

## Supporting Information

This document is associated with the paper titled:

### "Computational Insights in DNA Methylation: Catalytic and Mechanistic Elucidations for Forming 3-Methyl Cytosine"

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#### Path.A\_P\_B3LYP-6-31Gd.log.log

C -1.6965167888 2.3377375101 1.1170874495  
C -2.4290858841 0.8222211667 -1.1673586929  
C -3.2100203861 1.8399407491 -0.7205908282  
N -2.8526918188 2.5600017408 0.3727965569  
H -2.7062496973 0.242674659 -2.0377336247  
H -4.1385738019 2.1233118602 -1.2032903641  
O -1.4065631936 2.9955357783 2.0854203448  
N -0.8916089485 1.2684817786 0.6327056666  
C -1.2229128312 0.5253261469 -0.4619548893  
N -0.4287741039 -0.4622302288 -0.8624426628  
H 0.4558108844 -0.7550495015 -0.4226355635  
H -0.7015852669 -0.9952839227 -1.6782678556  
H -3.4294910719 3.3216429761 0.7147945269  
S 2.5176530633 -1.7865152311 0.2020220511  
C 3.6657691713 -1.8577557725 -1.2200831174  
H 3.8804037299 -0.8291651992 -1.5196804669  
H 4.5998026974 -2.3384095429 -0.9190515778  
H 3.2240818784 -2.3974370199 -2.0619668684  
C 0.3471403812 0.993667032 1.3850070529  
H 0.3971618113 1.708142979 2.2032315462  
H 1.2146966022 1.11870877 0.7325787853  
H 0.3225938841 -0.0232344675 1.7843138728  
C 2.2798775655 -3.569161659 0.535892878  
H 1.5904825957 -3.655425239 1.3791826106  
H 1.8592299259 -4.0840922579 -0.33182708  
H 3.2333196022 -4.0253171051 0.8132822501

Zero-point correction= 0.218524 (Hartree/Particle)  
Thermal correction to Energy= 0.233406

Thermal correction to Enthalpy= 0.234351  
 Thermal correction to Gibbs Free Energy= 0.173321  
 Sum of electronic and zero-point Energies= -912.441345  
 Sum of electronic and thermal Energies= -912.426462  
 Sum of electronic and thermal Enthalpies= -912.425518  
 Sum of electronic and thermal Free Energies= -912.486547  
 Entropy (Cal/Mol-Kelvin) = 128.447

**Path.A\_R\_B3LYP-6-31Gd.log.log**

C -0.5246550545 0.9255070898 0.5267079027  
 C -2.9691289744 1.9769006248 -0.3320268158  
 C -2.3256117474 2.540672759 0.7223799664  
 N -1.1362223961 2.0297761622 1.1415691055  
 H -3.9165442397 2.3625484056 -0.6865671963  
 H -2.7087817469 3.395844688 1.2679376207  
 O 0.562983797 0.5314525031 0.9789557416  
 N -1.1608213695 0.3536630702 -0.528145509  
 C -2.3278288132 0.847281284 -0.946664381  
 N -2.9139433471 0.240857841 -1.9978787557  
 H -2.4595091419 -0.553299346 -2.4243238971  
 H -3.7971960352 0.5521431692 -2.3716684695  
 H -0.6379009773 2.4335566127 1.9251081509  
 S 2.8014297607 -2.0867718356 0.1086376398  
 C 3.373055927 -0.3617320657 -0.0507815944  
 H 3.7261430443 -0.2348476273 -1.0768264868  
 H 2.5399684614 0.3054038182 0.1867963864  
 H 4.2098181289 -0.2349007146 0.6400759866  
 C 1.3401055005 -2.1129582085 -0.9820632651  
 H 0.6546442159 -1.3010638052 -0.7172803456  
 H 1.708082618 -2.0124773341 -2.0060973227  
 H 0.871701132 -3.0928847631 -0.8618246696  
 C 2.0483827819 -2.0967828913 1.7702470982  
 H 1.5699232494 -3.070393041 1.8994274288  
 H 2.8618600141 -1.9925338058 2.4919784704  
 H 1.3345052123 -1.2712705897 1.8348982102

Zero-point correction= 0.216972 (Hartree/Particle)  
 Thermal correction to Energy= 0.231816  
 Thermal correction to Enthalpy= 0.232760  
 Thermal correction to Gibbs Free Energy= 0.172753  
 Sum of electronic and zero-point Energies= -912.429001  
 Sum of electronic and thermal Energies= -912.414157  
 Sum of electronic and thermal Enthalpies= -912.413213  
 Sum of electronic and thermal Free Energies= -912.473219  
 Entropy (Cal/Mol-Kelvin) = 126.295

**Path.A\_TS\_B3LYP-6-31Gd.log.log**

C -0.70528871 1.46552062 0.78935792

C -3.07794371 1.61671662 -0.72151008  
 C -2.82676571 2.52646862 0.25728792  
 N -1.68325671 2.45395462 0.98431392  
 H -3.98383671 1.65823462 -1.31225508  
 H -3.50742671 3.33467662 0.50087092  
 O 0.30362129 1.44977362 1.47811492  
 N -0.96984271 0.54508462 -0.21079608  
 C -2.09031771 0.60070862 -0.93870108  
 N -2.28855671 -0.32386438 -1.89687508  
 H -1.60934171 -1.04675138 -2.07927708  
 H -3.12089371 -0.31037338 -2.46754408  
 H -1.47969271 3.12322162 1.71812992  
 S 2.47436229 -2.26630638 -0.32180608  
 C 3.81192629 -1.02414838 -0.25918108  
 H 3.91349329 -0.60138538 -1.26134408  
 H 3.57623429 -0.23229938 0.45692992  
 H 4.74787429 -1.51602938 0.01577492  
 C 0.59865029 -0.82038038 -0.33664008  
 H 1.00939929 -0.25001138 0.48441192  
 H 0.80135729 -0.52625338 -1.35596408  
 H -0.07136271 -1.64535038 -0.14307908  
 C 2.42770229 -2.80913438 1.42125492  
 H 1.63228029 -3.55245938 1.51193092  
 H 3.38106929 -3.27619738 1.67904792  
 H 2.22795929 -1.96593938 2.08816992

Zero-point correction=	0.215663 (Hartree/Particle)
Thermal correction to Energy=	0.230436
Thermal correction to Enthalpy=	0.231380
Thermal correction to Gibbs Free Energy=	0.172020
Sum of electronic and zero-point Energies=	-912.389506
Sum of electronic and thermal Energies=	-912.374733
Sum of electronic and thermal Enthalpies=	-912.373789
Sum of electronic and thermal Free Energies=	-912.433149
Entropy (Cal/Mol-Kelvin) =	124.934

#### Path.B\_P\_B3LYP-6-31Gd.log.log

C -0.1208281175 0.6963376049 -0.034599889  
 C -2.6924403644 0.6719834182 -1.2124329048  
 C -2.5781825961 1.0614585963 0.2174268827  
 N -1.1939280281 1.365311829 0.5098217768  
 H -3.6489334389 0.7695635403 -1.7107306965  
 H -3.1744366944 1.9513304141 0.4428861325  
 O 0.9923133299 0.7269046504 0.4844354532  
 N -0.3766346015 0.0293666687 -1.230866815  
 C -1.6336349515 0.1288441492 -1.8512242686  
 N -1.6924645762 -0.4207921764 -3.1334997161  
 H -0.9472233506 -0.1266944877 -3.7571510958

H -2.5978785938 -0.2895133073 -3.5689242196  
 H -0.9712042814 1.7451475693 1.4207997453  
 S 4.144662899 -1.6160564653 0.2863967637  
 C 4.412128427 0.184476095 0.1077692598  
 H 4.9498633866 0.3393961417 -0.8319330222  
 H 3.4527242513 0.7071826903 0.0733751828  
 H 5.022616278 0.5733432586 0.9291403946  
 C 0.7123480294 -0.7429326022 -1.8311915044  
 H 0.3145113206 -1.6739739422 -2.2383696011  
 H 1.4489668012 -0.9587206371 -1.0587538723  
 H 1.215091006 -0.1826863294 -2.6310851735  
 C 3.1926175391 -1.617573959 1.8479160694  
 H 2.8981024584 -2.6519162172 2.0458726192  
 H 3.8062754569 -1.2603910557 2.6812641495  
 H 2.2995663294 -0.9953276072 1.7470064273  
 C -3.3629548826 0.5454081568 2.9197672609  
 H -2.3569381443 0.7302387512 3.3106012972  
 H -3.9162684293 1.4891426337 2.861477416  
 H -3.8827466539 -0.116465968 3.617386713  
 S -3.3227988083 -0.3038754131 1.2982862351

Zero-point correction=	0.257152 (Hartree/Particle)
Thermal correction to Energy=	0.276068
Thermal correction to Enthalpy=	0.277012
Thermal correction to Gibbs Free Energy=	0.206156
Sum of electronic and zero-point Energies=	-1350.695694
Sum of electronic and thermal Energies=	-1350.676778
Sum of electronic and thermal Enthalpies=	-1350.675834
Sum of electronic and thermal Free Energies=	-1350.746690
Entropy (Cal/Mol-Kelvin) =	149.130

#### Path.B\_R\_B3LYP-6-31Gd.log.log

C -0.3519469309 0.2596445689 -1.8684296281  
 C -2.9022409495 1.412689127 -1.9502097132  
 C -2.3255558001 1.0892751398 -0.756505641  
 N -1.097434662 0.5337077049 -0.707879086  
 H -3.8928351309 1.8471235903 -2.0086489868  
 H -2.8021192411 1.2508569427 0.2056787875  
 O 0.7721454981 -0.2553388165 -1.7643773742  
 N -0.9108571176 0.5860258904 -3.0723874013  
 C -2.119752524 1.1262361989 -3.1133585536  
 N -2.6348468431 1.3814369033 -4.3555310656  
 H -1.9753332769 1.3291082509 -5.120193436  
 H -3.3890640365 2.0451259122 -4.4502375585  
 H -0.7087178217 0.3083299741 0.2405950661  
 S 3.0640153523 -1.5104269659 0.8495694671  
 C 2.7320097634 0.2634952454 0.578069879  
 H 3.6874688797 0.7795352072 0.6993924593

H 2.3434805046 0.3483451334 -0.4416007874  
 H 1.9732353657 0.5993019862 1.2996312755  
 C 1.4940888862 -2.3337333178 0.4149122619  
 H 0.7192699107 -2.0281678165 1.1327664019  
 H 1.2349993184 -1.984732269 -0.589484825  
 H 1.6911046128 -3.4081767493 0.4394975532  
 C 3.0576372704 -1.622262016 2.6705140534  
 H 3.1523562486 -2.6779227715 2.9353758471  
 H 3.9251650523 -1.0686318674 3.0372074725  
 H 2.111162013 -1.1906944449 3.0298987925  
 C -1.4433807323 0.4877670024 3.5651658087  
 H -1.6244725987 1.5658704113 3.4856445128  
 H -2.3937631738 -0.0326521799 3.399769532  
 H -1.1207210535 0.2773516922 4.5905897265  
 S -0.1654967836 -0.0621696668 2.3601321595

Zero-point correction= 0.254321 (Hartree/Particle)  
 Thermal correction to Energy= 0.273387  
 Thermal correction to Enthalpy= 0.274331  
 Thermal correction to Gibbs Free Energy= 0.204356  
 Sum of electronic and zero-point Energies= -1350.659070  
 Sum of electronic and thermal Energies= -1350.640003  
 Sum of electronic and thermal Enthalpies= -1350.639059  
 Sum of electronic and thermal Free Energies= -1350.709035  
 Entropy (Cal/Mol-Kelvin) = 147.276

#### Path.B\_TS\_B3LYP-6-31Gd.log.log

C -0.18968484 1.57507263 -0.81747223  
 C -2.51018084 0.03243263 -1.04384323  
 C -2.30972484 0.84583763 0.16441377  
 N -1.34683684 1.87074863 -0.07609223  
 H -3.42122584 -0.54392237 -1.15838623  
 H -3.22564784 1.27261763 0.57881077  
 O 0.86683816 2.17551763 -0.54732823  
 N -0.28050284 0.62757163 -1.79260623  
 C -1.46904784 -0.05646537 -1.92264023  
 N -1.47546784 -0.91878937 -3.02760123  
 H -0.94775484 -0.53137737 -3.80302923  
 H -2.40190184 -1.21216537 -3.31589123  
 H -1.13957084 2.50103963 0.68969877  
 S 3.04720116 -1.43334837 0.18329277  
 C 3.36598716 0.14809563 1.04272777  
 H 4.14280116 0.66624863 0.47613477  
 H 2.45888316 0.76126063 1.05131777  
 H 3.72747416 -0.05691037 2.05262877  
 C 1.45867016 -0.66126937 -1.03607223  
 H 0.68950716 -0.79275137 -0.28900223  
 H 1.86243816 0.33229963 -1.17646623

H 1.43934916 -1.33709737 -1.88269123  
 C 2.04593416 -2.31665337 1.42681877  
 H 1.73587116 -3.26270437 0.97663477  
 H 2.66088816 -2.51847737 2.30689177  
 H 1.15993616 -1.73028437 1.69314277  
 C -1.71315784 0.79277963 3.05915277  
 H -0.94267884 1.56250363 2.93899077  
 H -2.68824784 1.27602363 3.18695377  
 H -1.49341984 0.22620563 3.96860577  
 S -1.74001984 -0.37508837 1.64584877

Zero-point correction= 0.254458 (Hartree/Particle)  
 Thermal correction to Energy= 0.272632  
 Thermal correction to Enthalpy= 0.273577  
 Thermal correction to Gibbs Free Energy= 0.207197  
 Sum of electronic and zero-point Energies= -1350.604618  
 Sum of electronic and thermal Energies= -1350.586443  
 Sum of electronic and thermal Enthalpies= -1350.585499  
 Sum of electronic and thermal Free Energies= -1350.651878  
 Entropy (Cal/Mol-Kelvin) = 139.707

**Path.C\_P\_B3LYP-6-31Gd.log.log**

C -1.8925327579 3.3399112725 2.5475053582  
 C -3.3821067223 2.5421247274 0.2705537106  
 C -3.9190823621 3.3722966214 1.1859469077  
 N -3.1975209967 3.7569082567 2.2853598992  
 H -3.9435095414 2.2331825843 -0.6019934115  
 H -4.9233529223 3.7741801362 1.1099631174  
 O -1.3058827376 3.7189298765 3.5455203522  
 N -1.3501650296 2.4809965435 1.5916649884  
 C -2.0258707889 2.0466231594 0.4432884616  
 N -1.4156919996 1.2485024079 -0.3748679373  
 H 0.2025226413 0.5583134054 -0.5528316672  
 H -2.0249254339 1.0197148017 -1.1596318305  
 H -3.5813078237 4.3789497295 2.9831347695  
 C -0.0863126681 -1.467638732 -1.8814708065  
 H -0.7774140558 -1.6093527211 -1.0384654016  
 C 0.0911480636 -2.770101431 -2.6604765313  
 C 1.228160489 -0.9217826661 -1.3323420329  
 H 0.8000536746 -2.6088747997 -3.4825442516  
 H 0.5501351128 -3.5266462817 -2.0136955423  
 C -1.2396575601 -3.3030633161 -3.2261153752  
 O 1.1423018575 0.2190583737 -0.6395541674  
 O 2.2975140962 -1.4744165162 -1.5006168366  
 H -1.9278515466 -3.4545457468 -2.3767565558  
 C -1.0218622948 -4.6849931143 -3.8369444001  
 O -1.3112211153 -4.9704530015 -4.9784350218  
 N -1.8529867419 -2.3428640131 -4.1399793514

H -1.240195774 -2.2409143416 -4.9506399764  
 H -2.705397855 -2.7541506831 -4.5207793207  
 H -0.552275197 -0.7104827704 -2.5229369215  
 H -0.5711476672 -5.4414853416 -3.1541821005  
 S 3.1998658418 -0.0604505913 2.513456593  
 C 4.3537233735 -0.3308059774 1.1236658638  
 H 3.7505627875 -0.542861223 0.2369286951  
 H 4.9643982069 0.5600592084 0.9444752619  
 H 5.0048586241 -1.1876641 1.3251863655  
 C 0.0233823691 2.0071504816 1.8170007033  
 H 0.0391919385 0.9170064143 1.8647634533  
 H 0.3721727903 2.4295561527 2.7553217978  
 H 0.6692903016 2.3254371976 0.9963364367  
 C 4.3984553503 0.1773112711 3.8708149708  
 H 3.826009062 0.3510977802 4.7862314294  
 H 5.0219301452 -0.7120767575 4.0097998275  
 H 5.0399428658 1.0456257237 3.687935477

Zero-point correction= 0.352511 (Hartree/Particle)  
 Thermal correction to Energy= 0.379335  
 Thermal correction to Enthalpy= 0.380279  
 Thermal correction to Gibbs Free Energy= 0.284320  
 Sum of electronic and zero-point Energies= -1388.283921  
 Sum of electronic and thermal Energies= -1388.257097  
 Sum of electronic and thermal Enthalpies= -1388.256153  
 Sum of electronic and thermal Free Energies= -1388.352112  
 Entropy (Cal/Mol-Kelvin) = 201.962

#### Path.C\_R\_B3LYP-6-31Gd.log.log

C -0.2500855149 3.3172998903 2.7089204207  
 C -2.6499801944 3.9576500127 1.4051152546  
 C -2.1986701276 4.7497617369 2.4093241439  
 N -1.0349768321 4.4472794431 3.0485907577  
 H -3.572964055 4.1804552194 0.8835824119  
 H -2.7222576687 5.6382397197 2.7470505375  
 O 0.792904527 3.1242984749 3.3433379755  
 N -0.7033606155 2.5248547316 1.705131833  
 C -1.8409222726 2.8066417512 1.0673468193  
 N -2.2296185368 1.9826565254 0.0834892903  
 H -1.6680060636 1.1579089885 -0.1800644736  
 H -3.0815336043 2.1682556553 -0.422900128  
 H -0.6764884102 5.0221809039 3.799352791  
 C -0.5829027943 -2.0128133116 -2.2009744451  
 H -1.6280465781 -2.2601510482 -1.9694906639  
 C 0.2055517949 -3.2736503244 -2.5565508063  
 C -0.0077640176 -1.2283916586 -1.00782168  
 H 1.259000036 -3.0103624983 -2.7148940905  
 H 0.2001872228 -3.962614986 -1.7024910142

C -0.3321790401 -4.0017626008 -3.8055515061  
 O -0.6991543151 -0.2413603707 -0.6012606618  
 O 1.0916984106 -1.5976641288 -0.5215693983  
 H -1.4012991846 -4.2179262421 -3.6326051486  
 C 0.3451291758 -5.3603623457 -3.9380598214  
 O 0.9400405074 -5.7339214003 -4.9268231842  
 N -0.2235781925 -3.1704923314 -5.0009441346  
 H 0.762372089 -2.9455839755 -5.1411431526  
 H -0.4734455821 -3.7343700532 -5.8137247838  
 H -0.6264766873 -1.3400806188 -3.0657439117  
 H 0.2575420592 -6.0206239835 -3.0433104389  
 S 2.2073113633 -0.2350372808 1.5413778957  
 C 1.9784071102 1.1639440831 0.3947860781  
 H 1.0858734992 0.9252464164 -0.1879593141  
 H 1.8367989319 2.0769335503 0.9717958376  
 H 2.8710853156 1.1997907225 -0.2335345391  
 C 0.5554024678 -0.4623085575 2.2789028591  
 H 0.5876292759 -1.4064872285 2.827379843  
 H 0.3343045994 0.3875688277 2.9236423747  
 H -0.1393603451 -0.5064363948 1.4356116386  
 C 3.0346001311 0.6422708964 2.9249372659  
 H 3.1439658734 -0.0673792941 3.7493238994  
 H 4.0273948129 0.9440177576 2.580670431  
 H 2.4408324294 1.5104543269 3.2272599385

Zero-point correction= 0.351934 (Hartree/Particle)  
 Thermal correction to Energy= 0.378019  
 Thermal correction to Enthalpy= 0.378963  
 Thermal correction to Gibbs Free Energy= 0.290008  
 Sum of electronic and zero-point Energies= -1388.253219  
 Sum of electronic and thermal Energies= -1388.227134  
 Sum of electronic and thermal Enthalpies= -1388.226189  
 Sum of electronic and thermal Free Energies= -1388.315144  
 Entropy (Cal/Mol-Kelvin) = 187.221

#### Path.C\_TS\_B3LYP-6-31Gd.log.log

C -1.0196939009 3.2652324972 2.696664159  
 C -3.1023312664 3.0332952825 0.8246055017  
 C -3.1845263335 3.9538961253 1.8135404421  
 N -2.1752662501 4.0753203919 2.7182995779  
 H -3.8897445341 2.9255200878 0.0890927901  
 H -4.028145976 4.625523543 1.9321554792  
 O -0.1611148137 3.4336957282 3.5547663176  
 N -0.9481038373 2.3292068222 1.6936441276  
 C -1.9179238487 2.2019985696 0.7660578075  
 N -1.8008602289 1.3019111151 -0.2068551545  
 H -0.9011455661 0.7780770379 -0.4464424896  
 H -2.5333041427 1.2769226756 -0.9029402828



H -2.2058902298 4.7571045095 3.4646986485  
 C -0.293179361 -1.6702713636 -2.1281882457  
 H -1.1753550768 -1.8624104208 -1.497739033  
 C 0.1590347655 -2.9685193691 -2.7971308278  
 C 0.7858021422 -1.0194395921 -1.2394530322  
 H 1.0148347252 -2.7635016431 -3.4550528539  
 H 0.5370438601 -3.6528513893 -2.0293057995  
 C -0.9521748004 -3.6586528025 -3.6102144886  
 O 0.5013060089 0.1502864768 -0.7920395649  
 O 1.8370554781 -1.6449589542 -1.0113272043  
 H -1.7898584522 -3.8632585231 -2.9183625755  
 C -0.4794318561 -5.0295879063 -4.0795658845  
 O -0.5321297255 -5.4119011841 -5.2295003275  
 N -1.448434362 -2.8086154425 -4.6893791922  
 H -0.6481810478 -2.502378281 -5.2446661148  
 H -1.9936026302 -3.3884151609 -5.3285738104  
 H -0.6201393759 -0.9411965989 -2.8776098215  
 H -0.0821423714 -5.6927121668 -3.2762906532  
 S 2.6089798214 -0.2764638582 2.4493470398  
 C 3.6039274168 0.037162195 0.9546545955  
 H 3.1062016978 -0.5201834661 0.1461330741  
 H 3.6169787711 1.1071884334 0.7286822279  
 H 4.6201539788 -0.3325237596 1.1171093361  
 C 0.7222278182 1.0741066107 2.0123318337  
 H 0.1018610731 0.4683351119 2.6570622677  
 H 1.1928918672 1.9416756874 2.4485147863  
 H 0.7942426525 0.8245394324 0.9543704154  
 C 3.4661849627 0.7608436969 3.6821406475  
 H 2.8944563461 0.7139083498 4.6122956132  
 H 4.4733265364 0.3739148543 3.8586651174  
 H 3.5224059753 1.8001292377 3.3454889103

Zero-point correction= 0.350149 (Hartree/Particle)  
 Thermal correction to Energy= 0.375779  
 Thermal correction to Enthalpy= 0.376723  
 Thermal correction to Gibbs Free Energy= 0.289143  
 Sum of electronic and zero-point Energies= -1388.219962  
 Sum of electronic and thermal Energies= -1388.194332  
 Sum of electronic and thermal Enthalpies= -1388.193388  
 Sum of electronic and thermal Free Energies= -1388.280967  
 Entropy (Cal/Mol-Kelvin) = 184.327

**Path.D\_P\_B3LYP-6-31Gd.log.log**

C 0.1206433239 0.0862832117 0.2058714172  
 C 2.0576088821 -1.9356133284 -0.2657469043  
 C 2.4115327834 -0.6659108096 0.0905945353  
 N 1.4887882811 0.2915104867 0.3106021591  
 H 2.7990556144 -2.7031852733 -0.4420445016

H 3.445031524 -0.361042483 0.2155031311  
 O -0.7020045281 0.9457850168 0.4118548225  
 N -0.2419869048 -1.2445506282 -0.1690439527  
 C 0.6748169477 -2.2241662636 -0.3973369889  
 N 0.2512557197 -3.4457024754 -0.7423308513  
 H -0.7264721521 -3.6820538487 -0.8386449337  
 H 0.9233088519 -4.1811743236 -0.9119062761  
 H 1.7986201978 1.2489801911 0.5850268127  
 S -4.8550493428 -2.9682594213 -0.7524508571  
 C -5.9068934532 -3.0949610164 -2.2411742822  
 H -6.1685346986 -4.1364135908 -2.4482037816  
 H -6.8162969762 -2.4992333613 -2.1236640146  
 H -5.3326078622 -2.6990861411 -3.0825932347  
 C -5.9885513583 -3.6583697642 0.5038319536  
 H -6.8963903478 -3.0535177212 0.5791588225  
 H -6.2500202287 -4.6939389549 0.2688102512  
 H -5.4677293952 -3.6328104891 1.4643702262  
 C -1.6820089285 -1.5301102328 -0.2968049255  
 H -1.9788204761 -2.30760894 0.4119515441  
 H -1.9177706327 -1.8398120028 -1.3183044379  
 H -2.2208473028 -0.6139221942 -0.0683825751  
 N 3.5965775618 4.8713955295 2.633368029  
 H 4.3354675236 4.1734456552 2.5639314064  
 C 2.9657746011 5.0547379108 1.3430908803  
 H 2.134612731 5.7633311555 1.4729951636  
 C 3.9721152832 5.6601697104 0.3438196877  
 C 2.3695435558 3.7697396055 0.7480997558  
 H 4.8104044229 4.9734405682 0.1810888656  
 H 3.5185383791 5.8767349197 -0.6294236856  
 H 4.3652219031 6.5889889263 0.7629158122  
 O 2.6488516888 2.6512915212 1.152970262  
 O 1.5178190496 3.8901056478 -0.2834859396  
 H 2.9292775397 4.5161602895 3.3151681326  
 H 1.3540312227 4.8259349181 -0.495239528

Zero-point correction= 0.326978 (Hartree/Particle)  
 Thermal correction to Energy= 0.350375  
 Thermal correction to Enthalpy= 0.351319  
 Thermal correction to Gibbs Free Energy= 0.264354  
 Sum of electronic and zero-point Energies= -1236.084039  
 Sum of electronic and thermal Energies= -1236.060642  
 Sum of electronic and thermal Enthalpies= -1236.059698  
 Sum of electronic and thermal Free Energies= -1236.146663  
 Entropy (Cal/Mol-Kelvin) = 183.035

#### Path.D\_R\_B3LYP-6-31Gd.log.log

C 1.0445531781 -1.2345333126 -0.6756593394  
 C 3.17328965 -3.0008263991 -0.3486035947

C 3.3672797929 -1.6643327185 -0.1842089664  
 N 2.3321924695 -0.8013378988 -0.3397485159  
 H 3.9844176822 -3.7086659553 -0.2331985939  
 H 4.3267761459 -1.2273122294 0.0700983065  
 O 0.1587505379 -0.3684263022 -0.8270451863  
 N 0.8195672836 -2.567767345 -0.8109208012  
 C 1.8373602148 -3.4175090349 -0.6650714189  
 N 1.5621538492 -4.733747068 -0.8069392469  
 H 0.6426932196 -4.999691836 -1.1286492549  
 H 2.2945755816 -5.4266185426 -0.8233832412  
 H 2.4457823125 0.2018519882 -0.181696492  
 S -3.9776947673 -0.6703592883 0.1631473931  
 C -4.0627518902 0.3815152312 -1.324075952  
 H -4.896703047 1.0749393245 -1.1964279408  
 H -3.1183887399 0.9147126143 -1.4509511538  
 H -4.2570990606 -0.2721811267 -2.1771895765  
 C -3.474669616 0.5341974797 1.4396110982  
 H -2.5601583827 1.0721315037 1.1441225834  
 H -4.3153014132 1.2180723885 1.5810864967  
 H -3.3170318867 -0.032467924 2.3607712724  
 C -2.4447011518 -1.6034663808 -0.1376042968  
 H -2.2217066938 -2.1479213582 0.7836006568  
 H -2.6702587824 -2.3273142725 -0.9248899504  
 H -1.5995092963 -0.9643876677 -0.4311562647  
 N -0.442186614 1.9547352597 0.8639741757  
 H -0.034145595 1.7296630837 1.7732923078  
 C 0.1629051833 3.2006351716 0.4005783334  
 H -0.3056540422 3.4647717698 -0.5593924975  
 C -0.1014633925 4.3354350745 1.4050496321  
 C 1.6734165579 3.049863747 0.117541471  
 H 0.3909206711 4.1280718153 2.3621223432  
 H 0.2576665761 5.307909186 1.0515716415  
 H -1.1769636725 4.4177996446 1.5825820919  
 O 2.3036045896 2.040504711 0.3515213699  
 O 2.3023699785 4.1101420361 -0.4242274541  
 H -0.1403956781 1.1927175212 0.2451077334  
 H 1.6876952477 4.8517921099 -0.5565281686

Zero-point correction=	0.326806 (Hartree/Particle)
Thermal correction to Energy=	0.350107
Thermal correction to Enthalpy=	0.351051
Thermal correction to Gibbs Free Energy=	0.268268
Sum of electronic and zero-point Energies=	-1236.064965
Sum of electronic and thermal Energies=	-1236.041664
Sum of electronic and thermal Enthalpies=	-1236.040720
Sum of electronic and thermal Free Energies=	-1236.123502
Entropy (Cal/Mol-Kelvin) = 174.231	

**Path.D\_TS\_B3LYP-6-31Gd.log.log**

C 0.452939906 -0.5990497423 -0.1795937804  
C 2.482786089 -2.5225831731 -0.4104518956  
C 2.7847216589 -1.1983845295 -0.2941116253  
N 1.8068660557 -0.2721736788 -0.1748525313  
H 3.2545930929 -3.2753021718 -0.5064915798  
H 3.8005472137 -0.8183042783 -0.2917890065  
O -0.4051289258 0.2786035581 -0.0854090469  
N 0.1407706523 -1.9411600537 -0.2919119858  
C 1.0970190594 -2.8712917661 -0.4030186108  
N 0.7305359888 -4.1654763718 -0.5068892261  
H -0.2401495478 -4.4357622313 -0.5371674673  
H 1.4221879145 -4.892198844 -0.6135538183  
H 2.0499596726 0.7277510208 -0.0979839965  
S -4.2797564389 -2.3604878049 -0.1119775496  
C -4.7442366641 -1.0333253642 -1.2771414877  
H -5.8096085606 -0.8162999 -1.1705220484  
H -4.1534741127 -0.1314947934 -1.0956503984  
H -4.5556670768 -1.4041952479 -2.28723844  
C -4.597475544 -1.5428418033 1.4893871897  
H -4.0088100815 -0.6264205943 1.5838254006  
H -5.6631912895 -1.3179186542 1.574042954  
H -4.319362787 -2.2467769842 2.2771807235  
C -1.948552989 -2.1927679196 -0.2136136497  
H -1.834865558 -2.8255722101 0.6542193156  
H -1.9307572671 -2.6356431234 -1.1983890935  
H -1.9547594184 -1.1163756926 -0.1055401682  
N 0.4089254607 3.1670572796 1.0068739054  
H 0.8968366833 2.7543263293 1.8001271257  
C 1.2768219674 4.1024434918 0.322273505  
H 0.7112531045 4.5311628631 -0.5192318597  
C 1.6586918689 5.2480940142 1.2809521793  
C 2.5416763988 3.4704402227 -0.2959313084  
H 2.262286603 4.8700089266 2.1140779113  
H 2.2276741966 6.0479993504 0.7940148605  
H 0.7430575904 5.6815807404 1.6891500879  
O 2.8448684784 2.2951368907 -0.1971850747  
O 3.3551868295 4.2808537092 -0.9941735435  
H 0.1170415099 2.3946847327 0.4090270621  
H 3.019723266 5.1936468031 -0.9891480285

Zero-point correction= 0.325139 (Hartree/Particle)  
Thermal correction to Energy= 0.348615  
Thermal correction to Enthalpy= 0.349560  
Thermal correction to Gibbs Free Energy= 0.267571  
Sum of electronic and zero-point Energies= -1236.035031  
Sum of electronic and thermal Energies= -1236.011554  
Sum of electronic and thermal Enthalpies= -1236.010610

Sum of electronic and thermal Free Energies= -1236.092599  
Entropy (Cal/Mol-Kelvin) = 172.559

**Path.E\_P\_APFD-6-31Gd.log.log**

C -1.649499931 -0.7025267968 -0.2452995041  
O -1.3756669622 0.1633020612 0.5750112595  
O -2.76450027 -0.7078417018 -0.9812030407  
O -0.9020432942 -1.7501630664 -0.5439399553  
H -3.2157035922 0.1508074533 -0.8077606998  
C 3.9862558457 0.4796049874 -0.331203069  
C 3.992851164 -2.1702536038 0.6689201032  
C 5.1474085225 -1.5185396294 0.4363145428  
N 5.142283052 -0.2433985192 -0.0510479399  
H 3.9898930788 -3.1841839423 1.050044356  
H 6.124288017 -1.9558286272 0.6140983324  
O 4.0464139473 1.6180770125 -0.7559045963  
N 2.8061892485 -0.2052369966 -0.0821560507  
C 2.7281972109 -1.5156075202 0.3929465397  
N 1.5608840513 -2.0428606692 0.5527920398  
H -0.03664237 -1.7251408381 -0.0321387099  
H 1.6455603903 -2.9916395948 0.9095751037  
H 5.9987893336 0.2592323289 -0.2330185678  
S -3.6814964195 2.3343196443 -0.4943701362  
C -5.4055816192 2.7940029741 -0.8141295597  
H -6.098609872 2.0473981458 -0.4129593599  
H -5.6380877609 3.7743021943 -0.3860329179  
H -5.5335447411 2.8468324006 -1.8984141153  
C -3.6957487691 2.2515972184 1.3154301202  
H -3.7909676551 3.2483575857 1.7566895033  
H -4.5105074603 1.6113500146 1.6694782726  
H -2.7439885934 1.7981425705 1.5985601069  
C 1.5506569043 0.495197077 -0.3206439772  
H 0.9121715401 0.4334627977 0.5607160412  
H 1.0243672953 0.0345306486 -1.1605177743  
H 1.7852237086 1.530733391 -0.5574973471

Zero-point correction= 0.249396 (Hartree/Particle)  
Thermal correction to Energy= 0.268627  
Thermal correction to Enthalpy= 0.269571  
Thermal correction to Gibbs Free Energy= 0.196846  
Sum of electronic and zero-point Energies= -1176.306423  
Sum of electronic and thermal Energies= -1176.287192  
Sum of electronic and thermal Enthalpies= -1176.286248  
Sum of electronic and thermal Free Energies= -1176.358974  
Entropy (Cal/Mol-Kelvin) = 153.064

**Path.E\_R\_APFD-6-31Gd.log.log**

C -2.0176213969 -1.8106067562 -0.1022300937

O -2.7928506669 -0.9277970716 0.3571175332  
 O -2.0304046213 -3.0266489936 0.5535335868  
 O -1.2246950636 -1.7298842651 -1.0646965576  
 H -2.6891625795 -2.9187471874 1.2552786043  
 C 2.5484259229 0.9638656779 0.1254092942  
 C 3.6229188229 -1.6290384722 0.1193235022  
 C 4.4208406075 -0.5698562626 0.3959057298  
 N 3.9126042738 0.6870667141 0.3985369218  
 H 4.0115743045 -2.640868968 0.1094005836  
 H 5.4786286016 -0.6668184942 0.6219893173  
 O 2.176716901 2.1359049035 0.1580834719  
 N 1.7548403588 -0.0992313649 -0.1506347105  
 C 2.23691585 -1.3376834232 -0.1672658293  
 N 1.397009161 -2.3327563841 -0.4623474431  
 H 0.3984960782 -2.1497385678 -0.6885772506  
 H 1.7244277573 -3.2849043875 -0.4670031333  
 H 4.4896245663 1.4914203039 0.5997730207  
 S -2.5676621971 1.5731255039 -0.4625059666  
 C -2.337054452 3.333746072 -0.8676321026  
 H -3.3174490038 3.8092877225 -0.9567636994  
 H -1.7339237214 3.8398166393 -0.1088262959  
 H -1.8263383286 3.3806698075 -1.8324691385  
 C -3.213495222 1.7500273158 1.2140487266  
 H -2.5254130324 2.344182755 1.821179267  
 H -4.1912476265 2.2338045191 1.1531263891  
 H -3.3058135097 0.7281948434 1.5845244505  
 C -0.8391715589 1.0755998869 -0.2237224346  
 H -0.7372655108 0.7212502391 0.8004223495  
 H -0.6794893705 0.2212035775 -0.8835294563  
 H -0.1535153438 1.9050361172 -0.4083796366

Zero-point correction= 0.246695 (Hartree/Particle)  
 Thermal correction to Energy= 0.265804  
 Thermal correction to Enthalpy= 0.266748  
 Thermal correction to Gibbs Free Energy= 0.196334  
 Sum of electronic and zero-point Energies= -1176.262998  
 Sum of electronic and thermal Energies= -1176.243889  
 Sum of electronic and thermal Enthalpies= -1176.242945  
 Sum of electronic and thermal Free Energies= -1176.313359  
 Entropy (Cal/Mol-Kelvin) = 148.199

#### Path.E\_TS\_APFD-6-31Gd.log.log

C -2.1616356432 -1.9129985166 0.0433000295  
 O -2.0605364143 -1.2186310447 1.0858855062  
 O -3.3595320103 -2.5597803504 -0.1632770291  
 O -1.310278252 -2.0932175617 -0.8645560027  
 H -3.8957380157 -2.3169667364 0.6057611951  
 C 2.5246262805 1.2476813618 0.1442537257

C 3.4811895187 -1.3922322641 0.2255973544  
 C 4.3275820678 -0.3569999533 0.4281954672  
 N 3.8729260777 0.9208654317 0.3867713754  
 H 3.8283337273 -2.4182200527 0.2549911755  
 H 5.386220552 -0.4877097866 0.6290566994  
 O 2.1837514462 2.4242076665 0.1411427824  
 N 1.6837844719 0.1951116274 -0.0731268716  
 C 2.0941567102 -1.0810912777 -0.0338711425  
 N 1.2218203129 -2.0526358357 -0.2399768649  
 H 0.174156 -1.935957 -0.450004  
 H 1.5563407293 -3.003943893 -0.2016410138  
 H 4.4855351146 1.7089076839 0.5441238121  
 S -2.4663907781 1.3774647031 -0.3493764036  
 C -2.2881109854 3.0539023635 -1.011807617  
 H -3.2172561174 3.617739549 -0.8871543948  
 H -1.4648856357 3.5867143645 -0.5245024089  
 H -2.0708170277 2.9614207886 -2.0789142464  
 C -2.6750518192 1.7339691674 1.4080632686  
 H -1.8104361098 2.283789352 1.7942166572  
 H -3.591777026 2.3067984744 1.5733983123  
 H -2.7385888127 0.7513530379 1.8808863663  
 C -0.3084025845 0.7515889291 -0.2567871107  
 H -0.5723334056 0.0625711164 0.5422378926  
 H -0.3056391346 0.3589254508 -1.263867256  
 H 0.056955106 1.7547783391 -0.072377438

Zero-point correction= 0.246080 (Hartree/Particle)  
 Thermal correction to Energy= 0.264608  
 Thermal correction to Enthalpy= 0.265552  
 Thermal correction to Gibbs Free Energy= 0.197439  
 Sum of electronic and zero-point Energies= -1176.240911  
 Sum of electronic and thermal Energies= -1176.222383  
 Sum of electronic and thermal Enthalpies= -1176.221439  
 Sum of electronic and thermal Free Energies= -1176.289551  
 Entropy (Cal/Mol-Kelvin) = 143.355

#### Path.F\_P\_APFD-6-31Gd.log.log

C -1.4529565448 2.9203187231 1.0388821649  
 C -2.6237124496 1.0989138389 2.8581654242  
 C -3.0671443122 2.3676611057 2.774675639  
 N -2.4999552605 3.2431966316 1.8983593365  
 H -3.0683283278 0.3945323874 3.5503746482  
 H -3.8779833837 2.7564859792 3.3816142779  
 O -0.9905646256 3.7489239722 0.2809500424  
 N -1.008079709 1.6052018805 1.136595963  
 C -1.5396951924 0.6603460777 2.0037961516  
 N -1.0458005269 -0.5363277013 2.0107615474  
 H -0.0855580749 -1.3595868934 1.1207832883

H -1.5259695761 -1.1296098894 2.6811589338  
 H -2.8202694131 4.1975293729 1.8171531258  
 P -0.2821372231 -2.4475398218 -0.7697740875  
 O -0.7888522449 -1.4397143367 -1.7262660419  
 O 0.4834102561 -2.0038505794 0.5298862634  
 O -1.4696695048 -3.386466647 -0.1781521232  
 O 0.7752768064 -3.448796965 -1.4594651729  
 H -2.1975917054 -3.3961515005 -0.817335467  
 H 1.2533091296 -3.9564846507 -0.7873549842  
 S 2.9858705401 1.1996750984 -1.9341520447  
 C 2.4990998988 -0.5456130647 -1.9899417373  
 H 3.1725904737 -1.1273685988 -2.6278727816  
 H 2.4767999265 -0.9806741418 -0.9860415254  
 H 1.4881197493 -0.5969407221 -2.40073198  
 C 4.5993713187 1.034034885 -1.1245556103  
 H 5.0176743101 2.0382849909 -1.0151730439  
 H 4.5020528509 0.5842958012 -0.1302756144  
 H 5.2886079065 0.4319225247 -1.7266251255  
 C 0.0762573931 1.2038348889 0.2411308049  
 H 0.4353697995 2.089959735 -0.2747998436  
 H -0.2871218788 0.4710245285 -0.4837026836  
 H 0.8872985943 0.7661820907 0.8262362556

Zero-point correction=	0.257660 (Hartree/Particle)
Thermal correction to Energy=	0.279283
Thermal correction to Enthalpy=	0.280228
Thermal correction to Gibbs Free Energy=	0.202283
Sum of electronic and zero-point Energies=	-1555.311183
Sum of electronic and thermal Energies=	-1555.289559
Sum of electronic and thermal Enthalpies=	-1555.288615
Sum of electronic and thermal Free Energies=	-1555.366560
Entropy (Cal/Mol-Kelvin) =	164.049

#### Path.F\_R\_APFD-6-31Gd.log.log

C -0.801774346 2.7529928966 1.5117427679  
 C -2.7835738144 1.2363605395 2.7970165048  
 C -2.825047544 2.589372057 2.8561938823  
 N -1.8688181571 3.331217968 2.2452051883  
 H -3.537487326 0.6267392364 3.2815308942  
 H -3.6028985023 3.1365856235 3.3804435008  
 O -0.0018857925 3.5040098109 0.9565950056  
 N -0.7525893995 1.3990429112 1.4760112952  
 C -1.6809790293 0.655555475 2.0673638038  
 N -1.5631398993 -0.672277196 1.9830169262  
 H -0.8139722403 -1.1126377693 1.4173835071  
 H -2.2972464663 -1.2669366524 2.3317205425  
 H -1.8893854597 4.3410954806 2.2638979557  
 P -0.0030113313 -2.4109067392 -0.8824512889



O 0.21916348 -1.545507861 -2.0942233448  
 O 0.40974289 -1.9620764786 0.5002973733  
 O -1.5897911606 -2.8032387315 -0.7901625904  
 O 0.7485497855 -3.835870567 -1.1913482021  
 H -1.9529203904 -2.7740878046 -1.6870826928  
 H 0.835534084 -4.3136847575 -0.3539161993  
 S 2.0375195136 0.4000009857 -2.0744783259  
 C 2.9586928156 -1.0412910753 -1.4619077784  
 H 4.0271487042 -0.8412603593 -1.5743258006  
 H 2.690759054 -1.2191833536 -0.417935289  
 H 2.6403439122 -1.8928603702 -2.0605383899  
 C 3.2981229462 1.6841813413 -1.8137654718  
 H 2.8422333475 2.6477227209 -2.0526246102  
 H 3.6393059506 1.6879041563 -0.7749271831  
 H 4.135799222 1.5020677841 -2.4917530782  
 C 0.8789516801 0.8697442961 -0.7498506591  
 H 1.0596336612 1.9016731967 -0.438058307  
 H -0.1170712356 0.7465299607 -1.1657493547  
 H 0.9864910478 0.1748382752 0.0814204186

Zero-point correction= 0.257488 (Hartree/Particle)  
 Thermal correction to Energy= 0.278667  
 Thermal correction to Enthalpy= 0.279611  
 Thermal correction to Gibbs Free Energy= 0.205530  
 Sum of electronic and zero-point Energies= -1555.283546  
 Sum of electronic and thermal Energies= -1555.262367  
 Sum of electronic and thermal Enthalpies= -1555.261423  
 Sum of electronic and thermal Free Energies= -1555.335504  
 Entropy (Cal/Mol-Kelvin) = 155.917

#### Path.F\_TS\_APFD-6-31Gd.log.log

C -0.8399459001 2.8439673657 1.2183979775  
 C -2.6082779023 1.2453538258 2.708992276  
 C -2.6518852687 2.592991161 2.8194628469  
 N -1.792676734 3.3683178212 2.1120472493  
 H -3.277916146 0.6096523843 3.2756965993  
 H -3.3519645121 3.112444135 3.4660072774  
 O -0.1122811948 3.6099744172 0.5998441649  
 N -0.8072090932 1.4819052174 1.1105330053  
 C -1.6209697311 0.6834543144 1.8194432258  
 N -1.5007474665 -0.6272741535 1.698196603  
 H -0.747072 -1.115481 1.134886  
 H -2.1403078293 -1.2271583465 2.1967265453  
 H -1.8103734 4.3768692282 2.175981917  
 P -0.2058207774 -2.5437607244 -0.9140291661  
 O -0.3639070958 -1.6581522376 -2.1087520948  
 O 0.3508800027 -2.0230067337 0.4019493455  
 O -1.6555643442 -3.2110934706 -0.5188493422

O 0.718632561 -3.8219421913 -1.3513421966  
 H -2.1747718895 -3.275149262 -1.3335813451  
 H 1.0093107663 -4.2690411785 -0.5436096731  
 S 2.1086450731 0.706377189 -1.9903100492  
 C 2.6899024131 -1.0005889951 -1.8774785268  
 H 3.7284282872 -1.0644354173 -2.2154622868  
 H 2.5821269268 -1.3696993689 -0.8537970228  
 H 2.0331544457 -1.5870904737 -2.5213942258  
 C 3.2593650922 1.5329543895 -0.8651389602  
 H 2.9174822279 2.5636784732 -0.7390718796  
 H 3.2662362082 1.0390956924 0.1122948789  
 H 4.2694122355 1.5360026789 -1.2840977239  
 C 0.353825 0.849629 -0.477152  
 H 0.4933567765 1.9155635376 -0.568430389  
 H -0.3951829034 0.3241278951 -1.0613715758  
 H 0.9357127833 0.2641165876 0.21882266

Zero-point correction= 0.256774 (Hartree/Particle)  
 Thermal correction to Energy= 0.277543  
 Thermal correction to Enthalpy= 0.278487  
 Thermal correction to Gibbs Free Energy= 0.205126  
 Sum of electronic and zero-point Energies= -1555.255651  
 Sum of electronic and thermal Energies= -1555.234882  
 Sum of electronic and thermal Enthalpies= -1555.233938  
 Sum of electronic and thermal Free Energies= -1555.307299  
 Entropy (Cal/Mol-Kelvin) = 154.401

#### Path.G\_P\_B3LYP-6-31Gd.log.log

C -2.4214268026 -2.9683266459 -0.8521886256  
 O -2.5474813364 -2.2919286594 0.1601397477  
 O -3.4447661683 -3.3649772521 -1.6228250866  
 O -1.2805286613 -3.409621017 -1.359988146  
 H -4.2540920784 -2.9371475478 -1.2630355052  
 C 2.0948908298 0.7117704336 0.1714717531  
 C 3.3611144407 -1.815586238 0.2053780738  
 C 4.0667426325 -0.6803592537 0.3865275494  
 N 3.4550442275 0.5437020222 0.3705060264  
 H 3.8444676258 -2.784306853 0.2153595689  
 H 5.1385358765 -0.6664432162 0.5510789789  
 O 1.5840059495 1.8301352773 0.1604336312  
 N 1.3690250282 -0.4580995127 -0.0104806398  
 C 1.9283724501 -1.7476894333 -0.0184833888  
 N 1.142724064 -2.7569121705 -0.2201772276  
 H -0.499806208 -3.0889378139 -0.8153152058  
 H 1.675030993 -3.6262012586 -0.1963013877  
 H 3.9875610459 1.4076676827 0.4959394059  
 S -5.8421686528 -1.3137524243 -0.5176938529  
 C -7.6281089579 -1.6573798312 -0.6855014166

H -7.8688564668 -2.6744887834 -0.3615263535  
 H -8.219161626 -0.9386194289 -0.1100713753  
 H -7.8800082596 -1.5531496346 -1.7440750792  
 C -5.6162093613 -1.5836586039 1.274452458  
 H -6.0845349217 -0.783586027 1.8547867219  
 H -6.0303445198 -2.5513742591 1.5739634802  
 H -4.5371034829 -1.5930904669 1.4399197773  
 C -0.0823266328 -0.3531068421 -0.1993844674  
 H -0.6043975819 -0.9834041617 0.520391973  
 H -0.3477543691 -0.6920983976 -1.2042908445  
 H -0.3593417388 0.6909709039 -0.0747016091  
 N 2.1144990259 4.4414014111 1.8836495867  
 H 2.8816117446 4.2532890112 2.5299292418  
 C 2.6831517067 4.8840685509 0.6212343754  
 H 1.859248188 4.9548876459 -0.1022553504  
 C 3.3327869061 6.2700863907 0.7774259357  
 C 3.7259979863 3.906438077 0.0604859547  
 H 4.1633167218 6.2206797331 1.4906879285  
 H 3.7251376282 6.6475110671 -0.1737009844  
 H 2.588482995 6.9722882842 1.1618126281  
 O 4.4439890429 3.2208575889 0.7638962167  
 O 3.867800925 3.8497510718 -1.2811354693  
 H 1.6610997846 3.5412230114 1.7223109355  
 H 3.1738830076 4.37915357 -1.7094599331

Zero-point correction= 0.356554 (Hartree/Particle)  
 Thermal correction to Energy= 0.383981  
 Thermal correction to Enthalpy= 0.384925  
 Thermal correction to Gibbs Free Energy= 0.291401  
 Sum of electronic and zero-point Energies= -1500.669284  
 Sum of electronic and thermal Energies= -1500.641857  
 Sum of electronic and thermal Enthalpies= -1500.640913  
 Sum of electronic and thermal Free Energies= -1500.734437  
 Entropy (Cal/Mol-Kelvin) = 196.838

#### Path.G\_R\_B3LYP-6-3Gd.log.log

C -2.3921215487 -3.8085576974 -0.9282001312  
 O -3.4524814643 -3.2043142815 -0.6019488421  
 O -2.4157618835 -5.1885524203 -0.8131129684  
 O -1.3180623457 -3.3205144141 -1.3444985082  
 H -3.3159437737 -5.3913817654 -0.509513787  
 C 1.638274063 0.2402910693 -0.0260245481  
 C 3.3394486864 -1.9774072017 -0.0225848045  
 C 3.8291991221 -0.7451697563 0.2707996899  
 N 3.0118915681 0.3397463918 0.2761437289  
 H 3.9791471398 -2.8517873903 -0.0330148244  
 H 4.8719394388 -0.561758731 0.509554351  
 O 0.9524418697 1.2802421309 -0.0259190697

N 1.1356225256 -0.9862440696 -0.3004895109  
 C 1.9276643236 -2.0626924389 -0.31239184  
 N 1.3707226871 -3.2500328768 -0.5952245876  
 H 0.3731609729 -3.3286604496 -0.8580388914  
 H 1.9491696013 -4.0739472528 -0.6526113452  
 H 3.369413783 1.2678673524 0.5028315062  
 S -3.6363307432 -0.4413955057 -0.4544837662  
 C -3.8900848946 1.3483599902 -0.1499385186  
 H -4.964116143 1.540726249 -0.0891175524  
 H -3.391307327 1.664751117 0.76956139  
 H -3.4732991817 1.889634438 -1.0022694929  
 C -4.3032875273 -1.1001314196 1.1057235395  
 H -3.8157949738 -0.6108440382 1.9526810823  
 H -5.3793354016 -0.9102306054 1.1132936034  
 H -4.097045871 -2.1708133472 1.0558689667  
 C -1.8249623255 -0.5462116454 -0.2441230957  
 H -1.5833388676 -0.4673591732 0.8171622747  
 H -1.5107746577 -1.5071651406 -0.6714940168  
 H -1.3701398226 0.2888272371 -0.7788619785  
 N 0.643671239 3.6452046515 1.8043556894  
 H 1.3410556793 3.6441635289 2.5504101822  
 C 1.2414613888 4.2883999512 0.6424058436  
 H 0.5246797443 4.1971555934 -0.1849937265  
 C 1.5026855363 5.7776813303 0.9189106938  
 C 2.5584054289 3.6256524783 0.2125977261  
 H 2.2318620356 5.8893090208 1.72942859  
 H 1.8973948882 6.2919466032 0.035350699  
 H 0.568937198 6.2573436576 1.225356455  
 O 3.3698748847 3.1834671581 1.0025705453  
 O 2.8409905933 3.6005217817 -1.1094620509  
 H 0.512331974 2.6628488071 1.5520729698  
 H 2.0452203809 3.8328710832 -1.6163036697

Zero-point correction= 0.354782 (Hartree/Particle)  
 Thermal correction to Energy= 0.382024  
 Thermal correction to Enthalpy= 0.382968  
 Thermal correction to Gibbs Free Energy= 0.292199  
 Sum of electronic and zero-point Energies= -1500.621967  
 Sum of electronic and thermal Energies= -1500.594724  
 Sum of electronic and thermal Enthalpies= -1500.593780  
 Sum of electronic and thermal Free Energies= -1500.684550  
 Entropy (Cal/Mol-Kelvin) = 191.041

#### Path.G\_TS\_B3LYP-6-31Gd.log.log

C -2.0989159804 -4.0199402596 -0.1071094375  
 O -2.1140353213 -3.3351830804 0.9508599425  
 O -2.8804258617 -5.1628626856 -0.1157474572  
 O -1.4720061087 -3.8069168693 -1.175294584

H -3.2928393969 -5.1744560815 0.7635691121  
 C 1.5328799582 0.4551411837 -0.2177071557  
 C 3.1150225667 -1.7495417865 -0.9254019166  
 C 3.6915654835 -0.5622519328 -0.6105282705  
 N 2.9330545148 0.5085069042 -0.2559338647  
 H 3.7078750033 -2.6112877485 -1.2057261855  
 H 4.7643305368 -0.4009323505 -0.621773112  
 O 0.8887919473 1.4649126162 0.0919918755  
 N 0.9521083694 -0.738379679 -0.532496162  
 C 1.674645789 -1.8212930721 -0.8710759775  
 N 1.0331595362 -2.9478846323 -1.1617356562  
 H -0.0158029944 -3.0927610111 -1.0930110035  
 H 1.5740137637 -3.7679725466 -1.3965770624  
 H 3.3690040425 1.4086276607 -0.0440447475  
 S -3.4303195101 -0.7841379803 -0.0876619514  
 C -3.8318182854 0.954140097 -0.4788107057  
 H -4.8433490774 1.1908657087 -0.1379326116  
 H -3.114192809 1.6382313289 -0.0157616608  
 H -3.788414458 1.0650796101 -1.565214273  
 C -3.4951414 -0.7382719971 1.731784946  
 H -2.7882878854 -0.0002113139 2.1223903796  
 H -4.5110311278 -0.5010176175 2.0583942848  
 H -3.2077952745 -1.7452070564 2.0405188899  
 C -1.1730850056 -0.7891709889 -0.3618999965  
 H -1.1133741369 -1.6318301558 0.319739226  
 H -1.2281004466 -1.0031100452 -1.4187566487  
 H -1.0456369591 0.2335040106 -0.0347039944  
 N 2.1417353233 3.7076611708 1.7515574524  
 H 2.8216623774 3.1790697611 2.2965409215  
 C 2.8248630319 4.7149109239 0.9706496097  
 H 2.0755213518 5.210532284 0.3348810907  
 C 3.44558299 5.7739996423 1.9056314721  
 C 3.91038006 4.1666283672 0.0208556012  
 H 4.2165018899 5.3187210463 2.5381284634  
 H 3.9085741969 6.6075439204 1.3645727329  
 H 2.6615294347 6.1711967027 2.5544942613  
 O 4.3140612515 3.0220196897 0.0184677422  
 O 4.4540231194 5.0488902531 -0.8492414348  
 H 1.6601826057 3.0321421329 1.1516704398  
 H 4.0395853262 5.921458322 -0.7400644862

Zero-point correction=	0.354073 (Hartree/Particle)
Thermal correction to Energy=	0.381587
Thermal correction to Enthalpy=	0.382531
Thermal correction to Gibbs Free Energy=	0.289765
Sum of electronic and zero-point Energies=	-1500.599576
Sum of electronic and thermal Energies=	-1500.572061
Sum of electronic and thermal Enthalpies=	-1500.571117

Sum of electronic and thermal Free Energies= -1500.663883  
Entropy (Cal/Mol-Kelvin) = 195.243

**Path.H\_P\_M062X-6-31Gd.log.log**

C 0.1093999256 4.0108664154 1.1247183904  
C -2.1651429933 5.0019849724 -0.237464674  
C -1.6000919605 5.703503348 0.7554126579  
N -0.4927843999 5.2260149041 1.4088362907  
H -3.0364853991 5.3683098207 -0.7630753872  
H -1.9710291177 6.6640109048 1.0929183474  
O 1.0818886152 3.6424813649 1.7610392824  
N -0.4776807617 3.2924062951 0.1033617846  
C -1.5906822192 3.7235326449 -0.6340804612  
N -2.009745614 2.9705629515 -1.5828809244  
H -1.5601030971 1.4545507391 -2.2556483918  
H -2.8375955215 3.3467467374 -2.0396614125  
H -0.0529807364 5.7427660918 2.1571964421  
S 0.4750208958 -2.2184955108 0.7941043126  
C 1.7787024528 -1.6661840276 -0.3373789352  
H 1.4575966061 -0.7178973841 -0.7746950769  
H 2.7053583046 -1.5064250605 0.2184614189  
H 1.9273924885 -2.4101408406 -1.1264254069  
C 0.0914770495 1.9886181431 -0.2447222024  
H 0.9052304889 1.7517488708 0.4380723174  
H 0.4515537843 2.0140556946 -1.2764377762  
H -0.6899240946 1.2280235752 -0.176474202  
C 1.263894461 -3.7402481528 1.3923738221  
H 0.5886344448 -4.1974277245 2.1185565412  
H 1.4275923585 -4.4245851232 0.5558074231  
H 2.2085464066 -3.4999985485 1.8865434462  
C -2.1853605168 -1.488629495 -3.4376859578  
H -3.1587662293 -1.9568386073 -3.6055892789  
C -1.362244443 -2.2468615357 -2.3968969742  
C -2.4271403569 -0.0498129455 -3.0369788179  
H -0.4470763798 -1.6835982546 -2.1830914887  
H -1.9077594626 -2.3181255482 -1.4486556386  
C -0.9641292066 -3.6502560107 -2.8731146251  
O -3.4894998444 0.5235033163 -3.1333699152  
O -1.3210121797 0.5304442931 -2.5672830867  
H -1.8807342563 -4.2127784994 -3.1058171083  
C -0.2718552051 -4.364227024 -1.7227086292  
O 0.8905143922 -4.6973625444 -1.7642567835  
N -0.1513803353 -3.5654283832 -4.0747382458  
H 0.7450141167 -3.1525543753 -3.8150245641  
H 0.0785368768 -4.5064874806 -4.389293942  
H -1.6396690852 -1.4980478475 -4.3879805593  
H -0.8870208171 -4.5551769004 -0.8200530505  
N 2.5267125939 0.9232165335 1.8788895069

H 3.4828973833 0.6084230193 1.7315982364  
 C 2.0350295249 0.3766279251 3.1322740864  
 H 2.5388775672 0.8042480458 4.0208137289  
 C 0.5371441067 0.6479525247 3.2639559772  
 C 2.4199954445 -1.1018581932 3.1723867608  
 H -0.0155301682 0.0916823109 2.5017848297  
 H 0.1546072647 0.3977672388 4.2615513342  
 H 0.3620726173 1.7168122128 3.1151570762  
 O 3.3956616315 -1.5312562453 2.6107033054  
 O 1.6904076983 -1.9057196575 3.967625361  
 H 2.5094361738 1.9404003151 1.9205124769  
 H 0.8644747272 -1.4639042888 4.2150283598

Zero-point correction= 0.470207 (Hartree/Particle)  
 Thermal correction to Energy= 0.503589  
 Thermal correction to Enthalpy= 0.504534  
 Thermal correction to Gibbs Free Energy= 0.400919  
 Sum of electronic and zero-point Energies= -1711.322217  
 Sum of electronic and thermal Energies= -1711.288834  
 Sum of electronic and thermal Enthalpies= -1711.287890  
 Sum of electronic and thermal Free Energies= -1711.391505  
 Entropy (Cal/Mol-Kelvin) = 218.075

#### **Path.H\_R\_M062X-6-31Gd.log.log**

C 0.3167900388 3.9243385578 1.6855858114  
 C -1.555088223 4.6530776448 -0.258332506  
 C -1.2038503428 5.5391773673 0.6951211763  
 N -0.2879715772 5.1941603319 1.6397861349  
 H -2.2774690067 4.8949108867 -1.0262518539  
 H -1.6154623233 6.5403068498 0.7610348137  
 O 1.1043407529 3.7137491298 2.611665686  
 N -0.0154443099 3.0326611197 0.7244529669  
 C -0.9079403416 3.3566883633 -0.2200994008  
 N -1.2021232353 2.4684848124 -1.1570829641  
 H -0.838255208 1.5015658902 -1.1934867423  
 H -1.9460719052 2.5943100004 -1.8337143626  
 H -0.0100877504 5.8321590336 2.3722405325  
 S 1.6407962057 -1.2498606519 -0.5241788895  
 C 2.0357521961 -0.8911181232 -2.2496893449  
 H 1.0964982833 -0.5276359596 -2.6729586045  
 H 2.826333874 -0.1390712023 -2.2954529441  
 H 2.3569722689 -1.8203035273 -2.7240926114  
 C 1.2290857433 0.3845625739 0.1421513278  
 H 1.7550408081 0.5055459151 1.0945365244  
 H 1.5015530236 1.1469389334 -0.5880172354  
 H 0.1526138815 0.3834859513 0.2797705735  
 C 3.3142162016 -1.4545138539 0.1300363009  
 H 3.2072770518 -1.5450031595 1.2109022028

H 3.7420139366 -2.3638258907 -0.295388957  
 H 3.9205960808 -0.5842830523 -0.1297091632  
 C -2.1903988478 -1.6732750421 -2.9667213081  
 H -3.2353788251 -1.8368148845 -2.6764696389  
 C -1.310656995 -2.7968718936 -2.4372863773  
 C -1.7904946466 -0.2742770536 -2.4700508495  
 H -0.2683824724 -2.6300153358 -2.7457748172  
 H -1.3070003773 -2.7768926529 -1.3407115612  
 C -1.7386186018 -4.1856825513 -2.935390026  
 O -2.5099940007 0.6759816934 -2.8024213125  
 O -0.7338835322 -0.2023901813 -1.7465822654  
 H -2.7918183629 -4.336840994 -2.6560989309  
 C -0.9121945981 -5.2206799655 -2.1931134807  
 O -0.109759708 -5.9451000242 -2.7317915182  
 N -1.6194985864 -4.2804629369 -4.3810563608  
 H -0.6253670236 -4.2743068294 -4.6102199097  
 H -1.9457971849 -5.1976957628 -4.6810743128  
 H -2.1834906429 -1.6707518848 -4.0611169683  
 H -1.0559045562 -5.2535652624 -1.0910848849  
 N 2.0677355966 0.9636394126 3.1707117072  
 H 2.925007478 0.8931268515 3.7090952842  
 C 0.9607271995 0.3243842453 3.8465091422  
 H 1.0839841433 0.2977435824 4.9443327039  
 C -0.3526351848 1.0571592023 3.5326819321  
 C 0.8165558241 -1.1355199945 3.3999207875  
 H -0.4660926586 1.1684013915 2.4502353352  
 H -1.222323036 0.5251093373 3.9301151858  
 H -0.3173841641 2.0603673476 3.9620300723  
 O 1.3376942145 -1.6325042185 2.4347766911  
 O -0.0005476458 -1.8837171174 4.1681060157  
 H 1.8581671213 1.9518740733 2.9962470449  
 H -0.3404740495 -1.3553224925 4.9068851492

Zero-point correction= 0.467765 (Hartree/Particle)  
 Thermal correction to Energy= 0.501402  
 Thermal correction to Enthalpy= 0.502346  
 Thermal correction to Gibbs Free Energy= 0.396948  
 Sum of electronic and zero-point Energies= -1711.274446  
 Sum of electronic and thermal Energies= -1711.240809  
 Sum of electronic and thermal Enthalpies= -1711.239865  
 Sum of electronic and thermal Free Energies= -1711.345264  
 Entropy (Cal/Mol-Kelvin) = 221.830

**Path.H\_TS\_M062X-6-31Gd.log.log**

C 0.2427396618 3.7306753323 1.4307037075  
 C -1.4406748383 4.7360902735 -0.5774566118  
 C -1.0728660963 5.5217912919 0.4534915152  
 N -0.2527010266 5.0404790877 1.4296409566



H -2.093473515 5.0913244946 -1.3631035962  
H -1.4004676097 6.5492539597 0.563719767  
O 0.9461825213 3.3701124853 2.3697472242  
N -0.1064366924 2.948763905 0.3774019338  
C -0.9275236552 3.3816556301 -0.6018423686  
N -1.244717373 2.5607144592 -1.576420026  
H -1.0204389351 1.5128151715 -1.6177699021  
H -1.9347709798 2.8091068897 -2.2764015687  
H 0.0223015767 5.6058700226 2.2211779044  
S 1.4276056636 -1.067130953 -0.1001188364  
C 1.9113863892 -0.9303326876 -1.8373129604  
H 0.9947138571 -0.6719824373 -2.3727180952  
H 2.6621426914 -0.1428927335 -1.9499542991  
H 2.3155988464 -1.8833347056 -2.1847094193  
C 0.674310121 1.0469938117 0.2104855207  
H 1.2366689047 1.1908578701 1.125428398  
H 1.0818642818 1.3528591505 -0.744853578  
H -0.3377377368 0.6725107602 0.2259683052  
C 3.0653460612 -1.0834713315 0.6722644797  
H 2.9315817535 -1.223511568 1.7458542739  
H 3.6465041298 -1.9072407609 0.2519823007  
H 3.5734806706 -0.1324178954 0.4915153669  
C -2.3613443412 -1.6161464019 -3.020331055  
H -3.21783872 -1.8830829464 -2.3858052714  
C -1.2398073885 -2.6246108185 -2.8080687899  
C -1.9673610927 -0.1772563418 -2.6656976249  
H -0.3979407347 -2.3925566161 -3.4779968914  
H -0.856960876 -2.522458278 -1.7859601838  
C -1.670434139 -4.0744096242 -3.0571034409  
O -2.6209297119 0.75254808 -3.1511916284  
O -0.9822625469 -0.0438035988 -1.8462743593  
H -2.5034199115 -4.2984220133 -2.3712992974  
C -0.5255760126 -4.9934669873 -2.6666102166  
O -0.0180382708 -5.7895685334 -3.4185960978  
N -2.1287427135 -4.2657011325 -4.4219771925  
H -1.365270436 -4.0115801237 -5.049050991  
H -2.2729801142 -5.2617614319 -4.5823028341  
H -2.727318394 -1.637711675 -4.0489517482  
H -0.1566230373 -4.8813510263 -1.6228168307  
N 2.1264252897 0.7726103676 3.1977976035  
H 3.0637585208 0.6068350859 3.5558956333  
C 1.1412971216 0.2188001435 4.1041355499  
H 1.0840282097 0.7455772168 5.0756092032  
C -0.2413135057 0.2726818294 3.4430395053  
C 1.5374396993 -1.2188492095 4.4264629115  
H -0.2745643454 -0.4020367485 2.5819242875  
H -1.0510110438 0.0036211239 4.1299153074  
H -0.4235846144 1.2928144801 3.092890526

O 2.5424357294 -1.7453290027 4.0297554502  
O 0.6856939926 -1.8931479443 5.2237788968  
H 1.9700621329 1.7748172996 3.0923609545  
H -0.0730269377 -1.3357546157 5.4539481921

Zero-point correction= 0.466555 (Hartree/Particle)  
Thermal correction to Energy= 0.499770  
Thermal correction to Enthalpy= 0.500715  
Thermal correction to Gibbs Free Energy= 0.395666  
Sum of electronic and zero-point Energies= -1711.245262  
Sum of electronic and thermal Energies= -1711.212047  
Sum of electronic and thermal Enthalpies= -1711.211102  
Sum of electronic and thermal Free Energies= -1711.316151  
Entropy (Cal/Mol-Kelvin) = 221.094

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