -3.08840124 | -1.49212800 |
| O | -5.77344090 | -1.15332024 | 0.26757400 |
| H | -4.17801990 | -0.29424824 | -2.50085600 |
| O | -8.07194190 | -1.03731724 | 0.00511000 |
| H | -7.92033290 | -0.16267224 | 0.37063800 |

**Cyclam-5**

With$HCO_3$

SCF Energy: -1238.033144
Gibbs Energy: -1237.661996

| | | | |
|---|---|---|---|
| Ni | -2.19378420 | 0.68555758 | 0.00000000 |
| N | -2.41469620 | 2.65636758 | -0.59733300 |
| N | -0.22395720 | 0.87031758 | -0.68367000 |
| H | -0.21108120 | 0.29192258 | -1.53015200 |
| N | -1.90564020 | -1.25994042 | 0.67782800 |
| H | -0.89128820 | -1.99660642 | -3.10349700 |
| N | -3.70086520 | 0.79520858 | 1.42170900 |
| C | -2.55851520 | 3.61783058 | 0.50906500 |
| C | -3.79449220 | 3.30415358 | 1.35633200 |
| H | -4.67768320 | 3.25533558 | 0.70773300 |
| H | -3.95598620 | 4.14724458 | 2.03507100 |

| | | | |
|---|---|---|---|
| C | -3.71397820 | 2.04135958 | 2.21561900 |
| C | -3.61744820 | -0.42569842 | 2.24617700 |
| H | -2.89648220 | -0.23827842 | 3.04954500 |
| H | -4.57872220 | -0.65870942 | 2.71807900 |
| C | -3.15514620 | -1.60072442 | 1.38582100 |
| H | -3.91098620 | -1.81258042 | 0.62411600 |
| H | -3.03826320 | -2.49843642 | 2.00520000 |
| C | -0.66293020 | -1.44938942 | 1.44835200 |
| C | 0.57546280 | -1.13457642 | 0.60686200 |
| H | 1.45263080 | -1.46205042 | 1.17354800 |
| H | 0.55392080 | -1.73153242 | -0.31182300 |
| C | 0.78722680 | 0.33862058 | 0.25615100 |
| C | -0.01417420 | 2.29438258 | -1.01384900 |
| H | 0.29227980 | 2.80609958 | -0.09485400 |
| H | 0.79350680 | 2.42853758 | -1.74245700 |
| C | -1.31108220 | 2.90832658 | -1.54075500 |
| H | -1.17047720 | 3.98041558 | -1.72541700 |
| H | -1.57954120 | 2.43773758 | -2.49133500 |
| H | -4.55126020 | 0.76471758 | 0.85342100 |
| H | -3.30726020 | 2.61172458 | -1.09532800 |
| C | -6.73141720 | -0.38767542 | 0.44781900 |
| O | -7.68857020 | -0.55071742 | -0.13401700 |
| O | -1.03514520 | -1.45066642 | -2.32641400 |
| C | -4.31671920 | 0.40486558 | -1.94690300 |
| O | -4.85095920 | -0.23933242 | -2.99929700 |
| H | -5.69786320 | 0.17959658 | -3.19829800 |
| O | -3.17032820 | -0.05483042 | -1.60439300 |
| H | -1.93763920 | -1.07842942 | -2.38913000 |
| O | -4.92044320 | 1.33954558 | -1.40063500 |
| H | -0.60093420 | -2.48261142 | 1.81462600 |
| H | -4.55847920 | 2.02784058 | 2.91663800 |
| H | -2.64145820 | 4.63743558 | 0.11033300 |
| H | 1.79170780 | 0.46608158 | -0.16785500 |
| H | -1.65413720 | 3.58616158 | 1.13014000 |

| | | | |
|---|---|---|---|
| H | 0.74617880 | 0.94781658 | 1.16864800 |
| H | -2.79742220 | 2.06031758 | 2.81937100 |
| H | -0.69468120 | -0.79820342 | 2.33125600 |
| H | -1.83437620 | -1.80948642 | -0.17941000 |

Without$HCO_3$

SCF Energy: -897.0524899
Gibbs Energy: -896.7262079

| | | | |
|---|---|---|---|
| Ni | -1.60877508 | 0.61243144 | 0.00000000 |
| N | -3.57335508 | -0.18528556 | -0.17626600 |
| N | -1.02515108 | -1.21123256 | -0.83914700 |
| H | -0.67208108 | -1.63461956 | 0.02557900 |
| N | 0.32246092 | 1.47492144 | -0.15606500 |
| N | -2.25771608 | 2.61480844 | -0.49495700 |
| C | -4.42052308 | 0.40574944 | -1.23074600 |
| C | -4.59206508 | 1.91658744 | -1.06914400 |
| H | -4.91149908 | 2.14950444 | -0.04443900 |
| H | -5.41854608 | 2.22689744 | -1.71573000 |
| C | -3.37674308 | 2.76287944 | -1.44668100 |
| C | -1.05798408 | 3.38826944 | -0.86803400 |
| H | -0.86415608 | 3.20718044 | -1.93049300 |
| H | -1.21396808 | 4.46697844 | -0.74760600 |
| C | 0.12794292 | 2.93351344 | -0.02312400 |
| H | -0.06946508 | 3.14353444 | 1.03261200 |
| H | 1.02939192 | 3.48753244 | -0.31230600 |
| C | 1.11171992 | 1.07431544 | -1.33802400 |
| C | 1.28517892 | -0.44087156 | -1.42962000 |
| H | 2.06571192 | -0.64135756 | -2.16996900 |
| H | 1.66626992 | -0.83211756 | -0.47696400 |
| C | 0.04256792 | -1.21943456 | -1.85634600 |
| C | -2.23401508 | -1.93903456 | -1.26646900 |
| H | -2.48624308 | -1.60132956 | -2.27758200 |

| | | | |
|---|---|---|---|
| H | -2.05747808 | -3.01960956 | -1.32250500 |
| C | -3.37841708 | -1.64533156 | -0.30312400 |
| H | -4.29349108 | -2.14522656 | -0.64379500 |
| H | -3.13079708 | -2.03225256 | 0.68945100 |
| H | -2.57416008 | 2.93604244 | 0.42091900 |
| H | -4.00761908 | 0.00202844 | 0.72514500 |
| C | -1.34765108 | 0.04073444 | 1.92098000 |
| O | -1.40507308 | 0.13458944 | 3.10707400 |
| H | 2.09744192 | 1.55642744 | -1.30477700 |
| H | -3.67316208 | 3.81734844 | -1.52086300 |
| H | -5.40621608 | -0.07729256 | -1.22682300 |
| H | 0.32390592 | -2.25405056 | -2.09133100 |
| H | -3.96094508 | 0.18936744 | -2.20197900 |
| H | -0.37024008 | -0.78256156 | -2.77378400 |
| H | -3.01002008 | 2.46217744 | -2.43513100 |
| H | 0.60266992 | 1.44492844 | -2.23516300 |
| H | 0.80781092 | 1.13823444 | 0.67361100 |

**Cyclam-TS2-COOH**

SCF Energy: -1201.381174
Gibbs Energy: -1200.997513

| | | | |
|---|---|---|---|
| Ni | -0.09140768 | -0.33820840 | 0.00000000 |
| N | 0.84416632 | -2.24326840 | -0.06799400 |
| N | -1.18225468 | -1.13062940 | 1.56758800 |
| H | -2.10177668 | -1.25036340 | 1.10956100 |
| N | -0.95857368 | 1.55957760 | 0.23368200 |
| H | -1.90619568 | 1.44285860 | -0.13607800 |
| N | 1.56122032 | 0.69778260 | -0.72778500 |
| C | 2.24357032 | -2.22673640 | 0.39924000 |
| H | 2.67668732 | -3.23326340 | 0.33227400 |
| H | 2.25077732 | -1.94620440 | 1.45906200 |
| C | 3.10942632 | -1.24790840 | -0.39837000 |

| | | | |
|---|---|---|---|
| H | 3.02519932 | -1.46468640 | -1.47184600 |
| H | 4.15506632 | -1.43870640 | -0.13904500 |
| C | 2.83887432 | 0.23528860 | -0.14367700 |
| H | 2.79114232 | 0.42218960 | 0.93604700 |
| H | 3.66845132 | 0.83449660 | -0.53849300 |
| C | 1.30831232 | 2.14393060 | -0.52725500 |
| H | 1.66137532 | 2.39861260 | 0.47692600 |
| H | 1.88368032 | 2.75098560 | -1.23419500 |
| C | -0.18449268 | 2.44018460 | -0.66195100 |
| H | -0.51804368 | 2.23619560 | -1.68331000 |
| H | -0.37177068 | 3.49932960 | -0.44515700 |
| C | -1.06555068 | 2.03194960 | 1.62505300 |
| H | -1.49203868 | 3.04391860 | 1.63833400 |
| H | -0.05967968 | 2.10044760 | 2.05870200 |
| C | -1.94307868 | 1.10930360 | 2.46880500 |
| H | -2.08400468 | 1.59327760 | 3.44094200 |
| H | -2.93106768 | 1.01801460 | 2.00633100 |
| C | -1.37202068 | -0.27486040 | 2.75995500 |
| H | -0.39974368 | -0.17735340 | 3.25893300 |
| H | -2.04103468 | -0.78781040 | 3.46311600 |
| C | -0.58158068 | -2.42898640 | 1.93411800 |
| H | 0.23570732 | -2.22327740 | 2.63427400 |
| H | -1.29473568 | -3.07419340 | 2.45969900 |
| C | -0.05063968 | -3.14194540 | 0.69734100 |
| H | 0.46460932 | -4.06480940 | 0.99035300 |
| H | -0.87938968 | -3.40259240 | 0.03873500 |
| H | 1.57997132 | 0.50632960 | -1.72887600 |
| H | 0.83375132 | -2.54738340 | -1.03940500 |
| C | -1.35838268 | -0.72943340 | -1.67904200 |
| O | -1.75239968 | 0.20375360 | -2.33460800 |
| O | -1.81755668 | -1.93056840 | -1.53253300 |
| C | -4.70502368 | -0.72509140 | -0.28297000 |
| O | -4.59061868 | -1.63500040 | -1.15123500 |
| H | -3.17315068 | -1.93682340 | -1.64173400 |

| | | | |
|---|---|---|---|
| O | -3.71084468 | -0.29442440 | 0.39239400 |
| C | -6.04955568 | -0.10355540 | -0.03171300 |
| H | -6.24957068 | -0.03451340 | 1.04014800 |
| H | -6.05116768 | 0.90904860 | -0.44357300 |
| H | -6.82605168 | -0.68632540 | -0.52953300 |

**Cyclam-TS2-OH**

SCF Energy: -1087.99142
Gibbs Energy: -1087.619064

| | | | |
|---|---|---|---|
| Ni | -1.37111513 | -0.94149907 | 0.00000000 |
| N | -1.16528613 | 1.10265993 | -0.53344800 |
| N | 0.20412687 | -1.24879607 | -1.35816100 |
| H | -0.26700813 | -1.61386307 | -2.18699300 |
| N | -1.32040613 | -2.92014907 | 0.71464300 |
| H | -1.93215313 | -3.36401507 | 0.02611400 |
| N | -1.86192013 | -0.43898007 | 2.01994700 |
| C | -0.69898213 | 2.08888693 | 0.45478000 |
| H | -0.77864513 | 3.09998793 | 0.03501200 |
| H | 0.36299487 | 1.90333293 | 0.65390900 |
| C | -1.48776013 | 2.01930093 | 1.76114900 |
| H | -2.56018713 | 2.13329793 | 1.55482600 |
| H | -1.20436613 | 2.88578393 | 2.36623100 |
| C | -1.24400013 | 0.76842993 | 2.60317900 |
| H | -0.16746613 | 0.57937093 | 2.68867300 |
| H | -1.62598513 | 0.92860993 | 3.61997700 |
| C | -1.61458313 | -1.66142607 | 2.80911800 |
| H | -0.54124013 | -1.70581707 | 3.02408300 |
| H | -2.13951913 | -1.63590007 | 3.77172300 |
| C | -2.04379813 | -2.88172507 | 2.00442000 |
| H | -3.11272613 | -2.82210607 | 1.77840500 |
| H | -1.87396413 | -3.79820807 | 2.58112200 |
| C | -0.03583813 | -3.64342507 | 0.74889800 |

| | | | |
|---|---|---|---|
| H | -0.20723113 | -4.69034207 | 1.02935000 |
| H | 0.58759987 | -3.19577207 | 1.53094300 |
| C | 0.69296787 | -3.58470507 | -0.59225300 |
| H | 1.53242687 | -4.28488307 | -0.54506900 |
| H | 0.03789387 | -3.95724707 | -1.39114600 |
| C | 1.25403087 | -2.21433707 | -0.96909400 |
| H | 1.79488087 | -1.78627207 | -0.11705100 |
| H | 1.97613387 | -2.32467507 | -1.78809400 |
| C | 0.74415587 | 0.08805593 | -1.69078000 |
| H | 1.42515187 | 0.37707893 | -0.88294900 |
| H | 1.32620987 | 0.06391493 | -2.61953400 |
| C | -0.40046713 | 1.08734393 | -1.79528100 |
| H | -0.01335613 | 2.08282293 | -2.04207200 |
| H | -1.08658513 | 0.79205893 | -2.59541600 |
| H | -2.86928213 | -0.28556807 | 1.96886600 |
| H | -2.15089413 | 1.27664593 | -0.76093800 |
| C | -3.29600313 | -0.99375007 | -0.99986400 |
| O | -3.81927613 | 0.04732193 | -1.40924200 |
| O | -3.83679113 | -2.16720607 | -1.21444900 |
| C | -6.99528013 | -1.20545907 | 0.12147800 |
| O | -6.42499413 | -1.41224507 | -1.12485100 |
| H | -5.13573413 | -2.00440407 | -1.16605900 |
| H | -7.05506713 | -0.13951407 | 0.37077900 |
| H | -6.48343313 | -1.75466107 | 0.92387000 |
| H | -8.02665213 | -1.59064107 | 0.05564000 |

**Cyclam-TS4-COOH**

SCF Energy: -1202.064758
Gibbs Energy: -1201.671367

| | | | |
|---|---|---|---|
| Ni | -1.91956118 | -0.57586836 | 0.00000000 |
| N | -1.54376318 | -2.66802436 | -0.11537600 |
| N | -3.26720918 | -1.09511936 | 1.46332900 |

| | | | |
|---|---|---|---|
| H | -4.15123818 | -1.12238736 | 0.91748900 |
| N | -2.19836718 | 1.46635664 | 0.21402200 |
| H | -4.50571018 | 1.51783864 | -2.26017700 |
| N | 0.03615282 | -0.04116336 | -0.64090300 |
| C | -0.20403418 | -3.06441236 | 0.36372200 |
| C | 0.91509982 | -2.38910336 | -0.42860900 |
| H | 0.75809782 | -2.54346536 | -1.50487700 |
| H | 1.85075682 | -2.90385836 | -0.18980700 |
| C | 1.12559182 | -0.90614436 | -0.13214800 |
| C | 0.20892882 | 1.37804064 | -0.24758100 |
| H | 0.45260882 | 1.39386564 | 0.82032600 |
| H | 1.04478982 | 1.84396064 | -0.78190000 |
| C | -1.09293318 | 2.13104864 | -0.49004300 |
| H | -1.32941018 | 2.13221964 | -1.56039600 |
| H | -0.98416218 | 3.17763564 | -0.18152400 |
| C | -2.46295318 | 1.96432064 | 1.57421200 |
| C | -3.66839918 | 1.26191264 | 2.19884800 |
| H | -3.95536918 | 1.81889464 | 3.09589200 |
| H | -4.52317318 | 1.31686964 | 1.51282600 |
| C | -3.42522118 | -0.18703536 | 2.61363700 |
| C | -2.99812218 | -2.48754036 | 1.86419100 |
| H | -2.16545618 | -2.49415436 | 2.57800000 |
| H | -3.86715718 | -2.92792436 | 2.36653800 |
| C | -2.66643718 | -3.30128836 | 0.62133700 |
| H | -2.42805818 | -4.33774836 | 0.88701300 |
| H | -3.54060418 | -3.30273236 | -0.03603300 |
| H | 0.04927882 | -0.09069036 | -1.65944900 |
| H | -1.61216518 | -2.95757436 | -1.08908100 |
| C | -3.05312018 | -0.68472036 | -1.78085400 |
| O | -3.33785218 | -1.12064836 | -2.79573200 |
| O | -4.28067618 | 1.07235564 | -1.43639400 |
| C | -6.41152318 | -1.01942736 | -0.31622600 |
| O | -5.38479518 | -1.70870236 | -0.13235300 |
| H | -5.34365518 | 0.62660264 | -0.97906300 |

| | | | |
|---|---|---|---|
| O | -6.38177118 | 0.22938664 | -0.61849700 |
| H | -2.65133318 | 3.04497164 | 1.53480800 |
| H | 2.08466682 | -0.57748936 | -0.55167700 |
| H | -0.09511218 | -4.15434336 | 0.29668400 |
| H | -4.26051018 | -0.53251936 | 3.23630700 |
| H | -0.12395218 | -2.79993236 | 1.42432400 |
| H | -2.51828618 | -0.25052436 | 3.22940300 |
| H | 1.18378782 | -0.75403536 | 0.95192300 |
| H | -1.57173118 | 1.81372364 | 2.19792500 |
| H | -3.06370318 | 1.56756664 | -0.35719000 |
| C | -7.78342418 | -1.63078836 | -0.19538000 |
| H | -7.72663518 | -2.61915236 | 0.25990200 |
| H | -8.43580818 | -0.97580336 | 0.38622500 |
| H | -8.22039418 | -1.71836336 | -1.19468000 |

**Cyclam-TS4-OH**

SCF Energy: -1088.688964
Gibbs Energy: -1088.295856

| | | | |
|---|---|---|---|
| Ni | -2.52285183 | 0.42961608 | 0.00000000 |
| N | -3.49423983 | -1.44032992 | 0.17363400 |
| N | -1.23978583 | -0.57014392 | -1.29159500 |
| H | -0.36390183 | -0.64193792 | -0.73135900 |
| N | -1.63610683 | 2.30052808 | -0.33013000 |
| H | -0.05042583 | 1.12520508 | 2.93094300 |
| N | -4.29530983 | 1.53659108 | 0.32503900 |
| C | -4.80247183 | -1.50923692 | -0.50289900 |
| C | -5.78300083 | -0.47188292 | 0.04681800 |
| H | -5.85561983 | -0.56968392 | 1.13848800 |
| H | -6.77688783 | -0.71752192 | -0.33963000 |
| C | -5.49770483 | 0.98082308 | -0.33362500 |
| C | -4.00261383 | 2.92808108 | -0.08689300 |
| H | -4.15115183 | 2.98817808 | -1.17021000 |

| | | | |
|---|---|---|---|
| H | -4.69720783 | 3.64038908 | 0.37288400 |
| C | -2.56057683 | 3.28266708 | 0.26316700 |
| H | -2.41982883 | 3.25252408 | 1.34831400 |
| H | -2.33738383 | 4.30335308 | -0.07102300 |
| C | -1.24754283 | 2.57991608 | -1.72570400 |
| C | -0.28477983 | 1.52677008 | -2.27189100 |
| H | 0.11172017 | 1.90089308 | -3.22084200 |
| H | 0.56652217 | 1.41229108 | -1.59017300 |
| C | -0.90117183 | 0.15343608 | -2.53422600 |
| C | -1.79514983 | -1.90824492 | -1.54889900 |
| H | -2.50949083 | -1.83422492 | -2.37749500 |
| H | -1.01796383 | -2.61678392 | -1.85918100 |
| C | -2.49400383 | -2.42448392 | -0.29596000 |
| H | -2.95395083 | -3.40177992 | -0.48661400 |
| H | -1.75742583 | -2.54811692 | 0.50375800 |
| H | -4.45143683 | 1.52398408 | 1.33251600 |
| H | -3.64738883 | -1.59357792 | 1.16876400 |
| C | -1.85722983 | 0.30871208 | 1.93683800 |
| O | -2.21035783 | -0.09757792 | 2.98009500 |
| O | -0.34098783 | 1.13467608 | 2.00848600 |
| C | 2.23071217 | -0.45453592 | 0.68059700 |
| O | 0.89377817 | -0.11172592 | 0.38459500 |
| H | 0.44102917 | 0.43160108 | 1.15506000 |
| H | -0.78121883 | 3.57183408 | -1.78852100 |
| H | -6.37352883 | 1.59811408 | -0.09536500 |
| H | -5.23202083 | -2.51338292 | -0.39031900 |
| H | -0.19824183 | -0.44655292 | -3.12680600 |
| H | -4.64738583 | -1.34446292 | -1.57529500 |
| H | -1.81609183 | 0.25844408 | -3.13352800 |
| H | -5.34021783 | 1.05399208 | -1.41636300 |
| H | -2.15680883 | 2.61215108 | -2.33928900 |
| H | -0.79742283 | 2.25707408 | 0.25165800 |
| H | 2.81096317 | 0.43892608 | 0.94109800 |
| H | 2.28461917 | -1.15040592 | 1.52726100 |

| | | | |
|---|---|---|---|
| H | 2.70680517 | -0.93527592 | -0.18197500 |

**Cl-ver-1**

SCF Energy: -2810.73243
Gibbs Energy: -2810.44619

| | | | |
|---|---|---|---|
| Ni | -0.60329066 | 0.46617915 | 0.00000000 |
| N | 1.29669334 | 0.47336215 | -0.84126600 |
| N | -1.23546366 | -0.40565885 | -1.72691200 |
| H | -1.56340966 | 0.38420115 | -2.28853900 |
| N | -2.50148066 | 1.13643115 | 0.51119300 |
| H | -2.60842166 | 1.80937415 | -0.26702700 |
| N | 0.02982734 | 1.29348615 | 1.74779900 |
| C | 2.39111734 | -0.04195285 | -0.01579700 |
| C | 2.40401234 | 0.60272915 | 1.38363500 |
| H | 2.65378834 | 1.66264915 | 1.23306300 |
| H | 3.24396534 | 0.16950215 | 1.93214000 |
| C | 1.18115834 | 0.57180615 | 2.31855000 |
| C | -1.17417566 | 1.44513515 | 2.60686100 |
| H | -1.40014166 | 0.46748015 | 3.03337600 |
| H | -0.98709566 | 2.14760815 | 3.42620000 |
| C | -2.35557066 | 1.93353215 | 1.75927900 |
| H | -2.19646266 | 2.97072315 | 1.45044100 |
| H | -3.26907566 | 1.90110615 | 2.35962500 |
| C | -3.59350866 | 0.16507015 | 0.41396800 |
| C | -3.60852666 | -0.54563285 | -0.95294400 |
| H | -4.44513366 | -1.24862785 | -0.94383200 |
| H | -3.86508066 | 0.22152015 | -1.69722900 |
| C | -2.38613266 | -1.30001085 | -1.50670700 |
| C | -0.03034666 | -0.99040185 | -2.37290100 |
| H | 0.19643034 | -1.92725085 | -1.86328000 |
| H | -0.21667766 | -1.20571285 | -3.43056700 |
| C | 1.15064234 | -0.02098985 | -2.23709500 |

| | | | |
|---|---|---|---|
| H | 2.06379934 | -0.51456685 | -2.58105200 |
| H | 0.99148934 | 0.86000315 | -2.86556600 |
| H | 0.35794134 | 2.22133415 | 1.46752200 |
| H | 1.40016034 | 1.50138215 | -0.89384800 |
| C | -0.60215766 | 2.71985715 | -1.09991600 |
| O | 0.53951834 | 3.18503015 | -1.11835300 |
| O | -1.74262766 | 3.02742215 | -1.45229600 |
| H | -2.68821766 | -1.76654485 | -2.44938000 |
| H | -4.55689166 | 0.67402015 | 0.51754400 |
| H | 1.48105834 | 1.02809715 | 3.26691300 |
| H | 3.35332334 | 0.19134515 | -0.48225400 |
| Cl | 0.65891534 | -1.09034885 | 2.74422600 |
| Cl | 2.34678834 | -1.83745585 | 0.01815700 |
| Cl | -1.86135366 | -2.65921985 | -0.46077100 |
| Cl | -3.54353566 | -0.96223285 | 1.81175900 |

**Cl-ver-TS2**

SCF Energy: -3075.747538
Gibbs Energy: -3075.432722

| | | | |
|---|---|---|---|
| Ni | -0.95063982 | 0.17367459 | 0.00000000 |
| N | -1.38239482 | -1.76803541 | -0.56498000 |
| N | -0.89983682 | 0.62669659 | -2.00387600 |
| H | 0.08515118 | 0.69580559 | -2.26590000 |
| N | -0.13620082 | 1.99065759 | 0.57663800 |
| H | 0.79928418 | 1.81167459 | 0.18718300 |
| N | -1.29482682 | -0.17513741 | 1.99636600 |
| C | -2.55330982 | -2.43403941 | 0.01419600 |
| H | -2.50788482 | -3.50813941 | -0.19158300 |
| C | -2.58917482 | -2.27668941 | 1.54588200 |
| H | -1.73163782 | -2.84348741 | 1.93592500 |
| H | -3.48008782 | -2.79812141 | 1.90466400 |
| C | -2.55791082 | -0.90261341 | 2.23796000 |

| | | | |
|---|---|---|---|
| H | -2.68912882 | -1.07502841 | 3.31061500 |
| C | -1.13403982 | 1.12974459 | 2.69545400 |
| H | -2.06995782 | 1.67722759 | 2.59024000 |
| H | -0.93697782 | 0.98148359 | 3.76242100 |
| C | 0.00631118 | 1.92817859 | 2.05734200 |
| H | 0.96728418 | 1.44544059 | 2.25887600 |
| H | 0.04056118 | 2.92766259 | 2.49958600 |
| C | -0.60142282 | 3.23672559 | -0.04212900 |
| H | 0.12321118 | 4.03532659 | 0.14462000 |
| C | -0.72352482 | 3.09125059 | -1.57111700 |
| H | -1.12755882 | 4.03100959 | -1.95561500 |
| H | 0.30031318 | 3.02049559 | -1.96511000 |
| C | -1.52231482 | 1.94759559 | -2.21799000 |
| H | -1.60902282 | 2.15999959 | -3.28765600 |
| C | -1.52485082 | -0.51622241 | -2.72514900 |
| H | -2.60438582 | -0.36955941 | -2.70172600 |
| H | -1.20175482 | -0.54290341 | -3.77083900 |
| C | -1.16765282 | -1.83777241 | -2.03660700 |
| H | -1.74772182 | -2.64903941 | -2.48579200 |
| H | -0.10837782 | -2.06517441 | -2.18683000 |
| H | -0.53434082 | -0.79606841 | 2.28138100 |
| H | -0.55797682 | -2.20142641 | -0.13036200 |
| C | 1.31595918 | -0.58678241 | 0.07005000 |
| O | 1.36668418 | -1.77766041 | 0.35754100 |
| O | 2.07900318 | 0.34045459 | -0.23379700 |
| C | 5.65413718 | -0.04330341 | -0.00363000 |
| O | 4.74913418 | 0.20559959 | -0.93989700 |
| H | 3.63010318 | 0.20362259 | -0.47960900 |
| O | 5.07574018 | -0.19662241 | 1.21433800 |
| H | 5.79051218 | -0.38871841 | 1.83415000 |
| O | 6.83673118 | -0.12059941 | -0.20014500 |
| Cl | -2.10055782 | 3.82440459 | 0.74757700 |
| Cl | -3.21103282 | 1.85363859 | -1.61434700 |
| Cl | -4.05197482 | -1.89738041 | -0.80938800 |

| | | | |
|---|---|---|---|
| Cl | -3.93421682 | 0.14366259 | 1.76671000 |

**Cl-ver-3**

SCF Energy: -2811.381697
Gibbs Energy: -2811.081617

| | | | |
|---|---|---|---|
| Ni | 3.05301635 | -0.66727604 | 0.00000000 |
| N | 5.07056335 | -0.65720804 | -0.54648900 |
| N | 2.66153535 | -1.18063004 | -1.97632300 |
| H | 2.30323235 | -0.31817104 | -2.38710000 |
| N | 1.03475135 | -0.56494004 | 0.54541300 |
| H | 2.16410135 | 3.01856896 | -0.37434000 |
| N | 3.45558135 | -0.79195604 | 2.03856600 |
| C | 6.05320835 | -1.47915504 | 0.16042900 |
| H | 7.06475535 | -1.11282704 | -0.04405600 |
| C | 5.85953035 | -1.40830604 | 1.68608300 |
| H | 6.10408535 | -0.37754504 | 1.98085500 |
| H | 6.62768135 | -2.04045104 | 2.13875200 |
| C | 4.52485335 | -1.75254004 | 2.36808400 |
| H | 4.70478035 | -1.75737704 | 3.44813100 |
| C | 2.16209035 | -0.99602104 | 2.73885400 |
| H | 1.96289735 | -2.06621904 | 2.76040600 |
| H | 2.21189035 | -0.63795004 | 3.77341600 |
| C | 1.02920335 | -0.27303004 | 2.00242200 |
| H | 1.15521435 | 0.80898396 | 2.10009000 |
| H | 0.07291035 | -0.53796504 | 2.46412700 |
| C | 0.07234835 | -1.53448204 | 0.00993100 |
| H | -0.94792465 | -1.16094004 | 0.14757000 |
| C | 0.26317035 | -1.74674804 | -1.50366600 |
| H | -0.49699365 | -2.46305604 | -1.82577400 |
| H | 0.00071535 | -0.79423904 | -1.98640300 |
| C | 1.59946735 | -2.19484704 | -2.12104400 |
| H | 1.41339335 | -2.39288104 | -3.18177400 |

| | | | |
|---|---|---|---|
| C | 3.96399335 | -1.50603404 | -2.61614200 |
| H | 4.17429435 | -2.55563104 | -2.41670600 |
| H | 3.91536835 | -1.36566204 | -3.70181800 |
| C | 5.08392235 | -0.64011104 | -2.03006500 |
| H | 6.04417035 | -0.97972504 | -2.43093800 |
| H | 4.95167135 | 0.40310896 | -2.33117400 |
| H | 3.81263335 | 0.13665696 | 2.26632200 |
| H | 5.22862235 | 0.31098696 | -0.23911300 |
| C | 3.14864535 | 1.38249096 | -0.13864100 |
| O | 4.18270735 | 2.02463296 | -0.00905500 |
| O | 1.97960535 | 2.06283696 | -0.35640200 |
| H | 0.83139935 | 0.31897496 | 0.07362700 |
| Cl | 6.07629735 | -3.15598404 | -0.48225700 |
| Cl | 3.95932535 | -3.41285704 | 1.99489800 |
| Cl | 0.09636135 | -3.05479604 | 0.95971500 |
| Cl | 2.17862135 | -3.75755004 | -1.46189100 |

**Cl-ver-TS4**

SCF Energy: -3076.402233
Gibbs Energy: -3076.072954

| | | | |
|---|---|---|---|
| Ni | 4.38756840 | -0.59414990 | 0.00000000 |
| N | 3.49838140 | -2.47031190 | -0.36176500 |
| N | 5.53885740 | -0.98364990 | -1.63650500 |
| H | 6.45264640 | -1.24853690 | -1.21484400 |
| N | 5.33431340 | 1.19319610 | 0.45542800 |
| H | 7.56795740 | -0.82908590 | 2.56437900 |
| N | 2.81982240 | 0.08286210 | 1.19863900 |
| C | 2.04560640 | -2.55798490 | -0.60888700 |
| C | 1.24927340 | -1.70087690 | 0.39260400 |
| H | 1.37926440 | -2.16628890 | 1.38073400 |
| H | 0.19111240 | -1.82261190 | 0.14720000 |
| C | 1.50715640 | -0.19596790 | 0.57564000 |

| | | | |
|---|---|---|---|
| C | 3.09149940 | 1.51513310 | 1.50940400 |
| H | 2.67601440 | 2.11134210 | 0.69888200 |
| H | 2.60011240 | 1.81103910 | 2.44212700 |
| C | 4.59875640 | 1.76875510 | 1.60861200 |
| H | 5.00478740 | 1.29038610 | 2.50571700 |
| H | 4.77531040 | 2.84470610 | 1.70435100 |
| C | 5.74868840 | 2.09383210 | -0.63111000 |
| C | 6.46998540 | 1.33836310 | -1.75640900 |
| H | 6.77130840 | 2.07748610 | -2.50248100 |
| H | 7.40197740 | 0.94900710 | -1.32826100 |
| C | 5.83127240 | 0.16375510 | -2.50917400 |
| C | 5.01676740 | -2.18214090 | -2.33176400 |
| H | 4.24959340 | -1.87031090 | -3.03841800 |
| H | 5.81924440 | -2.68077290 | -2.88675000 |
| C | 4.43027840 | -3.15564190 | -1.30963100 |
| H | 3.93539040 | -3.98664290 | -1.82124700 |
| H | 5.23776840 | -3.57040490 | -0.69907100 |
| H | 2.84463140 | -0.44546290 | 2.07080000 |
| H | 3.61859640 | -2.93171390 | 0.53940400 |
| C | 5.41632840 | -1.51270090 | 1.63953600 |
| O | 5.29616640 | -2.26846790 | 2.50548500 |
| O | 7.09954340 | -0.62109890 | 1.74601700 |
| C | 8.87649840 | -1.25965090 | -1.02315000 |
| O | 10.00133940 | -1.06320490 | -0.31208400 |
| H | 10.70534640 | -0.84826690 | -0.93766700 |
| O | 7.85322240 | -1.57580890 | -0.27950600 |
| H | 7.64800440 | -1.10396190 | 0.80553000 |
| O | 8.82846840 | -1.13148190 | -2.23644500 |
| H | 6.20434840 | 0.80261310 | 0.84175300 |
| Cl | 4.35035340 | 0.64918810 | -3.41380000 |
| Cl | 1.64459940 | -2.22123790 | -2.31731700 |
| Cl | 1.39287640 | 0.71868210 | -0.95720100 |
| Cl | 4.36771540 | 3.09393410 | -1.19543400 |
| H | 6.45619340 | 2.83081510 | -0.23804300 |

| | | | |
|---|---|---|---|
| H | 6.54886740 | -0.14481290 | -3.27411600 |
| H | 1.71892140 | -3.59294590 | -0.46550300 |
| H | 0.70518140 | 0.19899310 | 1.20734800 |

**CN-ver-1**

SCF Energy: -1341.20594
Gibbs Energy: -1340.890725

| | | | |
|---|---|---|---|
| Ni | -1.46202159 | 0.68632481 | -0.02032326 |
| N | 0.52862941 | 0.80457881 | -0.61049126 |
| N | -1.89832259 | 0.40759481 | -2.02675726 |
| H | -2.19538459 | 1.32220681 | -2.37002526 |
| N | -3.45270659 | 0.80500981 | 0.56990774 |
| H | -3.61300359 | 1.75736581 | 0.21625574 |
| N | -1.02583059 | 0.40829081 | 1.98626074 |
| C | 1.53147241 | -0.07974619 | 0.01797274 |
| C | 1.40996241 | -0.06870619 | 1.55767774 |
| H | 1.60832241 | 0.95501881 | 1.89592474 |
| H | 2.21827941 | -0.68802419 | 1.95561474 |
| C | 0.09755841 | -0.53735619 | 2.22403074 |
| C | -2.30973559 | 0.03959881 | 2.64299574 |
| H | -2.49411759 | -1.02010419 | 2.45022174 |
| H | -2.25491259 | 0.18459481 | 3.72712674 |
| C | -3.44298059 | 0.88152981 | 2.05563674 |
| H | -3.30983359 | 1.93571481 | 2.31582574 |
| H | -4.39717459 | 0.55439781 | 2.48042774 |
| C | -4.45564359 | -0.07948119 | -0.05818926 |
| C | -4.33413459 | -0.06909219 | -1.59790126 |
| H | -5.14249359 | -0.68852619 | -1.99557626 |
| H | -4.53242459 | 0.95449481 | -1.93660626 |
| C | -3.02175659 | -0.53813519 | -2.26403426 |
| C | -0.61441859 | 0.03850281 | -2.68329926 |
| H | -0.43013359 | -1.02113819 | -2.49007526 |

| | | | |
|---|---|---|---|
| H | -0.66919059 | 0.18306281 | -3.76748926 |
| C | 0.51892641 | 0.88053281 | -2.09624826 |
| H | 1.47307141 | 0.55308581 | -2.52090626 |
| H | 0.38593441 | 1.93463081 | -2.35686026 |
| H | -0.72871459 | 1.32306081 | 2.32907474 |
| H | 0.68889841 | 1.75706681 | -0.25715626 |
| C | -1.46179659 | 3.01050481 | -0.02041626 |
| O | -0.31687359 | 3.43342781 | 0.14747374 |
| O | -2.60659059 | 3.43378781 | -0.18813126 |
| H | -3.22036359 | -0.60444719 | -3.34244726 |
| H | -5.46325359 | 0.29698081 | 0.16861874 |
| H | 0.29616541 | -0.60309619 | 3.30247974 |
| H | 2.53911941 | 0.29652781 | -0.20898426 |
| C | -4.39298859 | -1.42017219 | 0.54612474 |
| N | -4.38123159 | -2.43393919 | 1.10253274 |
| C | -2.60527359 | -1.88090419 | -1.83091426 |
| N | -2.23594659 | -2.92991619 | -1.51252226 |
| C | -0.31896259 | -1.88034919 | 1.79164674 |
| N | -0.68831859 | -2.92953919 | 1.47387774 |
| C | 1.46867741 | -1.42066219 | -0.58582726 |
| N | 1.45679541 | -2.43462319 | -1.14188126 |

**CN-ver-TS2**

SCF Energy: -1606.225572
Gibbs Energy: -1605.883326

| | | | |
|---|---|---|---|
| Ni | -2.68738565 | -0.77696525 | 0.00000000 |
| N | -3.20307565 | -2.68662725 | -0.66817200 |
| N | -3.43158765 | -0.08765825 | -1.80472500 |
| H | -2.59895165 | 0.02971675 | -2.38613700 |
| N | -1.94885265 | 1.08181375 | 0.60003700 |
| H | -1.13259465 | 1.14081375 | -0.01552400 |
| N | -2.46066165 | -1.35052325 | 1.97672200 |

| | | | |
|---|---|---|---|
| C | -4.08896665 | -3.53330625 | 0.16493500 |
| C | -3.62615065 | -3.55900625 | 1.63755600 |
| H | -2.62996165 | -4.01653925 | 1.66525700 |
| H | -4.28960565 | -4.24045725 | 2.17692400 |
| C | -3.56015765 | -2.24149625 | 2.43834200 |
| C | -2.30016365 | -0.09554925 | 2.76572500 |
| H | -3.29605665 | 0.31977275 | 2.93812500 |
| H | -1.84566465 | -0.30028225 | 3.74022000 |
| C | -1.43917165 | 0.89892175 | 1.98757800 |
| H | -0.40810965 | 0.53903675 | 1.89576800 |
| H | -1.40387565 | 1.84951175 | 2.52930200 |
| C | -2.76794265 | 2.28205875 | 0.32065700 |
| C | -3.19112065 | 2.34042875 | -1.16338100 |
| H | -3.69562465 | 3.29732775 | -1.32288600 |
| H | -2.27415265 | 2.37166475 | -1.76337600 |
| C | -4.10417565 | 1.23907075 | -1.74583000 |
| C | -4.25781465 | -1.19231425 | -2.36348300 |
| H | -5.22963465 | -1.17016325 | -1.86437200 |
| H | -4.42430165 | -1.05898025 | -3.43765400 |
| C | -3.56541065 | -2.53040825 | -2.10711400 |
| H | -4.21037265 | -3.34643725 | -2.44699800 |
| H | -2.63427465 | -2.59022225 | -2.67816400 |
| H | -1.59064465 | -1.88311625 | 2.03158200 |
| H | -2.27715565 | -3.11881825 | -0.63907600 |
| C | -0.62247665 | -1.06979425 | -0.85471400 |
| O | -0.28563965 | -2.22483025 | -0.69264600 |
| O | -0.07673965 | -0.03133325 | -1.29629800 |
| C | 2.33782935 | -0.87086725 | 0.29511200 |
| O | 2.37822335 | -0.68717925 | -0.98208000 |
| H | 1.09452635 | -0.27537325 | -1.38797100 |
| O | 3.55572935 | -1.16576525 | 0.79508300 |
| H | 3.43774835 | -1.29430225 | 1.74297200 |
| O | 1.35026735 | -0.82255425 | 1.04218700 |
| H | -4.03185965 | -4.57231325 | -0.18886600 |

| | | | |
|---|---|---|---|
| H | -4.36606565 | 1.55434475 | -2.76493800 |
| H | -2.16029165 | 3.18044475 | 0.49976200 |
| H | -3.39115965 | -2.51481825 | 3.48840300 |
| C | -5.49238265 | -3.13562125 | -0.02598900 |
| N | -6.59217865 | -2.86783125 | -0.26254200 |
| C | -3.88262565 | 2.36854175 | 1.27699200 |
| N | -4.69422765 | 2.45816475 | 2.09586100 |
| C | -5.37192065 | 1.10080775 | -1.01322700 |
| N | -6.38423565 | 0.96214375 | -0.47122000 |
| C | -4.81864865 | -1.48134625 | 2.38694700 |
| N | -5.78290165 | -0.84349325 | 2.34336800 |

**CN-ver-3**

SCF Energy: -1341.860593
Gibbs Energy: -1341.53214

| | | | |
|---|---|---|---|
| Ni | -6.06946962 | 0.22851919 | 0.00000000 |
| N | -4.03889762 | 0.21935719 | -0.54932500 |
| N | -6.44394362 | -0.27665881 | -1.99965800 |
| H | -6.72741562 | 0.59454719 | -2.44722700 |
| N | -8.10209762 | 0.27837419 | 0.55196800 |
| H | -6.95235662 | 3.91383219 | -0.12613900 |
| N | -5.68992762 | -0.06342781 | 2.04099200 |
| C | -3.06857162 | -0.63628481 | 0.15985000 |
| H | -2.04859762 | -0.27981781 | -0.04625300 |
| C | -3.24473862 | -0.54891981 | 1.69105700 |
| H | -3.06864962 | 0.49349119 | 1.98156200 |
| H | -2.44350762 | -1.13623681 | 2.14784300 |
| C | -4.57344062 | -0.99714881 | 2.33720300 |
| H | -4.39929262 | -1.02528181 | 3.42218400 |
| C | -6.98700362 | -0.42972581 | 2.66370400 |
| H | -7.15706962 | -1.49407481 | 2.48709600 |
| H | -6.97127762 | -0.26725681 | 3.74737500 |

| | | | |
|---|---|---|---|
| C | -8.11346362 | 0.39014719 | 2.03381900 |
| H | -7.98311062 | 1.45048919 | 2.26873600 |
| H | -9.07293562 | 0.07384719 | 2.45667100 |
| C | -9.05843862 | -0.66834081 | -0.06051800 |
| H | -10.08425062 | -0.31008881 | 0.11018400 |
| C | -8.88603062 | -0.74470881 | -1.59328400 |
| H | -9.68036862 | -1.38996481 | -1.97851800 |
| H | -9.07871462 | 0.25594419 | -1.99808700 |
| C | -7.55403562 | -1.24420081 | -2.19446000 |
| H | -7.73125762 | -1.38532481 | -3.27010200 |
| C | -5.14164162 | -0.70342481 | -2.57661200 |
| H | -4.96840862 | -1.74228981 | -2.28714500 |
| H | -5.15756762 | -0.65744681 | -3.67139900 |
| C | -4.01919762 | 0.18064619 | -2.03243900 |
| H | -3.05879262 | -0.17871381 | -2.41723500 |
| H | -4.14538662 | 1.21060919 | -2.37909800 |
| H | -5.40695462 | 0.85377019 | 2.38577300 |
| H | -3.85820162 | 1.18882919 | -0.26401500 |
| C | -5.95963062 | 2.26818919 | -0.05440800 |
| O | -4.91098862 | 2.89450819 | 0.00113100 |
| O | -7.13840662 | 2.95822919 | -0.12802600 |
| H | -8.32288962 | 1.20256719 | 0.17781200 |
| C | -8.99748362 | -1.97377481 | 0.61596800 |
| N | -9.01163262 | -2.96049381 | 1.21891200 |
| C | -4.96997062 | -2.36079281 | 1.95308600 |
| N | -5.31676662 | -3.43202681 | 1.68829800 |
| C | -7.14988962 | -2.55932481 | -1.67378800 |
| N | -6.80552262 | -3.59925281 | -1.30258900 |
| C | -3.10582662 | -2.00878181 | -0.37180500 |
| N | -3.08079762 | -3.05385581 | -0.86649600 |

**CN-ver-TS4**

SCF Energy: -1606.879609

Gibbs Energy: -1606.523759

| | | | |
|---|---|---|---|
| Ni | -2.43144416 | 0.94149907 | 0.00000000 |
| N | -1.65716916 | -0.86904293 | 0.78423200 |
| N | -3.54879616 | 1.01614907 | 1.71389000 |
| H | -4.47975516 | 0.68859707 | 1.38663400 |
| N | -3.21902616 | 2.69394407 | -0.80825900 |
| H | -5.62525716 | 0.42219707 | -2.45054100 |
| N | -0.78612316 | 1.27897207 | -1.26347100 |
| C | -0.19973416 | -0.97047293 | 1.04524700 |
| C | 0.62841784 | -0.50063493 | -0.16967600 |
| H | 0.36957384 | -1.14424293 | -1.01940800 |
| H | 1.67989684 | -0.70050993 | 0.05435100 |
| C | 0.53012084 | 0.96613907 | -0.64053100 |
| C | -0.91535616 | 2.68094107 | -1.75082600 |
| H | -0.50970916 | 3.34271007 | -0.98301300 |
| H | -0.33774716 | 2.83462207 | -2.66848700 |
| C | -2.38738416 | 3.01384007 | -1.99572400 |
| H | -2.77897916 | 2.42021407 | -2.82804600 |
| H | -2.47707816 | 4.06817407 | -2.27816100 |
| C | -3.54691916 | 3.82022507 | 0.09911900 |
| C | -4.38051716 | 3.35636707 | 1.30913800 |
| H | -4.67050516 | 4.24867207 | 1.87032600 |
| H | -5.30733016 | 2.91808707 | 0.92856500 |
| C | -3.77958716 | 2.35358407 | 2.31282800 |
| C | -3.02274116 | 0.01958107 | 2.67385300 |
| H | -2.18415516 | 0.45871007 | 3.21822700 |
| H | -3.79292616 | -0.25957993 | 3.40108800 |
| C | -2.57377416 | -1.22371393 | 1.91089900 |
| H | -2.10426816 | -1.93881693 | 2.59430800 |
| H | -3.44461416 | -1.71040093 | 1.46212700 |
| H | -0.88162616 | 0.65319607 | -2.06298100 |
| H | -1.83230916 | -1.54074393 | 0.03903300 |
| C | -3.51308316 | -0.20629293 | -1.41528300 |

| | | | |
|---|---|---|---|
| O | -3.45307216 | -1.12147493 | -2.11719500 |
| O | -5.12498516 | 0.76480607 | -1.69844500 |
| C | -6.87696516 | 0.77976607 | 1.16859300 |
| O | -8.02408516 | 0.84243107 | 0.47141700 |
| H | -8.70002116 | 1.21234207 | 1.05420100 |
| O | -5.88977016 | 0.27499407 | 0.48463300 |
| H | -5.67358916 | 0.51809607 | -0.69025600 |
| O | -6.77837916 | 1.17848207 | 2.32022800 |
| H | -4.11319116 | 2.32585207 | -1.15484900 |
| H | -4.17513416 | 4.53762607 | -0.44779500 |
| H | -4.52727016 | 2.24749407 | 3.11039200 |
| H | 0.05771284 | -2.02825093 | 1.19903400 |
| H | 1.32344584 | 1.10955107 | -1.38728600 |
| C | 0.16456084 | -0.31083493 | 2.30747100 |
| N | 0.45348084 | 0.11511307 | 3.34287600 |
| C | -2.53583616 | 2.84329307 | 2.92965300 |
| N | -1.55529316 | 3.19304007 | 3.43436600 |
| C | -2.32910616 | 4.56939907 | 0.44878400 |
| N | -1.37637816 | 5.19978307 | 0.62942800 |
| C | 0.79980584 | 1.93044707 | 0.43612700 |
| N | 1.02327284 | 2.71902507 | 1.25228300 |

**OMe-ver-1**

SCF Energy: -1430.408764
Gibbs Energy: -1429.958188

| | | | |
|---|---|---|---|
| Ni | -1.82815350 | -0.63071297 | 0.00000000 |
| N | 0.14991750 | -0.37692197 | -0.63131300 |
| N | -2.27201650 | -0.97011697 | -1.95877700 |
| H | -2.56112750 | -0.07787797 | -2.35868900 |
| N | -3.77966250 | -0.11670597 | 0.50823200 |
| H | -3.82381950 | 0.77751303 | -0.00649200 |
| N | -1.38573350 | -0.42012297 | 1.99119700 |

| | | | |
|---|---|---|---|
| C | 1.18102250 | -1.14096897 | 0.07794000 |
| C | 0.98801850 | -1.06534897 | 1.60811500 |
| H | 1.22525950 | -0.05014297 | 1.94918400 |
| H | 1.75124650 | -1.70988797 | 2.05534000 |
| C | -0.38576250 | -1.47865397 | 2.18197600 |
| C | -2.68291350 | -0.61499897 | 2.68096900 |
| H | -2.92003550 | -1.67893597 | 2.62075600 |
| H | -2.62274450 | -0.31695497 | 3.73360900 |
| C | -3.77172150 | 0.18551803 | 1.95903000 |
| H | -3.58471650 | 1.25846503 | 2.06356900 |
| H | -4.74310650 | -0.03145497 | 2.41351200 |
| C | -4.83574650 | -1.01079197 | 0.02962800 |
| C | -4.69491150 | -1.28747097 | -1.48185700 |
| H | -5.52195350 | -1.94685597 | -1.76433100 |
| H | -4.87121050 | -0.35099697 | -2.02616200 |
| C | -3.38960150 | -1.92343197 | -2.01224200 |
| C | -0.99794150 | -1.41782697 | -2.57154000 |
| H | -0.81106250 | -2.43347797 | -2.22007300 |
| H | -1.06458350 | -1.42141497 | -3.66576600 |
| C | 0.13389450 | -0.49537597 | -2.10904900 |
| H | 1.08703150 | -0.87620597 | -2.48693200 |
| H | -0.00962750 | 0.51212103 | -2.51140900 |
| H | -0.99813950 | 0.50088803 | 2.18443600 |
| H | 0.23953050 | 0.62320903 | -0.39177500 |
| C | -1.76671350 | 1.88546403 | -0.38236300 |
| O | -0.61848450 | 2.32111103 | -0.27010400 |
| O | -2.89893250 | 2.31390803 | -0.62256100 |
| H | -3.56791250 | -2.23677497 | -3.05631800 |
| H | -5.81486650 | -0.52414497 | 0.18180100 |
| H | -0.27032650 | -1.72137497 | 3.25126200 |
| H | 2.17062550 | -0.70867797 | -0.14917100 |
| O | -4.77938450 | -2.17082397 | 0.81449100 |
| O | -2.93152450 | -3.01168597 | -1.26463900 |
| O | 1.13538150 | -2.45171497 | -0.41511000 |

| | | | |
|---|---|---|---|
| O | -0.97003750 | -2.55948597 | 1.50314100 |
| C | -3.68657850 | -4.20002997 | -1.39942000 |
| H | -3.80934450 | -4.46935397 | -2.45640700 |
| H | -3.12526550 | -4.98476597 | -0.89287500 |
| H | -4.66941850 | -4.10595797 | -0.92596100 |
| C | -0.47137450 | -3.84577497 | 1.82378900 |
| H | -1.05118150 | -4.55176797 | 1.23081800 |
| H | 0.58618650 | -3.94405897 | 1.56011400 |
| H | -0.61413150 | -4.05781197 | 2.89047800 |
| C | -6.03954250 | -2.76783197 | 1.06607100 |
| H | -5.84779350 | -3.66834797 | 1.64963200 |
| H | -6.69032250 | -2.09440597 | 1.63870900 |
| H | -6.55100350 | -3.05065797 | 0.13635000 |
| C | 2.39127950 | -3.10544897 | -0.46613600 |
| H | 2.21382650 | -4.08915797 | -0.90093300 |
| H | 3.09982750 | -2.55275097 | -1.09647300 |
| H | 2.82843050 | -3.23268797 | 0.53336400 |

**OMe-ver-TS2**

SCF Energy: -1695.41326
Gibbs Energy: -1694.929461

| | | | |
|---|---|---|---|
| Ni | -3.80255928 | -1.38025592 | 0.00000000 |
| N | -3.82949628 | 0.68272508 | -0.47988800 |
| N | -2.33701028 | -1.54196292 | -1.47158500 |
| H | -2.84655628 | -1.88226692 | -2.28683900 |
| N | -3.87823628 | -3.44240592 | 0.39071200 |
| H | -4.35727028 | -3.80168692 | -0.43336600 |
| N | -4.78320928 | -1.16126392 | 1.85952800 |
| C | -3.51457228 | 1.67146808 | 0.56171700 |
| C | -4.15235428 | 1.25732208 | 1.89984900 |
| H | -5.23891628 | 1.38784208 | 1.83393000 |
| H | -3.81151928 | 1.96807808 | 2.65816000 |

| | | | |
|---|---|---|---|
| C | -3.83134528 | -0.17501592 | 2.37148000 |
| C | -4.68437528 | -2.47260792 | 2.53778900 |
| H | -3.70610128 | -2.52363292 | 3.01753700 |
| H | -5.45969928 | -2.57514492 | 3.30400100 |
| C | -4.79701728 | -3.62382492 | 1.54022500 |
| H | -5.80958728 | -3.65492292 | 1.13099700 |
| H | -4.60468328 | -4.57333492 | 2.05255100 |
| C | -2.57280128 | -4.10042092 | 0.47810100 |
| C | -1.78020528 | -3.90366492 | -0.83359800 |
| H | -0.91052328 | -4.56780792 | -0.80033500 |
| H | -2.39904128 | -4.28016592 | -1.65860800 |
| C | -1.24518228 | -2.51112592 | -1.20244300 |
| C | -1.87623328 | -0.15993992 | -1.74087000 |
| H | -1.20281828 | 0.12081308 | -0.93117200 |
| H | -1.33999428 | -0.09523992 | -2.69643800 |
| C | -3.07048228 | 0.79422008 | -1.74409900 |
| H | -2.71750428 | 1.81597008 | -1.91575900 |
| H | -3.75730828 | 0.53732308 | -2.55684300 |
| H | -5.74658028 | -0.83617792 | 1.78817900 |
| H | -4.82585428 | 0.77198208 | -0.68668200 |
| C | -5.67316828 | -1.57511992 | -1.02874300 |
| O | -6.38484528 | -0.56465392 | -0.95942000 |
| O | -6.22338128 | -2.74733692 | -1.27599900 |
| C | -8.85912628 | -1.44863492 | 0.35273800 |
| O | -8.45259328 | -1.57294292 | -0.86546300 |
| H | -7.21484628 | -2.57738392 | -1.26930300 |
| O | -7.85523828 | -1.44008792 | 1.30390300 |
| H | -8.33734128 | -1.39148192 | 2.14075400 |
| O | -10.02030228 | -1.37564592 | 0.69780700 |
| H | -3.93570528 | 2.64997508 | 0.27245300 |
| H | -0.65209328 | -2.62454492 | -2.12480300 |
| H | -2.71718728 | -5.19109292 | 0.60042900 |
| H | -3.77200328 | -0.20554392 | 3.46991000 |
| O | -0.42840728 | -2.00332992 | -0.18935100 |

| | | | |
|---|---|---|---|
| O | -1.96759428 | -3.59622592 | 1.62961200 |
| O | -2.12085628 | 1.79066208 | 0.63077500 |
| O | -2.62178228 | -0.66172392 | 1.82282600 |
| C | -0.78612128 | -4.26440492 | 2.02581300 |
| H | -0.53890228 | -3.89414992 | 3.02113900 |
| H | -0.94052228 | -5.35050592 | 2.07730400 |
| H | 0.04356372 | -4.03931492 | 1.34594400 |
| C | 0.91796272 | -1.75326892 | -0.56371000 |
| H | 0.98093072 | -1.01955992 | -1.37706100 |
| H | 1.41542972 | -1.35010892 | 0.31914000 |
| H | 1.42443172 | -2.67729892 | -0.86808700 |
| C | -1.43034228 | -0.50660092 | 2.57060700 |
| H | -1.54233228 | -0.96431892 | 3.56116000 |
| H | -0.66252728 | -1.03356692 | 2.00657900 |
| H | -1.16526228 | 0.55072508 | 2.66925800 |
| C | -1.65894728 | 3.05660008 | 1.06720800 |
| H | -0.57095128 | 3.02869108 | 1.00381400 |
| H | -2.03843728 | 3.86089808 | 0.42384200 |
| H | -1.94723828 | 3.26150508 | 2.10633200 |

**OMe-ver-3**

SCF Energy: -1431.055597
Gibbs Energy: -1430.592524

| | | | |
|---|---|---|---|
| Ni | -2.41316262 | 0.30164533 | 0.00000000 |
| N | -0.36919562 | -0.00891667 | -0.49033600 |
| N | -2.82149862 | -0.95234667 | -1.63196200 |
| H | -3.03605962 | -0.28014167 | -2.36814600 |
| N | -4.43524562 | 0.64485733 | 0.44972900 |
| H | -4.66705062 | 1.30082733 | -0.29543100 |
| N | -2.04325662 | 0.87793633 | 2.02695000 |
| C | 0.54160638 | -0.62588467 | 0.48091500 |
| C | 0.22191438 | -0.16092967 | 1.91247000 |

| | | | |
|---|---|---|---|
| H | 0.53722338 | 0.88226333 | 2.03373900 |
| H | 0.85469238 | -0.74283967 | 2.58921700 |
| C | -1.24976562 | -0.31184467 | 2.35010900 |
| C | -3.37000062 | 0.89719433 | 2.68408200 |
| H | -3.60573862 | -0.12683267 | 2.97582600 |
| H | -3.35588162 | 1.52432933 | 3.58200800 |
| C | -4.45816462 | 1.38735133 | 1.72700600 |
| H | -4.28946862 | 2.44004033 | 1.48290000 |
| H | -5.43528462 | 1.30587833 | 2.21808300 |
| C | -5.32350662 | -0.51139167 | 0.34482400 |
| C | -5.25427362 | -1.12379867 | -1.07132700 |
| H | -6.07630162 | -1.84082167 | -1.16426200 |
| H | -5.47881062 | -0.32670067 | -1.79189600 |
| C | -3.98516262 | -1.86166067 | -1.52314700 |
| C | -1.54196262 | -1.62025267 | -1.95453900 |
| H | -1.39546562 | -2.41299567 | -1.22069100 |
| H | -1.55842062 | -2.05750867 | -2.96206700 |
| C | -0.39174162 | -0.62055367 | -1.83529300 |
| H | 0.55133838 | -1.12670567 | -2.06538000 |
| H | -0.51837062 | 0.19328133 | -2.55584200 |
| H | -1.53012162 | 1.74052533 | 2.17522000 |
| H | -0.12525962 | 0.98051933 | -0.59730500 |
| C | -2.24591462 | 2.10307533 | -0.98018900 |
| O | -1.18806862 | 2.66234833 | -1.24205500 |
| O | -3.41216362 | 2.74551133 | -1.33062400 |
| H | -3.18331762 | 3.59401433 | -1.74879000 |
| H | 1.58009138 | -0.33030967 | 0.25067900 |
| H | -4.19275362 | -2.28022967 | -2.52227000 |
| H | -6.37189062 | -0.18868867 | 0.49833500 |
| H | -1.29937462 | -0.54369667 | 3.42548900 |
| O | -3.67864662 | -2.90905467 | -0.64851100 |
| O | -4.96622362 | -1.36980267 | 1.38734900 |
| O | 0.43898238 | -2.01923667 | 0.34561800 |
| O | -1.93306062 | -1.30642567 | 1.62219800 |

| | | | |
|---|---|---|---|
| C | -5.85929162 | -2.44238267 | 1.60814300 |
| H | -5.56490562 | -2.90462967 | 2.55093700 |
| H | -6.89532062 | -2.08693267 | 1.69349800 |
| H | -5.78914762 | -3.18976567 | 0.80959400 |
| C | -3.62513862 | -4.19472667 | -1.24575100 |
| H | -2.86109762 | -4.24492267 | -2.03158200 |
| H | -3.36596562 | -4.89759767 | -0.45293600 |
| H | -4.59716962 | -4.47730967 | -1.66872800 |
| C | -1.99648562 | -2.61040767 | 2.16659700 |
| H | -2.42165462 | -2.58151067 | 3.17770100 |
| H | -2.65921162 | -3.16796267 | 1.50650000 |
| H | -1.00598162 | -3.07644367 | 2.18445800 |
| C | 1.63268338 | -2.72449967 | 0.62936000 |
| H | 1.42288738 | -3.77950067 | 0.45115800 |
| H | 2.44997738 | -2.40237167 | -0.02919700 |
| H | 1.94470338 | -2.59801467 | 1.67441400 |

**OMe-ver-TS4**

SCF Energy: -1696.078071
Gibbs Energy: -1695.585792

| | | | |
|---|---|---|---|
| Ni | -1.86471657 | 1.45338206 | 0.00000000 |
| N | -1.31006257 | 1.13937006 | 2.01971100 |
| N | -3.37235057 | 2.64850906 | 0.78544500 |
| H | -4.20948157 | 2.04742906 | 0.71143200 |
| N | -2.42302457 | 1.77827606 | -1.96712300 |
| H | -4.55949957 | -1.19941394 | -1.52085000 |
| N | -0.00990457 | 0.73071206 | -0.81419400 |
| C | -0.08669557 | 1.93919506 | 1.94926200 |
| C | 1.07777643 | 1.06316506 | 1.43883600 |
| H | 0.95781743 | 0.03886906 | 1.81115800 |
| H | 2.02034243 | 1.42914006 | 1.85380000 |
| C | 1.26540443 | 1.04275006 | -0.08607200 |

| | | | |
|---|---|---|---|
| C | -0.01944657 | 1.19268306 | -2.22440000 |
| H | 0.29389543 | 2.23469006 | -2.21753300 |
| H | 0.67411443 | 0.60885406 | -2.84295200 |
| C | -1.42351357 | 1.10083306 | -2.81575200 |
| H | -1.73760857 | 0.05515106 | -2.90090900 |
| H | -1.41085157 | 1.52418706 | -3.82721300 |
| C | -2.68595457 | 3.18639006 | -2.25749200 |
| C | -3.89122257 | 3.68452506 | -1.44043700 |
| H | -4.20961057 | 4.64683606 | -1.85396300 |
| H | -4.72823357 | 3.00053906 | -1.62057600 |
| C | -3.73543957 | 3.89470406 | 0.07045600 |
| C | -3.09254957 | 2.87835906 | 2.21507900 |
| H | -2.42975657 | 3.73996606 | 2.29074700 |
| H | -4.01554757 | 3.10277906 | 2.76390100 |
| C | -2.43492857 | 1.64791006 | 2.83614400 |
| H | -2.11059557 | 1.88078206 | 3.85811100 |
| H | -3.16081657 | 0.83123806 | 2.89231800 |
| H | -0.09940557 | -0.28459494 | -0.80896200 |
| H | -1.10578657 | 0.18253306 | 2.28687000 |
| C | -2.76653057 | -0.48113794 | -0.09106500 |
| O | -2.61108157 | -1.58526094 | 0.22377500 |
| O | -4.22080357 | -0.32845094 | -1.27856800 |
| C | -6.58671757 | 1.69847306 | -0.12800100 |
| O | -7.37639357 | 1.08102106 | -1.03149000 |
| H | -8.13161957 | 1.66058606 | -1.19260900 |
| O | -5.53656157 | 0.99564106 | 0.18643700 |
| H | -5.03669857 | 0.27885706 | -0.58593700 |
| O | -6.84011157 | 2.80601906 | 0.31633100 |
| H | -2.94072857 | 3.30121006 | -3.32781500 |
| H | 1.99337843 | 0.25146106 | -0.32213000 |
| H | 0.15922843 | 2.39413006 | 2.92135000 |
| H | -4.71663057 | 4.21732006 | 0.44963500 |
| H | -3.29555457 | 1.24596106 | -2.03132500 |
| O | -1.47413257 | 3.84519806 | -2.01014900 |

| | | | |
|---|---|---|---|
| O | -2.77317157 | 4.88212406 | 0.34284200 |
| O | -0.43451557 | 2.94482406 | 1.02492800 |
| O | 1.77881443 | 2.27221006 | -0.49533600 |
| C | 0.19932043 | 4.21085606 | 1.13409000 |
| H | -0.25889657 | 4.82871506 | 0.36413900 |
| H | 0.00011543 | 4.64780906 | 2.12059200 |
| H | 1.27433743 | 4.12027606 | 0.96093500 |
| C | -3.31271757 | 6.10528806 | 0.81334200 |
| H | -3.83941957 | 5.96979906 | 1.76675800 |
| H | -2.47163657 | 6.78496606 | 0.95955000 |
| H | -4.00459557 | 6.54672306 | 0.08453000 |
| C | -1.42031557 | 5.18397506 | -2.46267100 |
| H | -0.38538057 | 5.50872106 | -2.34829600 |
| H | -1.70271257 | 5.25677906 | -3.52154500 |
| H | -2.06663457 | 5.83188306 | -1.86106200 |
| C | 2.95457043 | 2.21674606 | -1.29068400 |
| H | 2.77954543 | 1.69424006 | -2.23872100 |
| H | 3.23184543 | 3.25001406 | -1.49997000 |
| H | 3.77429243 | 1.72675406 | -0.75168500 |

**NHMe-ver-1**

SCF Energy: -1350.977777
Gibbs Energy: -1350.471132

| | | | |
|---|---|---|---|
| Ni | -5.02742213 | -0.39305301 | 0.00000000 |
| N | -7.14009913 | -0.28059301 | -0.25928000 |
| N | -4.93118513 | 1.08900599 | -1.44398700 |
| H | -4.78977613 | 0.54032099 | -2.29438000 |
| N | -3.01262213 | -0.85250901 | -0.14344900 |
| H | -3.04955313 | -1.28873001 | -1.07119500 |
| N | -5.07350513 | -1.68958001 | 1.63463100 |
| C | -8.00648713 | -0.10402201 | 0.92350200 |
| C | -7.41502913 | -0.96307601 | 2.06502200 |

| | | | |
|---|---|---|---|
| H | -7.57438913 | -2.01779001 | 1.81887700 |
| H | -8.00564313 | -0.78127301 | 2.96857200 |
| C | -5.91323813 | -0.74603801 | 2.40048200 |
| C | -3.65937713 | -1.81111601 | 2.05830200 |
| H | -3.38555413 | -0.91184301 | 2.60893300 |
| H | -3.51945313 | -2.67059201 | 2.72246800 |
| C | -2.74902013 | -1.93034401 | 0.83336100 |
| H | -2.94106913 | -2.88134301 | 0.32714000 |
| H | -1.70152113 | -1.93831901 | 1.15233300 |
| C | -2.05289513 | 0.27379499 | -0.20783100 |
| C | -2.45034713 | 1.20520899 | -1.37358500 |
| H | -1.64789113 | 1.94195199 | -1.47895900 |
| H | -2.44923113 | 0.61537999 | -2.29917300 |
| C | -3.76806113 | 2.01100299 | -1.30365700 |
| C | -6.27890013 | 1.69118299 | -1.49130700 |
| H | -6.39397913 | 2.32579899 | -0.60870400 |
| H | -6.41555413 | 2.31247399 | -2.38537400 |
| C | -7.32292413 | 0.57092799 | -1.45567500 |
| H | -8.33306513 | 0.98057399 | -1.52894000 |
| H | -7.18768813 | -0.07840801 | -2.32643100 |
| H | -5.50794013 | -2.60039701 | 1.52143800 |
| H | -7.24950613 | -1.25339501 | -0.57428000 |
| H | -9.01204413 | -0.49385201 | 0.68849800 |
| H | -5.76592213 | -0.88862701 | 3.47986600 |
| H | -1.06952413 | -0.14504601 | -0.47601200 |
| H | -3.75603613 | 2.69477999 | -2.16430100 |
| N | -1.94086213 | 0.94082499 | 1.07323100 |
| N | -3.86279513 | 2.82689299 | -0.11304800 |
| N | -5.44641513 | 0.59799699 | 1.99691900 |
| N | -8.10543513 | 1.28884899 | 1.36711700 |
| C | -0.64073813 | 0.82550399 | 1.72890800 |
| H | -0.44165113 | -0.21499301 | 2.00262300 |
| H | 0.19750787 | 1.17981399 | 1.11082000 |
| H | -0.65402413 | 1.40937399 | 2.65260200 |

| | | | |
|---|---|---|---|
| C | -4.33973713 | 4.19535499 | -0.28130500 |
| H | -3.62105313 | 4.76158999 | -0.87950200 |
| H | -5.32506813 | 4.28160799 | -0.76307100 |
| H | -4.39397413 | 4.67384399 | 0.69909300 |
| C | -9.07379813 | 2.15148299 | 0.67770500 |
| H | -9.38158813 | 2.94437499 | 1.36161600 |
| H | -8.63035113 | 2.63498699 | -0.19451200 |
| H | -9.97184713 | 1.60453699 | 0.35825600 |
| C | -4.61636813 | 1.32477799 | 2.97531100 |
| H | -4.93160713 | 1.12089099 | 4.00509800 |
| H | -3.56084013 | 1.07923299 | 2.84938200 |
| H | -4.72976713 | 2.39892999 | 2.80398800 |
| C | -5.31500713 | -2.13513501 | -1.69053200 |
| O | -4.29180913 | -2.17141401 | -2.38082400 |
| O | -6.41536313 | -2.68669801 | -1.63327500 |
| H | -2.20273113 | 1.91595399 | 0.96898400 |
| H | -4.35597513 | 2.33171599 | 0.62019800 |
| H | -8.37376613 | 1.26539599 | 2.34519400 |
| H | -6.26584013 | 1.17434199 | 1.78205400 |

**NHMe-ver-TS2**

SCF Energy: -1615.979556
Gibbs Energy: -1615.442854

| | | | |
|---|---|---|---|
| Ni | -3.58318086 | 0.30164533 | 0.00000000 |
| N | -4.44258986 | -1.48237567 | -0.82915200 |
| N | -4.13852686 | 1.20668033 | -1.77667700 |
| H | -3.29819686 | 1.09602933 | -2.34898000 |
| N | -2.30635986 | 1.83793733 | 0.55383900 |
| H | -1.56908786 | 1.71440733 | -0.14277200 |
| N | -3.20849686 | -0.50742567 | 1.87697900 |
| C | -5.42818986 | -2.23355467 | -0.02681700 |
| C | -4.95190686 | -2.22692167 | 1.44085900 |
| H | -4.05674986 | -2.85504767 | 1.49997500 |

| | | | |
|---|---|---|---|
| H | -5.70166386 | -2.73383167 | 2.05206100 |
| C | -4.63905086 | -0.84145467 | 2.06233100 |
| C | -2.69635586 | 0.62393333 | 2.68843800 |
| H | -3.54277486 | 1.23958333 | 2.99002300 |
| H | -2.20186486 | 0.25963533 | 3.59461700 |
| C | -1.73130086 | 1.48755133 | 1.87563900 |
| H | -0.80045486 | 0.94670733 | 1.68429400 |
| H | -1.49324686 | 2.39148833 | 2.44542600 |
| C | -2.85821686 | 3.19338133 | 0.39231500 |
| C | -3.23610886 | 3.42505433 | -1.09687700 |
| H | -3.43978986 | 4.49406433 | -1.22460200 |
| H | -2.34370786 | 3.22657433 | -1.70348900 |
| C | -4.42367686 | 2.67160833 | -1.73325400 |
| C | -5.20008386 | 0.34670633 | -2.33325100 |
| H | -6.09844186 | 0.51873333 | -1.73619600 |
| H | -5.41756986 | 0.59362933 | -3.38098400 |
| C | -4.77400786 | -1.12213167 | -2.22661800 |
| H | -5.54395986 | -1.77430767 | -2.65569500 |
| H | -3.87132886 | -1.28544267 | -2.82350700 |
| H | -2.59935986 | -1.31713267 | 1.94995700 |
| H | -3.58206486 | -2.03679267 | -0.84689600 |
| C | -1.63782086 | -0.61933967 | -1.14413600 |
| O | -1.57845686 | -1.83996367 | -1.06711200 |
| O | -1.00397986 | 0.30879833 | -1.67978100 |
| C | 2.05939914 | 0.07651033 | -0.02300400 |
| O | 1.87119814 | 0.13315833 | -1.32141200 |
| H | 0.52794214 | 0.23078633 | -1.57247600 |
| O | 3.35508214 | -0.07824867 | 0.24492200 |
| H | 3.44828014 | -0.11729467 | 1.20421800 |
| O | 1.19532614 | 0.15656233 | 0.83666500 |
| H | -5.45186086 | -3.28632467 | -0.36101800 |
| H | -4.48272386 | 3.01794033 | -2.78003000 |
| H | -2.07228986 | 3.92922933 | 0.62034100 |
| H | -4.89570586 | -0.85724567 | 3.13027700 |

| | | | |
|---|---|---|---|
| N | -6.75147386 | -1.62668167 | -0.17434300 |
| N | -3.89391686 | 3.38116833 | 1.38061300 |
| N | -5.68943086 | 2.93415733 | -1.07118400 |
| N | -5.36369686 | 0.25085733 | 1.37648500 |
| H | -5.58485186 | 3.73594133 | -0.46280700 |
| H | -4.70291786 | 2.82130333 | 1.13732000 |
| H | -7.00510786 | -1.63546967 | -1.15600700 |
| H | -6.04836986 | -0.16190867 | 0.73164600 |
| C | -7.81979886 | -2.30002767 | 0.57009300 |
| H | -8.78051786 | -1.93952767 | 0.19950300 |
| H | -7.79317386 | -3.39425967 | 0.46728800 |
| H | -7.76489486 | -2.04912567 | 1.63263200 |
| C | -6.11988386 | 1.16678333 | 2.24189200 |
| H | -6.84484686 | 0.62707333 | 2.86324000 |
| H | -5.46354986 | 1.74106933 | 2.89795200 |
| H | -6.66810386 | 1.86224633 | 1.60136100 |
| C | -6.81583786 | 3.20412633 | -1.97008200 |
| H | -7.68770886 | 3.47984133 | -1.37297500 |
| H | -6.61025886 | 4.01491733 | -2.68381000 |
| H | -7.07921986 | 2.31189633 | -2.54232300 |
| C | -4.26093886 | 4.76325833 | 1.65348400 |
| H | -3.39732786 | 5.29725933 | 2.05968100 |
| H | -4.61924686 | 5.32943733 | 0.77676100 |
| H | -5.04682586 | 4.78047333 | 2.41172200 |

**NHMe-ver-3**

SCF Energy: -1351.604607
Gibbs Energy: -1351.086225

| | | | |
|---|---|---|---|
| Ni | -1.24314438 | -0.31992687 | 0.00000000 |
| N | 0.52606262 | -1.46497387 | 0.20694800 |
| N | -1.68618338 | -1.11749687 | 1.97938400 |
| H | -2.50821638 | -1.70107287 | 2.08951600 |

| | | | |
|---|---|---|---|
| N | -3.05447138 | 0.66831413 | -0.27992000 |
| H | -3.14318538 | -2.49140487 | -2.53201300 |
| N | -0.50532838 | 1.08102313 | -1.35065300 |
| C | 1.82942062 | -0.82200387 | 0.03426100 |
| C | 1.79878762 | 0.04945813 | -1.24348000 |
| H | 1.48545662 | -0.60769987 | -2.06450300 |
| H | 2.83105162 | 0.33196613 | -1.47677100 |
| C | 0.97298162 | 1.35703713 | -1.28710100 |
| C | -1.33905438 | 2.29482213 | -1.20090700 |
| H | -0.86514538 | 2.86858913 | -0.40759200 |
| H | -1.30070438 | 2.90789713 | -2.11039000 |
| C | -2.82293538 | 2.01369213 | -0.84365100 |
| H | -3.44920438 | 2.13574513 | -1.73256700 |
| H | -3.17226738 | 2.76334313 | -0.12989300 |
| C | -3.96691138 | 0.49734913 | 0.87336500 |
| C | -3.33747138 | 0.72017013 | 2.26439300 |
| H | -3.38561938 | 1.78347413 | 2.51569000 |
| H | -3.98924638 | 0.21562313 | 2.98739700 |
| C | -1.90619438 | 0.23333113 | 2.52134500 |
| C | -0.47580338 | -1.80863987 | 2.47448900 |
| H | 0.12749862 | -1.08774487 | 3.03625600 |
| H | -0.74107538 | -2.60047087 | 3.18236600 |
| C | 0.33561662 | -2.41322887 | 1.31898200 |
| H | 1.28876562 | -2.80817887 | 1.69723700 |
| H | -0.21661438 | -3.26540787 | 0.91339300 |
| H | -0.68200738 | 0.65870813 | -2.26037000 |
| H | 0.33408062 | -1.99686187 | -0.65229100 |
| C | -1.78349738 | -1.80801787 | -1.36187900 |
| O | -1.02647538 | -2.67490287 | -1.79413600 |
| O | -3.05550038 | -1.77702887 | -1.87709700 |
| H | -1.74012738 | 0.25577913 | 3.61318500 |
| H | -4.23965238 | -0.57102787 | 0.80092500 |
| H | 1.24275762 | 1.85376713 | -2.23049000 |
| H | 2.59202062 | -1.60415687 | -0.15249700 |

| | | | |
|---|---|---|---|
| N | 2.18656662 | -0.08629887 | 1.25227200 |
| N | -0.92128538 | 1.07074813 | 1.82438800 |
| N | -5.13033138 | 1.34756013 | 0.75975100 |
| N | 1.28388662 | 2.27866913 | -0.22437900 |
| C | -6.08674138 | 0.94043213 | -0.26325100 |
| H | -6.95372638 | 1.60235613 | -0.22727500 |
| H | -5.63971438 | 1.04598213 | -1.25666000 |
| H | -6.42959938 | -0.09990387 | -0.15137600 |
| C | -0.96146938 | 2.49273213 | 2.18209400 |
| H | -1.82810538 | 2.98208613 | 1.73368300 |
| H | -0.99949638 | 2.64705513 | 3.26922100 |
| H | -0.06935338 | 2.97240213 | 1.78085800 |
| C | 3.58525962 | 0.36296713 | 1.26289700 |
| H | 4.29540862 | -0.44185587 | 1.02501200 |
| H | 3.73293262 | 1.16816813 | 0.53874000 |
| H | 3.82213762 | 0.75948313 | 2.25188300 |
| C | 2.20893962 | 3.34763213 | -0.57114100 |
| H | 2.43153262 | 3.93204013 | 0.32492800 |
| H | 3.16444162 | 2.99460613 | -0.99261800 |
| H | 1.74827262 | 4.02238013 | -1.29972800 |
| H | -3.42284638 | 0.07194213 | -1.01814400 |
| H | -5.59027438 | 1.45738513 | 1.65570100 |
| H | 0.02064962 | 0.73708013 | 2.02854200 |
| H | 2.08626562 | -0.72829487 | 2.03317600 |
| H | 1.57428362 | 1.76995313 | 0.60204300 |

**NHMe-ver-TS4**

SCF Energy: -1616.628334
Gibbs Energy: -1616.082623

| | | | |
|---|---|---|---|
| Ni | -2.23034727 | -0.19195612 | 0.00000000 |
| N | -2.72311827 | -0.35248612 | -2.01727400 |
| N | -0.58011727 | 0.91795088 | -0.62439300 |

| | | | |
|---|---|---|---|
| H | 0.17183173 | 0.21171888 | -0.62349100 |
| N | -1.72116427 | -0.05818412 | 1.99935400 |
| H | 0.24122373 | -3.11402912 | 1.48422000 |
| N | -4.15768827 | -0.92990512 | 0.75413400 |
| C | -3.98484927 | 0.41322688 | -1.91253800 |
| C | -5.11595327 | -0.56959812 | -1.51099100 |
| H | -4.87039927 | -1.56897612 | -1.88484400 |
| H | -6.03975927 | -0.28981812 | -2.02691800 |
| C | -5.42997527 | -0.67384712 | -0.00694800 |
| C | -4.16338427 | -0.51492112 | 2.17658000 |
| H | -4.42145527 | 0.54345888 | 2.21287900 |
| H | -4.89306527 | -1.09038112 | 2.75989200 |
| C | -2.78232127 | -0.70111112 | 2.79383700 |
| H | -2.53637927 | -1.76731012 | 2.85456300 |
| H | -2.80078927 | -0.30985212 | 3.81763400 |
| C | -1.30260927 | 1.28665688 | 2.42445200 |
| C | 0.01544973 | 1.64940188 | 1.69886400 |
| H | 0.48005573 | 2.48900688 | 2.22749300 |
| H | 0.71142973 | 0.81217288 | 1.82313500 |
| C | -0.02198127 | 2.03480088 | 0.21040500 |
| C | -0.83130927 | 1.30771488 | -2.01986100 |
| H | -1.40744927 | 2.22945788 | -2.00112400 |
| H | 0.10895073 | 1.50507788 | -2.55091800 |
| C | -1.58764727 | 0.21619388 | -2.77732300 |
| H | -1.91844727 | 0.60882788 | -3.74801000 |
| H | -0.91041427 | -0.62071912 | -2.97191200 |
| H | -4.02198927 | -1.93930812 | 0.72667200 |
| H | -2.90736827 | -1.28324712 | -2.37707700 |
| C | -1.45585727 | -2.20452712 | -0.00469200 |
| O | -1.66614427 | -3.27563612 | -0.38905300 |
| O | -0.01943827 | -2.21317712 | 1.25711100 |
| C | 2.56313373 | -0.43882012 | 0.15318300 |
| O | 3.24687573 | -1.16676512 | 1.06299000 |
| H | 4.07551973 | -0.70143512 | 1.23280900 |

| | | | |
|---|---|---|---|
| O | 1.42593273 | -0.98448212 | -0.17200300 |
| H | 0.86169673 | -1.66188312 | 0.57790300 |
| O | 2.97984773 | 0.61933088 | -0.28529400 |
| H | -1.07286127 | 1.26024688 | 3.50060800 |
| H | -6.08733627 | -1.54654112 | 0.14100400 |
| H | -4.22972127 | 0.86305988 | -2.88502900 |
| H | 1.02794673 | 2.14554288 | -0.10093000 |
| H | -0.90956827 | -0.68469912 | 2.02061000 |
| N | -3.75010827 | 1.46955288 | -0.91879600 |
| H | -4.43956027 | 1.41578188 | -0.16965900 |
| N | -6.10794727 | 0.53177088 | 0.44318700 |
| H | -6.54714927 | 0.97327988 | -0.35611300 |
| N | -2.42793427 | 2.18686988 | 2.26732400 |
| H | -2.55546227 | 2.40763188 | 1.28309700 |
| N | -0.72851527 | 3.28883388 | -0.01422300 |
| H | -0.91409727 | 3.73479788 | 0.87468700 |
| C | -2.36186227 | 3.40296988 | 3.06686400 |
| H | -1.45088727 | 4.00603688 | 2.91400100 |
| H | -3.22540527 | 4.02992988 | 2.83509500 |
| H | -2.41117227 | 3.14890488 | 4.12975800 |
| C | -0.00779127 | 4.25234788 | -0.85168100 |
| H | 0.10204973 | 3.86916588 | -1.86877800 |
| H | -0.58297827 | 5.17990988 | -0.90538500 |
| H | 0.99765473 | 4.48228488 | -0.47201100 |
| C | -7.13492727 | 0.35894088 | 1.47585300 |
| H | -7.83760427 | -0.45251012 | 1.23876500 |
| H | -6.68555127 | 0.15484588 | 2.44779300 |
| H | -7.69527227 | 1.29121188 | 1.56574400 |
| C | -3.77531327 | 2.84475188 | -1.43618300 |
| H | -4.79917427 | 3.21318288 | -1.57821200 |
| H | -3.23944527 | 3.50071588 | -0.74790800 |
| H | -3.26437827 | 2.90189988 | -2.39939200 |

**Cl-hor-1**

SCF Energy: -2810.762135
Gibbs Energy: -2810.477475

| | | | |
|---|---|---|---|
| Ni | 0.58500912 | 0.04570384 | 0.00000000 |
| N | -1.09815588 | -1.22721416 | -0.07989600 |
| N | 1.70574412 | -1.65780716 | -0.53429000 |
| H | 2.12903012 | -1.95476516 | 0.34882700 |
| N | 2.26816312 | 1.31862184 | -0.07987100 |
| H | 2.65773012 | 1.10208084 | 0.84564700 |
| N | -0.53574388 | 1.74922884 | -0.53421700 |
| C | -2.09350988 | -0.97057116 | -1.10740200 |
| H | -1.66144488 | -1.19349916 | -2.08661300 |
| C | -2.61244488 | 0.46712284 | -1.05137100 |
| H | -2.97850088 | 0.69340584 | -0.04262500 |
| H | -3.47377688 | 0.53146584 | -1.71760800 |
| C | -1.60766088 | 1.52757684 | -1.50155200 |
| H | -1.14913588 | 1.25473684 | -2.45617800 |
| C | 0.46845712 | 2.76297884 | -0.94820800 |
| H | 0.74195512 | 2.55033984 | -1.98756900 |
| H | 0.04077212 | 3.76874384 | -0.92232900 |
| C | 1.68167312 | 2.67958784 | -0.03821900 |
| H | 1.39523912 | 2.87000484 | 1.00015900 |
| H | 2.42056312 | 3.43496184 | -0.31862100 |
| C | 3.26350812 | 1.06200484 | -1.10739200 |
| H | 2.83143112 | 1.28496084 | -2.08659300 |
| C | 3.78244512 | -0.37569016 | -1.05140600 |
| H | 4.64377512 | -0.44000916 | -1.71764800 |
| H | 4.14850512 | -0.60200316 | -0.04266700 |
| C | 2.77766612 | -1.43613516 | -1.50161700 |
| H | 2.31914712 | -1.16327616 | -2.45623900 |
| C | 0.70154212 | -2.67155116 | -0.94829100 |
| H | 0.42803112 | -2.45889616 | -1.98764500 |
| H | 1.12922712 | -3.67731716 | -0.92243200 |

| | | | |
|---|---|---|---|
| C | -0.51165988 | -2.58818016 | -0.03828200 |
| H | -1.25055188 | -3.34355116 | -0.31868100 |
| H | -0.22520588 | -2.77861116 | 1.00008800 |
| H | -0.95903088 | 2.04617684 | 0.34890200 |
| H | -1.48772688 | -1.01072216 | 0.84562900 |
| C | 0.58506312 | 0.04558784 | 2.23201900 |
| O | -0.54866088 | -0.19813216 | 2.63671800 |
| O | 1.71882812 | 0.28925284 | 2.63664300 |
| Cl | -3.50982888 | -2.08393816 | -0.94297300 |
| Cl | -2.50860688 | 3.06260384 | -1.81757400 |
| Cl | 4.67982212 | 2.17537084 | -0.94294400 |
| Cl | 3.67862212 | -2.97115016 | -1.81766800 |

**Cl-hor-TS2**

SCF Energy: -3075.766543
Gibbs Energy: -3075.44298

| | | | |
|---|---|---|---|
| Ni | -1.84643504 | -0.90493600 | 0.00000000 |
| N | -0.72168204 | -2.18477700 | 1.29502300 |
| N | -2.12437304 | 0.25000800 | 1.73930800 |
| H | -3.07529804 | -0.00037200 | 2.01301200 |
| N | -2.79508804 | 0.51885200 | -1.28526500 |
| H | -3.79416604 | 0.35476500 | -1.18433400 |
| N | -0.67331504 | -1.33514100 | -1.69579400 |
| C | 0.72994696 | -2.19720200 | 1.03832100 |
| H | 1.12395496 | -1.19210600 | 1.22741500 |
| C | 1.05150796 | -2.61857700 | -0.39561100 |
| H | 0.53218896 | -3.55653500 | -0.63420500 |
| H | 2.12002696 | -2.85032200 | -0.44342600 |
| C | 0.76643596 | -1.57273700 | -1.47194700 |
| H | 1.21557696 | -0.61565400 | -1.18172400 |
| C | -0.92924004 | -0.26849800 | -2.68244600 |
| H | -0.30190504 | 0.58807500 | -2.41306900 |

| | | | |
|---|---|---|---|
| H | -0.64162704 | -0.57444700 | -3.69574700 |
| C | -2.40168204 | 0.12338800 | -2.65141600 |
| H | -3.01372904 | -0.73868000 | -2.93318300 |
| H | -2.59088904 | 0.92501900 | -3.37637800 |
| C | -2.53479504 | 1.93001300 | -0.94832000 |
| H | -1.46385004 | 2.12590900 | -1.07491200 |
| C | -2.95457104 | 2.26100800 | 0.48436700 |
| H | -2.96715804 | 3.35078000 | 0.58406900 |
| H | -3.98922404 | 1.93407300 | 0.65471700 |
| C | -2.04310104 | 1.71522400 | 1.58194100 |
| H | -1.00064904 | 1.96298300 | 1.34987200 |
| C | -1.19412904 | -0.26608900 | 2.76196600 |
| H | -0.21468104 | 0.18837400 | 2.57755500 |
| H | -1.50170904 | 0.02646200 | 3.77328900 |
| C | -1.10376304 | -1.78412400 | 2.66345400 |
| H | -0.39600104 | -2.16535800 | 3.41009500 |
| H | -2.08383904 | -2.22251900 | 2.87270200 |
| H | -1.09828704 | -2.19842400 | -2.03640700 |
| H | -1.07300404 | -3.12581500 | 1.13221000 |
| C | -3.39382104 | -2.14437000 | -0.08291300 |
| O | -3.60182004 | -2.84771700 | -1.07049600 |
| O | -4.14272304 | -2.12829500 | 0.97935300 |
| C | -6.71773404 | -3.70807500 | -0.04311200 |
| O | -5.91589604 | -3.71128900 | 0.94734600 |
| H | -5.06179904 | -2.90681800 | 0.95064400 |
| O | -6.65817504 | -2.66337300 | -0.87260900 |
| H | -7.28192604 | -2.80713000 | -1.59772900 |
| O | -7.52102404 | -4.62719700 | -0.22006900 |
| Cl | 1.53202696 | -2.06509000 | -2.97828600 |
| Cl | 1.53223496 | -3.28642500 | 2.16416500 |
| Cl | -3.38773204 | 2.98577300 | -2.06879700 |
| Cl | -2.43096104 | 2.50399800 | 3.10673600 |

**Cl-hor-3**

SCF Energy: -2810.743669
Gibbs Energy: -2810.461393

| | | | |
|---|---|---|---|
| Ni | 1.97440578 | -0.08226691 | 0.00000000 |
| N | 3.66442478 | 1.20949109 | -0.06633400 |
| N | 0.85617078 | 1.65560209 | -0.50840700 |
| H | 0.44361778 | 1.96860709 | 0.37190100 |
| N | 0.28589278 | -1.37658791 | -0.05312400 |
| H | 1.18794778 | -0.53255491 | 3.64158800 |
| N | 3.09290478 | -1.81423291 | -0.52519900 |
| C | 4.64452278 | 0.92879709 | -1.09294700 |
| H | 4.21056478 | 1.14014009 | -2.07431500 |
| C | 5.15922378 | -0.51133191 | -1.02337800 |
| H | 5.50804478 | -0.73376891 | -0.00781300 |
| H | 6.03075378 | -0.58027391 | -1.67536100 |
| C | 4.15959678 | -1.57293091 | -1.48491000 |
| H | 3.70338178 | -1.29159391 | -2.43842100 |
| C | 2.08552278 | -2.81238891 | -0.95488400 |
| H | 1.81294878 | -2.58369991 | -1.99144200 |
| H | 2.50110178 | -3.82412291 | -0.94713500 |
| C | 0.86986878 | -2.73764891 | -0.04450900 |
| H | 1.16049478 | -2.94834891 | 0.98852700 |
| H | 0.13125778 | -3.48883291 | -0.33849400 |
| C | -0.68316422 | -1.08831091 | -1.09183100 |
| H | -0.23246522 | -1.28439091 | -2.06854100 |
| C | -1.20859922 | 0.34760009 | -1.01135400 |
| H | -2.07882322 | 0.41508309 | -1.66531500 |
| H | -1.56371722 | 0.55956009 | 0.00432700 |
| C | -0.21757822 | 1.42218109 | -1.46155900 |
| H | 0.23238078 | 1.15766009 | -2.42273700 |
| C | 1.86383978 | 2.65261709 | -0.94560500 |
| H | 2.12665378 | 2.42258109 | -1.98442900 |
| H | 1.44895278 | 3.66459109 | -0.93337200 |

| | | | |
|---|---|---|---|
| C | 3.08845778 | 2.57192509 | -0.04784100 |
| H | 3.82652078 | 3.32052609 | -0.34984200 |
| H | 2.81312578 | 2.78502709 | 0.98895600 |
| H | 3.51484078 | -2.12434891 | 0.35182900 |
| H | 4.05408178 | 1.00838309 | 0.86041900 |
| C | 2.09473678 | -0.07363691 | 2.01411300 |
| O | 3.06024678 | 0.33448109 | 2.63599900 |
| O | 1.01888478 | -0.57802591 | 2.68414500 |
| Cl | 6.07966578 | 2.03586409 | -0.96871800 |
| Cl | 5.07446278 | -3.10079391 | -1.82964000 |
| Cl | -2.11047322 | -2.20733191 | -0.99944900 |
| Cl | -1.14555322 | 2.94838909 | -1.77606700 |
| H | -0.13547722 | -1.20077291 | 0.86074800 |

**Cl-hor-TS4**

SCF Energy: -3075.747767
Gibbs Energy: -3075.434511

| | | | |
|---|---|---|---|
| Ni | 0.74954294 | -0.04570384 | 0.00000000 |
| N | -0.30803606 | -1.88148584 | -0.25878000 |
| N | 2.13234394 | -0.88687884 | -1.32690400 |
| H | 2.88670594 | -1.12893984 | -0.65344200 |
| N | 1.75773694 | 1.80801616 | 0.12002600 |
| H | 2.97119994 | 0.32818016 | 3.31926000 |
| N | -1.01840806 | 1.10819416 | 0.26492000 |
| C | -1.52055306 | -1.74822284 | -1.05578200 |
| C | -2.51533806 | -0.76016984 | -0.44333400 |
| H | -2.68774606 | -1.00262984 | 0.61256100 |
| H | -3.47097406 | -0.89708184 | -0.95104400 |
| C | -2.13161406 | 0.71150516 | -0.59215600 |
| C | -0.59942106 | 2.52523416 | 0.10504200 |
| H | -0.57062606 | 2.74168316 | -0.96825300 |
| H | -1.32979206 | 3.20477216 | 0.55198800 |

| | | | |
|---|---|---|---|
| C | 0.76959994 | 2.72359316 | 0.73208000 |
| H | 0.73746894 | 2.49214516 | 1.80114900 |
| H | 1.08169094 | 3.76719916 | 0.63461700 |
| C | 2.36966194 | 2.26326016 | -1.12078000 |
| C | 3.35522194 | 1.24393416 | -1.68936700 |
| H | 3.92809594 | 1.74411016 | -2.47100100 |
| H | 4.06587894 | 0.92813216 | -0.91742000 |
| C | 2.69678594 | 0.01527816 | -2.31902600 |
| C | 1.54717394 | -2.12807484 | -1.87702500 |
| H | 0.93659694 | -1.86804684 | -2.75027400 |
| H | 2.33304794 | -2.81094884 | -2.20837300 |
| C | 0.72768594 | -2.80834984 | -0.79716100 |
| H | 0.26983594 | -3.72449584 | -1.17845700 |
| H | 1.39437494 | -3.07989484 | 0.02563100 |
| H | -1.30933906 | 0.96668516 | 1.23403100 |
| H | -0.58440906 | -2.21812584 | 0.66369200 |
| C | 1.05209394 | -0.43896284 | 2.02685200 |
| O | 0.59723494 | -0.89625984 | 2.98309600 |
| O | 2.71825694 | 0.38869016 | 2.38857100 |
| C | 4.00063094 | -2.27453284 | 1.11158700 |
| O | 4.49937594 | -2.49446484 | 2.34413200 |
| H | 4.58720594 | -3.44962684 | 2.45684500 |
| O | 3.85526494 | -1.01285484 | 0.84135700 |
| H | 3.39338194 | -0.27874484 | 1.75318300 |
| O | 3.69362994 | -3.19046684 | 0.35832900 |
| H | -1.24629906 | -1.44832284 | -2.07072000 |
| H | 1.91351894 | 0.30537616 | -3.02700700 |
| H | -1.86194106 | 0.93931216 | -1.62760000 |
| H | 1.58374294 | 2.49048216 | -1.84669200 |
| H | 2.48922194 | 1.62373016 | 0.81448600 |
| Cl | -2.36011906 | -3.34057684 | -1.23989700 |
| Cl | -3.59277906 | 1.71714316 | -0.24060100 |
| Cl | 3.24560994 | 3.82940116 | -0.87183300 |
| Cl | 3.94431094 | -0.82570484 | -3.32597400 |

**CN-hor-1**

SCF Energy: -1341.2191
Gibbs Energy: -1340.906704

| | | | |
|---|---|---|---|
| Ni | 3.16270556 | -0.92321754 | 0.00000000 |
| N | 1.46876756 | -2.17108954 | -0.08913800 |
| N | 4.25032056 | -2.64162354 | -0.52702000 |
| H | 4.64389656 | -2.95860154 | 0.36269200 |
| N | 4.85664356 | 0.32465446 | -0.08912000 |
| H | 5.23126256 | 0.12045946 | 0.84552500 |
| N | 2.07508756 | 0.79520246 | -0.52696400 |
| C | 0.43581856 | -1.88888754 | -1.10356700 |
| H | 0.87228256 | -2.06188454 | -2.09540200 |
| C | -0.06505544 | -0.43669254 | -1.00968800 |
| H | -0.38952144 | -0.21883654 | 0.01466400 |
| H | -0.95272244 | -0.34505254 | -1.64069600 |
| C | 0.95531856 | 0.61415746 | -1.48000600 |
| H | 1.39030556 | 0.29818746 | -2.43660700 |
| C | 3.08435256 | 1.79051246 | -0.97606700 |
| H | 3.34378756 | 1.55215546 | -2.01382300 |
| H | 2.67221356 | 2.80479646 | -0.96542000 |
| C | 4.30863556 | 1.70381246 | -0.07842200 |
| H | 4.03857356 | 1.93053046 | 0.95718700 |
| H | 5.05989656 | 2.43873546 | -0.38490500 |
| C | 5.88958556 | 0.04247846 | -1.10356500 |
| H | 5.45311356 | 0.21549746 | -2.09539200 |
| C | 6.39046056 | -1.40971854 | -1.00972400 |
| H | 7.27812356 | -1.50134154 | -1.64074100 |
| H | 6.71493356 | -1.62759854 | 0.01462000 |
| C | 5.37008556 | -2.46055754 | -1.48006300 |
| H | 4.93509456 | -2.14456554 | -2.43665500 |
| C | 3.24105356 | -3.63692454 | -0.97613900 |

| | | | |
|---|---|---|---|
| H | 2.98160956 | -3.39854454 | -2.01388800 |
| H | 3.65319456 | -4.65120754 | -0.96551900 |
| C | 2.01677856 | -3.55024754 | -0.07848100 |
| H | 1.26551556 | -4.28516454 | -0.38497500 |
| H | 2.28685056 | -3.77698854 | 0.95712000 |
| H | 1.68151456 | 1.11216346 | 0.36275600 |
| H | 1.09415356 | -1.96692754 | 0.84551600 |
| C | 3.16273556 | -0.92328954 | 2.22464500 |
| O | 2.02601756 | -1.15589854 | 2.62817000 |
| O | 4.29952456 | -0.69094354 | 2.62812500 |
| C | 7.02809456 | 0.97174146 | -0.96521800 |
| N | 7.90036856 | 1.72057046 | -0.83738600 |
| C | 6.04924656 | -3.74977454 | -1.71349300 |
| N | 6.55136856 | -4.78084754 | -1.86436600 |
| C | 0.27615656 | 1.90337946 | -1.71340600 |
| N | -0.22596344 | 2.93445646 | -1.86425400 |
| C | -0.70269144 | -2.81815154 | -0.96523200 |
| N | -1.57496544 | -3.56698254 | -0.83740900 |

**CN-hor-TS2**

SCF Energy: -1606.22606
Gibbs Energy: -1605.881694

| | | | |
|---|---|---|---|
| Ni | -0.58500912 | -0.55758683 | 0.00000000 |
| N | -1.14983412 | 1.45524217 | -0.27888600 |
| N | 1.34896488 | 0.12093317 | -0.53385700 |
| H | 1.45047688 | -0.10070383 | -1.52630200 |
| N | 0.02649688 | -2.55734483 | 0.37978300 |
| H | 0.02985988 | -2.98083383 | -0.54983500 |
| N | -2.13470412 | -0.99182783 | 1.34577300 |
| C | -1.70903412 | 2.12643917 | 0.91212000 |
| H | -0.94017812 | 2.14744417 | 1.69525400 |
| C | -2.95848012 | 1.38566717 | 1.42678600 |

| | | | |
|---|---|---|---|
| H | -3.63336912 | 1.16769817 | 0.59099400 |
| H | -3.49923512 | 2.05626717 | 2.09927200 |
| C | -2.65281512 | 0.09447917 | 2.20382300 |
| H | -1.90324912 | 0.30329717 | 2.97764800 |
| C | -1.69788212 | -2.18428783 | 2.11061300 |
| H | -0.96942212 | -1.85948783 | 2.86338100 |
| H | -2.53661712 | -2.64917183 | 2.64061200 |
| C | -1.08470012 | -3.18501483 | 1.14557800 |
| H | -1.83558012 | -3.49803783 | 0.41686700 |
| H | -0.74870212 | -4.07966183 | 1.67925800 |
| C | 1.36968088 | -2.71532283 | 0.97286300 |
| H | 1.35655988 | -2.25866483 | 1.97082000 |
| C | 2.46153988 | -2.04623583 | 0.11720700 |
| H | 3.43152488 | -2.40288683 | 0.47355800 |
| H | 2.37739088 | -2.37795883 | -0.92438200 |
| C | 2.47794688 | -0.50976983 | 0.18883300 |
| H | 2.40657888 | -0.19760883 | 1.23867200 |
| C | 1.30960688 | 1.60051817 | -0.38850100 |
| H | 1.39798988 | 1.82930717 | 0.67982200 |
| H | 2.15516088 | 2.07622817 | -0.89621400 |
| C | -0.00634212 | 2.12324917 | -0.94380300 |
| H | -0.05617212 | 3.21249417 | -0.84318900 |
| H | -0.07847912 | 1.89692217 | -2.01177000 |
| H | -2.90670112 | -1.28357883 | 0.72686900 |
| H | -1.90680312 | 1.34588417 | -0.95831600 |
| C | -1.79003112 | -1.18559783 | -1.61302600 |
| O | -2.71029112 | -0.39686383 | -1.85065000 |
| O | -1.85461912 | -2.44526683 | -1.91275300 |
| C | -5.05753312 | -2.22912583 | -1.41508700 |
| O | -4.22600612 | -2.24806683 | -2.40247600 |
| H | -2.85990012 | -2.57581483 | -2.22690300 |
| O | -4.47222312 | -2.04377483 | -0.16899000 |
| H | -5.20522512 | -2.11109383 | 0.46108000 |
| O | -6.25298512 | -2.38492083 | -1.50347300 |

| | | | |
|---|---|---|---|
| C | 3.76089088 | 0.00349617 | -0.33024600 |
| N | 4.73959388 | 0.43144917 | -0.77421500 |
| C | -2.04946912 | 3.53099517 | 0.61043600 |
| N | -2.29295612 | 4.63033217 | 0.34524900 |
| C | -3.87789512 | -0.37139583 | 2.88514500 |
| N | -4.84050112 | -0.80044383 | 3.36245100 |
| C | 1.69821188 | -4.14296783 | 1.15830500 |
| N | 1.92801588 | -5.26884883 | 1.29112600 |

**CN-hor-3**

SCF Energy: -1341.872905
Gibbs Energy: -1341.528539

| | | | |
|---|---|---|---|
| Ni | -0.34720743 | 0.26511203 | -0.00909191 |
| N | 1.35405957 | 1.52933203 | -0.08062691 |
| N | -1.42947443 | 2.01877403 | -0.50756791 |
| H | -1.81210443 | 2.35418003 | 0.37786609 |
| N | -2.04719643 | -1.00221497 | -0.06850891 |
| H | -2.45298343 | -0.84338697 | 0.85552209 |
| N | 0.73495257 | -1.48010997 | -0.53261491 |
| C | 2.37577757 | 1.22667303 | -1.09457091 |
| H | 1.93738457 | 1.39162603 | -2.08750191 |
| C | 2.86748957 | -0.22949297 | -0.99187791 |
| H | 3.17091657 | -0.44688897 | 0.03889609 |
| H | 3.76689157 | -0.32570897 | -1.60528691 |
| C | 1.85315157 | -1.28008397 | -1.47842391 |
| H | 1.42088657 | -0.95174297 | -2.43241491 |
| C | -0.27913143 | -2.45550197 | -1.00134891 |
| H | -0.53952543 | -2.19396097 | -2.03371691 |
| H | 0.11796957 | -3.47623497 | -1.01642291 |
| C | -1.50367543 | -2.38115297 | -0.09990691 |
| H | -1.22703843 | -2.63493897 | 0.92736609 |
| H | -2.25590043 | -3.10937097 | -0.42182991 |

| | | | |
|---|---|---|---|
| C | -3.05888543 | -0.68777197 | -1.09285391 |
| H | -2.60595343 | -0.83805697 | -2.08117891 |
| C | -3.55990943 | 0.76458603 | -0.97707991 |
| H | -4.45746143 | 0.86019703 | -1.59340691 |
| H | -3.87141143 | 0.96981103 | 0.05380609 |
| C | -2.55328943 | 1.82940103 | -1.44834591 |
| H | -2.12540343 | 1.52081603 | -2.41078591 |
| C | -0.41562143 | 2.99566303 | -0.97921191 |
| H | -0.16607143 | 2.73908703 | -2.01548791 |
| H | -0.81214943 | 4.01666903 | -0.98325591 |
| C | 0.81851357 | 2.90943103 | -0.09196991 |
| H | 1.56919857 | 3.63766503 | -0.41742191 |
| H | 0.55778157 | 3.15779603 | 0.94092409 |
| H | 1.12639657 | -1.81617897 | 0.34884509 |
| H | 1.72909957 | 1.33905103 | 0.85487409 |
| C | -0.21692643 | 0.26498803 | 2.00360209 |
| O | 0.76266557 | 0.65319303 | 2.61659409 |
| O | -1.29546243 | -0.22346897 | 2.67934509 |
| C | -3.25264443 | 3.11038503 | -1.67634391 |
| N | -3.77073443 | 4.13499403 | -1.81804291 |
| C | 3.52816257 | 2.14510903 | -0.98037791 |
| N | 4.41084757 | 2.88458603 | -0.86945691 |
| C | 2.54152757 | -2.56194397 | -1.73329991 |
| N | 3.04733957 | -3.58935797 | -1.89736591 |
| C | -4.20750043 | -1.61302597 | -1.00182891 |
| N | -5.08787843 | -2.35671597 | -0.90082291 |
| H | -1.12154643 | -0.18745097 | 3.63658609 |

**CN-hor-TS4**

SCF Energy: -1606.888338
Gibbs Energy: -1606.530983

| | | | |
|---|---|---|---|
| Ni | -3.65630700 | 1.10593811 | 0.01447751 |

| | | | |
|---|---|---|---|
| N | -2.12655400 | -0.35565989 | 0.61168951 |
| N | -4.58857600 | 0.35665811 | 1.80167551 |
| H | -5.26284200 | -0.29206789 | 1.35750251 |
| N | -5.11798100 | 2.74084411 | -0.13486449 |
| H | -3.64214400 | 0.24368111 | -3.80571749 |
| N | -2.31028400 | 2.78197111 | 0.35597651 |
| C | -0.83877900 | 0.05547711 | 1.23120551 |
| C | -0.30033400 | 1.42559011 | 0.80509751 |
| H | -0.16763800 | 1.47450911 | -0.28126249 |
| H | 0.69373100 | 1.53417911 | 1.24675851 |
| C | -1.17979300 | 2.59881511 | 1.27860151 |
| C | -3.12333900 | 3.99657311 | 0.55123551 |
| H | -3.46986300 | 4.01625011 | 1.59088851 |
| H | -2.53849400 | 4.90818211 | 0.38615551 |
| C | -4.29214700 | 3.94050511 | -0.42413249 |
| H | -3.91799200 | 3.86244011 | -1.44840149 |
| H | -4.88435700 | 4.86079911 | -0.36923449 |
| C | -6.10768500 | 3.04314511 | 0.93505551 |
| C | -6.54797300 | 1.85123611 | 1.78812151 |
| H | -7.33079200 | 2.20848711 | 2.46238351 |
| H | -6.99558100 | 1.06298711 | 1.17422351 |
| C | -5.40026200 | 1.26103211 | 2.62837851 |
| C | -3.63658300 | -0.49518689 | 2.53480051 |
| H | -2.98022200 | 0.14060511 | 3.14113851 |
| H | -4.15251300 | -1.17639989 | 3.22027251 |
| C | -2.85382100 | -1.29442589 | 1.50448651 |
| H | -2.16939400 | -1.99930889 | 1.98957551 |
| H | -3.54516400 | -1.87737489 | 0.89121351 |
| H | -1.90093800 | 2.84598611 | -0.57840049 |
| H | -1.91208500 | -0.83716289 | -0.25975249 |
| C | -2.94908400 | 1.30593411 | -1.99206649 |
| O | -2.00323100 | 1.74770111 | -2.54501549 |
| O | -3.99437700 | 0.59345311 | -2.97334249 |
| C | -5.91828000 | -1.12760489 | -0.77190949 |

| | | | |
|---|---|---|---|
| O | -6.46916300 | -1.67527089 | -1.85527749 |
| H | -7.23027100 | -2.20512389 | -1.58095649 |
| O | -4.87767200 | -0.39651289 | -1.05165949 |
| H | -4.53905400 | -0.06370589 | -2.24080749 |
| O | -6.35349700 | -1.30406989 | 0.36149351 |
| H | -0.99678600 | 0.08904811 | 2.31468051 |
| H | -4.75813600 | 2.06439911 | 3.01460551 |
| H | -1.58012000 | 2.39843911 | 2.28056651 |
| H | -5.64326000 | 3.77217911 | 1.60858251 |
| H | -5.63507100 | 2.48734611 | -0.97562349 |
| C | -5.95565700 | 0.56121911 | 3.80582451 |
| N | -6.36602300 | -0.00539689 | 4.72711451 |
| C | -7.28051000 | 3.70923211 | 0.33835051 |
| N | -8.18113500 | 4.21871811 | -0.17927749 |
| C | 0.17610900 | -0.98661289 | 0.98616951 |
| N | 0.93823400 | -1.82628289 | 0.75667351 |
| C | -0.36883600 | 3.83064811 | 1.37051551 |
| N | 0.23658400 | 4.81551311 | 1.41415851 |

**OMe-hor-1**

SCF Energy: -1430.425447
Gibbs Energy: -1429.979819

| | | | |
|---|---|---|---|
| Ni | -0.76782447 | -0.33820840 | 0.00000000 |
| N | 0.91756253 | 0.91407460 | -0.08449700 |
| N | -1.85328847 | 1.37342260 | -0.53642600 |
| H | -2.26224847 | 1.70545660 | 0.34036800 |
| N | -2.45319847 | -1.59044340 | -0.08455000 |
| H | -2.83107947 | -1.39816040 | 0.85062200 |
| N | 0.31767253 | -2.04977440 | -0.53646200 |
| C | 1.95638153 | 0.64076760 | -1.07540100 |
| H | 1.52999553 | 0.83321260 | -2.07582700 |
| C | 2.41723153 | -0.81617140 | -0.97074800 |

| | | | |
|---|---|---|---|
| H | 2.69609053 | -1.03774240 | 0.06648600 |
| H | 3.32989153 | -0.91546540 | -1.56314600 |
| C | 1.42202853 | -1.85939840 | -1.48257500 |
| H | 0.97616253 | -1.52199040 | -2.43540500 |
| C | -0.68606847 | -3.04193340 | -0.99341900 |
| H | -0.94798447 | -2.78740040 | -2.02708300 |
| H | -0.26483947 | -4.04995140 | -0.99969000 |
| C | -1.91129947 | -2.96892440 | -0.09644200 |
| H | -1.64066547 | -3.21719540 | 0.93414200 |
| H | -2.67463747 | -3.68193040 | -0.41762000 |
| C | -3.49204747 | -1.31711140 | -1.07543100 |
| H | -3.06569147 | -1.50951940 | -2.07588100 |
| C | -3.95284947 | 0.13984460 | -0.97073300 |
| H | -4.86552947 | 0.23918460 | -1.56309100 |
| H | -4.23166347 | 0.36139160 | 0.06652000 |
| C | -2.95760447 | 1.18303360 | -1.48257400 |
| H | -2.51169747 | 0.84556860 | -2.43536700 |
| C | -0.84955047 | 2.36559760 | -0.99333800 |
| H | -0.58763347 | 2.11111060 | -2.02701200 |
| H | -1.27077647 | 3.37361760 | -0.99957300 |
| C | 0.37567853 | 2.29255360 | -0.09635800 |
| H | 1.13902353 | 3.00556160 | -0.41752000 |
| H | 0.10504353 | 2.54080860 | 0.93423100 |
| H | 0.72661753 | -2.38185440 | 0.34032400 |
| H | 1.29543053 | 0.72175560 | 0.85067300 |
| C | -0.76784347 | -0.33810040 | 2.25305900 |
| O | 0.36025153 | -0.07520140 | 2.66457300 |
| O | -1.89598647 | -0.60098840 | 2.66446200 |
| O | -3.55677547 | 2.43619160 | -1.65755400 |
| O | -4.54696047 | -2.20441040 | -0.83186100 |
| O | 3.01130353 | 1.52808060 | -0.83182000 |
| O | 2.02127053 | -3.11253640 | -1.65747400 |
| C | 3.85652453 | 1.79311060 | -1.93758700 |
| H | 4.57211253 | 2.54463660 | -1.60637000 |

| | | | |
|---|---|---|---|
| H | 4.40816553 | 0.90038760 | -2.25742400 |
| H | 3.28198853 | 2.18768660 | -2.78679400 |
| C | 2.76978853 | -3.27690540 | -2.85003300 |
| H | 3.68239353 | -2.66874040 | -2.85004400 |
| H | 3.05077553 | -4.32842240 | -2.89591500 |
| H | 2.16432753 | -3.02506640 | -3.73137000 |
| C | -4.30529147 | 2.60053760 | -2.85011600 |
| H | -5.21804447 | 1.99259760 | -2.85000100 |
| H | -4.58602147 | 3.65211660 | -2.89617200 |
| H | -3.69991647 | 2.34841060 | -3.73143100 |
| C | -5.39246747 | -2.46907740 | -1.93749000 |
| H | -6.10783547 | -3.22087240 | -1.60640200 |
| H | -5.94435347 | -1.57629740 | -2.25674400 |
| H | -4.81813247 | -2.86317140 | -2.78705800 |

**OMe-hor-TS2**

SCF Energy: -1695.417044
Gibbs Energy: -1694.936908

| | | | |
|---|---|---|---|
| Ni | -0.65816734 | 1.03287468 | 0.00490545 |
| N | -1.51421734 | 2.88162668 | -0.53842355 |
| N | 1.13488066 | 1.88081968 | -0.72548355 |
| H | 1.26337966 | 1.51891268 | -1.67233155 |
| N | 0.24989166 | -0.77630332 | 0.64300945 |
| H | 0.28852666 | -1.34266732 | -0.20579155 |
| N | -2.05345634 | 0.63008568 | 1.51566445 |
| C | -2.10174834 | 3.66579468 | 0.54768045 |
| C | -3.16076734 | 2.83112068 | 1.27665245 |
| H | -3.83006134 | 2.36097268 | 0.54658045 |
| H | -3.77286034 | 3.51933468 | 1.86437045 |
| C | -2.61412734 | 1.77279068 | 2.23650845 |
| C | -1.42559134 | -0.36923332 | 2.40804245 |
| H | -0.71061734 | 0.15977668 | 3.05071945 |

| | | | |
|---|---|---|---|
| H | -2.16760134 | -0.83918332 | 3.05877845 |
| C | -0.72171134 | -1.41866532 | 1.56473545 |
| H | -1.45424334 | -1.94244632 | 0.94598245 |
| H | -0.22254334 | -2.15949432 | 2.19400345 |
| C | 1.61084966 | -0.66933132 | 1.16679845 |
| C | 2.52676266 | 0.02932968 | 0.15615545 |
| H | 3.55672266 | -0.14935332 | 0.47440845 |
| H | 2.42368666 | -0.44802832 | -0.82593755 |
| C | 2.34695366 | 1.54332168 | 0.02687845 |
| C | 0.88820266 | 3.34125368 | -0.81411055 |
| H | 0.97651966 | 3.75022868 | 0.19938645 |
| H | 1.64289766 | 3.83301868 | -1.43256455 |
| C | -0.50762334 | 3.58246368 | -1.36600755 |
| H | -0.72447634 | 4.65184268 | -1.42577155 |
| H | -0.58145434 | 3.17571268 | -2.37920255 |
| H | -2.83297934 | 0.17382468 | 1.02154645 |
| H | -2.28418034 | 2.58305068 | -1.14066455 |
| C | -1.80032634 | -0.00844332 | -1.43285155 |
| O | -2.84768934 | 0.57334668 | -1.73589655 |
| O | -1.67217534 | -1.29789932 | -1.57955655 |
| C | -4.89225034 | -1.38587032 | -0.94788455 |
| O | -4.11597934 | -1.42452932 | -1.97706055 |
| H | -2.62084134 | -1.61206132 | -1.83683555 |
| O | -4.27604634 | -0.95435132 | 0.21833145 |
| H | -4.96536134 | -1.00971732 | 0.89439545 |
| O | -6.05893734 | -1.71314332 | -0.92357455 |
| H | 1.56671366 | -0.08820132 | 2.10502645 |
| H | 2.24035466 | 1.99542168 | 1.02966945 |
| H | -1.29281934 | 3.95223368 | 1.24388745 |
| H | -1.80447034 | 2.20693768 | 2.85097345 |
| O | -2.65769334 | 4.81820268 | -0.02206855 |
| O | -3.61736634 | 1.26419468 | 3.07522445 |
| O | 2.06176766 | -1.96758332 | 1.43737445 |
| O | 3.41728766 | 2.14204268 | -0.64901055 |

| | | | |
|---|---|---|---|
| C | 4.59091766 | 2.36054168 | 0.11636745 |
| H | 5.09234466 | 1.42099168 | 0.37681345 |
| H | 5.25942166 | 2.95252668 | -0.50753255 |
| H | 4.36230466 | 2.91876068 | 1.03423045 |
| C | 3.07024366 | -2.07166532 | 2.42750045 |
| H | 3.25426066 | -3.13556932 | 2.57178145 |
| H | 4.00583966 | -1.59178832 | 2.11418245 |
| H | 2.73562966 | -1.62915832 | 3.37565945 |
| C | -3.95385034 | 2.06769768 | 4.19309645 |
| H | -4.45953834 | 2.99443668 | 3.89672245 |
| H | -4.63578034 | 1.47772268 | 4.80450145 |
| H | -3.05993134 | 2.31323568 | 4.78257145 |
| C | -2.82972734 | 5.91425868 | 0.85877945 |
| H | -3.18011234 | 6.74783468 | 0.25114145 |
| H | -3.57760934 | 5.70614868 | 1.63375245 |
| H | -1.87881834 | 6.18725968 | 1.33670745 |

**OMe-hor-3**

SCF Energy: -1431.073091
Gibbs Energy: -1430.612373

| | | | |
|---|---|---|---|
| Ni | -2.13893960 | -0.28336380 | 0.00000000 |
| N | -0.43899660 | 0.98312120 | -0.07461400 |
| N | -3.21360160 | 1.46788920 | -0.51958400 |
| H | -3.61677060 | 1.81678120 | 0.35115900 |
| N | -3.83740260 | -1.55289880 | -0.07762100 |
| H | -2.93359160 | -0.74014280 | 3.64269300 |
| N | -1.06357960 | -2.02478080 | -0.54885200 |
| C | 0.58376440 | 0.68781620 | -1.06770200 |
| H | 0.15342340 | 0.87541320 | -2.06799500 |
| C | 1.02967440 | -0.77479280 | -0.95784000 |
| H | 1.28745340 | -0.99985380 | 0.08401700 |
| H | 1.95251940 | -0.88181880 | -1.53294100 |

| | | | |
|---|---|---|---|
| C | 0.03498740 | -1.81007180 | -1.48895500 |
| H | -0.41165760 | -1.45135680 | -2.43411200 |
| C | -2.07462560 | -2.99280180 | -1.02940100 |
| H | -2.33405660 | -2.71214680 | -2.05738200 |
| H | -1.67088060 | -4.00809080 | -1.06286500 |
| C | -3.30295960 | -2.93153880 | -0.13278200 |
| H | -3.03007360 | -3.21067980 | 0.88914900 |
| H | -4.06704060 | -3.63554380 | -0.47371400 |
| C | -4.85214160 | -1.24124880 | -1.07734900 |
| H | -4.41050960 | -1.41129980 | -2.07530500 |
| C | -5.30413560 | 0.21766520 | -0.94704400 |
| H | -6.22620060 | 0.32850920 | -1.52277000 |
| H | -5.56672360 | 0.42763820 | 0.09682500 |
| C | -4.31467160 | 1.26782720 | -1.45932500 |
| H | -3.86995460 | 0.93052420 | -2.41296600 |
| C | -2.20127160 | 2.44054820 | -0.99245400 |
| H | -1.94771560 | 2.17144920 | -2.02501100 |
| H | -2.60465760 | 3.45638120 | -1.01055900 |
| C | -0.96755060 | 2.36304920 | -0.10438600 |
| H | -0.20400560 | 3.06971220 | -0.44101700 |
| H | -1.22987660 | 2.62949520 | 0.92374900 |
| H | -0.65581360 | -2.38037280 | 0.31712500 |
| H | -0.05882760 | 0.80263020 | 0.85949600 |
| C | -2.02644260 | -0.27860980 | 2.01858100 |
| O | -1.06949760 | 0.12623920 | 2.65855600 |
| O | -3.10799660 | -0.78570480 | 2.68654700 |
| H | -4.24646360 | -1.40501580 | 0.84641900 |
| O | 0.64314140 | -3.05662080 | -1.70304000 |
| O | 1.65984240 | 1.56259720 | -0.85139200 |
| O | -4.93312560 | 2.51357120 | -1.64536000 |
| O | -5.92686660 | -2.12285680 | -0.88383800 |
| C | 1.37265040 | -3.18346280 | -2.91006800 |
| H | 2.27132240 | -2.55417280 | -2.91737300 |
| H | 1.67696340 | -4.22721380 | -2.98136200 |

| | | | |
|---|---|---|---|
| H | 0.74599840 | -2.92955580 | -3.77624000 |
| C | -6.74091060 | -2.35236580 | -2.01917100 |
| H | -7.47801260 | -3.09935280 | -1.72668800 |
| H | -7.26885360 | -1.44506680 | -2.33906600 |
| H | -6.14636460 | -2.73863980 | -2.85859300 |
| C | -5.64899360 | 2.66653720 | -2.85771700 |
| H | -6.52810860 | 2.01155820 | -2.90302200 |
| H | -5.98394060 | 3.70270420 | -2.89258800 |
| H | -5.00265060 | 2.46541520 | -3.72304300 |
| C | 2.48630140 | 1.80300420 | -1.97455800 |
| H | 3.22196940 | 2.54490720 | -1.66576700 |
| H | 3.01612940 | 0.89845920 | -2.29955100 |
| H | 1.90232140 | 2.20026720 | -2.81652200 |

**OMe-hor-TS4**

SCF Energy: -1696.094156
Gibbs Energy: -1695.604853

| | | | |
|---|---|---|---|
| Ni | -3.16270556 | 0.63071297 | 0.00000000 |
| N | -1.99575156 | -1.07014403 | 0.51038100 |
| N | -4.40650756 | -0.02467703 | 1.54504100 |
| H | -5.19727956 | -0.43520203 | 1.01688200 |
| N | -4.26477156 | 2.38657697 | -0.35861000 |
| H | -5.61347056 | 0.28123097 | -3.14225100 |
| N | -1.49139056 | 1.80030797 | -0.58021600 |
| C | -0.71922956 | -0.76754303 | 1.16290300 |
| C | 0.13876344 | 0.15252897 | 0.28935700 |
| H | 0.20336044 | -0.25435003 | -0.72730100 |
| H | 1.15432444 | 0.12450997 | 0.69256100 |
| C | -0.29300256 | 1.61863297 | 0.24331900 |
| C | -1.96118856 | 3.20764997 | -0.62293600 |
| H | -1.93160756 | 3.59302597 | 0.40242300 |
| H | -1.29137856 | 3.82864197 | -1.22213200 |

| | | | |
|---|---|---|---|
| C | -3.38021856 | 3.25278097 | -1.16713000 |
| H | -3.40315056 | 2.87106697 | -2.19271200 |
| H | -3.75467456 | 4.27946797 | -1.19095800 |
| C | -4.86491956 | 3.04240697 | 0.80457400 |
| C | -5.72923556 | 2.05718497 | 1.59119400 |
| H | -6.33456456 | 2.63733497 | 2.29169400 |
| H | -6.42638456 | 1.54549997 | 0.91844900 |
| C | -4.95366156 | 1.02012297 | 2.40889400 |
| C | -3.71087256 | -1.09574503 | 2.28791000 |
| H | -3.06511556 | -0.62434503 | 3.03980300 |
| H | -4.42585756 | -1.73168603 | 2.81342200 |
| C | -2.90434756 | -1.93482203 | 1.31265600 |
| H | -2.33598356 | -2.70872403 | 1.83422500 |
| H | -3.59765256 | -2.42620103 | 0.62477000 |
| H | -1.23777056 | 1.52179397 | -1.52952000 |
| H | -1.76531556 | -1.57148103 | -0.34744400 |
| C | -3.57434356 | -0.11409503 | -1.90681500 |
| O | -3.15058056 | -0.67872003 | -2.82089400 |
| O | -5.31646956 | 0.52939097 | -2.25716000 |
| C | -6.24439056 | -1.99111903 | -0.54604900 |
| O | -6.64351156 | -2.43311703 | -1.76095800 |
| H | -6.60943956 | -3.39764003 | -1.74006500 |
| O | -6.26014456 | -0.69866703 | -0.45124600 |
| H | -5.90195056 | -0.08079903 | -1.46429200 |
| O | -5.88077156 | -2.76195503 | 0.33274300 |
| H | -0.94239656 | -0.27596003 | 2.12496100 |
| H | -4.10592156 | 1.50395497 | 2.93186500 |
| H | -0.54433256 | 1.96781597 | 1.26097800 |
| H | -4.04709656 | 3.41778997 | 1.44640100 |
| H | -5.02260656 | 2.05921997 | -0.96610500 |
| O | -0.06302556 | -1.98376203 | 1.39075100 |
| O | -5.77912756 | 0.39531397 | 3.35227300 |
| O | -5.61157656 | 4.12658097 | 0.32182500 |
| O | 0.70309344 | 2.43613597 | -0.30541600 |

| | | | |
|---|---|---|---|
| C | 0.81957144 | -1.99913303 | 2.49918700 |
| H | 1.23920144 | -3.00308103 | 2.54989600 |
| H | 1.64013744 | -1.27996803 | 2.38022600 |
| H | 0.28146244 | -1.78312103 | 3.43191600 |
| C | -5.95203756 | 1.09778497 | 4.56699000 |
| H | -6.46062356 | 2.05958097 | 4.42126100 |
| H | -6.57299056 | 0.46842197 | 5.20373400 |
| H | -4.98582756 | 1.27253497 | 5.06128300 |
| C | -5.88760456 | 5.14769397 | 1.26304400 |
| H | -6.36566056 | 5.95702297 | 0.71188000 |
| H | -6.57171056 | 4.80837097 | 2.04995300 |
| H | -4.96181156 | 5.52081597 | 1.72299000 |
| C | 1.73663544 | 2.82839497 | 0.58265100 |
| H | 2.34580244 | 1.97604797 | 0.90716600 |
| H | 2.37079344 | 3.52072497 | 0.03043400 |
| H | 1.32297644 | 3.33687097 | 1.46367200 |

**NHMe-hor-1**

SCF Energy: -1350.972215
Gibbs Energy: -1350.474135

| | | | |
|---|---|---|---|
| Ni | -3.89396696 | -0.59414990 | 0.00000000 |
| N | -2.24937096 | 0.69832510 | 0.01341000 |
| N | -5.02253096 | 1.11428910 | -0.41590400 |
| H | -5.38306796 | 1.41393510 | 0.49204100 |
| N | -5.53860396 | -1.88659690 | 0.01345100 |
| H | -5.87187796 | -1.68588690 | 0.96234400 |
| N | -2.76542696 | -2.30266790 | -0.41573700 |
| C | -1.16023296 | 0.44335510 | -0.95121000 |
| H | -1.57523596 | 0.58681210 | -1.95921700 |
| C | -0.67977496 | -1.01249790 | -0.81080600 |
| H | -0.42393596 | -1.20700990 | 0.24150300 |
| H | 0.25244804 | -1.09634590 | -1.37854000 |

| | | | |
|---|---|---|---|
| C | -1.61047696 | -2.12122590 | -1.32731200 |
| H | -2.03086796 | -1.81123290 | -2.29430100 |
| C | -3.74289096 | -3.31185590 | -0.88706400 |
| H | -3.99791696 | -3.05888690 | -1.92366200 |
| H | -3.30287296 | -4.31173790 | -0.89842400 |
| C | -4.98027996 | -3.25807190 | -0.00480400 |
| H | -4.71656596 | -3.51674290 | 1.02550400 |
| H | -5.73726696 | -3.96985690 | -0.34421200 |
| C | -6.62767496 | -1.63171490 | -0.95127400 |
| H | -6.21257896 | -1.77515590 | -1.95924500 |
| C | -7.10822996 | -0.17587890 | -0.81093300 |
| H | -8.04040996 | -0.09210490 | -1.37875700 |
| H | -7.36417596 | 0.01862710 | 0.24135100 |
| C | -6.17760096 | 0.93293110 | -1.32736700 |
| H | -5.75731096 | 0.62308310 | -2.29444100 |
| C | -4.04507496 | 2.12342510 | -0.88736800 |
| H | -3.79000296 | 1.87029410 | -1.92391700 |
| H | -4.48512596 | 3.12329310 | -0.89888100 |
| C | -2.80770896 | 2.06979710 | -0.00506600 |
| H | -2.05071496 | 2.78153810 | -0.34454600 |
| H | -3.07146296 | 2.32861810 | 1.02519300 |
| H | -2.40482096 | -2.60218590 | 0.49222000 |
| H | -1.91614296 | 0.49774610 | 0.96234500 |
| C | -3.89409796 | -0.59410990 | 2.29770100 |
| O | -2.77802996 | -0.29086790 | 2.72317000 |
| O | -5.01014096 | -0.89732590 | 2.72323700 |
| N | -0.10651396 | 1.42090510 | -0.79420700 |
| H | 0.45170004 | 1.22396110 | 0.03105100 |
| N | -0.94434296 | -3.38745690 | -1.54528400 |
| H | -0.29313596 | -3.58493690 | -0.79107000 |
| N | -7.68136096 | -2.60928190 | -0.79436000 |
| H | -8.23970596 | -2.41234990 | 0.03080600 |
| N | -6.84383596 | 2.19916210 | -1.54504700 |
| H | -7.49525396 | 2.39627810 | -0.79092200 |

| | | | |
|---|---|---|---|
| C | -8.52668596 | -2.82049290 | -1.96275200 |
| H | -9.28200696 | -3.57052490 | -1.72218900 |
| H | -9.04525696 | -1.91738290 | -2.32127100 |
| H | -7.91960796 | -3.21443390 | -2.78394100 |
| C | -7.50281496 | 2.34044010 | -2.83930000 |
| H | -8.25728996 | 1.56622310 | -3.04986800 |
| H | -7.99422296 | 3.31378610 | -2.88357500 |
| H | -6.75103296 | 2.31351510 | -3.63379900 |
| C | 0.73904004 | 1.63189510 | -1.96248700 |
| H | 1.49436004 | 2.38191910 | -1.72189300 |
| H | 1.25762004 | 0.72870510 | -2.32078300 |
| H | 0.13213204 | 2.02575910 | -2.78383700 |
| C | -0.28509996 | -3.52835190 | -2.83943800 |
| H | 0.46952904 | -2.75416590 | -3.04957400 |
| H | 0.20618504 | -4.50174790 | -2.88396300 |
| H | -1.03671796 | -3.50103690 | -3.63408100 |

**NHMe-hor-TS2**

```
SCF Energy: -1615.917198
Gibbs Energy: -1615.385908
```

| | | | |
|---|---|---|---|
| Ni | -4.60694682 | -0.31989945 | -0.00418770 |
| N | -5.35386682 | 1.55025955 | -0.61862170 |
| N | -2.77356782 | 0.37050055 | -0.78832770 |
| H | -2.69550082 | -0.04465945 | -1.71792470 |
| N | -3.81564782 | -2.16249645 | 0.68381530 |
| H | -3.82444782 | -2.74368845 | -0.15502570 |
| N | -6.02305782 | -0.57685445 | 1.51504130 |
| C | -5.86286782 | 2.44467455 | 0.44473330 |
| H | -5.02244182 | 2.66929155 | 1.11648130 |
| C | -6.96084182 | 1.71200255 | 1.23541630 |
| H | -7.69447682 | 1.28958655 | 0.53295930 |
| H | -7.48870482 | 2.46947855 | 1.82402530 |

| | | | |
|---|---|---|---|
| C | -6.51559282 | 0.62481755 | 2.22378030 |
| H | -5.66973482 | 1.00779855 | 2.81135130 |
| C | -5.45321082 | -1.58798145 | 2.43155730 |
| H | -4.69327882 | -1.08944245 | 3.04696230 |
| H | -6.21575282 | -1.97580045 | 3.11225030 |
| C | -4.83261482 | -2.70925145 | 1.61632630 |
| H | -5.60688382 | -3.19095545 | 1.01277630 |
| H | -4.38218982 | -3.46632145 | 2.26346930 |
| C | -2.43708982 | -2.14187145 | 1.21893430 |
| H | -2.45014782 | -1.50732345 | 2.11615630 |
| C | -1.48144182 | -1.51941345 | 0.18587430 |
| H | -0.46354782 | -1.73569045 | 0.52615730 |
| H | -1.60083982 | -2.03374945 | -0.77989870 |
| C | -1.55825682 | 0.00100055 | -0.02406070 |
| H | -1.65764482 | 0.48669955 | 0.95660730 |
| C | -2.93545782 | 1.83538755 | -0.95099470 |
| H | -2.81329182 | 2.28912255 | 0.03974030 |
| H | -2.15463182 | 2.25114555 | -1.59188470 |
| C | -4.32025682 | 2.13156455 | -1.50173170 |
| H | -4.47540482 | 3.20811855 | -1.61407370 |
| H | -4.43386482 | 1.67101255 | -2.48845170 |
| H | -6.82386182 | -1.00889845 | 1.03819130 |
| H | -6.15183482 | 1.26569755 | -1.18806570 |
| C | -5.80028482 | -1.34679745 | -1.41269670 |
| O | -6.87885282 | -0.77669145 | -1.61920170 |
| O | -5.66051082 | -2.62575445 | -1.64965870 |
| C | -8.85397582 | -2.80644245 | -0.83509470 |
| O | -8.15782882 | -2.71564845 | -1.91579170 |
| H | -6.60056982 | -2.94165345 | -1.88501570 |
| O | -8.18035082 | -2.41827945 | 0.31617430 |
| H | -8.79821582 | -2.62410045 | 1.03079730 |
| O | -9.99185082 | -3.21747245 | -0.75093070 |
| N | -0.38134382 | 0.56409955 | -0.65114870 |
| H | -0.06320282 | -0.02584545 | -1.41454470 |

| | | | |
|---|---|---|---|
| N | -2.03835582 | -3.46282945 | 1.65167530 |
| H | -1.77800882 | -4.04365545 | 0.86048230 |
| N | -6.29621082 | 3.70649455 | -0.11487470 |
| H | -7.21263582 | 3.61491355 | -0.54323570 |
| N | -7.55286782 | 0.25226755 | 3.16558530 |
| H | -8.45585182 | 0.21532955 | 2.70183430 |
| C | 0.72220918 | 0.86391955 | 0.25566630 |
| H | 1.08245018 | -0.00282245 | 0.83174030 |
| H | 1.55960518 | 1.25903955 | -0.32174370 |
| H | 0.41134718 | 1.64009755 | 0.96133230 |
| C | -1.01511582 | -3.50512445 | 2.68926230 |
| H | -0.78721382 | -4.54746945 | 2.91865930 |
| H | -0.07332882 | -3.00017645 | 2.42208430 |
| H | -1.40458582 | -3.04340045 | 3.60191530 |
| C | -7.62957082 | 1.07651355 | 4.36721430 |
| H | -7.78046182 | 2.14981255 | 4.17102230 |
| H | -8.45647482 | 0.72625855 | 4.98750830 |
| H | -6.70872182 | 0.95897055 | 4.94640830 |
| C | -6.26413682 | 4.83900655 | 0.80344930 |
| H | -6.65114282 | 5.72230755 | 0.29276030 |
| H | -6.84988682 | 4.69343155 | 1.72469030 |
| H | -5.22760682 | 5.04782555 | 1.08640030 |

**NHMe-hor-3**

SCF Energy: -1351.618002
Gibbs Energy: -1351.105677

| | | | |
|---|---|---|---|
| Ni | -2.15063780 | 0.15667308 | -0.16721019 |
| N | -0.46542780 | 1.43865208 | -0.24151219 |
| N | -3.25048780 | 1.89176508 | -0.67051419 |
| H | -3.62618180 | 2.22617308 | 0.21776881 |
| N | -3.83509980 | -1.12969392 | -0.22405919 |
| H | -2.92087980 | -0.24036492 | 3.49904781 |

| | | | |
|---|---|---|---|
| N | -1.05398580 | -1.57142392 | -0.69684619 |
| C | 0.57487720 | 1.16471408 | -1.24658619 |
| H | 0.12197820 | 1.31422208 | -2.23727119 |
| C | 1.03317920 | -0.30005992 | -1.12936419 |
| H | 1.30487420 | -0.51066292 | -0.08405619 |
| H | 1.95286220 | -0.39571692 | -1.71548119 |
| C | 0.06901820 | -1.38253692 | -1.63962619 |
| H | -0.37724180 | -1.04184092 | -2.58432019 |
| C | -2.05693380 | -2.55149092 | -1.16684419 |
| H | -2.32631280 | -2.27575192 | -2.19371719 |
| H | -1.63972780 | -3.56088192 | -1.20850119 |
| C | -3.28019480 | -2.50009892 | -0.26467619 |
| H | -2.99758780 | -2.76660792 | 0.75857481 |
| H | -4.04021080 | -3.21176592 | -0.59960519 |
| C | -4.86687080 | -0.84453092 | -1.23877819 |
| H | -4.39822180 | -0.97689292 | -2.22394819 |
| C | -5.33641580 | 0.61542808 | -1.10675719 |
| H | -6.25595580 | 0.70860408 | -1.69370319 |
| H | -5.61324680 | 0.81416808 | -0.06025219 |
| C | -4.38218380 | 1.71301208 | -1.60430219 |
| H | -3.94325580 | 1.39064708 | -2.55864419 |
| C | -2.24857380 | 2.87216908 | -1.14726519 |
| H | -1.99194680 | 2.59933908 | -2.17819519 |
| H | -2.66508080 | 3.88222008 | -1.17862519 |
| C | -1.01364680 | 2.81031608 | -0.26181519 |
| H | -0.25621780 | 3.52207508 | -0.60237819 |
| H | -1.27859580 | 3.07187008 | 0.76750281 |
| H | -0.66724080 | -1.90481892 | 0.18716881 |
| H | -0.09340480 | 1.24978308 | 0.69343181 |
| C | -2.01795880 | 0.15424908 | 1.85616781 |
| O | -1.02325480 | 0.48018208 | 2.48742781 |
| O | -3.12374380 | -0.26924292 | 2.54777881 |
| H | -4.23356880 | -0.97307592 | 0.70228281 |
| N | 0.71343820 | -2.65199292 | -1.91553719 |

| | | | |
|---|---|---|---|
| H | 1.37608020 | -2.88170292 | -1.18045619 |
| N | 1.65693720 | 2.12219308 | -1.14109019 |
| H | 2.24443020 | 1.91635108 | -0.33862819 |
| N | -5.03735580 | 2.98196608 | -1.85330219 |
| H | -5.69572380 | 3.19683508 | -1.11012119 |
| N | -5.94546880 | -1.80866792 | -1.16294719 |
| H | -6.56677880 | -1.59611892 | -0.38820119 |
| C | 2.45787320 | 2.30001908 | -2.34498119 |
| H | 3.23812920 | 3.03749708 | -2.14786819 |
| H | 2.94223820 | 1.38161408 | -2.71355119 |
| H | 1.82472420 | 2.69528508 | -3.14578419 |
| C | 1.35091120 | -2.75174792 | -3.22360019 |
| H | 2.11260420 | -1.97970492 | -3.41741919 |
| H | 1.82856920 | -3.72896592 | -3.31401619 |
| H | 0.58768120 | -2.68371792 | -4.00487719 |
| C | -6.69872980 | -2.00236292 | -2.39565119 |
| H | -7.48514980 | -2.73891992 | -2.22100619 |
| H | -7.16865680 | -1.08836092 | -2.79250619 |
| H | -6.03382780 | -2.40551092 | -3.16604219 |
| C | -5.68137280 | 3.10395108 | -3.15619019 |
| H | -6.44047480 | 2.33232508 | -3.36163419 |
| H | -6.16388080 | 4.08047408 | -3.22550519 |
| H | -4.92137480 | 3.05485708 | -3.94189019 |

**NHMe-hor-TS4**

SCF Energy: -1616.644794
Gibbs Energy: -1616.104879

| | | | |
|---|---|---|---|
| Ni | -3.07129788 | 0.72212065 | 0.00000000 |
| N | -1.86422588 | -1.01906035 | 0.06920300 |
| N | -4.36474088 | -0.35442335 | 1.21167600 |
| H | -5.10522288 | -0.61261235 | 0.53498200 |
| N | -4.22021188 | 2.46975565 | 0.05247600 |

| | | | |
|---|---|---|---|
| H | -5.41440388 | 0.89397765 | -3.26433400 |
| N | -1.42475788 | 2.02896865 | -0.23257700 |
| C | -0.62985588 | -0.87719335 | 0.87659800 |
| C | 0.23860712 | 0.25375165 | 0.29859200 |
| H | 0.37684612 | 0.09509965 | -0.78214000 |
| H | 1.23008112 | 0.15393565 | 0.75241400 |
| C | -0.21268088 | 1.69951765 | 0.55485600 |
| C | -1.94333788 | 3.39105065 | 0.04818800 |
| H | -1.94936688 | 3.51943165 | 1.13621000 |
| H | -1.27854388 | 4.15718365 | -0.35665200 |
| C | -3.35124488 | 3.52625365 | -0.50703700 |
| H | -3.34160388 | 3.40013965 | -1.59476500 |
| H | -3.76209588 | 4.51439665 | -0.28201500 |
| C | -4.82337288 | 2.78920565 | 1.37016200 |
| C | -5.72797688 | 1.63526065 | 1.81833000 |
| H | -6.33203188 | 2.01104365 | 2.64979100 |
| H | -6.43209788 | 1.38119465 | 1.01705400 |
| C | -5.05166588 | 0.34893665 | 2.32269800 |
| C | -3.66841588 | -1.57967235 | 1.65255200 |
| H | -3.06747988 | -1.33363835 | 2.53661700 |
| H | -4.38056488 | -2.34761635 | 1.96129800 |
| C | -2.78920288 | -2.08867335 | 0.52400700 |
| H | -2.22349488 | -2.97151135 | 0.83299500 |
| H | -3.41571588 | -2.35854335 | -0.33205100 |
| H | -1.16587988 | 1.99052565 | -1.21934300 |
| H | -1.57571288 | -1.23833135 | -0.88330700 |
| C | -3.43415788 | 0.42260265 | -2.03844700 |
| O | -2.92611288 | 0.12694565 | -3.03728300 |
| O | -5.17588388 | 0.96901465 | -2.33102700 |
| C | -7.51715288 | -0.54545335 | -0.48274300 |
| O | -8.34055288 | -0.21005035 | -1.50145100 |
| H | -9.24491088 | -0.27927435 | -1.17054600 |
| O | -6.26697788 | -0.50149935 | -0.80824900 |
| H | -5.80996488 | 0.26151065 | -1.70481000 |

| | | | |
|---|---|---|---|
| O | -7.95420888 | -0.83487035 | 0.62489700 |
| H | -0.94060888 | -0.60111735 | 1.89301900 |
| H | -4.28111188 | 0.62408065 | 3.06032000 |
| H | -0.50004388 | 1.79518765 | 1.61084900 |
| H | -3.99760988 | 2.89695865 | 2.08776800 |
| H | -4.97234688 | 2.28901265 | -0.61534500 |
| N | -5.95926688 | -0.56862035 | 2.96752900 |
| H | -6.75727388 | -0.75422235 | 2.35696300 |
| N | -5.49527388 | 4.07176065 | 1.31579300 |
| H | -6.41582088 | 3.96939665 | 0.89825200 |
| N | 0.06251412 | -2.14156335 | 0.98338600 |
| H | 0.60680112 | -2.33254835 | 0.14765400 |
| N | 0.82267212 | 2.68112365 | 0.31091000 |
| H | 1.33718512 | 2.45894165 | -0.53626500 |
| C | 0.87509412 | -2.31090835 | 2.18247500 |
| H | 1.36626812 | -3.28459035 | 2.14343400 |
| H | 1.65191712 | -1.54118135 | 2.31649400 |
| H | 0.22727612 | -2.30265935 | 3.06444900 |
| C | 1.74236512 | 2.91166065 | 1.42031400 |
| H | 2.26645112 | 2.00830365 | 1.76964600 |
| H | 2.49268812 | 3.64126965 | 1.11145600 |
| H | 1.19427412 | 3.33938665 | 2.26507600 |
| C | -6.37226088 | -0.20908735 | 4.31367600 |
| H | -6.89449288 | 0.75852565 | 4.39385400 |
| H | -7.04582288 | -0.98009935 | 4.69248500 |
| H | -5.49821688 | -0.17862835 | 4.97419500 |
| C | -5.59120888 | 4.77313965 | 2.59121300 |
| H | -6.12428988 | 5.71369865 | 2.44100800 |
| H | -6.10836288 | 4.20802965 | 3.38216400 |
| H | -4.58543688 | 5.01731965 | 2.94787800 |

**mesoCOOH-1**

SCF Energy: -1349.484845

Gibbs Energy: -1349.130722

| | | | |
|---|---|---|---|
| Ni | -3.74771468 | 0.46617915 | 0.00000000 |
| N | -5.18152368 | -1.05322585 | -0.03174800 |
| N | -2.38471768 | -1.06715185 | -0.43819600 |
| H | -1.97163268 | -1.32787685 | 0.45906000 |
| N | -2.31425968 | 1.98541415 | -0.02590800 |
| H | -1.90928568 | 1.88185215 | 0.91012800 |
| N | -5.11073568 | 2.00122315 | -0.43229000 |
| C | -6.25479068 | -0.93252485 | -1.03298600 |
| H | -6.97293168 | -1.75102485 | -0.91343800 |
| H | -5.81809668 | -1.00875985 | -2.03480000 |
| C | -7.00316968 | 0.40288615 | -0.90491400 |
| H | -7.85933168 | 0.33667515 | -1.58921700 |
| C | -6.21949268 | 1.64767215 | -1.34085300 |
| H | -5.79180568 | 1.45880215 | -2.33166100 |
| H | -6.90755168 | 2.49508415 | -1.43859500 |
| C | -4.29993368 | 3.13896615 | -0.91803900 |
| H | -4.02377168 | 2.93299115 | -1.95885000 |
| H | -4.87192668 | 4.07400215 | -0.90932800 |
| C | -3.05277668 | 3.26550415 | -0.05096500 |
| H | -3.33899168 | 3.49687115 | 0.97963800 |
| H | -2.41959468 | 4.08485115 | -0.40857200 |
| C | -1.24142868 | 1.86864115 | -1.02813100 |
| H | -0.52352168 | 2.68694215 | -0.90588300 |
| H | -1.67858068 | 1.94839415 | -2.02947100 |
| C | -0.49261068 | 0.53303315 | -0.90523000 |
| H | 0.36341332 | 0.60207715 | -1.58943100 |
| C | -1.27613568 | -0.71024885 | -1.34563300 |
| H | -1.70393868 | -0.51788485 | -2.33571600 |
| H | -0.58798368 | -1.55720685 | -1.44657100 |
| C | -3.19553768 | -2.20300985 | -0.92829700 |
| H | -3.47158468 | -1.99305585 | -1.96835500 |
| H | -2.62352568 | -3.13806685 | -0.92313400 |

| | | | |
|---|---|---|---|
| C | -4.44288468 | -2.33314985 | -0.06204200 |
| H | -5.07590968 | -3.15097285 | -0.42339600 |
| H | -4.15704568 | -2.56887485 | 0.96767200 |
| H | -5.52373968 | 2.25868815 | 0.46594000 |
| H | -5.58579368 | -0.95359485 | 0.90504800 |
| C | -3.74683068 | 0.45705315 | 2.27450300 |
| O | -4.81358168 | 0.00950215 | 2.69748700 |
| O | -2.67699268 | 0.90022015 | 2.69498800 |
| C | 0.13252032 | 0.43410515 | 0.48492600 |
| O | 0.53525932 | 1.38898315 | 1.09870700 |
| O | 0.19188732 | -0.82511485 | 0.94899700 |
| H | 0.59636132 | -0.80015485 | 1.83044700 |
| C | -7.62820068 | 0.49660915 | 0.48561000 |
| O | -8.03187068 | -0.46038485 | 1.09543100 |
| O | -7.68633768 | 1.75400015 | 0.95502700 |
| H | -8.09132368 | 1.72569715 | 1.83613900 |

**mesoCOOH-TS2**

```
SCF Energy: -1614.512557
Gibbs Energy: -1614.131223
```

| | | | |
|---|---|---|---|
| Ni | -5.97806195 | -2.86106029 | 0.00000000 |
| N | -4.99036095 | -4.10656929 | 1.43188400 |
| N | -7.00370895 | -2.17386629 | 1.66178600 |
| H | -7.84112295 | -2.75690329 | 1.55467300 |
| N | -6.83597295 | -1.41266329 | -1.34360400 |
| H | -7.64577095 | -1.86350929 | -1.77384800 |
| N | -4.18776995 | -2.28776229 | -0.95920400 |
| C | -3.59129495 | -3.77571529 | 1.77390900 |
| H | -3.17810595 | -4.56985929 | 2.40610800 |
| H | -3.58595695 | -2.85382029 | 2.36291600 |
| C | -2.68785095 | -3.57394429 | 0.55892200 |
| H | -1.65732095 | -3.52123829 | 0.93495900 |

| | | | |
|---|---|---|---|
| C | -2.92495295 | -2.26302629 | -0.20424800 |
| H | -2.97441195 | -1.43764729 | 0.51252800 |
| H | -2.08500695 | -2.07312929 | -0.88117800 |
| C | -4.44540995 | -1.05541629 | -1.73425800 |
| H | -4.41366295 | -0.21188629 | -1.03729600 |
| H | -3.66903495 | -0.89345429 | -2.49086100 |
| C | -5.81643595 | -1.18128829 | -2.38352900 |
| H | -5.83129295 | -2.03958829 | -3.06349500 |
| H | -6.04077595 | -0.28668629 | -2.97616800 |
| C | -7.34165995 | -0.15294729 | -0.75620400 |
| H | -7.89263095 | 0.40327571 | -1.52223000 |
| H | -6.48998795 | 0.46073371 | -0.44677200 |
| C | -8.24328895 | -0.39223529 | 0.45568500 |
| H | -8.74990695 | 0.55736171 | 0.66793000 |
| C | -7.48457895 | -0.78221329 | 1.73052200 |
| H | -6.62291095 | -0.12097129 | 1.86861400 |
| H | -8.14115895 | -0.66737929 | 2.59948200 |
| C | -6.32477995 | -2.64443729 | 2.88008000 |
| H | -5.48084895 | -1.97649829 | 3.08273800 |
| H | -6.99321095 | -2.60482629 | 3.74798800 |
| C | -5.86179095 | -4.07336129 | 2.62740500 |
| H | -5.35030495 | -4.47711029 | 3.50863600 |
| H | -6.72953995 | -4.70606829 | 2.41938200 |
| H | -4.10974495 | -3.04285629 | -1.64620100 |
| H | -4.98378695 | -5.05574529 | 1.05778900 |
| C | -7.23868495 | -4.41771629 | -0.99167500 |
| O | -7.19782895 | -4.70928429 | -2.16616100 |
| O | -8.01188695 | -4.52350229 | -0.00999900 |
| C | -9.34811595 | -1.39569129 | 0.10409700 |
| O | -9.65704195 | -1.64047429 | -1.04589900 |
| O | -9.87150695 | -1.96857229 | 1.16676700 |
| H | -10.64778195 | -2.81687629 | 0.86037100 |
| C | -2.73098595 | -4.80297529 | -0.33828900 |
| O | -3.24373595 | -5.85155429 | -0.02787600 |

| | | | |
|---|---|---|---|
| O | -2.15291295 | -4.58941129 | -1.52917200 |
| H | -2.16948295 | -5.41866329 | -2.03177000 |
| C | -11.52486195 | -4.71204429 | -0.25203700 |
| O | -10.50009595 | -5.33119929 | -0.80343300 |
| H | -9.46758895 | -4.95173129 | -0.37642600 |
| O | -12.68773095 | -5.11778429 | -0.73045500 |
| H | -12.55044295 | -5.79882329 | -1.40154500 |
| O | -11.47064395 | -3.86119029 | 0.62264800 |

**mesoCOOH-3**

SCF Energy: -1350.132283
Gibbs Energy: -1349.765729

| | | | |
|---|---|---|---|
| Ni | -1.86471657 | 1.41681899 | 0.00000000 |
| N | -0.39479957 | 2.94007199 | -0.02149600 |
| N | -3.19505957 | 2.99132599 | -0.48036200 |
| H | -3.64623657 | 3.25995099 | 0.39604100 |
| N | -3.34203657 | -0.11002201 | -0.15388800 |
| H | -3.75535157 | -0.09654701 | 0.77892300 |
| N | -0.53287557 | -0.11659501 | -0.61031500 |
| C | 0.65688543 | 2.84194299 | -1.04322800 |
| H | 1.39698143 | 3.63881699 | -0.90494100 |
| H | 0.20398043 | 2.97371999 | -2.03197300 |
| C | 1.37580143 | 1.48558999 | -1.00483500 |
| H | 2.22750543 | 1.57496999 | -1.69272300 |
| C | 0.56093943 | 0.28845399 | -1.51229100 |
| H | 0.11559843 | 0.56191999 | -2.47500400 |
| H | 1.23407243 | -0.55793201 | -1.69417300 |
| C | -1.37707557 | -1.18527201 | -1.17784200 |
| H | -1.68050157 | -0.87404401 | -2.18430100 |
| H | -0.82751057 | -2.12903701 | -1.28073800 |
| C | -2.60313757 | -1.38027001 | -0.29369100 |
| H | -2.28862557 | -1.68863001 | 0.70802200 |

| | | | |
|---|---|---|---|
| H | -3.24058557 | -2.17505101 | -0.69941000 |
| C | -4.40021057 | 0.08507799 | -1.15555800 |
| H | -5.14525057 | -0.71653701 | -1.08671700 |
| H | -3.95076657 | 0.03246199 | -2.15290600 |
| C | -5.10424357 | 1.44388399 | -1.00826300 |
| H | -5.96648057 | 1.40588599 | -1.68747300 |
| C | -4.27775457 | 2.66620899 | -1.42589800 |
| H | -3.82822057 | 2.46642399 | -2.40465200 |
| H | -4.94696557 | 3.52745299 | -1.54234400 |
| C | -2.35417157 | 4.11576399 | -0.93523800 |
| H | -2.04993857 | 3.91394299 | -1.96918200 |
| H | -2.90955557 | 5.06151299 | -0.93707300 |
| C | -1.13113757 | 4.21835599 | -0.03221500 |
| H | -0.49086557 | 5.04958799 | -0.35078000 |
| H | -1.44764757 | 4.42174299 | 0.99526300 |
| H | -0.10522157 | -0.46754901 | 0.24708900 |
| H | 0.02612243 | 2.83526699 | 0.90527500 |
| C | -1.76601757 | 1.32514099 | 2.01567000 |
| O | -0.91866657 | 1.87320999 | 2.69977000 |
| O | -2.72601557 | 0.56252499 | 2.63641200 |
| C | -5.69959257 | 1.64524699 | 0.37865900 |
| O | -6.30655457 | 0.54495899 | 0.83696100 |
| O | -5.64210757 | 2.67963899 | 1.00372000 |
| H | -2.57289457 | 0.59899599 | 3.59643400 |
| C | 2.01409643 | 1.28549499 | 0.36519300 |
| O | 2.41708743 | 2.18810599 | 1.05406600 |
| O | 2.09627443 | -0.00841901 | 0.72625000 |
| H | 2.53502943 | -0.04583901 | 1.59022500 |
| H | -6.68320957 | 0.74428099 | 1.70755900 |

**mesoCOOH-TS4**

SCF Energy: -1615.161548
Gibbs Energy: -1614.765027

| | | | |
|---|---|---|---|
| Ni | -3.56489933 | -0.48446069 | 0.00000000 |
| N | -4.64002633 | 0.82995331 | -1.22403600 |
| N | -1.92991733 | 0.05774831 | -1.23682400 |
| H | -1.80400533 | -0.68758969 | -1.92489800 |
| N | -2.37720933 | -1.69462369 | 1.31948800 |
| H | -2.27324833 | -2.61948369 | 0.90619400 |
| N | -4.71553833 | -0.16741869 | 1.69785700 |
| C | -5.17439833 | 2.01957631 | -0.52168500 |
| H | -5.73504333 | 2.63118231 | -1.23767200 |
| H | -4.34198433 | 2.62492731 | -0.14515700 |
| C | -6.09430133 | 1.62819831 | 0.64087300 |
| H | -6.63887933 | 2.53330131 | 0.93608000 |
| C | -5.36139833 | 1.14389231 | 1.89392200 |
| H | -4.58806033 | 1.87206331 | 2.16648700 |
| H | -6.07406533 | 1.08332431 | 2.72276000 |
| C | -3.93461933 | -0.57972569 | 2.87509200 |
| H | -3.23591433 | 0.22583331 | 3.13220700 |
| H | -4.58001433 | -0.73862869 | 3.74725700 |
| C | -3.18466633 | -1.86326469 | 2.55457700 |
| H | -3.90769533 | -2.65874569 | 2.36347300 |
| H | -2.55405933 | -2.16623069 | 3.39817100 |
| C | -1.01991933 | -1.17328469 | 1.57358000 |
| H | -0.47921833 | -1.84755869 | 2.24722500 |
| H | -1.10964433 | -0.20566969 | 2.07724400 |
| C | -0.20767633 | -0.98267769 | 0.28139800 |
| H | 0.82492167 | -0.79857869 | 0.60403100 |
| C | -0.62070033 | 0.21932531 | -0.57158800 |
| H | -0.67296033 | 1.10144931 | 0.07528000 |
| H | 0.15344867 | 0.41269431 | -1.32367200 |
| C | -2.34318433 | 1.28897731 | -1.94730100 |
| H | -2.24109933 | 2.12877631 | -1.25073100 |
| H | -1.69216533 | 1.49231631 | -2.80504500 |

| | | | |
|---|---|---|---|
| C | -3.79173233 | 1.14618531 | -2.38776500 |
| H | -4.12839733 | 2.05842131 | -2.89310600 |
| H | -3.88170333 | 0.32452431 | -3.10595300 |
| H | -5.43027933 | -0.90343869 | 1.51668500 |
| H | -5.48888233 | 0.35020231 | -1.54681700 |
| C | -4.33781733 | -2.19347969 | -0.94847100 |
| O | -4.47517133 | -3.04595669 | -1.68775100 |
| O | -5.88821033 | -2.41608169 | 0.63104700 |
| C | -0.15880733 | -2.25561969 | -0.55080400 |
| O | 0.22470267 | -3.31365669 | 0.16954300 |
| O | -0.44821633 | -2.32115669 | -1.72492300 |
| H | -5.87423433 | -3.26215869 | 1.09213000 |
| C | -7.15889033 | 0.61625431 | 0.19705300 |
| O | -7.29502333 | 0.30603431 | -0.98038700 |
| O | -7.83786033 | 0.13057731 | 1.19140700 |
| H | -8.46433333 | -0.64926269 | 0.87066100 |
| C | -8.95942233 | -2.45712769 | -0.50965200 |
| O | -7.76186233 | -2.81540169 | -0.82116600 |
| H | -6.91118333 | -2.54315569 | -0.09465600 |
| O | -9.91974233 | -2.98455669 | -1.27212000 |
| H | -9.50532033 | -3.56787269 | -1.91908300 |
| O | -9.30264633 | -1.70099469 | 0.40743200 |
| H | 0.28149867 | -4.08607469 | -0.41420500 |

**mesoCOOH-TS4’**

SCF Energy: -1615.151569
Gibbs Energy: -1614.755114

| | | | |
|---|---|---|---|
| Ni | -4.31444226 | -0.75868372 | 0.00000000 |
| N | -3.33237826 | -2.01797372 | 1.42525900 |
| N | -5.41033326 | -0.12876172 | 1.65787800 |
| H | -6.23440426 | -0.72688972 | 1.53607200 |
| N | -5.18399226 | 0.66276428 | -1.35430200 |

| | | | |
|---|---|---|---|
| H | -5.99916326 | 0.21429228 | -1.77385500 |
| N | -2.53006026 | -0.22381972 | -1.00996400 |
| C | -1.93428026 | -1.68209972 | 1.76025800 |
| H | -1.51176226 | -2.46727372 | 2.39843900 |
| H | -1.93001526 | -0.75391972 | 2.34015000 |
| C | -1.03220726 | -1.49542972 | 0.53344800 |
| H | -0.00000326 | -1.44337772 | 0.90436800 |
| C | -1.26718726 | -0.19722472 | -0.25266900 |
| H | -1.31368326 | 0.63718328 | 0.45415800 |
| H | -0.42564926 | -0.01994872 | -0.93194800 |
| C | -2.79147326 | 1.01011128 | -1.78046700 |
| H | -2.74490726 | 1.85493528 | -1.08528600 |
| H | -2.02678526 | 1.16950328 | -2.54997300 |
| C | -4.17479326 | 0.89225528 | -2.40459000 |
| H | -4.19802826 | 0.03419028 | -3.08435500 |
| H | -4.40536726 | 1.78765928 | -2.99464200 |
| C | -5.69717226 | 1.90674828 | -0.74699100 |
| H | -6.23027026 | 2.48540728 | -1.50998500 |
| H | -4.84867426 | 2.50969328 | -0.40676000 |
| C | -6.63164326 | 1.64497928 | 0.44137700 |
| H | -7.15862626 | 2.58804128 | 0.63203500 |
| C | -5.91015626 | 1.25592128 | 1.73509200 |
| H | -5.05857726 | 1.92597528 | 1.89725800 |
| H | -6.58903726 | 1.35298628 | 2.58873000 |
| C | -4.72782526 | -0.59460372 | 2.87675700 |
| H | -3.90514926 | 0.09533528 | 3.09694500 |
| H | -5.40482926 | -0.58674572 | 3.73930900 |
| C | -4.21643226 | -2.00429272 | 2.61624300 |
| H | -3.70118026 | -2.40101772 | 3.49894400 |
| H | -5.06752526 | -2.65482172 | 2.39675000 |
| H | -2.45178426 | -0.97650772 | -1.69668300 |
| H | -3.32232926 | -2.96525672 | 1.05081700 |
| C | -5.56919526 | -2.27989372 | -0.85798000 |
| O | -5.64402126 | -2.68874672 | -2.12825100 |

| | | | |
|---|---|---|---|
| O | -6.45350426 | -2.56124472 | -0.01725300 |
| C | -7.71798126 | 0.62423028 | 0.06192100 |
| O | -7.99175326 | 0.38538428 | -1.10690000 |
| O | -8.26403326 | 0.05472128 | 1.09993400 |
| H | -9.01795426 | -0.80600472 | 0.81157100 |
| C | -1.07687426 | -2.73509572 | -0.35066100 |
| O | -1.59091026 | -3.78315972 | -0.03614700 |
| O | -0.48789726 | -2.53809872 | -1.53924400 |
| H | -0.50275126 | -3.37418372 | -2.02982000 |
| C | -9.76845126 | -2.63065672 | -0.28403800 |
| O | -8.68771626 | -3.30118672 | -0.56154400 |
| H | -7.68429026 | -2.88639372 | -0.38524100 |
| O | -10.88112126 | -3.16456972 | -0.76102100 |
| H | -10.67049526 | -3.97641072 | -1.23833800 |
| O | -9.84136826 | -1.59001272 | 0.37660400 |
| H | -6.46193626 | -3.20069472 | -2.30901800 |

**$H_2CO_3$**

SCF Energy: -265.0265856
Gibbs Energy: -265.0123606

| | | | |
|---|---|---|---|
| C | -3.43280441 | 0.33450704 | -0.04493786 |
| O | -3.88356341 | 1.60867504 | -0.04439086 |
| H | -4.84810041 | 1.57362704 | -0.04404286 |
| O | -2.10044841 | 0.30394104 | -0.04396186 |
| H | -1.75066641 | 1.20324404 | -0.04404386 |
| O | -4.13020141 | -0.64128196 | -0.04392086 |

**$H_2O$**

SCF Energy: -76.44283475
Gibbs Energy: -76.43872275

| | | | |
|---|---|---|---|
| O | -1.86619719 | 1.54929575 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -1.86619719 | 2.31574875 | -0.57807500 |
| H | -1.86619719 | 0.78284275 | -0.57807500 |

**Methanol**

SCF Energy: -115.7336645
Gibbs Energy: -115.7045345

| | | | |
|---|---|---|---|
| C | -0.14084507 | 1.10915491 | 0.00000000 |
| H | 0.27850093 | 2.11681891 | -0.00011800 |
| H | 0.22078593 | 0.58417791 | 0.89406200 |
| H | 0.22076793 | 0.58398291 | -0.89395500 |
| O | -1.54846807 | 1.25198291 | 0.00000000 |
| H | -1.95186107 | 0.38069591 | -0.00000100 |

**$CH_3COOH$**

SCF Energy: -229.1015382
Gibbs Energy: -229.0651522

| | | | |
|---|---|---|---|
| C | 0.24542635 | 1.39068365 | -0.03109047 |
| H | -0.03492865 | 0.80880565 | -0.91290447 |
| H | -0.03487565 | 0.80880665 | 0.85073953 |
| H | -0.27628865 | 2.34602965 | -0.03107747 |
| C | 1.72788935 | 1.63049065 | -0.03114347 |
| O | 2.27284835 | 2.70926265 | -0.03113747 |
| O | 2.42412835 | 0.47406365 | -0.03104647 |
| H | 3.36291235 | 0.70800265 | -0.03103647 |

**$CO_2$**

SCF Energy: -188.5872255
Gibbs Energy: -188.5961395

| | | | |
|---|---|---|---|
| C | -3.64416852 | 0.66895675 | -0.03894818 |
| O | -3.64416852 | 0.66895675 | 1.12571782 |

| | | | |
|---|---|---|---|
| O | -3.64416852 | 0.66895675 | -1.20361418 |

CO

SCF Energy: -113.3108109
Gibbs Energy: -113.3248389

| | | | |
|---|---|---|---|
| C | -2.85211269 | 0.14084507 | 0.00000000 |
| O | -2.85211269 | 0.14084507 | 1.13457900 |