Supporting Information

DFT study of Ni-catalyzed (3+3)-Annulation between Donor-Acceptor Cyclopropanes and Diaziridines

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Calculation Method for GRI and LRI

The global electrophilicity index, ω,[s1] is expressed [$\omega = (\mu^2/2\eta)$] in terms of electronic chemical potential μ and the chemical hardness η.[s2] These parameters can be obtained in terms of one electron energies of HOMO and LUMO, ε_H and ε_L, as $\mu \approx (\varepsilon_H + \varepsilon_L)/2$ and $\eta \approx (\varepsilon_L - \varepsilon_H)$, correspondingly.[s3] Domingo et al. suggested an empirical (relative) nucleophilicity index, N,[s4] which is based on the HOMO energies obtained within the Kohn−Sham scheme and defined as $N = \varepsilon_{HOMO(Nu)} - \varepsilon_{HOMO(TCE)}$. The N index refers to TCE (tetracyanoethylene) due to its lowest HOMO energy within a considerable number of molecules studied in polar reactions. Such a selection permits it to have positive values of the nucleophilicity scale.[s5] The nucleophilic, P_k^+ , Parr functions, were obtained through the analysis of the Mulliken ASD of the radical cation by single-point energy calculations over the optimised neutral geometries. Local nucleophilicity $N_k = NP_k^+$.[s6]

Additional Energy Profiles of the Series A

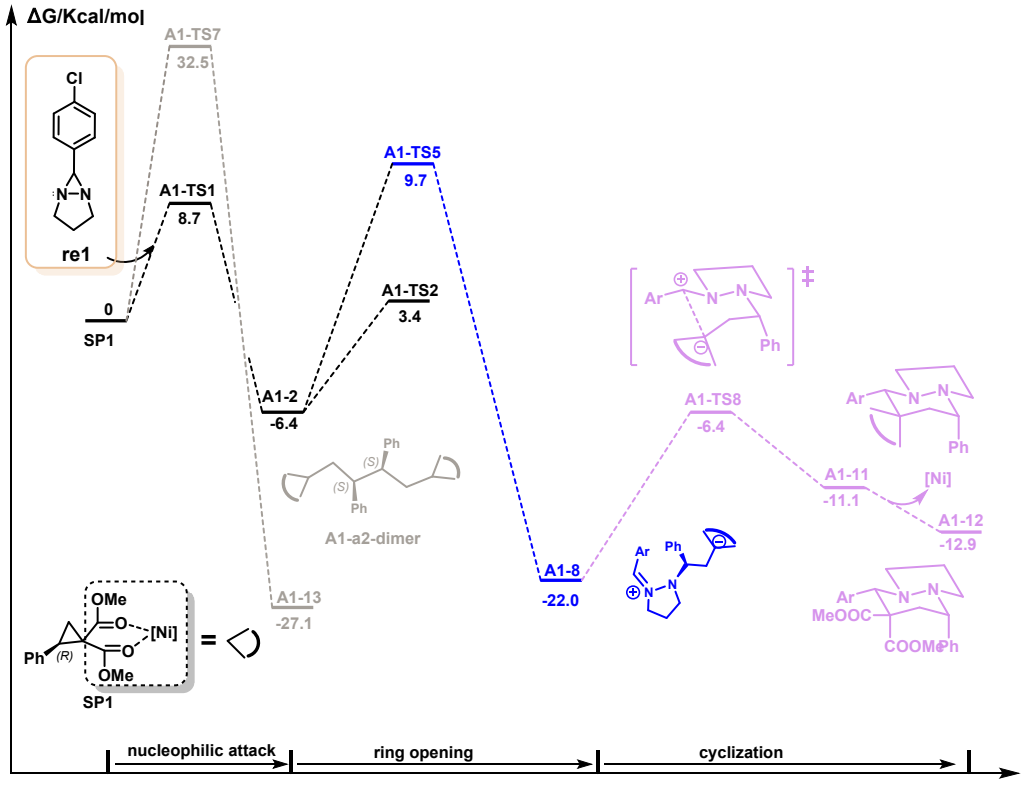


Figure S1. Additional energy profiles (kcal/mol) for possible reaction pathways beginnig with *R*-conformation DAC and **re1** (series **A1**). Energy profile shows that the first step is in favor of nucleophilic attack, rather than the dimerization.

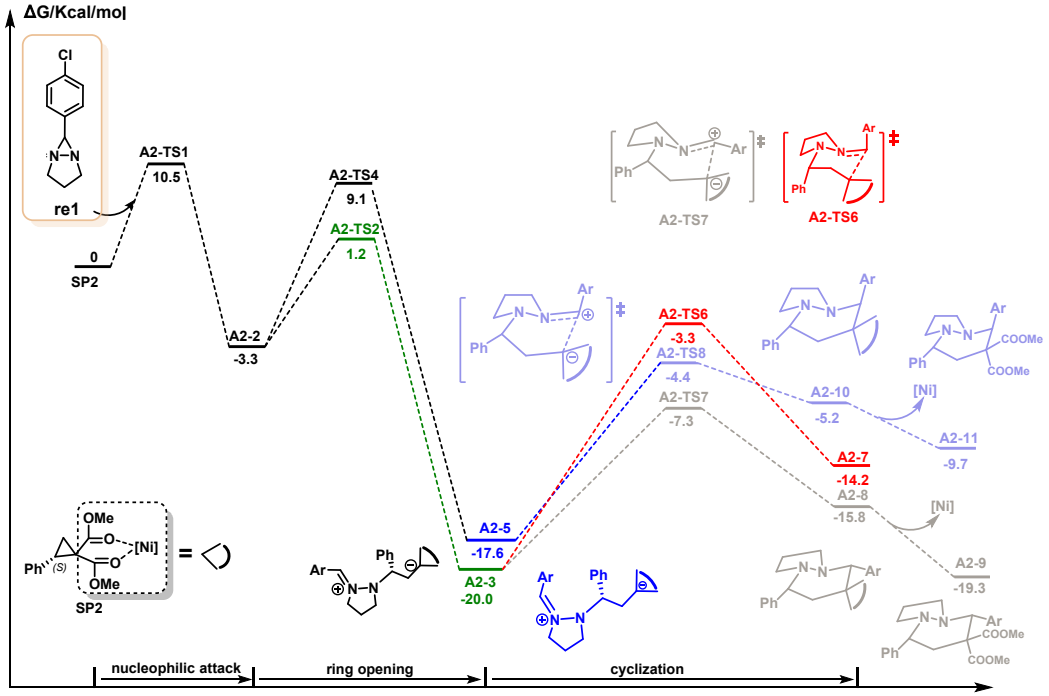


Figure S2. Additional energy profiles (kcal/mol) for possible reaction pathways beginning with *S*-conformation DAC and **re1** (series **A2**).

Additional Energy Profiles for the Series B

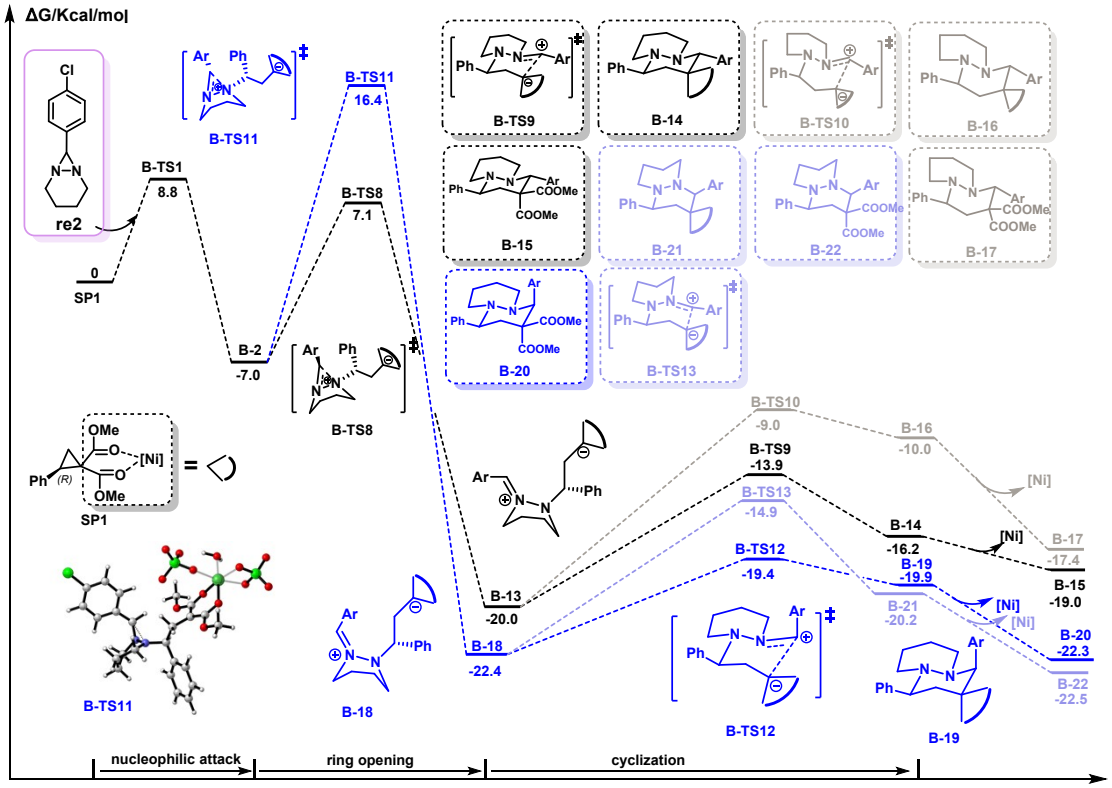
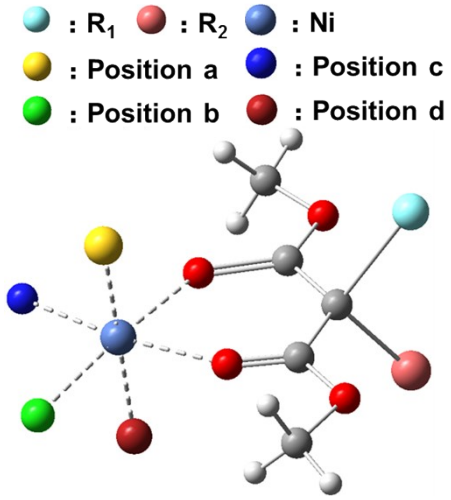


Figure S3. Additional energy profiles (kcal/mol) for possible reaction pathways beginning with *R*-conformation DAC and **re2** (series **B**).

Effect of Water Molecules in Catalyst Configuration

Table S1. Activation energies in the nucleophilic step with different position of water molecules in the catalyst.



Transition state[a]	E‡ (kcal/mol)
D1-Tsa	8.1
D1-Tsa2	8.7
D1-Tsa3	8.0
D1-TSb	7.9
D1-TSb2	8.4
D1-TSc	11.6
D1-TSc2	7.7
D1-TSd	7.6
D1-TSd2	10.0
D1-TSd3	10.7
D2-TSab	6.0
D2-Tsac	7.4
D2-TSad	7.9
D2-TSbc	9.3
D2-TSbd	8.8
D2-TScd	7.8

[a] The lowercase letters represent the position of the water molecules. When one H_2O is coordinated to Ni atom, one of ClO_4^- should act as a bidentate ligand. As a results, there might be several catalyst configurations. Calculation result shows that the free energy barrier of one water molecule catalyst model always is higher than that of the two water molecule catalyst model, regardless the positions of water molecules.

Table S2. Some constants: μ (Electronic Chemical Potential, in au), η (Chemical Hardness in au), ω (Global Electrophilicity, in eV), N (Global Nucleophilicity, in eV), N_k (Local Nucleophilicity, in eV), E_{HOMO} (HOMO Energy, in eV), and E_{LUMO} (LUMO Energy, in eV) for Re1 (6-(4-chlorophenyl)-1,5-diazabicyclo[3.1.0]hexane) and DAC (dimethyl (R)-2-phenylcyclopropane-1,1-dicarboxylate).

	E_{HOMO}	E_{LOMO}	μ	η	ω	N	N_k
Re1	-0.23564	-0.03178	-0.13371	0.20386	1.19	2.37	0.71
DAC	-0.25365	-0.02654	-0.1401	0.22711	1.18	2.06	-0.01

Additional Energy Profiles (Series E)

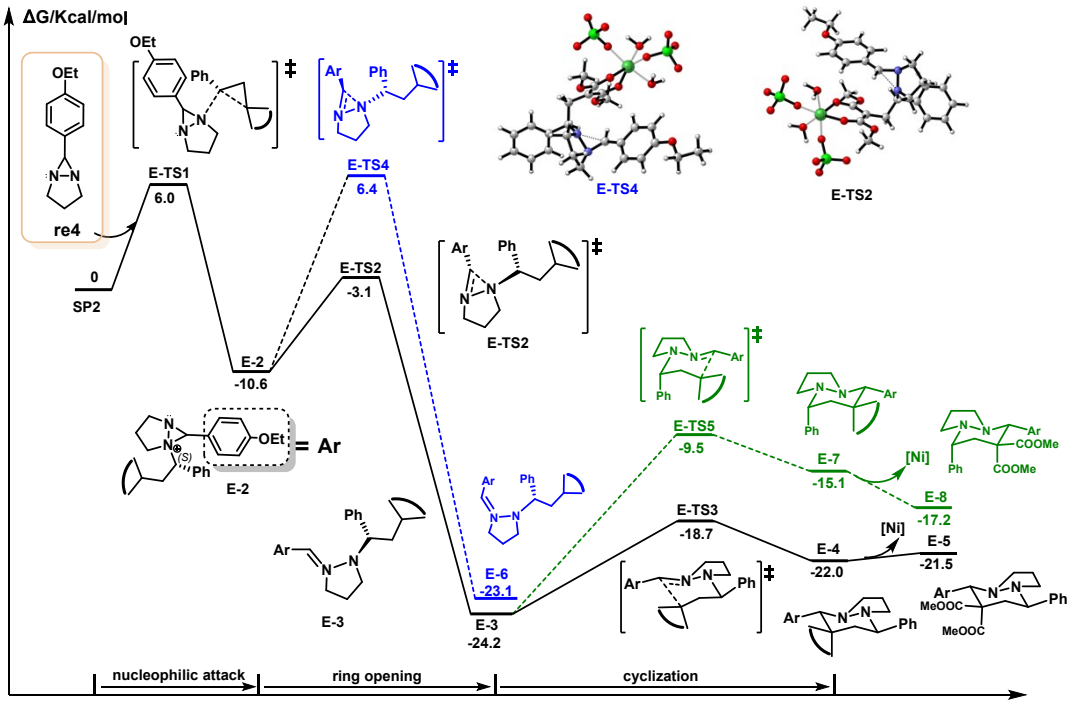


Figure S4. Additional energy profiles (kcal/mol) for possible reaction pathways beginning with *S*-conformation DAC and **re4** (series **E**).

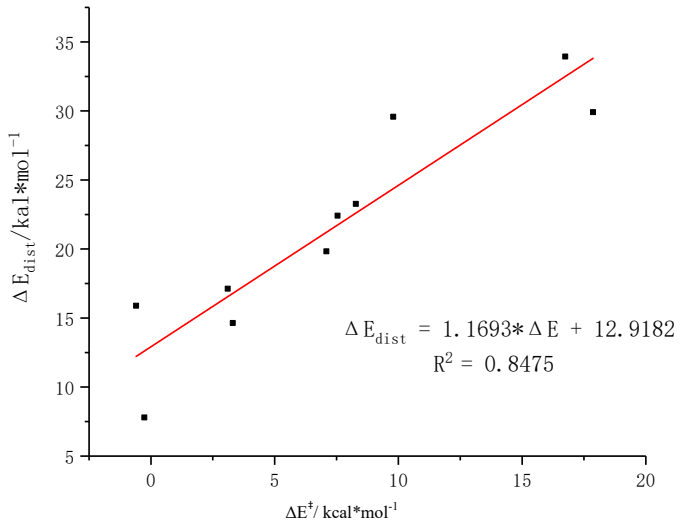


Figure S5. Linear fitting of $\Delta E^{\ddagger}$ and ΔE_{dist}. For definition of $\Delta E^{\ddagger}$, $\Delta E_{dist.}$ and $\Delta E_{dist\text{-}2}$, see Table 1.

Supporting References

(s1) Parr, R. G.; Szentpály, L. v.; Liu, S. Electrophilicity Index. *J. Am. Chem. Soc.* **1999**, *121*, 1922−1924.

(s2) (a) Parr, R. G.; Yang, W.; Density Functional Theory of Atoms and Molecules; Oxford University Press: New York, 1989. (b) Parr, R. G.; Pearson, R. G. Absolute hardness: companion parameter to absolute electronegativity. *J. Am. Chem. Soc.* **1983**, *105*, 7512−7516.

(s3) (a) Ayers, P. W.; Parr, R. G.; Pearson, R. G. Elucidating the hard/soft acid/base principle: A perspective based on half-reactions. *J. Chem. Phys.* **2006**, *124*, 194107. (b) Parr, R. G.; Bartolotti, L. J. On the Geometric Mean Principle for Electronegativity Equalization. *J. Am. Chem. Soc.* **1982**, *104*, 3801−3803. (c) Yang, W. T.; Zhang, Y. K.; Ayers, P. W. Degenerate Ground States and a Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory. *Phys. Rev. Lett.* **2000**, *84*, 5172−5175.

(s4) (a) Domingo, L. R.; Chamorro, E.; Pérez, P. Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. *J. Org. Chem.* **2008**, *73*, 4615−4624. (b) Domingo, L. R.; Pérez, P. The nucleophilicity N index in organic chemistry. *Org. Biomol. Chem.* **2011**, *9*, 7168−7175.

(s5) Domingo, L. R.; Aurell, M. J.; Perez, P.; Contreras, R. Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Diels−Alder Reactions. *J. Phys. Chem. A.* **2002**, *106*, 6871−6875.

(s6) Domingo, L. R.; Pérez, P.; Sáez, J. A. Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. *RSC Adv.* **2013**, *3*, 1486-1494.

1. Cartesian Coordinates and Thermodynamic Data for the Optimized Species: r1, r2, r3, r4, and A1-a1-s

SP1-s

C 5.81635700 -0.03206700 -0.07957400
C 5.69537800 -1.32459300 0.43343900
C 4.49486700 -2.02280500 0.29390200
C 3.40838900 -1.43783700 -0.36791600
C 3.53936100 -0.14336900 -0.88883000
C 4.73434600 0.55872900 -0.73671400
H 6.53296300 -1.78951200 0.94546000
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Ni -1.43698200 1.00054100 0.01179000
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O -0.24939900 3.56813400 0.74407500
Cl 0.57369000 3.13657700 -0.40566000
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O -4.87868000 -0.81143500 1.65798700
O 1.89472500 2.61969000 0.01933900
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O -4.28104600 -0.36213800 -0.68441300
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Thermal Correction to Free Energy: 0.245689 Hartree

Entropy: 204.047 cal/mol-kelvin

Single Point Energy with Solvent Effect: -2574.223475 Hartree

Thermal Free Energy with Correction: -2573.977786 Hartree

r1

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H 3.40286400 0.53340900 2.06252800

H 4.02462400 1.64989200 -0.00069000

H 5.30455900 0.44469300 -0.00016700

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Thermal Correction to Free Energy: 0.156038 Hartree

Entropy: 104.449 cal/mol-kelvin

Single Point Energy with Solvent Effect: -957.542189 Hartree

Thermal Free Energy with Correction: -957.386151 Hartree

r2

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C -1.12344200 0.31277400 -0.05901700
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H -4.74341500 -1.12834600 -0.26647300
H -2.86194700 0.56988100 -1.98025900
H -3.58039500 -0.76264500 1.99848900
H -5.01733400 0.94242900 1.14364200
H -5.15231800 0.25449700 -1.27984600
H -3.23911000 -1.13961600 -2.18844800
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C 0.98581600 -1.02355600 0.19102900
C 2.54835700 1.25748100 -0.23738200
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C 2.37383700 -1.12511300 0.20833300
H 0.36747500 -1.89884800 0.35598700
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H 3.16195500 2.13598200 -0.40190800
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Thermal Correction to Free Energy: 0.182962 Hartree
Entropy: 110.652 cal/mol-kelvin
Single Point Energy with Solvent Effect: -996.864556 Hartree
Thermal Free Energy with Correction: -996.681594 Hartree

r3

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Thermal Correction to Free Energy: 0.473505 Hartree

Entropy: 188.199 cal/mol-kelvin

Single Point Energy with Solvent Effect: -1303.692557 Hartree

Thermal Free Energy with Correction: -1303.219052 Hartree

r4

C -4.06394100 -0.02040800 -1.20091700

C -4.69046600 0.71642500 0.00030800

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Thermal Correction to Free Energy: 0.223054 Hartree

Entropy: 117.613 cal/mol-kelvin

Single Point Energy with Solvent Effect: -651.814475 Hartree

Thermal Free Energy with Correction: -651.591421 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Path-A1:

SP1

C 5.71247800 0.23623600 -0.06767100

C 5.70575200 -1.12983700 0.21941800

C 4.55322800 -1.88584200 -0.00114500

C 3.40159200 -1.28311600 -0.52145200

C 3.41654100 0.08795900 -0.81722400

C 4.56479400 0.84413300 -0.58252500

H 6.59508500 -1.60784000 0.61982700

H 4.54891400 -2.94813000 0.22677500

H 2.52610300 0.57320400 -1.20820300

H 4.55466300 1.90862100 -0.79527600

C 2.18004400 -2.10349500 -0.80565100

H 1.98299200 -2.27380100 -1.86302500

C 0.83047500 -1.84562900 -0.02639500

C 0.86981800 -0.84918900 1.08547500

C -0.37464500 -1.82189700 -0.90945300

O 1.76920000 -1.13104100 2.01161100

O -0.59905200 -2.97659700 -1.51047000

C 1.96022000 -0.13016500 3.04647600

H 2.78273900 -0.50729300 3.65092400

H 2.21031700 0.82804300 2.58875900

H 1.04867700 -0.03151900 3.63765700

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H -1.63140400 -2.37619800 -3.22925600

H -1.80868200 -4.08246900 -2.70112400

H -2.65158100 -2.76458200 -1.80843400

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O -1.07413700 -0.83405900 -1.14533600

Ni -1.23630600 0.92812500 -0.10252300

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O -0.79653400 2.87352200 0.70478100

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H -3.43414100 0.95270500 -1.24167400
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H 1.18035800 -4.02125600 -0.31300800
H 2.11794400 -3.26506100 1.07203800
H 6.60665300 0.82581500 0.11221400
Thermal Correction to Free Energy: 0.244391 Hartree
Entropy: 206.026 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.279628 Hartree
Thermal Free Energy with Correction: -2574.035237 Hartree

A1-TS1

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H -6.39727800 -1.53072100 2.64234000
H -5.89322100 -3.21254400 2.54623500
H -4.03915600 -1.17471700 3.10355900
H -3.58930400 -2.64493900 2.21391800
C -4.95714300 0.04338400 0.68064200
N -3.96232200 -1.00043500 0.99251400
N -5.03102200 -1.23636700 0.00469600
H -5.65727200 0.23493300 1.49528100
C -4.60234000 1.25888200 -0.10649200
C -4.58153600 2.50544100 0.53182200
C -4.33679900 1.18874100 -1.47970400
C -4.28963400 3.66642700 -0.18107700
H -4.79895000 2.57679400 1.59440900
C -4.04358100 2.34203800 -2.20465400
H -4.38294200 0.22710900 -1.97938400
C -4.02132100 3.57363400 -1.54811400
H -4.27678900 4.63191900 0.31206400
H -3.84308800 2.29157200 -3.26901800
Cl -3.65954500 5.02752800 -2.45483400
C -2.23130200 -4.97388400 -1.54383300
C -1.86396000 -4.89241900 -0.19765800
C -1.74592300 -3.65240400 0.42389900
C -1.99831300 -2.46656100 -0.29673200

C -2.37508800 -2.56767100 -1.65182000
C -2.48552000 -3.80781900 -2.27137600
H -1.65821000 -5.79835700 0.36432200
H -1.42428700 -3.59947100 1.45649800
H -2.56533500 -1.66033800 -2.21665500
H -2.76195800 -3.86772900 -3.31934400
C -1.94680000 -1.14139400 0.31355200
H -2.11438000 -0.31039000 -0.36215200
C 0.16022200 -0.53190200 0.83858800
C 1.20492900 -1.50942700 0.89957300
C 0.40707700 0.73651800 0.22146000
O 0.86612400 -2.64835900 1.54695700
O -0.64178900 1.58469600 0.28496200
C 1.91522400 -3.63036100 1.66667800
H 1.46001000 -4.47353300 2.18712500
H 2.27729800 -3.93051500 0.68166300
H 2.74981800 -3.22750400 2.24375000
C -0.38178300 2.93803900 -0.13716500
H -0.16146700 2.97283400 -1.20681600
H -1.30069100 3.48248400 0.07706900
H 0.45662600 3.34896100 0.42716000
O 2.36129700 -1.41298100 0.44662900
O 1.44730000 1.11749000 -0.35913000
Ni 3.27350400 0.26057100 -0.21061300
O 3.58031600 0.86923100 1.77592000
O 5.07417600 -0.86907500 -0.53268800
Cl 4.74997300 -1.21805400 -1.99223900
O 1.59614300 2.07620400 2.60401000
O 3.41076600 -0.47052000 -2.20169800
O 5.77445600 -0.68907200 -2.90381600
O 3.78849900 2.42108400 3.63765800
O 4.55255400 -2.66795700 -2.15141300
Cl 3.06073300 2.18849200 2.38208600
O 3.33672100 3.29343200 1.38910700
O 4.17637900 2.01384100 -0.84116800
H 3.72332600 2.33653000 -1.63107700
H 3.97946400 2.64690700 -0.11023900
C -1.16824800 -0.77053800 1.52647500
H -1.55002500 0.14192400 1.98680100
H -1.09463200 -1.56181400 2.27082100
H -2.31185400 -5.94335100 -2.02646400
Thermal Correction to Free Energy: 0.422093 Hartree
Entropy: 268.116 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.829626 Hartree

Thermal Free Energy with Correction: -3531.407533 Hartree

A1-2

C -5.95519700 -1.79289700 0.90764800
C -5.32580400 -2.20138800 2.25300100
C -3.81721800 -2.12478100 1.98325800
H -6.10418400 -2.65304200 0.25083900
H -6.90377400 -1.25977800 1.00823500
H -5.62288800 -1.52659200 3.05944100
H -5.62236400 -3.20966000 2.54888100
H -3.22942300 -1.76338200 2.82734700
H -3.40617600 -3.07144500 1.63089000
C -4.39090800 0.14363300 1.01949500
N -3.66983200 -1.15786000 0.83771800
N -4.98963700 -0.90589100 0.22189300
H -4.71488800 0.25302200 2.05498500
C -3.97597600 1.40687900 0.35051900
C -3.08578600 2.27856100 0.99346900
C -4.52464500 1.76305700 -0.88828800
C -2.73141000 3.48734200 0.40197600
H -2.63482300 2.01549900 1.94525000
C -4.20147800 2.98514100 -1.47264500
H -5.20962000 1.08671300 -1.38804200
C -3.30582600 3.83706600 -0.82164000
H -2.00556500 4.13465400 0.87888200
H -4.63441800 3.27550400 -2.42322100
Cl -2.89069000 5.36575400 -1.56206400
C -2.65776900 -5.11952500 -2.08005600
C -1.77795600 -4.95351700 -1.01016100
C -1.68862200 -3.72495800 -0.35097300
C -2.48500700 -2.64552400 -0.76135100
C -3.35555900 -2.81732600 -1.85016800
C -3.44623200 -4.04641800 -2.50187100
H -1.14597600 -5.77742000 -0.69246600
H -0.97159300 -3.60172400 0.45408900
H -3.95650800 -1.97940200 -2.19184100
H -4.11907300 -4.16219600 -3.34655000
C -2.43777200 -1.29773400 -0.07060900
H -2.56151400 -0.50268600 -0.80461300
C 0.13068700 -0.92247800 0.17800300
C 1.19673200 -1.66212800 0.75142600
C 0.42295600 0.06176200 -0.79675700
O 0.81201800 -2.64029700 1.62657500
O -0.67479600 0.67145300 -1.32068200

C 1.88213600 -3.34240300 2.28387500
H 1.39213500 -4.04720600 2.95748400
H 2.50361900 -3.87226500 1.55900100
H 2.51227800 -2.64963300 2.84542800
C -0.41548700 1.78428200 -2.19200100
H 0.16394000 1.46933300 -3.06285100
H -1.39732400 2.14321100 -2.50113500
H 0.12615400 2.56707100 -1.65645000
O 2.42674200 -1.53017000 0.55009600
O 1.54752100 0.41840300 -1.23603800
Ni 3.22400300 0.16879600 -0.15096000
O 2.43200500 1.21546100 1.55864600
O 5.14148300 -0.36094000 0.64953100
Cl 5.64420000 -1.02892200 -0.63987000
O 0.16202100 2.16852100 1.44382700
O 4.44187800 -0.81875900 -1.58929200
O 6.83273600 -0.33830100 -1.16268500
O 1.86533700 3.18609800 2.87232600
O 5.88175200 -2.46478500 -0.42439500
Cl 1.60781900 2.50636500 1.59237600
O 2.02906600 3.37265500 0.42992500
O 3.97001600 1.97224400 -0.86512900
H 3.83797000 1.98258300 -1.82234900
H 3.36405000 2.64647600 -0.48123000
C -1.23176400 -0.96271600 0.82877300
H -1.43447400 0.02153200 1.27003400
H -1.18023300 -1.67490400 1.65384300
H -2.71852400 -6.07486600 -2.59298000
Thermal Correction to Free Energy: 0.428138 Hartree
Entropy: 261.829 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.859714 Hartree
Thermal Free Energy with Correction: -3531.431576 Hartree

A1-TS7

C -1.02032400 4.70737000 0.88468100
C -1.09955700 4.37012600 -0.47014200
C -1.22078600 3.03961400 -0.85836200
C -1.27001700 2.01421000 0.10921700
C -1.19871000 2.37373600 1.47209800
C -1.06906500 3.70508600 1.85656100
H -1.05491300 5.14938400 -1.22519500
H -1.26896100 2.78493400 -1.90994500
H -1.20974300 1.59295100 2.22780100
H -0.99031900 3.95975400 2.90875400

C -1.40858800 0.59799400 -0.24753600
H -1.42559000 -0.07527800 0.60564000
C 0.64599300 -0.12645500 -0.92861900
C 1.64045900 0.85483700 -1.27583200
C 1.01108600 -1.21425600 -0.06310000
O 1.19508500 1.82469000 -2.09605100
O 0.06057900 -2.16439300 0.06398400
C 2.16818900 2.82522800 -2.46361100
H 1.61503500 3.55784100 -3.05115100
H 2.60358000 3.28101200 -1.57229000
H 2.96450500 2.37587300 -3.06051700
C 0.46111000 -3.34249000 0.79455800
H 0.63006200 -3.10305200 1.84769300
H -0.37100100 -4.03862300 0.69327200
H 1.37184400 -3.75957800 0.36281500
O 2.83865700 0.86974900 -0.93725600
O 2.07532900 -1.35691200 0.57576200
Ni 3.78395100 -0.29214900 0.40583000
O 4.61146300 -1.48300300 -1.08326100
O 5.30020900 1.24313700 0.57962700
Cl 4.56501200 2.02557300 1.67208600
O 2.93844500 -3.17021100 -1.75315300
O 3.35228900 1.10684800 1.95933200
O 5.39270700 2.16285700 2.87860600
O 5.32879000 -3.56243000 -2.11972400
O 4.09977900 3.32870900 1.16270700
Cl 4.31264200 -2.99216800 -1.22485700
O 4.40744900 -3.60644600 0.15452200
O 4.72292100 -1.49718800 1.80043300
H 4.17151000 -1.57042600 2.59004400
H 4.72138700 -2.37970400 1.35567500
C -0.75817000 -0.02319500 -1.46660200
H -1.17884400 -0.99876500 -1.70076400
H -0.81962800 0.60357700 -2.35186700
H -0.91104500 5.74630600 1.18077400
C -7.90452200 -2.73385500 1.90132500
C -6.63364500 -2.56750600 2.46790100
C -5.80607200 -1.54055800 2.03900500
C -6.24103500 -0.64439300 1.02639000
C -7.53516200 -0.83112800 0.46919300
C -8.35415500 -1.86260700 0.90140100
H -6.29695400 -3.24334600 3.24766100
H -4.82382100 -1.41962000 2.47855200
H -7.87599400 -0.15124900 -0.30641100

H -9.33918500 -1.99503700 0.46575800
C -5.47494000 0.47327500 0.58955600
H -5.96988900 1.16501800 -0.08434600
C -3.55477900 0.35299400 -0.49129900
C -3.56290800 -1.11208800 -0.80299900
C -3.77647400 1.26416000 -1.65802400
O -3.31731500 -1.83838800 0.32160100
O -4.43690200 2.39934300 -1.29528200
C -3.25772400 -3.26221400 0.11265200
H -3.05952400 -3.69303900 1.09400300
H -4.20458900 -3.63270300 -0.28591500
H -2.45523100 -3.50632700 -0.58527400
C -4.61502700 3.36588100 -2.34687700
H -5.14586000 2.92107100 -3.19129100
H -5.19687200 4.17411400 -1.90446400
H -3.64777700 3.73746500 -2.69105500
O -3.72379100 -1.61747500 -1.89080900
O -3.36778700 1.07664900 -2.78272700
C -4.07528500 0.79509600 0.88590100
H -3.89142400 1.85953700 1.03204000
H -3.62901900 0.21452700 1.69082600
H -8.54510800 -3.54179000 2.24192000
Thermal Correction to Free Energy: 0.4684 Hartree
Entropy: 294.522 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3379.250823 Hartree
Thermal Free Energy with Correction: -3378.782423 Hartree

A1-13

C -1.81353800 -5.73284000 0.03293100
C -2.69271800 -5.01978200 0.84781700
C -2.80490200 -3.63298100 0.72308000
C -2.05241100 -2.93491700 -0.23292200
C -1.17599100 -3.66630900 -1.04894700
C -1.05045600 -5.04849400 -0.91436700
H -3.29071200 -5.54016300 1.59086400
H -3.48643800 -3.10573600 1.38157700
H -0.57683900 -3.14292700 -1.78844200
H -0.35787700 -5.58906300 -1.55280100
C -2.08125800 -1.42400900 -0.40353800
H -1.77023300 -1.21618000 -1.42980500
C 0.36585600 -0.68153000 0.11061400
C 1.35669900 -1.32914100 0.90307200
C 0.77010700 0.12990500 -0.97052200
O 0.86307200 -2.14651500 1.86485600

O -0.26442400 0.71467600 -1.65559300
C 1.83721500 -2.78692000 2.70473700
H 1.25937200 -3.40146100 3.39635200
H 2.51255800 -3.40803700 2.11261600
H 2.42893800 -2.04729600 3.24945500
C 0.11709500 1.66591700 -2.66429000
H 0.66814100 1.17749100 -3.47153700
H -0.82040900 2.07540900 -3.04552400
H 0.72935100 2.45792700 -2.22958200
O 2.60298700 -1.22537200 0.81101300
O 1.93258500 0.36782200 -1.39259100
Ni 3.55039800 0.20798000 -0.20897300
O 2.80250700 1.69807700 1.15545200
O 5.39435200 -0.29270600 0.77076100
Cl 5.86240400 -1.27102300 -0.31682900
O 0.63299600 2.73570500 0.62953100
O 4.70770500 -1.17626700 -1.34160600
O 7.12124600 -0.81779900 -0.92787000
O 2.30510300 3.95177300 1.93243400
O 5.96138000 -2.63825600 0.21764100
Cl 2.08736200 3.00896300 0.82342400
O 2.65735600 3.55781100 -0.46304900
O 4.49263800 1.72234500 -1.27658800
H 4.41426500 1.50912300 -2.21567800
H 3.93606000 2.51635000 -1.10774200
C -1.07436400 -0.69233300 0.54514400
H -1.40044600 0.35394100 0.66202300
H -1.13816400 -1.15349000 1.53103000
H -1.72238400 -6.81010400 0.13597300
C -3.04232100 5.71607100 -0.13973700
C -2.09785600 4.69363100 -0.01552900
C -2.49839800 3.36137800 -0.09145500
C -3.85348400 3.04281300 -0.27827600
C -4.79660300 4.07454300 -0.39121500
C -4.39105200 5.40704700 -0.33122600
H -1.04756000 4.91441300 0.14273700
H -1.73843100 2.59207400 -0.00121900
H -5.84773000 3.83373600 -0.53117600
H -5.12554300 6.20055100 -0.42916300
C -4.31897400 1.62443200 -0.33286400
H -5.38730900 1.56771300 -0.55115100
C -3.48603200 -0.71714000 -0.30273300
C -3.82745600 -0.16656300 1.06499900
C -4.68074100 -1.59331400 -0.70592700

O -3.70635900 -0.84031000 2.14731100
O -4.51504400 -2.10178900 -1.92399300
C -4.05620000 -0.21490300 3.42414100
H -3.84284300 -0.97767200 4.16822400
H -3.43383800 0.66840700 3.56990200
H -5.11402400 0.04834800 3.41282800
C -5.55779100 -2.99107900 -2.38561500
H -6.52229900 -2.47966100 -2.38264100
H -5.26775800 -3.27332500 -3.39608800
H -5.60558200 -3.86838300 -1.73779500
O -4.25939200 1.03598200 1.09869000
O -5.66417600 -1.74184500 -0.00622400
C -3.49563900 0.60839200 -1.13056400
H -3.92390700 0.44992200 -2.12174600
H -2.46764600 0.94791200 -1.25796200
H -2.72687300 6.75387400 -0.08665400
Thermal Correction to Free Energy: 0.4684 Hartree
Entropy: 290.432 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3379.300524 Hartree
Thermal Free Energy with Correction: -3378.825672 Hartree

A1-TS2

C -1.99903400 1.34641800 1.54390600
C -0.57526300 -1.17893800 -0.31546400
C -1.95677500 -1.66889300 -0.68145400
C -3.10185400 -0.68419300 -0.32296400
H -2.03098500 -1.83175000 -1.76107700
H -2.12574900 -2.63514500 -0.20356900
H -2.89216000 0.25594600 -0.83707300
H -1.31837600 0.77693100 2.17255000
N -3.05826100 -0.33925400 1.11618600
N -3.36569800 0.98472300 1.50409700
C -3.37155400 -1.30079000 2.19675700
C -4.15200900 0.91487600 2.75244400
C -3.70878900 -0.40960300 3.40399200
H -4.23060100 -1.90577600 1.88153800
H -2.52015900 -1.96326200 2.36106100
C 0.05269000 -0.18360900 -1.10879700
O 1.19487500 0.32593200 -0.97684500
C 0.14061100 -1.76616100 0.75533100
O 1.30033400 -1.48873700 1.16735300
O -0.72556000 0.27193800 -2.12681300
C -0.08853600 1.15420300 -3.06565500
H -0.84380500 1.35875000 -3.82542600

H 0.22890000 2.08036900 -2.58155700
H 0.78437600 0.67505000 -3.51431300
O -0.53143700 -2.74167600 1.42963200
C 0.26323900 -3.56952400 2.29794400
H -0.41848100 -4.33960400 2.66175900
H 1.08329300 -4.02010200 1.73598800
H 0.66220400 -2.99233700 3.13621500
C -1.51027400 2.42569200 0.77186300
C -0.12492800 2.74334900 0.79114700
C -2.40066100 3.24510800 0.02289900
C 0.34685800 3.86258900 0.12363500
H 0.58526700 2.11076400 1.31604100
C -1.93415400 4.36796200 -0.63013700
H -3.44969900 2.97569900 -0.02126800
C -0.56134500 4.66985500 -0.57275700
H 1.40758400 4.08578400 0.12687200
H -2.60358900 5.00707900 -1.19450400
C -4.50036200 -1.14286100 -0.72765400
C -5.44526300 -0.17891800 -1.11080100
C -4.88885500 -2.49015700 -0.71187000
C -6.74221500 -0.54665500 -1.46703600
H -5.15546400 0.86841500 -1.13964200
C -6.18799400 -2.86083500 -1.06687800
H -4.17524500 -3.26139000 -0.44028100
C -7.11816300 -1.89155400 -1.44349700
H -7.45600100 0.21390800 -1.77032300
H -6.46857300 -3.90999900 -1.05576600
Ni 2.67224800 -0.47980300 0.11912300
O 2.96390500 -1.89107500 -1.38750700
O 4.10879400 1.03684300 -0.53402700
Cl 3.92935900 1.93713500 0.68392300
O 1.72838500 -3.94648500 -0.80938600
O 2.78287000 1.23114000 1.45082000
O 5.14164200 1.98739100 1.50965500
O 3.55077800 -3.99983100 -2.44436400
O 3.49117200 3.28963700 0.27438600
Cl 3.06338900 -3.41968400 -1.18603900
O 4.04452200 -3.67081800 -0.06569500
O 4.17080900 -1.34436500 1.26876000
H 3.79732600 -1.51929800 2.14277700
H 4.30863100 -2.22896800 0.84872600
H -8.12627400 -2.18185500 -1.72415600
Cl 0.01986900 6.07547700 -1.41253600
H -4.49534400 -0.84263800 4.02569400

H -2.82861300 -0.25795400 4.03563500

H -5.21050800 0.89312200 2.47830300

H -3.95861500 1.80136000 3.35998400

Thermal Correction to Free Energy: 0.423959 Hartree

Entropy: 265.554 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.839926 Hartree

Thermal Free Energy with Correction: -3531.415967 Hartree

A1-3

C 2.12432200 1.00339900 -0.56500900

C -0.00602900 -1.72174700 0.34036900

C 1.18386500 -2.62791000 0.55490400

C 2.52385800 -1.87427300 0.40121900

H 1.16932100 -3.05609300 1.56174500

H 1.13525300 -3.45742600 -0.15311500

H 2.48243400 -1.02337000 1.08604600

H 1.17905900 0.58134500 -0.22925500

N 2.56933100 -1.25219300 -0.97201600

N 2.94040800 0.09300500 -1.03588600

C 3.22699400 -1.90835700 -2.10107600

C 4.20881000 0.28260900 -1.79865000

C 4.54348200 -1.13066100 -2.30163500

H 5.33469600 -1.56841300 -1.68968300

H 4.87051900 -1.12079100 -3.34315600

H 4.02467700 1.00487400 -2.59815100

H 4.97399400 0.67732900 -1.12632800

H 3.38982000 -2.96096600 -1.87413800

H 2.57735700 -1.83793200 -2.98010700

C -0.41813300 -0.85260000 1.38151100

O -1.37548500 -0.03703800 1.40184500

C -0.72834800 -1.75720600 -0.87922000

O -1.70725300 -1.04040800 -1.22588000

O 0.37398300 -0.91168500 2.48939900

C -0.06340700 -0.13767500 3.61912400

H 0.67662000 -0.32377600 4.39847300

H -0.10660000 0.92626300 3.37447600

H -1.05347400 -0.46057800 3.94859800

O -0.27869600 -2.66894000 -1.77781100

C -1.13142100 -2.91095800 -2.90933800

H -0.66471300 -3.73688100 -3.44818800

H -2.13344600 -3.18834800 -2.57635300

H -1.19161500 -2.02860200 -3.55260200

C 2.29028400 2.42724600 -0.43252500

C 1.13244400 3.11277000 0.00728800

C 3.46561400 3.17606200 -0.68448000

C 1.13305000 4.49039500 0.17937800

H 0.21518300 2.56710900 0.20331800

C 3.47222400 4.55035700 -0.50786600

H 4.38322100 2.69896000 -1.00164200

C 2.30555000 5.20137300 -0.08009500

H 0.22934300 4.98775900 0.51229700

H 4.37216400 5.12526200 -0.69417200

C 3.77729200 -2.67202600 0.73444800

C 4.88508000 -2.01290600 1.29201800

C 3.87359000 -4.05179000 0.50032700

C 6.05846100 -2.70400300 1.59338400

H 4.81767400 -0.94958200 1.51331800

C 5.04736200 -4.74692500 0.80019200

H 3.02364900 -4.59406200 0.09801300

C 6.14347300 -4.07572700 1.34323200

H 6.89950700 -2.17682200 2.03455900

H 5.10026300 -5.81597400 0.61631500

Ni -2.78346500 0.12079800 -0.00648600

O -3.92039400 -1.37133700 0.88437900

O -3.61157200 1.87770200 1.04726800

Cl -2.77251400 2.89805100 0.29378600

O -3.25882700 -3.53720500 -0.09860500

O -1.94593800 2.01605900 -0.67165200

O -3.60689400 3.84108300 -0.46333700

O -5.42052800 -3.27897200 1.02332600

O -1.84762400 3.60297100 1.21534300

Cl -4.41382400 -2.64528700 0.16064500

O -5.03016400 -2.21301900 -1.15031000

O -4.21796300 0.32369100 -1.49376200

H -3.74781400 0.35293400 -2.33769200

H -4.67650900 -0.55283400 -1.46751900

Cl 2.33477400 6.92966800 0.13460300

H 7.05317100 -4.61866500 1.58168800

Thermal Correction to Free Energy: 0.426399 Hartree

Entropy: 264.889 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.883728 Hartree

Thermal Free Energy with Correction: -3531.457329 Hartree

A1-TS5

C 2.04529000 1.91643600 0.55927200

C 0.72207500 -1.41370900 0.04631400

C 2.14543900 -1.92606000 -0.00290400

C 3.18166400 -0.90903900 0.53440100

H 2.25233700 -2.82627900 0.61080600

H 2.38421100 -2.20993400 -1.02925000
H 2.87185600 -0.65638700 1.55070400
H 1.46817200 1.20413600 1.14087500
N 3.05515500 0.36707700 -0.21754100
N 3.38612000 1.57698700 0.54574600
C 3.53168000 0.51885400 -1.61026000
C 4.40930800 2.28745500 -0.23877500
C 4.09262900 1.95141200 -1.70623300
H 4.32325800 -0.21966900 -1.77553900
H 2.71662300 0.31852700 -2.30758800
C 0.05589800 -1.31487200 1.29441600
O -1.11592800 -0.92656000 1.53487100
C 0.03125000 -1.06648700 -1.13789800
O -1.15290700 -0.64212800 -1.25949700
O 0.82768500 -1.66510900 2.36039700
C 0.16175900 -1.70870700 3.63500800
H 0.92623500 -2.02254000 4.34669100
H -0.23706800 -0.72803300 3.90433600
H -0.66015900 -2.42761000 3.61514300
O 0.76020100 -1.19119700 -2.28285600
C 0.01518900 -1.15768500 -3.51185500
H 0.74464600 -1.36912000 -4.29527900
H -0.76346000 -1.92282000 -3.49978900
H -0.43573700 -0.17480200 -3.67356200
C 1.28337800 3.02687900 0.08046000
C -0.12043200 2.89779500 0.25910100
C 1.78399300 4.21720500 -0.51341600
C -0.99401900 3.89215700 -0.15486400
H -0.54362300 2.00447200 0.70935100
C 0.91889700 5.21927100 -0.90696900
H 2.84531500 4.37042400 -0.65228700
C -0.46757700 5.04914300 -0.73314300
H -2.06114600 3.75236100 -0.02956700
H 1.29610500 6.13483900 -1.34783100
C 4.62757800 -1.38476900 0.59264300
C 5.46819900 -0.88962600 1.60334700
C 5.16401400 -2.28324800 -0.34185300
C 6.80865700 -1.26969200 1.67126700
H 5.06090000 -0.21127300 2.34836700
C 6.50504000 -2.66738500 -0.27257500
H 4.53168200 -2.70556000 -1.11661400
C 7.33186600 -2.15918900 0.73019900
H 7.44036800 -0.88221700 2.46550900
H 6.90011100 -3.37136000 -0.99926500

Ni -2.55947800 -0.78005000 0.16117600
O -2.73001700 -2.85911900 0.17469300
O -3.98645300 -0.30354200 1.75065500
Cl -3.76615600 1.20354700 1.70230500
O -1.51027600 -3.74127400 -1.78045500
O -2.77030500 1.35021600 0.51842400
O -5.01063200 1.92348100 1.39705600
O -3.17384400 -5.11338900 -0.62030300
O -3.12781300 1.69226000 2.93822600
Cl -2.81510600 -3.76346800 -1.07491000
O -3.89139900 -3.19918600 -1.97241700
O -4.04045000 -0.61117300 -1.28506900
H -3.63504200 -0.15440400 -2.03451000
H -4.17872500 -1.54255100 -1.58994600
H 8.37312200 -2.46275100 0.78523800
Cl -1.53590000 6.31453900 -1.25059600
H 4.97874600 2.00216500 -2.34329000
H 3.34603300 2.63363500 -2.11933300
H 5.36960300 1.86024900 0.06165900
H 4.42034600 3.34789700 0.01513700
Thermal Correction to Free Energy: 0.423848 Hartree
Entropy: 267.182 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.829807 Hartree
Thermal Free Energy with Correction: -3531.405959 Hartree

A1-8

C 1.16357600 -2.11750400 0.88394400
C 1.11927400 0.31803100 0.15555400
C 2.63575800 0.48062600 0.21532300
C 3.57979700 -0.60609800 -0.37985100
H 2.90750300 1.40671000 -0.30567900
H 2.92071700 0.62910300 1.25700900
H 3.37431300 -0.69555400 -1.45215400
H 1.53229500 -1.65642200 1.79353700
N 3.42502700 -1.94445000 0.28526800
N 2.12406700 -2.47758300 0.05934400
C 4.28721700 -3.01295200 -0.26042800
C 2.05681100 -3.32106100 -1.15797300
C 3.54055300 -3.56967200 -1.49245700
H 3.82272900 -3.02862600 -2.39874600
H 3.75057500 -4.62864200 -1.65603900
H 1.49742700 -4.23048700 -0.92383700
H 1.54190400 -2.78378500 -1.95749500
H 5.27317100 -2.61419900 -0.49132700

H 4.39380800 -3.78475300 0.50881200
C 0.45491100 0.24842300 -1.11042600
O -0.77036200 0.30334400 -1.34987100
C 0.33593100 0.68653400 1.29956000
O -0.89863800 0.90068100 1.35812400
O 1.29176500 0.04606100 -2.16156600
C 0.68674700 0.12455700 -3.46832200
H 1.51094500 0.00654300 -4.17232700
H -0.05609200 -0.66445500 -3.60622300
H 0.19955800 1.09177400 -3.60452600
O 1.03797700 0.73659300 2.45463500
C 0.37354600 1.34608800 3.57753500
H 1.12262100 1.37823700 4.36896500
H 0.04953800 2.35436200 3.31351000
H -0.48803800 0.75221000 3.89189900
C -0.22077700 -2.55321900 0.87400900
C -0.85986000 -2.60357700 2.13129300
C -0.96108700 -2.91090400 -0.27187200
C -2.16722000 -3.05222700 2.25316700
H -0.31459200 -2.30228900 3.02073800
C -2.27768100 -3.33614600 -0.16127600
H -0.53666000 -2.80791800 -1.26184200
C -2.86719500 -3.42238100 1.10243800
H -2.64819300 -3.10440100 3.22307200
H -2.85937500 -3.55812000 -1.04743600
C 5.01627900 -0.14102200 -0.20062000
C 5.73098300 0.34990300 -1.29991600
C 5.63157000 -0.14274300 1.06006000
C 7.03120300 0.83591100 -1.14630300
H 5.26291400 0.36148900 -2.28124800
C 6.93311200 0.33372100 1.21276400
H 5.08942500 -0.52683900 1.91890600
C 7.63608400 0.82699900 0.11068100
H 7.56908600 1.21858600 -2.00875100
H 7.39805900 0.32492600 2.19443000
Ni -2.08963200 1.32125700 -0.21906500
O -1.08248200 3.08427800 -0.73579900
O -3.51005700 1.20278500 -1.86102900
Cl -4.18619100 -0.07061100 -1.34758800
O 0.72869500 3.56775600 0.86543800
O -3.43389200 -0.31500200 -0.01699800
O -5.61622000 0.14592400 -1.09310100
O -0.26592400 5.36043200 -0.47469900
O -3.94747100 -1.20010000 -2.26757900

Cl -0.51391600 4.11595500 0.26470400

O -1.54601900 4.32792000 1.34630100

O -3.40368200 2.42826900 0.92700300

H -3.62469200 1.94941400 1.73622200

H -2.87973600 3.22453800 1.18551600

Cl -4.51270200 -3.97675100 1.24500200

H 8.64787500 1.20229500 0.23238300

Thermal Correction to Free Energy: 0.426476 Hartree

Entropy: 265.76 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.882806 Hartree

Thermal Free Energy with Correction: -3531.45633 Hartree

A1-TS3

C 1.12193300 -2.00720400 0.77999400

C 1.09002600 0.14929000 0.20167400

C 2.60558600 0.38518400 0.23810300

C 3.56578700 -0.65533700 -0.40679500

H 2.82076200 1.34408100 -0.24624400

H 2.90266200 0.49943000 1.28066100

H 3.36657800 -0.69732800 -1.48379600

H 1.51688200 -1.67478300 1.73454100

N 3.40042100 -2.00712600 0.20833700

N 2.08113600 -2.50005000 -0.00909100

C 4.22551100 -3.07095900 -0.39268900

C 1.96711200 -3.29546700 -1.25143400

C 3.43856100 -3.56591300 -1.62726600

H 3.71439500 -2.99831800 -2.51961700

H 3.62186100 -4.62225300 -1.83501800

H 1.39705500 -4.20380700 -1.03811300

H 1.44894900 -2.73415200 -2.03330000

H 5.21581900 -2.68630100 -0.63193800

H 4.33066100 -3.87339600 0.34454200

C 0.41697500 0.18487700 -1.08266300

O -0.80307400 0.28044900 -1.30583300

C 0.31838400 0.62053800 1.34208200

O -0.89682600 0.90038900 1.38409800

O 1.24783600 0.03061400 -2.13448700

C 0.64478500 0.16549700 -3.44039200

H 1.47222500 0.08645700 -4.14510600

H -0.08964600 -0.62419800 -3.61340400

H 0.15056700 1.13430200 -3.52878400

O 1.02356100 0.66031800 2.48416200

C 0.37626300 1.27576900 3.61679300

H 1.13119100 1.28883400 4.40238000

H 0.06839400 2.29037800 3.35845600
H -0.49291200 0.69248500 3.92879300
C -0.26563400 -2.49144600 0.80408000
C -0.85310100 -2.64688800 2.07406800
C -1.03653300 -2.79868000 -0.33160700
C -2.14693800 -3.13528400 2.21379100
H -0.28070800 -2.39869900 2.96323800
C -2.33845400 -3.27002200 -0.20425400
H -0.64700300 -2.63363000 -1.32782700
C -2.88066600 -3.44873400 1.06890000
H -2.58686800 -3.26670600 3.19577600
H -2.94105200 -3.46106500 -1.08378300
C 4.99635900 -0.18393000 -0.19997200
C 5.70186700 0.38947000 -1.26459800
C 5.61609900 -0.26646400 1.05575800
C 6.99720900 0.87787500 -1.08145400
H 5.23092400 0.46183100 -2.24200800
C 6.91292200 0.21276900 1.23752700
H 5.08062100 -0.71769900 1.88554000
C 7.60654400 0.78892100 0.17035400
H 7.52842600 1.32430500 -1.91700300
H 7.38198700 0.14007800 2.21463500
Ni -2.09434300 1.36810600 -0.18795600
O -1.00638700 3.06868900 -0.73553400
O -3.50250500 1.32566700 -1.81525800
Cl -4.25407300 0.09078100 -1.30023900
O 0.91770000 3.39818900 0.76508300
O -3.50991000 -0.19035300 0.02926200
O -5.66645500 0.39396800 -1.04110300
O -0.04507700 5.28743500 -0.46213200
O -4.08219100 -1.04755800 -2.22099100
Cl -0.32335700 4.03822200 0.25637800
O -1.27616500 4.27190700 1.40320900
O -3.31914200 2.56046800 0.96553900
H -3.60819100 2.09340900 1.76017900
H -2.73267800 3.30207400 1.24668300
H 8.61492500 1.16547100 0.31472000
Cl -4.50960700 -4.05795200 1.23419600
Thermal Correction to Free Energy: 0.427979 Hartree
Entropy: 259.625 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.878457 Hartree
Thermal Free Energy with Correction: -3531.450478 Hartree

A1-4

C -1.12070300 1.86089200 0.68888000
C -0.90178400 0.34817000 0.24204000
C -2.30776300 -0.33175700 0.10848800
C -3.33030600 0.51174700 -0.67515300
H -2.20191200 -1.32301100 -0.34050700
H -2.69119600 -0.48011000 1.11896000
H -3.01812400 0.58970400 -1.72795900
H -1.54789400 1.77840500 1.70071300
N -3.39825000 1.84548100 -0.06654800
N -2.08534000 2.52320600 -0.18310100
C -4.27775300 2.77202200 -0.80015900
C -2.42238000 3.87989300 0.28967400
C -3.78291100 4.16852900 -0.37364200
H -3.68091500 4.82590100 -1.24033300
H -4.46351800 4.64987200 0.33253200
H -2.52086400 3.90006800 1.38747700
H -1.63899200 4.58099600 0.00000900
H -4.16859800 2.64174100 -1.88876000
H -5.31703000 2.57521600 -0.53299600
C -0.16686200 0.16869800 -1.09560100
O 0.70759700 -0.66050900 -1.33517900
C -0.12870000 -0.33273000 1.39053400
O 1.00308500 -0.81394200 1.35744000
O -0.63000300 0.93386300 -2.06709200
C -0.00944500 0.75730500 -3.37195600
H -0.46653300 1.52009300 -3.99956000
H 1.07076800 0.88978700 -3.29630800
H -0.22581000 -0.24329400 -3.74999600
O -0.81250700 -0.29993700 2.51979700
C -0.22795100 -0.97304200 3.66607500
H -0.97598200 -0.88272400 4.45153200
H -0.03850200 -2.01666900 3.41561400
H 0.69978600 -0.47440200 3.95319900
C 0.18638000 2.63478000 0.78369000
C 0.81156500 2.78103900 2.02896400
C 0.79771600 3.20810700 -0.34114900
C 2.02243500 3.46146300 2.15648500
H 0.34199600 2.36927100 2.91831900
C 2.00501000 3.89542800 -0.22962500
H 0.31044800 3.13232400 -1.30614400
C 2.61237400 4.01292300 1.02074300
H 2.49744700 3.57187600 3.12496700
H 2.47240600 4.33640800 -1.10296300
C -4.68823900 -0.17373900 -0.62320900

C -5.16124000 -0.87854900 -1.73546200
C -5.46427300 -0.15064500 0.54462800
C -6.38317200 -1.55226100 -1.68512300
H -4.56980100 -0.90126400 -2.64755500
C -6.68871900 -0.81610700 0.59365200
H -5.10705200 0.40792500 1.40463600
C -7.15043100 -1.52183900 -0.52022300
H -6.73537500 -2.09651900 -2.55658600
H -7.28266700 -0.78591900 1.50278000
Ni 2.05639700 -1.67638400 -0.19032700
O 0.93072000 -3.39906500 -0.30001600
O 3.25774100 -2.00288400 -1.91094400
Cl 4.02642900 -0.67498200 -1.78904400
O -0.95867500 -3.19252300 1.26272200
O 3.45515300 -0.12302200 -0.45605200
O 5.46920700 -0.90300200 -1.67403800
O -0.15289900 -5.40042300 0.56397900
O 3.67986700 0.23127600 -2.89754900
Cl 0.22254700 -4.03010200 0.92100200
O 1.19972000 -4.01041200 2.07234900
O 3.33623600 -2.63947100 1.09313200
H 3.76271000 -2.03943200 1.71882700
H 2.75302100 -3.25050600 1.60020900
H -8.10245700 -2.04302600 -0.48002000
Cl 4.12935500 4.88059300 1.16880000
Thermal Correction to Free Energy: 0.429567 Hartree
Entropy: 259.872 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.881461 Hartree
Thermal Free Energy with Correction: -3531.451894 Hartree

A1-TS4

C 1.79275700 1.82095600 2.44673800
C 2.90753100 1.51439200 3.46458600
C 3.58639100 0.23543700 2.91264000
H 0.85099700 1.34143000 2.73396500
H 1.62600000 2.88523600 2.28194200
H 3.62461600 2.33745000 3.50731700
H 2.49820300 1.37128800 4.46614200
H 4.65964700 0.39470900 2.74607000
H 3.46818200 -0.63050400 3.57124500
C 1.79750500 1.24466100 -0.01543600
N 2.86061200 -0.03839000 1.66711200
N 2.32929200 1.20593400 1.22431400
H 2.49308500 0.93989500 -0.79100100

C 0.88410600 2.32517600 -0.43335200
C 1.21503800 3.04610200 -1.59534100
C -0.31342600 2.62996800 0.23434700
C 0.40386800 4.07933300 -2.05315600
H 2.12494100 2.80437500 -2.13735300
C -1.14040600 3.65267400 -0.22356300
H -0.64636000 2.03744700 1.07736200
C -0.76869200 4.37826500 -1.35557100
H 0.67090900 4.64501000 -2.93866000
H -2.07755600 3.85662300 0.27992400
Cl -1.80065800 5.67169400 -1.93078300
C 7.35052200 -0.26453300 -0.96768600
C 6.55224500 0.81329100 -0.58448800
C 5.28895000 0.59371200 -0.02948900
C 4.80679600 -0.70949200 0.15486700
C 5.62410800 -1.78486000 -0.22203000
C 6.88144700 -1.56711400 -0.78455400
H 6.91186200 1.83017900 -0.71438600
H 4.68433900 1.44367800 0.27146700
H 5.27105800 -2.80300300 -0.07453300
H 7.49749200 -2.41420800 -1.07214500
C 3.41584000 -1.01173300 0.71639000
H 3.51064600 -1.90222600 1.34626800
C 1.00521700 -0.77656900 -0.19803600
C 0.27726400 -1.22022600 0.99294100
C 0.16463800 -0.49604400 -1.35088400
O 0.84898200 -2.23192700 1.65086900
O 0.84502900 -0.40463300 -2.49967000
C 0.09863000 -2.77362100 2.75988000
H 0.70601100 -3.59542500 3.13755300
H -0.04927200 -2.01338000 3.53016400
H -0.87044000 -3.13364100 2.41126000
C 0.06066900 -0.22365600 -3.69668800
H -0.44921800 0.74202500 -3.67608600
H 0.77910400 -0.26066900 -4.51499000
H -0.66907500 -1.03008900 -3.78535500
O -0.80585800 -0.74759500 1.39301200
O -1.06513100 -0.27502000 -1.35208300
Ni -2.40739100 -0.72947600 0.11441700
O -2.15306200 -2.79368500 -0.07460100
O -3.74688300 -0.77698100 1.78748100
Cl -3.90034500 0.74588700 1.88718000
O -0.49185500 -3.31895300 -1.81694700
O -3.03800600 1.21841600 0.68329900

O -5.29716500 1.15591600 1.70340800

O -2.19746700 -4.95920400 -1.18407700

O -3.31867000 1.25473300 3.13950300

Cl -1.90250100 -3.53940200 -1.41065300

O -2.82887200 -2.94822400 -2.44273100

O -3.95749000 -0.80159300 -1.24403400

H -3.95479500 -0.02127600 -1.81380200

H -3.73691000 -1.58027600 -1.80809500

C 2.38457700 -1.38441300 -0.41412900

H 2.76757100 -1.05452900 -1.37956200

H 2.31245700 -2.47458300 -0.47181000

H 8.33185400 -0.09227800 -1.39956600

Thermal Correction to Free Energy: 0.428628 Hartree

Entropy: 258.519 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.861238 Hartree

Thermal Free Energy with Correction: -3531.43261 Hartree

A1-6

C 1.80483800 2.01018600 2.19818000

C 2.82380800 1.71291800 3.31423300

C 3.49093800 0.39055400 2.86154900

H 0.82586100 1.58644900 2.45702700

H 1.68935200 3.07414200 1.98961900

H 3.56937100 2.50839000 3.38438900

H 2.33165700 1.62558000 4.28537000

H 4.56361800 0.53693900 2.67755100

H 3.37458500 -0.42504500 3.58222700

C 1.62592000 1.11842800 -0.17467900

N 2.76387000 0.04013300 1.63576100

N 2.41686400 1.33525100 1.03950200

H 2.34609600 1.09535600 -0.99930600

C 0.69943400 2.27654200 -0.51324900

C 1.14749700 3.18808200 -1.48213800

C -0.54281000 2.50893200 0.09248100

C 0.39074800 4.30258000 -1.83959900

H 2.10881800 3.02982900 -1.96420500

C -1.31819900 3.61278000 -0.26164100

H -0.93254900 1.82129300 0.82986900

C -0.84293700 4.50400600 -1.22237000

H 0.74989100 5.00229300 -2.58602700

H -2.28634900 3.76358000 0.20109500

Cl -1.81332700 5.89715200 -1.67067800

C 7.43122500 -0.25887500 -0.71770400

C 6.54258400 0.81453900 -0.63183100

C 5.24357300 0.62212800 -0.15781500
C 4.81534300 -0.65190100 0.24790000
C 5.72190500 -1.71813400 0.17118900
C 7.01660900 -1.52870500 -0.31399500
H 6.86143500 1.80863000 -0.93308900
H 4.56470600 1.46441500 -0.07139500
H 5.40963700 -2.70954400 0.49239600
H 7.70133700 -2.37026800 -0.36918600
C 3.39317000 -0.93282400 0.73238200
H 3.43855000 -1.84172800 1.34148300
C 1.09507300 -0.41893100 -0.25312600
C 0.31114500 -0.93623300 0.95398600
C 0.16688500 -0.46178400 -1.46585200
O 0.76738400 -2.06161100 1.46492800
O 0.82560000 -0.48424400 -2.60701100
C 0.02938700 -2.62565600 2.57859300
H 0.60948700 -3.49467900 2.88427500
H -0.03814300 -1.89410500 3.38566200
H -0.96586800 -2.91864000 2.24621200
C 0.03385800 -0.55157100 -3.81986900
H -0.57029400 0.35202100 -3.91927200
H 0.76135900 -0.62313300 -4.62623900
H -0.60467700 -1.43512700 -3.78538500
O -0.74377400 -0.41733700 1.34912800
O -1.06664600 -0.39709800 -1.43801500
Ni -2.40999400 -0.80042000 0.09590300
O -1.94816100 -2.82372200 0.06800900
O -3.70806800 -0.91089700 1.74708000
Cl -4.12723600 0.57297500 1.70427400
O -0.15954400 -3.28639500 -1.56273500
O -3.29030400 1.07076400 0.48872000
O -5.55936700 0.71137200 1.42574500
O -1.70331400 -5.05723700 -0.86537400
O -3.70638900 1.27194300 2.92378200
Cl -1.55670400 -3.63755200 -1.19689500
O -2.48972100 -3.22888100 -2.30497500
O -3.91143500 -1.15978800 -1.26179200
H -4.06719600 -0.41416700 -1.85614400
H -3.59503800 -1.92235100 -1.79788700
C 2.40285800 -1.22401000 -0.44781200
H 2.85003100 -0.92675600 -1.39602800
H 2.18543800 -2.29061600 -0.51164400
H 8.43993300 -0.10569800 -1.09019800

Thermal Correction to Free Energy: 0.430582 Hartree

Entropy: 258.385 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.881461 Hartree

Thermal Free Energy with Correction: -3531.450879 Hartree

A1-5

C 0.41624400 -0.29554600 -0.50601200

C -0.15683700 1.03670600 0.11672500

C -1.69963000 1.02869200 -0.06346800

C -2.36440600 -0.27013400 0.42313500

H -2.12720800 1.87882400 0.47245400

H -1.91974400 1.15137200 -1.12890700

H -2.23046300 -0.34402800 1.51138600

H 0.15693400 -0.24465400 -1.57493900

N -1.71595800 -1.40057700 -0.25030500

N -0.27594600 -1.44093200 0.10750100

C -2.18228400 -2.70584500 0.24486600

C 0.11470700 -2.73022600 -0.50193400

C -1.05242100 -3.67317500 -0.15424400

H -0.80256600 -4.34310400 0.67217200

H -1.32127300 -4.29100400 -1.01459200

H 0.21378700 -2.62953300 -1.59469000

H 1.07113700 -3.06304000 -0.09965000

H -2.30801100 -2.69115800 1.33942700

H -3.14528000 -2.94440300 -0.20940300

C 0.17404700 1.22435000 1.61132700

O -0.63290600 1.16496400 2.51347100

C 0.31756900 2.30666300 -0.60520600

O 0.39329100 3.39282400 -0.07578700

O 1.47582000 1.49104900 1.80239800

C 1.86268600 1.76215700 3.15993700

H 2.94080400 1.91501600 3.13044300

H 1.35618700 2.65928400 3.52308000

H 1.60799500 0.92162000 3.80952500

O 0.52506400 2.11277300 -1.92575000

C 0.85660900 3.30012100 -2.67151100

H 0.97234800 2.97337100 -3.70443800

H 0.05664300 4.03878900 -2.58759700

H 1.78472700 3.73771700 -2.29777200

C 1.92680500 -0.47207300 -0.39897100

C 2.74956900 -0.12512500 -1.47572100

C 2.52791500 -1.01404000 0.74660100

C 4.13458500 -0.28900400 -1.41451600

H 2.30380300 0.28112900 -2.37727700

C 3.90613800 -1.19555600 0.82219200

H 1.90286300 -1.31125500 1.58180600
C 4.70158700 -0.82300800 -0.26146900
H 4.76268300 -0.01563300 -2.25502700
H 4.36134000 -1.62182400 1.70929600
C -3.85141400 -0.23536200 0.10728500
C -4.77339000 0.06892700 1.11505200
C -4.32209400 -0.45514600 -1.19506400
C -6.13744000 0.15569200 0.83079300
H -4.41804200 0.23998200 2.12800800
C -5.68507500 -0.37694300 -1.47890300
H -3.60963500 -0.70467600 -1.97555800
C -6.59734300 -0.06860000 -0.46709600
H -6.83974300 0.39275100 1.62489000
H -6.03640600 -0.55631200 -2.49127400
H -7.65882500 -0.00663700 -0.68896600
Cl 6.44602100 -1.04388600 -0.17177800
Thermal Correction to Free Energy: 0.430582 Hartree
Entropy: 258.385 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.881461 Hartree
Thermal Free Energy with Correction: -3531.450879 Hartree

A1-7

C -0.15087000 -0.75676500 -2.40019000
C 1.04113300 -0.91250300 -3.36549100
C 2.25201900 -0.40454500 -2.54807100
H -0.68705000 0.17645000 -2.60038800
H -0.85215300 -1.59141500 -2.45072200
H 1.19012000 -1.95566300 -3.65525900
H 0.88133900 -0.33149900 -4.27680000
H 2.93553700 -1.23339100 -2.31701800
H 2.82240900 0.38039800 -3.05474500
C -0.27686100 -0.23846800 0.08660000
N 1.64358200 0.15794300 -1.33965900
N 0.50398100 -0.74894200 -1.07484800
H 0.05961500 -0.83601100 0.94156500
C -1.76729600 -0.55029100 -0.01001000
C -2.16482200 -1.84092200 0.37383600
C -2.75575900 0.34337000 -0.44312500
C -3.49720000 -2.24346100 0.32159200
H -1.41611900 -2.54750100 0.72204700
C -4.09769500 -0.03966400 -0.48727200
H -2.47788300 1.34038000 -0.75873900
C -4.45770200 -1.32996100 -0.10902600
H -3.78851300 -3.24459100 0.61913200

H -4.85583600 0.66151200 -0.81798400
Cl -6.14942600 -1.81485800 -0.16736200
C 5.10519600 -2.81105500 1.23258600
C 3.77443300 -3.08647700 0.91195000
C 2.93513900 -2.07490300 0.44366200
C 3.41932400 -0.76725500 0.27760000
C 4.76066800 -0.50814500 0.58818100
C 5.59736500 -1.51616500 1.06932300
H 3.38667300 -4.09505600 1.02602900
H 1.90811500 -2.29496300 0.17182200
H 5.15427900 0.49725300 0.45475200
H 6.63272300 -1.29103500 1.30931700
C 2.53311600 0.38512600 -0.19404800
H 3.20339100 1.17596800 -0.54984200
C 0.20730900 1.20545600 0.49502400
C 0.13178500 2.25625100 -0.62523600
C -0.63757900 1.73772600 1.65627500
O 1.09421300 3.18969400 -0.48075700
O -0.62243400 0.88779800 2.70345800
C 1.04557900 4.26603000 -1.43142100
H 1.86199200 4.93462100 -1.15901300
H 1.18178000 3.88574200 -2.44673200
H 0.08607500 4.78392800 -1.37080600
C -1.42244200 1.28638400 3.83219900
H -2.47136100 1.37563000 3.54129300
H -1.29448200 0.49830100 4.57336500
H -1.07849700 2.24577800 4.22492800
O -0.71533400 2.32075100 -1.49178500
O -1.24308400 2.78716100 1.65279800
C 1.67476000 0.98894600 0.96345900
H 1.65589400 0.30982800 1.81731200
H 2.11095500 1.92980500 1.30168000
H 5.75379700 -3.60038100 1.60140700
Thermal Correction to Free Energy: 0.388626 Hartree
Entropy: 186.892 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1762.592139 Hartree
Thermal Free Energy with Correction: -1762.203513 Hartree

A1-10

C 0.62523600 0.71426400 1.09959300
C -0.08982500 1.37227900 -0.16273900
C -1.05745500 0.36235000 -0.81699500
C -1.99600100 -0.30675100 0.20385100
H -1.64480300 0.86085800 -1.59054300

H -0.46940300 -0.41809100 -1.30375500
H -2.61361800 0.46894700 0.68982300
H 0.92167300 1.55351600 1.73259500
N -1.12474100 -1.00780000 1.18279800
N -0.27703700 -0.09249300 1.90750700
C -1.83563600 -1.65962900 2.29166800
C -1.06332500 0.53301300 3.00243000
C -2.11314200 -0.54831300 3.33807600
H -3.12687700 -0.15007100 3.23802900
H -2.01104900 -0.92871300 4.35751900
H -0.38235700 0.73880400 3.83426600
H -1.53578100 1.48083000 2.72619500
H -2.73610200 -2.15441100 1.92671800
H -1.16605700 -2.41529100 2.71220600
C 0.97584500 1.88990800 -1.14272600
O 1.57209800 2.93526200 -0.97791600
C -0.82666500 2.65692500 0.27565900
O -0.75378500 3.19007500 1.36044400
O 1.19609400 1.06059000 -2.17399500
C 2.25674900 1.45309900 -3.06600200
H 2.27109900 0.69764100 -3.85058700
H 2.05934700 2.44312300 -3.48213500
H 3.20853100 1.46993000 -2.53082300
O -1.56306200 3.14970400 -0.74039900
C -2.20320600 4.41321000 -0.48494100
H -2.73914500 4.65998400 -1.40079300
H -2.89511500 4.33026800 0.35631200
H -1.45516100 5.17586900 -0.25776200
C 1.89698900 -0.05613800 0.74117200
C 3.12234900 0.62337800 0.70351500
C 1.89241000 -1.43338600 0.48414700
C 4.31142700 -0.03982000 0.39636400
H 3.15414200 1.68835500 0.91331300
C 3.07163800 -2.11116200 0.17776100
H 0.95371300 -1.97303900 0.53749100
C 4.27283000 -1.40613100 0.13127400
H 5.25471500 0.49469400 0.37720200
H 3.06070500 -3.17764300 -0.01873500
C -2.93109900 -1.27930400 -0.49184700
C -4.29537000 -0.98847100 -0.60884200
C -2.44673900 -2.46808100 -1.05790300
C -5.15818300 -1.85714800 -1.27984900
H -4.68532800 -0.07251700 -0.17141400
C -3.30749400 -3.33962600 -1.72336300

H -1.39349500 -2.71149300 -0.96219400
C -4.66609000 -3.03627800 -1.83906400
H -6.21364900 -1.61351200 -1.36085800
H -2.91729300 -4.25790400 -2.15304700
Cl 5.76628100 -2.25803800 -0.25674900
H -5.33524800 -3.71561300 -2.35894600
Thermal Correction to Free Energy: 0.388849 Hartree
Entropy: 185.699 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1762.606893 Hartree
Thermal Free Energy with Correction: -1762.218044 Hartree

A1-12

C 0.59232600 1.06013500 0.92666900
C -0.21714600 1.50001400 -0.39187300
C -1.75528900 1.41609800 -0.15479000
C -2.31972400 0.25118200 0.70767400
H -2.03722500 2.35541900 0.32376700
H -2.26387300 1.42610500 -1.12078600
H -3.12106800 0.72209500 1.30077800
H 1.06921700 1.97010100 1.29842100
N -1.28940900 -0.31485300 1.62053900
N -0.27416000 0.62178200 1.99693000
C -1.85389300 -0.63877100 2.93905700
C -0.84404700 1.58139900 2.96099600
C -1.85589600 0.70285700 3.73611600
H -2.84590200 1.16607800 3.75284000
H -1.55175100 0.54262200 4.77328300
H -0.04122200 1.97082000 3.59476300
H -1.34633100 2.44366500 2.49293700
H -2.84513700 -1.08271000 2.82578300
H -1.20017300 -1.36774700 3.42626300
C 0.08777900 2.96457900 -0.77582100
O -0.73685700 3.74993900 -1.18658300
C 0.18497700 0.69247800 -1.63504400
O 0.77303200 1.15508600 -2.59111300
O 1.38561900 3.28587300 -0.60173500
C 1.76040900 4.59949600 -1.05639500
H 2.81969800 4.69908400 -0.82216600
H 1.59374900 4.68382200 -2.13230300
H 1.17593700 5.36468800 -0.54130700
O -0.22260800 -0.57917800 -1.55015400
C 0.11617900 -1.42340100 -2.66618500
H -0.39687600 -2.36538300 -2.47991900
H -0.22396400 -0.97413800 -3.60115000

H 1.19788000 -1.57009800 -2.70846200
C 1.72889100 0.06025400 0.67166500
C 2.84279500 0.44054700 -0.08967800
C 1.71163100 -1.22322100 1.22875400
C 3.90744500 -0.43637000 -0.30098600
H 2.88225200 1.43167900 -0.52692700
C 2.76695700 -2.11171500 1.02570800
H 0.86109200 -1.52746100 1.82423200
C 3.85890000 -1.70982400 0.25973800
H 4.76601000 -0.13069100 -0.88848900
H 2.74362300 -3.10529100 1.45979700
C -3.00601800 -0.86012500 -0.08509400
C -4.22846500 -0.58451000 -0.71363500
C -2.48177100 -2.15357000 -0.18335700
C -4.90091500 -1.56642000 -1.44053600
H -4.66243700 0.40995500 -0.63124000
C -3.15827400 -3.14162200 -0.90204500
H -1.53900500 -2.37007500 0.30433600
C -4.36686800 -2.85257100 -1.53689700
H -5.84540500 -1.32962200 -1.92218400
H -2.73899000 -4.14246900 -0.96310900
Cl 5.19841300 -2.82597200 0.00152500
H -4.89153200 -3.62270500 -2.09491000
Thermal Correction to Free Energy: 0.388187 Hartree
Entropy: 186.389 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1762.593046 Hartree
Thermal Free Energy with Correction: -1762.204859 Hartree

A1-TS6

C 1.07625200 0.16526600 1.32445700
C 0.66801800 -0.50457700 -0.71629300
C 2.10581600 -0.53309100 -1.25684400
C 3.24546500 -1.13717000 -0.38564300
H 2.13295200 -1.08210500 -2.20551500
H 2.38543200 0.49334100 -1.49441800
H 3.02991100 -2.19847100 -0.21903600
H 0.17161900 -0.23102800 1.77522400
N 3.37208700 -0.42591400 0.92402200
N 2.15723900 -0.56586400 1.65123400
C 4.34248400 -1.04231100 1.84917300
C 2.11950000 -1.81971700 2.44750300
C 3.60213800 -2.24168700 2.49065900
H 3.76312400 -3.15516600 1.91236700
H 3.94552900 -2.43080300 3.50986200

H 1.70354100 -1.59048700 3.43072500
H 1.47997600 -2.57106000 1.98007600
H 5.24889700 -1.32058700 1.31262300
H 4.59798200 -0.29627200 2.60767000
C -0.18686400 0.58608400 -1.19281200
O -1.39423900 0.73859200 -0.93541500
C -0.03077000 -1.77531800 -0.54749100
O -1.25555200 -1.98068500 -0.44292000
O 0.44468100 1.51145500 -1.91444600
C -0.35286300 2.63104700 -2.37355500
H 0.30574200 3.18859100 -3.03806400
H -1.24076000 2.27627600 -2.89841600
H -0.65384500 3.24571900 -1.52360300
O 0.79446800 -2.83691700 -0.50175700
C 0.17571600 -4.12011200 -0.27281000
H 0.99983200 -4.83229300 -0.24127300
H -0.37129800 -4.11264100 0.67247800
H -0.50792100 -4.36411500 -1.08832600
C 1.09399200 1.64256100 1.21772000
C -0.11936500 2.30675900 1.48206500
C 2.24423600 2.41073100 0.96279100
C -0.18711800 3.69804400 1.48910100
H -1.01529200 1.73123600 1.69202900
C 2.18536700 3.80067100 0.97468100
H 3.18472100 1.90861500 0.77517500
C 0.96846900 4.43578400 1.23304400
H -1.12361900 4.20136900 1.70141300
H 3.07497400 4.39145000 0.78629200
C 4.55562200 -1.03472900 -1.14971700
C 5.13964900 -2.18811100 -1.68805400
C 5.18503000 0.20050800 -1.36319700
C 6.32185400 -2.11345300 -2.42755700
H 4.66286800 -3.15261400 -1.53024000
C 6.36944800 0.27654500 -2.09522400
H 4.74715500 1.10408400 -0.95051400
C 6.94089000 -0.88009800 -2.63142100
H 6.75874200 -3.01856600 -2.83942900
H 6.84640900 1.24020200 -2.24946600
Ni -2.77527800 -0.63607100 -0.40916500
O -2.54351100 -0.22603500 1.64809700
O -4.29373200 0.77915400 -0.91313800
Cl -4.34599900 0.39252600 -2.40106300
O -1.05253500 -1.86083700 2.72388400
O -3.34310400 -0.78806900 -2.44707400

O -5.68768500 -0.06112500 -2.78333900

O -2.64688700 -0.56276900 4.05535400

O -3.86221200 1.49805900 -3.24550300

Cl -2.41949400 -1.26597400 2.78778400

O -3.44693600 -2.33776500 2.56715500

O -4.19402600 -2.07075300 -0.00285200

H -4.07936600 -2.85569700 -0.55340000

H -4.07924900 -2.33436700 0.93850300

Cl 0.89752400 6.18736900 1.24165100

H 7.86225100 -0.81904200 -3.20305800

Thermal Correction to Free Energy: 0.429229 Hartree

Entropy: 257.693 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.874609 Hartree

Thermal Free Energy with Correction: -3531.44538 Hartree

A1-9

C 0.93457100 0.53509400 0.89413400

C 0.76995400 -0.56498700 -0.32064700

C 2.17778800 -0.90803200 -0.85183500

C 3.19136800 -1.28394100 0.25373300

H 2.12526800 -1.71836500 -1.58247800

H 2.55799200 -0.02969200 -1.37507400

H 2.85771000 -2.20823300 0.74577800

H 0.00296600 0.49468800 1.46080100

N 3.26219800 -0.14713600 1.20987400

N 1.98089400 0.14978100 1.79901100

C 4.05826900 -0.42208200 2.41628100

C 1.70069000 -0.83426200 2.86602300

C 3.11170300 -1.17124600 3.39761900

H 3.28820500 -2.25025900 3.38614600

H 3.25576200 -0.82624500 4.42403200

H 1.04359800 -0.37124400 3.60544100

H 1.19472300 -1.74413600 2.50659700

H 4.95505000 -0.98563600 2.15636400

H 4.35888200 0.53923800 2.84099300

C -0.12886200 0.07868600 -1.37864400

O -1.33797200 0.26776300 -1.23979200

C 0.00275300 -1.78704900 0.19352500

O -1.13795800 -1.76274700 0.66166700

O 0.50739700 0.46640100 -2.46318100

C -0.28621000 1.16071500 -3.46765100

H 0.39045600 1.29905600 -4.30854300

H -1.15296500 0.55755000 -3.74082000

H -0.61106200 2.12104300 -3.06418800

O 0.66669400 -2.92922300 0.08813300
C -0.02215300 -4.12933800 0.51665900
H 0.67521500 -4.94112300 0.31836800
H -0.25415000 -4.06612100 1.58171200
H -0.94109100 -4.25485900 -0.05832200
C 1.09127800 1.96031300 0.36026200
C -0.05518800 2.76037800 0.23359500
C 2.33421500 2.51865200 0.02552700
C 0.02693400 4.06912600 -0.24505800
H -1.02590600 2.37010900 0.52108700
C 2.42959300 3.82586100 -0.44943700
H 3.23209000 1.92969000 0.16784600
C 1.27167000 4.58943700 -0.59138000
H -0.86553400 4.67916100 -0.33022600
H 3.39484100 4.25101000 -0.70217700
C 4.55442800 -1.55631500 -0.36079700
C 5.04846900 -2.86532700 -0.41666900
C 5.32792000 -0.52190700 -0.90798000
C 6.28239900 -3.14101800 -1.00937300
H 4.46136200 -3.67657600 0.00750800
C 6.56258400 -0.79406000 -1.49643500
H 4.96415200 0.49959500 -0.86223700
C 7.04335100 -2.10464700 -1.55071300
H 6.64895100 -4.16297900 -1.04340000
H 7.15124800 0.01838800 -1.91291500
Ni -2.75231700 -0.65588700 -0.04890500
O -2.74491200 0.92825600 1.25374100
O -4.24464100 -0.02140800 -1.41771500
Cl -4.05789900 -1.20642300 -2.38353800
O -1.63573200 0.03595000 3.26078800
O -2.99067600 -2.04226500 -1.62643700
O -5.29780300 -1.97128300 -2.53454000
O -2.88585600 2.14978800 3.35339200
O -3.51115100 -0.74863000 -3.67186900
Cl -2.82818200 0.79290100 2.80496300
O -4.08098300 0.02271200 3.11986400
O -4.10555600 -1.71342400 1.07789800
H -3.76632000 -2.57244000 1.36062100
H -4.28500500 -1.18714700 1.89539200
Cl 1.38783500 6.23453800 -1.20034500
H 8.00503500 -2.31486500 -2.00954900
Thermal Correction to Free Energy: 0.431607 Hartree
Entropy: 253.236 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.879201 Hartree

Thermal Free Energy with Correction: -3531.447594 Hartree

A1-TS8

C -1.41496600 -1.05628200 0.81682200
C -0.91340400 0.82729200 -0.23132200
C -2.31678700 1.22419300 -0.69377900
C -3.47990500 1.25092500 0.33549100
H -2.29074800 2.21429700 -1.16501400
H -2.58613100 0.53018300 -1.48844900
H -3.38554900 2.15054500 0.94796800
H -1.01315000 -0.62005900 1.72575400
N -3.35393500 0.12442000 1.28863200
N -2.77620400 -1.02615600 0.67439600
C -4.54088800 -0.30800600 2.05264000
C -3.68573200 -2.17895700 0.80660500
C -4.42460500 -1.84100900 2.11184000
H -3.82272900 -2.15379100 2.97048900
H -5.40065800 -2.32757700 2.17784000
H -4.37861700 -2.21843100 -0.04080100
H -3.12001100 -3.10880100 0.84746400
H -4.53133300 0.14510700 3.04901200
H -5.46801400 -0.00937800 1.54978100
C -0.27120600 1.65248000 0.80034500
O 0.94123400 1.88449200 0.95188300
C -0.00920300 0.30978300 -1.25851600
O 1.21011000 0.10158900 -1.13279900
O -1.13248000 2.19130800 1.66439900
C -0.55933600 2.94695900 2.75717200
H -1.41104200 3.25342400 3.36318800
H 0.12348800 2.31521000 3.32692200
H -0.02270500 3.81750800 2.37483400
O -0.61371800 -0.03933000 -2.40071500
C 0.24439400 -0.55823900 -3.44656300
H -0.40839000 -0.67337500 -4.31130200
H 1.05596900 0.13991700 -3.65501500
H 0.66251800 -1.52049500 -3.14567200
C -0.68214000 -2.19183400 0.24462100
C 0.44029600 -2.69264000 0.92649100
C -1.08709200 -2.81959800 -0.95007000
C 1.13357100 -3.79928300 0.44433700
H 0.76105900 -2.21817500 1.84563100
C -0.40139100 -3.92531800 -1.43990400
H -1.93142300 -2.42724500 -1.50613200
C 0.70580300 -4.40876200 -0.73495500

H 1.99890600 -4.17810100 0.97567000
H -0.71296600 -4.41041300 -2.35823000
C -4.81309900 1.35171600 -0.41005200
C -5.66201800 2.43570500 -0.15289300
C -5.22681900 0.39522000 -1.35107000
C -6.88613700 2.56786200 -0.81261400
H -5.35837800 3.18839300 0.57102500
C -6.45123000 0.51824200 -2.00719300
H -4.58443500 -0.44989700 -1.58173200
C -7.28543800 1.60704500 -1.74109900
H -7.52487300 3.42027800 -0.59987900
H -6.75183700 -0.23222800 -2.73293000
Ni 2.53611300 1.14426200 -0.00880100
O 2.67316100 2.49846200 -1.69360000
O 3.24480000 1.00051800 3.36029600
Cl 2.61365200 -0.28033900 2.89262100
O 3.48022600 1.17791400 -3.62572900
O 2.83645000 -0.40083100 1.36962600
O 3.24616900 -1.44946700 3.52051500
O 5.02305900 2.67362700 -2.45375400
O 1.14690900 -0.24980300 3.15933300
Cl 3.86710600 1.77437500 -2.33647300
O 4.15989300 0.67200900 -1.29030200
O 3.83872200 2.34020300 1.06838000
H 3.78053400 1.99796100 1.98934500
H 4.73376000 2.14803700 0.75275400
Cl 1.56692300 -5.80319900 -1.35021000
H -8.23627900 1.70521500 -2.25650200
Thermal Correction to Free Energy: 0.427282 Hartree
Entropy: 261.191 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.858805 Hartree
Thermal Free Energy with Correction: -3531.431523 Hartree

A1-11

C 1.43528700 0.95840200 0.72744400
C 0.94733900 -0.43901500 0.02782500
C 2.18180800 -1.21974900 -0.53538000
C 3.39147700 -1.35963800 0.41834600
H 1.86431100 -2.21012300 -0.87890100
H 2.50576500 -0.67406400 -1.41787900
H 3.24709200 -2.23819600 1.05858200
H 1.11835100 0.88202000 1.77506500
N 3.37606500 -0.20844000 1.32312600
N 2.90125400 1.00107400 0.62752000

C 4.57843100 0.13882700 2.06744900
C 3.53491100 2.14404600 1.34604100
C 4.23405800 1.53812800 2.57436200
H 3.54764500 1.47560500 3.42395800
H 5.11225200 2.11267100 2.87873700
H 4.26507300 2.61403400 0.67855000
H 2.79345300 2.89978200 1.61141300
H 4.73500700 -0.59013700 2.86969000
H 5.48700000 0.16255400 1.44426500
C 0.21469300 -1.32369200 1.05206300
O -0.91678600 -1.80349300 0.93627900
C -0.00219100 -0.09308000 -1.13224400
O -1.22152300 0.04229000 -1.04601300
O 0.95588700 -1.61638400 2.09668500
C 0.34338000 -2.43154200 3.13206700
H 1.11173700 -2.52670500 3.89700300
H -0.54017800 -1.92383300 3.51822800
H 0.07221400 -3.40694200 2.72451800
O 0.62389000 0.12929100 -2.27193500
C -0.19579700 0.54930000 -3.39865700
H 0.49064900 0.57950300 -4.24278600
H -1.00298400 -0.16419700 -3.56470100
H -0.60757700 1.53865100 -3.19359200
C 0.81395400 2.20985500 0.12707000
C -0.31035000 2.78625400 0.73227400
C 1.35718900 2.82590500 -1.01075200
C -0.89404000 3.94125200 0.21089600
H -0.73846600 2.32852700 1.61827300
C 0.78920200 3.98453800 -1.53822300
H 2.23842800 2.40024500 -1.47790100
C -0.33781300 4.53135800 -0.92241300
H -1.76780100 4.37685700 0.68212500
H 1.21757500 4.46431200 -2.41153900
C 4.66935000 -1.59190600 -0.38760800
C 5.36197300 -2.80164500 -0.26335600
C 5.18176100 -0.61145000 -1.25283100
C 6.53048500 -3.03923300 -0.99077300
H 4.98098700 -3.56854600 0.40763500
C 6.35383500 -0.84158000 -1.97253300
H 4.65899600 0.33566100 -1.35023700
C 7.02999300 -2.05826900 -1.84731400
H 7.04938000 -3.98781600 -0.88559400
H 6.73973100 -0.07170700 -2.63502600
Ni -2.56965200 -1.13899200 -0.04375800

O -2.48294100 -2.44794900 -1.73595500
O -3.30572300 -1.04909600 3.26620800
Cl -2.84278900 0.30778100 2.80437400
O -3.33444200 -1.21565900 -3.70615800
O -3.04735200 0.38104000 1.27322400
O -3.63838000 1.37996500 3.41070200
O -4.77720200 -2.84678100 -2.58557100
O -1.38885200 0.46159500 3.08915000
Cl -3.71849900 -1.84249300 -2.43179600
O -4.14644600 -0.77069700 -1.39944000
O -3.79298000 -2.43781900 0.98485700
H -3.78642200 -2.08529500 1.90490600
H -4.69524600 -2.33537700 0.64835200
Cl -1.05625600 5.99125100 -1.58305400
H 7.93948100 -2.23813000 -2.41313300
Thermal Correction to Free Energy: 0.430235 Hartree
Entropy: 258.111 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.868413 Hartree
Thermal Free Energy with Correction: -3531.438178 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Path-A2:

SP2

C 5.12449700 -0.47844100 -2.18441700
C 5.37525000 -1.21231700 -1.02428400
C 4.61649400 -0.98604900 0.12549100
C 3.60113200 -0.02185700 0.12559300
C 3.35712600 0.71712100 -1.04351600
C 4.11368500 0.48664400 -2.19143300
H 6.16449100 -1.95823800 -1.01032300
H 4.82492600 -1.55127100 1.02886900
H 2.56587700 1.46266400 -1.05375700
H 3.91549400 1.06292600 -3.09027300
C 2.79776700 0.27479300 1.35208600
H 2.79724600 1.32081700 1.64864000
C 1.34963200 -0.34093600 1.53319600
C 0.31253400 0.60709700 2.02788900
C 0.91673800 -1.30909700 0.47833300
O 0.70993700 1.30932100 3.07887500
O 1.56225000 -2.45623100 0.51519300
C -0.20820900 2.33452700 3.55115000

H 0.32276000 2.83165100 4.36083400
H -0.43741700 3.02504500 2.73825800
H -1.12553500 1.86768300 3.91275900
C 1.21061600 -3.43701300 -0.50025700
H 1.48010300 -3.05445200 -1.48619200
H 1.80131700 -4.31652700 -0.25155800
H 0.14132900 -3.64228000 -0.44749200
O -0.80590900 0.76551400 1.53940700
O 0.07908500 -1.06970400 -0.39512000
Ni -1.38978200 0.36448100 -0.39517900
O -2.89933900 -0.83841200 0.27813400
O -2.37505500 2.28327000 -0.40566200
Cl -1.12509800 3.06499900 -0.82200700
O -1.91119100 -3.02907400 0.83746800
O -0.10610100 1.91041300 -1.05147800
O -1.34061000 3.80526400 -2.06779200
O -4.29534800 -2.82991400 0.30579500
O -0.65128600 3.92652300 0.27692900
Cl -2.93943000 -2.36435000 -0.00042000
O -2.61023100 -2.56001700 -1.46092900
O -1.93375100 -0.09221000 -2.32140800
H -1.18530200 -0.09212300 -2.93229500
H -2.25908800 -1.02183500 -2.24382800
C 2.52558400 -0.69455500 2.43835900
H 2.88722000 -1.71005600 2.33187800
H 2.46475800 -0.32397400 3.45445600
H 5.71599000 -0.65396300 -3.07814400
Thermal Correction to Free Energy: 0.245079 Hartree
Entropy: 204.863 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.27969 Hartree
Thermal Free Energy with Correction: -2574.034611 Hartree

A2-TS1

C 5.06917800 -3.09314900 0.69483200
C 4.71611300 -3.77434500 -0.64221000
C 3.44892500 -3.02244900 -1.08457300
H 4.59109300 -3.59281400 1.54121900
H 6.14338700 -3.03425000 0.88929400
H 5.52169700 -3.67125500 -1.37355200
H 4.52718200 -4.84259500 -0.51809500
H 3.36754700 -2.87992800 -2.16491400
H 2.54557900 -3.52063400 -0.72534200
C 4.78387200 -0.98505000 -0.57010200
N 3.49159900 -1.68880200 -0.41358200

N 4.51430100 -1.72043200 0.64689600
H 5.42859000 -1.45080400 -1.31746200
C 4.90471100 0.49977600 -0.51216200
C 5.04248300 1.22345300 -1.70383900
C 4.92942700 1.18067500 0.71027500
C 5.18024300 2.60942300 -1.68256900
H 5.03907700 0.70518600 -2.65936700
C 5.07682300 2.56582300 0.74575400
H 4.83859000 0.61760600 1.63269600
C 5.19635100 3.27081100 -0.45297300
H 5.27878700 3.17202900 -2.60395500
H 5.10015400 3.09655000 1.69095300
Cl 5.38015200 5.01091400 -0.41495800
C 0.69780600 -3.59583700 3.30271400
C 1.51421400 -2.47817600 3.50496700
C 1.80243000 -1.62063200 2.44645100
C 1.28602100 -1.88175700 1.16360500
C 0.46508500 -3.00998300 0.97097500
C 0.16721600 -3.85623300 2.03709200
H 1.91986500 -2.27329600 4.49123000
H 2.43392400 -0.75472600 2.60634900
H 0.01069600 -3.18147200 -0.00044500
H -0.48766200 -4.70775800 1.88161200
C 1.59437300 -1.01986600 0.01293700
H 1.25921600 -1.40072900 -0.94661600
C 0.08333800 0.59575200 -0.04455200
C -0.52687200 0.53756400 -1.33693700
C -0.73267300 0.72892400 1.12460100
O 0.35881400 0.42945900 -2.35637700
O -0.04575900 1.02597900 2.24623900
C -0.21989500 0.32961600 -3.67538400
H 0.62973200 0.22146100 -4.35056900
H -0.88198900 -0.53639400 -3.73537300
H -0.78438400 1.23313200 -3.91402400
C -0.83747800 1.24780700 3.42920100
H -1.32797100 0.32303900 3.74359000
H -0.12898500 1.57735000 4.18939800
H -1.59281400 2.01278200 3.24088900
O -1.74317100 0.59163300 -1.60988600
O -1.97404300 0.59629000 1.20579700
Ni -3.19345200 0.07575300 -0.31590700
O -4.16431700 1.87443400 -0.55379800
O -4.05908900 -1.14890100 -1.95582400
Cl -3.21097600 -2.37523300 -1.64734900

O -3.13570900 3.45123500 1.04729600
O -2.46957300 -1.95561900 -0.35469300
O -4.04348300 -3.55925900 -1.39136100
O -5.37229000 3.86626900 0.13756700
O -2.21590500 -2.62239700 -2.71498700
Cl -4.41957700 2.85577700 0.61768000
O -5.01977600 2.05153800 1.74951500
O -4.67507200 -0.49976300 1.00432100
H -4.27285100 -0.99287600 1.73120600
H -4.96980000 0.36904800 1.37818300
C 1.58857200 0.47159300 0.07207700
H 1.96056900 0.88123600 1.00808100
H 2.10816300 0.92558300 -0.76955600
H 0.46818500 -4.25630800 4.13385000
Thermal Correction to Free Energy: 0.42202 Hartree
Entropy: 268.542 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.826038 Hartree
Thermal Free Energy with Correction: -3531.404018 Hartree

A2-2

C 5.11076000 -2.91572800 0.81994600
C 4.89703200 -3.64142200 -0.52326300
C 3.57966000 -3.05152500 -1.04354600
H 4.63189900 -3.44376100 1.64742500
H 6.16132600 -2.74714200 1.06889000
H 5.72289600 -3.46207300 -1.21581700
H 4.81689700 -4.72162700 -0.38675000
H 3.54980200 -2.88497400 -2.12187400
H 2.71470300 -3.64239200 -0.74292100
C 4.66358900 -0.84889700 -0.49169200
N 3.42989100 -1.71370700 -0.34969000
N 4.43901200 -1.60174900 0.71706100
H 5.30750500 -1.28841800 -1.25460100
C 4.73220800 0.63361300 -0.44616100
C 4.86478800 1.34244800 -1.64821600
C 4.75822500 1.32417300 0.77206500
C 4.98944000 2.72832600 -1.64082500
H 4.86126300 0.81440200 -2.59814500
C 4.89576600 2.70878900 0.79070900
H 4.66605700 0.77500700 1.70238900
C 5.00430800 3.40243300 -0.41711300
H 5.07917200 3.28243900 -2.56801000
H 4.91532600 3.24982300 1.72983200
Cl 5.17475100 5.13956900 -0.39771600

C 0.18534000 -4.07026100 2.73039700
C 1.24626500 -3.25219500 3.12959300
C 1.82408600 -2.36140900 2.22566900
C 1.36083600 -2.29718800 0.90155300
C 0.29058200 -3.11428400 0.51179200
C -0.29934000 -3.99068100 1.42515900
H 1.61133700 -3.29445100 4.15180500
H 2.62344300 -1.70484000 2.55279200
H -0.12349800 -3.03175100 -0.48871100
H -1.14617100 -4.59328000 1.11334000
C 1.94690400 -1.32244000 -0.10294400
H 1.52263700 -1.51676100 -1.09117100
C 0.18116200 0.38107200 0.07709800
C -0.40424100 0.41518900 -1.21177000
C -0.63508700 0.50955300 1.23001100
O 0.49671300 0.28211000 -2.23391800
O 0.05172500 0.64029100 2.39383700
C -0.07241800 0.28374400 -3.55745200
H 0.77218300 0.13482800 -4.23299000
H -0.80310400 -0.52077800 -3.66316200
H -0.56043300 1.23810100 -3.76678900
C -0.74289000 0.85846900 3.56943400
H -1.34752000 -0.02288800 3.80104700
H -0.02650300 1.04184000 4.37163100
H -1.40147200 1.71904000 3.43498200
O -1.60848100 0.55763000 -1.52427200
O -1.89110200 0.51306200 1.29396100
Ni -3.11329500 0.18576000 -0.26642500
O -3.87291500 2.09544700 -0.50109400
O -4.07947000 -0.91295400 -1.97486200
Cl -3.37631100 -2.22569700 -1.66954700
O -2.83429000 3.51691200 1.23246400
O -2.65086400 -1.92802300 -0.33883700
O -4.33635300 -3.32587300 -1.48771600
O -4.91969100 4.19201900 0.13935100
O -2.36741200 -2.54923400 -2.70681400
Cl -4.12761800 3.07232600 0.67054600
O -4.91486700 2.31804000 1.71993400
O -4.68124200 -0.25354700 1.01293800
H -4.30280600 -0.72646000 1.76594500
H -4.93793600 0.64228800 1.35001300
C 1.67306100 0.16445100 0.19550000
H 2.01875300 0.43442300 1.19309900
H 2.19718000 0.78017100 -0.53564400

H -0.27116300 -4.75363100 3.44047000

Thermal Correction to Free Energy: 0.425477 Hartree

Entropy: 267.042 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.851541 Hartree

Thermal Free Energy with Correction: -3531.426064 Hartree

A2-TS2

C 4.23381500 2.30276300 1.98986700

C 4.82590300 1.02231400 2.60834200

C 3.72401900 -0.02243300 2.37479700

H 3.67771000 2.89240200 2.72549100

H 4.99021900 2.93906600 1.52662100

H 5.73404800 0.72783600 2.07665200

H 5.06316000 1.15315800 3.66626300

H 4.08741800 -1.04787400 2.30700500

H 2.94801400 0.01448000 3.14659900

C 1.90397800 1.93220600 1.08946800

N 3.15539800 0.38786600 1.08541300

N 3.29755500 1.79104900 0.94086100

H 1.44021700 1.57024400 2.00531400

C 1.10833700 2.60041400 0.12288000

C -0.29457300 2.68602800 0.31343400

C 1.69812700 3.23707700 -1.00085700

C -1.07824300 3.41614400 -0.56574100

H -0.77726900 2.16232400 1.13261700

C 0.91987000 3.97644500 -1.87106700

H 2.76556100 3.13813100 -1.16336600

C -0.46454800 4.06308300 -1.64416000

H -2.15136000 3.45408700 -0.42397600

H 1.35832200 4.47725100 -2.72665000

Cl -1.43973700 4.98297700 -2.75397000

C 7.24263100 -1.74927400 -0.94347300

C 6.35027800 -2.62860300 -0.33025600

C 5.03729800 -2.23046300 -0.06636300

C 4.59802000 -0.94581700 -0.41471600

C 5.50486200 -0.07159700 -1.03528000

C 6.81563100 -0.46705700 -1.29820400

H 6.67113400 -3.63075400 -0.06152500

H 4.35285500 -2.93542800 0.39410300

H 5.17296100 0.92316900 -1.32199200

H 7.50012200 0.21988800 -1.78753800

C 3.17978700 -0.45915900 -0.13132400

H 2.87693400 0.21002800 -0.93969600

C 0.69574300 -1.03394400 0.08785100

C 0.02316100 -0.97016000 1.33185100

C 0.00790500 -0.65452200 -1.09451500

O 0.77877700 -1.32706000 2.41200200

O 0.77400700 -0.71014900 -2.21018200

C 0.05832700 -1.48038000 3.64956800

H 0.80322800 -1.80641000 4.37716300

H -0.39959600 -0.53890700 3.96085500

H -0.72693600 -2.23243600 3.54715200

C 0.08676400 -0.58408100 -3.46538600

H -0.36729700 0.40511000 -3.56632300

H 0.85351900 -0.72612000 -4.22782700

H -0.68190200 -1.35492200 -3.54977100

O -1.15880500 -0.60669200 1.55959300

O -1.18254500 -0.25465700 -1.21442800

Ni -2.60681900 -0.59836100 0.17115300

O -2.49384200 -2.68417800 0.11044700

O -4.09314200 -0.40740600 1.74947100

Cl -4.08183300 1.12002700 1.77778200

O -1.12697800 -3.38019500 -1.82170200

O -3.11356900 1.45447700 0.61205500

O -5.41391700 1.67376200 1.50209400

O -2.66512600 -4.95291700 -0.74648300

O -3.51561500 1.62365800 3.04257900

Cl -2.44310300 -3.56104800 -1.16040400

O -3.54532700 -3.09447700 -2.08084500

O -4.07069400 -0.58172800 -1.29649300

H -3.75272900 -0.01959000 -2.01565500

H -4.06017500 -1.50469300 -1.65273700

C 2.10317600 -1.56663700 -0.01200100

H 2.19936700 -2.19675200 -0.90031900

H 2.31340500 -2.19595600 0.85599100

H 8.26135500 -2.06247400 -1.15177900

Thermal Correction to Free Energy: 0.423169 Hartree

Entropy: 266.964 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.842013 Hartree

Thermal Free Energy with Correction: -3531.418844 Hartree

A2-3

C 4.76607300 -1.80993500 -2.24766500

C 3.88327200 -2.31638400 -3.38527900

C 2.77504300 -3.06634100 -2.63942100

H 5.47807900 -2.56856100 -1.90778100

H 5.29358700 -0.88133400 -2.46122800

H 3.46862900 -1.47193700 -3.94216500

H 4.43603900 -2.95262200 -4.07817400
H 1.80339000 -2.96266200 -3.12794500
H 2.99581500 -4.13400600 -2.52998600
C 3.89714600 -0.68710900 -0.19582300
N 2.72473200 -2.44568400 -1.29768000
N 3.78475900 -1.56534100 -1.16051200
H 3.03947800 -0.60752900 0.45902900
C 5.00970200 0.20665300 0.07433000
C 4.67535900 1.41004600 0.73398100
C 6.36746100 -0.04965700 -0.20899900
C 5.64880000 2.34659400 1.05439100
H 3.63540000 1.61243900 0.97307100
C 7.34846100 0.87731900 0.12344100
H 6.67763500 -0.99201400 -0.64420100
C 6.98421400 2.07632800 0.74271900
H 5.38156400 3.27552900 1.54485700
H 8.39239100 0.67052400 -0.08278800
Cl 8.21684200 3.24002200 1.14916700
C 1.09138500 -3.00938500 3.51556200
C 2.30229200 -3.18887000 2.84818500
C 2.40647700 -2.88380900 1.48953000
C 1.31176300 -2.37628500 0.77183100
C 0.08743700 -2.23733600 1.44836900
C -0.01573800 -2.54258300 2.80562700
H 3.16768600 -3.57770400 3.37757400
H 3.34680200 -3.07615300 0.98094200
H -0.80141300 -1.90829700 0.92722100
H -0.97857800 -2.42434700 3.29304200
C 1.39161200 -2.09465400 -0.73138900
H 0.72458500 -2.81303100 -1.21550800
C -0.41359000 -0.22322900 -0.90222900
C -1.55197700 -0.82162300 -1.50273700
C -0.57145100 0.81019800 0.05400300
O -1.24627400 -1.82525000 -2.37593500
O 0.59199500 1.40233200 0.45821400
C -2.37963900 -2.48410000 -2.97651200
H -1.95727300 -3.28859200 -3.58064200
H -3.04517900 -2.88149500 -2.20760200
H -2.93934800 -1.78891300 -3.60626100
C 0.42750200 2.55644300 1.30091600
H 0.02467900 2.27427800 2.27719800
H 1.42890200 2.97614800 1.41785100
H -0.23911800 3.28204800 0.83137300
O -2.76029700 -0.54523600 -1.33745000

O -1.63258100 1.22836200 0.57903600
Ni -3.48085300 0.56468700 0.16766400
O -4.02126500 2.11150700 -1.11221300
O -5.25866900 -0.73009900 0.13413800
Cl -4.66214400 -1.78654800 1.06007200
O -2.03683200 3.55253000 -1.41985200
O -3.31913100 -1.13640900 1.48085800
O -5.50773900 -2.00037600 2.24373400
O -4.28956500 4.41646800 -1.83465800
O -4.39909600 -3.04352000 0.33148900
Cl -3.45583700 3.54401200 -0.99375400
O -3.55608500 3.95128100 0.45937000
O -4.24383700 1.68306600 1.73948000
H -3.66928500 1.55263700 2.50513100
H -4.09183300 2.60799800 1.42373200
C 0.95587700 -0.68838800 -1.29420000
H 1.66579100 0.08304900 -1.00513200
H 1.02238900 -0.78772400 -2.38476700
H 1.00610800 -3.24966000 4.57120100
Thermal Correction to Free Energy: 0.42431 Hartree
Entropy: 271.205 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.877068 Hartree
Thermal Free Energy with Correction: -3531.452758 Hartree

A2-TS4

C -4.58661600 2.16799800 1.25390000
C -4.69735300 2.98449100 -0.06296700
C -4.00677200 2.08842000 -1.11645100
H -4.07772900 2.74321200 2.02873800
H -5.53998100 1.82878300 1.66225300
H -5.73093900 3.21160400 -0.34017300
H -4.16285800 3.93065000 0.04270700
H -4.73634200 1.48919100 -1.67238500
H -3.40980400 2.64485700 -1.83957900
C -4.19344500 -0.24324800 0.50806900
N -3.11242000 1.19885800 -0.35098500
N -3.73272300 1.00172900 0.93806500
H -3.41692100 -0.99957200 0.57373800
C -5.47516900 -0.72233000 0.09192700
C -5.55427600 -2.11933700 -0.16388600
C -6.65157300 0.05272400 -0.09200500
C -6.73630000 -2.71750600 -0.56344600
H -4.66555400 -2.73091500 -0.03886100
C -7.83609400 -0.54074800 -0.49636300

H -6.64441000 1.12137300 0.07110200
C -7.87818600 -1.92290000 -0.72706600
H -6.78377600 -3.78383100 -0.75174800
H -8.73078800 0.05502300 -0.63640300
Cl -9.37015900 -2.65830600 -1.22789600
C -0.64412500 4.97158800 1.88861300
C -0.83121400 3.76430600 2.56529400
C -1.13325600 2.59777000 1.86093300
C -1.25899300 2.62582100 0.46276200
C -1.06058400 3.84401200 -0.20671300
C -0.75187900 5.00825900 0.49724200
H -0.72561700 3.72609600 3.64568500
H -1.23694700 1.66079900 2.39422400
H -1.11971800 3.87524800 -1.29234400
H -0.58287200 5.93661700 -0.04027900
C -1.63784700 1.39785300 -0.34577200
H -1.38665900 1.56810700 -1.39488300
C 0.54924800 0.07633700 0.02597800
C 1.21490000 0.08341100 -1.23402000
C 1.31287700 -0.04901800 1.22173200
O 0.37074700 0.22154400 -2.29434700
O 0.57743300 -0.12545700 2.35734300
C 0.99343800 0.17129700 -3.59121200
H 0.18139600 0.31129700 -4.30608600
H 1.74176900 0.95998000 -3.69383400
H 1.47925900 -0.79443300 -3.74752800
C 1.30539300 -0.43858300 3.55695700
H 1.99531300 0.36935500 3.81434800
H 0.54575200 -0.54663500 4.33242900
H 1.86040900 -1.36957700 3.42945400
O 2.43541600 -0.02340700 -1.47627700
O 2.56302500 -0.08787900 1.33316200
Ni 3.86566900 -0.49440700 -0.15060600
O 3.35010200 -2.53143500 -0.28397200
O 5.32995400 -0.41250400 -1.72611800
Cl 5.66654300 1.07065700 -1.52039800
O 1.52459400 -3.08454800 1.27800300
O 4.77552600 1.43207900 -0.31007900
O 7.08577100 1.24840600 -1.17875100
O 3.05433300 -4.82147800 0.48145900
O 5.27280200 1.86314600 -2.69770900
Cl 2.92178000 -3.41751000 0.90049600
O 3.84268800 -3.11794000 2.06099100
O 5.30906800 -0.98839900 1.25604500

H 5.31172700 -0.29753700 1.93155900

H 4.93954300 -1.80125400 1.67566800

C -0.95219700 0.06419200 0.06543300

H -1.27410500 -0.20979300 1.07179600

H -1.33445100 -0.69176300 -0.63159700

H -0.39874400 5.87421800 2.44034000

Thermal Correction to Free Energy: 0.422281 Hartree

Entropy: 268.401 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.821737 Hartree

Thermal Free Energy with Correction: -3531.399456 Hartree

A2-5

C 4.41273400 -3.26952300 0.89373000

C 4.43634100 -4.00162400 -0.44871500

C 3.39487600 -3.22638100 -1.28112400

H 3.57523000 -3.58376700 1.52119700

H 5.34769100 -3.31126400 1.45319700

H 5.43110600 -3.93802500 -0.89837300

H 4.17240800 -5.05513900 -0.34078900

H 3.69758000 -3.12226500 -2.32584900

H 2.42254000 -3.72179400 -1.24510900

C 4.80636200 -0.83948900 0.88992300

N 3.28301800 -1.86699600 -0.66748500

N 4.14992000 -1.87848700 0.43804800

H 5.34624800 -1.05015400 1.80976000

C 4.97356100 0.48508300 0.34915200

C 5.59114800 1.43302500 1.19716000

C 4.67662400 0.85408800 -0.98350400

C 5.88397700 2.71151600 0.74872500

H 5.83697300 1.16127000 2.22000900

C 4.99680500 2.12173300 -1.44541300

H 4.20909900 0.13644800 -1.64440400

C 5.58655000 3.04845900 -0.57660200

H 6.34263500 3.44076800 1.40614200

H 4.77855300 2.40467700 -2.46873000

Cl 5.96204800 4.64381300 -1.15611200

C -0.11868700 -4.09661300 2.50409500

C 0.80396200 -3.14570400 2.94941100

C 1.42390900 -2.28971500 2.03875100

C 1.14957200 -2.38339600 0.66295500

C 0.20339100 -3.32608700 0.23531900

C -0.42790900 -4.17491100 1.14686300

H 1.02300000 -3.05523800 4.00974800

H 2.09273400 -1.51845300 2.40869900

H -0.08704400 -3.36052900 -0.81122100
H -1.17590000 -4.87803200 0.79465500
C 1.81959400 -1.47454600 -0.35699300
H 1.36519400 -1.65524700 -1.33324900
C 0.15630400 0.35493000 -0.10516500
C -0.52448200 0.36663300 -1.34990500
C -0.56051100 0.61535300 1.08984700
O 0.28508500 0.14301300 -2.42652800
O 0.21884900 0.77963500 2.19391700
C -0.38283600 0.10308300 -3.70205500
H 0.39937900 -0.12678100 -4.42774200
H -1.15747200 -0.66673100 -3.70629100
H -0.83975900 1.06875600 -3.92951700
C -0.47692500 1.13360600 3.39860600
H -1.10621900 0.30792400 3.74314900
H 0.30356500 1.34042500 4.13295100
H -1.10080700 2.01531400 3.23929200
O -1.73900100 0.57199400 -1.57677500
O -1.80453600 0.70757200 1.24637700
Ni -3.16239800 0.36525000 -0.19338600
O -3.82372600 2.31207700 -0.45690000
O -4.33347300 -0.74274500 -1.74051500
Cl -3.69543700 -2.08714900 -1.41857400
O -2.47030400 3.76681000 1.01266600
O -2.83690100 -1.76974300 -0.17598800
O -4.71020800 -3.10050500 -1.08796000
O -4.66237300 4.49543000 0.20005900
O -2.81331700 -2.53840600 -2.52020400
Cl -3.85276200 3.36279400 0.67612600
O -4.50566500 2.71205800 1.87619800
O -4.64391800 0.10874400 1.23579700
H -4.25318600 -0.40301100 1.95626900
H -4.75625800 1.03152300 1.57710600
C 1.63072900 0.03011300 -0.07812000
H 2.05100600 0.31377400 0.88835300
H 2.15946500 0.59376900 -0.85107800
H -0.61123900 -4.75292000 3.21540900
Thermal Correction to Free Energy: 0.424468 Hartree
Entropy: 269.571 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.873199 Hartree
Thermal Free Energy with Correction: -3531.448731 Hartree

A2-TS3

C -2.28460800 -2.94042200 -1.77029500

C -3.80503600 -3.14877800 -1.93353100
C -4.35602700 -2.93377900 -0.50592700
H -1.70927600 -3.86509400 -1.86613500
H -1.90138200 -2.21221200 -2.49006500
H -4.21878700 -2.41231000 -2.62712900
H -4.04429200 -4.14154500 -2.32075100
H -5.36257400 -2.51884200 -0.48480500
H -4.35306400 -3.87432700 0.05411400
C -1.07157300 -2.12023500 0.33135200
N -3.41192800 -2.01320900 0.15177900
N -2.16218100 -2.44241500 -0.38260200
H -1.29676600 -2.06080700 1.39140000
C 0.28971600 -2.57885400 0.00508600
C 1.12443400 -2.91474700 1.08728300
C 0.81233100 -2.69103200 -1.29648800
C 2.42025900 -3.37704900 0.88801700
H 0.74996700 -2.81797600 2.10201900
C 2.10389500 -3.16020100 -1.50835000
H 0.22623900 -2.39373700 -2.15653700
C 2.89851400 -3.50787100 -0.41507600
H 3.05777200 -3.61833500 1.72994700
H 2.50132800 -3.24256300 -2.51346600
Cl 4.51870700 -4.10075300 -0.68610200
C -7.50908900 0.73532400 1.25702400
C -6.69953300 -0.05387100 2.07790300
C -5.45228700 -0.48589800 1.62820800
C -4.99993700 -0.14220400 0.34540700
C -5.82049200 0.64469000 -0.47141200
C -7.06566800 1.08563800 -0.01842100
H -7.03900600 -0.33032000 3.07208600
H -4.82640700 -1.10268500 2.26610400
H -5.47887000 0.92158500 -1.46582100
H -7.68743700 1.69980100 -0.66327700
C -3.62501300 -0.56566100 -0.14495700
H -3.56947500 -0.38240100 -1.22496500
C -1.06244100 0.05812400 0.32313600
C -0.17675700 0.23450500 1.46948200
C -0.51430600 0.42621800 -0.97449700
O -0.76758700 -0.03187300 2.64900900
O -1.43376300 0.41860300 -1.95445300
C 0.04646300 0.15982000 3.82740400
H -0.60334800 -0.09388000 4.66420000
H 0.92377900 -0.48902000 3.80112300
H 0.37514600 1.19860300 3.89250100

C -1.01190100 0.94314000 -3.23208100
H -0.24654700 0.30342600 -3.67820900
H -1.91127200 0.94812800 -3.84741200
H -0.62364700 1.95448600 -3.10539000
O 1.03529100 0.50268200 1.46502500
O 0.67235600 0.66487700 -1.27062600
Ni 2.10153300 1.38488400 -0.00692100
O 1.10413900 3.17569300 0.41596300
O 3.75703800 1.60045100 1.34070900
Cl 4.43652900 0.28902700 0.92074800
O -1.06068200 3.24871700 -0.75235500
O 3.48126900 -0.20547000 -0.19648800
O 5.77597600 0.53496200 0.37289800
O 0.05898300 5.31965300 -0.07238800
O 4.44878100 -0.67528600 2.03327900
Cl 0.23639600 3.95888800 -0.59118100
O 0.96401900 3.97244400 -1.91507000
O 3.10190100 2.35913500 -1.52643600
H 3.28926300 1.76514600 -2.26459400
H 2.46282500 3.04194800 -1.83805900
C -2.55813400 0.31529800 0.56465100
H -2.77598300 1.35064700 0.28068100
H -2.74038000 0.23894200 1.63664000
H -8.47835800 1.07460400 1.61041900
Thermal Correction to Free Energy: 0.429336 Hartree
Entropy: 257.07 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.878023 Hartree
Thermal Free Energy with Correction: -3531.448687 Hartree

A2-4

C -2.23536900 -2.77953200 -1.84407500
C -3.74865900 -3.00983500 -2.06737500
C -4.35414400 -2.86954200 -0.64803500
H -1.63925300 -3.67236800 -2.05205700
H -1.86912300 -1.97090900 -2.48565200
H -4.15644400 -2.25542600 -2.74598300
H -3.95953600 -3.98963700 -2.50248500
H -5.35461700 -2.43628700 -0.64165300
H -4.38962400 -3.84304600 -0.15022500
C -1.04824600 -1.93564700 0.30806700
N -3.42051800 -2.01729500 0.10144400
N -2.15784500 -2.48385000 -0.39589600
H -1.27647500 -2.11083700 1.36183700
C 0.28270900 -2.59874300 0.00400600

C 0.92456200 -3.29599500 1.03744700
C 0.90672400 -2.56034300 -1.25147200
C 2.14701700 -3.93481900 0.83687400
H 0.45824700 -3.34973900 2.01739500
C 2.12731000 -3.19573500 -1.47113100
H 0.45001600 -2.03342900 -2.08147900
C 2.74015100 -3.87990500 -0.42246500
H 2.63278000 -4.46873200 1.64569900
H 2.60307200 -3.15446800 -2.44428800
Cl 4.27225500 -4.68634800 -0.69456500
C -7.37393800 0.86410500 1.42680000
C -6.60727500 -0.03905900 2.16737400
C -5.39423100 -0.50891800 1.66474600
C -4.93336500 -0.08747800 0.40851800
C -5.71124900 0.81373100 -0.32800700
C -6.92228100 1.29068200 0.17749900
H -6.95497800 -0.37757900 3.13941600
H -4.80292800 -1.21977100 2.23371200
H -5.36434500 1.14845300 -1.30272300
H -7.51180000 1.99184000 -0.40614900
C -3.59508800 -0.56045600 -0.13614100
H -3.55340300 -0.31555300 -1.20522700
C -1.00003100 -0.27467100 0.30115200
C -0.08519500 0.09024500 1.47068100
C -0.48033200 0.30312700 -1.00702300
O -0.59660200 -0.28684100 2.63797800
O -1.40462100 0.34220000 -1.95343500
C 0.21533900 -0.02628400 3.81180900
H -0.35632200 -0.43345400 4.64382500
H 1.18386300 -0.51930900 3.71480800
H 0.36489500 1.04833500 3.92716600
C -1.02394700 0.95525600 -3.21406200
H -0.22533800 0.37850000 -3.68429400
H -1.92914900 0.93154600 -3.81826500
H -0.69434000 1.97823800 -3.03383100
O 1.02590400 0.61341800 1.43724500
O 0.66910700 0.67190000 -1.25870000
Ni 2.10515200 1.47464500 -0.05900700
O 1.09625000 3.24690600 0.36150900
O 3.75722500 1.95009200 1.15164400
Cl 4.47288100 0.58431300 0.97664000
O -1.11005000 3.16361200 -0.72169300
O 5.78787100 0.78224300 0.35472100
O 4.54133500 -0.13028600 2.25696400

O -0.08894800 5.31512700 -0.13786800
O 3.50865700 -0.12475800 0.00390600
Cl 0.14690900 3.95487200 -0.63051900
O 0.83018200 3.97003900 -1.97583900
O 3.03079100 2.38177600 -1.66230700
H 2.38560300 3.07408500 -1.93571700
H 3.81482900 2.84154000 -1.32783600
C -2.46344000 0.19811100 0.59942200
H -2.54614900 1.26579200 0.38034700
H -2.63177600 0.06759400 1.66894000
H -8.31713500 1.23114800 1.82096300
Thermal Correction to Free Energy: 0.430311 Hartree
Entropy: 259.041 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.883724 Hartree
Thermal Free Energy with Correction: -3531.453413 Hartree

A2-TS5

C -3.25459400 3.00195400 0.62152100
C -4.44833400 3.07387100 1.58735000
C -4.90286900 1.60949200 1.68304800
H -3.58702400 3.01315900 -0.42082500
H -2.51703500 3.79062700 0.76806200
C -1.42836600 1.45278000 1.43272100
N -3.66189300 0.82080800 1.51860700
N -2.67221800 1.69898700 0.98258700
H -1.39398600 0.94010600 2.38894000
C -0.28611500 2.27554000 1.05443300
C 0.71899200 2.49979600 2.01412200
C -0.14542000 2.85929800 -0.21987100
C 1.80444100 3.31991700 1.73259500
H 0.63699100 2.03992200 2.99428900
C 0.94406600 3.66822200 -0.51591600
H -0.87808400 2.65360100 -0.99344800
C 1.90618900 3.90473500 0.46921800
H 2.57240200 3.49891200 2.47609800
H 1.06674800 4.09415200 -1.50442700
Cl 3.26732900 4.93429400 0.10884300
C -6.06973700 -0.56741200 -2.90502900
C -5.09410600 0.41721900 -2.73504300
C -4.33640900 0.46660200 -1.56411200
C -4.54311500 -0.45543700 -0.52831700
C -5.53504400 -1.43019000 -0.71241800
C -6.28382700 -1.49743800 -1.88870000
H -4.91703700 1.14791700 -3.51971800

H -3.55675000 1.21117500 -1.47276700
H -5.72509100 -2.15276400 0.07838500
H -7.03961400 -2.26909200 -2.00298000
C -3.78627800 -0.46586700 0.80680700
H -4.43953000 -1.03534300 1.47779500
C -1.06798600 -0.68088500 0.61691500
C -0.59480600 -0.46696700 -0.73735800
C -0.05124500 -0.97564800 1.61149400
O -1.58248100 -0.45186200 -1.64269300
O -0.55281400 -1.24401600 2.82998100
C -1.18466200 -0.35347800 -3.02643900
H -2.11734100 -0.37749700 -3.58849000
H -0.63943100 0.57487100 -3.20784100
H -0.54599000 -1.19747900 -3.29357500
C 0.38432500 -1.71360800 3.82073000
H 1.11478300 -0.93781700 4.06102100
H -0.22192100 -1.95140600 4.69436300
H 0.89729700 -2.60274700 3.45051900
O 0.57130800 -0.25745000 -1.12023400
O 1.18945600 -0.91012500 1.48652500
Ni 2.23590900 -0.99846900 -0.24940600
O 1.57308400 -2.92595600 -0.73769600
O 3.35982900 -0.56673200 -2.02793600
Cl 3.84461000 0.80801400 -1.54748800
O 0.02916300 -3.79770500 0.97187800
O 3.22143700 0.87583800 -0.12990200
O 5.30966900 0.85712200 -1.46158500
O 1.29878500 -5.32801900 -0.45884000
O 3.29346300 1.88247200 -2.39061600
Cl 1.31827100 -4.05979100 0.27996000
O 2.44207300 -4.03757100 1.28857900
O 3.87931800 -1.83885600 0.67705600
H 4.14127400 -1.32278600 1.45023700
H 3.55169300 -2.71384700 0.99368500
C -2.45117000 -1.30498000 0.82724700
H -2.42154700 -1.78663600 1.80287300
H -2.58536100 -2.10276300 0.09110200
H -4.11613500 3.44405600 2.56184200
H -5.24060300 3.72903200 1.21890700
H -5.62533800 1.37557700 0.89183400
H -5.36020400 1.37775600 2.64937400
H -6.65532400 -0.60712400 -3.81872100
Thermal Correction to Free Energy: 0.428552 Hartree
Entropy: 258.429 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.863559 Hartree

Thermal Free Energy with Correction: -3531.435007 Hartree

A2-6

C -4.43171000 1.55097900 -0.80843700

C -4.81401400 3.00663100 -0.52804600

C -3.51795500 3.78218100 -0.84302700

H -5.01159200 0.83354300 -0.22827900

H -4.55384500 1.32100300 -1.88021500

H -5.66105100 3.32958000 -1.13757800

H -5.08952200 3.13159500 0.52273700

H -3.60350700 4.39088700 -1.74949800

H -3.24575200 4.44737100 -0.01443000

C -2.30778100 0.36248000 -1.03524100

N -2.50910600 2.73273200 -1.08542200

N -3.00895100 1.50263600 -0.42212900

H -2.37936500 0.46949400 -2.12768900

C -2.94285500 -0.97761900 -0.66592400

C -3.01020800 -1.98986400 -1.63451600

C -3.51520500 -1.23314400 0.58984200

C -3.58914700 -3.22911200 -1.35856900

H -2.61665400 -1.80695600 -2.62879600

C -4.10927000 -2.46019800 0.87833200

H -3.50676800 -0.45712900 1.34371900

C -4.13288200 -3.45687800 -0.09702900

H -3.63114400 -4.00174100 -2.11828400

H -4.55194800 -2.64318700 1.85132600

Cl -4.87357500 -5.00673900 0.26364000

C -0.11737600 4.48175400 3.26623600

C -1.30306100 3.77050200 3.08203000

C -1.64877600 3.28091400 1.81825900

C -0.81656600 3.50872600 0.71388200

C 0.36727900 4.23747700 0.91162000

C 0.72193800 4.71101100 2.17346000

H -1.96638900 3.59303700 3.92446300

H -2.55508000 2.70242200 1.68712300

H 1.02131100 4.43765500 0.06550500

H 1.64737500 5.26470100 2.30125000

C -1.13420800 3.04896100 -0.71787100

H -0.86612100 3.89579900 -1.36397800

C -0.75130800 0.47053700 -0.75098300

C -0.28421500 0.28194400 0.70250100

C 0.01586000 -0.53743900 -1.63432500

O -1.22757300 0.19114400 1.60652500

O -0.43812400 -0.57277600 -2.87196400
C -0.79736500 0.03914600 2.99000000
H -1.71782800 -0.12684300 3.54698900
H -0.11569300 -0.80537400 3.08292000
H -0.30627200 0.95706700 3.31386500
C 0.30262800 -1.38064300 -3.82685300
H 0.28267600 -2.42745000 -3.51894400
H -0.22148000 -1.24249800 -4.77077200
H 1.32651600 -1.01262600 -3.88716700
O 0.90789100 0.26155400 1.01399200
O 0.97214500 -1.23330900 -1.29019100
Ni 2.41027600 -0.87467600 0.17177600
O 3.24498300 0.74438400 -0.80060100
O 3.51576500 -0.81048500 1.98284300
Cl 2.85773300 -2.06340000 2.58689600
O 2.29857400 1.07705300 -3.04723900
O 1.86709900 -2.45420800 1.45496900
O 3.83790500 -3.13162200 2.80116300
O 4.52189500 1.94303800 -2.48821700
O 2.10931700 -1.72586400 3.80878600
Cl 3.57014100 0.84327200 -2.31229100
O 4.16512600 -0.47080600 -2.74957300
O 3.77172400 -2.13630400 -0.69233700
H 3.40420000 -3.00056400 -0.91750000
H 4.06897800 -1.69293200 -1.52200200
C -0.25701000 1.88605000 -1.22584200
H -0.30681800 1.88772700 -2.31590000
H 0.78643700 2.01805800 -0.93781300
H 0.15035000 4.85668700 4.24968800
Thermal Correction to Free Energy: 0.432044 Hartree
Entropy: 255.378 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.87255 Hartree
Thermal Free Energy with Correction: -3531.440506 Hartree

A2-TS6

C 2.93447100 -0.05575400 2.26564800
C 4.34098500 0.56488200 2.41680100
C 4.62404800 1.28002700 1.05977900
H 2.96798400 -1.12075500 2.02059000
H 2.30020600 0.06989600 3.14293200
H 4.34840600 1.28887900 3.23456100
H 5.09244300 -0.19590200 2.63996400
H 4.84572400 2.33931100 1.22483400
H 5.46301600 0.83496700 0.52197000

C 1.11357600 1.06779500 0.94712600
N 3.39009100 1.15214900 0.25942400
N 2.39248100 0.73134400 1.15091600
H 0.44251100 0.51026600 1.59212200
C 0.63023900 2.41719800 0.59135200
C -0.68903400 2.72059400 0.98449800
C 1.40105100 3.42485500 -0.01739800
C -1.22263400 3.99115000 0.78547300
H -1.29917400 1.95711900 1.45737500
C 0.87642500 4.69865900 -0.21202200
H 2.41605700 3.20825300 -0.32415400
C -0.43343000 4.97351200 0.18715900
H -2.23569000 4.21674900 1.09885400
H 1.47546300 5.47533100 -0.67442000
Cl -1.09247800 6.57693400 -0.06924100
C 5.98536100 -2.99683500 -1.84147300
C 5.55276200 -2.13846500 -2.85360600
C 4.73751300 -1.05098500 -2.54544600
C 4.30555100 -0.79989200 -1.23194600
C 4.75650100 -1.66614800 -0.23031900
C 5.58868700 -2.74939100 -0.52847000
H 5.86013500 -2.30613600 -3.88180800
H 4.43189800 -0.37941900 -3.34509500
H 4.46236400 -1.51478700 0.79872800
H 5.92610600 -3.39922600 0.27447700
C 3.42670800 0.45282900 -1.04710400
H 3.91953800 1.19063700 -1.69270100
C 0.72551700 -0.06523600 -0.94707000
C -0.51945200 0.55545200 -1.39066600
C 0.58338800 -1.41295200 -0.42748500
O -0.37829500 1.49567700 -2.32893100
O 1.75713400 -2.03692000 -0.26672900
C -1.58937200 2.16246100 -2.76052700
H -1.27969800 2.79285000 -3.59313800
H -2.33714400 1.43155800 -3.07100800
H -1.99102400 2.76863500 -1.94674100
C 1.70944700 -3.36751500 0.28760800
H 1.27052300 -3.34204800 1.28745200
H 1.11934100 -4.02474200 -0.35413400
H 2.74706800 -3.69642400 0.31747700
O -1.65656400 0.33199000 -0.93449900
O -0.46092000 -2.02386500 -0.11431000
Ni -2.35110500 -1.31360900 -0.00574800
O -2.03973100 -0.45230200 1.90635100

O -4.33842200 -0.63642600 -0.39419500
Cl -4.42859400 -1.27930200 -1.78874600
O 0.04373300 -1.21430400 2.96846000
O -3.07229800 -2.02193300 -1.87389000
O -5.54113800 -2.23318400 -1.86049400
O -1.79354900 -0.33064400 4.32446100
O -4.50442800 -0.24548800 -2.83562200
Cl -1.43681500 -1.13944900 3.15249000
O -2.00121700 -2.52578700 3.25492300
O -3.06440800 -3.05472800 0.83511300
H -2.68941500 -3.82944200 0.39689700
H -2.76500700 -3.06239500 1.77233700
C 1.99609100 0.34344700 -1.70855200
H 1.78299900 1.33191800 -2.11311200
H 2.12685400 -0.31282300 -2.57530000
H 6.62996000 -3.83957800 -2.07222400
Thermal Correction to Free Energy: 0.429935 Hartree
Entropy: 256.427 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.855936 Hartree
Thermal Free Energy with Correction: -3531.426001 Hartree

A2-7

C 2.63863900 1.16207800 2.22858700
C 4.09002600 0.75576400 2.49346000
C 4.67794600 0.61017500 1.07301000
H 1.94353200 0.89191100 3.02709700
H 2.57004400 2.24552900 2.05022100
H 4.62476400 1.49550800 3.09340000
H 4.12764300 -0.20005200 3.02343000
H 5.28539100 1.47924000 0.79647400
H 5.30873600 -0.28211900 0.99376400
C 1.11486400 0.84447200 0.31100900
N 3.50846200 0.54140600 0.16745800
N 2.31374600 0.39014600 1.02260100
H 0.29149300 0.67064100 1.00558900
C 1.02778600 2.31522000 -0.12512900
C -0.14190100 3.02387400 0.19873500
C 2.04268100 3.00242700 -0.81582400
C -0.31078100 4.36011700 -0.16597200
H -0.93967300 2.52948200 0.74319400
C 1.89037200 4.34103700 -1.17733500
H 2.97110900 2.49441400 -1.03955900
C 0.70974900 5.00895400 -0.85670200
H -1.22080400 4.88947700 0.09382500

H 2.68297300 4.86139200 -1.70411500
Cl 0.51136800 6.69153500 -1.32565600
C 4.55173600 -4.59677400 0.12212200
C 4.82545100 -4.06266200 -1.13842300
C 4.48460300 -2.74040500 -1.42502900
C 3.84664900 -1.92944200 -0.47496900
C 3.57845000 -2.47730700 0.78847800
C 3.93274100 -3.79638700 1.08391300
H 5.31757800 -4.66938400 -1.89346200
H 4.72199400 -2.32981900 -2.40465300
H 3.07639900 -1.87065500 1.53287000
H 3.72443900 -4.19712400 2.07243700
C 3.51756900 -0.48311200 -0.87597600
H 4.32387900 -0.18481400 -1.55881200
C 0.92110900 -0.18872600 -0.87452900
C -0.30007300 0.30010000 -1.67491800
C 0.45663700 -1.53922800 -0.29437100
O -0.03432100 0.75429700 -2.87811900
O 0.95104000 -2.58187800 -0.92151100
C -1.16402300 1.27484900 -3.63765500
H -0.75859500 1.49610800 -4.62283400
H -1.95611100 0.52647000 -3.68438000
H -1.53387600 2.17981300 -3.15320500
C 0.48357800 -3.89401500 -0.51462100
H -0.59397900 -3.96126700 -0.67294400
H 1.02335400 -4.59007600 -1.15287800
H 0.73426500 -4.06164000 0.53329400
O -1.44160200 0.29697100 -1.21336800
O -0.37519200 -1.64746300 0.61111300
Ni -2.29739500 -0.83921600 0.33028100
O -2.26928100 0.79943200 1.54737800
O -4.18115000 -0.59451200 -0.59717200
Cl -4.00153000 -1.74970500 -1.60150600
O -0.78560200 0.10209700 3.38261400
O -2.62192800 -2.31020900 -1.16066300
O -5.04541900 -2.76331200 -1.43940700
O -2.20086500 2.10150100 3.59933900
O -3.91522600 -1.23490500 -2.97802700
Cl -2.09950000 0.72769800 3.09888800
O -3.21154500 -0.13389200 3.62757000
O -3.03222500 -2.09511900 1.78488100
H -2.32475700 -2.67495800 2.09987000
H -3.28423500 -1.52952500 2.55466300
C 2.21338900 -0.30089600 -1.71266800

H 2.31244800 0.63076500 -2.27129500
H 2.12465800 -1.10727300 -2.44237900
H 4.82655800 -5.62160100 0.35459500
Thermal Correction to Free Energy: 0.430293 Hartree
Entropy: 259.334 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.873682 Hartree
Thermal Free Energy with Correction: -3531.443389 Hartree

A2-TS8

C -2.50531000 -1.92054100 -2.58735700
C -4.02192100 -1.98314700 -2.76660000
C -4.49801000 -1.57116200 -1.37265500
H -2.13592900 -2.81515200 -2.07255500
H -1.94839600 -1.79419400 -3.51911800
H -4.34921200 -1.26253500 -3.52169200
H -4.37612900 -2.97698500 -3.04903600
H -5.52475200 -1.20105200 -1.35262900
H -4.43746500 -2.43296700 -0.69325200
C -1.19221600 -0.10462900 -1.44852000
N -3.57338500 -0.48305700 -0.97212700
N -2.37413900 -0.70904900 -1.77490700
H -0.38330700 -0.50728400 -2.05464800
C -1.13062800 1.39754500 -1.39532300
C 0.12434000 2.01877100 -1.51367200
C -2.27884300 2.20646900 -1.35193800
C 0.23789300 3.40773200 -1.54741900
H 1.02613500 1.42158200 -1.58764400
C -2.17555500 3.59509400 -1.39099500
H -3.25795300 1.74153900 -1.32008900
C -0.91546600 4.18740300 -1.47765200
H 1.21195000 3.87488800 -1.63941400
H -3.06567700 4.21399100 -1.36428300
Cl -0.78531700 5.93743900 -1.51837900
C -6.85076200 -0.91502300 2.81826800
C -5.91526800 -1.94846000 2.77675900
C -4.74111700 -1.80594500 2.03315100
C -4.48211400 -0.62621200 1.32366200
C -5.42898000 0.40786100 1.37865500
C -6.60387100 0.26662200 2.11518000
H -6.09529900 -2.86877300 3.32491700
H -4.02554300 -2.62222000 2.01824900
H -5.23684200 1.33143400 0.83897600
H -7.32243500 1.08053100 2.14709100
C -3.22745300 -0.41393500 0.48972600

H -2.91964000 0.61967400 0.66628000
C -0.67362100 -0.84103700 0.31879900
C -0.02898300 0.25950800 1.07204100
C 0.26723900 -1.95113200 0.01220700
O -0.86247400 0.93368200 1.85801200
O -0.33146600 -3.02070000 -0.51530500
C -0.31092700 2.08470100 2.55041800
H -1.11843700 2.43896400 3.18899400
H 0.56257900 1.79315100 3.13483900
H -0.02586900 2.84651400 1.82283500
C 0.53063700 -4.10484800 -0.93786900
H 1.03830800 -4.53823900 -0.07398400
H -0.13836600 -4.83409700 -1.39290100
H 1.26199300 -3.73698500 -1.65816100
O 1.15031800 0.62665800 0.96716600
O 1.49591600 -1.98343600 0.18522600
Ni 2.81044400 -0.47673900 0.55725200
O 2.90214900 0.05770000 -1.46698900
O 3.99171200 1.06638200 1.42920900
Cl 3.88490500 0.52396200 2.86465200
O 1.48312800 -1.39597000 -2.86360900
O 3.06864700 -0.77612600 2.63783700
O 5.20803600 0.20631100 3.41143400
O 3.40740500 -0.22944900 -3.83041900
O 3.12614000 1.45114700 3.72072200
Cl 2.88609000 -0.93481800 -2.65606600
O 3.74708000 -2.11374800 -2.29520300
O 4.45590700 -1.67907500 0.27500600
H 4.44649600 -2.44460900 0.86404100
H 4.39888200 -1.99775200 -0.65389800
C -2.04194000 -1.31514700 0.87490400
H -1.97910200 -1.35837500 1.96666600
H -2.22282300 -2.33353400 0.52753100
H -7.76220900 -1.02595400 3.39821400
Thermal Correction to Free Energy: 0.431142 Hartree
Entropy: 253.496 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.858959 Hartree
Thermal Free Energy with Correction: -3531.427817 Hartree

A2-10

C -2.56951300 -0.82504400 -3.08822300
C -4.08789300 -0.90371000 -3.23398400
C -4.50592700 -1.07040500 -1.77302000
H -2.14847200 -1.83155100 -2.95974900

H -2.06986600 -0.34722100 -3.93655400
H -4.48289700 0.02821500 -3.64867500
H -4.41521700 -1.73804300 -3.85887900
H -5.55035500 -0.81493800 -1.58300200
H -4.35634900 -2.11762200 -1.46799300
C -1.18846400 0.36320300 -1.32918000
N -3.62787400 -0.13482700 -1.03416100
N -2.44226300 0.03053900 -1.90927100
H -0.44169600 0.24164800 -2.11564000
C -1.11116700 1.82024200 -0.86575600
C 0.13504700 2.46195900 -0.81068100
C -2.26441700 2.56997500 -0.59127800
C 0.23783600 3.80530100 -0.44670600
H 1.04241000 1.92177600 -1.05877800
C -2.17429400 3.91243800 -0.22543100
H -3.23919700 2.10431300 -0.69201800
C -0.92099100 4.51856700 -0.14715800
H 1.20647200 4.29132500 -0.41151200
H -3.06955700 4.48758100 -0.01557900
Cl -0.80526300 6.21024600 0.31610300
C -6.74617500 -2.01031100 2.44451400
C -5.76137600 -2.91683200 2.05386100
C -4.62393700 -2.47161500 1.37525300
C -4.45123300 -1.11315500 1.08271200
C -5.44744400 -0.21049700 1.48562800
C -6.58594100 -0.65243500 2.15686900
H -5.87449000 -3.97398100 2.27658700
H -3.87082600 -3.19641200 1.08159100
H -5.32351800 0.84650700 1.26598900
H -7.34472300 0.06255000 2.46173700
C -3.24043500 -0.56539100 0.34247100
H -2.95487900 0.35030700 0.86700600
C -0.72156300 -0.74851800 -0.12532800
C -0.04541800 -0.00297600 1.01539900
C 0.25242300 -1.74953200 -0.74197200
O -0.87967300 0.36712200 1.96988700
O -0.31794500 -2.50769100 -1.66362600
C -0.32603800 1.18360400 3.04002300
H -1.14847000 1.31684500 3.74012800
H 0.51935700 0.67449600 3.50379200
H -0.00122100 2.14055500 2.62875200
C 0.54102500 -3.42761400 -2.38664900
H 0.93927400 -4.17792200 -1.70123900
H -0.10830500 -3.88900000 -3.12862500

H 1.35148800 -2.87326200 -2.85952100
O 1.14521100 0.31027600 1.07038600
O 1.44252100 -1.91900300 -0.46064500
Ni 2.81606300 -0.66522500 0.40812300
O 3.00898100 0.51877000 -1.28795700
O 3.98731900 0.44476400 1.79079300
Cl 3.78281500 -0.53774200 2.95745500
O 1.58054800 -0.31745400 -3.11120300
O 2.93203800 -1.64208000 2.27153400
O 5.05962300 -1.09016200 3.41811000
O 3.57075200 1.02616200 -3.60172800
O 3.00927300 0.08873700 4.04191600
Cl 2.99169200 -0.01081600 -2.74494200
O 3.80239000 -1.27882800 -2.78901100
O 4.42535100 -1.77846500 -0.21045800
H 4.37514400 -2.69977000 0.07550400
H 4.40724100 -1.75277600 -1.19425000
C -2.01627800 -1.48990100 0.34074100
H -1.85476200 -1.89815300 1.34184000
H -2.19124400 -2.33232200 -0.33045200
H -7.62938500 -2.35685900 2.97306500
Thermal Correction to Free Energy: 0.431059 Hartree
Entropy: 256.105 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.860183 Hartree
Thermal Free Energy with Correction: -3531.429124 Hartree

A2-TS7

C -2.00174400 -3.36785600 1.26523500
C -3.45891500 -3.78149200 1.48393400
C -4.20066100 -2.50611200 1.08973400
H -1.62305100 -2.81631400 2.13378900
H -1.33362000 -4.20753000 1.05932000
H -3.72824600 -4.60470300 0.81598000
H -3.65629900 -4.08390100 2.51438200
H -5.25050300 -2.67239600 0.84533000
H -4.15085000 -1.77205300 1.90961100
C -1.11855300 -1.85643100 -0.58410600
N -3.48439800 -2.05735200 -0.12050900
N -2.10548800 -2.51174100 0.08229500
H -1.46922800 -1.54196000 -1.56471400
C 0.25163500 -2.44463300 -0.66522800
C 0.81175100 -2.59392000 -1.94406200
C 1.01274400 -2.84560300 0.44411700
C 2.07636500 -3.14811700 -2.12047400

H 0.24597500 -2.28553700 -2.81877600
C 2.28323100 -3.39169400 0.28363200
H 0.63136400 -2.71808500 1.45023700
C 2.80400100 -3.54705400 -1.00051700
H 2.49569300 -3.26570600 -3.11318000
H 2.87482600 -3.67302700 1.14635700
Cl 4.39425000 -4.24529700 -1.20913200
C -7.70688200 0.62006500 -0.19620100
C -6.80966700 1.08942100 0.76207500
C -5.46461000 0.71232700 0.71393500
C -4.99801200 -0.13394300 -0.29844300
C -5.90957300 -0.59622600 -1.26061900
C -7.25210100 -0.22712800 -1.21023000
H -7.15185500 1.75354900 1.55043000
H -4.78451800 1.09491200 1.46789800
H -5.55663500 -1.25509400 -2.04961600
H -7.94187800 -0.59339200 -1.96524400
C -3.54672500 -0.58540500 -0.40978400
H -3.28898900 -0.47861000 -1.46644500
C -1.05077900 0.00121100 0.09746800
C -0.16237300 0.00042300 1.27637700
C -0.51370000 0.73081000 -1.06845300
O -0.75928900 -0.43314200 2.39949500
O -1.44285100 0.94347800 -2.00287300
C 0.05301900 -0.41113500 3.59692600
H -0.60364000 -0.76445500 4.39096700
H 0.92073500 -1.06396700 3.48464300
H 0.39659100 0.60479700 3.79831600
C -1.04771000 1.73803900 -3.14511100
H -0.28290300 1.21568300 -3.72383700
H -1.95738700 1.85977800 -3.73139500
H -0.66851400 2.70279400 -2.80588400
O 1.04061500 0.28388400 1.32070100
O 0.66543200 1.04656700 -1.29923800
Ni 2.13094100 1.44538800 0.06295300
O 1.19956300 3.12137000 0.88588100
O 3.78939200 1.34834900 1.39879200
Cl 4.43425300 0.12726000 0.72113000
O -1.03333800 3.38387500 -0.11270100
O 3.46249100 -0.10563800 -0.46486500
O 5.77853500 0.44207200 0.22498600
O 0.12707400 5.30723400 0.86553500
O 4.42023800 -1.03556200 1.62354700
Cl 0.27175400 4.06799400 0.09445000

O 0.91869200 4.33002100 -1.24427200

O 3.10122200 2.70160800 -1.25351600

H 3.27364400 2.26543000 -2.09810800

H 2.44984600 3.42346100 -1.41127900

C -2.55162400 0.25500900 0.40662300

H -2.75679700 1.31508000 0.23200100

H -2.71091500 0.07291800 1.46987000

H -8.75128900 0.91559200 -0.15819600

Thermal Correction to Free Energy: 0.428739 Hartree

Entropy: 258.203 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3531.861154 Hartree

Thermal Free Energy with Correction: -3531.432415 Hartree

A2-8

C -1.93885900 -3.28060500 1.32315700

C -3.37635700 -3.74258300 1.56559600

C -4.16332800 -2.51291000 1.11865900

H -1.60007100 -2.65271600 2.15815300

H -1.23635400 -4.10950900 1.20339700

H -3.61320000 -4.60267700 0.93252300

H -3.56421400 -4.00817200 2.60844700

H -5.20969800 -2.72472700 0.89079600

H -4.13882500 -1.74868800 1.91256200

C -1.07396200 -1.74106800 -0.53265500

N -3.47048200 -2.08531600 -0.11288400

N -2.06978600 -2.55927800 0.05562000

H -1.41481800 -1.54609700 -1.55215100

C 0.28744500 -2.40214300 -0.64716800

C 0.76609700 -2.70368100 -1.92996000

C 1.08759700 -2.74470000 0.45186500

C 1.99757800 -3.32712500 -2.11976300

H 0.16264100 -2.45949300 -2.80009200

C 2.32497000 -3.36244200 0.28136400

H 0.75740400 -2.53494700 1.46276800

C 2.77046700 -3.65232400 -1.00690500

H 2.35373600 -3.55791800 -3.11741500

H 2.94444200 -3.60035600 1.13777300

Cl 4.32146000 -4.43643400 -1.23115800

C -7.68411500 0.62986800 -0.15588900

C -6.76426500 1.12878000 0.76498200

C -5.42368300 0.73668500 0.70628300

C -4.98430800 -0.15423000 -0.27921800

C -5.91889300 -0.64691200 -1.20378800

C -7.25654600 -0.26298400 -1.14249000

H -7.08509600 1.82705400 1.53263800
H -4.72663000 1.14196500 1.43267200
H -5.58651800 -1.34364400 -1.96858700
H -7.96459900 -0.65441400 -1.86746300
C -3.54003800 -0.62236900 -0.40625300
H -3.29361500 -0.51547300 -1.46618400
C -1.03674100 -0.15311400 0.06697200
C -0.14745600 -0.01669300 1.29005300
C -0.49912900 0.66646400 -1.09465500
O -0.73652400 -0.41617700 2.41600500
O -1.42629400 0.87498700 -2.01664900
C 0.04855900 -0.29354700 3.62970500
H -0.59692100 -0.67133800 4.42066900
H 0.96380100 -0.88252100 3.55021600
H 0.30713000 0.75281600 3.79855600
C -1.04912700 1.68305000 -3.16007300
H -0.27802100 1.17132900 -3.73944500
H -1.96365000 1.78818900 -3.74100500
H -0.68537400 2.65162400 -2.81587200
O 1.01689900 0.37484900 1.33037100
O 0.66472900 1.02825000 -1.29170900
Ni 2.14275200 1.49855300 0.05021500
O 1.21298900 3.18863000 0.81952300
O 3.77496800 1.45765700 1.39987600
Cl 4.43357700 0.21288400 0.77388400
O -1.05248700 3.29850400 -0.13027700
O 3.47164800 -0.06004500 -0.41361700
O 5.78078100 0.51511200 0.28122200
O 0.04201000 5.32135400 0.71628100
O 4.40890600 -0.91518900 1.71713800
Cl 0.22439900 4.05250400 0.00612400
O 0.82822300 4.26858300 -1.36011000
O 3.08663900 2.72001900 -1.31147300
H 3.29539400 2.26176500 -2.13606400
H 2.42107300 3.41777300 -1.50748600
C -2.52681700 0.20333300 0.39846300
H -2.67730900 1.27026300 0.21977400
H -2.68571300 0.02918200 1.46264500
H -8.72500900 0.93641900 -0.10976800
Thermal Correction to Free Energy: 0.427904 Hartree
Entropy: 262.357 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3531.873921 Hartree
Thermal Free Energy with Correction: -3531.446017 Hartree

A2-9

C 0.25910400 -2.80897100 -0.14644200
C -0.92312000 -3.67763500 -0.61870600
C -2.08850700 -2.67256400 -0.71252300
H 0.42575500 -2.94438400 0.93448300
H 1.19043700 -3.02507500 -0.66950600
H -0.72706700 -4.13610900 -1.59094100
H -1.12582000 -4.47999400 0.09487900
C 0.52905300 -0.40966800 0.33288300
N -1.59164700 -1.49578500 0.01773700
N -0.18134800 -1.43312600 -0.44431900
H 0.28825000 -0.54658100 1.40020600
C 2.04536000 -0.52072100 0.21631300
C 2.81309000 -0.36561000 1.37843000
C 2.71167800 -0.80488600 -0.98446400
C 4.20458000 -0.46489000 1.35412200
H 2.31688200 -0.16715600 2.32397900
C 4.09960500 -0.92072100 -1.02381300
H 2.13793200 -0.91947100 -1.89371800
C 4.83669000 -0.74391900 0.14626100
H 4.78654600 -0.34079200 2.26046700
H 4.60667300 -1.14130700 -1.95651400
Cl 6.59120300 -0.88566100 0.09764200
C -6.43298900 -0.36045000 0.95976600
C -5.42640400 -0.83918700 1.80163400
C -4.09552500 -0.82016800 1.38641000
C -3.75153200 -0.32920000 0.11887600
C -4.76735700 0.14317300 -0.71916300
C -6.09968600 0.13161900 -0.30224700
H -5.67890200 -1.22800800 2.78415700
H -3.31052000 -1.20206200 2.03173500
H -4.51291200 0.52214600 -1.70586600
H -6.87594100 0.50149600 -0.96600100
C -2.29805500 -0.25683600 -0.32224000
H -2.27217200 -0.08940700 -1.41444600
C -0.09375100 0.99282900 -0.02295500
C 0.61628700 2.09749800 0.77232200
C 0.04912500 1.39268600 -1.50717300
O 0.46083100 1.93006700 2.10379700
O -0.81499900 2.38828800 -1.80447600
C 1.11684100 2.91596000 2.92395800
H 0.88020700 2.64456400 3.95227100
H 2.19581200 2.89347100 2.75548900
H 0.74206200 3.91521900 2.69245700

C -0.68590800 2.93493000 -3.12759500
H -0.85008200 2.16209000 -3.88207100
H -1.44724300 3.71124100 -3.19914800
H 0.31083600 3.36030100 -3.26429700
O 1.24498700 3.00939200 0.28431700
O 0.81519000 0.93031100 -2.31840900
C -1.59101200 0.91965800 0.37472000
H -2.09731700 1.85205900 0.12110700
H -1.65638400 0.78075000 1.45643800
H -7.46935800 -0.37443900 1.28443200
H -3.01136100 -3.02644300 -0.24981900
H -2.29925700 -2.42551500 -1.76568100
Thermal Correction to Free Energy: 0.38797 Hartree
Entropy: 187.372 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1762.607914 Hartree
Thermal Free Energy with Correction: -1762.219944 Hartree

A2-10

C 0.08596600 -2.46647700 1.59436000
C -0.87674500 -3.55367100 1.11039300
C -1.10427100 -3.17947100 -0.36992300
H 0.02369600 -2.27432600 2.66927000
H 1.12509900 -2.73111300 1.34248900
H -0.46771600 -4.55947400 1.23182800
H -1.81711300 -3.49769100 1.66519900
H -0.53541600 -3.82853300 -1.04476200
H -2.16387600 -3.25888700 -0.63766200
C 0.50188800 -0.12461400 0.87955800
N -0.60254500 -1.79209900 -0.51325400
N -0.38566000 -1.29313600 0.86275800
H 0.50111100 0.20826300 1.92078100
C 1.96574900 -0.33019700 0.47585400
C 2.95916300 0.21771800 1.30229000
C 2.37798000 -1.04404300 -0.66184400
C 4.31535500 0.07868900 1.00963900
H 2.66761300 0.77715800 2.18637800
C 3.73128300 -1.20324000 -0.96207700
H 1.62850400 -1.49859800 -1.29756800
C 4.68982200 -0.63531900 -0.12605600
H 5.06990100 0.51192200 1.65670100
H 4.03857700 -1.76205000 -1.83930000
Cl 6.39920300 -0.82519100 -0.50797800
C -5.71878600 -0.59930600 -0.35691100
C -5.24278600 -0.51540200 -1.66610100

C -3.87456300 -0.61168800 -1.91694600
C -2.94873100 -0.77574000 -0.87481400
C -3.44064100 -0.86069400 0.43734700
C -4.81272800 -0.77624400 0.68918200
H -5.93587100 -0.38637900 -2.49276700
H -3.51706400 -0.55973100 -2.94344400
H -2.74288200 -0.97873600 1.25676600
H -5.17096400 -0.84896400 1.71249500
C -1.46217700 -0.85964800 -1.25117600
H -1.44413200 -1.22440500 -2.28630100
C -0.23517500 1.01262700 0.08532000
C 0.72353900 2.21483300 -0.03143400
C -1.38679800 1.55613200 0.96627200
O 1.16742300 2.42958700 -1.28024400
O -2.15228900 2.40797500 0.25489500
C 2.11059000 3.50950300 -1.41868600
H 2.35336700 3.54961600 -2.47988000
H 1.66488400 4.44957200 -1.08659900
H 3.00485200 3.30821300 -0.82516600
C -3.24332000 3.00614900 0.97809900
H -2.87304500 3.53162200 1.86092400
H -3.70992800 3.70126400 0.28077500
H -3.95437100 2.23605600 1.28515200
O 1.05297300 2.88661900 0.92342000
O -1.56497000 1.31115500 2.13606700
C -0.72374900 0.50264200 -1.28947400
H 0.15704900 0.37813200 -1.92225000
H -1.35744700 1.25691900 -1.75865300
H -6.78414200 -0.53286100 -0.15564500
Thermal Correction to Free Energy: 0.389837 Hartree
Entropy: 184.078 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1762.604551 Hartree
Thermal Free Energy with Correction: -1762.214714 Hartree

A2-11

C -1.06837400 1.60316800 2.57830300
C -2.16925000 0.81857900 3.28394200
C -2.61450200 -0.12823200 2.16708900
H -1.51016800 2.37854700 1.92631100
H -0.37106600 2.09518000 3.26383200
H -1.74995300 0.26257100 4.12745700
H -2.98623900 1.44765700 3.64597500
H -3.09186200 -1.03830800 2.53856800
H -3.34168400 0.38565600 1.52327000

C 0.61516800 0.94344000 0.87773600
N -1.37369200 -0.48127800 1.43034700
N -0.36598800 0.53485100 1.86428900
H 1.11412900 1.80372400 1.32497200
C 1.71387800 -0.10596700 0.69605500
C 2.96216100 0.28617200 0.19068400
C 1.55080300 -1.43233300 1.11412400
C 4.00991800 -0.62548100 0.06277400
H 3.12553600 1.31744400 -0.10665700
C 2.58976500 -2.35563200 0.99182300
H 0.60440300 -1.73705000 1.54851000
C 3.81004100 -1.94583100 0.46037700
H 4.97271000 -0.31124200 -0.32477900
H 2.45557100 -3.38198700 1.31525000
Cl 5.12556200 -3.10752500 0.30455200
C -4.95183800 -2.98886400 -1.05777800
C -4.97635900 -1.62906100 -1.36221800
C -3.88515700 -0.81578400 -1.04435200
C -2.75123200 -1.35069700 -0.42238400
C -2.73839600 -2.72196600 -0.12308800
C -3.82645600 -3.53396400 -0.43431700
H -5.84504500 -1.19494900 -1.84896000
H -3.92580500 0.24018400 -1.29175800
H -1.86443200 -3.14678900 0.36238500
H -3.79537100 -4.59328100 -0.19557600
C -1.53115500 -0.51912500 -0.05555800
H -0.66562600 -1.07419700 -0.43170900
C -0.06491000 1.51273300 -0.47536100
C 0.82852500 1.26382800 -1.70214100
C -0.21443000 3.04657000 -0.42111900
O 0.64179000 0.03536300 -2.21670900
O 0.82865000 3.65220800 0.17585400
C 1.49195600 -0.30937200 -3.32715500
H 1.16883300 -1.30029600 -3.64338600
H 1.37611200 0.41459800 -4.13608500
H 2.53584100 -0.32976400 -3.00674000
C 0.81234800 5.09022700 0.13497500
H -0.08838500 5.47793400 0.61597700
H 1.70520100 5.40853700 0.67192600
H 0.84258900 5.43597500 -0.90049800
O 1.61106100 2.06877800 -2.16290600
O -1.15777100 3.64913700 -0.88621300
C -1.47284400 0.88003100 -0.67203400
H -1.71023000 0.83952900 -1.73685100

H -2.22003500 1.53542200 -0.21770400

H -5.79962000 -3.62070100 -1.30602900

Thermal Correction to Free Energy: 0.388979 Hartree

Entropy: 184.755 cal/mol-kelvin

Single Point Energy with Solvent Effect: -1762.589758 Hartree

Thermal Free Energy with Correction: -1762.200779 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Path-B:

B-TS1

C -2.23927600 -4.79312400 -1.68684300

C -1.93970800 -4.75267000 -0.32165600

C -1.78759200 -3.53094000 0.32740200

C -1.93936500 -2.32168000 -0.38331500

C -2.24939700 -2.38122500 -1.75762400

C -2.39187300 -3.60410400 -2.40506800

H -1.81341600 -5.67726900 0.23342000

H -1.52223900 -3.51058100 1.37706000

H -2.35956900 -1.45614200 -2.31446700

H -2.61436100 -3.63276300 -3.46711800

C -1.84934900 -1.01319100 0.25351800

H -1.96617200 -0.16147900 -0.40630900

C 0.24587600 -0.50300000 0.85596500

C 1.24256200 -1.53089200 0.91455800

C 0.56625100 0.76921600 0.27943800

O 0.83698200 -2.66544100 1.52872400

O -0.43586900 1.66934800 0.36102400

C 1.83406400 -3.70122900 1.64135100

H 1.32535000 -4.53692600 2.12271400

H 2.20674100 -3.98692100 0.65602900

H 2.67169800 -3.35781300 2.25164300

C -0.10239000 3.01836200 -0.02244600

H 0.12382900 3.07085000 -1.09014000

H -0.99244000 3.60426200 0.20384000

H 0.75452500 3.36821100 0.55506100

O 2.41157100 -1.47869600 0.48858000

O 1.63079900 1.11055600 -0.28076100

Ni 3.40532800 0.14622800 -0.16983400

O 3.79595100 0.71844600 1.80973400

O 5.12903800 -1.08534400 -0.54110400
Cl 4.74797000 -1.40796500 -1.99267600
O 1.87502100 1.98524600 2.69578700
O 3.45511400 -0.57477000 -2.16879700
O 5.78194300 -0.94367600 -2.92841800
O 4.10314400 2.24859200 3.67593300
O 4.45297900 -2.84169600 -2.14936700
Cl 3.33622600 2.04998800 2.43793800
O 3.62513800 3.15168400 1.44474800
O 4.39324500 1.85272200 -0.80319000
H 3.94896200 2.20178000 -1.58688200
H 4.23175700 2.48945600 -0.06678200
C -1.10932900 -0.70023400 1.50454100
H -1.46795700 0.21799700 1.97165100
H -1.08802800 -1.51032400 2.23147100
C -5.68524800 -1.57107700 2.55307200
C -6.68699400 -1.80066800 1.38715800
C -5.98851200 -1.94439300 0.02683200
C -4.21847000 -1.54635400 2.09429800
C -4.85484300 0.27950900 0.43840300
H -6.70266800 -1.82526800 -0.79337100
H -3.85922500 -2.56404300 1.90904700
H -5.54448300 -2.93918500 -0.08444400
H -3.57842800 -1.11108300 2.86629300
H -5.63112100 0.49026400 1.17228300
N -3.93563700 -0.80169900 0.84332600
N -4.89359800 -0.99161400 -0.24977600
C -4.37848200 1.49062300 -0.29187300
C -4.34861400 2.72382100 0.37133100
C -4.01363800 1.43205700 -1.64229800
C -3.95088200 3.88177700 -0.29364300
H -4.64267100 2.78706200 1.41588500
C -3.61530800 2.58259800 -2.32051400
H -4.06456600 0.48136000 -2.16212000
C -3.58616000 3.80011100 -1.63895600
H -3.93081500 4.83706300 0.21879300
H -3.33823900 2.54091900 -3.36796200
Cl -3.09138000 5.25116800 -2.48645800
H -5.77585800 -2.36016200 3.30589100
H -5.92224000 -0.63690700 3.07271100
H -7.40163000 -0.97236500 1.34334200
H -7.28379400 -2.70165500 1.55893000
H -2.34573000 -5.74929600 -2.19056100
Thermal Correction to Free Energy: 0.449418 Hartree

Entropy: 274.216 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.152278 Hartree

Thermal Free Energy with Correction: -3570.70286 Hartree

B-2

C -2.55163100 -5.00215600 -2.19407300

C -1.76359300 -4.85874400 -1.05136400

C -1.69037600 -3.63014200 -0.39125500

C -2.41004300 -2.52640600 -0.87264000

C -3.18621500 -2.67610500 -2.03365800

C -3.26230100 -3.90578800 -2.68701500

H -1.19036600 -5.70155500 -0.67679200

H -1.04412700 -3.52683600 0.47403800

H -3.72320300 -1.81920000 -2.42984400

H -3.86124200 -4.00335400 -3.58780500

C -2.37806600 -1.17533400 -0.18593200

H -2.45403800 -0.38809100 -0.93434500

C 0.18535800 -0.87170400 0.15512400

C 1.19716900 -1.64651300 0.77830500

C 0.55512400 0.07863400 -0.82673300

O 0.74055200 -2.58299800 1.66529700

O -0.49453100 0.73176200 -1.39488000

C 1.75639500 -3.31508100 2.37368300

H 1.21397500 -3.97874000 3.04903600

H 2.37473300 -3.89186400 1.68273100

H 2.40036400 -2.63692000 2.93739300

C -0.15145200 1.81248100 -2.27758800

H 0.43051100 1.44971800 -3.12803700

H -1.10376600 2.22011800 -2.61684900

H 0.42033200 2.57353100 -1.74208000

O 2.43772000 -1.57894200 0.61251000

O 1.70892000 0.37173500 -1.23633400

Ni 3.34333000 0.05630000 -0.10533100

O 2.58449300 1.17943900 1.56330400

O 5.21410100 -0.56248500 0.74560000

Cl 5.70680500 -1.27875800 -0.52113400

O 0.36646800 2.23829300 1.38331400

O 4.53575700 -1.02721800 -1.49867000

O 6.93857800 -0.65838600 -1.03231600

O 2.09531100 3.21267100 2.81117600

O 5.86822900 -2.72050200 -0.27528500

Cl 1.82337700 2.50984200 1.54649500

O 2.30658200 3.32057800 0.36782800

O 4.20609300 1.79739200 -0.84200200

H 4.09986600 1.78846700 -1.80244000

H 3.62477500 2.51070000 -0.49166300

C -1.20164300 -0.84563600 0.75421100

H -1.38979600 0.15755900 1.15606200

H -1.19157900 -1.53178000 1.60116200

C -5.15351900 -1.81600000 2.56647600

C -6.41295400 -1.53297400 1.70364500

C -6.08402300 -1.44558900 0.20884700

C -3.87098700 -2.00260500 1.75023000

C -4.34916500 0.33791900 0.74691900

H -6.89849600 -0.97670800 -0.35080200

H -3.84709000 -2.97543200 1.25463400

H -5.92692000 -2.43537700 -0.23060900

H -2.99195400 -1.93200800 2.38975000

H -4.80479800 0.45237100 1.72829600

N -3.67639600 -1.00498500 0.64235500

N -4.87857800 -0.66641700 -0.14111600

C -3.78783700 1.59199700 0.17350100

C -2.95552100 2.40817500 0.95189500

C -4.15856400 2.00526300 -1.11243400

C -2.47725400 3.61430900 0.44896800

H -2.64853600 2.10024300 1.94687200

C -3.71691100 3.22853300 -1.61035600

H -4.79882900 1.37262100 -1.71789700

C -2.87700300 4.02193900 -0.82517600

H -1.79024900 4.21550600 1.03162700

H -4.01388200 3.56397100 -2.59769200

Cl -2.31092800 5.55041000 -1.45696500

H -5.27820000 -2.73548200 3.14582000

H -5.01088300 -1.02111600 3.30519500

H -6.88442700 -0.60037000 2.02931600

H -7.16460300 -2.31529100 1.84201800

H -2.59944400 -5.95820700 -2.70706300

Thermal Correction to Free Energy: 0.455534 Hartree

Entropy: 267.653 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.183501 Hartree

Thermal Free Energy with Correction: -3570.727967 Hartree

B-TS5

C -1.57937800 -2.10340000 0.21081400

C -1.92999200 -1.15511300 1.37517800

C -1.93788800 -0.18254500 -1.37749200

C -1.00891400 -1.33360200 -0.98539400

H -2.57987100 -1.62053700 2.12254900

H -1.01746300 -0.84859000 1.88907300
H -0.89759300 -2.00247500 -1.84460200
H -0.01519100 -0.95367000 -0.74701000
C -3.87693900 0.36858100 0.56661400
C -0.26545900 2.07663000 0.84931800
C -1.46661200 2.05732200 -0.13016700
H -4.13743500 1.41900400 0.65881900
H -0.61551100 1.85513500 1.85764300
H 0.05403000 3.12716800 0.85528000
H -1.08130600 2.22071000 -1.13734300
N -2.58888400 0.11057600 0.98372800
N -2.18085600 0.73874000 -0.23631300
C -2.47502800 3.16923600 0.15760500
C -3.06828000 3.85117000 -0.91470100
C -2.84265600 3.52617600 1.46352500
C -4.00650900 4.86003600 -0.69364900
H -2.78243100 3.59711200 -1.93259800
C -3.78428500 4.53375100 1.68708200
H -2.39188200 3.02149600 2.31161100
C -4.36887300 5.20299800 0.61072400
H -4.44498600 5.38428500 -1.53787900
H -4.05352200 4.80030600 2.70500700
H -5.09366300 5.99228300 0.78699100
C -4.97474600 -0.48856100 0.17788300
C -6.10031600 0.17205300 -0.37089800
C -5.03345000 -1.89064500 0.34475000
C -7.22599400 -0.53243300 -0.76844900
H -6.07426400 1.25124300 -0.49261000
C -6.16393200 -2.60122700 -0.03223200
H -4.20957500 -2.42691500 0.79388000
C -7.25051300 -1.92101500 -0.59573700
H -8.07978500 -0.02295200 -1.19990000
H -6.21253800 -3.67491000 0.10827400
Cl -8.66060600 -2.81683000 -1.07797500
C 0.89901000 1.16704500 0.52888500
C 1.62123400 1.32732500 -0.68342600
O 2.55230100 0.61980900 -1.14810200
O 1.20418900 2.37917400 -1.43977700
C 1.42066900 0.29519800 1.52058000
O 2.42368100 -0.45299700 1.45166300
C 2.02082400 2.69508600 -2.58313100
H 1.96811900 1.90076800 -3.33283200
H 1.60484900 3.62036400 -2.98398500
H 3.05937600 2.83564400 -2.27882400

O 0.73560200 0.29062600 2.70298800
C 1.29658400 -0.53553600 3.74182800
H 0.61162900 -0.43612000 4.58512300
H 1.36902300 -1.57530600 3.41576400
H 2.29260200 -0.18196800 4.01665900
Ni 3.48182100 -0.86868700 -0.17889100
O 5.09825700 0.23076800 0.51593000
O 3.81844500 -2.88961100 0.74994400
Cl 2.55205400 -3.48873900 0.16226500
O 4.78914900 2.57894600 -0.18696900
O 2.04842300 -2.37009300 -0.78007700
O 2.83500900 -4.70796200 -0.60967600
O 7.01421400 1.71823700 0.36442700
O 1.53534000 -3.73061000 1.21476800
Cl 5.71286300 1.42283900 -0.25250700
O 5.89061200 0.98995700 -1.69102600
O 4.60914100 -1.36278300 -1.84109900
H 4.03337900 -1.38246900 -2.61642600
H 5.19823500 -0.57319800 -1.93887400
H -0.83711400 -2.81999400 0.57557300
H -2.45383800 -2.67776800 -0.11453700
H -2.90017500 -0.57065100 -1.73156000
H -1.51545300 0.42758300 -2.17752400
Thermal Correction to Free Energy: 0.453697 Hartree
Entropy: 267.663 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.158272 Hartree
Thermal Free Energy with Correction: -3570.704575 Hartree

B-TS2

C -0.67949000 -1.79647700 -3.05917100
C -0.92510700 -1.83506000 -1.55240400
C -1.53982700 0.56341700 -3.11032500
C -0.36401000 -0.35282300 -3.46980400
H -1.33266600 -2.79102400 -1.21378800
H 0.01071500 -1.65727600 -1.02523200
H -0.19075800 -0.27760500 -4.54832800
H 0.54894300 -0.02249400 -2.96348400
C -3.26843900 -0.82954500 -1.28837300
C -1.13494900 1.43648000 0.57637300
C -1.76972500 1.71171600 -0.80415400
H -3.68278300 -0.74410500 -2.29506800
H -1.76753800 0.77812100 1.16901900
H -1.13719200 2.41124200 1.07859900
H -1.04408600 2.31607000 -1.35364700

N -1.89432000 -0.80684900 -1.10595800
N -1.90545000 0.47582900 -1.67588400
C -3.07509100 2.49818800 -0.77534700
C -3.33296300 3.43850200 -1.78326300
C -4.03063900 2.32971700 0.23699500
C -4.51988900 4.17178600 -1.79949100
H -2.58919400 3.61462900 -2.55681400
C -5.21670300 3.06532600 0.22708800
H -3.84728200 1.63470300 1.04890200
C -5.46835400 3.98409000 -0.79333200
H -4.69597500 4.89720500 -2.58837300
H -5.94065900 2.92679300 1.02495000
H -6.38971400 4.55893800 -0.79624000
C -4.18508200 -1.09844000 -0.21889900
C -5.57053500 -1.13934700 -0.49337200
C -3.72523800 -1.38731600 1.08683100
C -6.47648500 -1.47971500 0.49871600
H -5.92783100 -0.90833700 -1.49288700
C -4.62837800 -1.73069200 2.08168400
H -2.66154000 -1.32662400 1.29894400
C -5.99687100 -1.77439700 1.78197300
H -7.54046000 -1.51855900 0.29586000
H -4.28919400 -1.95707400 3.08611800
Cl -7.12970300 -2.19506700 3.03503100
C 0.26486000 0.86811500 0.50594600
C 1.31093300 1.66227700 -0.03543600
O 2.50387200 1.34723200 -0.27969000
O 0.93469400 2.93636300 -0.33250700
C 0.58992200 -0.37448100 1.10279000
O 1.69243300 -0.97465500 1.09618200
C 1.99478700 3.83689100 -0.70130800
H 2.43458700 3.55231200 -1.66125400
H 1.52326800 4.81731600 -0.77844200
H 2.77345300 3.83918500 0.06367400
O -0.43010900 -0.98962000 1.77756600
C -0.06640600 -2.20516100 2.45897800
H -0.98650000 -2.55971900 2.92737900
H 0.32099700 -2.94802100 1.75851500
H 0.69290200 -2.00946300 3.21886900
Ni 3.32720700 -0.43545000 0.08946000
O 4.31955900 0.01926000 1.84645100
O 3.78838500 -2.61522100 -0.16332300
Cl 3.03587500 -2.74347500 -1.47655000
O 3.78295500 2.37467900 2.36376100

O 2.55312200 -1.29492700 -1.73898900
O 3.91420400 -3.18789400 -2.56848000
O 5.74737000 1.29068200 3.34657700
O 1.85202900 -3.62403200 -1.33153000
Cl 4.89637200 1.42195000 2.15523100
O 5.71752000 1.84212100 0.95682800
O 5.03711100 0.08869000 -0.95743300
H 4.77022300 0.58422200 -1.74268700
H 5.46688300 0.73979200 -0.34764200
H 0.15798100 -2.46064200 -3.28457000
H -1.55580900 -2.16540400 -3.61051300
H -2.41854200 0.27730600 -3.70593500
H -1.33197100 1.61060200 -3.33048900
Thermal Correction to Free Energy: 0.452505 Hartree
Entropy: 269.055 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.164673 Hartree
Thermal Free Energy with Correction: -3570.712168 Hartree

B-TS8

C -2.10857200 -5.35831200 -2.18285500
C -1.31318600 -5.10503900 -1.06520000
C -1.36685800 -3.86543800 -0.42243500
C -2.21883100 -2.86094900 -0.89981900
C -3.01067000 -3.12318500 -2.02930300
C -2.95997100 -4.36152100 -2.66677700
H -0.63869900 -5.87080900 -0.69346900
H -0.72631900 -3.67862500 0.43275000
H -3.66076100 -2.34253100 -2.41867900
H -3.57254800 -4.54507400 -3.54486100
C -2.33798600 -1.49938700 -0.22992300
H -2.45833200 -0.74470700 -1.00635700
C 0.21520900 -0.99533500 0.16749900
C 1.26767100 -1.64072100 0.87199300
C 0.54373800 -0.09095800 -0.87253000
O 0.85852600 -2.56569100 1.78820000
O -0.53362900 0.44016800 -1.51285300
C 1.90187100 -3.17210600 2.57109700
H 1.39012300 -3.85430000 3.25155600
H 2.60114300 -3.71713400 1.93356100
H 2.45550900 -2.41517900 3.13078900
C -0.24278000 1.48001900 -2.45820800
H 0.36070500 1.09869100 -3.28560800
H -1.21383400 1.81474100 -2.82563700
H 0.28419000 2.30276600 -1.97030600

O 2.50291400 -1.46556300 0.75112100
O 1.68358500 0.26095600 -1.27586200
Ni 3.30531200 0.16430900 -0.08803100
O 2.40394200 1.38215400 1.43964800
O 5.18765400 -0.23497700 0.86034800
Cl 5.76762600 -1.02911600 -0.32042800
O 0.13631600 2.26002900 1.03185000
O 4.61317600 -0.95341200 -1.34570800
O 6.96931800 -0.37270800 -0.85750500
O 1.68997800 3.46270600 2.48560600
O 6.01942200 -2.42649400 0.06519600
Cl 1.55655800 2.64660000 1.26674500
O 2.06533700 3.40079900 0.06112400
O 4.06864200 1.88374000 -0.96963600
H 3.97983300 1.78010500 -1.92621100
H 3.44014200 2.58968700 -0.69354500
C -1.18960500 -1.04896300 0.70704600
H -1.47412600 -0.04078500 1.03628300
H -1.18658300 -1.67662900 1.60057000
C -5.12600800 -2.15273300 2.40404300
C -6.35833700 -1.58656600 1.65053500
C -6.00550700 -1.15063600 0.21262600
C -3.98282200 -2.54286700 1.45969500
C -4.16553900 0.44979500 0.87928600
H -6.68565700 -0.37698100 -0.15377300
H -4.27468700 -3.40188700 0.84105800
H -6.06275400 -1.99216300 -0.48408000
H -3.09162900 -2.83764400 2.01700900
H -4.13407100 0.32587300 1.95861100
N -3.60649300 -1.43567300 0.56271600
N -4.64261100 -0.61344500 0.08464500
C -3.73950000 1.68371700 0.31500000
C -3.14880200 2.66662400 1.14851100
C -3.93754300 1.97482300 -1.05855300
C -2.78761600 3.90144100 0.63980300
H -2.95104700 2.43976300 2.19145800
C -3.61067800 3.22013500 -1.56339200
H -4.34951600 1.20874700 -1.70606400
C -3.03381100 4.17634600 -0.71178600
H -2.30442500 4.64085500 1.26679500
H -3.77569500 3.45999100 -2.60764800
Cl -2.59706700 5.72782000 -1.35889400
H -5.40065400 -3.04087000 2.97979700
H -4.75764500 -1.42492400 3.13457900

H -6.76736900 -0.73545800 2.20373000

H -7.15691000 -2.33318800 1.59562000

H -2.05904400 -6.32207200 -2.68111600

Thermal Correction to Free Energy: 0.451288 Hartree

Entropy: 271.362 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.156805 Hartree

Thermal Free Energy with Correction: -3570.705517 Hartree

B-TS11

C -1.43694600 6.46161800 -0.11540800

C -0.73862100 5.66103800 -1.01747800

C -0.76107900 4.26749200 -0.89869400

C -1.48610800 3.65722800 0.13180200

C -2.16876600 4.47594100 1.04885800

C -2.15111300 5.86344100 0.92670200

H -0.16260200 6.11818800 -1.81679700

H -0.17718800 3.66840800 -1.58787400

H -2.70092200 4.01863400 1.87997500

H -2.67996000 6.47793300 1.64979300

C -1.56450700 2.14300400 0.31823200

H -1.35170600 1.91220500 1.36171000

C 0.77554700 1.05247800 -0.10068400

C 1.86454800 1.29991200 -0.98168500

C 1.01360100 0.31749500 1.08343400

O 1.56496200 2.07877000 -2.05570900

O -0.09578600 0.12222800 1.86419500

C 2.63040000 2.27915000 -3.00126700

H 2.19556100 2.88197900 -3.79965200

H 3.46809600 2.80379100 -2.53678700

H 2.98715300 1.32387800 -3.39189200

C 0.08612100 -0.72918900 3.00752800

H 0.81533600 -0.30190800 3.69951900

H -0.89409900 -0.78254000 3.48554500

H 0.41440900 -1.72303500 2.69664900

O 3.04293900 0.88002100 -0.88699400

O 2.09722900 -0.16227700 1.51188400

Ni 3.55768500 -0.69213800 0.23571700

O 2.21339500 -1.97055700 -0.91243900

O 5.34020500 -0.97556900 -0.91035000

Cl 6.23388800 -0.14045400 0.02160000

O -0.13231000 -2.16118000 -0.20018900

O 5.22732500 0.28399600 1.11738000

O 7.30219500 -0.96554200 0.60503800

O 0.94982900 -3.99923000 -1.39278000

O 6.75790600 1.04114500 -0.67944400
Cl 1.13765400 -2.92601800 -0.40352200
O 1.57989000 -3.49122300 0.92391100
O 4.01105900 -2.34175500 1.41676700
H 4.10559100 -2.03365000 2.32771300
H 3.20536300 -2.90363500 1.37798100
C -0.64116500 1.26190500 -0.57103800
H -1.11881400 0.27673400 -0.62726300
H -0.62854500 1.64388100 -1.59243100
C -5.17798400 1.97342900 -0.97336700
C -5.49210000 2.66743600 0.35758500
C -4.97386600 1.85053700 1.55712900
C -3.65761600 1.80799400 -1.16578300
C -3.38699100 -0.10256300 0.91512500
H -5.67398100 1.06866500 1.86020900
H -3.23650000 2.71819700 -1.60456400
H -4.83530700 2.49935500 2.42889700
H -3.42596500 0.97866000 -1.84434400
H -2.33781600 -0.33074100 1.09448000
N -2.96026200 1.66212700 0.12640100
N -3.68462200 1.20349800 1.25955300
C -4.16384500 -1.21546400 0.43731000
C -3.40262200 -2.35315700 0.05777800
C -5.57721100 -1.28849500 0.34711000
C -4.02105000 -3.50510700 -0.40758900
H -2.31584400 -2.32549200 0.11091300
C -6.19714100 -2.44130000 -0.10348900
H -6.19862100 -0.45372600 0.64274700
C -5.41575600 -3.54355100 -0.48433200
H -3.42953700 -4.36237900 -0.70790500
H -7.27777300 -2.50177300 -0.16216900
Cl -6.20732000 -4.98167100 -1.05682000
H -5.57070700 2.55996500 -1.80927400
H -5.67459300 1.00040700 -1.02228700
H -6.56830800 2.83152000 0.47093200
H -5.01632800 3.65401100 0.36768500
H -1.41427500 7.54314000 -0.21149600
Thermal Correction to Free Energy: 0.453419 Hartree
Entropy: 268.487 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.144178 Hartree
Thermal Free Energy with Correction: -3570.690759 Hartree

B-8

C -6.11865200 -2.23146600 -2.46525100

C -5.48109700 -3.13936200 -1.61539800
C -4.28405700 -2.79126200 -0.99029000
C -3.70672500 -1.53004400 -1.20033600
C -4.35146800 -0.63000100 -2.05683100
C -5.54865900 -0.97763700 -2.68735600
H -5.91221200 -4.12234500 -1.44782300
H -3.78255600 -3.50603900 -0.34342200
H -3.90712900 0.34488900 -2.23781000
H -6.03412500 -0.26829600 -3.35156400
C -2.36200500 -1.16572400 -0.57840800
H -2.17537700 -0.10471600 -0.76224400
C 0.18496000 -1.35925200 -1.12644800
C 1.24618000 -2.14261600 -0.60378000
C 0.49289900 -0.08192500 -1.65796300
O 0.89798300 -3.41828200 -0.26715500
O -0.52045300 0.48042800 -2.37707100
C 1.96092600 -4.24781700 0.23346200
H 1.49278100 -5.20623500 0.46194300
H 2.74015000 -4.37465500 -0.52111300
H 2.40887100 -3.81217500 1.12923900
C -0.22559400 1.73633900 -3.00646800
H 0.60760100 1.63422900 -3.70545600
H -1.13589100 2.01328700 -3.54004400
H 0.02971400 2.49798900 -2.26640400
O 2.44583700 -1.81414300 -0.42983500
O 1.55946100 0.57847100 -1.55704500
Ni 3.07887700 0.07701300 -0.36597900
O 1.93060000 0.14875600 1.46486400
O 4.95025900 -0.40151400 0.54559000
Cl 5.73777900 -0.53700000 -0.77832800
O 1.48959000 2.57316600 1.41707400
O 4.64086900 -0.27277700 -1.82020100
O 6.77452800 0.50888900 -0.84223600
O 0.14991600 1.09006600 2.82883500
O 6.28971900 -1.89041800 -0.92120300
Cl 1.52334200 1.35432600 2.31205500
O 2.48978400 1.54587200 3.40566300
O 3.66162100 2.07156000 -0.19491200
H 2.98010400 2.50052700 0.36568000
H 4.49446300 2.09443800 0.29907200
C -1.20772300 -1.92670000 -1.30316300
H -1.22811500 -2.98294400 -1.02810000
H -1.49292400 -1.88203100 -2.35973500
C -1.79033400 -2.86265600 2.81656400

C -2.97845200 -2.26580700 3.57723000
C -4.05928700 -1.83330200 2.58469300
C -1.29093200 -1.90638600 1.72964700
C -4.02748000 0.27427800 1.38540700
H -4.87833500 -1.31206300 3.08383000
H -4.45254200 -2.68536600 2.02231700
H -5.02827300 0.34942100 1.80182700
N -2.41609000 -1.44736600 0.88169800
N -3.46551700 -0.89865300 1.59160100
C -3.50442500 1.46425700 0.75713500
C -4.43554500 2.42134800 0.29460100
C -2.12973100 1.78079600 0.73261900
C -4.00826500 3.63764300 -0.21496000
H -5.49850400 2.19929000 0.32719900
C -1.69712100 3.01431900 0.25904000
H -1.39343100 1.10657700 1.15257900
C -2.63697600 3.92570200 -0.22807400
H -4.71998600 4.36692400 -0.58453200
H -0.64092400 3.25795800 0.29763700
Cl -2.10180600 5.46685400 -0.84454300
H -7.04934200 -2.50330700 -2.95448900
H -2.65939300 -1.39480100 4.16211100
H -3.41288400 -2.98818000 4.27594000
H -2.08874100 -3.81257400 2.35591400
H -0.96500900 -3.07721100 3.50236700
H -0.76972500 -1.04601900 2.16686900
H -0.59425400 -2.42881800 1.08346500
Thermal Correction to Free Energy: 0.455019 Hartree
Entropy: 269.692 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.212201 Hartree
Thermal Free Energy with Correction: -3570.757182 Hartree

B-18

C -2.28731000 -5.16556800 -1.98274300
C -1.67945800 -5.03805000 -0.73282900
C -1.65065000 -3.80318900 -0.08165900
C -2.23653700 -2.67132900 -0.66982700
C -2.82175200 -2.80977800 -1.93951400
C -2.85390200 -4.04382800 -2.59060400
H -1.20972300 -5.89955300 -0.26725800
H -1.12506800 -3.71390500 0.86297900
H -3.23258100 -1.93342700 -2.43628700
H -3.30215300 -4.12461800 -3.57683400
C -2.26511300 -1.31196400 0.01498700

H -2.31167500 -0.54563100 -0.75794200
C 0.29242100 -0.92434600 0.26194900
C 1.37230200 -1.64706400 0.83881800
C 0.57333200 0.03284000 -0.74097400
O 1.00510500 -2.61757400 1.72308200
O -0.52647700 0.65239000 -1.25932900
C 2.08496100 -3.30166700 2.38134600
H 1.60568100 -4.00463800 3.06447100
H 2.70793200 -3.83269100 1.65836500
H 2.71184400 -2.59791000 2.93318000
C -0.26426400 1.73620200 -2.16283400
H 0.25744300 1.38276800 -3.05565800
H -1.24554100 2.13010200 -2.43301800
H 0.33341100 2.50739400 -1.67253200
O 2.60057900 -1.49570800 0.63523600
O 1.69102900 0.36566100 -1.21960600
Ni 3.38121000 0.16772600 -0.15336800
O 2.59722200 1.33256200 1.49188400
O 5.31074900 -0.32228000 0.64923600
Cl 5.79893000 -1.05266400 -0.61101700
O 0.33234100 2.28264600 1.30689600
O 4.58616400 -0.89240300 -1.55641000
O 6.98013100 -0.38690500 -1.18159900
O 2.03521200 3.38885500 2.67035000
O 6.04280200 -2.47567400 -0.32764500
Cl 1.77945500 2.62546100 1.43881500
O 2.20590800 3.41294300 0.22211900
O 4.13308700 1.92072600 -0.97946500
H 4.00419900 1.86542500 -1.93547800
H 3.52846300 2.62078300 -0.64254400
C -1.06506700 -0.97576900 0.92185600
H -1.27032500 -0.00102900 1.38242000
H -1.00741200 -1.68950800 1.74382500
C -5.16798200 -1.87678900 2.51423400
C -6.21019800 -2.27263900 1.44550000
C -5.63061800 -2.04807500 0.03476200
C -3.75136200 -2.03760100 1.96565700
C -4.95377300 0.22645300 -0.52524300
H -6.40365300 -1.82741800 -0.70317100
H -3.57809700 -3.07584700 1.64852800
H -5.05966800 -2.91174000 -0.31252200
H -3.00857400 -1.79893900 2.72898000
H -5.83957200 0.16315200 -1.15114300
N -3.52255400 -1.08567700 0.85331300

N -4.67741000 -0.90982200 0.07475100
C -4.31046500 1.51156200 -0.49459300
C -4.88688900 2.49916700 -1.33437100
C -3.20784700 1.87574100 0.31409500
C -4.38767200 3.78931800 -1.36690600
H -5.73558800 2.24404400 -1.96335900
C -2.70065300 3.16731300 0.28657000
H -2.75002400 1.14516800 0.96186400
C -3.29233100 4.11643200 -0.55417000
H -4.82978400 4.54112400 -2.01034300
H -1.82810300 3.41546600 0.88212500
Cl -2.65640300 5.73300700 -0.60525000
H -5.28332100 -2.48889000 3.41244900
H -5.31270300 -0.83405500 2.81714500
H -7.12869300 -1.69229000 1.57361900
H -6.48024800 -3.32970400 1.53259400
H -2.30012300 -6.12628300 -2.48892400
Thermal Correction to Free Energy: 0.455415 Hartree
Entropy: 268.737 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.208017 Hartree
Thermal Free Energy with Correction: -3570.752602 Hartree

B-8

C 0.85556700 6.19043800 -1.95892500
C -0.04548000 5.66156700 -1.03635600
C 0.18021100 4.40814600 -0.45887600
C 1.31697200 3.66679200 -0.80414800
C 2.21391700 4.20542900 -1.74108700
C 1.99058300 5.45577500 -2.31231700
H -0.93554000 6.22072800 -0.76305700
H -0.54526900 4.01280800 0.24310300
H 3.09602200 3.63549400 -2.02176300
H 2.69543900 5.85384900 -3.03674700
C 1.61461300 2.28338400 -0.22800000
H 1.75329000 1.61060700 -1.07723300
C -0.73869400 1.16036200 0.11223400
C -1.98231900 1.51465200 0.70745400
C -0.73082500 0.12125600 -0.84170000
O -1.93093300 2.58987000 1.54132200
O 0.50334200 -0.16627300 -1.37205300
C -3.16016300 2.92646500 2.20903300
H -2.91584500 3.77712200 2.84654400
H -3.93358600 3.19597600 1.48679300
H -3.51696000 2.08647000 2.80858800

C 0.55011100 -1.28444100 -2.27553100
H -0.07196200 -1.09859500 -3.15367700
H 1.59725800 -1.37253600 -2.57063900
H 0.21462600 -2.19469200 -1.77459700
O -3.09826900 0.96249800 0.55669800
O -1.69576700 -0.56131500 -1.27833300
Ni -3.32142700 -0.89405700 -0.14613200
O -2.11930400 -1.66848300 1.49208000
O -5.26419800 -1.03645700 0.74472100
Cl -6.02197800 -0.58352600 -0.51331900
O 0.33132800 -1.79205400 1.32628500
O -4.86169900 -0.37745600 -1.51676800
O -6.92493100 -1.64051200 -0.99317700
O -0.90354000 -3.43072600 2.65593400
O -6.72277500 0.68629000 -0.27194600
Cl -0.91893400 -2.60896500 1.43637500
O -1.03522300 -3.47738200 0.20567700
O -3.47039100 -2.83775700 -0.86677200
H -3.48978300 -2.79644600 -1.83195100
H -2.62651800 -3.26503000 -0.60154700
C 0.54624400 1.68674600 0.72228200
H 1.01114300 0.87370200 1.29677300
H 0.28548000 2.43917900 1.46686400
C 4.43228000 3.52573500 2.05131200
C 5.26427300 2.24847200 2.13913300
C 5.14793600 1.44301400 0.84400100
C 3.00038800 3.15608800 1.68467600
C 3.26291700 0.01814200 0.12737200
H 5.62868300 0.47406400 0.94964400
H 5.59643800 1.98564200 0.00594000
H 2.18879400 -0.06631600 0.00833400
N 2.95727300 2.36424100 0.43412200
N 3.72334900 1.19351600 0.48424300
C 4.01699500 -1.19737900 -0.15382800
C 3.35879900 -2.40948000 0.15107600
C 5.28244700 -1.24633800 -0.77588900
C 3.97624900 -3.63073400 -0.09629100
H 2.36567400 -2.39009500 0.59536100
C 5.89013500 -2.46572100 -1.04696300
H 5.77821900 -0.33724400 -1.09810100
C 5.23982000 -3.65177300 -0.69039200
H 3.47551800 -4.55820400 0.15699900
H 6.85401700 -2.50364000 -1.54155600
Cl 6.01393400 -5.18032700 -1.02025100

H 0.67371000 7.16363000 -2.40547600

H 6.32486400 2.46196600 2.30650100

H 4.92326900 1.63041300 2.97850900

H 4.84324500 4.19757600 1.28893900

H 4.43966800 4.06221000 3.00506500

H 2.40144300 4.04520500 1.48312000

H 2.52389600 2.60181600 2.50575900

Thermal Correction to Free Energy: 0.457495 Hartree

Entropy: 265.311 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.206579 Hartree

Thermal Free Energy with Correction: -3570.749084 Hartree

B-13

C 0.39659600 6.30658800 -1.86619800

C -0.41741200 5.69133200 -0.91672400

C -0.08137400 4.43706200 -0.39727100

C 1.07840900 3.78359100 -0.82985000

C 1.88694200 4.40708700 -1.79393900

C 1.55414900 5.65867000 -2.30612500

H -1.32489900 6.18217300 -0.57760000

H -0.73851600 3.97015400 0.32724500

H 2.78481600 3.90277300 -2.14293500

H 2.19089200 6.12489100 -3.05256000

C 1.49236200 2.40639800 -0.31794800

H 1.63678500 1.78084700 -1.20195600

C -0.76590000 1.12283000 0.08550200

C -1.99713500 1.38900100 0.74762100

C -0.74627500 0.12093100 -0.90766200

O -1.95974000 2.42991900 1.62578700

O 0.47625800 -0.07777600 -1.50389500

C -3.17327300 2.67595100 2.35895200

H -2.94512200 3.51620000 3.01601200

H -3.99245600 2.92738100 1.68216000

H -3.45704900 1.79758400 2.94240900

C 0.54459500 -1.16803700 -2.44078100

H -0.11457100 -0.98701100 -3.29242000

H 1.58427300 -1.19843000 -2.77202900

H 0.26844000 -2.10587600 -1.95532400

O -3.09088700 0.78955300 0.61987000

O -1.69176600 -0.59585600 -1.32950000

Ni -3.26277000 -1.04420900 -0.15766900

O -1.98528500 -1.83904700 1.40328600

O -5.16826800 -1.30288400 0.78656800

Cl -5.98387400 -0.82199600 -0.42412200

O 0.45691300 -1.82566100 1.11118500
O -4.86641800 -0.52655400 -1.45326200
O -6.86380100 -1.88906700 -0.92379100
O -0.62033000 -3.56216300 2.45407900
O -6.72145300 0.40836300 -0.10109500
Cl -0.73997000 -2.71142100 1.26025600
O -0.87596000 -3.55242600 0.01323200
O -3.35980500 -2.95749500 -0.96287700
H -3.40127200 -2.87482000 -1.92469800
H -2.49525700 -3.36481900 -0.73423800
C 0.51936300 1.69230700 0.65375700
H 1.06730100 0.87446600 1.14062300
H 0.26409000 2.38446400 1.45777400
C 3.33994600 2.79182400 2.73315900
C 4.62715600 1.95544600 2.58310700
C 4.91462900 1.65089000 1.09995100
C 3.02677000 3.49796600 1.41328800
C 3.28965100 0.23298700 -0.10292700
H 5.53973400 0.77099200 0.99239500
H 3.82303300 4.20720000 1.15520100
H 5.39939000 2.49218800 0.59924000
H 2.10278500 4.07279700 1.46983300
H 2.25592300 0.11365500 -0.41053000
N 2.84769800 2.53793300 0.29765200
N 3.63702300 1.40269500 0.38152400
C 4.15395400 -0.93439300 -0.27443600
C 3.57740100 -2.19208800 -0.00071700
C 5.46674700 -0.88034400 -0.78343800
C 4.31576600 -3.35877500 -0.17459000
H 2.55537300 -2.25179100 0.36739600
C 6.20077800 -2.04564800 -0.97517400
H 5.90497300 0.06818400 -1.07841200
C 5.62372700 -3.27826000 -0.65658900
H 3.87651000 -4.32306400 0.05453700
H 7.20517500 -2.00502400 -1.38123300
Cl 6.55082900 -4.74078000 -0.88914700
H 3.44342500 3.53425500 3.52971900
H 2.49700100 2.14816200 3.00125200
H 4.54601000 1.01717800 3.13852000
H 5.49820900 2.48916700 2.97648000
H 0.12967800 7.27978000 -2.26764300
Thermal Correction to Free Energy: 0.452905 Hartree
Entropy: 272.802 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.20163 Hartree

Thermal Free Energy with Correction: -3570.748725 Hartree

B-TS3

C -2.87207100 -0.79240300 3.97501900
C -1.70023500 -0.74476900 2.98994200
C -4.36446400 -0.17218400 2.05337800
C -4.17068600 -1.13409000 3.23273400
H -0.79570900 -0.35777700 3.46385100
H -1.48269000 -1.74406200 2.60058400
H -5.03073500 -1.05941000 3.90677600
H -4.14025000 -2.16991300 2.87280500
C -1.10278500 0.93026100 1.30725600
C -1.90008200 -1.05390800 -0.85837800
C -3.00384100 -1.29772000 0.22066600
H -0.13292600 0.86577900 1.79280600
H -2.24978300 -0.26019300 -1.51771200
H -1.89114900 -1.97039300 -1.46129700
H -2.71760700 -2.17612900 0.80862100
N -2.03463400 0.15759200 1.86381200
N -3.21444700 -0.11641200 1.12384700
C -4.30506200 -1.62843300 -0.49486300
C -4.84694800 -2.91545100 -0.39399800
C -4.96290100 -0.68346600 -1.29719600
C -6.01683200 -3.25539900 -1.07697400
H -4.34444000 -3.66128900 0.21683200
C -6.13586900 -1.01769700 -1.97276300
H -4.55511400 0.31849300 -1.39304200
C -6.66612800 -2.30604400 -1.86580700
H -6.41868200 -4.26068500 -0.99059700
H -6.63378500 -0.27398700 -2.58821300
H -7.57724400 -2.56680400 -2.39602900
C -1.30045100 2.14099500 0.51963800
C -0.17225200 2.98269500 0.41870900
C -2.51824900 2.56800100 -0.05076000
C -0.24941200 4.21363600 -0.22316000
H 0.77491300 2.68007100 0.84979000
C -2.60335600 3.80069800 -0.68394900
H -3.38825500 1.92965900 0.01672900
C -1.46838800 4.61523600 -0.76987700
H 0.62747400 4.84741500 -0.28805000
H -3.54054500 4.13414900 -1.11530700
Cl -1.58664900 6.16210100 -1.57701300
C -0.47776800 -0.71101400 -0.42620000
C 0.27687300 -1.67060400 0.34006400

O 1.44345200 -1.55968600 0.78126000
O -0.40802900 -2.79479600 0.63227900
C 0.28922000 0.20401500 -1.23882700
O 1.48853200 0.52710100 -1.09660700
C 0.33825000 -3.85282100 1.27247900
H 0.63438000 -3.55768700 2.28304100
H -0.34837900 -4.69842600 1.31020800
H 1.22307100 -4.09424900 0.68314700
O -0.40835800 0.77371500 -2.23546700
C 0.32299300 1.65840800 -3.10826000
H -0.40686400 1.99694200 -3.84316100
H 0.72891400 2.50287000 -2.54946600
H 1.13989600 1.12115500 -3.59389200
Ni 2.87132000 -0.31252100 0.09716400
O 3.53421000 -1.46866700 -1.48936100
O 4.18358800 1.42153800 -0.12058600
Cl 3.68748000 2.12477400 1.13898300
O 1.99550900 -3.38771600 -1.66355000
O 2.58978700 1.14370300 1.64463700
O 4.74715700 2.25214600 2.14612600
O 4.24834800 -3.50063300 -2.62077600
O 3.06907000 3.42516500 0.81147400
Cl 3.42267800 -3.01045100 -1.51050100
O 3.94231500 -3.51690000 -0.18427800
O 4.28816500 -1.26232300 1.27631700
H 3.95571200 -1.38527000 2.17491200
H 4.34176300 -2.15786800 0.86310000
H -2.65157300 -1.52879900 4.75474000
H -2.97025800 0.18325800 4.46662000
H -4.50445200 0.84810700 2.43100300
H -5.24604100 -0.43068000 1.46705300
Thermal Correction to Free Energy: 0.457896 Hartree
Entropy: 260.606 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.212625 Hartree
Thermal Free Energy with Correction: -3570.754729 Hartree

B-4

C -2.75060400 -0.26806600 4.00741100
C -1.63982400 -0.40599700 2.95978800
C -4.28069700 0.33456400 2.10925100
C -4.11836100 -0.53432000 3.36654000
H -0.68170700 -0.07742100 3.37425300
H -1.53313600 -1.46814000 2.68336700
H -4.92787600 -0.31427200 4.07171200

H -4.21099900 -1.59627300 3.10260000
C -0.86083100 0.75733500 0.89887700
C -2.03984400 -0.86585300 -0.74319800
C -3.13271200 -1.05622000 0.33937500
H 0.05750500 0.76746100 1.48938400
H -2.37524700 -0.08302400 -1.42353000
H -1.94746500 -1.78240900 -1.33030400
H -2.87988300 -1.93118000 0.95150900
N -1.94362100 0.46753300 1.81206200
N -3.18192500 0.18931300 1.14336000
C -4.46427100 -1.34882600 -0.33489300
C -5.06441500 -2.60393700 -0.17804300
C -5.10066500 -0.39956100 -1.14942200
C -6.26711300 -2.90976500 -0.81862700
H -4.58345200 -3.35103400 0.44861300
C -6.30510800 -0.69920000 -1.78465600
H -4.65493800 0.58180400 -1.28044300
C -6.89165700 -1.95701400 -1.62326900
H -6.71461300 -3.89063000 -0.68640500
H -6.78560500 0.04896200 -2.40865600
H -7.82805900 -2.19077900 -2.12123700
C -0.97112000 2.13696100 0.24813500
C 0.16402200 2.96129400 0.26744700
C -2.14468000 2.63889800 -0.33560000
C 0.14717800 4.23814400 -0.29439700
H 1.08085300 2.61472000 0.73026700
C -2.17900500 3.91623000 -0.89344100
H -3.04340400 2.03676700 -0.31908500
C -1.02884300 4.70475800 -0.87627400
H 1.03709300 4.85682300 -0.26832000
H -3.09251800 4.29862600 -1.33575800
Cl -1.06990200 6.31042600 -1.59079900
C -0.66061100 -0.45062200 -0.18944300
C 0.08130400 -1.60874400 0.49131700
O 1.22615600 -1.53256400 0.94977900
O -0.62379100 -2.71533100 0.59575300
C 0.28031100 0.10128100 -1.26444900
O 1.46557300 0.37854300 -1.07379900
C 0.02122000 -3.86450300 1.20727800
H 0.23214500 -3.64775800 2.25680200
H -0.70633200 -4.66905200 1.11823500
H 0.94042300 -4.09792800 0.67158700
O -0.30009800 0.33207400 -2.42255900
C 0.53219300 0.91835400 -3.45933400

H -0.11168100 0.97702600 -4.33456800
H 0.86207500 1.90972700 -3.14545100
H 1.39608200 0.27850600 -3.64284500
Ni 2.84886400 -0.47955200 0.18835600
O 3.35421000 -1.65622300 -1.43228300
O 4.32511800 1.00879800 -0.16071100
Cl 4.02347600 1.80229000 1.12143800
O 1.39229400 -3.11174200 -1.69733600
O 2.82818500 0.98001900 1.69683700
O 5.15293100 1.76762600 2.05457100
O 3.54949100 -3.73873800 -2.68157700
O 3.58379900 3.16824500 0.80404200
Cl 2.87265300 -3.12009600 -1.53913900
O 3.24165300 -3.80046300 -0.24295700
O 4.11910100 -1.67198600 1.29889200
H 3.86274700 -1.72913000 2.22884400
H 4.00121500 -2.56350300 0.90049600
H -2.56058500 -0.95577000 4.83909300
H -2.72581800 0.75161600 4.41006700
H -4.29757300 1.39210900 2.39692300
H -5.21665000 0.11194000 1.59397100
Thermal Correction to Free Energy: 0.460267 Hartree
Entropy: 259.168 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.21731 Hartree
Thermal Free Energy with Correction: -3570.757043 Hartree

B-TS4

C 7.35259400 -1.42851800 -0.92351000
C 6.45895100 -0.62620300 -1.63619800
C 5.15950800 -0.43117500 -1.16683100
C 4.72375100 -1.02561900 0.02779200
C 5.62939300 -1.84358100 0.71925600
C 6.93115500 -2.04235500 0.25587000
H 6.77075000 -0.15819500 -2.56565100
H 4.48126800 0.18038600 -1.75410900
H 5.30567500 -2.34047100 1.63100700
H 7.61034200 -2.68223300 0.81183200
C 3.31791300 -0.83978000 0.61304200
H 3.17562900 -1.65569100 1.32470300
C 0.80454900 -0.59558600 -0.11244000
C 0.16887100 -1.22960200 1.03608900
C -0.09771000 -0.26836100 -1.20654600
O 0.94925800 -2.07840700 1.71006800
O 0.52493000 -0.03423500 -2.36930600

C 0.33713700 -2.74863700 2.83609400
H 1.10914000 -3.41228300 3.22356800
H 0.03019700 -2.02350300 3.59200600
H -0.53357300 -3.31540300 2.50274000
C -0.32264000 0.15148600 -3.52234400
H -0.90526200 1.06999600 -3.42307900
H 0.36160000 0.22082000 -4.36768800
H -0.98919300 -0.70508800 -3.63261300
O -0.97757100 -0.99070800 1.46000000
O -1.33825600 -0.13958300 -1.15396900
Ni -2.60838400 -0.87518800 0.24924100
O -2.28235600 -2.88345200 -0.22675900
O -3.89897700 -1.18057300 1.93613400
Cl -4.12270200 0.31131600 2.21183700
O -0.56238000 -3.05536900 -1.98026500
O -3.31263500 0.96036600 1.05541200
O -5.54182400 0.66911700 2.09921900
O -2.19850800 -4.85065000 -1.65767700
O -3.53900200 0.70361800 3.50439700
Cl -1.96888700 -3.40104800 -1.65092500
O -2.90157200 -2.69847500 -2.60730600
O -4.18582500 -0.85663700 -1.08311900
H -4.25530900 0.00164300 -1.52131300
H -3.91732800 -1.51647900 -1.76504300
C 2.23269700 -0.97119500 -0.48392300
H 2.50900700 -0.34660400 -1.33320300
H 2.27042300 -2.00275800 -0.85260400
C 4.43263800 2.95834900 1.24049800
C 5.14271900 1.76877600 1.89739700
C 3.43166300 2.49141400 0.17165800
C 4.09623900 0.77912500 2.43086100
C 1.18258800 1.44439700 0.74472900
H 0.75402000 1.06745300 1.66579200
N 3.09652500 0.38185000 1.43650000
N 2.53702000 1.47086500 0.74285700
C 0.34520100 2.41057000 0.01970700
C -0.85886900 2.80365100 0.63039500
C 0.64990100 2.92342800 -1.25769000
C -1.71300100 3.71626800 0.01724300
H -1.14990200 2.37613000 1.58348300
C -0.19460200 3.83742100 -1.87759900
H 1.53100700 2.58480500 -1.78961600
C -1.36718500 4.23661000 -1.22856000
H -2.64242600 4.00137600 0.49539700

H 0.04429300 4.23414100 -2.85801100
Cl -2.42587200 5.39091500 -2.01057500
H 8.36272700 -1.58238400 -1.29122400
H 3.96492700 2.08556500 -0.69547300
H 2.82393800 3.33162100 -0.15977800
H 3.56288700 1.23652900 3.27576400
H 4.56703300 -0.13501300 2.80052700
H 5.79411100 1.27113000 1.17218100
H 5.77499600 2.11231400 2.72372200
H 5.15165100 3.63810200 0.77074300
H 3.89111200 3.53486700 2.00140900
Thermal Correction to Free Energy: 0.456957 Hartree
Entropy: 262.576 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.200899 Hartree
Thermal Free Energy with Correction: -3570.743942 Hartree

B-6

C 7.17586100 -1.73189200 -0.95794400
C 6.79412100 -0.61314900 -0.21546800
C 5.49297700 -0.50499500 0.27929700
C 4.55527900 -1.51351500 0.03706700
C 4.94803700 -2.63580100 -0.70475900
C 6.24773200 -2.74649300 -1.20006200
H 7.51282500 0.17712600 -0.01598800
H 5.19876600 0.35435400 0.87102000
H 4.23374500 -3.43546900 -0.89071600
H 6.53671600 -3.62699600 -1.76711800
C 3.11170400 -1.41238200 0.52743300
H 2.82194600 -2.40063900 0.89378600
C 0.82924400 -0.47812900 -0.18620500
C -0.00135200 -1.48173700 0.63445400
C -0.09352500 -0.09051800 -1.35651800
O 0.45873900 -2.71298900 0.63122500
O 0.52548200 -0.00067300 -2.50777800
C -0.35507700 -3.71746500 1.30395000
H 0.15889300 -4.65862300 1.11997300
H -0.40114100 -3.49488100 2.37122800
H -1.35678300 -3.71601600 0.87470100
C -0.27659000 0.36406400 -3.66343000
H -0.64500100 1.38390900 -3.54007700
H 0.40699000 0.29811900 -4.50746300
H -1.10529500 -0.33644600 -3.76566800
O -1.03270500 -1.16874400 1.23164500
O -1.29721300 0.15819600 -1.24032800

Ni -2.68673500 -0.42542400 0.18994200
O -2.89818300 -2.34524600 -0.56483200
O -3.91818700 -0.66998000 1.89108200
Cl -3.74141700 0.77265800 2.39870400
O -1.22367800 -2.66812600 -2.33559600
O -2.81485900 1.35187300 1.28273300
O -5.01774700 1.49203200 2.41586100
O -3.25458700 -4.03927300 -2.27809300
O -3.04544800 0.79774800 3.68950300
Cl -2.68411200 -2.70702900 -2.06067800
O -3.39069700 -1.66169900 -2.88236300
O -4.22660800 0.17493300 -1.03345500
H -4.14484100 1.09572600 -1.31510000
H -4.13865500 -0.39434200 -1.83151400
C 2.17625900 -1.05570700 -0.66099100
H 2.65912000 -0.30793800 -1.28963400
H 2.01169000 -1.93758300 -1.28313500
C 2.21673200 1.45117700 3.60633500
C 2.65941700 0.03911500 4.01331100
C 2.78442200 1.80660500 2.22194200
C 2.34101200 -0.95846600 2.89291000
C 1.08479800 0.85069200 0.68944200
H 0.32158900 0.84072700 1.47788100
N 2.93589500 -0.47451400 1.64079400
N 2.47948100 0.79660400 1.19295900
C 0.91997900 2.14822100 -0.09789100
C -0.21734100 2.94554000 0.08420400
C 1.90601300 2.57847300 -0.99912200
C -0.38436300 4.13355400 -0.62972600
H -0.98643600 2.64053800 0.78720000
C 1.75160400 3.76065400 -1.72095000
H 2.81481500 1.99791300 -1.11178800
C 0.60092200 4.52785200 -1.53308800
H -1.26500200 4.74826400 -0.47908000
H 2.51735200 4.08984600 -2.41480500
Cl 0.39929400 6.01849500 -2.44114800
H 8.18966500 -1.81640700 -1.33861600
H 3.87675800 1.87389200 2.27975500
H 2.40872900 2.77300100 1.87771300
H 1.24651400 -1.10186800 2.83986100
H 2.78606300 -1.93393700 3.11216800
H 3.74196400 0.02898400 4.18954600
H 2.16833700 -0.27219400 4.94181700
H 2.55547200 2.19181700 4.33960700

H 1.12048500 1.50764000 3.59092600

Thermal Correction to Free Energy: 0.458526 Hartree

Entropy: 261.941 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.211901 Hartree

Thermal Free Energy with Correction: -3570.753375 Hartree

B-TS6

C -7.46730700 -2.16178200 0.26087400

C -6.75136300 -1.67820300 1.35930900

C -5.56182500 -0.97685100 1.16804200

C -5.07301500 -0.73851800 -0.12601800

C -5.80069400 -1.22351000 -1.21881900

C -6.98820300 -1.93404400 -1.02893000

H -7.11816700 -1.85197900 2.36682600

H -5.01210700 -0.59979100 2.02569700

H -5.43176200 -1.05059000 -2.22682200

H -7.53682200 -2.30699800 -1.88892700

C -3.75250900 -0.01815700 -0.35371300

H -3.61710700 0.10179100 -1.43440800

C -1.15194700 -0.46256800 0.11791700

C -0.27180900 -0.78336500 1.23614000

C -0.52960500 -0.45089700 -1.19623100

O -0.91824000 -0.94328600 2.40337600

O -1.41954200 -0.35467600 -2.20756700

C -0.09937500 -1.31801100 3.53755100

H 0.62268300 -0.53050300 3.76131100

H -0.80210600 -1.44645900 4.36025100

H 0.43141600 -2.24736400 3.32494500

C -0.87765500 -0.42995500 -3.54314200

H -0.32531600 -1.36159600 -3.67768400

H -1.74330900 -0.39578400 -4.20419700

H -0.20869000 0.41106400 -3.73828000

O 0.97040300 -0.83280100 1.22917900

O 0.68029000 -0.49677200 -1.48579500

Ni 2.12453300 -1.36460500 -0.35631700

O 3.26116700 0.34169000 -0.12153900

O 3.24279800 -2.77530400 0.79494200

Cl 2.20032100 -3.91070000 0.72242700

O 3.93717800 0.50354300 -2.48938300

O 1.13607100 -3.29942400 -0.20641500

O 2.79295700 -5.10968300 0.11604700

O 4.70929900 2.15490100 -0.85494000

O 1.62823600 -4.17561100 2.05463900

Cl 4.42061700 0.72767300 -1.07460800

O 5.57623900 -0.14832300 -0.79461800

O 3.15913100 -2.02747800 -2.02179200

H 3.94529200 -2.49812800 -1.70550100

H 3.49052200 -1.20679100 -2.45911400

C -2.61154500 -0.92964200 0.19352500

H -2.83888500 -1.14263200 1.23795900

H -2.70749000 -1.87993500 -0.34463300

C -4.99553800 2.87611500 -1.20059800

C -3.70571800 3.67237800 -1.41663800

C -2.47765300 2.77659100 -1.22510000

C -4.92846400 2.17842200 0.16222800

C -1.51356600 1.64874800 0.79260600

H -1.84559400 1.21578200 1.73011400

N -3.75430300 1.30354800 0.33281900

N -2.56231000 2.03435600 0.04787900

C -0.21340100 2.34105600 0.85993900

C 0.61787900 2.65791000 -0.22890800

C 0.20452400 2.71202000 2.15202900

C 1.80207800 3.36327600 -0.04011800

H 0.37666600 2.31460300 -1.22782700

C 1.37632300 3.43296100 2.35036700

H -0.40961100 2.45394600 3.01001400

C 2.16427300 3.76428800 1.24742000

H 2.46307500 3.56660300 -0.87328000

H 1.68131600 3.73102200 3.34695800

Cl 3.62963100 4.67989400 1.48881300

H -8.39104400 -2.71263500 0.41124400

H -2.38738800 2.06279400 -2.05242300

H -1.56910500 3.37738100 -1.19455700

H -5.81504000 1.57306000 0.34751100

H -4.87327600 2.93379700 0.95612200

H -3.66040700 4.50064400 -0.69867800

H -3.66372800 4.11104100 -2.41904200

H -5.86882200 3.53648700 -1.23322500

H -5.12671700 2.13428200 -1.99858300

Thermal Correction to Free Energy: 0.455679 Hartree

Entropy: 265.41 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.201637 Hartree

Thermal Free Energy with Correction: -3570.745958 Hartree

B-9

C -7.39188100 -1.14556100 0.61578700

C -6.66976000 -0.39036800 1.54377100

C -5.41139300 0.11075700 1.21373700

C -4.85710100 -0.12767000 -0.05310700
C -5.59101300 -0.88072300 -0.97636200
C -6.84871400 -1.39010300 -0.64545900
H -7.08776300 -0.19268300 2.52686400
H -4.85613000 0.70809100 1.93093600
H -5.17370600 -1.07408800 -1.96163400
H -7.40259900 -1.97478900 -1.37432500
C -3.46645500 0.37578900 -0.41076400
H -3.31255400 0.19574200 -1.48218500
C -0.94796700 0.03110900 0.28090800
C -0.31474800 -0.41846200 -1.03540000
C -0.10318600 -0.50162200 1.44424900
O -1.18747300 -0.81965600 -1.94321200
O -0.74752000 -0.43385700 2.59623800
C -0.63678900 -1.36410000 -3.17320800
H -0.00216500 -2.21862700 -2.93575800
H -1.50453900 -1.66456900 -3.75733100
H -0.05582600 -0.60052000 -3.69278100
C -0.05923200 -0.95257300 3.76081100
H 0.82964800 -0.35336300 3.96665700
H -0.77979600 -0.87066000 4.57249800
H 0.21844200 -1.99265100 3.58391700
O 0.89302800 -0.43579300 -1.28317900
O 1.06724000 -0.89058900 1.41069400
Ni 2.28579500 -1.46055900 -0.14362400
O 1.18510900 -3.16668900 -0.58916800
O 3.62702300 -1.51348400 -1.78529100
Cl 4.41017900 -0.25897600 -1.35101700
O -0.78216700 -3.27340700 0.88357100
O 3.68404200 0.09113000 -0.02270400
O 5.81936200 -0.57211200 -1.09904800
O 0.13380300 -5.31268900 -0.12174100
O 4.22817200 0.83275200 -2.31987700
Cl 0.44345400 -4.01302400 0.48021300
O 1.36015700 -4.15700500 1.66579700
O 3.49529100 -2.59060900 1.06944300
H 3.86909600 -2.08140100 1.80059600
H 2.90396000 -3.28384000 1.44158700
C -2.42833100 -0.44963400 0.39499800
H -2.70950000 -0.38706500 1.44602800
H -2.49389600 -1.49939600 0.10424500
C -4.10521000 3.05202100 -2.09532100
C -2.66872500 3.52407600 -2.34675900
C -1.67047400 2.52298500 -1.75356400

C -4.29289100 2.74849900 -0.60115700
C -1.02816000 1.65479300 0.52660200
H -1.51182600 1.66618300 1.50588700
N -3.30595500 1.80570400 -0.05463500
N -1.98675400 2.30070400 -0.33285000
C 0.26887800 2.43935100 0.68396500
C 1.35194400 2.42839400 -0.20529200
C 0.34383700 3.29019400 1.79995400
C 2.47300300 3.23237100 0.01039100
H 1.36233400 1.77675500 -1.06754200
C 1.45071100 4.10296700 2.02790100
H -0.48634200 3.32777800 2.50023000
C 2.51228400 4.06672600 1.12358800
H 3.30915300 3.18861300 -0.67758200
H 1.49181400 4.75535600 2.89310500
Cl 3.91676000 5.08269100 1.40192700
H -8.37071500 -1.53850400 0.87476800
H -1.69084100 1.59548200 -2.34568600
H -0.65698100 2.92730300 -1.80488900
H -5.28805700 2.34799700 -0.40042600
H -4.18345600 3.67696000 -0.02815700
H -2.51282900 4.49980700 -1.87056400
H -2.47050900 3.64606800 -3.41740100
H -4.82735600 3.81496700 -2.40788900
H -4.31734200 2.15487500 -2.69217700
Thermal Correction to Free Energy: 0.458503 Hartree
Entropy: 262.734 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.209012 Hartree
Thermal Free Energy with Correction: -3570.750509 Hartree

B-TS7

C -6.67061000 2.54972400 -0.49738000
C -5.74532500 2.17404100 -1.47327300
C -4.80847500 1.17315900 -1.21102800
C -4.78767300 0.51927500 0.02765600
C -5.73244800 0.89390100 0.99256100
C -6.65900900 1.90668500 0.74060000
H -5.75040600 2.66249200 -2.44386800
H -4.08294000 0.89812000 -1.96786400
H -5.74531900 0.38683100 1.95509800
H -7.37735300 2.18279800 1.50704300
C -3.80302600 -0.59112000 0.38850700
H -4.37837400 -1.27862600 1.02874000
C -1.20164800 0.04630800 0.74439000

C -0.96232500 1.14335500 -0.19795900
C -0.07829300 -0.21286200 1.63869800
O -2.06123100 1.81155100 -0.53545300
O -0.41037800 -0.85843400 2.77182800
C -1.88390600 2.94700800 -1.41767200
H -1.47454100 2.61999900 -2.37565500
H -2.88376800 3.35941300 -1.54044700
H -1.20871100 3.67366800 -0.96370900
C 0.66110600 -1.08612000 3.71250400
H 1.11230900 -0.13750200 4.00845700
H 0.18922700 -1.57161900 4.56650400
H 1.42664800 -1.72789000 3.27331400
O 0.12569600 1.46103900 -0.70990500
O 1.12061700 0.05914800 1.44220500
Ni 1.93439800 1.45480900 0.20716100
O 2.56333400 0.27833800 -1.36639900
O 2.47814200 3.40177600 -0.54174400
Cl 1.77595100 4.19762200 0.57503900
O 4.73014300 -0.47302800 -0.46657100
O 1.22311200 3.06645000 1.46241000
O 2.75628600 5.00272000 1.31779300
O 3.99559700 -1.15597500 -2.70176200
O 0.67435200 5.00912100 0.02941000
Cl 4.03610400 -0.04071800 -1.73502200
O 4.66828800 1.17043200 -2.28488500
O 3.75703200 1.43078400 1.18265000
H 4.21075000 2.26104600 0.97286600
H 4.28433900 0.71473200 0.75254000
C -2.61251700 -0.11251600 1.31444300
H -2.93296900 0.83170500 1.76648100
H -2.53823600 -0.82754300 2.13349700
C -4.96735500 -3.22626200 -0.96167500
C -3.84387200 -4.19346400 -0.58212400
C -2.75823700 -3.48467500 0.23916800
C -4.36417100 -1.98418900 -1.62755500
C -1.06533900 -1.76366600 -0.54359800
H -0.93751600 -1.10358600 -1.39317600
N -3.32602400 -1.31327700 -0.81478500
N -2.32399600 -2.25483700 -0.44513700
C 0.12902500 -2.55122700 -0.18164900
C 0.24905700 -3.32030100 0.99435900
C 1.21553000 -2.52357400 -1.07286200
C 1.38952500 -4.07546000 1.24056700
H -0.53118900 -3.30190600 1.74509100

C 2.36376700 -3.27714300 -0.83737300
H 1.18222300 -1.89385900 -1.95470400
C 2.43547300 -4.05952500 0.31281600
H 1.47501300 -4.66832800 2.14444000
H 3.19594200 -3.22272300 -1.52861700
Cl 3.86141600 -5.02394900 0.62120400
H -7.39632500 3.33104600 -0.70260800
H -3.13082500 -3.25034600 1.24645400
H -1.89422200 -4.13630100 0.34394700
H -5.13262100 -1.24629400 -1.85577400
H -3.88428900 -2.26731300 -2.57187700
H -3.38531600 -4.60012200 -1.49198200
H -4.22177000 -5.04233600 -0.00240300
H -5.67299200 -3.70224500 -1.65092700
H -5.54223300 -2.94084900 -0.07203300
Thermal Correction to Free Energy: 0.458548 Hartree
Entropy: 260.073 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.194555 Hartree
Thermal Free Energy with Correction: -3570.736007 Hartree

B-11

C -6.66839500 2.48015000 0.26010600
C -5.64047600 2.57015100 -0.68032700
C -4.66092000 1.57800500 -0.75338800
C -4.69606500 0.47046700 0.10423900
C -5.74264000 0.38546100 1.03312800
C -6.71531600 1.38225800 1.11995900
H -5.60090600 3.41414800 -1.36357600
H -3.86419600 1.65925900 -1.48385700
H -5.79920900 -0.47490500 1.69664300
H -7.51465500 1.29384700 1.85013300
C -3.65924500 -0.64957300 0.09365100
H -4.22160700 -1.56189100 0.34011900
C -1.15281300 -0.23530600 0.66656100
C -1.01149200 1.15794600 0.03204700
C -0.06504200 -0.23441400 1.74194000
O -1.96913100 1.99711200 0.35954500
O -0.44908100 -0.71228900 2.91270100
C -1.84095400 3.36781600 -0.11105100
H -1.68855200 3.37706100 -1.19083900
H -2.78292900 3.84033400 0.15845700
H -0.99573800 3.84356200 0.38568900
C 0.57057900 -0.80331200 3.94175700
H 1.02349900 0.17487100 4.10729200

H 0.04431800 -1.14945700 4.82946800
H 1.33506700 -1.51869800 3.63410700
O -0.04221000 1.49573000 -0.64931200
O 1.08726500 0.16147500 1.55619000
Ni 1.91756500 1.43403300 0.11839500
O 2.40563500 0.06556600 -1.28056400
O 2.45764500 3.27262500 -0.84081500
Cl 2.15965800 4.14626700 0.38716900
O 4.83413000 -0.10706500 -0.85426800
O 1.40701800 3.15148700 1.30120300
O 3.42535300 4.54423700 1.03710900
O 3.76139300 -1.46233200 -2.58661900
O 1.30156200 5.28525300 0.04603200
Cl 3.80339900 -0.13354400 -1.95258500
O 4.02561600 0.95726300 -2.91182200
O 3.73521100 1.37925800 1.07190600
H 4.11286300 2.26672000 1.17952300
H 4.32967600 0.87051600 0.46671400
C -2.57011000 -0.50213200 1.21569800
H -2.85814000 0.28756000 1.91074100
H -2.53117800 -1.42600100 1.79515600
C -4.46216900 -2.46287800 -2.33696000
C -3.40029600 -3.54381800 -2.10807000
C -2.50085100 -3.19184400 -0.91420500
C -3.80066700 -1.07744400 -2.37740900
C -0.75801000 -1.35384600 -0.44426800
H -0.16551800 -0.79860500 -1.17621000
N -2.95296700 -0.79940400 -1.20004400
N -1.96634200 -1.83677000 -1.10849400
C 0.12787000 -2.48800500 0.06331100
C -0.16908200 -3.26181600 1.19823300
C 1.28302200 -2.80101000 -0.66410900
C 0.66884500 -4.29864300 1.60544800
H -1.06651300 -3.07366600 1.77737000
C 2.13355100 -3.83515300 -0.27092200
H 1.54423200 -2.22031000 -1.54015500
C 1.81953600 -4.57580200 0.86549900
H 0.42905200 -4.89235300 2.48077100
H 3.03190800 -4.04553300 -0.83996000
Cl 2.87778200 -5.87889400 1.38007900
H -7.42909700 3.25321800 0.31574500
H -3.06124300 -3.31932700 0.02944200
H -1.66028600 -3.88320000 -0.87733900
H -4.55341900 -0.29229600 -2.46023100

H -3.13975600 -1.00703000 -3.24763500
H -2.76766600 -3.62718200 -2.99998700
H -3.86273800 -4.52324700 -1.94063800
H -4.99828800 -2.63616700 -3.27695900
H -5.21631600 -2.49613000 -1.54003500
Thermal Correction to Free Energy: 0.457774 Hartree
Entropy: 264.509 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.196408 Hartree
Thermal Free Energy with Correction: -3570.738634 Hartree

B-TS12

C 6.55318200 -1.86989600 -2.64288200
C 6.05975100 -0.59245300 -2.36656200
C 4.90292500 -0.43693800 -1.60364200
C 4.22425300 -1.55479500 -1.09611600
C 4.72965400 -2.82959700 -1.37811700
C 5.88319100 -2.98897900 -2.14882600
H 6.57429700 0.28394900 -2.75006400
H 4.52341000 0.56063500 -1.40442300
H 4.21326700 -3.70610600 -0.99490800
H 6.25718000 -3.98661600 -2.35970700
C 2.94021700 -1.41244400 -0.29011900
H 2.65508700 -2.41187200 0.06030200
C 0.41833600 -0.63454400 -0.65548900
C -0.32095300 -1.75567400 -0.10127300
C -0.40439500 0.38508600 -1.28891200
O 0.39169000 -2.89391500 -0.01516600
O 0.21440500 1.06551900 -2.25543600
C -0.30530400 -4.03706700 0.52928700
H 0.42791100 -4.84317000 0.52864100
H -0.65655500 -3.82514900 1.54123400
H -1.16058700 -4.29159100 -0.09894000
C -0.57021200 2.05656900 -2.95624700
H -0.82973400 2.87732400 -2.28433200
H 0.07713500 2.41114900 -3.75744500
H -1.47585300 1.59768200 -3.35500900
O -1.49274200 -1.76704900 0.31624800
O -1.57555800 0.70145900 -0.98417100
Ni -2.86731600 -0.30722700 0.19424900
O -3.84111300 -1.36884300 -1.27738500
O -3.73741500 -1.17950800 2.06022900
Cl -2.85875100 -0.35388300 2.98473700
O -2.72930200 -0.81407800 -3.41015800
O -2.15590700 0.61526800 1.98485200

O -3.64915200 0.41443900 3.95196800
O -5.02111200 -1.67988400 -3.38061800
O -1.82747800 -1.18925800 3.63729900
Cl -4.03682600 -0.81898900 -2.71405900
O -4.55501600 0.59461500 -2.58253000
O -4.33578900 1.12634300 0.03927600
H -3.99356600 2.01611800 0.19353100
H -4.58988900 1.07059400 -0.91603100
C 1.81453400 -0.88063800 -1.23041000
H 2.15993200 0.05316500 -1.67452600
H 1.75959500 -1.60258400 -2.05410800
C 4.08226500 -0.56962100 3.20473600
C 2.82122500 -1.23333900 3.80024200
C 1.75732900 -1.42212300 2.69374300
C 4.29846600 -1.01778800 1.75908500
C 1.05436600 0.44359400 1.23293000
H 0.73878000 -1.30602600 3.06994900
H 4.36660600 -2.11729200 1.72270000
H 1.83578400 -2.41461600 2.23924900
H 5.23345700 -0.62808000 1.35071500
H 0.10531900 0.31373800 1.74551800
N 3.18872300 -0.53579200 0.89343800
N 2.00087600 -0.40202700 1.66100400
C 1.28781800 1.82317300 0.76263500
C 2.50925100 2.32835700 0.27921500
C 0.20291700 2.71269600 0.90373500
C 2.64215000 3.67307700 -0.05252700
H 3.35481600 1.66131000 0.18605600
C 0.32663300 4.05743200 0.56679100
H -0.73711000 2.34922400 1.30454600
C 1.54809300 4.52907500 0.08537800
H 3.58762400 4.05784900 -0.41823100
H -0.50944400 4.73661500 0.69062900
Cl 1.71532900 6.21934700 -0.34263300
H 4.96771400 -0.81939800 3.79667200
H 3.98138100 0.52100000 3.22713300
H 2.42031100 -0.61849800 4.61126100
H 3.06466000 -2.21187700 4.22780200
H 7.45208800 -1.99029600 -3.24022700
Thermal Correction to Free Energy: 0.456722 Hartree
Entropy: 262.962 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.20447 Hartree
Thermal Free Energy with Correction: -3570.747748 Hartree

B-19

C 6.64338000 -2.81546200 -1.21533000
C 6.27332300 -1.48073700 -1.39809100
C 5.07952300 -1.00286700 -0.85876000
C 4.23809500 -1.84868200 -0.12119500
C 4.62142200 -3.18298400 0.05854200
C 5.81289500 -3.66648800 -0.48611400
H 6.91579600 -0.81086300 -1.96257800
H 4.80095100 0.03641000 -1.00367300
H 3.98064200 -3.85065300 0.62929400
H 6.09189000 -4.70555000 -0.33653600
C 2.91216400 -1.35566700 0.44034000
H 2.51435000 -2.15305200 1.08750000
C 0.57608600 -0.52431700 -0.25031700
C -0.27906700 -1.53074500 0.52786700
C -0.30723300 -0.03020100 -1.39582300
O 0.19332100 -2.76085200 0.55475800
O 0.30901700 0.05543000 -2.55106000
C -0.64644300 -3.76049500 1.19822800
H -0.13700800 -4.70622700 1.02472700
H -0.72424000 -3.54373700 2.26499400
H -1.63710000 -3.74972100 0.74317300
C -0.47000900 0.53939100 -3.67799900
H -0.74446500 1.58174700 -3.50635200
H 0.19502700 0.44988600 -4.53464000
H -1.36011000 -0.07851000 -3.79609300
O -1.33047300 -1.23275900 1.09609000
O -1.48614300 0.31975800 -1.26255000
Ni -2.86268700 -0.15740400 0.20500300
O -3.42959900 -1.97038400 -0.60728500
O -3.95798700 -0.23498100 2.03732200
Cl -3.41645800 1.10208400 2.56535100
O -1.88943000 -2.41991200 -2.47195900
O -2.56033900 1.56968600 1.34470700
O -4.49774200 2.05782600 2.81604500
O -4.09311700 -3.49019100 -2.39032400
O -2.54398400 0.89811800 3.73027100
Cl -3.32731600 -2.26825700 -2.12733900
O -3.90938800 -1.08470600 -2.85587000
O -4.37222600 0.73321100 -0.87040900
H -4.17188500 1.64644400 -1.11434400
H -4.40869900 0.20149300 -1.69916300
C 1.92102000 -1.10550500 -0.71971600
H 2.37317900 -0.39688200 -1.41492500

H 1.76476700 -2.03690900 -1.26817700
C 3.71473000 0.66073600 3.48687400
C 2.37872200 0.19828000 4.09997600
C 1.40531000 -0.23459000 2.97426500
C 4.08502700 -0.22395500 2.29874400
C 0.87121400 0.74763900 0.72772900
H 0.38446100 0.09017600 3.18919300
H 4.14171900 -1.27028200 2.64329500
H 1.38081800 -1.33393500 2.89122700
H 5.07211900 0.02884300 1.90129300
H -0.06505800 0.92877100 1.25694800
N 3.08918400 -0.09776800 1.20188900
N 1.84785300 0.41097600 1.72989000
C 1.19033900 2.02770800 -0.04570000
C 2.46560500 2.35098500 -0.53332300
C 0.15169500 2.95107300 -0.24583700
C 2.69193800 3.54191600 -1.22242800
H 3.28979500 1.67756400 -0.33665400
C 0.36272100 4.14420000 -0.93831400
H -0.83330700 2.75060400 0.16372200
C 1.63476900 4.42634700 -1.43069600
H 3.68256900 3.78427800 -1.59140400
H -0.44658700 4.85272500 -1.07700500
Cl 1.91478600 5.92211800 -2.31054500
H 4.51686400 0.61531000 4.23094000
H 3.63848300 1.69996100 3.15433200
H 1.93856800 1.00909400 4.68838000
H 2.54400300 -0.64144000 4.78479300
H 7.57258700 -3.18718100 -1.63716400
Thermal Correction to Free Energy: 0.459229 Hartree
Entropy: 260.989 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.207772 Hartree
Thermal Free Energy with Correction: -3570.748543 Hartree

B-TS13

C 7.28377300 -1.46053000 -1.13843600
C 6.38382000 -0.55093500 -1.69760700
C 5.09277500 -0.43138200 -1.18177800
C 4.67414100 -1.20985500 -0.09065700
C 5.58957900 -2.12120600 0.45418300
C 6.88087800 -2.24949600 -0.06110400
H 6.68331500 0.05899200 -2.54525100
H 4.40446700 0.26553700 -1.65100100
H 5.28287100 -2.74469700 1.29081300

H 7.56793400 -2.96750200 0.37733700
C 3.27541700 -1.10673800 0.52557300
H 3.16068900 -1.96089100 1.19714800
C 0.77177200 -0.78583700 -0.19117200
C 0.13388100 -1.36908100 0.97431800
C -0.11762700 -0.34524500 -1.24499900
O 0.87737100 -2.27107400 1.62452200
O 0.49632000 -0.12392700 -2.41701700
C 0.25720800 -2.89844200 2.76913000
H 0.99391500 -3.61324300 3.13412600
H 0.02270900 -2.15525200 3.53360300
H -0.66004500 -3.40551400 2.46535100
C -0.35762200 0.16920900 -3.54128200
H -0.86000600 1.12889900 -3.40076900
H 0.31100900 0.21051100 -4.40096500
H -1.09591200 -0.62468900 -3.66371500
O -0.98158900 -1.05668800 1.43650800
O -1.34465700 -0.11775200 -1.15944900
Ni -2.62159400 -0.75986600 0.27776100
O -2.50338000 -2.77594700 -0.24926900
O -3.88476800 -0.96818100 2.00979100
Cl -3.94518500 0.53115700 2.31838800
O -0.91378600 -3.06982400 -2.10747000
O -3.10982800 1.11999900 1.14660300
O -5.32242700 1.03597400 2.25967400
O -2.68622900 -4.71372000 -1.71007600
O -3.28377300 0.83666700 3.59699300
Cl -2.32297400 -3.29138600 -1.69739500
O -3.24319300 -2.48912600 -2.58561000
O -4.24153000 -0.55114000 -0.98799600
H -4.21965700 0.31068200 -1.42415200
H -4.07394000 -1.23385700 -1.68091900
C 2.18030600 -1.20294700 -0.57089700
H 2.47491700 -0.58755900 -1.42034300
H 2.19001600 -2.23554500 -0.93992500
C 3.87124900 1.71960200 3.03004200
C 4.02061200 2.82628300 1.96276000
C 3.60571900 2.30693600 0.56296800
C 4.10829100 0.34180900 2.41231400
C 1.27788700 1.32945700 0.70662800
H 0.75658800 0.93153800 1.56902800
N 3.05590100 0.06217100 1.42240700
N 2.62502500 1.21722200 0.72094000
C 0.57535300 2.35030400 -0.06634400

C -0.64106700 2.83842400 0.44534600
C 1.03110100 2.83748600 -1.30893200
C -1.35922700 3.82071500 -0.23033200
H -1.04678100 2.43319600 1.36565900
C 0.32163200 3.81847900 -1.99040500
H 1.92429700 2.42285700 -1.76276000
C -0.86578600 4.31265200 -1.43836700
H -2.29718200 4.18562100 0.17149100
H 0.67239400 4.19377700 -2.94522900
Cl -1.75509200 5.55079900 -2.29691200
H 4.46649900 1.90357200 0.02567000
H 3.17041600 3.10092300 -0.03998000
H 3.41162000 3.69344400 2.23682800
H 5.05956000 3.16938600 1.90604900
H 8.28611600 -1.55808000 -1.54473400
H 4.05971100 -0.44959500 3.16817800
H 5.11544500 0.30216500 1.96938200
H 4.57450400 1.88132400 3.85196100
H 2.86529900 1.74472200 3.46364200
Thermal Correction to Free Energy: 0.455939 Hartree
Entropy: 264.438 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.196486 Hartree
Thermal Free Energy with Correction: -3570.740547 Hartree

B-21

C 7.07222300 -1.79100600 -0.81856000
C 6.44725800 -0.63043400 -0.35681000
C 5.07388900 -0.61697200 -0.11029000
C 4.29898900 -1.77176200 -0.31023500
C 4.94245600 -2.93193600 -0.76263300
C 6.31407300 -2.94392900 -1.02252400
H 7.03116700 0.27049100 -0.18926800
H 4.59392000 0.28299600 0.25625100
H 4.36079900 -3.83806200 -0.91772400
H 6.78842700 -3.85413900 -1.37840100
C 2.79235700 -1.81854000 -0.07133900
H 2.49898000 -2.87161200 -0.11305800
C 0.68304900 -0.49689400 -0.52129600
C -0.15789600 -1.60551600 0.13972700
C -0.26558600 0.18148300 -1.51363500
O 0.09858800 -2.82144800 -0.29738200
O 0.26001800 0.41331900 -2.69139300
C -0.75718300 -3.88592600 0.19896900
H -0.43790700 -4.77476400 -0.34189900

H -0.60529700 -4.00536200 1.27339000
H -1.79930100 -3.64538800 -0.00940200
C -0.59378500 1.04430100 -3.68514800
H -0.83499800 2.05917800 -3.36438200
H 0.00251100 1.05744800 -4.59526500
H -1.50139700 0.45414400 -3.81033700
O -1.08587900 -1.36794100 0.91882300
O -1.41824200 0.52255000 -1.22678700
Ni -2.68311600 -0.18270900 0.27744600
O -3.34057800 -1.82563600 -0.79600500
O -3.70763600 -0.56442400 2.10540900
Cl -3.18931900 0.69662000 2.81330500
O -1.96718700 -2.00110700 -2.82834400
O -2.34550000 1.34277100 1.66765500
O -4.28804700 1.59026700 3.18989200
O -4.19704800 -3.01538700 -2.74053700
O -2.31479600 0.35231000 3.94163900
Cl -3.36743200 -1.87202500 -2.34878400
O -3.95871500 -0.57187900 -2.82722300
O -4.24148700 0.88886400 -0.53843400
H -4.03713000 1.82834200 -0.63429100
H -4.34356100 0.50882200 -1.44129500
C 1.97228600 -1.05861200 -1.15426500
H 2.54983200 -0.23102900 -1.56577200
H 1.73574600 -1.72590500 -1.98475100
C 2.14078200 -1.57613900 3.67742200
C 1.70382800 -0.08881800 3.66041300
C 2.47995400 0.67997700 2.58392100
C 2.92553300 -1.93296400 2.40733100
C 1.05146700 0.58093800 0.59270600
H 0.21022500 0.58439600 1.29601400
N 2.27892600 -1.34876400 1.23106600
N 2.31116400 0.12565700 1.22299000
C 1.22461300 2.00252700 0.06621800
C 0.21889400 2.95237700 0.29684700
C 2.37404900 2.40568000 -0.63038300
C 0.33795000 4.26047700 -0.17542300
H -0.66357600 2.67351300 0.86414600
C 2.50589400 3.70714600 -1.11178800
H 3.18560900 1.70464900 -0.78331100
C 1.48078700 4.62545200 -0.88399600
H -0.44142100 4.98981500 0.01626700
H 3.39690500 4.01005000 -1.65058500
Cl 1.64210900 6.26826700 -1.48522700

H 3.55039000 0.68237300 2.81792100
H 2.17021200 1.72727700 2.53908500
H 0.62859400 -0.01373200 3.47007700
H 1.87505000 0.38421000 4.63294100
H 8.14046300 -1.79634500 -1.01494200
H 2.93902700 -3.01657100 2.25149800
H 3.97776000 -1.61840900 2.48999700
H 2.77223400 -1.79145300 4.54630200
H 1.25907000 -2.21952800 3.75603800
Thermal Correction to Free Energy: 0.46013 Hartree
Entropy: 260.035 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.209216 Hartree
Thermal Free Energy with Correction: -3570.749086 Hartree

B-TS9

C -7.40719500 -1.48449300 0.28634100
C -6.70593700 -0.89603900 1.34187200
C -5.46020600 -0.31167600 1.11727300
C -4.90008200 -0.29703300 -0.16875900
C -5.61216400 -0.88636600 -1.21977800
C -6.85589900 -1.48078100 -0.99487300
H -7.12832000 -0.89678100 2.34265100
H -4.91793500 0.14272900 1.94165400
H -5.18745100 -0.88586900 -2.22056100
H -7.39199600 -1.93813300 -1.82136000
C -3.51890300 0.29042900 -0.42286200
H -3.35890200 0.33185700 -1.50791900
C -0.98440300 -0.35357900 0.15372600
C -0.32343800 -0.36539000 -1.12927900
C -0.17329500 -0.68577400 1.30536100
O -1.17429500 -0.33663900 -2.17975400
O -0.86528000 -0.73553300 2.45901400
C -0.57134400 -0.47428400 -3.48417700
H 0.01726300 -1.39178800 -3.53401900
H -1.40784300 -0.51256900 -4.18178800
H 0.07834000 0.37576300 -3.70516300
C -0.16214100 -1.25878100 3.60311500
H 0.66319800 -0.60091900 3.88464600
H -0.90575000 -1.30182900 4.39873900
H 0.21925700 -2.25607800 3.37717200
O 0.90110500 -0.35466100 -1.36570800
O 1.06400100 -0.86001500 1.35177600
Ni 2.27216600 -1.29808700 -0.21452000
O 1.31012300 -3.09585500 -0.68472600

O 3.66803100 -1.18932700 -1.86780200
Cl 4.31953600 0.11338200 -1.39249500
O -0.52088600 -3.54848300 0.90019900
O 3.57658900 0.36578100 -0.05750000
O 5.75715100 -0.06198000 -1.15378000
O 0.53379500 -5.37610600 -0.34432100
O 4.03655500 1.21577600 -2.33206600
Cl 0.74374000 -4.09845600 0.34755700
O 1.75802500 -4.24271500 1.45575500
O 3.60642800 -2.34366700 0.96010400
H 3.84515500 -1.82965200 1.74238200
H 3.09556900 -3.13243800 1.26117900
C -2.47623400 -0.68285000 0.20557700
H -2.75297300 -0.82269600 1.25021100
H -2.63732100 -1.65009900 -0.28418400
C -4.16006800 3.92266700 -0.65788200
C -3.24080800 3.66957900 -1.85204900
C -1.95137900 2.98753800 -1.36634000
C -4.59043800 2.57287100 -0.08215300
C -1.22721200 1.91244200 0.75534900
H -1.62854100 1.52223900 1.68374900
N -3.44090800 1.65801500 0.16103000
N -2.19161100 2.27993400 -0.08898100
C 0.13123300 2.46035900 0.82562000
C 0.99193300 2.68787100 -0.26528600
C 0.59546000 2.76797500 2.12060200
C 2.25435500 3.23828100 -0.07450700
H 0.71412400 2.38484300 -1.26610600
C 1.84578400 3.34091000 2.31904600
H -0.04170500 2.57524700 2.97881200
C 2.66584900 3.57927800 1.21456800
H 2.92741800 3.36041100 -0.91439400
H 2.18754800 3.59373200 3.31623700
Cl 4.24255500 4.29043700 1.45690700
H -5.05510000 4.47692700 -0.95629800
H -3.64539600 4.52859000 0.09747200
H -8.37545400 -1.94345000 0.46303900
H -1.55907600 2.28715000 -2.11026800
H -1.18055800 3.73350700 -1.16201600
H -2.98030600 4.59530800 -2.37304400
H -3.75978900 3.03167200 -2.57682800
H -5.27376300 2.09716000 -0.79246600
H -5.14337500 2.70326600 0.85465500
Thermal Correction to Free Energy: 0.456874 Hartree

Entropy: 262.497 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.195841 Hartree

Thermal Free Energy with Correction: -3570.738967 Hartree

B-14

C -7.41472900 -1.15774200 0.53216800

C -6.70474600 -0.41204600 1.47695800

C -5.44613200 0.09980400 1.16528600

C -4.87854800 -0.11923800 -0.09909800

C -5.60055400 -0.86276600 -1.03956500

C -6.85878600 -1.38247700 -0.72722600

H -7.13276200 -0.22960500 2.45869700

H -4.89934900 0.68687300 1.89739100

H -5.17373300 -1.03942600 -2.02383000

H -7.40321300 -1.95955100 -1.46916500

C -3.48650800 0.39399000 -0.43588300

H -3.32609800 0.25151800 -1.51421700

C -0.97597100 0.02204400 0.26852700

C -0.32641500 -0.39782900 -1.04595600

C -0.14391900 -0.52825700 1.43095700

O -1.18912000 -0.78258700 -1.97316000

O -0.80671600 -0.49914800 2.57464400

C -0.62206900 -1.29884500 -3.20683000

H 0.01878200 -2.15179900 -2.98049800

H -1.48116400 -1.59614300 -3.80530700

H -0.04304400 -0.52094300 -3.70750000

C -0.12871000 -1.04082100 3.73461100

H 0.74964200 -0.43668200 3.96951800

H -0.86177600 -0.98986100 4.53765000

H 0.16466500 -2.07215900 3.53370200

O 0.88417600 -0.40503400 -1.27994800

O 1.03366600 -0.89585500 1.40701000

Ni 2.27475700 -1.42538400 -0.14457600

O 1.19711200 -3.14224100 -0.61843500

O 3.62678600 -1.45143600 -1.77689800

Cl 4.39405000 -0.19216400 -1.32812500

O -0.78349100 -3.28735500 0.83321800

O 3.65779400 0.13895900 -0.00142400

O 5.80524400 -0.49267100 -1.07095600

O 0.16427600 -5.30469000 -0.18643800

O 4.20742600 0.90340200 -2.29184700

Cl 0.45436400 -4.00845200 0.43277800

O 1.36101100 -4.15686300 1.62607600

O 3.48489700 -2.55854700 1.06627400

H 3.84570200 -2.05463600 1.80751900

H 2.89597400 -3.26148900 1.42377500

C -2.45669800 -0.45826100 0.35355600

H -2.75034100 -0.42432600 1.40234200

H -2.52016600 -1.49953500 0.03281400

C -3.83622600 3.80940600 -1.46768900

C -2.90484900 3.10517400 -2.45442200

C -1.66513000 2.58032500 -1.70849400

C -4.34702400 2.78927700 -0.43682000

C -1.04495100 1.65310300 0.54489100

H -1.51159000 1.65271500 1.53195700

N -3.31566700 1.80558100 -0.03360600

N -2.00682000 2.30631400 -0.29763600

C 0.27491500 2.39816400 0.68285600

C 1.26511500 2.49251600 -0.30561100

C 0.48582800 3.08317500 1.89087200

C 2.42527000 3.23889700 -0.09754700

H 1.16768600 1.96904000 -1.24692100

C 1.63513300 3.83764500 2.11397400

H -0.26943800 3.03755500 2.67094000

C 2.60007300 3.90950500 1.11028000

H 3.19140000 3.27480300 -0.86309100

H 1.78068000 4.36373300 3.05091200

Cl 4.05549600 4.85310100 1.37885300

H -4.69000900 4.26313600 -1.98226100

H -3.29480800 4.61959000 -0.96703900

H -8.39426600 -1.55822800 0.77652500

H -1.25021900 1.71153400 -2.23988200

H -0.88581300 3.34823500 -1.69557700

H -2.58643400 3.77429400 -3.25982300

H -3.44250000 2.27535800 -2.93003500

H -5.19000700 2.23707500 -0.86001200

H -4.72075400 3.30825200 0.45497100

Thermal Correction to Free Energy: 0.458006 Hartree

Entropy: 263.417 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3571.200703 Hartree

Thermal Free Energy with Correction: -3570.742697 Hartree

B-TS10

C 6.56117900 -2.60782700 -0.76400700

C 5.71841500 -2.02937200 -1.71474200

C 4.83116000 -1.01557700 -1.34828600

C 4.77789200 -0.55520600 -0.02715300

C 5.64167000 -1.13135000 0.91457700

C 6.51796600 -2.15584100 0.55566100
H 5.74974300 -2.36770200 -2.74685600
H 4.16725000 -0.58245700 -2.08757700
H 5.63063900 -0.77415500 1.94220300
H 7.17340700 -2.59161000 1.30414800
C 3.84833100 0.56318500 0.43886200
H 4.45296400 1.16047900 1.14371600
C 1.21370700 -0.01260200 0.71415300
C 0.94885200 -1.06845800 -0.27073800
C 0.09644300 0.25352400 1.61952300
O 2.04671500 -1.68645000 -0.69390900
O 0.43930900 0.91856300 2.73776800
C 1.85921600 -2.77383200 -1.63316000
H 1.40101500 -2.40258600 -2.55209000
H 2.86277700 -3.15071900 -1.82147700
H 1.22209500 -3.54238000 -1.19328800
C -0.62411300 1.16275100 3.68403600
H -1.07146400 0.21938500 4.00191600
H -0.14515300 1.66474300 4.52439100
H -1.39393000 1.79523500 3.23896600
O -0.15301400 -1.37932700 -0.75540100
O -1.10351200 -0.01643200 1.43621700
Ni -1.92149200 -1.44304100 0.23554900
O -2.66893400 -0.29116800 -1.30290300
O -2.41892800 -3.41023100 -0.48830700
Cl -1.62698500 -4.17587200 0.58907100
O -4.76819500 0.45701700 -0.25685900
O -1.08874400 -3.02225500 1.45704400
O -2.52879900 -5.03288000 1.37096600
O -4.26335800 1.01136300 -2.59139100
O -0.51281200 -4.92799700 -0.01383300
Cl -4.17884600 -0.03537700 -1.55572100
O -4.81812300 -1.29975500 -1.96264700
O -3.69965200 -1.48783500 1.29126000
H -4.15528100 -2.30783500 1.04674000
H -4.25080800 -0.75405000 0.92652800
C 2.62657600 0.06310700 1.30808700
H 2.90542800 -0.92230200 1.69473400
H 2.56249800 0.72000800 2.17447700
C 4.49080600 3.64196700 -1.20054500
C 4.17505500 3.92637000 0.26784800
C 2.75278500 3.43216800 0.59065500
C 4.50576800 2.12363600 -1.43007100
C 1.15651000 1.79987300 -0.49745000

H 1.11501400 1.19593900 -1.39572800
N 3.42501800 1.41512400 -0.69134300
N 2.40038700 2.30673500 -0.29610600
C -0.08142200 2.55621100 -0.22106400
C -0.29584000 3.37787300 0.90488200
C -1.12042000 2.43836500 -1.16157300
C -1.47688600 4.09621700 1.05106900
H 0.44218200 3.43883600 1.69277800
C -2.30929400 3.15072900 -1.02529200
H -1.01461300 1.76622900 -2.00603000
C -2.47202900 3.98858600 0.07564000
H -1.63157700 4.73217700 1.91562800
H -3.10472500 3.02356100 -1.74965000
Cl -3.94825600 4.90716000 0.25938200
H 7.24898200 -3.39803100 -1.05002600
H 4.42029700 1.89599400 -2.49875600
H 5.46055800 1.71351100 -1.09093800
H 3.73925900 4.12072300 -1.83900800
H 5.46202600 4.05761300 -1.48633200
H 4.91191900 3.42528600 0.90586900
H 4.23720100 4.99449100 0.49605100
H 2.03335300 4.22881700 0.39109700
H 2.66278600 3.15456400 1.64932800
Thermal Correction to Free Energy: 0.457432 Hartree
Entropy: 262.438 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.188559 Hartree
Thermal Free Energy with Correction: -3570.731127 Hartree

B-16

C 6.69508100 -2.30184000 0.16678100
C 5.71572400 -2.32322500 -0.82756200
C 4.72381900 -1.34071700 -0.86383300
C 4.69777200 -0.31336100 0.08769800
C 5.69712200 -0.29464600 1.07123400
C 6.68124800 -1.28201800 1.11976200
H 5.72339400 -3.10530300 -1.58187600
H 3.96496000 -1.36953100 -1.63734800
H 5.70733600 0.50620300 1.80759600
H 7.44291200 -1.24704300 1.89344600
C 3.65007800 0.79618600 0.11152900
H 4.20555900 1.71207000 0.37255500
C 1.15980700 0.29036600 0.69080000
C 1.07762100 -1.10042900 0.04165600
C 0.07581900 0.23473900 1.76642100

O 2.07689500 -1.89674000 0.34958900
O 0.44301200 0.71364000 2.94277700
C 2.01305600 -3.26490600 -0.14126000
H 1.84401200 -3.26555200 -1.21850600
H 2.98265400 -3.69152800 0.10543900
H 1.20185600 -3.79213300 0.36053200
C -0.57770500 0.75117800 3.97411700
H -0.98910300 -0.24678800 4.12975000
H -0.06475500 1.10938000 4.86486000
H -1.37214200 1.43702600 3.67515900
O 0.12098600 -1.47410200 -0.63915100
O -1.06087700 -0.20219000 1.57708400
Ni -1.83648000 -1.49691700 0.12696400
O -2.37417000 -0.14240800 -1.26741900
O -2.29830900 -3.35573600 -0.83545900
Cl -1.95499100 -4.21930300 0.38798900
O -4.81041600 -0.07512300 -0.86248200
O -1.25329600 -3.19214100 1.30635800
O -3.19774300 -4.68556500 1.03609800
O -3.78524700 1.30980200 -2.60102100
O -1.03939900 -5.31085900 0.04020200
Cl -3.77300200 -0.01278700 -1.95304700
O -3.93801100 -1.12225000 -2.90278000
O -3.66064700 -1.51813100 1.07060700
H -4.00371400 -2.42027200 1.17049000
H -4.27151700 -1.03039900 0.46439200
C 2.56915600 0.60976900 1.23798500
H 2.88743200 -0.16893500 1.93233300
H 2.49647800 1.53207000 1.81691400
C 3.64163000 2.72006700 -2.83098900
C 3.62420500 3.63883700 -1.60721600
C 2.40409000 3.31468800 -0.71290200
C 3.75371100 1.25642000 -2.37591700
C 0.72347200 1.40351400 -0.41516700
H 0.18557700 0.82640500 -1.17139400
N 2.93050800 0.96682600 -1.16885800
N 1.91765200 1.96180600 -1.03765300
C -0.23491400 2.48544400 0.07497400
C -0.02774200 3.24864900 1.23630500
C -1.36788400 2.76119400 -0.70116600
C -0.92737900 4.24293700 1.61800000
H 0.84312800 3.08260200 1.86039100
C -2.27960400 3.75133100 -0.33379500
H -1.56424100 2.18261500 -1.59539100

C -2.05092300 4.48597100 0.82688800
H -0.75601000 4.82941800 2.51402200
H -3.15990800 3.93113400 -0.94016200
Cl -3.18631300 5.73594700 1.30804100
H 7.46576700 -3.06651100 0.19334900
H 3.44796100 0.58255400 -3.18501600
H 4.79535400 1.02480000 -2.13872400
H 2.72621500 2.86412100 -3.41310300
H 4.48480900 2.95914400 -3.48826800
H 4.55609500 3.50499800 -1.04417300
H 3.59077200 4.69210800 -1.90260100
H 1.58624900 4.00297100 -0.93370900
H 2.66458000 3.46559400 0.34764700
Thermal Correction to Free Energy: 0.457337 Hartree
Entropy: 265.292 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3571.190096 Hartree
Thermal Free Energy with Correction: -3570.732759 Hartree

B-12

C 5.97681500 -0.41771900 -0.51274500
C 4.97755900 -0.22830300 -1.46824700
C 3.70736300 0.21152000 -1.08736400
C 3.41866800 0.47060800 0.25865200
C 4.43371100 0.28874800 1.20804700
C 5.69979500 -0.15733900 0.83068100
H 5.18583200 -0.41728300 -2.51788900
H 2.93097900 0.35864900 -1.82930300
H 4.23025500 0.50260800 2.25526500
H 6.47196300 -0.29111400 1.58308600
C 2.03942100 0.93248000 0.72796400
H 2.21614500 1.58394600 1.60059400
C 0.19350000 -0.83796400 0.19870500
C 0.98220900 -1.64107800 -0.86671800
C -0.73984700 -1.89228700 0.80596200
O 1.74996300 -2.57029600 -0.26772600
O -0.92065700 -1.74669500 2.13772700
C 2.50630200 -3.41685400 -1.15177700
H 3.25076900 -2.82699400 -1.69072300
H 2.99350500 -4.14883000 -0.50833600
H 1.84278800 -3.90909100 -1.86575600
C -1.81769900 -2.70178800 2.73508400
H -1.46197100 -3.71923900 2.56072300
H -1.82296900 -2.47136800 3.80015700
H -2.81902700 -2.59811200 2.31079700

O 0.92725000 -1.48954700 -2.06585000
O -1.27199500 -2.76726300 0.15831800
C 1.14754000 -0.22720300 1.25293100
H 1.78199700 -1.00896100 1.67371500
H 0.52804800 0.14519200 2.06986200
C 1.38686100 4.01813200 0.44593900
C -0.12834600 3.93641800 0.67187500
C -0.57488600 2.48497400 0.90709200
C 1.81457300 3.00218400 -0.62708400
C -0.61444000 0.33721800 -0.54065600
H -0.34365700 0.19451600 -1.58765500
N 1.32977100 1.64325700 -0.35724900
N -0.08962200 1.66584900 -0.20905300
C -2.13425200 0.26996900 -0.47737700
C -2.87397100 0.26996600 0.71578900
C -2.84334800 0.22463000 -1.68441600
C -4.26778200 0.22798400 0.70673400
H -2.36425900 0.29256600 1.67258600
C -4.23670900 0.18019000 -1.71538900
H -2.29576800 0.21804600 -2.62197200
C -4.93925900 0.18404900 -0.51352000
H -4.82742000 0.23181100 1.63552600
H -4.76916800 0.14116700 -2.65895600
Cl -6.69789900 0.13143100 -0.53253800
H 6.96447600 -0.75665500 -0.81188600
H -0.22497400 2.14399600 1.89830200
H -1.66437700 2.44027000 0.91668200
H 2.90363000 2.96017000 -0.72075600
H 1.40485900 3.29895500 -1.59899800
H -0.65119800 4.31474400 -0.21501300
H -0.43185500 4.55767600 1.52253300
H 1.68128800 5.02767000 0.13632100
H 1.91418800 3.81678600 1.38763600
Thermal Correction to Free Energy: 0.41799 Hartree
Entropy: 187.665 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.932734 Hartree
Thermal Free Energy with Correction: -1801.514744 Hartree

B-10

C -6.29615400 -0.15850000 -1.35779700
C -5.22547700 -0.28549800 -2.24644900
C -3.91721300 -0.33004300 -1.76787900
C -3.65681700 -0.25623500 -0.39096800
C -4.73697500 -0.13427000 0.49002200

C -6.04818600 -0.08248600 0.01239400
H -5.41069100 -0.34919300 -3.31499700
H -3.08610900 -0.44128300 -2.45769700
H -4.54979700 -0.07709200 1.55950400
H -6.87369000 0.01337900 0.71186700
C -2.23138400 -0.25723600 0.13595300
H -2.28255000 -0.30721300 1.23581000
C -0.04330500 1.15289300 0.14886100
C 0.12425600 1.37820000 1.66397500
C 0.56421400 2.39757900 -0.51556800
O -0.87102000 2.13679700 2.16400900
O 0.53935500 2.30430300 -1.85898300
C -0.72487600 2.50737100 3.54642900
H 0.18785800 3.09093600 3.68480700
H -1.60375800 3.10633000 3.78270000
H -0.67970100 1.61907100 4.18052100
C 1.11737200 3.41727100 -2.56726300
H 2.17160900 3.52736000 -2.30400000
H 1.00790900 3.17801400 -3.62427200
H 0.58958500 4.34148300 -2.32251200
O 1.03626600 0.96075600 2.34294400
O 1.01068100 3.35600000 0.07996100
C -1.54563600 1.07027400 -0.26179900
H -1.59725800 1.16391600 -1.34898500
H -2.09490600 1.90561300 0.17486800
C -1.88299400 -3.34086300 1.06044100
C -0.43693200 -3.25418700 1.56281300
C 0.07256600 -1.81570600 1.43644500
C -1.98182000 -2.72295900 -0.34317400
C 0.61979000 -0.17080400 -0.40603800
H 0.38518200 -0.11945900 -1.47520900
N -1.43355900 -1.36328000 -0.44409900
N -0.07888600 -1.37506700 0.03706600
C 2.13734900 -0.35797200 -0.33212800
C 3.04615600 0.57863300 0.17162900
C 2.65176700 -1.53183700 -0.90704800
C 4.42380300 0.35586700 0.10360100
H 2.70128800 1.48648400 0.64630700
C 4.02066900 -1.77332100 -0.97527700
H 1.95736400 -2.26920600 -1.29632000
C 4.90081000 -0.81845100 -0.46800100
H 5.11615400 1.08831300 0.50325400
H 4.40182700 -2.68586300 -1.42013000
Cl 6.63691200 -1.10618800 -0.55123200

H -7.31510800 -0.12151800 -1.73184200
H -0.46598200 -1.17988500 2.15513800
H 1.13173800 -1.74414500 1.69051500
H -3.01622100 -2.69940000 -0.69131400
H -1.40665800 -3.33637500 -1.04701900
H 0.20270200 -3.91286500 0.96194500
H -0.35964200 -3.58289400 2.60549100
H -2.22876400 -4.38080600 1.02766500
H -2.55092100 -2.80924100 1.75158700
Thermal Correction to Free Energy: 0.417512 Hartree
Entropy: 188.805 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.937784 Hartree
Thermal Free Energy with Correction: -1801.520272 Hartree

B-7

C -5.37639000 -1.65893500 -2.50455800
C -4.39611500 -2.48865900 -1.95788100
C -3.42076300 -1.96267500 -1.10936300
C -3.41090700 -0.59988400 -0.79767600
C -4.40092700 0.22508000 -1.34677300
C -5.37725600 -0.29764700 -2.19479100
H -4.39294000 -3.55035600 -2.18932600
H -2.66686600 -2.60260900 -0.66378600
H -4.41100700 1.28573800 -1.10326200
H -6.14152800 0.35516000 -2.60732600
C -2.32605200 0.01012600 0.08777700
H -2.80676300 0.79501700 0.68974900
C -0.07927200 1.18574400 0.11975100
C -0.56619100 2.23158700 1.14913600
C 0.98570800 1.94801000 -0.68713500
O -1.26854400 3.20343400 0.53476600
O 1.02148900 1.57856600 -1.97820100
C -1.69241400 4.28883800 1.38065200
H -2.23849900 4.97062500 0.72965900
H -2.33654100 3.92095400 2.18242000
H -0.82435500 4.78623100 1.81861200
C 2.04745300 2.20845800 -2.76929300
H 3.03471100 1.95474700 -2.37763800
H 1.92017700 1.81489800 -3.77704400
H 1.92492400 3.29349500 -2.75831700
O -0.35717300 2.21617400 2.34163900
O 1.71676400 2.78719000 -0.20551900
C -1.24479500 0.69559300 -0.76623900
H -0.85564800 -0.00644800 -1.50372600

H -1.68467600 1.53418300 -1.30845000
C -1.63885600 -2.01636600 3.22638500
C -0.17613900 -2.37879700 2.94401300
C 0.06238300 -2.43919000 1.42662300
C -2.03272700 -0.76478700 2.43650300
C 0.56908500 -0.05301900 0.88228800
H 0.66950200 0.26593200 1.92641000
N -1.72006300 -0.96258100 1.01053600
N -0.34030300 -1.21737600 0.71246000
C 1.95967500 -0.41228300 0.37559100
C 3.08943600 0.02599700 1.07586800
C 2.14816900 -1.16131000 -0.79497900
C 4.37804300 -0.26814200 0.62944400
H 2.96328300 0.61557300 1.97926900
C 3.42780500 -1.46910700 -1.25306000
H 1.28119700 -1.52146400 -1.33799800
C 4.53459700 -1.01642000 -0.53471000
H 5.24730000 0.07626200 1.17822000
H 3.56785900 -2.05529300 -2.15459500
Cl 6.15425600 -1.40156800 -1.10840600
H -0.53159700 -3.25597500 0.99983400
H 1.11218000 -2.64003000 1.20519700
H 0.48962800 -1.63396400 3.39924800
H 0.08180900 -3.34541100 3.39260700
H -1.80584700 -1.84960400 4.29657600
H -2.28617000 -2.84635200 2.91638000
H -3.11410200 -0.60521800 2.50282300
H -1.53977800 0.12412400 2.86083300
H -6.13763800 -2.07004600 -3.16136700
Thermal Correction to Free Energy: 0.415809 Hartree
Entropy: 191.765 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.939695 Hartree
Thermal Free Energy with Correction: -1801.523886 Hartree

B-5

C 1.73989600 -0.33860700 3.77789600
C 1.10059600 0.67310000 2.82353300
C 1.73276800 -1.94400100 1.85610700
C 2.58310200 -1.34148700 2.98370000
H 0.40926200 1.32944200 3.35683400
H 1.88368000 1.32236800 2.40461900
H 2.95726900 -2.14423500 3.63004400
H 3.46398700 -0.84028800 2.56017900
C -0.65163200 0.72550800 1.02801700

C 0.96625500 0.48991600 -0.96200300
C 1.93665400 -0.23384400 -0.00503200
H -0.96973900 1.53880900 1.68239400
H 0.37470100 -0.26572400 -1.48132600
H 1.53173000 1.03954900 -1.71739500
H 2.59191200 0.51266100 0.47397800
N 0.32002600 -0.04807400 1.79851400
N 1.09433500 -0.94716900 0.98506400
C 2.82694400 -1.18015800 -0.79251200
C 4.20627000 -0.95432900 -0.86404100
C 2.29012300 -2.27150200 -1.49317900
C 5.03286400 -1.79098000 -1.61682300
H 4.63719800 -0.11294800 -0.32691400
C 3.11364400 -3.11247400 -2.23959000
H 1.22317900 -2.46639800 -1.44262600
C 4.48855400 -2.87372500 -2.30649400
H 6.10066200 -1.59666500 -1.66095400
H 2.68167700 -3.95467800 -2.77270700
H 5.12868700 -3.52774000 -2.89130900
C -1.90407100 -0.08462400 0.69152100
C -3.15290800 0.54952300 0.76343400
C -1.87170500 -1.44228300 0.34525600
C -4.33588800 -0.13558700 0.48308600
H -3.20810500 1.59844300 1.03927400
C -3.04469200 -2.14321000 0.06782700
H -0.91494700 -1.94864000 0.30527300
C -4.26913500 -1.48163800 0.13397500
H -5.29506900 0.36601000 0.54845000
H -3.00992800 -3.19469000 -0.19572200
Cl -5.75419800 -2.36227500 -0.22042200
C -0.00141900 1.44569400 -0.23355300
C 0.70616400 2.73835400 0.23182200
O 0.60955900 3.25136500 1.32372000
O 1.43881100 3.26712700 -0.76969500
C -1.12055100 1.96926100 -1.14979700
O -1.74633900 2.98337500 -0.91499300
C 2.04946200 4.53830600 -0.48239900
H 2.73991200 4.45108100 0.35969000
H 2.58339800 4.81820300 -1.38991200
H 1.28412500 5.27888000 -0.24011800
O -1.35246200 1.18135300 -2.21118800
C -2.45893400 1.57941300 -3.04305000
H -2.48368700 0.85787300 -3.85871600
H -3.38872900 1.54608300 -2.47120600

H -2.30628300 2.59163000 -3.42319700
H 2.34774800 0.19036400 4.52101700
H 0.94695700 -0.87092400 4.31801900
H 0.91603700 -2.52901500 2.29590600
H 2.32449200 -2.61358400 1.22959600
Thermal Correction to Free Energy: 0.417814 Hartree
Entropy: 188.252 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.942441 Hartree
Thermal Free Energy with Correction: -1801.524627 Hartree

B-17

C 5.95802400 -0.44346600 -0.64209100
C 4.92475100 -0.24335400 -1.55841600
C 3.67436900 0.20735200 -1.12812400
C 3.43915900 0.46369600 0.22852700
C 4.48790700 0.27074100 1.13838100
C 5.73495000 -0.18423600 0.71165800
H 5.09124800 -0.43150500 -2.61560500
H 2.87170600 0.36281600 -1.83979400
H 4.32594000 0.48295400 2.19315500
H 6.53432900 -0.32638800 1.43350200
C 2.08085100 0.93361000 0.74768600
H 2.29292900 1.57710300 1.62107400
C 0.20272800 -0.82614300 0.25552600
C 0.95018700 -1.66480100 -0.81130000
C -0.74992000 -1.83834300 0.90136200
O 1.71870700 -2.59514800 -0.21628500
O -0.96881200 -1.60572600 2.21490400
C 2.44220000 -3.46485300 -1.10510500
H 3.17531100 -2.89185700 -1.67698200
H 2.94174700 -4.18874400 -0.46198500
H 1.75440500 -3.96498700 -1.79004600
C -1.89453100 -2.51147600 2.84448200
H -1.54745300 -3.54182300 2.74415100
H -1.92657700 -2.21488900 3.89261000
H -2.88207400 -2.42276800 2.38602500
O 0.86929600 -1.53209800 -2.01172400
O -1.27203300 -2.74880200 0.29572900
C 1.19556800 -0.22724000 1.28556600
H 1.83743600 -1.01917400 1.67530400
H 0.60785300 0.13914900 2.12702400
C 0.91076600 4.11929100 -0.13624800
C 0.29267500 3.70606300 1.20259900
C -0.56212000 2.43082700 1.03017200

C 1.84202800 3.00221400 -0.64671600
C -0.58975100 0.35845500 -0.49318200
H -0.29200700 0.22467700 -1.53327200
N 1.34219500 1.65837500 -0.29939000
N -0.06794600 1.67508400 -0.13329300
C -2.11127400 0.28637900 -0.47254800
C -2.89189900 0.36472800 0.69138000
C -2.77818000 0.14461500 -1.69660300
C -4.28426400 0.31108500 0.63706300
H -2.41697900 0.45879300 1.66087100
C -4.16916500 0.08519200 -1.77208200
H -2.19831600 0.07151600 -2.61162200
C -4.91298400 0.17235300 -0.59864100
H -4.87579700 0.37798200 1.54346300
H -4.66800300 -0.02829100 -2.72793300
Cl -6.66991100 0.10433600 -0.67372600
H 6.93072200 -0.78958500 -0.97959600
H 1.96820700 3.08144000 -1.73378600
H 2.83729600 3.10976000 -0.20208100
H 0.11277300 4.30103000 -0.86375100
H 1.47417300 5.05372000 -0.03685300
H 1.09337300 3.53039500 1.93146300
H -0.32918700 4.50672900 1.61585600
H -1.59806000 2.70796600 0.81350400
H -0.57595300 1.86411800 1.97635700
Thermal Correction to Free Energy: 0.416767 Hartree
Entropy: 190.261 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.92513 Hartree
Thermal Free Energy with Correction: -1801.508363 Hartree

B-15

C -6.32549000 -0.38116100 -1.27111800
C -5.25769800 -0.69458500 -2.11567000
C -3.94903500 -0.65482800 -1.63728200
C -3.68706600 -0.30883900 -0.30361700
C -4.76356800 -0.00095700 0.53506900
C -6.07478000 -0.03321600 0.05599500
H -5.44551400 -0.97116600 -3.14934900
H -3.11734100 -0.90992000 -2.28700100
H -4.57391000 0.26540100 1.57201100
H -6.89851600 0.20832400 0.72166300
C -2.25746400 -0.22053900 0.20896100
H -2.29855300 -0.14389700 1.31155500
C -0.10334800 1.19602200 0.06786200

C 0.01453400 1.53337400 1.56427300
C 0.53287200 2.36995000 -0.68546900
O -0.90785000 2.44435600 1.93104100
O 0.43733800 2.20885400 -2.02003900
C -0.80189300 2.91791800 3.28514800
H 0.16430200 3.40334000 3.43935600
H -1.61459700 3.63283400 3.40911700
H -0.90267300 2.09073900 3.99137700
C 1.06207700 3.23564700 -2.81340300
H 2.13014300 3.28916100 -2.59168900
H 0.89802000 2.94298400 -3.84978900
H 0.60589100 4.20669800 -2.60905200
O 0.82445300 1.07040300 2.33781100
O 1.07451900 3.32262100 -0.16423300
C -1.59556000 1.05549900 -0.35098500
H -1.63950800 1.01927800 -1.44208400
H -2.16207300 1.92791500 -0.02126900
C -1.00340200 -3.74030200 0.48297200
C -0.04502600 -3.30843000 1.61196800
C 0.14345100 -1.77384800 1.58240200
C -2.07529200 -2.67562900 0.26129000
C 0.56675500 -0.17204200 -0.36270900
H 0.31537100 -0.22184400 -1.42948700
N -1.47586000 -1.40348600 -0.21429500
N -0.09491600 -1.33374900 0.20152500
C 2.08718000 -0.32632300 -0.29723300
C 2.97651100 0.58906800 0.27464600
C 2.62203000 -1.46500400 -0.92258500
C 4.35763900 0.37983700 0.22169900
H 2.61217600 1.47070600 0.78241500
C 3.99337400 -1.69218400 -0.97800300
H 1.94301200 -2.18716200 -1.36512300
C 4.85500300 -0.75841100 -0.40228400
H 5.03637300 1.09602000 0.67107900
H 4.39157700 -2.57593900 -1.46406300
Cl 6.59457400 -1.02788800 -0.46855600
H -1.48726900 -4.69290600 0.72423700
H -0.44953500 -3.88712800 -0.44907200
H -7.34482400 -0.41144900 -1.64487000
H -0.53031200 -1.28635900 2.30222100
H 1.15431700 -1.48411800 1.86829000
H 0.92029700 -3.81114500 1.49085800
H -0.44242600 -3.61020600 2.58849900
H -2.61832800 -2.51937200 1.20986700

H -2.81694800 -3.00204200 -0.47308000

Thermal Correction to Free Energy: 0.416588 Hartree

Entropy: 190.227 cal/mol-kelvin

Single Point Energy with Solvent Effect: -1801.929215 Hartree

Thermal Free Energy with Correction: -1801.512627 Hartree

B-20

C -4.46019900 -2.82456800 -2.42249500

C -3.09765500 -3.09915800 -2.28232600

C -2.29165400 -2.27361200 -1.50020500

C -2.83479200 -1.16257500 -0.83778700

C -4.20151600 -0.89990300 -0.98245400

C -5.01006200 -1.72112500 -1.77082500

H -2.66190900 -3.95824000 -2.78458700

H -1.23432300 -2.49427200 -1.39012500

H -4.63721800 -0.04407800 -0.47281900

H -6.06879100 -1.49978300 -1.87101500

C -1.95609900 -0.23452500 -0.01409300

H -2.61943100 0.48319900 0.50355500

C -0.07202700 1.48876300 -0.15784900

C -0.85128400 2.68891800 0.42040800

C 1.00563900 2.13653800 -1.03852500

O -1.58724900 3.28383900 -0.54089000

O 1.23761900 1.46191600 -2.17542900

C -2.28207200 4.47780300 -0.13698600

H -2.81309300 4.82163600 -1.02398100

H -2.98315900 4.25868500 0.67157000

H -1.57018600 5.23288300 0.20364400

C 2.30777900 1.97639500 -2.99035000

H 3.25374000 1.91643700 -2.44786700

H 2.33161200 1.34068200 -3.87456000

H 2.11460700 3.01590400 -3.26331700

O -0.81231200 3.08312900 1.56427800

O 1.60343700 3.14458400 -0.71861300

C -0.99866100 0.53894800 -0.93937200

H -0.38256600 -0.18047100 -1.48226700

H -1.57398200 1.10017100 -1.67852900

C -1.27643600 -2.07887400 3.18930600

C -1.22751900 -0.73991700 3.95147100

C -1.02063600 0.42041000 2.95027200

C -1.94595800 -1.88372200 1.83105000

C 0.61826000 0.69995000 1.03780500

H -0.41267300 1.21816800 3.37755700

H -2.95425400 -1.46428800 1.99062600

H -1.98494400 0.88209000 2.68875600
H -2.08370900 -2.83578500 1.31114500
H 0.94643700 1.47229400 1.73495600
N -1.13893400 -0.99117100 0.96060600
N -0.32034800 -0.12502200 1.78029400
C 1.86948900 -0.07187700 0.61193100
C 1.84141100 -1.41901500 0.22697000
C 3.11015000 0.58133200 0.64581400
C 3.01045000 -2.09017400 -0.13052400
H 0.89220000 -1.94141400 0.22433500
C 4.28840100 -0.07418800 0.28630000
H 3.16246300 1.62096700 0.95532600
C 4.22567400 -1.40927100 -0.10392700
H 2.97983800 -3.13358100 -0.42479800
H 5.24199700 0.44080700 0.32297700
Cl 5.70530400 -2.25167900 -0.55941000
H -1.82974700 -2.83351200 3.75857300
H -0.26406400 -2.46450200 3.03765300
H -0.41466300 -0.76061800 4.68487200
H -2.15842300 -0.58114200 4.50917300
H -5.08700700 -3.46739400 -3.03359100
Thermal Correction to Free Energy: 0.417035 Hartree
Entropy: 189.409 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.933277 Hartree
Thermal Free Energy with Correction: -1801.516242 Hartree

B-22

C -4.11571700 -2.98375400 -1.85328000
C -4.75581400 -1.75154300 -1.71228700
C -4.15779200 -0.73605600 -0.96621400
C -2.90588700 -0.92237500 -0.36428900
C -2.27404600 -2.16274600 -0.50923400
C -2.87564400 -3.18534700 -1.24518900
H -5.72534400 -1.58380400 -2.17271600
H -4.67331500 0.21474600 -0.84732900
H -1.30619200 -2.31202200 -0.04553300
H -2.37409700 -4.14484100 -1.34031300
C -2.29850800 0.22552900 0.44190500
H -3.14888700 0.68351400 0.97882700
C -0.16343700 1.50521900 -0.56215100
C 0.13368800 2.98100800 -0.91058200
C 0.33135900 0.72534400 -1.79055200
O 1.42815200 3.30220000 -0.71056900
O -0.01914400 -0.56491700 -1.73664800

C 1.80743100 4.62398500 -1.13533900
H 2.86365700 4.71976300 -0.88611500
H 1.65450200 4.72878500 -2.21154600
H 1.21638600 5.37951900 -0.61339900
C 0.40798900 -1.37663800 -2.84607700
H 1.49582800 -1.47730900 -2.83721800
H -0.07213700 -2.34256200 -2.69799200
H 0.09467400 -0.92828900 -3.79077100
O -0.68732500 3.77318500 -1.31566900
O 0.93529000 1.22324200 -2.71911600
C -1.71437100 1.37643300 -0.43116100
H -2.15120400 1.32257700 -1.43049400
H -2.06452100 2.32441600 -0.02184100
C -1.75038900 -0.22851700 3.86611600
C -1.99985000 1.25888900 3.59845400
C -0.92197700 1.81169600 2.64444100
C -1.82807900 -1.02258100 2.54737100
C 0.57988300 1.08531200 0.80713300
H -0.08731100 2.22971500 3.22035500
H -1.33529100 2.63511200 2.03913600
H 1.05544700 1.99964000 1.16993700
N -1.28973900 -0.26974400 1.39279600
N -0.35975600 0.70576600 1.84273600
C 1.71646300 0.07130400 0.63794800
C 1.70307700 -1.17010400 1.28194900
C 2.84319300 0.40976900 -0.12572000
C 2.76798100 -2.06197800 1.15562200
H 0.85426300 -1.43919200 1.89508700
C 3.91623200 -0.47121100 -0.26353400
H 2.88769500 1.37293300 -0.62183100
C 3.86724900 -1.70595400 0.37836500
H 2.74581000 -3.02253600 1.65862600
H 4.78259100 -0.19712000 -0.85524400
Cl 5.21676000 -2.82757600 0.21296800
H -4.58246600 -3.78092800 -2.42458400
H -1.99741900 1.83417400 4.52966400
H -2.99642200 1.38622600 3.15937800
H -2.48317400 -0.62677900 4.57645300
H -0.76215100 -0.35442600 4.32106200
H -2.86966800 -1.27206800 2.32194300
H -1.29368100 -1.97640100 2.65111100
Thermal Correction to Free Energy: 0.416537 Hartree
Entropy: 190.805 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1801.933083 Hartree

Thermal Free Energy with Correction: -1801.516546 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Path-C1:

C1-TS1

C 2.20568600 -3.87131900 1.29875600
C 1.46897900 -2.87816700 1.94674100
C 1.01333500 -1.77168100 1.23376300
C 1.26193800 -1.64985300 -0.14592200
C 1.96894300 -2.68410700 -0.79286000
C 2.45302000 -3.77281800 -0.07585800
H 1.23124600 -2.97004100 3.00132900
H 0.43319000 -1.01247500 1.74070500
H 2.14289100 -2.63696900 -1.86242900
H 3.00432000 -4.55589500 -0.58801700
C 0.72564000 -0.49345800 -0.88098500
H 0.15181200 0.19401400 -0.28295800
C -1.34835600 -0.93315200 -1.87881800
C -1.82820600 -2.20153600 -1.43269500
C -2.22852200 0.18604200 -1.87937200
O -0.98600600 -3.22946200 -1.67088000
O -1.71624300 1.30039700 -2.46738600
C -1.38250100 -4.50358200 -1.12956200
H -0.55906600 -5.18020500 -1.35930400
H -1.53271200 -4.43029500 -0.05023900
H -2.30642000 -4.84987800 -1.59736100
C -2.62301900 2.40748100 -2.61021500
H -3.03956600 2.70080600 -1.64601600
H -2.02445600 3.21567900 -3.03190500
H -3.44036900 2.14531500 -3.28680100
O -2.92420100 -2.44814200 -0.87737200
O -3.40113300 0.24748100 -1.43638800
Ni -4.04172500 -1.01675000 -0.01780700
O -5.69246600 -1.75473600 -1.01357400
O -4.18686500 -2.08220900 1.88777900
Cl -2.86472200 -1.58192400 2.47255900
O -6.94073300 0.36924800 -1.10853500
O -2.34519100 -0.63854100 1.37009400
O -3.09317400 -0.82963100 3.71744800
O -7.99759000 -1.73683600 -1.80052900

O -1.91755000 -2.69808000 2.66538300
Cl -7.08780200 -1.10676900 -0.83559700
O -7.51470400 -1.30213000 0.57469100
O -5.12027600 0.50104100 0.92812900
H -5.75016000 0.80144900 0.23354600
H -5.68552300 0.04684200 1.57465800
C 0.10504300 -0.72314500 -2.25018600
H 0.18635400 0.13198500 -2.91466300
H 0.52627100 -1.59426900 -2.75021200
H 2.56801700 -4.73091000 1.85517600
C 4.13332000 0.06081200 0.19970800
C 2.04613800 2.01274700 0.26698400
H 3.63810900 -0.90818000 0.35331200
H 2.80936600 2.78663200 0.06952000
C 5.62383300 -0.16129000 0.03782400
C 6.15109500 -1.45865400 -0.01691700
C 6.49978400 0.92366100 -0.06544900
C 7.51579500 -1.66781700 -0.17363700
H 5.48395900 -2.31281900 0.06724800
C 7.87238900 0.73030700 -0.22342100
H 6.09613800 1.92945500 -0.01198600
C 8.38833400 -0.57356900 -0.27969600
H 7.93345000 -2.66832900 -0.21428800
H 8.52605200 1.59101500 -0.29817500
C 0.69468700 2.68551000 0.38001300
C -0.42597500 2.09938000 1.00085200
C 0.55573200 3.98870900 -0.11092300
C -1.63789200 2.76816700 1.08258700
H -0.36950400 1.11010200 1.43882700
C -0.65374400 4.68209900 -0.03268500
H 1.41133500 4.48843800 -0.55816000
C -1.76547400 4.06578900 0.55750700
H -2.50097400 2.29262000 1.53635000
H -0.71446600 5.69003700 -0.42483600
O 9.70475100 -0.87990600 -0.43139400
O -2.99504300 4.62835900 0.66555700
C 10.65631900 0.18120800 -0.54080600
H 10.41185500 0.81263400 -1.40649300
H 10.61624600 0.81172900 0.35840300
C 12.02813400 -0.44986700 -0.69958600
H 12.06476700 -1.07311400 -1.59728600
H 12.79161500 0.32915600 -0.78596800
H 12.26687900 -1.07558900 0.16474500
C -3.20315300 5.95480600 0.17159700

H -2.53257300 6.65258600 0.69229800
H -2.96434100 5.99365500 -0.90064300
C -4.65848600 6.31028100 0.41669500
H -4.89000000 6.27204600 1.48441800
H -4.86312500 7.32130400 0.05160800
H -5.31905700 5.61183900 -0.10393100
N 2.19741800 1.06656100 -0.92873300
N 3.61079100 0.74288200 -0.99762900
N 2.42687200 1.24058800 1.43551200
N 3.87935300 0.96296700 1.32744700
C 3.81318600 0.14328000 -2.31865200
H 4.86418600 0.24327900 -2.59279700
H 3.55577500 -0.92412000 -2.34267300
C 2.01916500 1.78211700 -2.22256000
H 0.95992100 1.86421400 -2.46054500
C 2.86438500 0.96745300 -3.22067800
H 3.41473900 1.63628100 -3.88575800
H 2.24921900 0.31495800 -3.84278500
H 2.42988900 2.79103800 -2.11362900
C 4.18169600 0.36573200 2.63826000
C 2.38628300 2.00098700 2.70093000
H 2.75839900 3.02645300 2.55438500
H 1.36426500 2.05134000 3.07568100
C 3.33880900 1.20935300 3.61972100
H 3.95420300 1.88731300 4.21544200
H 2.78862700 0.56464700 4.30887000
H 5.25607800 0.42495800 2.82109900
H 3.87664600 -0.69119700 2.67939600
Thermal Correction to Free Energy: 0.745931 Hartree
Entropy: 341.726 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.976581 Hartree
Thermal Free Energy with Correction: -3877.23065 Hartree

C1-2

C 2.22930600 -4.08515800 1.07320500
C 1.45399500 -3.15100200 1.76009400
C 1.08085400 -1.95793000 1.13891500
C 1.46151800 -1.68054100 -0.18075500
C 2.19033900 -2.65696200 -0.87855600
C 2.59102400 -3.83689800 -0.25422000
H 1.11769600 -3.35102100 2.77238900
H 0.46800500 -1.24973500 1.68177100
H 2.43688300 -2.51296100 -1.92522200
H 3.16235400 -4.57369100 -0.81177600

C 0.96238100 -0.41107000 -0.84734800
H 0.23962600 0.05348200 -0.18991500
C -1.28126300 -0.91250900 -1.83142200
C -1.79338700 -2.16714400 -1.39915600
C -2.14136500 0.20867400 -1.87111800
O -0.95046100 -3.20887800 -1.58158900
O -1.60144800 1.31846400 -2.46545400
C -1.39309500 -4.47393900 -1.06011200
H -0.56632100 -5.16180000 -1.24040500
H -1.60321700 -4.39592100 0.00885600
H -2.29350600 -4.81276600 -1.57754400
C -2.50277100 2.41855900 -2.66316100
H -2.94610200 2.73990600 -1.71988900
H -1.89523200 3.21690300 -3.09255000
H -3.30375900 2.14027400 -3.35311200
O -2.92121100 -2.40460700 -0.89776100
O -3.32375600 0.30504000 -1.44879900
Ni -4.00917500 -0.95711800 -0.05474500
O -5.68740700 -1.62042300 -1.07022300
O -4.22807700 -2.06542100 1.83921800
Cl -2.89876400 -1.63210700 2.45374500
O -6.83379200 0.56124500 -1.15687700
O -2.33046900 -0.67284400 1.39052300
O -3.11594000 -0.91057100 3.71978500
O -7.97912100 -1.48479500 -1.88607600
O -1.99051600 -2.78449600 2.62401300
Cl -7.05125800 -0.90992800 -0.90350400
O -7.50661600 -1.09924200 0.49962900
O -5.04680200 0.58301300 0.91360900
H -5.64477800 0.92298900 0.20907700
H -5.64847400 0.13395400 1.53047600
C 0.18142000 -0.73529300 -2.17217400
H 0.25853700 0.05566800 -2.91131600
H 0.58108800 -1.64213300 -2.62571400
H 2.52572500 -5.01204200 1.55560700
C 4.09160500 -0.07994600 0.26313600
C 1.91994900 1.80309600 0.32325500
H 3.70229100 -1.08502600 0.46005100
H 2.70161900 2.53401300 0.07190300
C 5.59458100 -0.16684700 0.07720700
C 6.22408000 -1.41593900 -0.01748300
C 6.37849900 0.98799000 -0.00435900
C 7.59903600 -1.50898600 -0.19202800
H 5.62961900 -2.32342100 0.05026700

C 7.76041900 0.91109300 -0.17931300
H 5.89721400 1.95654300 0.08455800
C 8.37955600 -0.34503200 -0.27506700
H 8.09578300 -2.47090000 -0.26233800
H 8.34174100 1.82365900 -0.23380900
C 0.59284700 2.50373100 0.42641400
C -0.55811000 1.94145100 1.01587100
C 0.51204300 3.82587900 -0.03123600
C -1.74213100 2.65583000 1.10134900
H -0.55612000 0.93558900 1.41834600
C -0.66777500 4.56457900 0.05732100
H 1.39168700 4.30433400 -0.45487300
C -1.81020400 3.97443900 0.61755300
H -2.63128600 2.19791300 1.52149300
H -0.68451400 5.58523000 -0.30472600
O 9.71374700 -0.53921600 -0.44404200
O -3.01383400 4.58306800 0.73373900
C 10.57776600 0.59771900 -0.52263800
H 10.28287600 1.23096100 -1.37105000
H 10.48714700 1.19714600 0.39384100
C 11.99541300 0.08299300 -0.69679400
H 12.08099800 -0.51064800 -1.61103300
H 12.69357300 0.92296200 -0.76131200
H 12.28458500 -0.54456200 0.15057100
C -3.17005400 5.92776700 0.26836000
H -2.47877800 6.58841500 0.80994800
H -2.92172300 5.98049100 -0.80088700
C -4.61346400 6.32930900 0.51194500
H -4.85415500 6.27452700 1.57690600
H -4.77881400 7.35533300 0.16954400
H -5.29427100 5.66732000 -0.02962900
N 2.06553100 0.80645700 -0.91566000
N 3.49373700 0.51085500 -0.94762800
N 2.31518800 1.03314700 1.47138700
N 3.78085800 0.82485500 1.37915600
C 3.84389800 0.07355000 -2.30210200
H 4.87960700 0.35911100 -2.49201600
H 3.76391100 -1.00982500 -2.44800900
C 1.95968300 1.60668600 -2.19444000
H 0.91544000 1.73961200 -2.46563000
C 2.83697300 0.84073400 -3.19347900
H 3.33724900 1.53896400 -3.86781400
H 2.24966400 0.15242400 -3.80282600
H 2.39689000 2.58047800 -1.97419600

C 4.10902100 0.23703500 2.69181800

C 2.20576500 1.74869000 2.76063900

H 2.52847800 2.79498300 2.65617600

H 1.17418900 1.73375800 3.10996200

C 3.17337400 0.97453200 3.67439700

H 3.71597200 1.65807900 4.33112600

H 2.63865000 0.25977700 4.30370200

H 5.16940600 0.39527700 2.89609600

H 3.90787800 -0.84441600 2.70821500

Thermal Correction to Free Energy: 0.745931 Hartree

Entropy: 341.726 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3877.976581 Hartree

Thermal Free Energy with Correction: -3877.23065 Hartree

C1-3

C 2.46665300 1.32126800 4.64978800

C 1.38405400 0.85646200 5.39829600

C 0.20797500 0.46296400 4.75709000

C 0.09391900 0.51348000 3.36212900

C 1.18809300 0.98453200 2.61925600

C 2.36248000 1.38509000 3.25778200

H 1.45085800 0.80611400 6.48166200

H -0.63223500 0.10571500 5.34790200

H 1.11546700 1.03560200 1.53881300

H 3.19761100 1.74739900 2.66443500

C -1.19899000 0.07432200 2.69153000

H -1.96956500 0.00212700 3.47530200

C 0.04814600 -1.70948900 1.18446900

C -0.11071700 -2.05475700 -0.17451600

C 1.32730100 -1.97564100 1.76129000

O -1.41508100 -2.20019800 -0.60143700

O 1.30661200 -2.19785100 3.08953200

C -1.58346200 -3.01220500 -1.77700000

H -2.65374000 -2.99563300 -1.99000100

H -1.01182700 -2.62382000 -2.62143900

H -1.25635600 -4.03704200 -1.58015900

C 2.55780500 -2.54758300 3.70304400

H 3.25588700 -1.70772300 3.65591800

H 2.31265600 -2.76814600 4.74225000

H 2.99677500 -3.41854300 3.21207400

O 0.77296000 -2.29947600 -1.04095800

O 2.44246200 -2.06127200 1.17684600

Ni 2.72776300 -2.02676700 -0.78875200

O 3.05800400 -4.04079800 -1.14821100

O 3.11897600 -1.40233800 -2.84726800
Cl 2.87066900 0.08527600 -2.65163300
O 3.51731800 -5.11245100 1.02553600
O 2.43790500 0.17700400 -1.17406100
O 4.08914400 0.88014300 -2.87430300
O 4.10192400 -6.23357800 -1.07353900
O 1.76098100 0.54540800 -3.52163100
Cl 4.02307900 -4.95312100 -0.35619600
O 5.37307000 -4.27347100 -0.33910600
O 4.72862100 -1.67065700 -0.32471000
H 4.68147600 -1.53602100 0.63339200
H 5.15202300 -2.55989700 -0.42604500
C -1.11880500 -1.37140100 2.09075900
H -1.10586400 -2.03447100 2.96285300
H -2.06311600 -1.56242400 1.57999000
H 3.38120700 1.63436500 5.14563200
C -3.18063500 0.52119600 -0.11471000
C -1.36234900 3.31118400 -0.78223800
H -2.43729300 -0.24514200 -0.33831200
H -2.23080100 3.87779000 -0.45877000
C -4.57291400 -0.07725900 -0.29852400
C -4.73178000 -1.46531400 -0.14960200
C -5.71254600 0.69144400 -0.55189800
C -5.98243900 -2.05933900 -0.24946600
H -3.86043000 -2.08119500 0.04939500
C -6.97789600 0.10748600 -0.66190100
H -5.62103800 1.76527400 -0.68269400
C -7.11959400 -1.27734700 -0.50760300
H -6.10642500 -3.13112600 -0.13434200
H -7.83557700 0.73747400 -0.86479300
C -0.07819300 3.95212300 -0.74432400
C 1.17442200 3.28861400 -0.84391100
C -0.07825600 5.35629100 -0.57979100
C 2.35059200 4.00849500 -0.82407700
H 1.24535300 2.20998300 -0.90897500
C 1.09883600 6.08622900 -0.56541200
H -1.02485700 5.88026000 -0.47557400
C 2.33028000 5.41329300 -0.69671200
H 3.30624100 3.50275300 -0.90955600
H 1.06066400 7.16192400 -0.44973200
O -8.29774700 -1.95238700 -0.59288100
O 3.53028300 6.01526700 -0.69663300
C -9.49694700 -1.22027300 -0.85148000
H -9.65293900 -0.47034200 -0.06309700

H -9.40926800 -0.68811200 -1.80934300
C -10.64258900 -2.21603300 -0.88697200
H -10.72730100 -2.74029500 0.06883700
H -11.58548600 -1.69668100 -1.08337700
H -10.48433700 -2.95826200 -1.67417900
C 3.61721500 7.44587900 -0.57749100
H 3.05686400 7.91298500 -1.39757100
H 3.16515800 7.75922400 0.37246800
C 5.08719600 7.81638500 -0.63563500
H 5.52880900 7.49589500 -1.58271500
H 5.19954200 8.90110300 -0.54837700
H 5.63777900 7.34312000 0.18152700
N -1.62900000 1.13101400 1.70096600
N -2.99497000 0.88742100 1.26016300
N -1.65239900 2.10697600 -1.19282400
N -3.01111300 1.67191100 -1.14838700
C -3.93717700 1.85670300 1.86581400
H -4.27531900 2.59004200 1.12142900
H -4.82130700 1.34442900 2.25593000
C -1.70475700 2.46274200 2.34350900
H -0.90438300 2.59389600 3.06690500
C -3.11028000 2.54758000 2.94868000
H -3.43780400 3.57344300 3.13860700
H -3.15635100 1.99947400 3.89465600
H -1.58189300 3.23628700 1.57717400
C -3.17909300 1.19853400 -2.55090600
C -0.80709800 1.21781700 -2.04135100
H -0.09994500 1.82856300 -2.59922500
H -0.24285600 0.52839900 -1.41280900
C -1.84661300 0.52145700 -2.93746400
H -1.61052900 0.65258700 -3.99491300
H -1.87342900 -0.54659600 -2.72877500
H -3.36534900 2.08177600 -3.17164600
H -4.03994200 0.53873100 -2.62212400
Thermal Correction to Free Energy: 0.74399 Hartree
Entropy: 347.699 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3878.005014 Hartree
Thermal Free Energy with Correction: -3877.261024 Hartree

C1-TS3

C 0.68318900 2.14791900 4.63910700
C 0.53889200 0.86082200 5.16048600
C -0.07820600 -0.13420200 4.39928500
C -0.55924100 0.13650000 3.11205700

C -0.41874900 1.43606400 2.60352200
C 0.20208900 2.43173100 3.35879400
H 0.90337800 0.63064300 6.15809400
H -0.18065000 -1.13776500 4.80608300
H -0.79482600 1.66739700 1.61420400
H 0.31985500 3.42509400 2.93667300
C -1.21047000 -0.96553600 2.29041600
H -1.32876800 -1.83257200 2.96286900
C 0.74903500 -0.62190800 0.50700700
C 0.69746800 -0.08140000 -0.79347400
C 1.96400300 -0.48322200 1.23790400
O -0.43515300 -0.36377200 -1.52064800
O 2.06272200 -1.31401000 2.30118900
C -0.47113300 0.22133700 -2.83267700
H -1.46829200 -0.00314000 -3.21956800
H -0.31214500 1.30040200 -2.79011300
H 0.29573500 -0.21489100 -3.47879200
C 3.26858400 -1.21897100 3.07344000
H 3.32843100 -0.24990000 3.57602800
H 3.19824100 -2.01709500 3.81410700
H 4.14569600 -1.35591200 2.43809400
O 1.56736900 0.59232900 -1.40637000
O 2.93323900 0.29303800 1.02147600
Ni 3.12079400 1.46924000 -0.57470200
O 4.43675800 0.22242100 -1.64861600
O 2.82712800 3.12632300 -2.03423300
Cl 1.82319900 3.87112900 -1.16273700
O 4.64570900 -1.91480400 -0.42834500
O 1.85275600 3.07380200 0.15321600
O 2.24157300 5.26234700 -0.92995600
O 6.37246300 -1.20493200 -2.00577300
O 0.46279100 3.81050000 -1.75619800
Cl 5.40975900 -0.76393200 -0.98238900
O 6.11050600 -0.03355200 0.13475600
O 4.78317900 2.35411700 0.30643600
H 4.54614900 2.50654300 1.23145100
H 5.42589500 1.60580800 0.30913000
C -0.35470000 -1.48562400 1.07731300
H 0.08960400 -2.42502100 1.41784300
H -1.05974500 -1.74115700 0.29030800
H 1.16469300 2.92483500 5.22660800
C -4.24842500 -0.86253500 0.16805700
C -3.13708600 -2.92737500 -1.90412700
H -5.27260500 -1.09280400 0.50241900

H -3.15003000 -2.56249400 -2.93116500
C -4.14959500 0.62959200 -0.04815900
C -5.24522500 1.45552500 0.24771400
C -2.98282800 1.22530400 -0.53744700
C -5.17319700 2.83291700 0.06712000
H -6.16611200 1.02182900 0.63358000
C -2.89250700 2.60175300 -0.72635400
H -2.12171400 0.60692900 -0.75287100
C -3.99217100 3.41989000 -0.41753700
H -6.01450400 3.47649000 0.30168600
H -1.96124300 3.02333300 -1.08731200
C -1.93366100 -3.52244500 -1.45691200
C -1.86605500 -4.37403600 -0.32101800
C -0.75020000 -3.29043400 -2.20142300
C -0.67032500 -4.93718900 0.05421000
H -2.77053600 -4.56836200 0.24325200
C 0.46200100 -3.82093000 -1.81169800
H -0.79387600 -2.66156800 -3.08445000
C 0.52195100 -4.62646700 -0.65296400
H -0.59273400 -5.58749000 0.91858900
H 1.35760000 -3.59575100 -2.37557800
O -4.00648000 4.76716200 -0.55366700
O 1.64390100 -5.13413200 -0.15096800
C -2.81684500 5.42717800 -1.02082700
H -1.97392500 5.18604300 -0.36250500
H -2.56567000 5.06600600 -2.02621400
C -3.09786300 6.91800600 -1.02912500
H -3.34155400 7.27202400 -0.02340900
H -2.21423200 7.45758800 -1.38205300
H -3.93674300 7.15261000 -1.69083800
C 2.93220700 -4.70562400 -0.68019100
H 3.03032800 -5.08323300 -1.70497500
H 2.96895900 -3.61291700 -0.69439200
C 4.00780900 -5.26885600 0.22422900
H 3.99999100 -6.36261800 0.22333700
H 4.98125100 -4.91679400 -0.12669700
H 3.86923600 -4.91373700 1.24857900
N -2.56752200 -0.48522700 1.86862500
N -3.27927200 -1.45860900 1.08129600
N -4.37111100 -3.00147200 -1.20893000
N -4.18443400 -1.55873600 -1.20732500
C -3.87958800 -2.41816400 2.04568400
H -4.76940000 -2.88093900 1.61309400
H -3.15728700 -3.21811600 2.23431300

C -3.45922100 -0.24725400 3.02996000
H -2.89259000 0.14968300 3.87096000
C -4.15017100 -1.60184600 3.33369700
H -5.21977200 -1.47324300 3.52434200
H -3.72094500 -2.09497300 4.21017400
H -4.19866600 0.50570900 2.73941700
C -5.07032700 -0.95971200 -2.26445300
C -5.57064100 -3.30202800 -2.01704100
H -5.45409800 -4.28662600 -2.47676200
H -6.42526600 -3.33986000 -1.33570000
C -5.69455500 -2.14361200 -3.02106700
H -5.15582700 -2.35790600 -3.94783500
H -6.73417100 -1.94485500 -3.29066000
H -4.48610800 -0.28947100 -2.89648300
H -5.83029700 -0.35622900 -1.76313600
Thermal Correction to Free Energy: 0.745395 Hartree
Entropy: 345.702 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.998902 Hartree
Thermal Free Energy with Correction: -3877.253507 Hartree

C1-TS5

C 2.48243500 0.68937700 4.83473200
C 1.80959800 -0.39359800 5.40310900
C 0.73793700 -0.98072000 4.72685100
C 0.32127300 -0.49908200 3.47926800
C 0.99856300 0.59636500 2.92296100
C 2.07358300 1.18177600 3.59289900
H 2.11794400 -0.78356300 6.36943000
H 0.22439900 -1.83242400 5.16766000
H 0.69095800 0.98204100 1.95822700
H 2.60320200 2.00790500 3.12837700
C -0.82746200 -1.16991000 2.74581000
H -1.29202900 -1.87350800 3.45647400
C 0.86974400 -1.67043700 0.77595100
C 0.85226000 -1.00368500 -0.46647700
C 2.11977100 -2.09768200 1.30005000
O -0.39349600 -0.70574000 -0.96448800
O 2.02071400 -2.94188200 2.35419300
C -0.38747100 -0.13493200 -2.28413500
H -1.43834500 0.03484200 -2.52858400
H 0.17408200 0.80053700 -2.30085100
H 0.05845400 -0.82488200 -3.00488600
C 3.25254200 -3.45556600 2.87756400
H 3.84549100 -2.65600700 3.33085000

H 2.96068900 -4.17918100 3.64011200
H 3.83542300 -3.93891500 2.09045100
O 1.82358400 -0.67643200 -1.19809900
O 3.28550000 -1.79712000 0.91751400
Ni 3.72735700 -0.65775700 -0.64609200
O 4.23116900 -2.09937800 -2.04927600
O 4.05840500 1.09536500 -1.95324600
Cl 3.51877700 2.11384600 -0.96153700
O 4.29633600 -4.26374200 -0.86308200
O 3.35422900 1.31728600 0.33119200
O 4.46485300 3.23380100 -0.77131700
O 5.36781500 -3.99890400 -3.05056700
O 2.19780700 2.62536500 -1.41086700
Cl 5.06295400 -3.36862600 -1.75678100
O 6.33764400 -2.92291300 -1.07531200
O 5.67935200 -0.58689700 0.06889200
H 5.57237400 -0.84182700 0.99658900
H 6.10244500 -1.37207700 -0.36153500
C -0.39363300 -2.04345500 1.51612000
H -0.26992800 -3.05670300 1.90692500
H -1.24139000 -2.07952500 0.83216800
H 3.32122300 1.14513600 5.35376500
C -3.43539400 0.03671600 0.56697000
C -3.42986900 3.05338000 0.38741500
H -2.54202900 0.35411000 0.02590300
H -3.71199400 3.57415400 1.30334800
C -4.28718600 -0.84510400 -0.34792600
C -3.59167900 -1.75045000 -1.17263500
C -5.68140300 -0.85615500 -0.40492900
C -4.26581600 -2.61670300 -2.01835600
H -2.50674200 -1.76818900 -1.14154000
C -6.37817200 -1.72466900 -1.25460100
H -6.27440000 -0.19003700 0.21144500
C -5.66987900 -2.61282900 -2.06992500
H -3.72593400 -3.31041700 -2.65440500
H -7.46110400 -1.69775200 -1.26507900
C -2.21386700 3.41312500 -0.24042600
C -1.99129400 3.14380900 -1.62067600
C -1.26820400 4.21057500 0.45575300
C -0.92370900 3.70577600 -2.27588200
H -2.69768100 2.51512400 -2.15088500
C -0.17456700 4.74920900 -0.18725700
H -1.41684600 4.40750400 1.51419100
C -0.00283000 4.52626500 -1.57597000

H -0.74644400 3.53389500 -3.33143900
H 0.53766200 5.34982600 0.36313600
O -6.23491900 -3.49725800 -2.93303800
O 0.96111200 5.06145700 -2.31101100
C -7.65905600 -3.55736300 -3.03081600
H -8.08916700 -3.80135900 -2.04910400
H -8.05281300 -2.57786200 -3.33768500
C -8.00275800 -4.62480600 -4.05437000
H -7.60992600 -5.59670300 -3.74385300
H -9.08867200 -4.70646400 -4.16135800
H -7.57512000 -4.37576400 -5.02932400
C 2.07118100 5.75323800 -1.68351100
H 1.69267700 6.67975800 -1.23311000
H 2.49148400 5.10525800 -0.91096400
C 3.09467600 6.02957700 -2.76543800
H 2.66641000 6.63288600 -3.57102200
H 3.94057700 6.57230700 -2.33378300
H 3.46690100 5.08958300 -3.17796000
N -1.84455700 -0.11162900 2.38916100
N -2.96102000 -0.68590500 1.70266000
N -4.38676600 2.23733700 -0.25797200
N -4.12352200 1.39005300 0.88361000
C -3.85961000 -1.30473700 2.69893900
H -4.89555700 -1.29792400 2.35630700
H -3.58138600 -2.35618700 2.82476700
C -2.45023600 0.44865700 3.62251600
H -1.69699400 0.55035900 4.40313500
C -3.60799300 -0.51158400 4.00932200
H -4.49428200 0.03185800 4.35074900
H -3.31594500 -1.18416600 4.81978800
H -2.82635200 1.45208900 3.39692600
C -5.22385100 1.55275300 1.88377100
C -5.79813900 2.65168300 -0.21072100
H -5.88981700 3.65107600 -0.64282600
H -6.36508700 1.95206500 -0.82814800
C -6.20675800 2.57577400 1.27365100
H -6.10763900 3.54772500 1.76384200
H -7.24538000 2.25863100 1.39235800
H -4.81479000 1.89693700 2.83510300
H -5.69021700 0.58369700 2.05660300
Thermal Correction to Free Energy: 0.744609 Hartree
Entropy: 341.451 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.957568 Hartree
Thermal Free Energy with Correction: -3877.212959 Hartree

C1-6

C -2.51944000 4.72381300 -1.04425000
C -1.53923700 4.91510100 -2.01944200
C -0.36457800 4.16172000 -1.98374200
C -0.15685400 3.20329500 -0.98282200
C -1.14754700 3.01968500 -0.00401000
C -2.31949500 3.77655600 -0.03723100
H -1.68571700 5.64913200 -2.80674300
H 0.39254700 4.31034200 -2.75074400
H -1.01876400 2.28479700 0.78167300
H -3.07557500 3.60445800 0.72225700
C 1.11287500 2.37556100 -1.00160000
H 1.78579700 2.81968600 -1.75234900
C -0.31898100 0.16143200 -0.88180500
C -0.26959500 -0.59992700 0.30577900
C -1.54959800 0.20364800 -1.60515500
O 0.96483100 -0.68472100 0.91634800
O -1.45357700 0.75374200 -2.83871100
C 0.95842300 -1.35823600 2.19281300
H 1.97521300 -1.25223000 2.58009600
H 0.23964600 -0.89480900 2.87085000
H 0.70482800 -2.41351700 2.07371600
C -2.64960500 0.73695400 -3.63346800
H -3.41741100 1.37767300 -3.19164600
H -2.35159100 1.12733100 -4.60743900
H -3.03564400 -0.28032400 -3.72425200
O -1.18948700 -1.23354400 0.87341500
O -2.68588700 -0.19066500 -1.24061600
Ni -3.13835000 -1.02704500 0.51646100
O -3.30080100 -2.99851600 -0.12166100
O -3.48590700 -1.29561700 2.67557000
Cl -3.27351000 0.17359500 3.02640000
O -2.76442300 -3.04202200 -2.53312800
O -3.13791600 0.83457400 1.63577900
O -4.43333400 0.72819400 3.74042800
O -4.04832900 -4.85369700 -1.50181300
O -2.01892500 0.35892800 3.78809400
Cl -3.78963700 -3.40533400 -1.52968400
O -5.06794600 -2.64336200 -1.79912700
O -5.16021300 -0.76816100 0.12487300
H -5.25022200 0.08659000 -0.31713700
H -5.32137500 -1.45353700 -0.57121500
C 0.87374300 0.89341500 -1.44907500

H 0.75119600 0.95043000 -2.53295000
H 1.79507700 0.32109500 -1.29750500
H -3.43415600 5.30923700 -1.06858000
C 3.50136100 0.82733700 0.36153900
H 2.64433100 0.20750500 0.62410700
C 4.76973600 0.17122900 0.20663900
C 6.00996600 0.75095400 -0.17219000
C 4.74433300 -1.22309100 0.45239900
C 7.14571700 -0.02296500 -0.27720300
H 6.09010300 1.80589000 -0.39577800
C 5.88026400 -2.00879000 0.34825000
H 3.80073300 -1.69064100 0.71672600
C 7.10047800 -1.41096000 -0.01617500
H 8.09621900 0.41105300 -0.56734800
H 5.81329900 -3.07170000 0.54169800
O 8.26410400 -2.06287800 -0.14953800
C 8.31996900 -3.48537100 0.08471000
H 7.99342700 -3.69352800 1.11110000
H 7.63481200 -3.99041000 -0.60721200
C 9.75372100 -3.92573700 -0.13842400
H 10.42879400 -3.41389800 0.55243700
H 9.83803900 -5.00331900 0.02916100
H 10.07121100 -3.70872400 -1.16168000
N 1.80778000 2.46466400 0.35247000
N 3.17680900 2.08609100 0.22279700
C 4.07338700 3.26438900 0.03196800
H 4.86899200 3.21148300 0.77977000
H 4.51815200 3.23029200 -0.96621300
C 1.92190400 3.81708800 0.93632800
H 0.99408100 4.36387800 0.79406400
C 3.13631600 4.46187100 0.24334100
H 3.60285000 5.24092700 0.84949000
H 2.84498600 4.90228400 -0.71346100
H 2.10023300 3.70219400 2.01078900
Thermal Correction to Free Energy: 0.494126 Hartree
Entropy: 277.955 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.15513 Hartree
Thermal Free Energy with Correction: -3225.661004 Hartree

C1-4

C 6.34755000 -2.85364000 -2.35875400
C 5.46488300 -3.87646700 -2.01160800
C 4.28571200 -3.57942000 -1.32485300
C 3.96703700 -2.25915600 -0.98192600

C 4.85951700 -1.23860900 -1.34146600
C 6.04104100 -1.53321200 -2.02079000
H 5.69208300 -4.90595600 -2.27264100
H 3.60007800 -4.38056300 -1.06006900
H 4.62633000 -0.20820900 -1.09130600
H 6.72211400 -0.73122700 -2.29105300
C 2.65007200 -1.95583000 -0.28328500
H 2.18490700 -2.90698800 -0.00710200
C 0.26613300 -0.92934500 -0.88146700
C -0.60438200 -1.95099800 -0.42629300
C -0.29399100 0.33886400 -1.19499400
O -0.05253400 -3.20096700 -0.42258000
O 0.51704800 1.15522200 -1.91139500
C -0.94485400 -4.27780000 -0.08075100
H -0.33874600 -5.18271600 -0.14257200
H -1.34922900 -4.14992100 0.92629000
H -1.77612200 -4.32734500 -0.78709500
C -0.07707600 2.36702200 -2.40246400
H -0.32767200 3.04258400 -1.58034500
H 0.68309400 2.81859700 -3.04144600
H -0.98009800 2.14557900 -2.97503700
O -1.79265900 -1.86052500 -0.02932400
O -1.43566100 0.78896200 -0.89747900
Ni -2.83755100 -0.18326600 0.12904900
O -4.07556600 -0.80048500 -1.40655300
O -3.76517900 -1.15203200 2.01877300
Cl -2.73862800 -0.55321800 2.94969300
O -3.07258700 0.02882000 -3.50559800
O -1.92710600 0.39080600 2.01606000
O -3.35787700 0.22977300 4.02840700
O -5.44130900 -0.59024400 -3.40592900
O -1.81157800 -1.58394000 3.47788700
Cl -4.31009600 0.02376700 -2.69663700
O -4.65314100 1.43406700 -2.26793900
O -4.02424700 1.49691800 0.32528100
H -3.45383500 2.26037500 0.48196300
H -4.39516800 1.60568100 -0.58824100
C 1.69873300 -1.24040900 -1.28814100
H 2.17546700 -0.31436900 -1.61105500
H 1.70746100 -1.90060300 -2.16569800
H 7.26671200 -3.08174100 -2.89024100
C 1.16686200 0.20106200 1.81652300
H 0.22912500 0.14123800 2.36509100
C 1.53115500 1.50523600 1.34300100

C 0.60030800 2.53984300 1.62625800
C 2.74771700 1.84999300 0.71323700
C 0.87643700 3.85136900 1.29989400
H -0.34272500 2.28519700 2.10025200
C 3.03497200 3.16704500 0.39456100
H 3.46370300 1.06860900 0.49640200
C 2.09904900 4.18165000 0.68147500
H 0.17321600 4.64879600 1.51345500
H 3.97854600 3.40400000 -0.08084600
O 2.27936500 5.48527700 0.40589900
C 3.49440300 5.92332400 -0.22701400
H 4.35087100 5.65184100 0.40340000
H 3.60336300 5.41621500 -1.19418700
C 3.39684900 7.42701000 -0.40308900
H 3.28547900 7.92348400 0.56448200
H 4.30443300 7.80337000 -0.88411000
H 2.53912200 7.68840900 -1.02836200
N 2.96865800 -1.17557400 0.98312600
N 1.79086100 -0.94272200 1.74466000
C 1.40634700 -2.14583100 2.54266100
H 0.96460300 -1.82103900 3.48422500
H 0.65820500 -2.71276900 1.98792400
C 3.76092100 -1.97837500 1.94922100
H 4.54422000 -2.52210300 1.42435000
C 2.74686900 -2.89506600 2.68278600
H 3.02505600 -3.03987800 3.72865900
H 2.69004600 -3.87946700 2.21336000
H 4.22914000 -1.28168700 2.65129900
Thermal Correction to Free Energy: 0.49275 Hartree
Entropy: 280.731 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.162268 Hartree
Thermal Free Energy with Correction: -3225.669518 Hartree

C1-TS4

C -6.33837900 -2.98437400 2.18615400
C -5.42314400 -3.97785200 1.83796800
C -4.26583900 -3.64501200 1.13095300
C -4.00200600 -2.31818900 0.76818900
C -4.92752100 -1.32710700 1.12661000
C -6.08695400 -1.65789300 1.82723600
H -5.60885200 -5.01217300 2.11259800
H -3.55612600 -4.42370900 0.86206200
H -4.73941100 -0.29357000 0.85351400
H -6.79503700 -0.87900000 2.09569300

C -2.71299100 -1.97799300 0.03735900
H -2.23535000 -2.91802100 -0.25962400
C -0.37301000 -0.81536800 0.49605400
C 0.56258100 -1.86228500 0.09768300
C 0.26478600 0.32556400 1.14899700
O 0.03434600 -3.10002300 0.09332000
O -0.50668900 0.94560600 2.04064900
C 0.93056800 -4.16918900 -0.28355400
H 0.33098800 -5.07692400 -0.22231500
H 1.30683100 -4.01518800 -1.29745200
H 1.77516800 -4.21452900 0.40590300
C 0.08015500 2.07053100 2.73344800
H 0.26334600 2.88742100 2.03231200
H -0.66383100 2.36209400 3.47393600
H 1.01300600 1.76733400 3.21038500
O 1.74967000 -1.73056300 -0.24484300
O 1.40440100 0.77971800 0.91566400
Ni 2.90648600 -0.08388700 -0.12380000
O 3.90180900 -0.92088000 1.47484000
O 4.05518500 -0.89784400 -1.82493100
Cl 3.15909500 -0.26379400 -2.88156600
O 2.52307100 -0.49734900 3.47736500
O 2.22194600 0.62741300 -2.00883500
O 3.92305400 0.57584600 -3.81051500
O 4.92043300 -0.95988000 3.68277900
O 2.34230700 -1.27886700 -3.57397600
Cl 3.87130100 -0.30106200 2.89481700
O 4.15574700 1.17512000 2.74254400
O 4.12415400 1.56986400 0.07674000
H 3.65557800 2.38339800 -0.15017600
H 4.29077000 1.59200600 1.05157600
C -1.75389800 -1.23211800 1.01202000
H -2.26542200 -0.33535800 1.36331800
H -1.64751000 -1.88374100 1.88709300
H -7.24102000 -3.24026100 2.73318800
C -0.99576300 0.10375900 -1.41015400
H -0.01806000 0.06324400 -1.88523200
C -1.41704500 1.46631700 -1.03826400
C -0.44675000 2.48745300 -1.15327600
C -2.71854100 1.83314000 -0.65698500
C -0.76408500 3.80939400 -0.88795800
H 0.55613100 2.23386000 -1.48009500
C -3.04702800 3.16033100 -0.39348900
H -3.48115400 1.06826900 -0.58944400

C -2.06810600 4.16066200 -0.49916100
H -0.02522900 4.59704100 -0.99230800
H -4.06307900 3.40544700 -0.10884200
O -2.27897100 5.47782800 -0.26021700
C -3.58695000 5.91958600 0.12019100
H -4.30924100 5.65248700 -0.66313700
H -3.89143000 5.41711700 1.04842800
C -3.52215300 7.42408500 0.31148900
H -3.21774400 7.91790600 -0.61525100
H -4.50496600 7.80675400 0.60262200
H -2.80322900 7.68339000 1.09339300
N -3.03155700 -1.15648400 -1.17515900
N -1.83561600 -0.83939200 -1.87797700
C -1.43074700 -1.92130500 -2.80851600
H -1.07971900 -1.46599600 -3.73772400
H -0.61429100 -2.52285700 -2.39875200
C -3.78574900 -1.89429500 -2.20588100
H -4.56862500 -2.49360800 -1.74210800
C -2.73283400 -2.73182800 -2.97680800
H -3.00608000 -2.85652400 -4.02666400
H -2.62797700 -3.72877200 -2.54167700
H -4.25183300 -1.15903700 -2.86863800
Thermal Correction to Free Energy: 0.495211 Hartree
Entropy: 272.985 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.149764 Hartree
Thermal Free Energy with Correction: -3225.654553 Hartree

C1-5

C 5.98768100 -4.16718900 -0.86392000
C 4.85297800 -4.89167600 -0.49651800
C 3.73347800 -4.22865700 0.00884300
C 3.72505300 -2.83509200 0.14727300
C 4.86952600 -2.11669100 -0.22654800
C 5.99305200 -2.77775700 -0.72399700
H 4.84000000 -5.97325400 -0.59666900
H 2.85428900 -4.79863300 0.29932100
H 4.88211200 -1.03761700 -0.11086700
H 6.87426900 -2.20672300 -1.00305000
C 2.46756900 -2.13965000 0.64583300
H 1.85338500 -2.88088800 1.17965300
C 0.41056500 -0.79211000 -0.11632000
C -0.67844700 -1.66452600 0.53763800
C -0.26739500 -0.06138600 -1.28354400
O -0.45985300 -2.96121400 0.48934500

O 0.43069600 -0.04938700 -2.39273500
C -1.51606900 -3.81252300 1.01316000
H -1.18730100 -4.82804900 0.80134200
H -1.62067800 -3.64779200 2.08672600
H -2.45383600 -3.58240100 0.50705400
C -0.15774400 0.63170200 -3.53317500
H -0.22286800 1.70041500 -3.32100200
H 0.52887100 0.44084700 -4.35558800
H -1.14637900 0.21866600 -3.73359800
O -1.69776700 -1.19941300 1.04870100
O -1.35467100 0.51712200 -1.19268000
Ni -2.92209900 0.20202900 0.12558000
O -3.74762700 -1.41873100 -0.86484600
O -4.22409600 0.24456400 1.80641300
Cl -3.56967100 1.47817900 2.45022300
O -2.09233800 -2.09383000 -2.55182700
O -2.46091700 1.79682100 1.39642700
O -4.51203800 2.59773200 2.53745000
O -4.45033300 -2.71504500 -2.80295000
O -2.95339500 1.14027800 3.73794200
Cl -3.50885900 -1.67628300 -2.37406800
O -3.75678000 -0.37606200 -3.09509900
O -4.12260700 1.41269800 -1.03587200
H -3.72700100 2.28035400 -1.19255700
H -4.16005900 0.94084800 -1.89872900
C 1.65339800 -1.59397400 -0.54957100
H 2.29462500 -0.93817500 -1.14061000
H 1.36006300 -2.42330200 -1.19667600
H 6.86212200 -4.68083500 -1.25281800
C 0.81044900 0.30234900 0.96164100
H -0.12833500 0.62779100 1.41761200
C 1.46603000 1.55989700 0.38682500
C 0.68192500 2.72720100 0.29662200
C 2.79829400 1.64161300 -0.04120300
C 1.19427500 3.90849000 -0.22308200
H -0.34426700 2.71064400 0.65269500
C 3.32975600 2.82602200 -0.55831300
H 3.44008600 0.77726300 0.06520900
C 2.52563000 3.96793700 -0.66107000
H 0.58691000 4.80580500 -0.28421300
H 4.36698500 2.84515000 -0.87134200
O 2.93636700 5.16870600 -1.15412300
C 4.28999100 5.31212300 -1.58658600
H 4.97297100 5.08657100 -0.75561100

H 4.50069600 4.60042800 -2.39745400
C 4.46855600 6.74339600 -2.06166400
H 4.26214500 7.44691500 -1.25044800
H 5.49557300 6.90032300 -2.40514600
H 3.78818900 6.96280300 -2.88915300
N 2.78409600 -1.02639700 1.55264500
N 1.49871800 -0.45026600 2.01512400
C 1.84495200 0.36170700 3.20201600
C 3.36911100 -1.47773400 2.82290800
C 3.12266600 -0.29689900 3.76988900
H 2.85105300 -2.37888900 3.19247400
H 4.42504700 -1.71543000 2.68269700
H 3.95826600 0.40692900 3.73872700
H 3.00153800 -0.62861900 4.80363900
H 0.99973700 0.33456200 3.89551000
H 2.03708400 1.40854500 2.93561200
Thermal Correction to Free Energy: 0.496395 Hartree
Entropy: 274.491 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.157923 Hartree
Thermal Free Energy with Correction: -3225.661528 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Path-C2.

C2-TS1

C 1.24240600 0.86424200 4.72956500
C 1.50856100 1.72743800 3.66405500
C 0.91378000 1.50804300 2.42373800
C 0.04678100 0.41420300 2.22237100
C -0.20041100 -0.45385700 3.30354000
C 0.38848700 -0.22728700 4.54509400
H 2.18777200 2.56414200 3.79406500
H 1.14200400 2.16654800 1.59178600
H -0.84185100 -1.31687200 3.16675000
H 0.18837600 -0.90634600 5.36867000
C -0.52923800 0.20186300 0.87974700
H -0.16840300 0.91059000 0.15286200
C 0.83361300 -1.46785100 -0.01173000
C 1.39099800 -1.03575900 -1.25057700
C 1.66252600 -2.16568100 0.91681300
O 0.50424000 -0.43665300 -2.08625600

O 0.98610100 -2.82408500 1.88481500
C 1.03128200 -0.04903200 -3.37119600
H 0.19812400 0.43241200 -3.88510200
H 1.86967100 0.63985700 -3.25156700
H 1.36597900 -0.92686800 -3.92840200
C 1.78556600 -3.61419300 2.78486800
H 2.40780800 -2.97144400 3.41348300
H 1.06875500 -4.16112900 3.39850700
H 2.42272800 -4.30044000 2.22442500
O 2.56499300 -1.18431900 -1.65681700
O 2.91468700 -2.23372200 0.92759100
Ni 4.13276600 -1.38121900 -0.42917000
O 4.76554800 -3.12086100 -1.34720900
O 5.16503100 0.13692500 -1.66491300
Cl 4.55930000 1.32681700 -0.93223000
O 3.59063200 -5.01679600 -0.28187500
O 3.79134100 0.65930800 0.22765500
O 5.59715800 2.22535100 -0.40666000
O 5.69334200 -5.36168700 -1.48900400
O 3.60406100 2.04962100 -1.80795100
Cl 4.92656500 -4.46967000 -0.60707700
O 5.69342100 -4.19348300 0.66761100
O 5.73447300 -1.52211300 0.87465000
H 5.42490300 -1.28159600 1.75776500
H 5.89682800 -2.49933300 0.89197100
C -0.62445500 -1.18883500 0.29014400
H -1.04262600 -1.93031400 0.97110700
H -1.19439100 -1.17061500 -0.63481700
H 1.70481100 1.03463200 5.69741800
C -3.84836300 -0.32052800 -0.43330200
C -2.44187600 2.17539400 -0.31502400
H -3.09015600 -1.10809200 -0.57013300
H -3.40941600 2.68728700 -0.17087600
C -5.21842500 -0.96877300 -0.38448200
C -5.35028700 -2.36405900 -0.38445600
C -6.37599700 -0.18580000 -0.33848300
C -6.60339300 -2.96248100 -0.33871700
H -4.46233700 -2.99004300 -0.42433200
C -7.64139600 -0.77113100 -0.29284800
H -6.27836500 0.89476100 -0.34906000
C -7.76072500 -2.16958700 -0.29255400
H -6.71431300 -4.04162500 -0.34196300
H -8.51979900 -0.13780100 -0.26154600
C -1.33326500 3.20752000 -0.31710400

C -0.07281100 2.99321500 -0.91089300
C -1.57259000 4.45717000 0.26480800
C 0.91359600 3.96826900 -0.88191300
H 0.14125800 2.05478400 -1.41173100
C -0.59414400 5.45266000 0.30236500
H -2.54777900 4.67380100 0.69321800
C 0.66313000 5.20825000 -0.26688600
H 1.88884700 3.78180400 -1.31977800
H -0.82412700 6.40589000 0.76245800
O -8.93959900 -2.84536200 -0.25162100
O 1.68788500 6.09374700 -0.28759600
C -10.16260300 -2.10542000 -0.22070500
H -10.18374000 -1.45885100 0.66781400
H -10.22933100 -1.46087000 -1.10826500
C -11.30285300 -3.10727200 -0.19033200
H -11.23342900 -3.74460300 0.69546100
H -12.26253500 -2.58223200 -0.16618300
H -11.27878200 -3.74600200 -1.07745900
C 1.52099400 7.37338300 0.32906000
H 0.69330100 7.91251500 -0.15284100
H 1.26720500 7.24281500 1.39048900
C 2.82846000 8.12844700 0.17082700
H 3.07396200 8.25592700 -0.88682000
H 2.74803400 9.11769100 0.63165200
H 3.64694700 7.58531700 0.65054300
N -2.38387000 1.19568100 0.86311000
N -3.62196100 0.43260500 0.80630800
N -2.49016600 1.35647900 -1.51263800
N -3.79436700 0.65382100 -1.52451300
C -3.71468800 -0.24879700 2.09449900
H -4.74185900 -0.58027500 2.24868100
H -3.05763200 -1.13037200 2.15219000
C -2.56386600 1.88926000 2.17744900
H -1.60071500 2.22476600 2.55338700
C -3.27047400 0.85263600 3.07752000
H -4.12984700 1.30982400 3.57270200
H -2.60396900 0.46201500 3.84645700
H -3.20556000 2.75948600 2.01689600
C -3.80973500 0.03745000 -2.86092600
C -2.58781600 2.13295100 -2.76619600
H -3.26058500 2.99481800 -2.64055900
H -1.60469100 2.49926800 -3.05913400
C -3.18902400 1.12403800 -3.76464100
H -3.93308600 1.60663300 -4.40235200

H -2.42267100 0.69276000 -4.41274100
H -4.83631600 -0.22026800 -3.12662400
H -3.20059500 -0.87933800 -2.88969900
Thermal Correction to Free Energy: 0.745416 Hartree
Entropy: 342.673 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.979734 Hartree
Thermal Free Energy with Correction: -3877.234318 Hartree

C2-2

C -4.92832200 -0.52936600 5.09530500
C -3.68319900 -0.17189400 5.61408400
C -2.57713000 -0.07354600 4.76772700
C -2.68582800 -0.32749800 3.39158900
C -3.94230200 -0.70295400 2.88833000
C -5.05182500 -0.79612400 3.73006300
H -3.57018800 0.02525500 6.67665600
H -1.60849000 0.19563100 5.18306300
H -4.05883600 -0.91951500 1.83270800
H -6.01442900 -1.08644700 3.31773300
C -1.44920900 -0.20821300 2.50759100
H -0.60273000 -0.00846600 3.16643800
C 0.18892300 -1.57180600 1.02917200
C 0.21637200 -1.91237400 -0.33813800
C 1.42269200 -1.37596900 1.70328100
O -0.99316500 -2.28296300 -0.87302100
O 1.30715100 -1.26556900 3.04949700
C -0.93743100 -2.92531500 -2.15666300
H -1.97084900 -3.18186500 -2.39510400
H -0.52057000 -2.26467500 -2.92062100
H -0.32326700 -3.82761300 -2.10849800
C 2.53025300 -1.28575500 3.80068900
H 3.14097100 -0.40517800 3.58110800
H 2.22322100 -1.27649000 4.84732000
H 3.09783900 -2.19111700 3.57592800
O 1.19338700 -1.91843100 -1.14048200
O 2.58870300 -1.29932000 1.22098800
Ni 3.11559700 -1.83518800 -0.62164300
O 3.08488300 -3.90426900 -0.40292800
O 3.74814100 -1.76139900 -2.72856900
Cl 3.74083800 -0.24300100 -2.83759600
O 3.01196900 -4.35718800 2.02066500
O 3.31260200 0.19427800 -1.41812400
O 5.07220600 0.28851300 -3.15820200
O 3.62260900 -6.12178800 0.43422300

O 2.72251500 0.20964300 -3.81540000
Cl 3.72184400 -4.69339900 0.76371500
O 5.16852000 -4.26857300 0.85848000
O 5.09694900 -1.71959800 0.00750600
H 5.03255800 -1.24718700 0.84971900
H 5.32263300 -2.65026000 0.25717900
C -1.10940600 -1.55531700 1.81431900
H -1.07346700 -2.29615400 2.62243500
H -1.92948400 -1.86527700 1.16605600
H -5.79208700 -0.60873600 5.74933800
C -2.58095300 0.61988600 -0.57414800
C -0.50859500 3.09253000 -0.81188900
H -1.93251200 -0.25629100 -0.58500700
H -1.42134300 3.60178600 -0.51804500
C -3.98328500 0.21507400 -1.02071500
C -4.36994500 -1.13270700 -0.92674800
C -4.91919600 1.13732000 -1.49453000
C -5.65167900 -1.53687400 -1.27618000
H -3.65149300 -1.87239800 -0.58534500
C -6.21226500 0.74608700 -1.85355200
H -4.63631600 2.17960700 -1.60399000
C -6.58752100 -0.59868100 -1.74060200
H -5.95200700 -2.57722100 -1.20696900
H -6.90908500 1.49087200 -2.21889400
C 0.75186300 3.68101100 -0.43922700
C 1.99588600 3.00015400 -0.40830500
C 0.72673100 5.04223800 -0.06306300
C 3.15079900 3.67067500 -0.05862700
H 2.07151100 1.94304500 -0.63186400
C 1.88430500 5.72320100 0.28195100
H -0.21986600 5.57651100 -0.05824400
C 3.11446200 5.03823200 0.28018800
H 4.10261000 3.15156400 -0.03749500
H 1.82862100 6.77016600 0.55191900
O -7.81417700 -1.09285800 -2.05981200
O 4.29819100 5.59302900 0.59986200
C -8.81438400 -0.19734600 -2.54898900
H -9.00989300 0.58599500 -1.80313800
H -8.45863300 0.29271200 -3.46634200
C -10.06588400 -1.01313200 -2.82018100
H -10.41812600 -1.49502600 -1.90404900
H -10.86150300 -0.36508300 -3.20012400
H -9.86606200 -1.78996400 -3.56328600
C 4.36247600 6.98352100 0.95479200

H 3.97571400 7.58955300 0.12510800
H 3.73281000 7.16473100 1.83581200
C 5.81568500 7.31117600 1.24273300
H 6.43542100 7.12405300 0.36193700
H 5.91127800 8.36574000 1.51781400
H 6.19298800 6.70133800 2.06781800
N -1.41213600 0.96973600 1.57213400
N -2.58403200 1.12746100 0.74679400
N -0.72016600 2.00975900 -1.51000100
N -2.04661900 1.57077200 -1.71254400
C -3.43057900 2.25734700 1.16350400
H -3.46743200 3.02318900 0.37539900
H -4.45872600 1.93321400 1.35494900
C -1.30894100 2.25175900 2.29065800
H -0.81223700 2.10675300 3.25135600
C -2.74599600 2.79062100 2.43165500
H -2.78305600 3.88228200 2.49373900
H -3.22319200 2.38270400 3.32450900
H -0.69498300 2.94614300 1.70709400
C -2.02389700 0.84333500 -3.02368200
C 0.24132500 1.28545900 -2.37514700
H 1.12032900 1.89563700 -2.56101100
H 0.55107400 0.35528000 -1.89264500
C -0.62149300 1.05334100 -3.61246300
H -0.59300400 1.93427900 -4.26045000
H -0.26927600 0.19491600 -4.18595100
H -2.81522200 1.23501800 -3.66579000
H -2.22177900 -0.21967500 -2.85912800
Thermal Correction to Free Energy: 0.748617 Hartree
Entropy: 340.761 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.991107 Hartree
Thermal Free Energy with Correction: -3877.24249 Hartree

C2-TS2

C 1.11948500 -0.21712300 4.68984000
C 1.51861600 0.82009300 3.84678500
C 0.88756600 1.00041300 2.61508900
C -0.15127200 0.15206600 2.19978900
C -0.51951100 -0.90518800 3.04518100
C 0.10242300 -1.08319200 4.28161000
H 2.32932000 1.48200800 4.13510100
H 1.23000200 1.79082100 1.95384000
H -1.27143100 -1.61925000 2.72865300
H -0.19989400 -1.90798100 4.92072900

C -0.76915400 0.38882100 0.82408800
H -0.16394900 1.17025900 0.37090300
C 0.77865300 -1.23462200 -0.32502200
C 1.53850400 -0.69516800 -1.38768000
C 1.40117600 -2.20706900 0.50933900
O 0.85157600 0.11217100 -2.26307100
O 0.54110400 -3.00570000 1.18779300
C 1.63683400 0.57465500 -3.38409400
H 0.96209200 1.19753400 -3.97491300
H 2.49611000 1.15255500 -3.04076000
H 1.98722000 -0.26934100 -3.98146100
C 1.14108800 -4.04188500 1.98369400
H 1.68765200 -3.61363300 2.82875300
H 0.30680800 -4.64553200 2.34442900
H 1.82369100 -4.64294200 1.38025900
O 2.74602100 -0.90427500 -1.66153000
O 2.63056900 -2.41142400 0.67420500
Ni 4.07718800 -1.37877200 -0.25823800
O 4.86584800 -2.93554400 -1.37353600
O 5.34675900 0.28263300 -1.00505600
Cl 4.62862400 1.36227500 -0.20772200
O 3.57292100 -4.97950700 -0.86132100
O 3.66343900 0.55432200 0.68000700
O 5.56410500 2.13394100 0.62459100
O 5.82644600 -5.12429500 -1.80699900
O 3.84991100 2.24789400 -1.11012600
Cl 4.93429100 -4.40138100 -0.88770000
O 5.51505800 -4.38415600 0.50943900
O 5.39880900 -1.81993600 1.27812600
H 4.87933000 -1.81147100 2.09325400
H 5.60439000 -2.77296200 1.10022700
C -0.66979200 -0.84529800 -0.11706800
H -1.22838800 -1.69031700 0.29378600
H -1.10568100 -0.58314600 -1.07927400
H 1.60651300 -0.36101400 5.64993800
C -3.77691500 -0.25047000 -0.57811900
C -2.36583900 2.32620800 -0.51349600
H -3.05780700 -1.02639200 -0.87255700
H -3.31336900 2.68223000 -0.10053500
C -5.14892200 -0.88736600 -0.46788200
C -5.28815300 -2.28213600 -0.50707700
C -6.29871900 -0.10356500 -0.32635200
C -6.53868700 -2.87810000 -0.40222900
H -4.40799800 -2.90985900 -0.62203000

C -7.56125100 -0.68687400 -0.21935900
H -6.19949500 0.97676900 -0.30626100
C -7.68750200 -2.08448900 -0.25609600
H -6.65429000 -3.95623900 -0.43414700
H -8.43288100 -0.05236500 -0.11321000
C -1.29272600 3.34681300 -0.46888400
C 0.03108100 3.14988800 -0.92370400
C -1.61451400 4.59486000 0.08852300
C 0.98263800 4.14967800 -0.80725200
H 0.33553500 2.20126300 -1.35174700
C -0.67444100 5.61789200 0.19078700
H -2.62662000 4.78103100 0.43816000
C 0.63851600 5.39688900 -0.25298500
H 2.00787800 3.97498600 -1.11640600
H -0.96810500 6.56953700 0.61618800
O -8.86331500 -2.75764700 -0.16239600
O 1.63484600 6.30677200 -0.19060900
C -10.07973100 -2.01744900 -0.02453200
H -10.03778600 -1.40047800 0.88389200
H -10.20401700 -1.34478800 -0.88450200
C -11.21809800 -3.01893700 0.05076900
H -11.09100000 -3.68423100 0.90909900
H -12.17219000 -2.49387900 0.15647700
H -11.25596500 -3.62868700 -0.85599500
C 1.38134900 7.59263600 0.38729700
H 0.59060500 8.10264300 -0.18011000
H 1.03236400 7.46881400 1.42168400
C 2.68053900 8.37583000 0.33929200
H 3.02153000 8.49382600 -0.69264400
H 2.53400000 9.36939400 0.77359800
H 3.46188800 7.85999000 0.90340400
N -2.18393300 1.10616800 0.85777700
N -3.42228600 0.36558900 0.71352400
N -2.55704400 1.53306400 -1.60746500
N -3.83105900 0.84475900 -1.57741000
C -3.74701200 -0.24392200 2.00372400
H -4.82188100 -0.41706200 2.05105300
H -3.24494300 -1.20750400 2.16908800
C -2.45170100 1.81443600 2.15058600
H -1.51390100 2.12677000 2.60216600
C -3.27104800 0.82719400 3.00947000
H -4.11734900 1.34149800 3.47084900
H -2.66351000 0.38857500 3.80110600
H -3.04412500 2.69986700 1.91016000

C -4.07242400 0.41819100 -2.97478900
C -2.02318100 1.65709300 -2.96901600
H -2.30023500 2.62419300 -3.41061800
H -0.94116100 1.55800600 -2.96884000
C -2.70855300 0.48925800 -3.68040000
H -2.80189800 0.65575800 -4.75583200
H -2.13457300 -0.42889100 -3.52325400
H -4.78137900 1.11705600 -3.43224700
H -4.52036300 -0.57643200 -2.99670700
Thermal Correction to Free Energy: 0.747554 Hartree
Entropy: 339.427 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.9809 Hartree
Thermal Free Energy with Correction: -3877.233346 Hartree

C2-3

C -4.92832200 -0.52936600 5.09530500
C -3.68319900 -0.17189400 5.61408400
C -2.57713000 -0.07354600 4.76772700
C -2.68582800 -0.32749800 3.39158900
C -3.94230200 -0.70295400 2.88833000
C -5.05182500 -0.79612400 3.73006300
H -3.57018800 0.02525500 6.67665600
H -1.60849000 0.19563100 5.18306300
H -4.05883600 -0.91951500 1.83270800
H -6.01442900 -1.08644700 3.31773300
C -1.44920900 -0.20821300 2.50759100
H -0.60273000 -0.00846600 3.16643800
C 0.18892300 -1.57180600 1.02917200
C 0.21637200 -1.91237400 -0.33813800
C 1.42269200 -1.37596900 1.70328100
O -0.99316500 -2.28296300 -0.87302100
O 1.30715100 -1.26556900 3.04949700
C -0.93743100 -2.92531500 -2.15666300
H -1.97084900 -3.18186500 -2.39510400
H -0.52057000 -2.26467500 -2.92062100
H -0.32326700 -3.82761300 -2.10849800
C 2.53025300 -1.28575500 3.80068900
H 3.14097100 -0.40517800 3.58110800
H 2.22322100 -1.27649000 4.84732000
H 3.09783900 -2.19111700 3.57592800
O 1.19338700 -1.91843100 -1.14048200
O 2.58870300 -1.29932000 1.22098800
Ni 3.11559700 -1.83518800 -0.62164300
O 3.08488300 -3.90426900 -0.40292800

O 3.74814100 -1.76139900 -2.72856900
Cl 3.74083800 -0.24300100 -2.83759600
O 3.01196900 -4.35718800 2.02066500
O 3.31260200 0.19427800 -1.41812400
O 5.07220600 0.28851300 -3.15820200
O 3.62260900 -6.12178800 0.43422300
O 2.72251500 0.20964300 -3.81540000
Cl 3.72184400 -4.69339900 0.76371500
O 5.16852000 -4.26857300 0.85848000
O 5.09694900 -1.71959800 0.00750600
H 5.03255800 -1.24718700 0.84971900
H 5.32263300 -2.65026000 0.25717900
C -1.10940600 -1.55531700 1.81431900
H -1.07346700 -2.29615400 2.62243500
H -1.92948400 -1.86527700 1.16605600
H -5.79208700 -0.60873600 5.74933800
C -2.58095300 0.61988600 -0.57414800
C -0.50859500 3.09253000 -0.81188900
H -1.93251200 -0.25629100 -0.58500700
H -1.42134300 3.60178600 -0.51804500
C -3.98328500 0.21507400 -1.02071500
C -4.36994500 -1.13270700 -0.92674800
C -4.91919600 1.13732000 -1.49453000
C -5.65167900 -1.53687400 -1.27618000
H -3.65149300 -1.87239800 -0.58534500
C -6.21226500 0.74608700 -1.85355200
H -4.63631600 2.17960700 -1.60399000
C -6.58752100 -0.59868100 -1.74060200
H -5.95200700 -2.57722100 -1.20696900
H -6.90908500 1.49087200 -2.21889400
C 0.75186300 3.68101100 -0.43922700
C 1.99588600 3.00015400 -0.40830500
C 0.72673100 5.04223800 -0.06306300
C 3.15079900 3.67067500 -0.05862700
H 2.07151100 1.94304500 -0.63186400
C 1.88430500 5.72320100 0.28195100
H -0.21986600 5.57651100 -0.05824400
C 3.11446200 5.03823200 0.28018800
H 4.10261000 3.15156400 -0.03749500
H 1.82862100 6.77016600 0.55191900
O -7.81417700 -1.09285800 -2.05981200
O 4.29819100 5.59302900 0.59986200
C -8.81438400 -0.19734600 -2.54898900
H -9.00989300 0.58599500 -1.80313800

H -8.45863300 0.29271200 -3.46634200
C -10.06588400 -1.01313200 -2.82018100
H -10.41812600 -1.49502600 -1.90404900
H -10.86150300 -0.36508300 -3.20012400
H -9.86606200 -1.78996400 -3.56328600
C 4.36247600 6.98352100 0.95479200
H 3.97571400 7.58955300 0.12510800
H 3.73281000 7.16473100 1.83581200
C 5.81568500 7.31117600 1.24273300
H 6.43542100 7.12405300 0.36193700
H 5.91127800 8.36574000 1.51781400
H 6.19298800 6.70133800 2.06781800
N -1.41213600 0.96973600 1.57213400
N -2.58403200 1.12746100 0.74679400
N -0.72016600 2.00975900 -1.51000100
N -2.04661900 1.57077200 -1.71254400
C -3.43057900 2.25734700 1.16350400
H -3.46743200 3.02318900 0.37539900
H -4.45872600 1.93321400 1.35494900
C -1.30894100 2.25175900 2.29065800
H -0.81223700 2.10675300 3.25135600
C -2.74599600 2.79062100 2.43165500
H -2.78305600 3.88228200 2.49373900
H -3.22319200 2.38270400 3.32450900
H -0.69498300 2.94614300 1.70709400
C -2.02389700 0.84333500 -3.02368200
C 0.24132500 1.28545900 -2.37514700
H 1.12032900 1.89563700 -2.56101100
H 0.55107400 0.35528000 -1.89264500
C -0.62149300 1.05334100 -3.61246300
H -0.59300400 1.93427900 -4.26045000
H -0.26927600 0.19491600 -4.18595100
H -2.81522200 1.23501800 -3.66579000
H -2.22177900 -0.21967500 -2.85912800
Thermal Correction to Free Energy: 0.744611 Hartree
Entropy: 346.35 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3878.010448 Hartree
Thermal Free Energy with Correction: -3877.265837 Hartree

C2-TS3

C -3.75728300 -2.27295100 5.41029000
C -2.68592400 -1.48812100 5.83807300
C -1.84770900 -0.88006800 4.90075900
C -2.06128700 -1.03395700 3.52293200

C -3.13242600 -1.84330600 3.10898900
C -3.97376600 -2.45160700 4.04183000
H -2.49533700 -1.35673800 6.89979100
H -1.00360200 -0.28583900 5.24375000
H -3.30285700 -2.00068600 2.04918100
H -4.79358800 -3.07785600 3.69974800
C -1.12169700 -0.36033700 2.52395400
H -0.24747400 -0.02188100 3.08427400
C 0.68652000 -0.98273300 0.76753600
C 0.74907600 -0.75139100 -0.62108500
C 1.90187000 -1.05192000 1.49653500
O -0.45452400 -0.78783500 -1.27969700
O 1.73521500 -1.32910000 2.81499900
C -0.36257900 -0.95404300 -2.70532000
H -1.38217700 -1.15448500 -3.03698700
H 0.03018400 -0.05613100 -3.18998300
H 0.28916800 -1.79426700 -2.95308000
C 2.91790400 -1.65603900 3.55560000
H 3.60799100 -0.80816100 3.59211900
H 2.56958000 -1.89948400 4.56049600
H 3.41633800 -2.51860200 3.10821600
O 1.76069600 -0.51211400 -1.33831500
O 3.08710200 -0.88964800 1.08525500
Ni 3.60826100 -1.08461600 -0.84111500
O 2.96994900 -3.07036000 -1.09879000
O 4.31665000 -0.78245900 -2.86995600
Cl 4.71543100 0.68139800 -2.67202800
O 2.73191500 -4.07901800 1.13827100
O 4.41478800 0.90140500 -1.17198100
O 6.14607500 0.88592600 -2.94251000
O 2.84668100 -5.48706700 -0.86327100
O 3.86454000 1.57232500 -3.48453400
Cl 3.33944000 -4.26959300 -0.20235100
O 4.84428900 -4.30216200 -0.08265900
O 5.49645600 -1.68629600 -0.19440900
H 5.48999400 -1.44775000 0.74348100
H 5.45693500 -2.67383100 -0.20637900
C -0.60781500 -1.36298600 1.45956300
H -0.46443500 -2.31901600 1.97468600
H -1.38542900 -1.52623700 0.71069100
H -4.40874100 -2.75277100 6.13519400
C -2.97243700 1.00969400 -0.09775700
C -1.71819700 3.77829400 -0.59940200
H -1.98237400 0.77099200 -0.48117000

H -2.29072700 4.64678400 -0.26579600
C -4.01204300 0.22690200 -0.88844400
C -3.88198500 0.15217700 -2.28914700
C -5.07175800 -0.46741000 -0.29815400
C -4.78338600 -0.56297500 -3.06358100
H -3.04398200 0.64399500 -2.77369400
C -5.98971300 -1.19288800 -1.06418900
H -5.17982300 -0.47908700 0.77918700
C -5.85420200 -1.24165100 -2.45651300
H -4.67162500 -0.63147700 -4.14075300
H -6.79077100 -1.72286000 -0.56340400
C -0.36974100 3.68802900 -0.18734000
C 0.53467200 2.72087300 -0.70861200
C 0.11992300 4.65787300 0.72535700
C 1.86243300 2.74011600 -0.35500800
H 0.17100700 1.96522300 -1.39387800
C 1.45021600 4.68676700 1.08999000
H -0.56156700 5.40297700 1.12846600
C 2.33475400 3.72303900 0.54792400
H 2.56811100 2.01726200 -0.75101100
H 1.80645700 5.44432500 1.77656300
O -6.68231300 -1.91245800 -3.29721700
O 3.63713400 3.66323500 0.83068100
C -7.76191100 -2.67374500 -2.74688000
H -7.36669000 -3.42574300 -2.05042800
H -8.43397400 -2.01066400 -2.18422000
C -8.49170400 -3.33345700 -3.90306400
H -7.81925500 -3.99483300 -4.45586500
H -9.33025200 -3.92674300 -3.52631400
H -8.88151400 -2.58075600 -4.59386300
C 4.24148300 4.61475100 1.72478400
H 4.09319600 5.62724800 1.32773400
H 3.75179400 4.55117800 2.70511400
C 5.71524600 4.26819400 1.81788900
H 6.18555800 4.32006000 0.83292500
H 6.21977000 4.97251600 2.48621900
H 5.84892700 3.25654700 2.20904500
N -1.64350500 0.89278900 1.89046900
N -2.94497000 0.72736200 1.30316700
N -2.29930600 2.95456400 -1.58436100
N -3.11935900 2.52909600 -0.46037800
C -3.98308900 1.27914800 2.21592600
H -4.65663000 1.95118000 1.67991900
H -4.58419100 0.47031000 2.64052600

C -1.76774000 2.04064100 2.80214000
H -1.01807800 1.97810900 3.59360200
C -3.21444400 2.02191100 3.33192100
H -3.60800700 3.02839800 3.50497700
H -3.27976300 1.46758400 4.26971900
H -1.58141000 2.96098100 2.23857700
C -4.45807800 3.16196400 -0.61086100
C -3.15184300 3.62464900 -2.60617300
H -2.85064400 4.67364600 -2.69079000
H -2.99007400 3.14470800 -3.57320200
C -4.60252500 3.46767300 -2.11027700
H -5.19796500 4.36603100 -2.28895200
H -5.08467100 2.62788700 -2.61394900
H -4.50282800 4.06985600 -0.00018400
H -5.21879900 2.46833200 -0.25496600
Thermal Correction to Free Energy: 0.741253 Hartree
Entropy: 348.405 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.965448 Hartree
Thermal Free Energy with Correction: -3877.224195 Hartree

C2-4

C 4.21797100 -5.88912700 1.30967400
C 3.21338100 -6.37830900 0.47417200
C 2.21205300 -5.52229400 0.01032800
C 2.19315300 -4.16569700 0.36637600
C 3.20019200 -3.69361800 1.22492800
C 4.20540300 -4.54420900 1.68701800
H 3.20272600 -7.42632800 0.18902400
H 1.42358700 -5.91619500 -0.62671400
H 3.19230800 -2.65783400 1.55267500
H 4.97160500 -4.16028100 2.35476800
C 1.09291000 -3.25741300 -0.17712900
H 0.34386000 -3.88480600 -0.66233500
C -0.61659100 -1.40470700 0.58642800
C -0.60282700 -0.17960600 1.30414500
C -1.65976300 -1.64096600 -0.34608200
O 0.41770500 -0.05497200 2.20174500
O -1.75962900 -2.92881100 -0.75757900
C 0.40128000 1.13560500 3.00641900
H 1.27772500 1.05654500 3.65154500
H 0.45774700 2.03285400 2.38595500
H -0.50972500 1.18353800 3.60736200
C -2.88500400 -3.24120900 -1.59812000
H -2.80605600 -2.72964500 -2.56156300

H -2.84192200 -4.32170000 -1.74241700
H -3.81565800 -2.95401800 -1.10581700
O -1.39533700 0.79171800 1.21615700
O -2.46465900 -0.80964300 -0.84612300
Ni -2.80569400 1.03958000 -0.16603800
O -4.33181600 0.56978500 1.15845600
O -2.77347700 3.19817200 0.18848900
Cl -1.64254600 3.50342700 -0.78471400
O -4.73191000 -1.86477700 1.04863300
O -1.31433800 2.11524200 -1.37792500
O -2.07220500 4.42580400 -1.84496300
O -6.44689500 -0.35128000 1.92213900
O -0.45696300 4.02163100 -0.05900800
Cl -5.38240000 -0.53869700 0.92607300
O -5.92501900 -0.36108600 -0.47384000
O -4.19076100 1.29165900 -1.69720400
H -3.86002100 0.77376500 -2.44364100
H -4.97013200 0.78758900 -1.35391000
C 0.36891700 -2.49517800 0.96054600
H -0.11890200 -3.28581700 1.54784400
H 1.10781800 -2.05584500 1.63092500
H 4.99627600 -6.55203000 1.67584500
C 2.10471000 -0.19416400 -0.72116700
H 1.02128300 -0.10939200 -0.68169200
C 2.87766900 0.97003600 -0.42085500
C 2.13751900 2.18274300 -0.35922400
C 4.27087500 1.02313100 -0.17539000
C 2.76018800 3.38581600 -0.10715800
H 1.06446000 2.17288500 -0.52304300
C 4.89999500 2.22696000 0.09318700
H 4.86674200 0.11909600 -0.15534600
C 4.15037900 3.42414400 0.11800500
H 2.18533800 4.30410900 -0.07073000
H 5.96422700 2.23685000 0.29208500
O 4.67182300 4.63683700 0.35996800
C 6.07991100 4.78102900 0.61561600
H 6.35082900 4.18869400 1.49911500
H 6.64606400 4.39938600 -0.24380200
C 6.34992400 6.25685700 0.84012100
H 5.77782500 6.62848000 1.69411600
H 7.41418400 6.41248300 1.04000800
H 6.07306300 6.83895700 -0.04265700
N 1.50706200 -2.37913600 -1.32851600
N 2.49985300 -1.39970200 -1.05481500

C 3.85342700 -1.81747600 -1.51698800

H 4.29302200 -0.98585000 -2.07323800

H 4.48126700 -2.05123500 -0.65466700

C 2.03371300 -3.07158200 -2.51534200

H 1.61964100 -4.07825800 -2.57107200

C 3.57418600 -3.05796600 -2.38382200

H 4.06524400 -2.98510000 -3.35662900

H 3.92998700 -3.95878800 -1.88215500

H 1.71710200 -2.51792500 -3.40621600

Thermal Correction to Free Energy: 0.4943 Hartree

Entropy: 277.946 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3226.159626 Hartree

Thermal Free Energy with Correction: -3225.665326 Hartree

C2-TS5

C -2.39278200 -4.15354900 4.47529100

C -1.84864300 -2.97432300 4.98553600

C -1.57330600 -1.90394300 4.13196300

C -1.83860800 -1.97615700 2.75629900

C -2.36733200 -3.17696200 2.25975900

C -2.64579100 -4.25176400 3.10562300

H -1.63043000 -2.88852200 6.04655800

H -1.12662900 -0.99947900 4.53806400

H -2.54706800 -3.27825100 1.19526800

H -3.05249800 -5.17190600 2.69374400

C -1.53849400 -0.76224500 1.86667900

H -0.89996800 -0.10748800 2.46568400

C 0.59410100 -0.44098300 0.39930900

C 0.91753300 0.31953700 -0.74265800

C 1.62128500 -0.71604400 1.34077300

O -0.07733000 0.44220200 -1.68660600

O 1.24767300 -1.59462200 2.30248200

C 0.25845600 1.26846900 -2.81203300

H -0.66244500 1.35078000 -3.39539100

H 0.59639400 2.25689300 -2.49505000

H 1.05014100 0.81215200 -3.41228400

C 2.26647200 -2.01303600 3.22035600

H 2.62590200 -1.17035300 3.81795300

H 1.78499100 -2.75110800 3.86293100

H 3.10797900 -2.45582300 2.68311200

O 1.99603400 0.89745000 -1.03297700

O 2.79683100 -0.26154900 1.40225300

Ni 3.65730100 0.88852200 0.02293700

O 4.40352400 -0.67547600 -1.19614900

O 4.25863300 2.67452400 -1.14494100
Cl 3.57442000 3.65772100 -0.19878400
O 3.48131500 -2.79513000 -0.33080700
O 3.15032200 2.75528300 0.97459200
O 4.51170000 4.69379900 0.26228000
O 5.49987900 -2.78668100 -1.70787200
O 2.37322700 4.25390300 -0.83201600
Cl 4.74253800 -2.07517800 -0.66265700
O 5.57338600 -1.90347400 0.58226800
O 5.43888600 0.79848800 1.09231900
H 5.20581900 0.93523200 2.02063400
H 5.67857500 -0.15329800 1.00566200
C -0.75287000 -1.12045000 0.56789500
H -0.60708700 -2.20463700 0.55165600
H -1.38318400 -0.87908000 -0.28408900
H -2.60566500 -4.99047900 5.13415900
C -4.11268400 0.83188800 -0.24980400
C -3.34445400 -0.93623000 -2.74588400
H -5.19717200 0.94634400 -0.10143400
H -3.06939800 -0.32968000 -3.60902800
C -3.46668600 2.17914900 -0.01902100
C -4.23140800 3.25158300 0.46654700
C -2.10742600 2.39424000 -0.26515400
C -3.65148400 4.49294100 0.70902800
H -5.29265700 3.11691700 0.66831900
C -1.50939200 3.62887800 -0.02974500
H -1.50004200 1.58288600 -0.64039300
C -2.28079900 4.69126500 0.46946100
H -4.23699600 5.32301700 1.09015700
H -0.44822900 3.74597600 -0.21753400
C -2.48262500 -2.01166300 -2.43263900
C -2.86820100 -3.09944200 -1.60299800
C -1.19377000 -2.03320900 -3.02421800
C -1.99927700 -4.14021400 -1.37814400
H -3.85459400 -3.09039500 -1.15326000
C -0.29828100 -3.04940600 -2.76659700
H -0.89729900 -1.21937300 -3.67671600
C -0.68293900 -4.10689100 -1.91272200
H -2.26992200 -4.98516700 -0.75466200
H 0.69354800 -3.01977100 -3.19787100
O -1.79693600 5.92622700 0.74206400
O 0.11267600 -5.11056900 -1.55724400
C -0.39033900 6.17176300 0.55993700
H 0.19000000 5.46752600 1.16786300

H -0.11724000 6.00623500 -0.48941500
C -0.12105600 7.60564100 0.97537200
H -0.38783500 7.76257500 2.02443100
H 0.94192100 7.83071100 0.84952500
H -0.69973200 8.30381500 0.36348200
C 1.52640300 -5.07618500 -1.90997800
H 1.61230400 -5.15031200 -3.00071500
H 1.95715000 -4.12808300 -1.57381900
C 2.19356600 -6.24713800 -1.21942400
H 1.77101500 -7.19997400 -1.55098500
H 3.26186800 -6.23438600 -1.45224000
H 2.08173400 -6.16669500 -0.13529700
N -2.70952800 0.12843900 1.57628200
N -3.63211500 -0.29022300 0.56472400
N -4.62967000 -0.74152500 -2.18016600
N -4.01495000 0.50125500 -1.74816600
C -4.73763100 -1.01711200 1.25524800
H -5.67601300 -0.88034300 0.71082900
H -4.51321100 -2.08467400 1.25724300
C -3.53836100 0.47525100 2.74499700
H -2.96413600 0.37975800 3.66708000
C -4.77163100 -0.46188700 2.70090200
H -5.69716900 0.08244300 2.91151900
H -4.68550800 -1.27240700 3.42816400
H -3.84850400 1.52186800 2.64921400
C -4.47211500 1.60595800 -2.66104900
C -5.72079800 -0.40416600 -3.11695300
H -5.84967000 -1.22422100 -3.82782300
H -6.63943500 -0.31018900 -2.53099200
C -5.31500600 0.93357000 -3.75858500
H -4.73446700 0.77813500 -4.67191200
H -6.18332800 1.53933700 -4.02701300
H -3.60638100 2.15103700 -3.04007000
H -5.06460000 2.30715800 -2.06912000
Thermal Correction to Free Energy: 0.743275 Hartree
Entropy: 344.186 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3877.956418 Hartree
Thermal Free Energy with Correction: -3877.213143 Hartree

C2-6

C -5.63017400 -1.76766700 -0.28942600
C -5.69658300 -2.62861700 0.98419800
C -4.77954400 -1.88010900 1.98512100
H -5.23485700 -2.32221200 -1.14261100

H -6.58456800 -1.30912200 -0.55531800
H -6.71758000 -2.70986700 1.36339700
H -5.31961100 -3.63105700 0.78241100
H -5.37408700 -1.22623100 2.63213200
H -4.19753300 -2.54892000 2.61904800
C -4.69192100 0.50200200 -0.49836000
N -3.86656300 -1.03344000 1.19136000
N -4.66102200 -0.68410500 0.07216500
H -5.33075700 0.51295600 -1.37983300
C -4.03465000 1.72675600 -0.20023300
C -4.06240100 2.72014500 -1.22019700
C -3.34068700 2.02479300 1.00135500
C -3.36095600 3.89455500 -1.08973000
H -4.61691300 2.52959000 -2.13542500
C -2.64816500 3.20782300 1.14614700
H -3.35091100 1.30214900 1.80607100
C -2.59914100 4.13544100 0.07845400
H -3.34042100 4.63759200 -1.87870100
H -2.10781900 3.40128800 2.06344900
C -2.76134600 -5.21839900 -1.63618500
C -2.68640700 -3.95920500 -2.23575800
C -2.59085400 -2.80743900 -1.45233800
C -2.58103200 -2.89420600 -0.05065000
C -2.62707100 -4.16855600 0.53597500
C -2.72051700 -5.32172800 -0.24515300
H -2.68076000 -3.87372200 -3.31876300
H -2.47059100 -1.84371100 -1.93550500
H -2.56752600 -4.26058900 1.61813900
H -2.74590100 -6.29744000 0.23140700
C -2.51201300 -1.66186800 0.83893400
H -2.15685200 -1.97555500 1.82274100
C -0.13309000 -0.90169000 0.07380500
C 0.73476700 -1.21338900 1.15116100
C 0.41965400 -0.63633900 -1.19941300
O 0.08896900 -1.43525100 2.33265800
O -0.49004300 -0.36693900 -2.18024900
C 0.93482800 -1.68467700 3.46716200
H 0.25614800 -1.79660600 4.31447900
H 1.52123000 -2.59522100 3.32421900
H 1.62035800 -0.85082400 3.63324100
C 0.04728700 0.13324000 -3.41152000
H 0.68145800 -0.61308200 -3.89677000
H -0.81952200 0.35196800 -4.03793900
H 0.62642000 1.04303900 -3.23622300

O 1.98662900 -1.30635500 1.15471000
O 1.63736200 -0.61306100 -1.53313200
Ni 3.12066100 -0.38034400 -0.20438700
O 2.38692400 1.50954100 0.55543500
O 4.85026400 -0.53410900 1.05001300
Cl 5.36772000 -1.83223200 0.40978400
O 0.32731600 2.44108500 -0.42546500
O 4.29842200 -2.09325300 -0.67490100
O 6.68471100 -1.62414900 -0.21163500
O 1.99654400 3.91299400 0.57816600
O 5.38114900 -2.92754800 1.39196600
Cl 1.78110500 2.68123100 -0.21599000
O 2.47298600 2.78853000 -1.55077900
O 4.20619000 0.66795800 -1.64507800
H 4.09717100 0.18058000 -2.47258400
H 3.71162300 1.51193600 -1.74605800
C -1.57173700 -0.54149700 0.35688900
H -1.97912400 -0.07477400 -0.53907700
H -1.58838400 0.22119500 1.13998700
H -2.82615000 -6.11263100 -2.24903500
O -1.89035100 5.25861000 0.08785500
C -0.93237700 5.50850900 1.15302800
H -1.48673600 5.67602400 2.08492400
H -0.28458000 4.63416700 1.25429200
C -0.12613900 6.72733400 0.75517200
H -0.77101400 7.59697300 0.59920500
H 0.58917700 6.95919700 1.54931900
H 0.43823000 6.52670000 -0.15811000
Thermal Correction to Free Energy: 0.495188 Hartree
Entropy: 276.57 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.155344 Hartree
Thermal Free Energy with Correction: -3225.660156 Hartree

C2-TS4

C 2.76218900 -3.38564400 1.46326700
C 4.10877100 -3.36280400 2.21262000
C 4.81057600 -2.14914300 1.60601500
H 2.77064700 -4.10749200 0.64099000
H 1.93671600 -3.65732100 2.12774100
C 1.34259400 -1.37156600 1.34491500
N 3.69843300 -1.21892900 1.43647900
N 2.57583300 -2.01448000 0.89608300
H 1.38160100 -1.23012700 2.43559200
C 0.11106800 -2.18081900 0.98350700

C -0.99204500 -2.20203500 1.84142000
C 0.02227800 -2.90194700 -0.22117800
C -2.16740100 -2.87759300 1.50926600
H -0.94283100 -1.68169000 2.79512400
C -1.13465700 -3.58777300 -0.56067100
H 0.87566400 -2.92422700 -0.89054400
C -2.25032400 -3.56454700 0.29179700
H -3.00444100 -2.85813600 2.19621000
H -1.20980800 -4.14017700 -1.49143100
C 5.73485500 -0.30016900 -3.32647900
C 4.99496000 -1.38045500 -2.84126500
C 4.38283200 -1.31581000 -1.58716200
C 4.51200200 -0.17335600 -0.78467900
C 5.27228300 0.89685900 -1.27882100
C 5.86761600 0.84460800 -2.53983000
H 4.89118500 -2.28071100 -3.44163200
H 3.78153900 -2.14294200 -1.23133000
H 5.40253100 1.78746600 -0.66687700
H 6.44393700 1.69210200 -2.90003800
C 3.92713100 -0.02745900 0.62764800
H 4.69309000 0.52893800 1.18392600
C 1.26032300 0.13260200 0.74893800
C 0.70696000 0.10493800 -0.68137600
C 0.30268400 0.87556500 1.70188300
O 1.58520200 -0.38509400 -1.53154700
O 0.84960600 1.07839600 2.88805700
C 1.18988700 -0.43377900 -2.92574600
H 2.06384500 -0.82091200 -3.44530600
H 0.32679000 -1.09147300 -3.04178100
H 0.93468100 0.56799600 -3.27429100
C 0.07335200 1.83674700 3.84818300
H -0.82386700 1.28005500 4.12644700
H 0.73262700 1.95924500 4.70563800
H -0.19826800 2.80078900 3.41654600
O -0.39446900 0.48120200 -1.07757300
O -0.86798800 1.19968200 1.49976600
Ni -1.88257500 1.58520000 -0.24005100
O -0.81294100 3.31078200 -0.69015400
O -3.04746400 1.47259900 -2.00950900
Cl -3.86930300 0.25258300 -1.55449400
O 0.97751100 3.59631000 0.97205900
O -3.26260000 -0.00450600 -0.14809100
O -5.29434400 0.58543800 -1.43526200
O 0.11961100 5.52176200 -0.27889700

O -3.62613200 -0.90006500 -2.43138500
Cl -0.21754800 4.25526500 0.37703600
O -1.26214900 4.45455100 1.44893200
O -3.26315900 2.77259500 0.72297600
H -3.70786400 2.31211300 1.44619600
H -2.73246300 3.51014800 1.10312300
C 2.65620800 0.85794300 0.76744500
H 2.73365200 1.34476500 1.73719200
H 2.65524400 1.65105500 0.01696200
H 3.94983500 -3.20666500 3.28325900
H 4.67227000 -4.28961300 2.08129200
H 5.30734600 -2.41242900 0.66006700
H 5.55530400 -1.70140000 2.27145800
H 6.20658400 -0.35215700 -4.30349900
O -3.34111200 -4.24520800 -0.14084600
C -4.56780400 -4.11621200 0.58437700
H -4.81480900 -3.05272400 0.69990000
H -4.45491200 -4.55256900 1.58732700
C -5.64184700 -4.84326700 -0.20458200
H -6.60054200 -4.77705200 0.31883800
H -5.75546700 -4.39746500 -1.19620500
H -5.38463500 -5.89939200 -0.32575800
Thermal Correction to Free Energy: 0.497032Hartree
Entropy: 272.039 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.145888 Hartree
Thermal Free Energy with Correction: -3225.648856 Hartree

C2-5

C 2.76218900 -3.38564400 1.46326700
C 4.10877100 -3.36280400 2.21262000
C 4.81057600 -2.14914300 1.60601500
H 2.77064700 -4.10749200 0.64099000
H 1.93671600 -3.65732100 2.12774100
C 1.34259400 -1.37156600 1.34491500
N 3.69843300 -1.21892900 1.43647900
N 2.57583300 -2.01448000 0.89608300
H 1.38160100 -1.23012700 2.43559200
C 0.11106800 -2.18081900 0.98350700
C -0.99204500 -2.20203500 1.84142000
C 0.02227800 -2.90194700 -0.22117800
C -2.16740100 -2.87759300 1.50926600
H -0.94283100 -1.68169000 2.79512400
C -1.13465700 -3.58777300 -0.56067100
H 0.87566400 -2.92422700 -0.89054400

C -2.25032400 -3.56454700 0.29179700
H -3.00444100 -2.85813600 2.19621000
H -1.20980800 -4.14017700 -1.49143100
C 5.73485500 -0.30016900 -3.32647900
C 4.99496000 -1.38045500 -2.84126500
C 4.38283200 -1.31581000 -1.58716200
C 4.51200200 -0.17335600 -0.78467900
C 5.27228300 0.89685900 -1.27882100
C 5.86761600 0.84460800 -2.53983000
H 4.89118500 -2.28071100 -3.44163200
H 3.78153900 -2.14294200 -1.23133000
H 5.40253100 1.78746600 -0.66687700
H 6.44393700 1.69210200 -2.90003800
C 3.92713100 -0.02745900 0.62764800
H 4.69309000 0.52893800 1.18392600
C 1.26032300 0.13260200 0.74893800
C 0.70696000 0.10493800 -0.68137600
C 0.30268400 0.87556500 1.70188300
O 1.58520200 -0.38509400 -1.53154700
O 0.84960600 1.07839600 2.88805700
C 1.18988700 -0.43377900 -2.92574600
H 2.06384500 -0.82091200 -3.44530600
H 0.32679000 -1.09147300 -3.04178100
H 0.93468100 0.56799600 -3.27429100
C 0.07335200 1.83674700 3.84818300
H -0.82386700 1.28005500 4.12644700
H 0.73262700 1.95924500 4.70563800
H -0.19826800 2.80078900 3.41654600
O -0.39446900 0.48120200 -1.07757300
O -0.86798800 1.19968200 1.49976600
Ni -1.88257500 1.58520000 -0.24005100
O -0.81294100 3.31078200 -0.69015400
O -3.04746400 1.47259900 -2.00950900
Cl -3.86930300 0.25258300 -1.55449400
O 0.97751100 3.59631000 0.97205900
O -3.26260000 -0.00450600 -0.14809100
O -5.29434400 0.58543800 -1.43526200
O 0.11961100 5.52176200 -0.27889700
O -3.62613200 -0.90006500 -2.43138500
Cl -0.21754800 4.25526500 0.37703600
O -1.26214900 4.45455100 1.44893200
O -3.26315900 2.77259500 0.72297600
H -3.70786400 2.31211300 1.44619600
H -2.73246300 3.51014800 1.10312300

C 2.65620800 0.85794300 0.76744500
H 2.73365200 1.34476500 1.73719200
H 2.65524400 1.65105500 0.01696200
H 3.94983500 -3.20666500 3.28325900
H 4.67227000 -4.28961300 2.08129200
H 5.30734600 -2.41242900 0.66006700
H 5.55530400 -1.70140000 2.27145800
H 6.20658400 -0.35215700 -4.30349900
O -3.34111200 -4.24520800 -0.14084600
C -4.56780400 -4.11621200 0.58437700
H -4.81480900 -3.05272400 0.69990000
H -4.45491200 -4.55256900 1.58732700
C -5.64184700 -4.84326700 -0.20458200
H -6.60054200 -4.77705200 0.31883800
H -5.75546700 -4.39746500 -1.19620500
H -5.38463500 -5.89939200 -0.32575800
Thermal Correction to Free Energy: 0.497032Hartree
Entropy: 272.039 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.145888 Hartree
Thermal Free Energy with Correction: -3225.648856 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of different catalyst configuration (Series D):

D1-a

C 5.53473000 -0.85839700 -1.35165700
C 4.23073200 -1.13736700 -1.76769000
C 3.20281300 -0.23167600 -1.50926100
C 3.46809600 0.95766600 -0.81568300
C 4.77783500 1.23162300 -0.40079500
C 5.80713700 0.32900900 -0.67031500
H 4.00958700 -2.06277600 -2.29016500
H 2.18882500 -0.45816200 -1.82332900
H 4.99701000 2.15867900 0.12092700
H 6.81998600 0.55527200 -0.34991500
C 2.37629200 1.95789700 -0.60066600
H 1.92308700 2.33379000 -1.51497200
C 1.24009600 1.77142800 0.49825800
C -0.13260100 2.15813000 0.06052700
C 1.33740700 0.63057200 1.45464800
O -0.16867900 3.31259400 -0.58575400

O 2.54653500 0.47930200 1.96400200
C -1.46559800 3.73654400 -1.10066800
H -1.23799100 4.53868700 -1.80014700
H -1.97699200 2.90265000 -1.58056500
H -2.07430000 4.10521400 -0.27294500
C 2.77381600 -0.71796800 2.75619200
H 2.48235100 -1.59708400 2.18003600
H 3.84221800 -0.71439500 2.96274700
H 2.19625000 -0.66591700 3.68062900
O -1.16097100 1.50426400 0.24972200
O 0.40956400 -0.11815700 1.77474600
Ni -1.30705500 -0.51240600 0.64115100
O -4.37685500 0.78093600 0.70374900
O -0.91204600 -2.59535100 0.77966000
Cl -4.12669500 0.20138100 -0.67252100
Cl 0.08532600 -2.63350400 -0.38916200
O -5.29113500 -0.55565900 -1.14185000
O -2.94932000 -0.79952800 -0.53655900
O -0.00112900 -1.16942900 -0.89937800
O 1.45103600 -2.90509700 0.10201600
O -3.74173800 1.27928700 -1.60859000
O -0.33397800 -3.57277600 -1.42909700
O -2.52226100 -0.28379000 2.27814500
H -2.20502700 0.38774300 2.89532100
H -3.35094500 0.07540700 1.86362600
H 6.33465700 -1.56334400 -1.55818300
C 2.31175000 2.87457900 0.55204400
H 3.04005500 2.74972800 1.34503600
H 1.94481900 3.88296300 0.40218800
Thermal Correction to Free Energy: 0.244576 Hartree
Entropy: 205.301 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.275357 Hartree
Thermal Free Energy with Correction: -2574.030781 Hartree

D1-TSa

C -3.93959100 -2.73660000 2.39522700
C -3.00355500 -1.74778100 2.70630900
C -2.47416000 -0.95234400 1.69615300
C -2.85671700 -1.14966600 0.35342600
C -3.79393100 -2.16171900 0.05341500
C -4.33716300 -2.93961800 1.06870000
H -2.67927900 -1.60591700 3.73195500
H -1.72997500 -0.19877400 1.92649100
H -4.09385500 -2.33634800 -0.97396300

H -5.06189900 -3.71246600 0.83083100
C -2.30774100 -0.28166500 -0.67003800
H -1.67065200 0.52473700 -0.33169400
C -0.70103500 -1.12468600 -1.93422300
C 0.35707200 -0.17575000 -2.11861400
C -0.36658200 -2.47091900 -1.57911500
O -0.04084700 1.00618000 -2.62493400
O -1.40790700 -3.32237600 -1.59738000
C 1.00008800 1.97337800 -2.88536700
H 0.47711000 2.91165200 -3.06846600
H 1.68146700 2.05133200 -2.03874700
H 1.56552800 1.67685800 -3.77316300
C -1.14413500 -4.65646200 -1.11254700
H -0.72269700 -4.61725600 -0.10672400
H -2.11432300 -5.15331700 -1.10981100
H -0.45229100 -5.17454900 -1.78024400
O 1.57465700 -0.35611200 -1.88343200
O 0.77374700 -2.90491100 -1.29085300
Ni 2.16634300 -1.65284800 -0.44262600
O 4.96957200 0.00576400 -1.45326200
O 2.37726900 -2.95746900 1.24556200
Cl 4.37959400 0.71227500 -0.25624100
Cl 1.16002100 -2.42242800 2.00766400
O 5.43262700 1.09791600 0.69601500
O 3.44502600 -0.28032100 0.45808100
O 0.71821600 -1.24567800 1.10912500
O 0.09031900 -3.44142000 2.06118200
O 3.59890200 1.89306500 -0.70465700
O 1.52624300 -1.94266900 3.34510500
O 3.70638700 -2.36912000 -1.61259000
H 3.36909000 -2.46177100 -2.51370500
H 4.32776500 -1.59819800 -1.62819900
H -4.35382300 -3.35732700 3.18438400
C -2.13642200 -0.66412500 -2.09748800
H -2.79504800 -1.46479200 -2.42939900
H -2.20156700 0.18565700 -2.77564800
C -4.98846600 1.19677600 -1.74495200
C -6.19601500 1.97749500 -1.19243500
C -5.93623600 1.96482400 0.32748800
H -5.20936100 0.12838000 -1.82953900
H -4.63874100 1.55520600 -2.71691500
H -6.22716700 2.99589200 -1.58790200
H -7.14404300 1.50087200 -1.45168400
H -6.27476200 2.87083000 0.83779800

H -6.41095600 1.10429700 0.80731000
C -3.65606200 2.70572300 -0.26934600
N -4.47727600 1.81442600 0.52665000
N -3.89836500 1.32744800 -0.74450500
H -4.16016100 3.47058200 -0.86360600
C -2.31751800 3.10081800 0.25226100
C -1.45553500 3.86874100 -0.53732900
C -1.88638000 2.71107200 1.53208500
C -0.17854200 4.21405200 -0.09276900
H -1.77829400 4.20377400 -1.52092300
C -0.62165800 3.04886900 1.98793600
H -2.55914100 2.13790300 2.16053000
C 0.25650700 3.78835600 1.17366500
H 0.46788700 4.80652300 -0.72836800
H -0.27467100 2.74384300 2.96943200
O 1.47163400 4.04302200 1.70050200
C 2.48088100 4.66339600 0.88584800
H 2.17608800 5.69491800 0.65761700
H 2.58551300 4.10643200 -0.05119900
C 3.78223900 4.62980300 1.66444100
H 4.10786700 3.59883400 1.82021100
H 4.56117100 5.15037400 1.09889500
H 3.66879400 5.12227800 2.63463200
Thermal Correction to Free Energy: 0.491914 Hartree
Entropy: 275.021 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.101244 Hartree
Thermal Free Energy with Correction: -3225.60933 Hartree

D1-a2

C -4.17026700 -2.29529700 2.25647100
C -3.02865900 -1.55177300 2.56558600
C -2.62133400 -0.51051700 1.73253600
C -3.34850000 -0.21134600 0.56978900
C -4.49437200 -0.95875200 0.26769900
C -4.90460000 -1.99415700 1.10845200
H -2.45169600 -1.78135800 3.45614600
H -1.73056000 0.06194900 1.97439700
H -5.07659200 -0.72362700 -0.61848100
H -5.79818100 -2.56234200 0.86686900
C -2.92760000 0.93565700 -0.29432600
H -2.85287800 1.89054100 0.21994900
C -1.72478000 0.80097300 -1.32777000
C -0.79454900 1.96438000 -1.39820100
C -1.10385200 -0.54631200 -1.47802100

O -1.42522600 3.12754800 -1.44633100
O -1.95043400 -1.48765000 -1.84585400
C -0.59640700 4.32222600 -1.39834700
H -1.30356700 5.14963300 -1.39558400
H 0.00807700 4.31038000 -0.49075000
H 0.04525700 4.36144400 -2.27994400
C -1.44394400 -2.85396400 -1.88040000
H -0.80002000 -3.04286000 -1.02173900
H -2.33365400 -3.48050100 -1.87070700
H -0.87691700 -2.99906400 -2.80198200
O 0.43824600 1.89909700 -1.42111500
O 0.08562800 -0.80110700 -1.26843400
Ni 1.49208000 0.40043800 -0.37636300
O 3.00641800 -2.39768400 -1.36851900
O 2.48426300 1.89404600 0.77412500
Cl 2.60238800 -2.54940400 0.08251900
Cl 1.35282700 2.07530900 1.79640500
O 3.67890300 -3.16488100 0.86463900
O 1.33493500 -3.30441900 0.17541900
O 0.34507000 0.99513700 1.31689200
O 1.80310100 1.80033400 3.16006900
O 2.38686500 -1.11843000 0.64585400
O 0.73829200 3.41146300 1.66171300
O 2.84966300 0.19843700 -1.89867500
H 3.09226700 -0.76249400 -1.82432200
H 2.45135500 0.31882500 -2.77028900
H -4.48685600 -3.10365500 2.90895800
C -3.18503600 1.01004800 -1.74600300
H -3.63836000 0.15412300 -2.23164500
H -3.40697900 1.97422500 -2.18747100
Thermal Correction to Free Energy: 0.244766 Hartree
Entropy: 205.074 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.276875 Hartree
Thermal Free Energy with Correction: -2574.032109 Hartree

D1-TSa2

C 0.84102800 -2.87953100 -3.53262400
C 0.81629400 -1.51962400 -3.21473400
C 1.07313500 -1.10515800 -1.91103300
C 1.33028400 -2.05262300 -0.90011300
C 1.33852400 -3.42267900 -1.23218500
C 1.10838600 -3.83008700 -2.54089600
H 0.58912200 -0.78362300 -3.97918200
H 1.03340400 -0.05226500 -1.65492800

H 1.53169600 -4.16495200 -0.46488000
H 1.12547700 -4.88659000 -2.79113600
C 1.58325900 -1.58838900 0.45552100
H 1.71966300 -0.52075900 0.58009500
C -0.22501200 -1.63237000 1.71320000
C -0.38300500 -0.39071800 2.40947700
C -1.35291200 -2.19411200 1.03262100
O 0.72023100 0.00754500 3.07558100
O -1.17471200 -3.45136100 0.59696200
C 0.62938400 1.27965200 3.75150800
H 1.61509200 1.43698500 4.19051100
H 0.38576700 2.06930600 3.03926600
H -0.13217400 1.24265400 4.53352600
C -2.26751600 -4.03383800 -0.15157800
H -2.66511000 -3.32633200 -0.87944200
H -1.84298300 -4.91271500 -0.63652400
H -3.06793600 -4.32774700 0.53211800
H 0.64403900 -3.20172000 -4.55095400
C 1.13278700 -2.30656500 1.67816200
H 1.05008900 -3.38610300 1.56143800
H 1.72124800 -2.06048600 2.56073800
C 4.36933400 -2.75471800 1.54318600
C 5.78109100 -3.10626300 1.03726200
C 5.68793300 -2.78707200 -0.46821900
H 3.70950100 -3.62649500 1.52545300
H 4.35652800 -2.33507800 2.55271500
H 6.54423000 -2.49978900 1.53128600
H 6.03125200 -4.15348200 1.22147200
H 6.62104200 -2.40899300 -0.89508700
H 5.37876400 -3.66340100 -1.04511200
C 4.70899900 -0.64312800 0.27004100
N 4.63041600 -1.76699200 -0.64141500
N 3.80401600 -1.76529600 0.58658000
H 5.57615800 -0.58243000 0.93143200
C 4.16316800 0.67098900 -0.17195700
C 3.95975200 1.69692800 0.75802000
C 3.85410300 0.91198600 -1.51973000
C 3.42372100 2.92531500 0.37430300
H 4.21185400 1.53729900 1.80425500
C 3.33519300 2.13501700 -1.91736900
H 4.01305100 0.12322700 -2.24671200
C 3.09399600 3.14827900 -0.97258000
H 3.25726100 3.69365000 1.11868400
H 3.08692700 2.33239600 -2.95491200

O 2.55780600 4.28804200 -1.45902900
C 2.12088400 5.30908200 -0.54679400
H 2.99811400 5.76683900 -0.06740000
H 1.48763500 4.85917000 0.22466000
C 1.33828500 6.32694400 -1.35580900
H 0.45527200 5.85650800 -1.79573600
H 1.00921700 7.14440000 -0.70682900
H 1.95336100 6.74576000 -2.15758800
O -1.41975100 0.31038300 2.47387900
O -2.45317800 -1.62963600 0.83135900
Ni -2.68314200 0.38539800 0.85982600
O -5.62725900 -1.00316100 0.06615500
O -2.48730200 2.53362000 0.78293500
Cl -4.93003800 -0.59362800 -1.21215400
Cl -1.16658400 2.55800500 0.01432300
O -5.87043400 0.06883900 -2.12622100
O -4.28471000 -1.76938900 -1.83591900
O -0.93597700 1.06628800 -0.29092500
O -1.27354100 3.33854400 -1.22470500
O -3.84695500 0.44465000 -0.83431800
O -0.07404300 3.06462500 0.88179100
O -4.36181600 0.26103900 2.04942200
H -5.00126700 -0.17157600 1.42590400
H -4.18021700 -0.38731800 2.74289900
Thermal Correction to Free Energy: 0.490868 Hartree
Entropy: 277.298 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.100566 Hartree
Thermal Free Energy with Correction: -3225.609698 Hartree

D1-TSa2

C 0.84102800 -2.87953100 -3.53262400
C 0.81629400 -1.51962400 -3.21473400
C 1.07313500 -1.10515800 -1.91103300
C 1.33028400 -2.05262300 -0.90011300
C 1.33852400 -3.42267900 -1.23218500
C 1.10838600 -3.83008700 -2.54089600
H 0.58912200 -0.78362300 -3.97918200
H 1.03340400 -0.05226500 -1.65492800
H 1.53169600 -4.16495200 -0.46488000
H 1.12547700 -4.88659000 -2.79113600
C 1.58325900 -1.58838900 0.45552100
H 1.71966300 -0.52075900 0.58009500
C -0.22501200 -1.63237000 1.71320000
C -0.38300500 -0.39071800 2.40947700

C -1.35291200 -2.19411200 1.03262100
O 0.72023100 0.00754500 3.07558100
O -1.17471200 -3.45136100 0.59696200
C 0.62938400 1.27965200 3.75150800
H 1.61509200 1.43698500 4.19051100
H 0.38576700 2.06930600 3.03926600
H -0.13217400 1.24265400 4.53352600
C -2.26751600 -4.03383800 -0.15157800
H -2.66511000 -3.32633200 -0.87944200
H -1.84298300 -4.91271500 -0.63652400
H -3.06793600 -4.32774700 0.53211800
H 0.64403900 -3.20172000 -4.55095400
C 1.13278700 -2.30656500 1.67816200
H 1.05008900 -3.38610300 1.56143800
H 1.72124800 -2.06048600 2.56073800
C 4.36933400 -2.75471800 1.54318600
C 5.78109100 -3.10626300 1.03726200
C 5.68793300 -2.78707200 -0.46821900
H 3.70950100 -3.62649500 1.52545300
H 4.35652800 -2.33507800 2.55271500
H 6.54423000 -2.49978900 1.53128600
H 6.03125200 -4.15348200 1.22147200
H 6.62104200 -2.40899300 -0.89508700
H 5.37876400 -3.66340100 -1.04511200
C 4.70899900 -0.64312800 0.27004100
N 4.63041600 -1.76699200 -0.64141500
N 3.80401600 -1.76529600 0.58658000
H 5.57615800 -0.58243000 0.93143200
C 4.16316800 0.67098900 -0.17195700
C 3.95975200 1.69692800 0.75802000
C 3.85410300 0.91198600 -1.51973000
C 3.42372100 2.92531500 0.37430300
H 4.21185400 1.53729900 1.80425500
C 3.33519300 2.13501700 -1.91736900
H 4.01305100 0.12322700 -2.24671200
C 3.09399600 3.14827900 -0.97258000
H 3.25726100 3.69365000 1.11868400
H 3.08692700 2.33239600 -2.95491200
O 2.55780600 4.28804200 -1.45902900
C 2.12088400 5.30908200 -0.54679400
H 2.99811400 5.76683900 -0.06740000
H 1.48763500 4.85917000 0.22466000
C 1.33828500 6.32694400 -1.35580900
H 0.45527200 5.85650800 -1.79573600

H 1.00921700 7.14440000 -0.70682900
H 1.95336100 6.74576000 -2.15758800
O -1.41975100 0.31038300 2.47387900
O -2.45317800 -1.62963600 0.83135900
Ni -2.68314200 0.38539800 0.85982600
O -5.62725900 -1.00316100 0.06615500
O -2.48730200 2.53362000 0.78293500
Cl -4.93003800 -0.59362800 -1.21215400
Cl -1.16658400 2.55800500 0.01432300
O -5.87043400 0.06883900 -2.12622100
O -4.28471000 -1.76938900 -1.83591900
O -0.93597700 1.06628800 -0.29092500
O -1.27354100 3.33854400 -1.22470500
O -3.84695500 0.44465000 -0.83431800
O -0.07404300 3.06462500 0.88179100
O -4.36181600 0.26103900 2.04942200
H -5.00126700 -0.17157600 1.42590400
H -4.18021700 -0.38731800 2.74289900
Thermal Correction to Free Energy: 0.490868 Hartree
Entropy: 277.298 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.100566 Hartree
Thermal Free Energy with Correction: -3225.609698 Hartree

D1-a3

C 4.99073300 -0.95458200 -2.51390400
C 3.90443400 -0.09052900 -2.67307800
C 3.24489500 0.42161300 -1.55683700
C 3.66001100 0.06326300 -0.26388100
C 4.75561300 -0.79742000 -0.11204700
C 5.41815000 -1.30259900 -1.23138600
H 3.57038700 0.19014300 -3.66734200
H 2.40785000 1.10181100 -1.67729300
H 5.10459900 -1.06213400 0.88142900
H 6.27134500 -1.96203500 -1.10040000
C 2.95696600 0.66198400 0.91135700
H 2.77635300 1.72880500 0.82514600
C 1.65504400 -0.01640700 1.54855100
C 0.56048100 0.92387700 1.91513600
C 1.25751900 -1.33781600 0.99240400
O 0.99466300 2.00939700 2.52838300
O 2.20016300 -2.26110800 1.10837500
C 0.01921400 3.06315800 2.75583900
H 0.60110900 3.90273500 3.13153900
H -0.47553700 3.30720200 1.81565000

H -0.71123500 2.73525600 3.49758700
C 1.95119500 -3.53062400 0.45645900
H 1.79134800 -3.37455000 -0.61137500
H 2.84926200 -4.11903700 0.63439700
H 1.07415100 -4.00933900 0.89468300
O -0.64869600 0.74110600 1.72350200
O 0.18847400 -1.59628000 0.43469400
Ni -1.47983300 -0.43160100 0.26616400
O -1.70436200 2.73526400 -0.48708300
O -2.58407600 -1.66661300 -1.04642400
Cl -0.54817600 2.18106500 -1.22720900
Cl -3.94444700 -1.00708600 -0.74149600
O 0.72504300 2.49790900 -0.50125200
O -0.48887900 2.62793600 -2.62531100
O -4.70358000 -0.72808100 -1.95542100
O -4.68354700 -1.88436900 0.21192400
O -0.66858700 0.62424300 -1.25766400
O -3.51402100 0.27467400 -0.01315300
O -2.34499000 -1.55179800 1.89059300
H -2.68734600 -0.89017000 2.50910100
H -3.14140200 -1.99932800 1.54216300
H 5.50631700 -1.34840700 -3.38502400
C 2.99661700 0.12061800 2.28213000
H 3.51048900 -0.81638000 2.45932800
H 2.99615600 0.81714800 3.11206700
Thermal Correction to Free Energy: 0.244624 Hartree
Entropy: 205.865 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.271135 Hartree
Thermal Free Energy with Correction: -2574.026511 Hartree

D1-TSa3

C -0.66297200 -4.83149700 2.18226400
C -0.78894300 -3.51764700 2.63954600
C -1.01156600 -2.48405400 1.73479600
C -1.09504000 -2.74966800 0.35115900
C -0.95113800 -4.08179100 -0.09774800
C -0.74500400 -5.11207000 0.81318300
H -0.69870800 -3.29280400 3.69720400
H -1.07933900 -1.46181800 2.08735900
H -0.98324900 -4.30250000 -1.15839400
H -0.63673900 -6.13346000 0.46036400
C -1.37182600 -1.64406900 -0.54960400
H -1.47420800 -0.67244100 -0.08456200
C 0.36052900 -1.01414500 -1.78825900

C 0.50026300 0.40811800 -1.69224000
C 1.50688300 -1.85660700 -1.64001500
O -0.63887800 1.08212100 -1.91951300
O 1.28098400 -3.15514800 -1.93686800
C -0.59152900 2.50681200 -1.70699700
H -1.61125500 2.85102300 -1.87492100
H -0.27522100 2.71800100 -0.68481400
H 0.09530500 2.97671800 -2.41484800
C 2.39346200 -4.04810600 -1.74770900
H 2.74744700 -4.01196100 -0.71554700
H 2.00973800 -5.03975900 -1.98858900
H 3.21543400 -3.78347300 -2.41624700
O 1.54989200 1.06062600 -1.46576700
O 2.66094400 -1.52231500 -1.29255400
Ni 3.12967500 0.26824600 -0.52448800
O 1.72260200 1.98837900 2.22186100
O 5.01633500 -0.20016900 0.39100200
Cl 1.10258200 0.67162600 1.99243400
Cl 5.45786900 1.26426800 0.52759800
O -0.16503500 0.82235800 1.19624400
O 0.82024300 -0.05440800 3.25070000
O 6.02626000 1.54603200 1.84402400
O 6.41018600 1.57892400 -0.57996800
O 2.06780600 -0.22831800 1.18020000
O 4.14921800 2.02367700 0.28366800
O 4.24241600 0.74620100 -2.31005100
H 3.82558400 1.56529100 -2.61326100
H 5.14974700 0.99593600 -2.04606300
H -0.48845500 -5.63780200 2.88904900
C -1.02485100 -1.60543700 -1.99420800
H -0.98604100 -2.57911900 -2.47978100
H -1.67029900 -0.93007500 -2.55418700
C -4.15421700 -3.01319500 -1.21917800
C -5.35357300 -3.49880200 -0.38198100
C -5.04130500 -2.92843300 1.01661300
H -3.35649900 -3.75995600 -1.22929000
H -4.40874200 -2.75806800 -2.25141100
H -6.29904800 -3.11466000 -0.77365200
H -5.42689400 -4.58854500 -0.37218600
H -5.93160200 -2.63792800 1.58115900
H -4.46762700 -3.63735400 1.61987500
C -4.64000000 -0.80719600 -0.18732300
N -4.18110300 -1.73982100 0.82460700
N -3.60769500 -1.81141500 -0.53356800

H -5.60587400 -1.00655700 -0.65515800
C -4.34008700 0.64172500 -0.05397000
C -5.03673300 1.55516300 -0.85038300
C -3.40536500 1.13252800 0.87308800
C -4.81489700 2.92933100 -0.74382700
H -5.77358100 1.19668000 -1.56598600
C -3.17100800 2.49360300 0.98796000
H -2.86526500 0.44544700 1.51328900
C -3.87641700 3.40533800 0.18332200
H -5.37671900 3.60989400 -1.37194200
H -2.43835000 2.87205300 1.69197500
O -3.58024500 4.71698700 0.37811500
C -4.27025600 5.70790000 -0.38595600
H -5.35229400 5.62508800 -0.21166800
H -4.08860500 5.54529800 -1.45793600
C -3.75130400 7.06567300 0.05289400
H -2.67490600 7.14236300 -0.12278600
H -4.25344800 7.85896100 -0.50920100
H -3.93773200 7.22265500 1.11868900
Thermal Correction to Free Energy: 0.491649 Hartree
Entropy: 276.216 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.096894 Hartree
Thermal Free Energy with Correction: -3225.605245 Hartree

D1-b

C 5.12572600 -0.47354200 -2.18367600
C 4.11449800 0.49111900 -2.19016600
C 3.35748700 0.72024100 -1.04228300
C 3.60143600 -0.01966800 0.12625200
C 4.61720600 -0.98342500 0.12561600
C 5.37643400 -1.20834100 -1.02411300
H 3.91636900 1.06807800 -3.08857900
H 2.56591100 1.46544500 -1.05211600
H 4.82557200 -1.54936200 1.02856400
H 6.16599900 -1.95392100 -1.01060400
C 2.79754000 0.27557900 1.35271400
H 2.79644400 1.32135800 1.65011700
C 1.34952800 -0.34084700 1.53284600
C 0.31190400 0.60643200 2.02782600
C 0.91754800 -1.30824400 0.47691500
O 0.70885400 1.30850800 3.07909800
O 1.56389600 -2.45492100 0.51276200
C -0.20992100 2.33300900 3.55166700
H 0.32062700 2.83006000 4.36166700

H -0.43935400 3.02377900 2.73904600
H -1.12708300 1.86553900 3.91287300
C 1.21359000 -3.43476100 -0.50400900
H 1.48300300 -3.05068900 -1.48937500
H 1.80509600 -4.31399600 -0.25623600
H 0.14451000 -3.64119600 -0.45183200
O -0.80659100 0.76441200 1.53934300
O 0.08012300 -1.06841200 -0.39662900
Ni -1.39067300 0.36384500 -0.39526500
O -2.89928400 -0.84075600 0.27754800
O -2.37774100 2.28170500 -0.40452900
Cl -1.12873200 3.06467300 -0.82143200
O -1.90608200 -3.02892100 0.83809500
O -0.10879000 1.91108400 -1.05155000
O -1.34560700 3.80481600 -2.06707200
O -4.29070200 -2.83548900 0.30639900
O -0.65522900 3.92655800 0.27733400
Cl -2.93587700 -2.36695900 -0.00009900
O -2.60622700 -2.56247100 -1.46054600
O -1.93561600 -0.09288000 -2.32124700
H -1.18776100 -0.09062800 -2.93284700
H -2.25859000 -1.02332200 -2.24381900
H 5.71758200 -0.64802100 -3.07738400
C 2.52528500 -0.69470000 2.43812800
H 2.88732000 -1.71000500 2.33112700
H 2.46395900 -0.32490000 3.45448400
Thermal Correction to Free Energy: 0.245083 Hartree
Entropy: 204.857 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.279686 Hartree
Thermal Free Energy with Correction: -2574.034603 Hartree

D1-TSb

C -0.43436700 -4.42562700 2.73021600
C -0.82037700 -3.10820500 2.99046600
C -1.08330900 -2.23939800 1.93553000
C -0.95341800 -2.67019800 0.60072300
C -0.54711100 -3.99702500 0.35262000
C -0.29684700 -4.86698500 1.41060300
H -0.90822200 -2.75606800 4.01339900
H -1.34979100 -1.20716000 2.13565800
H -0.40573200 -4.34041000 -0.66599500
H 0.01534600 -5.88721800 1.20815200
C -1.28024400 -1.73347600 -0.47559200
H -1.61463400 -0.75310000 -0.16167800

C 0.54533600 -0.95167400 -1.38774800
C 0.46367100 0.48002700 -1.37063600
C 1.74965300 -1.59766500 -0.95639400
O -0.69091300 0.96373700 -1.87169900
O 1.83919100 -2.89534900 -1.31072400
C -0.83272300 2.40008900 -1.84774200
H -1.83177300 2.58853800 -2.23961500
H -0.73743400 2.77327700 -0.82670400
H -0.07316000 2.86633800 -2.47890600
C 3.06980800 -3.55989300 -0.96031100
H 3.15419500 -3.66423100 0.12435800
H 3.00855100 -4.54107800 -1.43150100
H 3.92417500 -2.99649600 -1.33898000
O 1.33359000 1.28420700 -0.97893900
O 2.68986100 -1.09183200 -0.30587800
Ni 2.73063700 0.80616200 0.38697700
O 4.25817300 1.50439300 -0.80583600
O 2.12881400 2.63334700 1.48867600
Cl 1.00425900 1.94784000 2.25429200
O 4.95252600 -0.36415900 -2.26795800
O 1.15645800 0.46941700 1.82333000
O 1.18376700 2.07259100 3.70773100
O 6.45689900 1.52069400 -1.83953400
O -0.31908200 2.44895000 1.81822900
Cl 5.43970800 0.62106800 -1.27797200
O 5.97627100 -0.09549300 -0.05856400
O 4.12450700 0.31696600 1.82928700
H 3.88245400 -0.52489900 2.23654500
H 4.93880200 0.15110500 1.28968600
H -0.23039000 -5.10468600 3.55298700
C -0.65947400 -1.75606000 -1.82943000
H -0.38389500 -2.74597000 -2.18866700
H -1.25780700 -1.23264800 -2.57449100
C -3.56381800 -3.50765200 -1.58815200
C -4.85914100 -4.13869000 -1.04311400
C -4.92513500 -3.58634300 0.39508000
H -2.70422100 -4.16039100 -1.41717100
H -3.60527000 -3.25360300 -2.65038500
H -5.72960300 -3.83809600 -1.63178900
H -4.81770600 -5.22989800 -1.06140200
H -5.94349700 -3.41093000 0.75237500
H -4.42194300 -4.24996800 1.10347400
C -4.51017300 -1.39053500 -0.66744900
N -4.18203100 -2.30606500 0.40881900

N -3.32655900 -2.27338600 -0.79239800
H -5.32316000 -1.66828800 -1.34041900
C -4.38436500 0.07436200 -0.45189200
C -4.91076900 0.95339200 -1.40228200
C -3.76732500 0.61049400 0.69195800
C -4.82076000 2.33675800 -1.23861600
H -5.40605200 0.56035700 -2.28737200
C -3.65795900 1.98104200 0.86384700
H -3.38867000 -0.06207900 1.45383000
C -4.18596800 2.85827800 -0.10125700
H -5.24695200 2.99069700 -1.98944200
H -3.15670000 2.40043200 1.72916400
O -4.03638700 4.17932100 0.16104400
C -4.52436300 5.14037100 -0.77970200
H -5.60916700 5.01737400 -0.90622800
H -4.04925200 4.97599300 -1.75702300
C -4.19071600 6.51850800 -0.23783600
H -3.11057900 6.63230500 -0.11396600
H -4.54559700 7.28848600 -0.92952800
H -4.66750700 6.67680500 0.73325400
Thermal Correction to Free Energy: 0.489575 Hartree
Entropy: 280.281 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.103085 Hartree
Thermal Free Energy with Correction: -3225.61351 Hartree

D1-b2

C 5.35556800 1.12068000 -1.57712500
C 4.23011000 1.81631000 -1.12864500
C 3.38839300 1.25034800 -0.17192800
C 3.66154600 -0.02794300 0.34135100
C 4.79655400 -0.71666300 -0.10746100
C 5.63923100 -0.14510500 -1.06153500
H 4.00458500 2.80405200 -1.51898500
H 2.51681800 1.79905200 0.17107500
H 5.03486700 -1.69438300 0.30004600
H 6.51999700 -0.68607700 -1.39537000
C 2.76510300 -0.59230700 1.39685200
H 2.53064800 0.09962600 2.20090200
C 1.45513900 -1.42291500 1.03071800
C 0.24224100 -1.12250200 1.84068300
C 1.22890700 -1.70810400 -0.41471300
O 0.50381600 -0.94010000 3.12699100
O 2.19111100 -2.43146900 -0.96520000
C -0.61266500 -0.50546100 3.95110100

H -0.18823800 -0.36250700 4.94303100
H -1.01798100 0.42671500 3.55392100
H -1.38795500 -1.27257600 3.96167700
C 2.11603300 -2.62898500 -2.39892600
H 2.12387500 -1.66317700 -2.90621200
H 3.00173400 -3.20939400 -2.64990200
H 1.20462400 -3.17213300 -2.65303800
O -0.90940000 -1.05643100 1.40697600
O 0.27724600 -1.30235800 -1.08590900
Ni -1.35005700 -0.23155100 -0.42872500
O -0.07470600 1.27060400 0.12686100
O -2.80741900 -1.69683800 -0.91712100
Cl -4.00408600 -0.79499500 -0.54565700
O -1.37551700 2.83300400 1.51601400
O -3.30441400 0.33084300 0.23775200
O -4.59190800 -0.23924600 -1.78754600
O 0.71999500 3.54022900 0.45467700
O -4.97645500 -1.50671600 0.28212500
Cl -0.52079400 2.75556300 0.31714600
O -1.27359400 3.14168900 -0.92040600
O -1.71965700 0.74296700 -2.21778100
H -2.64755800 0.61775100 -2.48120200
H -1.61975800 1.69155900 -1.97657200
H 6.01206300 1.56595000 -2.31908300
C 2.67096600 -2.02458700 1.74354900
H 3.23082600 -2.74139000 1.15516700
H 2.51048700 -2.29533800 2.78056900
Thermal Correction to Free Energy: 0.244879 Hartree
Entropy: 205.895 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.276852 Hartree
Thermal Free Energy with Correction: -2574.031973 Hartree

D1-TSb2

C -2.43746300 -4.53882800 1.99962700
C -2.07697900 -3.27622000 2.47656300
C -1.88117700 -2.22281600 1.58740800
C -2.03294600 -2.42294600 0.19961200
C -2.38247700 -3.70833600 -0.26950200
C -2.58981500 -4.75306000 0.62517700
H -1.93888200 -3.11086800 3.54036800
H -1.57224000 -1.25333900 1.96142200
H -2.47842000 -3.89077600 -1.33387800
H -2.86088400 -5.73722000 0.25458800
C -1.87953600 -1.28622200 -0.69759000

H -1.64634200 -0.33718800 -0.23502000
C -0.00711500 -1.25782600 -1.85778100
C 0.59030600 0.04624500 -1.85914200
C 0.80068500 -2.38926200 -1.51880900
O -0.24685800 1.03363200 -2.23028800
O 0.24227600 -3.57999500 -1.82045600
C 0.30281000 2.36650500 -2.20420900
H -0.53027200 3.01938000 -2.46224900
H 0.68449300 2.60137600 -1.20907400
H 1.11146000 2.45946000 -2.93242300
C 0.99207300 -4.74611900 -1.43334200
H 1.17719100 -4.74774400 -0.35726400
H 0.37033100 -5.59511100 -1.71793400
H 1.94820400 -4.77808100 -1.95971600
H -2.59092100 -5.35907400 2.69517200
C -1.49245600 -1.39147000 -2.13105700
H -1.75104800 -2.33853200 -2.60215900
H -1.86355900 -0.55980200 -2.72789500
C -4.96315700 -1.44925700 -1.44032600
C -6.28350000 -1.40071400 -0.64770600
C -5.80601500 -1.06732900 0.78055000
H -4.55284100 -2.46257300 -1.46105100
H -5.04833000 -1.08457900 -2.46746500
H -6.95676600 -0.63309500 -1.03784800
H -6.81834700 -2.35209100 -0.68991700
H -6.50669600 -0.44495400 1.34385500
H -5.60942200 -1.97372400 1.35977900
C -4.50082500 0.72519100 -0.31344800
N -4.51596900 -0.35282000 0.65703500
N -3.98731100 -0.61073200 -0.69620400
H -5.44361500 0.97837400 -0.80177400
C -3.60390200 1.89314100 -0.11093300
C -3.77216800 3.02413100 -0.91474600
C -2.60605900 1.91333500 0.87997100
C -2.96547700 4.15284100 -0.75816600
H -4.54912100 3.03565400 -1.67618600
C -1.78998200 3.02226800 1.04208100
H -2.47875200 1.06224000 1.53941300
C -1.96349600 4.15309000 0.22366200
H -3.12811600 5.01629800 -1.39164900
H -1.00433200 3.03037700 1.78977800
O -1.11920400 5.18775900 0.46343900
C -1.22641600 6.37583600 -0.32358300
H -2.22980200 6.80946900 -0.20758000

H -1.08552500 6.13249300 -1.38636600
C -0.15701500 7.33981000 0.15829700
H 0.83750400 6.90145500 0.04059900
H -0.20043400 8.26765400 -0.42024000
H -0.30383600 7.58063000 1.21456500
O 1.77848400 0.33017200 -1.59226900
O 1.93484800 -2.37591700 -0.98909800
Ni 2.77147300 -0.71866500 -0.19248100
O 1.10263000 -0.39293400 1.05288900
O 4.63151100 -0.80430200 -1.27757700
Cl 5.28729400 0.32949600 -0.47331900
O 1.47032400 1.81692600 2.08399400
O 4.08253600 0.96359800 0.23391400
O 6.19495000 -0.26457100 0.54407700
O -0.19224800 0.27290900 2.99740800
O 5.96987500 1.28676000 -1.34631700
Cl 1.15040900 0.40625800 2.37650000
O 2.19817900 -0.22624900 3.24166900
O 3.69544600 -1.71074200 1.39956200
H 4.64437000 -1.49377000 1.40748000
H 3.30632400 -1.29099300 2.19703300
Thermal Correction to Free Energy: 0.49236 Hartree
Entropy: 274.992 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.102295 Hartree
Thermal Free Energy with Correction: -3225.609935 Hartree

D1-c

C 5.36757800 1.30974500 -0.91499400
C 4.23446200 1.86208500 -0.31241800
C 3.34565500 1.04668500 0.38727700
C 3.57730400 -0.33438200 0.48263200
C 4.71342100 -0.88114000 -0.12607700
C 5.60635600 -0.06194200 -0.81892500
H 4.03841700 2.92731000 -0.38819000
H 2.46082100 1.48288900 0.84407900
H 4.90331900 -1.94789700 -0.05041400
H 6.48650800 -0.49655100 -1.28374000
C 2.63938700 -1.19534600 1.27191600
H 2.61437900 -0.97986200 2.33843400
C 1.18937900 -1.50579700 0.73007500
C 0.11026800 -1.38840200 1.75174100
C 0.87677700 -0.99741500 -0.64144300
O 0.32630100 -2.15137400 2.81514000
O 1.56938800 -1.58315400 -1.59368200

C -0.65459700 -2.07364600 3.87863700
H -0.29332600 -2.75641300 4.64553800
H -0.71666700 -1.05259100 4.25898700
H -1.63019300 -2.38605100 3.50346600
C 1.31563800 -1.12729700 -2.95230700
H 1.57814100 -0.07199900 -3.04024700
H 1.95969000 -1.74457700 -3.57557300
H 0.26167400 -1.27826700 -3.18909300
O -0.86989800 -0.64395900 1.70309600
O 0.09788500 -0.07444800 -0.89137900
Ni -1.44527700 0.61903900 0.21507200
O -2.85503800 -0.54724000 -0.64988100
O -1.64294300 2.38013200 -1.04199300
Cl -0.99444800 3.30841500 -0.00870100
O -1.52396700 -2.61869600 -0.44987500
O -0.33543800 2.29914800 0.95662200
O 0.00158800 4.19345300 -0.61206100
O -3.86968100 -2.69476400 -1.16034800
O -2.05890900 4.04387100 0.72044300
Cl -2.59535400 -1.96824000 -1.26022600
O -2.15262100 -1.78501300 -2.65955500
O -3.11054100 1.29232400 1.29586900
H -3.17383600 2.26374400 1.25996600
H -3.86070400 0.93146800 0.79751100
H 6.06007800 1.94626400 -1.45789200
C 2.25741000 -2.57870200 0.89443200
H 2.63758400 -2.98032100 -0.03702200
H 2.08529400 -3.30214200 1.68149000
Thermal Correction to Free Energy: 0.243789 Hartree
Entropy: 207.833 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.276381 Hartree
Thermal Free Energy with Correction: -2574.032592 Hartree

D1-TSc

C -1.18120700 -4.84926900 2.45725200
C -1.67395400 -3.63155700 2.93489400
C -1.80600200 -2.55051500 2.06992000
C -1.44084500 -2.66192300 0.71264300
C -0.94553200 -3.89718100 0.24532500
C -0.81882300 -4.97824000 1.11359400
H -1.94629500 -3.52527100 3.98029200
H -2.18139100 -1.60190900 2.44049000
H -0.62682000 -3.99682400 -0.78481200
H -0.42650800 -5.92130600 0.74526000

C -1.64936200 -1.51045900 -0.16107100
H -1.98480000 -0.60383500 0.32872700
C 0.28451800 -0.65181100 -0.85938600
C 0.30218100 0.74809300 -0.56513800
C 1.48936800 -1.41567700 -0.72257500
O -0.87956300 1.36502300 -0.80015800
O 1.42262200 -2.66349100 -1.22404200
C -0.89631600 2.78953600 -0.60392500
H -1.90587600 3.09959400 -0.87162800
H -0.68110800 3.03923800 0.43750700
H -0.15665800 3.27219700 -1.24600800
C 2.66737100 -3.39921400 -1.23086400
H 3.01475700 -3.57246600 -0.21023300
H 2.43490200 -4.34307300 -1.72477900
H 3.42326400 -2.84075800 -1.78541300
O 1.25288600 1.43775700 -0.14006400
O 2.56236800 -1.04400900 -0.20412000
Ni 3.11762800 0.81711500 0.25283800
O 4.11869300 1.23179200 -1.47639500
O 4.90158400 0.10989700 1.33732900
Cl 4.30519100 0.39751000 2.71521600
O 2.31406400 0.59528600 -3.03052400
O 2.81188400 0.56286300 2.40996500
O 4.54316100 -0.70063100 3.65650600
O 4.41480200 1.54929400 -3.86452400
O 4.84398900 1.69601300 3.21242600
Cl 3.79330600 0.63716600 -2.88650600
O 4.36958300 -0.72602300 -2.95221400
O 3.79202200 2.77851900 0.67229800
H 4.30950500 2.77629600 1.49874200
H 4.41512900 2.91217800 -0.05966900
H -1.07192900 -5.69304400 3.13214800
C -0.96213300 -1.26830900 -1.45715200
H -0.73190800 -2.16849200 -2.02464600
H -1.51035700 -0.56155100 -2.08098900
C -3.83051600 -3.02932400 -1.72715600
C -5.19203200 -3.68311900 -1.42647700
C -5.42522600 -3.31638700 0.05289000
H -3.00740900 -3.72347100 -1.53943400
H -3.73748900 -2.64135300 -2.74458700
H -5.97958400 -3.28373300 -2.07058000
H -5.16530200 -4.76390600 -1.58092700
H -6.47668700 -3.15392300 0.30500600
H -5.02449200 -4.08017500 0.72471500

C -4.84668900 -1.01923500 -0.65907300
N -4.66727000 -2.07288100 0.32102700
N -3.67223400 -1.91272700 -0.75574000
H -5.57560800 -1.18205000 -1.45484800
C -4.73358100 0.40057400 -0.22999600
C -5.02445300 1.41976900 -1.14112500
C -4.39067500 0.75180000 1.08636900
C -4.96800800 2.76370500 -0.76928600
H -5.30707500 1.16939900 -2.16101400
C -4.33114900 2.08245600 1.47096000
H -4.19710600 -0.03443300 1.80835400
C -4.61887600 3.10269100 0.54654500
H -5.20461100 3.52805000 -1.49907300
H -4.07420200 2.36493700 2.48639500
O -4.53900300 4.36943600 1.02364400
C -4.82719800 5.46551400 0.14811200
H -5.85412300 5.37415900 -0.23172300
H -4.14439600 5.44154900 -0.71242700
C -4.65175900 6.74533000 0.94493200
H -3.62814300 6.82938600 1.31961000
H -4.86138200 7.61165900 0.31049900
H -5.33513300 6.76616600 1.79818600
Thermal Correction to Free Energy: 0.491703 Hartree
Entropy: 274.37 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.097197 Hartree
Thermal Free Energy with Correction: -3225.605494 Hartree

D1-c2

C 4.87432300 -1.32152200 -2.25969300
C 4.02257400 -0.22166000 -2.38434700
C 3.35754200 0.28040900 -1.26718300
C 3.52704900 -0.31966700 -0.00905400
C 4.39202200 -1.41676200 0.10857000
C 5.06153600 -1.91409300 -1.00972400
H 3.87438300 0.25106000 -3.35032200
H 2.70845900 1.14264700 -1.37335300
H 4.55853700 -1.87606200 1.07768400
H 5.73468700 -2.75968400 -0.90173700
C 2.82623900 0.27057900 1.17085300
H 2.81887700 1.35657800 1.18335600
C 1.39098800 -0.25040100 1.65973600
C 0.42619200 0.81802500 2.04076400
C 0.82829300 -1.44172600 0.96649600
O 0.95991500 1.73602400 2.83029200

O 1.59353500 -2.51826800 1.06238100
C 0.13459600 2.89096400 3.13511300
H 0.75181000 3.51158200 3.78223000
H -0.11114600 3.40805500 2.20721500
H -0.77533100 2.57442600 3.64663600
C 1.17037700 -3.68214100 0.30800200
H 1.10004300 -3.43199500 -0.75141400
H 1.94366200 -4.42744500 0.48394700
H 0.20085000 -4.02794500 0.66944700
O -0.75947800 0.88038900 1.70270500
O -0.22710200 -1.47220900 0.33105500
Ni -1.59969300 0.02722700 0.05072900
O 0.80200000 2.82437500 -0.12609700
O -3.11827200 -1.20442700 0.92841200
Cl -3.73232600 -1.59246500 -0.43022000
O 0.82586400 2.65229600 -2.56537400
O -2.64467200 -1.10246200 -1.40826000
O -3.93314700 -3.03857400 -0.53253500
O -0.27384100 0.92547600 -1.25778600
O -4.97103900 -0.81487300 -0.65472200
Cl 0.03619000 2.43958200 -1.34487000
O -1.26625000 3.18013300 -1.39964400
O -2.99034700 1.54181600 -0.07211400
H -2.60285500 2.24354200 -0.64005200
H -3.81774300 1.23551100 -0.47618100
H 5.39541200 -1.70947400 -3.13006700
C 2.67504200 -0.38961500 2.48208200
H 3.02828300 -1.40720600 2.59667300
H 2.71981300 0.22114200 3.37584600
Thermal Correction to Free Energy: 0.245325 Hartree
Entropy: 204.476 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.28093 Hartree
Thermal Free Energy with Correction: -2574.035605 Hartree

D1-TSc2

C -0.28497600 -4.80897900 2.13265300
C -0.63516800 -3.54159500 2.60488100
C -0.93249000 -2.52228200 1.70561300
C -0.86886300 -2.75073300 0.31508700
C -0.50373300 -4.03415400 -0.14735000
C -0.22042300 -5.05311500 0.75646100
H -0.66196000 -3.34044900 3.67080500
H -1.18095700 -1.53348300 2.07234100
H -0.42153500 -4.22466200 -1.21098200

H 0.06174500 -6.03629500 0.39166000
C -1.23396800 -1.66498600 -0.58362100
H -1.48142200 -0.72461200 -0.10777800
C 0.49666300 -0.80400100 -1.67842500
C 0.46888100 0.61984900 -1.52266100
C 1.73051800 -1.50447300 -1.50217300
O -0.72540000 1.17387100 -1.80377200
O 1.68868000 -2.80575300 -1.86336600
C -0.83211000 2.59359500 -1.58401200
H -1.86279900 2.84058500 -1.83569100
H -0.62454100 2.82605900 -0.53848600
H -0.13378000 3.13411200 -2.22653700
C 2.90425000 -3.55220600 -1.66652200
H 3.21598100 -3.51546900 -0.62089400
H 2.66449500 -4.57379800 -1.96250000
H 3.70539000 -3.15069700 -2.29045200
H -0.05046300 -5.60421300 2.83447400
C -0.79194600 -1.53841100 -1.99880900
H -0.60894000 -2.48516400 -2.50437000
H -1.47212500 -0.92357400 -2.58741800
C -3.73840800 -3.34129100 -1.45928400
C -4.93504200 -3.97240200 -0.72145300
C -4.79035500 -3.40423000 0.70485800
H -2.86234500 -3.99337700 -1.41858400
H -3.94263000 -3.09200500 -2.50389500
H -5.88552600 -3.68249100 -1.17666100
H -4.88985300 -5.06359000 -0.73381500
H -5.74572700 -3.22725500 1.20641600
H -4.18481700 -4.05826100 1.33812600
C -4.54154700 -1.22268000 -0.43389100
N -4.05799100 -2.12334200 0.59452000
N -3.38259600 -2.10182900 -0.71650300
H -5.44072100 -1.51463000 -0.97944500
C -4.41070500 0.24624700 -0.25217600
C -5.09060400 1.10287600 -1.12266800
C -3.65639900 0.80701400 0.79219600
C -5.02387600 2.48942500 -0.97656300
H -5.69144000 0.68874500 -1.92943000
C -3.57798000 2.18177900 0.94859300
H -3.13936500 0.15983900 1.49087200
C -4.26216300 3.03642500 0.06645900
H -5.56816400 3.12443300 -1.66484000
H -2.98455900 2.61700600 1.74493100
O -4.12468300 4.36592700 0.30714700

C -4.79413900 5.30082300 -0.54253000
H -5.87817300 5.12302200 -0.50890700
H -4.46205000 5.16320200 -1.58125000
C -4.45546100 6.69442000 -0.04445700
H -3.37615100 6.86501600 -0.08070900
H -4.94776800 7.44570200 -0.66935200
H -4.79062600 6.82681300 0.98779800
O 1.41541900 1.37001700 -1.19222200
O 2.81149900 -1.04158100 -1.07749300
Ni 3.02102000 0.74331600 -0.17265600
O -0.37976500 0.96554700 1.52362200
O 4.69432300 1.27519900 -1.46939900
Cl 5.74700500 0.95523400 -0.40175900
O 0.60320900 -0.05359500 3.51546700
O 4.92956000 0.17111800 0.63751400
O 6.84133100 0.14701600 -0.94707600
O 1.88436200 -0.00097100 1.44924400
O 6.22385400 2.21858200 0.21773100
Cl 0.87014000 0.76189600 2.31628800
O 1.46333400 2.08730200 2.69066700
O 3.24845300 2.62050200 0.68522400
H 2.74909800 2.61151300 1.52918400
H 4.18267400 2.80319400 0.87908400
Thermal Correction to Free Energy: 0.49176 Hartree
Entropy: 275.946 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.106553 Hartree
Thermal Free Energy with Correction: -3225.614793 Hartree

D1-d

C -6.17060700 -1.62015600 0.31004000
C -5.39887400 -1.23614600 1.40945600
C -4.41689200 -0.25774500 1.26405100
C -4.18420200 0.34187600 0.01714500
C -4.96726500 -0.04483000 -1.07713500
C -5.95527100 -1.01934000 -0.93111000
H -5.56442800 -1.69529100 2.37946700
H -3.82406000 0.04445800 2.12414100
H -4.81117000 0.42330700 -2.04402000
H -6.55791700 -1.30684600 -1.78754000
C -3.16002700 1.42618000 -0.09250000
H -3.28897600 2.22622900 0.63186800
C -1.60584600 1.12480300 -0.26312600
C -0.71388500 1.96385500 0.59249400
C -1.18200500 -0.28757600 -0.50305000

O -1.11232900 3.22547000 0.66466100
O -1.92016100 -0.91096300 -1.39882500
C -0.26705200 4.13356700 1.42394700
H -0.73875800 5.10824100 1.31352700
H -0.24225500 3.82867100 2.47149800
H 0.73925300 4.12672200 1.00418900
C -1.59810500 -2.30766300 -1.66322700
H -1.89873700 -2.91261700 -0.80627900
H -2.18467000 -2.56352300 -2.54327900
H -0.52850600 -2.42502000 -1.83255500
O 0.27292200 1.56874500 1.21732800
O -0.25395200 -0.85896900 0.07750800
Ni 1.54497800 0.03466500 0.55663000
O 1.63365900 1.11816700 -1.26810500
O 2.71769800 -1.46632200 -0.16574800
Cl 2.82726000 2.01058400 -0.83988800
Cl 2.46432900 -2.98326400 0.03971100
O 3.94451900 1.87602700 -1.77317600
O 3.16319500 1.41481000 0.53820400
O 1.94488700 -3.16045600 1.45061800
O 1.44671100 -3.43924200 -0.93038200
O 2.37132700 3.40889700 -0.69975400
O 3.74979000 -3.66647100 -0.13350300
O 1.69599200 -0.72174900 2.45161900
H 0.86161200 -0.67176000 2.93552200
H 1.86696800 -1.68545100 2.27623200
H -6.93846600 -2.37969600 0.42224800
C -2.46084500 1.82278300 -1.32979200
H -2.61643400 1.23483600 -2.22669900
H -2.23864400 2.87147300 -1.48768300
Thermal Correction to Free Energy: 0.243306 Hartree
Entropy: 207.878 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.271132 Hartree
Thermal Free Energy with Correction: -2574.027826 Hartree

D1-TSd

C -1.72755900 -5.29730400 1.94887500
C -2.27031900 -4.14559900 2.52651100
C -2.25160300 -2.94509700 1.82509600
C -1.68444400 -2.86909700 0.53517900
C -1.14217300 -4.04074500 -0.03456800
C -1.16564000 -5.24108500 0.66998300
H -2.70287200 -4.18584700 3.52136100
H -2.67223100 -2.04894500 2.27035200

H -0.67602800 -3.99985000 -1.01076100
H -0.73811200 -6.13471300 0.22560700
C -1.75013600 -1.59953000 -0.17399700
H -2.15355600 -0.76442000 0.38630100
C 0.24756700 -0.67503800 -0.52763200
C 0.20771900 0.65716200 0.00806300
C 1.43974700 -1.45461400 -0.36076700
O -0.95623700 1.29916500 -0.21728100
O 1.39412200 -2.68058300 -0.91496700
C -0.99409700 2.69154100 0.16671600
H -1.97155400 3.04283600 -0.16104200
H -0.89573200 2.79201800 1.24996300
H -0.18867800 3.23792400 -0.32674100
C 2.60179300 -3.47205200 -0.80136300
H 2.74282000 -3.79471600 0.23265800
H 2.43805600 -4.33151200 -1.45174300
H 3.47476300 -2.89683000 -1.10840200
O 1.11089800 1.24184400 0.64328500
O 2.48468500 -1.09851300 0.22577000
Ni 3.10449000 0.83644200 0.33550900
O 2.79032100 1.34802200 -1.72572200
O 5.09058700 0.38740500 -0.00739500
Cl 3.06746500 2.85377000 -1.53622700
Cl 5.86254600 -0.81287300 0.58227300
O 4.15398000 3.30217000 -2.41233500
O 3.47864900 2.91126400 -0.05782800
O 5.36370100 -1.02083400 1.99752600
O 5.59061700 -2.02068300 -0.22728300
O 1.82479000 3.62529000 -1.75735100
O 7.28922900 -0.46111100 0.58583900
O 3.43832300 0.77702500 2.37006100
H 2.69015300 0.31987200 2.77579000
H 4.20811900 0.15158300 2.42175800
H -1.73760900 -6.23544900 2.49586900
C -0.92405900 -1.19340900 -1.33743700
H -0.62723800 -2.01080800 -1.99279600
H -1.40126700 -0.40033100 -1.91436900
C -3.77911800 -2.81964000 -2.22675600
C -5.16476700 -3.49196400 -2.19719700
C -5.57898500 -3.34784100 -0.71887500
H -2.98264300 -3.54774100 -2.05055200
H -3.56473800 -2.28463700 -3.15546300
H -5.86866500 -2.98871300 -2.86485100
H -5.11525000 -4.53750500 -2.50872500

H -6.65378000 -3.20686700 -0.57553600
H -5.26387700 -4.21188600 -0.12759200
C -4.92264100 -0.98061200 -0.99668800
N -4.86077600 -2.17313200 -0.17327900
N -3.74245800 -1.86531900 -1.08634000
H -5.55385400 -1.00962200 -1.88651500
C -4.85898300 0.35643700 -0.34750600
C -5.01299900 1.50794800 -1.12478400
C -4.69108000 0.49860400 1.03994500
C -4.98770700 2.77999000 -0.55142300
H -5.15989300 1.42005100 -2.19875500
C -4.66629100 1.75563300 1.62450300
H -4.60643100 -0.39175300 1.65418700
C -4.81192900 2.91016200 0.83446300
H -5.11263900 3.65088100 -1.18289000
H -4.54525700 1.87762100 2.69573200
O -4.77555500 4.08914200 1.50236800
C -4.91170600 5.31294300 0.76930200
H -5.87712900 5.32311400 0.24507400
H -4.11524400 5.38317700 0.01599700
C -4.82000100 6.45449700 1.76529000
H -3.85670400 6.43965500 2.28203900
H -4.91939900 7.41183000 1.24521000
H -5.61521100 6.38055400 2.51207800
Thermal Correction to Free Energy: 0.488807 Hartree
Entropy: 281.615 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.095982 Hartree
Thermal Free Energy with Correction: -3225.607175 Hartree

D1-d2

C 5.31585200 0.35016000 2.49730400
C 3.99034500 -0.02295000 2.73446800
C 3.23553300 -0.61201000 1.72060900
C 3.79950000 -0.82572700 0.45315600
C 5.12790300 -0.44877300 0.22223200
C 5.88341300 0.13468900 1.24072600
H 3.54394700 0.14441600 3.71020100
H 2.20083100 -0.89132700 1.90272300
H 5.57500100 -0.62133300 -0.75239800
H 6.91435000 0.41905100 1.05172500
C 2.99322400 -1.50179800 -0.61252200
H 2.69169000 -2.52064300 -0.37991600
C 1.81885900 -0.73639400 -1.33906500
C 0.56570300 -1.51620800 -1.54740300

C 1.64308600 0.70400000 -0.97448500
O 0.78134200 -2.74282200 -1.99948400
O 2.65933200 1.47059500 -1.33207600
C -0.39520700 -3.58951900 -2.15013300
H 0.00087900 -4.57611400 -2.38298100
H -0.97465100 -3.59245300 -1.22568000
H -1.01109000 -3.21315200 -2.96850400
C 2.59009100 2.86316900 -0.91951000
H 2.69843300 2.92503000 0.16472100
H 3.42585100 3.34606200 -1.42206000
H 1.63505500 3.29680800 -1.21746800
O -0.57629900 -1.11022700 -1.33127400
O 0.67921500 1.16164500 -0.36470500
Ni -1.20481700 0.34979700 -0.01988700
O -1.95816400 1.81743100 -1.34250700
O -3.05179700 -0.56079900 0.03706400
Cl -2.13097300 2.89100100 -0.24543700
Cl -3.35926000 -1.77492000 0.94321900
O -1.17993100 3.99503900 -0.45508800
O -1.73697300 2.07850700 1.01703200
O -3.60582600 -1.28913000 2.31612200
O -4.48941900 -2.50113000 0.35899500
O -3.51887600 3.34516500 -0.16034000
O -2.11458800 -2.65900400 0.95383700
O -0.45146000 -0.71929500 1.61219000
H -0.78712400 -0.31749000 2.42768700
H -0.93482600 -1.58646700 1.52583800
H 5.90302000 0.80585500 3.28908000
C 3.09425800 -1.18387100 -2.05466000
H 3.74784600 -0.37524200 -2.35955800
H 2.97180900 -1.98710400 -2.77130800
Thermal Correction to Free Energy: 0.243124 Hartree
Entropy: 208.84 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.271552 Hartree
Thermal Free Energy with Correction: -2574.028428 Hartree

D1-TSd2

C -2.57799900 -4.29073000 3.09749700
C -2.78733900 -2.92625500 3.31719000
C -2.59634100 -2.02072700 2.27925200
C -2.18284300 -2.45891500 1.00418500
C -1.97336400 -3.83879300 0.79903100
C -2.17246200 -4.74295700 1.83843900
H -3.09455600 -2.57181800 4.29611400

H -2.75314000 -0.95996800 2.44804900
H -1.62779600 -4.19629400 -0.16298400
H -2.00237800 -5.80219700 1.67109300
C -2.05009100 -1.47303700 -0.06125100
H -2.21461000 -0.44070300 0.22320500
C 0.06482500 -1.15648900 -0.69235600
C 0.34188600 0.24798300 -0.63346900
C 1.05914500 -2.08496100 -0.23311400
O -0.67787600 1.02695900 -1.06115700
O 0.75029900 -3.38095900 -0.44890900
C -0.40880700 2.44411400 -1.09714800
H -1.35046400 2.90035600 -1.40012200
H -0.09475100 2.80455400 -0.11609700
H 0.38171900 2.66150900 -1.81883300
C 1.76824300 -4.33552000 -0.07280700
H 1.91905400 -4.32434100 1.00898400
H 1.38272000 -5.30298300 -0.39567700
H 2.71065600 -4.10160400 -0.57071400
H -2.72441100 -4.99964800 3.90708300
C -1.24042200 -1.63274700 -1.29658200
H -1.16381900 -2.65638000 -1.65953700
H -1.58403900 -0.97400000 -2.09514100
C -4.38241800 -2.67649100 -1.73366200
C -5.87402300 -3.01376800 -1.55239800
C -6.17091500 -2.47930300 -0.13718600
H -3.74670500 -3.50285800 -1.40445400
H -4.10770000 -2.41066300 -2.75750700
H -6.49067600 -2.52076700 -2.30816500
H -6.06047500 -4.08679900 -1.63295200
H -7.18435700 -2.08619600 -0.01920900
H -6.00990300 -3.24755100 0.62397000
C -5.05597500 -0.41630400 -0.92233900
N -5.19881600 -1.39673100 0.13711400
N -4.09105600 -1.53237100 -0.82831300
H -5.72421700 -0.49342700 -1.78173500
C -4.68299700 0.98046900 -0.57062300
C -4.63741000 1.95648000 -1.57019200
C -4.41670900 1.36198100 0.75531400
C -4.32136500 3.28366600 -1.27514000
H -4.85668500 1.68630100 -2.60060900
C -4.10160300 2.67615800 1.06391900
H -4.48552700 0.61723800 1.54107600
C -4.04956500 3.65146500 0.05172300
H -4.30035200 4.01641300 -2.07254700

H -3.90053000 2.98377800 2.08464600
O -3.74135400 4.90573000 0.45960700
C -3.66096200 5.95871700 -0.50883000
H -4.62844300 6.06499500 -1.01854600
H -2.90400900 5.70831500 -1.26452000
C -3.29019100 7.23110100 0.23085900
H -2.32674200 7.11744000 0.73466600
H -3.21680900 8.06443800 -0.47415400
H -4.04716900 7.47596700 0.98084900
O 1.39113500 0.80456100 -0.25309600
O 2.13940700 -1.81006400 0.32240000
Ni 3.17108600 -0.05266800 0.16109400
O 3.73783500 -0.70031500 -1.80938300
O 4.11973800 1.76452100 -0.21043300
Cl 4.97514800 -1.48256200 -1.33078100
Cl 4.23567200 2.83640600 0.89291300
O 4.77562500 -2.93115600 -1.54131000
O 4.98559300 -1.15805800 0.17589900
O 5.18589900 2.33873500 1.92639500
O 4.68154900 4.08717400 0.26602200
O 6.19348500 -0.99424300 -1.98360300
O 2.87315900 3.00091200 1.52221100
O 3.03884900 0.33928000 2.20905200
H 3.95008700 0.46848400 2.52410900
H 2.68224700 1.25601900 2.20977000
Thermal Correction to Free Energy: 0.48906 Hartree
Entropy: 282.022 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.09304 Hartree
Thermal Free Energy with Correction: -3225.60398 Hartree

D1-d3

C 5.32516300 2.52506800 -0.93229500
C 4.16853400 2.88355000 -0.23491000
C 3.43776000 1.91587200 0.45302100
C 3.85176400 0.57475100 0.44597800
C 5.01142200 0.22394200 -0.25518300
C 5.74520400 1.19449500 -0.93962000
H 3.83684900 3.91771800 -0.22576200
H 2.53329600 2.19620600 0.98752500
H 5.34626400 -0.80901500 -0.25778800
H 6.64511000 0.90959800 -1.47669700
C 3.07993100 -0.44229200 1.22825000
H 3.02726500 -0.23946200 2.29619500
C 1.70189600 -1.00271200 0.70002600

C 0.63294100 -1.08781900 1.73888000
C 1.28111200 -0.58462200 -0.67391200
O 0.99170400 -1.82156000 2.78223400
O 2.10054100 -0.98799100 -1.61995700
C 0.01353400 -1.96427900 3.84176300
H 0.48734600 -2.61215800 4.57693000
H -0.22074400 -0.98912200 4.27237900
H -0.89416500 -2.41948400 3.44335700
C 1.73813300 -0.64407100 -2.98606400
H 1.74185000 0.44048800 -3.10617900
H 2.50796800 -1.10652400 -3.60072700
H 0.74996300 -1.05029700 -3.20414200
O -0.45356300 -0.50589900 1.72557300
O 0.30332800 0.12282700 -0.93891700
Ni -1.35403100 0.43517000 0.16951900
O -2.45801400 1.73827300 -1.11790400
O -2.35153000 -1.22952500 -0.40135500
Cl -3.50237300 2.11933700 -0.04545100
Cl -1.67835400 -2.47796600 -1.04536200
O -3.26747100 3.51714300 0.38376800
O -3.11214300 1.17029900 1.11160900
O -1.32893000 -2.15335100 -2.44822000
O -0.43375600 -2.77932500 -0.26414700
O -4.86618900 1.87867000 -0.50664300
O -2.65000400 -3.57452900 -0.94591500
O -0.45804300 2.29478800 0.86309800
H -0.57440300 2.88751500 0.10345800
H -1.09035400 2.63130800 1.51885900
H 5.89546700 3.27976100 -1.46567000
C 2.94268600 -1.87033600 0.84818700
H 3.37595400 -2.19772600 -0.08866500
H 2.90964500 -2.61470900 1.63367600
Thermal Correction to Free Energy: 0.242984 Hartree
Entropy: 209.168 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2574.271631 Hartree
Thermal Free Energy with Correction: -2574.028647 Hartree

D1-TSd3

C 1.98086600 -4.53968200 -2.95344100
C 2.34732700 -3.23431100 -3.29366400
C 2.29721700 -2.22801300 -2.33464700
C 1.87265400 -2.50356400 -1.01862700
C 1.50556800 -3.82519900 -0.69059800
C 1.56109600 -4.83069600 -1.65246600

H 2.66760600 -3.00332400 -4.30493700
H 2.57745800 -1.21291100 -2.59789200
H 1.14669900 -4.05502400 0.30480100
H 1.26843300 -5.84288700 -1.39004200
C 1.89378200 -1.42007100 -0.03892700
H 2.14750600 -0.44024100 -0.42645400
C -0.15615500 -0.85604300 0.60992300
C -0.32391700 0.56029500 0.46014900
C -1.26262400 -1.73335500 0.37277400
O 0.77495300 1.27122400 0.80071400
O -1.05816400 -3.00887700 0.74773500
C 0.63270400 2.70287700 0.76698100
H 1.59319500 3.08969700 1.10548300
H 0.41611800 3.04576200 -0.24731900
H -0.17352400 3.02141100 1.43075700
C -2.21777900 -3.87130600 0.70408000
H -2.54039100 -4.02742700 -0.32797400
H -1.88645300 -4.81159000 1.14545100
H -3.03004500 -3.42788600 1.28225300
H 2.01687900 -5.32658000 -3.70110200
C 1.12169300 -1.38035900 1.22943500
H 0.96844400 -2.34911600 1.70132600
H 1.54881900 -0.67709700 1.94492100
C 4.15441000 -2.79964600 1.55646700
C 5.59668300 -3.27781100 1.30450400
C 5.87071600 -2.78636100 -0.13086900
H 3.42813700 -3.56650700 1.27549500
H 3.96012600 -2.49443300 2.58765100
H 6.29540600 -2.83952200 2.02162900
H 5.68463200 -4.36299300 1.38964000
H 6.90950400 -2.49275200 -0.30465100
H 5.59799600 -3.54171200 -0.87278800
C 4.99047300 -0.62076300 0.68114300
N 4.99232300 -1.61895700 -0.37093200
N 3.92466800 -1.64463100 0.64666900
H 5.68727800 -0.75306600 1.51068800
C 4.73294200 0.80249100 0.33237800
C 4.82050000 1.78171700 1.32583000
C 4.44764100 1.20225000 -0.98392600
C 4.61798100 3.13144200 1.03448700
H 5.05531100 1.49554300 2.34839900
C 4.24535300 2.53947900 -1.28901500
H 4.41190900 0.45163500 -1.76640300
C 4.32708500 3.51838700 -0.28247300

H 4.69808400 3.86483700 1.82733300
H 4.03175000 2.86079900 -2.30296100
O 4.11948800 4.79569900 -0.68583700
C 4.19568400 5.85506700 0.27558800
H 5.19242500 5.86270000 0.73765400
H 3.45495000 5.68857400 1.06972500
C 3.92373700 7.15624400 -0.45702700
H 2.93016600 7.14226400 -0.91292000
H 3.97243600 7.99576800 0.24275600
H 4.66413700 7.31736700 -1.24525200
O -1.33318700 1.18332000 0.07431400
O -2.36839600 -1.43806700 -0.13707000
Ni -3.12861400 0.40458700 -0.34662300
O -5.12725900 -0.03455000 -1.17252200
O -3.90418500 0.66988900 1.50866100
Cl -5.32088100 1.39264500 -1.69042400
Cl -3.64697400 -0.27390200 2.71903900
O -5.04347300 1.41289800 -3.16015300
O -4.20175400 2.16361100 -0.97778000
O -4.26551100 -1.59336100 2.43135100
O -2.17096100 -0.41866300 2.88490700
O -6.64506700 1.92363500 -1.37190700
O -4.26104800 0.37890800 3.88831200
O -2.53709700 0.18081600 -2.43572200
H -2.76039200 -0.74826400 -2.59099500
H -3.17932800 0.68476000 -2.97380000
Thermal Correction to Free Energy: 0.489356 Hartree
Entropy: 281.087 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3226.092446 Hartree
Thermal Free Energy with Correction: -3225.60309 Hartree

D2-ab

C 5.71679500 -1.39076100 -0.62757500
C 4.55064900 -1.49746100 -1.38825300
C 3.60634900 -0.47336700 -1.36610100
C 3.80803900 0.66227100 -0.56897600
C 4.98198000 0.76358400 0.18925300
C 5.93260500 -0.25671400 0.15789900
H 4.36585900 -2.37926100 -1.99320800
H 2.70087200 -0.56849200 -1.95755300
H 5.16200100 1.64759400 0.79358500
H 6.84231300 -0.16348300 0.74410900
C 2.80967500 1.77216900 -0.61763100
H 2.54793800 2.08004400 -1.62650400

C 1.48654100 1.81730600 0.27976700
C 0.26960300 2.26506700 -0.45352000
C 1.29427200 0.81761800 1.37203300
O 0.49569400 3.31884700 -1.23422500
O 2.39201700 0.61519300 2.08017700
C -0.61771800 3.77056700 -2.04567300
H -0.21540800 4.58304600 -2.64809500
H -0.97982700 2.95478400 -2.67309300
H -1.42706000 4.12303400 -1.40424100
C 2.34545100 -0.44859000 3.06562800
H 2.02683000 -1.37326700 2.58455900
H 3.36490400 -0.52614300 3.43889100
H 1.65550600 -0.18030900 3.86794700
O -0.84849200 1.75518200 -0.40597900
O 0.24267400 0.23665200 1.64734600
Ni -1.44475900 0.00356600 0.47922100
O -0.24643900 -0.96431700 -0.92684000
O -3.05967900 -0.03302300 -0.85956400
Cl -4.52392000 -0.09538300 -0.38731400
O 1.46714000 -2.22005000 0.31951800
O -4.78814800 1.13078200 0.44687400
O -5.39546300 -0.13593600 -1.56061000
O -0.65983200 -3.29553700 -0.23061000
O -4.67448900 -1.31789100 0.46942200
Cl 0.40706000 -2.35467600 -0.71048400
O 0.95145600 -2.77963700 -2.00863000
O -2.10941500 -1.70256500 1.42886500
H -3.04638800 -1.79384400 1.14665900
H -1.62941000 -2.44908300 1.00029200
O -2.51153600 1.10445600 1.90861500
H -3.39885100 1.29188100 1.51665300
H -2.66946100 0.51823500 2.66226500
H 6.45497800 -2.18720000 -0.64755000
C 2.64921900 2.81834700 0.40728800
H 3.21275800 2.72519300 1.32799000
H 2.42765200 3.83096100 0.09195200
Thermal Correction to Free Energy: 0.270493 Hartree
Entropy: 211.968 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2650.771197 Hartree
Thermal Free Energy with Correction: -2650.500704 Hartree

D2-TSab

C -1.97786500 -4.58827500 2.02799500
C -1.95423000 -3.28993200 2.54144900

C -1.92661000 -2.20498300 1.67352100
C -1.90859300 -2.39905500 0.27685800
C -1.91980200 -3.71846700 -0.22644400
C -1.95979900 -4.80044300 0.64517500
H -1.93427600 -3.12460800 3.61328000
H -1.88161300 -1.19653300 2.07018400
H -1.86892800 -3.89096100 -1.29495400
H -1.96193100 -5.81249300 0.25162600
C -1.93650100 -1.23342100 -0.58546300
H -1.89976200 -0.27197500 -0.08741300
C -0.03289800 -0.86149100 -1.75162300
C 0.33875800 0.50175100 -1.53029300
C 0.97144000 -1.88054500 -1.74113600
O -0.69064600 1.37322200 -1.65740000
O 0.51214100 -3.10938900 -2.06159800
C -0.37161300 2.75856900 -1.43589000
H -1.32009700 3.28605900 -1.53256700
H 0.05206100 2.90353600 -0.44015000
H 0.34655000 3.11035900 -2.18023800
C 1.46323000 -4.18482100 -1.94479100
H 1.85419300 -4.22824300 -0.92720000
H 0.90316400 -5.08914500 -2.18561000
H 2.28526400 -4.04907700 -2.65115500
O 1.46822300 0.95760400 -1.25598300
O 2.19292700 -1.74106200 -1.51024200
Ni 3.00897000 -0.14040000 -0.57360800
O 1.82357200 -0.54970900 1.14905600
O 3.71670200 1.62124800 0.40388800
Cl 5.14680200 2.15330000 0.26443600
O 1.24861600 -2.94610100 1.20519100
O 5.39563600 2.44062100 -1.19305200
O 5.28399100 3.37006500 1.06999800
O 3.30002700 -2.16502900 2.28471300
O 6.08744000 1.07666500 0.72357100
Cl 1.86210100 -1.84057100 1.98631100
O 1.11470000 -1.58167900 3.23126700
O 4.65079800 -1.21519100 0.11690800
H 5.26985800 -0.54209400 0.47465700
H 4.31609500 -1.71284600 0.89786500
O 4.16353000 0.26597300 -2.28679800
H 4.64627700 1.10598700 -2.10510600
H 4.83592800 -0.42992300 -2.30045100
H -1.99309000 -5.43779100 2.70460300
C -1.49251100 -1.19159800 -2.00588500

H -1.60308800 -2.13682900 -2.53463400
H -1.99238100 -0.39550000 -2.55893400
C -4.77507600 -1.99372500 -1.62721500
C -6.14542400 -2.29960800 -0.99377700
C -5.91257800 -1.96035900 0.49224200
H -4.13819200 -2.88208000 -1.63855800
H -4.83378100 -1.59066500 -2.64150300
H -6.93547100 -1.68253900 -1.42960700
H -6.43451800 -3.34320700 -1.13564300
H -6.79500900 -1.55492800 0.99474000
H -5.56643500 -2.83215300 1.05399800
C -4.95361400 0.15119700 -0.37404700
N -4.82239300 -0.96081600 0.54723300
N -4.10585600 -1.00483100 -0.74009500
H -5.86883200 0.21820900 -0.96494500
C -4.37754300 1.47228300 -0.00660800
C -4.63241900 2.58279000 -0.81583300
C -3.61826000 1.65082500 1.16233800
C -4.13802300 3.84726700 -0.49074800
H -5.23234000 2.46931900 -1.71596400
C -3.12029600 2.90000200 1.49869800
H -3.44523200 0.80178500 1.81479800
C -3.37412200 4.01118500 0.67456400
H -4.35982600 4.68830900 -1.13604900
H -2.53544400 3.04922500 2.40007900
O -2.84758800 5.18759300 1.09544000
C -3.05389200 6.36757500 0.31224300
H -4.13057200 6.56847500 0.22286200
H -2.65251400 6.21550500 -0.69937400
C -2.34182900 7.51052700 1.01285400
H -1.27169700 7.30390600 1.09767300
H -2.47338700 8.43665100 0.44530500
H -2.74585600 7.65846500 2.01796700
Thermal Correction to Free Energy: 0.515502 Hartree
Entropy: 286.298 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.598123 Hartree
Thermal Free Energy with Correction: -3302.082621 Hartree

D2-ac

C -4.62869000 -2.35187700 2.14290100
C -3.71845300 -1.37164900 2.54469800
C -3.23853500 -0.43996900 1.62553900
C -3.65434700 -0.48551200 0.28522200
C -4.57649900 -1.46614200 -0.10684000

C -5.06137800 -2.39291000 0.81627300
H -3.38136600 -1.32642900 3.57568700
H -2.54378700 0.32639800 1.95003500
H -4.93151700 -1.49851500 -1.13215800
H -5.78181600 -3.14172900 0.49978400
C -3.15443300 0.55241900 -0.66694700
H -3.14563900 1.55911600 -0.26071100
C -1.81650100 0.35414900 -1.53124200
C -0.93448300 1.55393500 -1.62336600
C -1.14719300 -0.96901000 -1.45964000
O -1.60618800 2.66021500 -1.90230700
O -1.95339000 -1.98220800 -1.74027400
C -0.85807400 3.90270400 -1.85123600
H -1.58487500 4.67629800 -2.09268100
H -0.45875900 4.03579100 -0.84538900
H -0.04939200 3.88234300 -2.58312400
C -1.42840100 -3.31565100 -1.52865100
H -1.01573800 -3.40005900 -0.52272400
H -2.28174800 -3.97803200 -1.66019700
H -0.65177100 -3.53211400 -2.26463900
O 0.29149000 1.56828300 -1.48958000
O 0.03428700 -1.16922400 -1.16009500
Ni 1.47076100 0.18891700 -0.50272600
O 0.33593900 0.49794800 1.23487800
O 2.43431300 -1.39608100 0.45669900
Cl 3.97092400 -1.54777600 0.48069700
O -1.12355900 2.47191900 1.10459200
O 4.54709700 -0.32460100 1.12006900
O 4.30256000 -2.76392500 1.22284800
O -0.42719900 1.58131900 3.27170000
O 4.43621300 -1.63533500 -0.94916700
Cl -0.01471100 1.85239500 1.88834900
O 1.19637700 2.73558800 1.83698200
O 2.87139900 1.58585600 0.01027000
H 2.42677600 2.15493900 0.67650000
H 3.59718700 1.12427100 0.48245900
O 2.49578700 -0.27717700 -2.27067800
H 3.34296600 -0.68416500 -1.96843100
H 2.00577600 -1.01155900 -2.66630300
C -3.22514500 0.44963700 -2.13517700
H -5.00490000 -3.07428000 2.86139600
H -3.41676400 1.34879100 -2.70829500
H -3.58976300 -0.47059900 -2.57536100
Thermal Correction to Free Energy: 0.26989 Hartree

Entropy: 213.195 cal/mol-kelvin

Single Point Energy with Solvent Effect: -2650.773855 Hartree

Thermal Free Energy with Correction: -2650.503965 Hartree

D2-TSac

C -0.13854000 -4.80596800 2.07254100

C -0.47466400 -3.54301700 2.56665500

C -0.85939700 -2.53296700 1.69035900

C -0.89993000 -2.76723600 0.29911500

C -0.54764900 -4.04656800 -0.18599700

C -0.17686100 -5.05590300 0.69619700

H -0.42327000 -3.33859600 3.63107500

H -1.09808400 -1.54741500 2.07190200

H -0.54603800 -4.24058900 -1.25209900

H 0.09304700 -6.03608300 0.31440200

C -1.35542300 -1.69457000 -0.56985400

H -1.59114300 -0.75949500 -0.07828400

C 0.24960600 -0.79496500 -1.82214800

C 0.19971400 0.63382300 -1.67042000

C 1.50743700 -1.46038100 -1.75513100

O -1.02702300 1.15170700 -1.86170800

O 1.46236100 -2.77728900 -2.05773500

C -1.16005700 2.56756500 -1.62945400

H -2.21400700 2.78365800 -1.80004700

H -0.88048700 2.80328600 -0.60180500

H -0.52982000 3.12946600 -2.32213600

C 2.69998300 -3.49974000 -1.92775600

H 3.11504800 -3.38045300 -0.92533100

H 2.44592700 -4.54241600 -2.11992000

H 3.43034500 -3.14793600 -2.66011000

O 1.14991100 1.40571300 -1.41928800

O 2.62178900 -0.95441500 -1.47728400

Ni 2.88935500 0.84273800 -0.54092500

O 1.78763500 0.11991900 1.15600500

O 4.62346600 0.03006100 0.37186400

Cl 5.96707800 0.77041100 0.46054800

O -0.53579400 0.91994300 1.31364700

O 5.74502500 2.05418400 1.19981200

O 6.93268600 -0.09081100 1.14897900

O 0.65106700 0.15674500 3.30638100

O 6.41635300 1.07126300 -0.94519700

Cl 0.77972000 0.87786400 2.02654400

O 1.27708900 2.27572100 2.24204500

O 3.18866400 2.69129400 0.30780000

H 2.53592000 2.74655000 1.03800600
H 4.07348500 2.68438700 0.73023800
O 4.02675300 1.33821200 -2.24067100
H 4.96320400 1.37195800 -1.93491700
H 3.95877500 0.51370100 -2.74382900
C -1.04383800 -1.56733100 -2.01813900
H 0.16414900 -5.59353800 2.75667300
H -1.78939400 -0.97393600 -2.54614400
H -0.88202300 -2.51304700 -2.53294900
C -3.89883200 -3.46651400 -1.19310100
C -4.99062400 -4.12660100 -0.32894300
C -4.73705700 -3.51272800 1.06279500
H -2.99654400 -4.08225500 -1.22364000
H -4.21335400 -3.25359700 -2.21827500
H -5.99208500 -3.89048700 -0.69779300
H -4.89789200 -5.21482400 -0.31917900
H -5.64776400 -3.36085500 1.64868400
H -4.04741100 -4.12385100 1.65149900
C -4.69226400 -1.35790000 -0.14816200
N -4.07418800 -2.20661200 0.85212200
N -3.52568100 -2.19397200 -0.51749000
H -5.62429900 -1.70548900 -0.59755700
C -4.61770000 0.12014600 -0.01888200
C -5.43372300 0.91361800 -0.83067700
C -3.78502800 0.75057200 0.92069400
C -5.42716500 2.30560700 -0.72834600
H -6.09532500 0.44386800 -1.55527700
C -3.76568700 2.13180800 1.03258400
H -3.15751800 0.15488500 1.57280500
C -4.58825100 2.92243200 0.21113200
H -6.07591600 2.89052500 -1.36865400
H -3.11485000 2.62142000 1.74839200
O -4.49967900 4.26413300 0.40421200
C -5.31737400 5.13668700 -0.37903400
H -6.37748300 4.89245000 -0.22261200
H -5.09354800 4.99841000 -1.44632400
C -5.01716900 6.55902800 0.05913100
H -3.96184000 6.79697200 -0.09913700
H -5.62327200 7.26469900 -0.51704500
H -5.24441200 6.69095800 1.12041900
Thermal Correction to Free Energy: 0.516323 Hartree
Entropy: 284.769 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.599939 Hartree
Thermal Free Energy with Correction: -3302.083616 Hartree

D2-ad

C -5.41508800 0.28120700 -1.79919100
C -4.11507300 0.34555800 -2.30660800
C -3.12340000 -0.49090400 -1.79725000
C -3.41696600 -1.39130800 -0.76223900
C -4.72374700 -1.45371500 -0.26224900
C -5.71818100 -0.62265600 -0.77989700
H -3.87180500 1.04922100 -3.09666500
H -2.11101800 -0.43713200 -2.18606700
H -4.96895000 -2.16110900 0.52432100
H -6.72907900 -0.68371700 -0.38756800
C -2.34797400 -2.31133900 -0.26386600
H -1.86515300 -2.90039700 -1.03971800
C -1.25371500 -1.84419600 0.79129800
C 0.13942100 -2.30585600 0.52106600
C -1.39552500 -0.49303800 1.40957000
O 0.20252400 -3.58304900 0.17319400
O -2.58884000 -0.27408000 1.92718400
C 1.52178300 -4.11271700 -0.14569400
H 1.32851400 -5.06871400 -0.62893800
H 2.06356500 -3.42570300 -0.79551100
H 2.08329200 -4.25495600 0.77975600
C -2.85003700 1.06350800 2.44295300
H -2.49746500 1.81783900 1.73997300
H -3.92958500 1.10171200 2.57459800
H -2.33629000 1.18637200 3.39824800
O 1.15644800 -1.61524800 0.60520900
O -0.51077000 0.36592300 1.45565000
Ni 1.24772000 0.46587100 0.37422900
O 4.32881800 -0.82105800 0.71011500
O 1.18935400 2.52235600 0.19036800
Cl 4.08876000 -0.57535900 -0.75624300
Cl -0.08731200 3.35791000 -0.06234600
O 5.25690100 0.04105700 -1.39253300
O 2.91320500 0.43945700 -0.86011500
O 0.33130800 4.63690100 -0.64585300
O -0.94708000 2.57831400 -1.04193800
O 3.68250300 -1.83078700 -1.42923500
O -0.82551800 3.52739900 1.20731600
O 0.23669400 0.26379800 -1.44542600
H -0.23049200 1.14151200 -1.49625700
H 0.98629200 0.30304800 -2.06150900
O 2.45419300 0.59935900 2.04605500

H 2.13182700 0.06948000 2.78619900
H 3.28400500 0.16528700 1.73163700
H -6.18775400 0.93163400 -2.19809800
C -2.32206300 -2.90875900 1.08467100
H -1.94946100 -3.91967400 1.19875500
H -3.07573800 -2.59991800 1.79912000
Thermal Correction to Free Energy: 0.267704 Hartree
Entropy: 216.848 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2650.766407 Hartree
Thermal Free Energy with Correction: -2650.498703 Hartree

D2-TSad

C -3.22541300 -3.45765500 2.29981800
C -2.48199600 -2.31980000 2.62222300
C -2.23247300 -1.35691600 1.64985400
C -2.69763600 -1.53138400 0.33101600
C -3.43896500 -2.68994200 0.01861000
C -3.70940600 -3.63735700 0.99944500
H -2.08924700 -2.19088400 3.62542300
H -1.64241500 -0.47854500 1.88537700
H -3.79889200 -2.84863900 -0.99214100
H -4.28457800 -4.52441200 0.75172100
C -2.41757000 -0.50412600 -0.66040700
H -1.91576200 0.38491100 -0.30340800
C -0.74514100 -0.95771900 -2.02601100
C 0.10468000 0.18059600 -2.20635500
C -0.14710000 -2.22400600 -1.72184000
O -0.54197800 1.29000400 -2.62039000
O -0.98827800 -3.26874000 -1.80140100
C 0.28119500 2.44337700 -2.89240200
H -0.41842700 3.26953100 -3.02013100
H 0.97699400 2.63023200 -2.07500300
H 0.84896400 2.28700400 -3.81380800
C -0.44237900 -4.55851100 -1.43928700
H 0.09938700 -4.50249000 -0.49455700
H -1.30527100 -5.22033900 -1.36567900
H 0.23795200 -4.90684900 -2.22019500
O 1.34756900 0.22426000 -2.05437900
O 1.05163500 -2.42683700 -1.42073200
Ni 2.24694100 -0.96994600 -0.64609700
O 4.71729200 1.28163100 -1.62959000
O 3.16578900 -2.23256700 0.73765100
Cl 4.00304100 1.83088500 -0.42807100
Cl 2.48039000 -3.22464500 1.69538900

O 4.94935500 2.41344400 0.53642800
O 3.29392100 0.64797400 0.26785900
O 3.42655900 -3.52265600 2.77906700
O 1.24387100 -2.53978800 2.25277000
O 2.98060100 2.82534500 -0.84657200
O 2.07703100 -4.43929400 0.95468300
O 0.86195400 -0.35461500 0.82383100
H 0.93575700 -1.10108100 1.47717700
H 1.37681800 0.38331300 1.18995600
O 3.79333200 -1.28080000 -2.00030400
H 3.38431300 -1.24801600 -2.87595700
H 4.31661800 -0.44941700 -1.92658700
H -3.42088700 -4.20980500 3.05840500
C -2.24769400 -0.77935400 -2.11444400
H -2.50733800 0.07104500 -2.74339000
H -2.75429100 -1.67801900 -2.46255900
C -5.33514000 0.47624500 -1.55291800
C -6.64544400 0.99500200 -0.93196700
C -6.35604900 0.91191800 0.58019200
H -5.36976600 -0.60542400 -1.71329000
H -5.07398400 0.95795900 -2.49884200
H -6.85644100 2.02024500 -1.24648600
H -7.50391800 0.38464700 -1.22089600
H -6.83538600 1.70337100 1.16294500
H -6.66339700 -0.05221500 0.99490700
C -4.25240500 2.08259500 0.02362500
N -4.88882200 1.00497900 0.75596300
N -4.26310900 0.72337200 -0.55445900
H -4.89353500 2.79071000 -0.50520000
C -2.98919000 2.66214900 0.56285100
C -2.26677300 3.59354600 -0.19028500
C -2.49129500 2.28627700 1.82167500
C -1.05757200 4.11731400 0.26847500
H -2.64522200 3.91554900 -1.15800400
C -1.29316600 2.80222200 2.29250700
H -3.05630500 1.58091900 2.42113300
C -0.55058100 3.70957900 1.51373800
H -0.51761600 4.83058600 -0.34150600
H -0.90050600 2.51931300 3.26374500
O 0.61530100 4.12787500 2.04993000
C 1.46405200 5.01245400 1.29425500
H 0.93984400 5.96632600 1.14170500
H 1.68381500 4.56316800 0.32019700
C 2.74395300 5.20572000 2.08514200

H 3.29095300 4.26374300 2.17016800

H 3.38810000 5.92300700 1.56777100

H 2.52991400 5.58928200 3.08694600

Thermal Correction to Free Energy: 0.513556 Hartree

Entropy: 289.725 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3302.591125 Hartree

Thermal Free Energy with Correction: -3302.077569 Hartree

D2-bc

H -1.26382300 -0.81591800 4.47707000

C 0.63297800 -2.64335300 -2.28408500

H 0.99454300 -1.76920000 -2.82835400

H 1.09771100 -3.55327800 -2.65896900

H -0.45455500 -2.69888900 -2.33195400

O -0.81945200 -0.17238900 1.98362900

O -0.20487000 -0.73504800 -0.69784200

Ni -1.40842500 0.66589500 0.19258800

O -3.09962800 -0.52438500 0.14315100

O 0.27658900 1.89543000 0.40073000

Cl 0.35544800 3.28097700 -0.28312900

O -2.44040900 -2.78194700 -0.59455000

O -0.79225900 4.09336200 0.23403000

O 1.65136500 3.87606300 0.06830600

O -4.74309900 -1.99054900 -0.88656000

O 0.22733100 3.07884900 -1.75794900

Cl -3.31943000 -1.63324900 -0.92200100

O -2.93558100 -1.05832200 -2.26022400

O -2.56891800 2.11029000 1.12841100

H -2.12260000 2.95766900 0.91149000

H -3.41770200 2.11349600 0.66278700

O -2.00748300 1.43244500 -1.62431300

H -1.26860100 1.88568800 -2.07135000

H -2.29944700 0.64659100 -2.13565600

C 5.10955500 -0.07263600 -1.89459200

C 4.30533000 0.87469100 -1.25547400

C 3.48937200 0.49557000 -0.19105700

C 3.46263700 -0.84027600 0.24068500

C 4.27247700 -1.78397800 -0.40350500

C 5.09370500 -1.40060500 -1.46514000

H 4.30835700 1.90985700 -1.58268800

H 2.86065800 1.23522600 0.29587400

H 4.27325900 -2.81640200 -0.06713300

H 5.72279300 -2.13947000 -1.95302900

C 2.60277500 -1.20669800 1.40775200

H 2.74755600 -0.57925300 2.28392300
C 1.05540300 -1.51578600 1.21701300
C 0.16332300 -0.87291200 2.22119900
C 0.55744500 -1.55884300 -0.19169300
O 0.54534800 -1.10966500 3.47264200
O 1.05160800 -2.55901200 -0.89461800
C -0.23017600 -0.46872100 4.51529100
H 0.24827900 -0.76703000 5.44644100
H -0.20388300 0.61498600 4.38938900
H 5.74783500 0.22404800 -2.72175600
C 2.06737100 -2.55958200 1.68096700
H 2.25919100 -3.34817100 0.96364600
H 1.97651200 -2.87859300 2.71207500
Thermal Correction to Free Energy: 0.269045 Hartree
Entropy: 214.861 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2650.776387 Hartree
Thermal Free Energy with Correction: -2650.507342 Hartree

D2-TSbc

H -0.25795100 2.92819900 -2.78034700
C 2.97242500 -3.38764500 -1.00612600
H 3.05425800 -3.43628600 0.08239000
H 2.91650700 -4.39091800 -1.42909800
H 3.82321000 -2.83751700 -1.41075300
O 1.18780700 1.44006400 -1.19765700
O 2.57463700 -0.89857700 -0.46400200
Ni 2.66689300 1.02915800 0.11834900
O 4.23790300 1.50283300 -1.17251000
O 1.05061800 0.68910200 1.50354200
Cl 1.20729000 0.88248300 3.01789300
O 4.69371700 -0.41392600 -2.66225100
O 1.65418600 2.29355000 3.25427500
O -0.10451700 0.62786100 3.64741100
O 6.43652500 1.23726100 -2.17030900
O 2.23712600 -0.07928900 3.51445100
Cl 5.29601700 0.47118900 -1.64163500
O 5.71162200 -0.33728500 -0.43703200
O 2.78241100 3.01694200 0.76622700
H 2.46641800 2.98124300 1.69387600
H 3.73456000 3.18761900 0.80541100
O 4.12916000 0.61243200 1.53928300
H 3.77086400 0.05648400 2.25351500
H 4.80279100 0.11701000 1.01980100
C -0.39148900 -4.18972600 2.67515300

C -0.78038500 -2.86757000 2.90231300
C -1.11003700 -2.04706100 1.82768500
C -1.02886700 -2.52673400 0.50625700
C -0.61471300 -3.85700300 0.28987500
C -0.31116200 -4.68280200 1.36842600
H -0.80984800 -2.46463300 3.90914800
H -1.37740900 -1.01198600 2.00941800
H -0.50759900 -4.23643500 -0.72039600
H 0.00496800 -5.70673200 1.19209100
C -1.38849800 -1.62715200 -0.58884100
H -1.74924200 -0.64962200 -0.29362200
C 0.42382000 -0.81990400 -1.53075300
C 0.32689400 0.60768400 -1.55123700
C 1.63779500 -1.43964000 -1.08524000
O -0.84769400 1.06189900 -2.04964400
O 1.73726300 -2.74784600 -1.39027000
C -0.99700000 2.49085500 -2.10507600
H -2.00782400 2.65623400 -2.47767700
H -0.87665800 2.93110900 -1.11309800
H -0.13580600 -4.83236300 3.51265700
C -0.76903400 -1.65737400 -1.94359000
H -0.47235400 -2.64755700 -2.28527600
H -1.38222400 -1.16224800 -2.69610500
C -3.60582800 -3.45450900 -1.75036100
C -4.89379300 -4.13110500 -1.24555600
C -4.99371300 -3.62413500 0.20702900
H -2.73351800 -4.09035600 -1.58107300
H -3.63460600 -3.17322100 -2.80609200
H -5.76226400 -3.83268300 -1.83836100
H -4.82656900 -5.22001200 -1.29605600
H -6.02083900 -3.48541900 0.55522800
H -4.48234200 -4.29525200 0.90228900
C -4.61732700 -1.38911600 -0.78477400
N -4.28394900 -2.32681700 0.26943000
N -3.41162900 -2.23661300 -0.91733800
H -5.41413700 -1.66247400 -1.47863500
C -4.52519300 0.07051000 -0.51364800
C -4.97704500 0.97967600 -1.47391800
C -4.02208500 0.56676300 0.70135700
C -4.92291100 2.35664900 -1.25100700
H -5.38501100 0.61563400 -2.41419900
C -3.95868000 1.93157300 0.93580600
H -3.69831600 -0.13220900 1.46489700
C -4.40855700 2.84046700 -0.03865000

H -5.28808700 3.03429300 -2.01294700
H -3.56991400 2.32349300 1.86962600
O -4.31233100 4.15233900 0.29117200
C -4.75388800 5.14265900 -0.64229800
H -5.81606800 4.98441000 -0.87539500
H -4.18464600 5.05009600 -1.57779900
C -4.53288100 6.50197500 -0.00358700
H -3.47475500 6.65245800 0.22642200
H -4.85656900 7.29328400 -0.68637300
H -5.10373400 6.58859800 0.92482100
Thermal Correction to Free Energy: 0.514599 Hartree
Entropy: 288.185 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.598494 Hartree
Thermal Free Energy with Correction: -3302.083895 Hartree

D2-bd

C -5.58151600 -1.10862000 -2.06959600
C -4.28742600 -1.61252400 -2.22481000
C -3.40867000 -1.63264300 -1.14249900
C -3.81494800 -1.14125900 0.10814100
C -5.11234600 -0.63684000 0.25584300
C -5.99216900 -0.62220100 -0.82784100
H -3.96317100 -1.99186700 -3.18944100
H -2.39761700 -2.01251600 -1.26822500
H -5.43827700 -0.26466900 1.22264400
H -6.99783700 -0.23269500 -0.69997800
C -2.87578600 -1.21696200 1.27135200
H -2.56782400 -2.22573000 1.53745700
C -1.65209600 -0.22320900 1.39094500
C -0.36924500 -0.86545700 1.79831600
C -1.57316500 0.86200500 0.36111500
O -0.48966200 -1.63452700 2.87085800
O -2.58719000 1.70181900 0.41212500
C 0.71729600 -2.32132100 3.30985900
H 0.38146600 -3.00392000 4.08817000
H 1.17949800 -2.84954000 2.47585300
H 1.42408600 -1.59078400 3.70633600
C -2.60581100 2.76507600 -0.57921000
H -2.68709600 2.33230700 -1.57779000
H -3.48954600 3.35256400 -0.33772300
H -1.69441900 3.35561600 -0.48979000
O 0.71225200 -0.75329700 1.22346300
O -0.69732400 0.96267000 -0.49957400
Ni 1.18538800 0.13556100 -0.54108500

O 3.33799700 -2.50228800 0.94818800
O 2.00171600 1.74953100 0.49101800
Cl 3.48387000 -2.14802500 -0.47664500
Cl 1.51467000 3.20705800 0.32057200
O 4.85461900 -2.30984700 -0.97134400
O 3.09942100 -0.65480600 -0.67163700
O 2.57747000 4.09268600 0.80809100
O 1.26174800 3.42883900 -1.15444300
O 2.52049900 -2.96383800 -1.31462300
O 0.24826500 3.38040800 1.07528600
O 0.36689000 -1.46584000 -1.62150400
H 0.35219500 -1.15066900 -2.53690400
H 1.08445200 -2.15456400 -1.57937500
O 1.67410800 1.05108500 -2.34057700
H 1.56411700 2.00768300 -2.10587300
H 2.63005600 0.89537100 -2.40215100
C -2.82231300 -0.22839000 2.37272500
H -6.26599000 -1.09681700 -2.91264400
H -2.59602700 -0.57954900 3.37202700
H -3.46140200 0.64383000 2.31236800
Thermal Correction to Free Energy: 0.26806 Hartree
Entropy: 216.526 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2650.769737 Hartree
Thermal Free Energy with Correction: -2650.501677 Hartree

D2-TSbd

C -2.89084800 -4.22354700 3.22981400
C -3.09864400 -2.85593200 3.43105200
C -2.79829600 -1.95346800 2.41654100
C -2.27516300 -2.39784900 1.18453900
C -2.07031600 -3.78081900 0.99714700
C -2.37809400 -4.68172800 2.01283400
H -3.49045200 -2.49676800 4.37760400
H -2.95539700 -0.89050900 2.57099500
H -1.64342200 -4.14240500 0.07017900
H -2.21017900 -5.74355600 1.85993200
C -2.03576400 -1.41251800 0.13698600
H -2.20435300 -0.37867200 0.41436800
C 0.13180600 -1.13617500 -0.33286400
C 0.42326800 0.26375600 -0.23205300
C 1.09254000 -2.09935200 0.12202600
O -0.55314200 1.06563500 -0.70745100
O 0.71799400 -3.38075800 -0.05647500
C -0.27006500 2.48208400 -0.67394200

H -1.09570200 2.94360100 -1.21413900
H -0.23768200 2.83884000 0.35787200
H 0.68983000 2.69602800 -1.14487400
C 1.71940800 -4.37616500 0.23344800
H 1.98694700 -4.35527600 1.29224900
H 1.25618200 -5.32915800 -0.02423200
H 2.60580500 -4.19967100 -0.37696000
O 1.44962100 0.79695800 0.23613600
O 2.20271100 -1.86982000 0.64893000
Ni 3.20200100 -0.11328300 0.53575100
O 3.03681400 3.68349100 0.05603600
O 3.47740100 -0.37063700 -1.56215700
Cl 4.03524800 3.02758400 0.92139700
Cl 3.82452700 -1.69485200 -2.26365800
O 5.30016400 3.77666000 0.99142700
O 4.36726200 1.62728400 0.34800500
O 4.44907400 -1.37332100 -3.55569500
O 4.79552400 -2.44780700 -1.37862100
O 3.47007100 2.82182100 2.30810700
O 2.58635200 -2.49650100 -2.43162400
O 3.08025100 0.18224800 2.60536000
H 3.89647700 -0.20447500 2.95229900
H 3.18947900 1.16358700 2.67330800
O 5.09256200 -0.96218200 0.84503100
H 5.13922600 -1.60938200 0.09715800
H 5.66630900 -0.22221900 0.58920100
C -1.13751600 -1.57635800 -1.03378400
H -3.12277200 -4.93021800 4.02127600
H -1.40650400 -0.89997300 -1.84622700
H -1.05268100 -2.59557900 -1.40653000
C -4.24868600 -2.61723900 -1.67889500
C -5.75741700 -2.91736500 -1.60930000
C -6.15780800 -2.32246800 -0.24435700
H -3.66134900 -3.44354000 -1.26978700
H -3.88480100 -2.39458300 -2.68504600
H -6.29887900 -2.44242700 -2.43134000
H -5.96099900 -3.98889600 -1.66496600
H -7.16791500 -1.90414900 -0.22650100
H -6.07891400 -3.06377200 0.55551200
C -4.93314000 -0.31585300 -1.01033200
N -5.18603000 -1.25036000 0.07016700
N -4.00610700 -1.44636400 -0.79386900
H -5.52932100 -0.41441200 -1.91916800
C -4.55845800 1.08655000 -0.68511000

C -4.40108400 2.01514200 -1.71784300
C -4.39985100 1.52130000 0.64141600
C -4.07855000 3.34694700 -1.45368500
H -4.53447300 1.70288800 -2.75103900
C -4.08095100 2.84147800 0.91955500
H -4.55380200 0.81378600 1.44932700
C -3.91438800 3.76810700 -0.12528200
H -3.96689100 4.04147400 -2.27714500
H -3.96174100 3.19051800 1.93982400
O -3.60871300 5.03257400 0.25360800
C -3.40220800 6.03446700 -0.74966700
H -4.31472300 6.14741200 -1.35120600
H -2.58916700 5.72409200 -1.41989100
C -3.05439400 7.32849600 -0.03681900
H -2.14443900 7.20878400 0.55700900
H -2.88846200 8.12454100 -0.76873000
H -3.86630300 7.63250400 0.62950100
Thermal Correction to Free Energy: 0.512604 Hartree
Entropy: 292.041 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.591742 Hartree
Thermal Free Energy with Correction: -3302.079138 Hartree

D2-cd

C 5.23535500 3.04332900 -0.56344100
C 4.40095700 3.06238900 0.55709800
C 3.81030600 1.88275600 1.00623700
C 4.03784600 0.66783900 0.33965200
C 4.88113800 0.65878300 -0.77834500
C 5.47586200 1.83932900 -1.22642100
H 4.21503500 3.99401300 1.08328100
H 3.16834700 1.89926100 1.88401900
H 5.08484600 -0.27409300 -1.29363800
H 6.13169600 1.81558100 -2.09169300
C 3.40736900 -0.57650000 0.87677000
H 3.48843100 -0.67799900 1.95632300
C 1.97261700 -1.05809800 0.39570000
C 1.05971300 -1.49488700 1.49202900
C 1.34518800 -0.32084200 -0.74186700
O 1.63625200 -2.36483200 2.31494100
O 2.04095500 -0.37551300 -1.85715600
C 0.82624400 -2.84782700 3.41348300
H 1.46922300 -3.53858200 3.95614300
H 0.51843900 -2.01591900 4.04941700
H -0.05610600 -3.35795700 3.02432400

C 1.46515400 0.28883700 -3.01703700
H 1.37102700 1.35813100 -2.82225800
H 2.17185700 0.09929900 -3.82260600
H 0.48886700 -0.14906800 -3.22722900
O -0.08502800 -1.09739800 1.69988000
O 0.30520500 0.34319100 -0.67056300
Ni -1.31673200 0.08759100 0.55175800
O -2.14489900 -1.52206900 -0.39587900
O -2.33650800 1.49125300 -0.65910600
Cl -3.56862400 2.26529300 -0.15262300
O -0.08275400 -2.79325200 -0.84414200
O -3.37377900 2.43593900 1.36203400
O -3.58723300 3.57736700 -0.80813100
O -2.27148400 -3.66897900 -1.51929800
O -4.78402700 1.46745800 -0.38029200
Cl -1.43027900 -2.46909600 -1.40783500
O -1.28683200 -1.75188200 -2.69449900
O -2.92803400 -0.23836500 1.82751000
H -3.41447900 0.60886800 1.89937300
H -3.49668000 -0.85363900 1.33748800
O -0.72912000 1.80480000 1.64616900
H -0.23825600 2.33642800 1.00254400
H -1.59733900 2.26280700 1.73386000
C 3.24557200 -1.85196200 0.13947400
H 5.69947700 3.96072500 -0.91286700
H 3.34126800 -2.77882700 0.69120500
H 3.54257300 -1.89752400 -0.90083900
Thermal Correction to Free Energy: 0.267359 Hartree
Entropy: 218.525 cal/mol-kelvin
Single Point Energy with Solvent Effect: -2650.764148 Hartree
Thermal Free Energy with Correction: -2650.496789 Hartree

D2-TScd

C 2.17386300 -4.90791500 -2.65741900
C 2.61711800 -3.65823900 -3.10000800
C 2.51580400 -2.55186500 -2.26370300
C 1.96324700 -2.66965300 -0.97139700
C 1.52060900 -3.93741000 -0.53919800
C 1.62686800 -5.04320200 -1.37824800
H 3.03654300 -3.54914900 -4.09538700
H 2.85726200 -1.57948000 -2.60489700
H 1.06577200 -4.04590900 0.43718500
H 1.27486600 -6.01252000 -1.03835200
C 1.94288400 -1.48841900 -0.11675700

H 2.26293600 -0.56413200 -0.58353500
C -0.12873600 -0.78164500 0.36350700
C -0.22011600 0.61405900 0.05544500
C -1.27993400 -1.62142900 0.21252300
O 0.92810900 1.29207200 0.26907200
O -1.09638700 -2.89828600 0.60283900
C 0.83217500 2.72572500 0.20855900
H 1.82668700 3.08658800 0.46952200
H 0.55752600 3.05518400 -0.79626500
H 0.08834600 3.07686100 0.92613200
C -2.28557400 -3.71191100 0.65197400
H -2.73239300 -3.80536000 -0.33966500
H -1.95191900 -4.68365200 1.01726000
H -3.01037600 -3.26879300 1.33703900
O -1.21213400 1.24217500 -0.37483500
O -2.40348900 -1.29141300 -0.22129100
Ni -3.11979200 0.57540100 -0.30983200
O -3.34756200 0.93373500 1.75646900
O -5.10355100 -0.22183300 -0.30139800
Cl -6.22705300 0.26461800 -1.22044800
O -1.12114800 1.34958900 2.73605900
O -6.41426300 1.73877400 -0.98687400
O -5.79031500 0.04225900 -2.64507500
O -3.08635700 1.06571100 4.16645500
O -7.45074900 -0.48266600 -0.92206100
Cl -2.39822900 0.60974800 2.94620600
O -2.15523700 -0.85582700 2.95790900
O -3.88640900 2.54012200 -0.30603900
H -4.85009700 2.44455200 -0.48690700
H -3.81110100 2.67936800 0.65378400
O -3.13341200 0.59552600 -2.41627300
H -4.04215400 0.33521900 -2.69761200
H -3.02512800 1.52018800 -2.67785700
C 1.10090000 -1.28886200 1.08781900
H 2.24895200 -5.77298800 -3.30978000
H 1.51161400 -0.52779500 1.75247800
H 0.88256700 -2.19638900 1.64754400
C 3.98463300 -2.72743900 1.84711700
C 5.41758200 -3.29022400 1.83377600
C 5.87695800 -3.01150800 0.38845500
H 3.25465100 -3.49707500 1.58293300
H 3.69047500 -2.27892700 2.79915200
H 6.05406300 -2.78475300 2.56444800
H 5.43701900 -4.35600900 2.07129600

H 6.94277700 -2.78296300 0.30202100
H 5.65092300 -3.85179000 -0.27364800
C 5.03008600 -0.72452100 0.79833000
N 5.09368900 -1.85649600 -0.10740300
N 3.92100500 -1.69859200 0.77443600
H 5.62593400 -0.76844800 1.71161500
C 4.88713000 0.64641500 0.23765900
C 4.92335700 1.74908600 1.09552900
C 4.75824500 0.87117400 -1.14295200
C 4.82311800 3.05269500 0.60675500
H 5.03505100 1.59783600 2.16657800
C 4.65810600 2.16043300 -1.64324900
H 4.76270700 0.02154900 -1.81758100
C 4.68887400 3.26473600 -0.77339400
H 4.85899500 3.88449400 1.29936100
H 4.56636000 2.34678700 -2.70810400
O 4.59236000 4.48226400 -1.36398600
C 4.62863200 5.65907400 -0.54901000
H 5.56881000 5.68685600 0.01877700
H 3.79873000 5.63745900 0.17065800
C 4.51546400 6.85785100 -1.47334800
H 3.57776700 6.82553800 -2.03465500
H 4.53886700 7.78307800 -0.88995500
H 5.34470400 6.87511700 -2.18575600
Thermal Correction to Free Energy: 0.513249 Hartree
Entropy: 291.021 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.588983 Hartree
Thermal Free Energy with Correction: -3302.075734 Hartree

Cartesian coordinates and thermodynamic data of the optimized species of Series E:

E-2

C -0.09444100 -4.08724400 2.72637000
C -1.19762300 -3.38019300 3.21165200
C -1.87855400 -2.49635400 2.37664500
C -1.47764200 -2.32060600 1.04089000
C -0.36995200 -3.03464600 0.56397200
C 0.32145300 -3.90837300 1.40733400
H -1.51230400 -3.49908600 4.24457800
H -2.71888100 -1.92707500 2.76425100

H 0.00073400 -2.88052600 -0.44226400
H 1.20754700 -4.40953700 1.03471700
C -2.26201500 -1.35864200 0.17348000
H -2.61668500 -0.53463500 0.78787500
C -0.23650100 -0.18341700 -0.96897300
C 0.05956500 0.75646300 0.04661400
C 0.75908700 -0.50320300 -1.92967800
O -1.02322300 1.12474300 0.79531400
O 0.35766400 -1.38405300 -2.88740500
C -0.75480700 2.02894400 1.87793600
H -1.71923300 2.19249400 2.36175400
H -0.03910500 1.59667400 2.58104700
H -0.35168000 2.97356800 1.50588400
C 1.36577400 -1.79947900 -3.82425200
H 2.19899500 -2.26941600 -3.29989700
H 0.86798100 -2.51680700 -4.47924600
H 1.72958500 -0.94856600 -4.40548100
O 1.16157500 1.27576600 0.34204300
O 1.92968000 -0.05343900 -2.01543600
Ni 2.91664900 0.82914000 -0.50702700
O 2.99331800 -1.06173400 0.52264000
O 3.86924300 1.70815800 1.19464800
Cl 4.99230000 2.74411200 1.10931900
O 2.47617300 -2.99073000 -0.92939900
O 4.47103700 3.93255200 0.34368300
O 5.39088000 3.13027400 2.46673300
O 4.76714200 -2.14219700 -0.80981400
O 6.13559900 2.13061000 0.35402000
Cl 3.50586100 -2.39618100 -0.02789600
O 3.77538800 -3.28791500 1.11573600
O 4.76419900 0.50168700 -1.42273800
H 5.43355400 0.92338900 -0.84227800
H 4.89709200 -0.47068700 -1.34233500
O 2.95302000 2.66879100 -1.55592600
H 3.40886300 3.30327500 -0.95592000
H 3.58918100 2.47537900 -2.26002400
H 0.45437400 -4.75689500 3.38183900
C -1.61811100 -0.78549500 -1.11017900
H -1.53929400 -1.57465900 -1.85990600
H -2.33841400 -0.05303900 -1.50440400
C -3.43932700 -3.31035800 -1.10511600
C -4.70265400 -4.12140600 -0.78202000
C -5.12702900 -3.59746100 0.60341700
H -2.52606000 -3.80556200 -0.77341500

H -3.34424800 -3.03568300 -2.15599000
H -5.48306000 -3.96132800 -1.53031200
H -4.48849400 -5.19178600 -0.76054200
H -6.20820200 -3.59631300 0.76272600
H -4.65348300 -4.15907900 1.41192000
C -4.87304800 -1.33312800 -0.40908700
N -4.63348400 -2.20853700 0.71619500
N -3.55456800 -2.05665700 -0.27985000
H -5.42911000 -1.72718500 -1.26008100
C -5.01997900 0.12309500 -0.18873700
C -5.21513000 0.96178200 -1.29324800
C -5.00024700 0.68741200 1.09917100
C -5.36089800 2.33735300 -1.13612200
H -5.24935500 0.54071400 -2.29519800
C -5.15531700 2.05284500 1.26866300
H -4.87251300 0.04334100 1.96243900
C -5.32596500 2.89418700 0.15309700
H -5.50109900 2.96150100 -2.00952800
H -5.14738400 2.50231000 2.25571300
O -5.45652500 4.20953900 0.42660100
C -5.58643900 5.14573000 -0.65427000
H -6.49186900 4.91476200 -1.23155400
H -4.72029600 5.05428700 -1.32260200
C -5.66441000 6.53404300 -0.04699900
H -4.76035800 6.75560000 0.52617800
H -5.76404300 7.28120300 -0.83984000
H -6.52739900 6.61750400 0.61907500
Thermal Correction to Free Energy: 0.519915 Hartree
Entropy: 283.734 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.629009 Hartree
Thermal Free Energy with Correction: -3302.109094 Hartree

E-TS4

C 4.86683800 1.90410900 -0.34509700
C 4.64567500 1.77301400 1.17215700
C 3.97891100 0.38832200 1.29773300
H 4.92629000 2.92325600 -0.72889500
H 5.77474400 1.37812800 -0.65279200
H 5.58183100 1.82913500 1.73275700
H 3.98401400 2.55701200 1.54748900
H 4.72280300 -0.38607800 1.51376400
H 3.20012000 0.34686700 2.06143700
C 2.42590200 1.61450300 -0.91388800
N 3.39770800 0.10701800 -0.03148100

N 3.74701600 1.17944100 -0.96766900
H 1.76262000 0.88567400 -1.36871900
C 1.77810500 2.80880700 -0.49940400
C 0.35043600 2.75954600 -0.52102300
C 2.39372300 4.03303200 -0.12256500
C -0.40716400 3.85562200 -0.18150800
H -0.16017300 1.83727700 -0.78226200
C 1.63819700 5.14203300 0.20059800
H 3.47105500 4.12851300 -0.10498000
C 0.22421100 5.06446800 0.17708000
H -1.48857300 3.79553800 -0.18835100
H 2.13564300 6.06641300 0.46562200
C 7.31007300 -3.01362600 -0.75935400
C 6.46689800 -3.29982700 0.31499500
C 5.18374600 -2.75048600 0.36915800
C 4.72300600 -1.90669300 -0.65215500
C 5.57873700 -1.63397100 -1.73202200
C 6.86137800 -2.17945000 -1.78590100
H 6.80302600 -3.95839200 1.11069800
H 4.53453400 -2.99898300 1.20273200
H 5.22669100 -0.99816600 -2.54017700
H 7.50532500 -1.96390300 -2.63387600
C 3.34500300 -1.25629900 -0.61740300
H 3.02727800 -1.09410000 -1.64971500
C 0.86333700 -1.41260400 -0.00590300
C 0.26157300 -0.85314900 1.14833000
C 0.13792300 -1.42236800 -1.22095000
O 1.04666100 -0.85105400 2.26019000
O 0.81606200 -1.97699200 -2.26481400
C 0.37271500 -0.58348700 3.50270100
H 1.12584900 -0.74229100 4.27628700
H 0.00604500 0.44589200 3.53751300
H -0.46179600 -1.27386900 3.63453300
C 0.07338700 -2.14771000 -3.48318100
H -0.21605500 -1.18241100 -3.90641400
H 0.74884200 -2.67255200 -4.15995600
H -0.82859400 -2.73761100 -3.30795400
C 2.22290000 -2.07171600 0.06911500
H 2.20209100 -3.04765700 -0.42662900
H 2.46777400 -2.25211000 1.11733000
H 8.30558100 -3.44570400 -0.80220900
Ni -2.39121100 -0.69277400 -0.03381500
O -2.44719600 -2.75945900 0.38475700
O -3.88175700 -1.03890200 -1.52871500

Cl -5.17534600 -0.23262900 -1.66147200
O -0.90141000 -3.42733600 2.18712800
O -4.79188800 1.21154000 -1.89029100
O -5.95099600 -0.74849500 -2.79241700
O -3.10576500 -2.53432200 2.75545200
O -5.93387200 -0.34249100 -0.37304800
Cl -2.32891700 -3.39539800 1.78409400
O -2.91068300 -4.74377100 1.71171300
O -3.82770000 -0.30650800 1.44134900
H -4.70172300 -0.44700700 1.02033300
H -3.67499500 -1.06054600 2.06204500
O -2.60361300 1.44641500 -0.31795700
H -3.34613500 1.51583700 -0.96860600
H -3.01817000 1.59176000 0.54771700
O -0.88838000 -0.34623800 1.25875700
O -1.01176800 -0.96104800 -1.45809300
O -0.58909600 6.08161700 0.47615300
C -0.04922900 7.36751600 0.84564200
H 0.58027800 7.74042300 0.02831900
H 0.57349000 7.25116000 1.74119300
C -1.22314500 8.29199100 1.10403000
H -0.85632500 9.28299400 1.38677300
H -1.84040300 8.39292600 0.20771700
H -1.84726600 7.90837300 1.91513900
Thermal Correction to Free Energy: 0.518943 Hartree
Entropy: 282.516 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.6008 Hartree
Thermal Free Energy with Correction: -3302.081857 Hartree

E-TS2

C 4.54468000 1.09791600 2.67143400
C 5.10289400 -0.33542600 2.61852600
C 3.95317100 -1.13056700 1.98180900
H 4.01907600 1.29177700 3.61279400
H 5.31539600 1.85956800 2.53666500
H 5.98431100 -0.37770900 1.97375500
H 5.37414800 -0.70452800 3.61023100
H 4.27048300 -2.02606200 1.44765700
H 3.20154000 -1.43074400 2.72025800
C 2.20040300 1.28707200 1.78869100
N 3.36831100 -0.17161500 1.03755800
N 3.58129700 1.15101200 1.52927400
H 1.73569200 0.58243400 2.47785000
C 1.41448300 2.29543600 1.20560800

C 0.00691200 2.31556000 1.44113400
C 1.98730700 3.31797700 0.39902500
C -0.77468500 3.32099500 0.92562300
H -0.46512100 1.51474100 2.00212400
C 1.20964100 4.33710200 -0.10784600
H 3.05133200 3.28407400 0.19247200
C -0.18455200 4.34715300 0.15184600
H -1.85052800 3.32920100 1.06424700
H 1.66312500 5.11250100 -0.71238300
C 7.49678100 -0.87943200 -1.78129300
C 6.68704800 -1.99814300 -1.58468100
C 5.36429500 -1.84531400 -1.16176500
C 4.82992200 -0.57012500 -0.92803000
C 5.65452000 0.54719300 -1.13625500
C 6.97500300 0.39712400 -1.55809900
H 7.08001500 -2.99404000 -1.76766800
H 4.74523600 -2.72756100 -1.03547800
H 5.25063600 1.54249400 -0.97061200
H 7.59390600 1.27496700 -1.72126100
C 3.40107400 -0.35675200 -0.43487000
H 3.04074400 0.59444300 -0.83269900
C 0.97180300 -1.17388000 -0.38211500
C 0.40686600 -1.93180700 0.67268000
C 0.18870700 -0.19202900 -1.03048700
O 1.25626800 -2.83035300 1.24357400
O 0.83562300 0.44029100 -2.05120000
C 0.64470800 -3.81733800 2.09240100
H 1.45030300 -4.50210000 2.36255000
H 0.22213600 -3.35807400 2.99005700
H -0.14182300 -4.34544400 1.55033100
C 0.03567800 1.31554500 -2.85809700
H -0.30877600 2.17853800 -2.28232800
H 0.68971500 1.63724700 -3.67017500
H -0.83608100 0.79087300 -3.25484300
C 2.38100100 -1.44310900 -0.85501200
H 2.41679000 -1.48961600 -1.94801800
H 2.69300000 -2.42082200 -0.48467900
H 8.52341700 -0.99952800 -2.11457400
Ni -2.29046100 -0.90321100 0.28376500
O -2.43721700 -2.26800100 -1.31427700
O -3.82341600 0.29307200 -0.63277700
Cl -5.00905600 0.89580600 0.11869700
O -0.89725700 -4.17425800 -1.02329700
O -4.45560000 1.78468000 1.21579000

O -5.82200800 1.68349100 -0.81265700
O -3.09919400 -4.22038100 0.04486900
O -5.79024300 -0.21922300 0.73989100
Cl -2.32363300 -3.80082600 -1.18359500
O -2.91429000 -4.39389200 -2.39288600
O -3.69951900 -1.98449400 1.39707700
H -4.58032100 -1.64599600 1.14007900
H -3.60194300 -2.89091600 1.01353300
O -2.35202800 0.33484100 2.05795300
H -3.11504200 0.94586500 1.90357800
H -2.68409900 -0.35708500 2.65098900
O -0.75846100 -1.86652900 1.14838800
O -0.98739300 0.17881000 -0.77502500
O -1.02497900 5.27874000 -0.30507800
C -0.54977900 6.35053700 -1.14483400
H -0.07728500 5.92293700 -2.03754600
H 0.20219700 6.93089000 -0.59578900
C -1.75052600 7.20216500 -1.50934900
H -1.43448400 8.02863700 -2.15263400
H -2.49589400 6.60893100 -2.04487800
H -2.21685300 7.61811200 -0.61256900
Thermal Correction to Free Energy: 0.5202 Hartree
Entropy: 278.856 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.61719 Hartree
Thermal Free Energy with Correction: -3302.09699 Hartree

E-3

C -4.50479100 3.26263700 -0.20882800
C -3.42779100 4.26872700 -0.61015000
C -2.32725200 4.01532600 0.42587500
H -5.15249300 3.64349300 0.58778900
H -5.11553500 2.90438600 -1.03664200
H -3.06667700 4.04629000 -1.61797800
H -3.80051400 5.29429100 -0.59391200
H -1.32400900 4.11963800 0.00591200
H -2.41465200 4.68551400 1.28874200
C -4.05554600 0.86708900 0.32146800
N -2.53296900 2.62241100 0.88002500
N -3.71081000 2.13131900 0.32164300
H -3.29069900 0.19347800 0.68832100
C -5.29992000 0.26563100 -0.10187400
C -5.23342000 -1.11659100 -0.41569000
C -6.56158100 0.89231600 -0.17600000
C -6.34881500 -1.81481400 -0.82975700

H -4.28058800 -1.63223600 -0.33900400
C -7.69339300 0.19341000 -0.57915100
H -6.68822200 1.92395800 0.12848300
C -7.59562300 -1.16621000 -0.92424900
H -6.29291300 -2.86823700 -1.08088600
H -8.64706000 0.70550000 -0.60740500
C -1.72433300 -1.16325600 4.16082900
C -2.27465200 0.11531300 4.28519700
C -2.15847200 1.03113400 3.24129400
C -1.50653300 0.68013700 2.04625600
C -0.96475100 -0.60487400 1.92839900
C -1.06616900 -1.51635500 2.98420700
H -2.78295600 0.40496100 5.20091200
H -2.57220900 2.02993800 3.35147700
H -0.42988800 -0.90533100 1.03833200
H -0.59889400 -2.48916000 2.87442400
C -1.33634100 1.73719400 0.95232000
H -0.56487300 2.42863000 1.29888600
C 0.51866700 0.84682900 -0.65993000
C 1.58689400 1.72110800 -0.34348400
C 0.81161800 -0.39749100 -1.28316300
O 1.18879200 2.97909500 0.03824400
O -0.28425300 -1.13444100 -1.61216200
C 2.24924400 3.87581800 0.41191600
H 1.75330800 4.79290900 0.73495600
H 2.84824000 3.45702600 1.22315100
H 2.90469800 4.07788200 -0.43822800
C -0.02414600 -2.43597800 -2.16391300
H 0.54348800 -3.04043300 -1.45482600
H -1.00874800 -2.87237100 -2.34199700
H 0.52766500 -2.35702400 -3.10376000
C -0.91617400 1.29045200 -0.48373400
H -1.56255900 0.48596900 -0.83483900
H -1.12009700 2.15455500 -1.13404600
H -1.79791000 -1.87180400 4.98070400
O -8.62473800 -1.93074700 -1.33491700
C -9.93776200 -1.35705700 -1.44985900
H -9.90573900 -0.51289400 -2.15106300
H -10.25685900 -0.97904900 -0.46978200
C -10.86803300 -2.44772700 -1.94635900
H -11.88276400 -2.05188500 -2.04773200
H -10.54176200 -2.82010300 -2.92095600
H -10.89105000 -3.28542400 -1.24443700
O 2.81980900 1.50289900 -0.36597200

O 1.93550500 -0.86885100 -1.58757900
Ni 3.68118900 -0.25155100 -0.80676000
O 3.09437300 -1.06028100 1.09489800
O 5.46078200 0.48121500 0.12679100
Cl 6.84650600 0.44406200 -0.52190600
O 1.24511600 -2.68559900 0.91747300
O 6.77683000 1.22001600 -1.81199300
O 7.82071500 1.04276000 0.39604700
O 3.55286800 -3.44210700 0.63931800
O 7.18074000 -0.98818300 -0.82281500
Cl 2.64914700 -2.49807700 1.38849200
O 2.75374200 -2.72110100 2.83966400
O 4.65526700 -2.00797000 -1.37055800
H 5.59805300 -1.88324000 -1.12967700
H 4.29722200 -2.68368100 -0.74895300
O 4.30219200 0.46611600 -2.69887100
H 5.18929700 0.86862200 -2.55056700
H 4.46730800 -0.35776200 -3.18005800
Thermal Correction to Free Energy: 0.517718 Hartree
Entropy: 289.552 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.64469 Hartree
Thermal Free Energy with Correction: -3302.126972 Hartree

E-6

Ni -2.93282800 -1.04156600 -0.30352400
O -3.09208700 1.03681200 0.16420000
O -4.46028200 -1.40569300 1.17103400
Cl -5.59115400 -2.42023300 1.00300400
O -2.02200800 2.39784600 -1.59407200
O -4.97241600 -3.78053000 0.80546600
O -6.43636900 -2.40138400 2.20209200
O -4.38097300 1.78111000 -1.80168400
O -6.37183400 -2.04993600 -0.22513300
Cl -3.28541800 2.17884900 -0.84457200
O -3.67675900 3.38308800 -0.08743400
O -4.37961600 -0.92968900 -1.80574600
H -5.22458100 -1.19117300 -1.38149400
H -4.45189100 0.03696100 -1.98568100
O -2.84883700 -3.10395400 -0.78296900
H -3.52642800 -3.54021000 -0.21611500
H -3.21028000 -3.11787700 -1.68091700
C 4.25519800 3.72870800 0.61334200
C 4.19932500 3.94815400 2.12657900
C 3.25183900 2.82772000 2.61177300

H 3.40637200 4.18328200 0.09762600
H 5.19290400 4.03196500 0.14609600
H 5.19570700 3.83870800 2.56368200
H 3.82025700 4.94076800 2.37632200
H 3.60626000 2.37103000 3.53956100
H 2.24498400 3.21460600 2.77500700
C 4.86375900 1.48413800 -0.19877600
N 3.21654800 1.78994900 1.53771600
N 4.10401400 2.25231500 0.54479500
H 5.39894900 2.04222300 -0.96362200
C 5.13305900 0.07875400 -0.14567500
C 5.86322400 -0.46161400 -1.22907900
C 4.81838300 -0.77537000 0.94521500
C 6.24113300 -1.79358200 -1.26067400
H 6.12823300 0.17951800 -2.06574000
C 5.22070800 -2.09242800 0.93585100
H 4.26831300 -0.37716100 1.78749900
C 5.91765100 -2.62607400 -0.17172400
H 6.78439400 -2.17699800 -2.11470000
H 4.99310300 -2.75461500 1.76383800
C -0.09648500 4.96895700 -0.73511500
C 0.80029500 4.20896500 -1.48888300
C 1.39071600 3.07000700 -0.94212800
C 1.11470500 2.68393700 0.38049100
C 0.19632100 3.44734100 1.11602500
C -0.41004300 4.57705100 0.56462600
H 1.01456500 4.48555100 -2.51739400
H 2.03886900 2.45871600 -1.56207500
H -0.07995300 3.13005300 2.11878200
H -1.14694400 5.12860200 1.13905100
C 1.78702900 1.48715500 1.03016700
H 1.28516900 1.27547200 1.97662500
C 0.31280600 -0.30341900 0.00921100
C -0.40916300 -0.82193200 1.11106700
C -0.29026400 -0.28577500 -1.27453400
O 0.31554800 -0.86847300 2.27378300
O 0.51223500 0.18461900 -2.26871600
C -0.38106600 -1.38306400 3.41782200
H 0.32621500 -1.30776700 4.24598700
H -1.28079800 -0.79966300 3.62623400
H -0.67231100 -2.42488400 3.26247900
C -0.11518900 0.34456700 -3.55006200
H -0.97365300 1.01379000 -3.47019200
H 0.65304800 0.77694500 -4.19442700

H -0.44104800 -0.61910700 -3.95025400
O -1.59120800 -1.23746300 1.16299200
O -1.44059500 -0.67535700 -1.59864300
C 1.73144000 0.17902300 0.21630800
H 2.21092500 0.30225500 -0.75611000
H 2.29886000 -0.57493600 0.76863200
H -0.57718400 5.83809200 -1.17321100
O 6.22915300 -3.92712400 -0.08730100
C 6.88963400 -4.58275400 -1.18760700
H 6.28107600 -4.46642800 -2.09292600
H 7.86336800 -4.10650200 -1.35911500
C 7.04910700 -6.04412000 -0.81454300
H 6.07439800 -6.50753600 -0.64188300
H 7.54897400 -6.57973200 -1.62685700
H 7.65076300 -6.14944000 0.09205300
Thermal Correction to Free Energy: 0.518227 Hartree
Entropy: 287.715 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.647108 Hartree
Thermal Free Energy with Correction: -3302.128881 Hartree

E-TS3

Ni -1.86639100 -1.17375100 0.12202100
O -0.71372700 -2.88572000 -0.34246600
O -3.06944600 -1.62939900 -1.55171900
Cl -4.60340600 -1.69815400 -1.49770000
O 1.18833000 -3.18430800 1.19044500
O -5.10178500 -0.33416700 -1.08915000
O -5.10675900 -2.06526100 -2.82288400
O -1.01968100 -4.02557000 1.82577200
O -4.99011700 -2.70321900 -0.45707700
Cl -0.05301400 -3.82999300 0.68534300
O 0.22757200 -5.10245700 0.00838500
O -3.03179400 -2.24714300 1.45927500
H -3.76294700 -2.63796900 0.93566900
H -2.43326900 -2.98430400 1.72408000
O -3.11006900 0.45365800 0.58698600
H -3.89639800 0.35182300 -0.00043700
H -3.42158000 0.24369700 1.47928300
O -0.57420600 -0.61141400 1.58605200
O -0.63401300 -0.16063200 -1.13713900
C 2.39982400 3.19160600 -1.54014200
C 3.87241300 3.36008100 -1.97189300
C 4.66952600 2.89896600 -0.72952000
H 1.87961000 4.14240900 -1.39530900

H 1.83784300 2.59511700 -2.26491000
H 4.09181700 2.72694100 -2.83541500
H 4.10482200 4.39081600 -2.24870700
H 5.62621200 2.43777000 -0.97133900
H 4.84800500 3.74138300 -0.05360800
C 1.54135500 2.10177800 0.60861200
N 3.80149500 1.93516500 -0.03176400
N 2.51030300 2.50352700 -0.23730000
H 1.95371500 1.85736400 1.58302000
C 0.19432300 2.69264600 0.63962100
C -0.36791700 2.94357800 1.90955200
C -0.57773700 3.00793300 -0.49011300
C -1.62659700 3.50255200 2.04284700
H 0.20369500 2.70389200 2.80190700
C -1.84693200 3.56544300 -0.37017000
H -0.21017600 2.79240000 -1.48546200
C -2.38501400 3.81212800 0.90108200
H -2.05449000 3.70293500 3.01933700
H -2.41644800 3.77726700 -1.26628900
C 7.81048000 -1.13810200 -0.06733100
C 7.20342700 -0.45701900 0.99080100
C 5.93301600 0.09590800 0.83377400
C 5.25290200 -0.01742200 -0.38800500
C 5.87194000 -0.69706700 -1.44374100
C 7.14073100 -1.25856800 -1.28510900
H 7.71949700 -0.35960500 1.94176300
H 5.46503400 0.62954800 1.65542700
H 5.35392100 -0.79388900 -2.39490500
H 7.60409700 -1.78692700 -2.11329600
C 3.85005600 0.54112100 -0.56268600
H 3.60059600 0.52417500 -1.63063400
C 1.36152600 -0.00623900 0.23688900
C 0.63982800 -0.36925000 1.45719400
C 0.60089300 -0.11868400 -0.99977900
O 1.40712100 -0.33504000 2.55585300
O 1.37031100 -0.10233000 -2.10592600
C 0.81107000 -0.84310000 3.76834000
H 1.60679200 -0.80738500 4.51174800
H -0.03158100 -0.21950600 4.07426000
H 0.47416700 -1.86839800 3.60802400
C 0.68122100 -0.31401200 -3.35760500
H 0.00717400 0.51818000 -3.57362200
H 1.46820300 -0.37745100 -4.10863100
H 0.10315200 -1.23852000 -3.31866800

C 2.85333800 -0.37606200 0.19866100

H 2.95383100 -1.37828400 -0.23093000

H 3.20424400 -0.45030200 1.22780300

H 8.79828100 -1.57188100 0.05782900

O -3.61091600 4.33671500 1.13164100

C -4.47807000 4.60181500 0.02043000

H -4.00942500 5.34020100 -0.64446100

H -4.63455700 3.67773800 -0.55106800

C -5.78729700 5.12749600 0.57976100

H -6.48045600 5.34679700 -0.23773000

H -6.25105500 4.38701200 1.23694800

H -5.62324500 6.04477000 1.15204800

Thermal Correction to Free Energy: 0.520782 Hartree

Entropy: 279.777 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3302.642782 Hartree

Thermal Free Energy with Correction: -3302.122 Hartree

E-4

Ni -1.86652800 -1.25963100 0.17610600

O -0.61146800 -2.90010400 -0.25389000

O -2.99813800 -1.82573100 -1.47862700

Cl -4.53186100 -1.98320400 -1.42724100

O 1.35329300 -2.96752600 1.22464500

O -5.10773300 -0.63890700 -1.06920500

O -4.99708000 -2.42893000 -2.74048200

O -0.76431400 -3.92723900 1.98469200

O -4.85886400 -2.97328700 -0.35257700

Cl 0.15017500 -3.73606100 0.80522700

O 0.50363300 -5.01877100 0.18797700

O -2.94428100 -2.35881200 1.54793600

H -3.65800600 -2.80262400 1.04132500

H -2.30683000 -3.05121400 1.83626800

O -3.15911900 0.31996000 0.57484200

H -3.94051000 0.17936400 -0.01042400

H -3.47744800 0.18382800 1.47865800

O -0.56153300 -0.58842300 1.61248100

O -0.61697400 -0.21456200 -1.09802800

C 2.08480500 2.78539100 -1.92470100

C 3.50024200 3.06249800 -2.48425500

C 4.41678000 2.91365800 -1.24135200

H 1.41636500 3.64398700 -2.02306100

H 1.61936900 1.93787600 -2.44770200

H 3.75888700 2.33656000 -3.25990500

H 3.58134700 4.05778600 -2.92786100

H 5.39150500 2.48019500 -1.46764200
H 4.56698200 3.88449300 -0.76042000
C 1.40071500 1.94298800 0.41220600
N 3.68075400 2.05566500 -0.30264300
N 2.33796600 2.53803400 -0.48888900
H 1.87086600 2.03693500 1.39451900
C 0.05911200 2.64611800 0.48316200
C -0.31793100 3.21963300 1.71081300
C -0.82470100 2.78932700 -0.59293100
C -1.52097000 3.89546000 1.86160800
H 0.35170500 3.14187900 2.56382400
C -2.03342100 3.47411500 -0.46288500
H -0.59704400 2.35307900 -1.55753800
C -2.39422800 4.02720100 0.77168200
H -1.80440200 4.33714600 2.81132900
H -2.68696400 3.55392900 -1.32278500
C 7.81196400 -0.84203800 0.13971300
C 7.21697100 0.05759700 1.02763800
C 5.92897800 0.53524100 0.78702200
C 5.21835900 0.12522500 -0.35069400
C 5.82553800 -0.77201900 -1.23728900
C 7.11213000 -1.25672600 -0.99387600
H 7.75745200 0.38759300 1.91050100
H 5.46921100 1.24336900 1.46923000
H 5.28559700 -1.09776100 -2.12321400
H 7.56679600 -1.95451800 -1.69125000
C 3.79736800 0.60406300 -0.60349100
H 3.54454100 0.38634300 -1.64984900
C 1.34539900 0.28886400 0.28221300
C 0.59760400 -0.17630200 1.53375200
C 0.60756700 -0.20175700 -0.95436800
O 1.32103100 -0.02156200 2.63139700
O 1.40359900 -0.61632200 -1.92862500
C 0.73407700 -0.49691000 3.86748400
H 1.50456100 -0.34419200 4.62118300
H -0.16247400 0.07954600 4.10272100
H 0.48456200 -1.55403600 3.76691300
C 0.75028000 -1.20115500 -3.08696000
H 0.13098900 -0.45375400 -3.58588000
H 1.56468400 -1.52856600 -3.73067300
H 0.13292300 -2.04165200 -2.76796900
C 2.83289100 -0.17363400 0.32122500
H 2.88875700 -1.23956500 0.09329800
H 3.18804900 -0.04453200 1.34394300

H 8.81420100 -1.21510500 0.32974100

O -3.54988100 4.70219200 1.01277200

C -4.49474500 4.85585300 -0.04989700

H -4.02930400 5.39624700 -0.88598200

H -4.80478100 3.86804600 -0.41771400

C -5.68079600 5.62743100 0.50048200

H -6.43177100 5.76864200 -0.28265400

H -6.14309100 5.08496100 1.32980400

H -5.36760200 6.61045900 0.86297400

Thermal Correction to Free Energy: 0.521734 Hartree

Entropy: 281.095 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3302.648854 Hartree

Thermal Free Energy with Correction: -3302.12712 Hartree

E-TS5

Ni 2.03975100 -0.88740800 -0.10717700

O 1.39586700 -2.87770300 0.21459000

O 3.73946300 -1.34737400 1.06107900

Cl 5.17779200 -1.02003600 0.63379500

O -0.76514300 -3.40546200 -0.83669500

O 5.27492200 0.47572900 0.47421100

O 6.09856200 -1.49982900 1.66641100

O 1.28334600 -3.52059200 -2.16616500

O 5.43310600 -1.68049900 -0.68761100

Cl 0.67508100 -3.77700300 -0.80928700

O 0.87287300 -5.17375600 -0.40100600

O 2.95704600 -1.40959400 -1.89734900

H 3.86456200 -1.69882400 -1.66175800

H 2.45369700 -2.21137300 -2.17243700

O 2.79626100 1.03639400 -0.51202400

H 3.70094900 1.04890900 -0.11891300

H 2.93683400 0.97908700 -1.46870100

C -3.75038900 2.90232100 0.48079700

C -4.84514900 3.01813200 1.55335000

C -5.16227900 1.55064100 1.86909300

H -4.18663700 2.75045000 -0.51182800

H -3.07467300 3.75639200 0.44372000

H -4.44980800 3.53008000 2.43603400

H -5.72143000 3.56449300 1.19735600

H -5.53037800 1.41084200 2.88983400

H -5.91396400 1.15903800 1.17205400

C -1.72245000 1.64790400 1.31239600

N -3.87000100 0.85250500 1.70755200

N -3.02040500 1.70460400 0.92955600

H -1.57634000 1.34670600 2.34583300
C -0.70693900 2.49465600 0.70458500
C 0.36481200 2.94829100 1.50450400
C -0.74166500 2.89278100 -0.64394200
C 1.33044000 3.79311600 0.99128500
H 0.42463400 2.63832100 2.54334200
C 0.22783700 3.73731900 -1.17354000
H -1.52670600 2.51908600 -1.29388400
C 1.27241300 4.19716000 -0.35413700
H 2.15277300 4.14847500 1.60237700
H 0.17418100 4.01909900 -2.21784900
C -6.45007600 -1.42834600 -2.22601900
C -5.57917400 -0.33850000 -2.28613000
C -4.74893700 -0.03564200 -1.20580100
C -4.77841100 -0.80393200 -0.03318600
C -5.66805300 -1.88764700 0.01338300
C -6.48720300 -2.20769700 -1.07055300
H -5.54071900 0.27719200 -3.18098500
H -4.05061400 0.78617700 -1.28991500
H -5.71936500 -2.49620200 0.91372600
H -7.15884100 -3.05886100 -1.00569000
C -3.92981600 -0.53565400 1.21757100
H -4.47457300 -1.04272100 2.02249500
C -1.22184300 -0.51785300 0.85979800
C -0.83952200 -0.50480300 -0.54446700
C -0.13045300 -0.55745000 1.82037400
O -1.89174800 -0.56985900 -1.36427500
O -0.54002500 -0.67210400 3.09917000
C -1.61036800 -0.78190400 -2.76310800
H -2.58800200 -0.89343700 -3.23050600
H -1.07327100 0.07233500 -3.18179900
H -1.01562600 -1.68850500 -2.88240100
C 0.50026800 -0.77560900 4.09418300
H 1.09609100 0.13881300 4.12803700
H -0.02341700 -0.93024000 5.03709400
H 1.15656000 -1.61827200 3.86994800
O 0.30149800 -0.39389700 -1.03499600
O 1.08452400 -0.39333600 1.60561000
C -2.52019500 -1.23805500 1.24595200
H -2.38425300 -1.57569000 2.27244800
H -2.60426300 -2.13544200 0.62688800
H -7.09113200 -1.66566600 -3.06991200
O 2.26370000 5.02140300 -0.76165600
C 2.29983200 5.46232500 -2.12437800

H 2.35934700 4.59209400 -2.79183200
H 1.37672400 6.00960800 -2.35966800
C 3.51797700 6.35401600 -2.28190900
H 4.43218400 5.80314200 -2.04559500
H 3.58582800 6.71450700 -3.31267000
H 3.45267100 7.21814400 -1.61523900
Thermal Correction to Free Energy: 0.520109 Hartree
Entropy: 280.855 cal/mol-kelvin
Single Point Energy with Solvent Effect: -3302.627304 Hartree
Thermal Free Energy with Correction: -3302.107195 Hartree

E-7

Ni 2.20778900 -0.76006200 -0.03380800
O 1.67791400 -2.77871700 0.08141200
O 3.91887000 -1.25340500 1.05980300
Cl 5.33757700 -0.84346100 0.61918300
O -0.54180000 -3.24670100 -0.86542300
O 5.37834300 0.66248600 0.58590700
O 6.29840100 -1.37894700 1.58334400
O 1.39457300 -3.09928500 -2.34912100
O 5.57026000 -1.38186900 -0.75866200
Cl 0.90635000 -3.56414200 -1.00026200
O 1.17773200 -4.99159400 -0.80023900
O 3.07254300 -1.00981500 -1.88402200
H 4.00260400 -1.27804700 -1.72185200
H 2.59659400 -1.79249300 -2.24531300
O 2.80888300 1.23792600 -0.06582700
H 3.76094000 1.23428200 0.19658700
H 2.78305200 1.53356500 -0.98634300
C -3.98513200 2.55714200 1.17153500
C -5.17750700 2.19146600 2.07747100
C -5.32946900 0.68966200 1.84412300
H -4.31739700 2.99032900 0.22313700
H -3.32747400 3.28782000 1.65172100
H -4.93439500 2.38361200 3.12615100
H -6.07887300 2.75511400 1.82524700
H -5.79829000 0.16603100 2.68316400
H -5.92079500 0.48768000 0.93857000
C -1.86175100 1.30567200 1.30367300
N -3.93692000 0.26712100 1.73436400
N -3.26500900 1.27732700 0.88819200
H -1.81162800 1.43852700 2.39258600
C -1.08841700 2.42847900 0.63247500
C -0.09003000 3.11378700 1.34409000

C -1.33072900 2.81339300 -0.69108100
C 0.65006300 4.12869500 0.75334300
H 0.10660500 2.85407400 2.38125400
C -0.60169700 3.83878100 -1.29805600
H -2.11303100 2.31385800 -1.25271300
C 0.40155500 4.50042300 -0.57699200
H 1.42206500 4.65626600 1.30333400
H -0.82686900 4.11497100 -2.32126600
C -5.53959200 -2.56867800 -2.39428200
C -5.32605000 -1.19620300 -2.25179900
C -4.70469200 -0.68942700 -1.10775800
C -4.29943000 -1.54545900 -0.07418900
C -4.53451900 -2.91970400 -0.22529900
C -5.13477300 -3.43200300 -1.37567100
H -5.64267300 -0.51313700 -3.03601200
H -4.50840900 0.37171000 -1.02004100
H -4.24072100 -3.60353600 0.56850400
H -5.29330100 -4.50237500 -1.47020700
C -3.67042000 -1.08094300 1.24751700
H -4.12056300 -1.73307200 2.00785400
C -1.18096100 -0.12963300 1.04148500
C -0.74226900 -0.24963100 -0.42532700
C 0.02855800 -0.22924900 1.99455600
O -1.77201600 -0.36067200 -1.23063800
O -0.33173400 -0.05517500 3.26271300
C -1.49439400 -0.58616800 -2.63691800
H -2.47223700 -0.75698800 -3.08216100
H -1.01294800 0.29714700 -3.06146600
H -0.85112400 -1.45911200 -2.74443500
C 0.71269500 -0.19594900 4.25760000
H 1.49182700 0.55033800 4.09346300
H 0.21380000 -0.03890900 5.21224600
H 1.15080400 -1.19368100 4.20103900
O 0.40768000 -0.22974900 -0.86816900
O 1.20099300 -0.46139300 1.72452500
C -2.14280100 -1.32113800 1.41877400
H -1.99293100 -1.50781900 2.48254900
H -1.82690700 -2.21346300 0.87383500
H -6.01834800 -2.96024400 -3.28718200
O 1.17441100 5.50817500 -1.06457800
C 0.96759700 5.95413300 -2.40671200
H 1.12461200 5.11987900 -3.10505200
H -0.06726700 6.30397500 -2.52766100
C 1.95484300 7.07671700 -2.67215600

H 2.98252600 6.72316900 -2.55207700

H 1.83294800 7.44996600 -3.69343600

H 1.79193600 7.90529900 -1.97755400

Thermal Correction to Free Energy: 0.521584 Hartree

Entropy: 281.369 cal/mol-kelvin

Single Point Energy with Solvent Effect: -3302.637772 Hartree

Thermal Free Energy with Correction: -3302.116188 Hartree

E-8

C -0.07807000 -2.29606300 1.80161400

C 1.07668900 -3.25733300 2.10243400

C 2.30199100 -2.32364300 2.21436600

H -0.87330700 -2.74394000 1.20625100

H -0.51151600 -1.91284500 2.74056200

H 0.89715500 -3.83348700 3.01340400

H 1.21156200 -3.96423300 1.27932800

H 2.72311100 -2.29619600 3.22527400

H 3.09612900 -2.64183100 1.52677400

C -0.20459600 0.03509100 1.05578700

N 1.77464500 -0.98497000 1.89593900

N 0.57611800 -1.21472300 1.04671500

H -0.25923300 0.38576200 2.09972000

C -1.64155700 -0.15095800 0.58772500

C -2.66950700 0.44454500 1.33791300

C -2.00992200 -0.91772400 -0.52324000

C -4.00605200 0.30366500 0.98553700

H -2.41580900 1.02821500 2.21890000

C -3.34881400 -1.08181300 -0.88221700

H -1.23908500 -1.38018500 -1.12448900

C -4.35709700 -0.46413100 -0.13215400

H -4.79550200 0.76798900 1.56737600

H -3.58964900 -1.68521500 -1.74912300

C 5.17787500 -1.25413300 -2.08756800

C 3.88748800 -1.76932700 -1.96202900

C 3.07212700 -1.39437000 -0.89059300

C 3.54023700 -0.49719100 0.08035300

C 4.84513100 0.00152500 -0.05133000

C 5.65547100 -0.36193900 -1.12574600

H 3.50680200 -2.46816500 -2.70184700

H 2.06416400 -1.78240500 -0.80804400

H 5.23293500 0.68456700 0.70201100

H 6.66124000 0.04125600 -1.20545500

C 2.71913000 -0.04272200 1.29600500

H 3.45424600 0.14709400 2.08976500

C 0.63140900 1.16118700 0.33263400
C 0.88404300 0.92726800 -1.17128300
C -0.17093000 2.47239800 0.40551000
O 1.78299900 1.82340700 -1.62656000
O -0.29313600 2.91746200 1.67581200
C 2.06868400 1.74699100 -3.03262600
H 2.77357400 2.55391100 -3.23143400
H 2.51363100 0.77969100 -3.27615100
H 1.15386000 1.88280800 -3.61380400
C -1.08594600 4.10908200 1.82935200
H -2.10589600 3.93389900 1.47973100
H -1.07575300 4.33157700 2.89601200
H -0.65223100 4.93318300 1.25870700
O 0.37267700 0.09105400 -1.87899700
O -0.66603800 3.03561900 -0.54422300
C 1.97355000 1.29973000 1.10531700
H 1.73650800 1.68390900 2.09978400
H 2.62097000 2.02038900 0.60320900
H 5.80753000 -1.54805700 -2.92254300
O -5.69319900 -0.55373600 -0.39879800
C -6.11725300 -1.31432000 -1.52909800
H -5.66306700 -0.91028300 -2.44468100
H -5.78760600 -2.35784400 -1.42449000
C -7.63186000 -1.23082700 -1.59419800
H -7.95577200 -0.19220600 -1.70372200
H -8.00422100 -1.80318500 -2.44930700
H -8.07985500 -1.63670100 -0.68293100
Thermal Correction to Free Energy: 0.456833 Hartree
Entropy: 197.072 cal/mol-kelvin
Single Point Energy with Solvent Effect: -1456.874678 Hartree
Thermal Free Energy with Correction: -1456.417845 Hartree

E-5

O -0.85637400 3.07432200 -0.26827400
O -0.51502400 0.91078800 2.30081100
C -0.05776300 -2.76382500 0.03548400
C 1.07739800 -3.68481500 0.52447800
C 2.27540400 -2.72546200 0.67415100
C -0.22753100 -0.34635900 -0.39744800
N 1.84380300 -1.51618000 -0.04404800
N 0.42262900 -1.41280000 0.37603000
H 0.05212200 -0.46266600 -1.45786000
C -1.74886600 -0.40809500 -0.34787100
C -2.46322400 -0.23470800 -1.54522800

C -2.48372000 -0.66151600 0.81556800
C -3.85123600 -0.28562200 -1.58041000
H -1.91919000 -0.05874300 -2.46924100
C -3.87781200 -0.72960700 0.79495100
H -1.95929600 -0.79245600 1.75231800
C -4.57199200 -0.53368800 -0.40526500
H -4.39790300 -0.14881200 -2.50767700
H -4.40761700 -0.92859600 1.71878400
C 6.74652900 -0.52805900 -0.82107100
C 5.74894700 -0.95675700 -1.69982900
C 4.40816100 -0.90146100 -1.32128700
C 4.04438500 -0.42380200 -0.05419300
C 5.05119500 -0.00171400 0.82080300
C 6.39374900 -0.04950000 0.44086500
H 6.01627200 -1.33482900 -2.68268000
H 3.62916700 -1.24438500 -1.99511000
H 4.78133000 0.36636200 1.80756900
H 7.16257800 0.28154700 1.13323800
C 2.58197200 -0.31160100 0.34751200
H 2.53058500 -0.17135100 1.44289700
C 0.43225300 1.02238700 0.01974000
C -0.22336800 2.16829400 -0.76220300
C 0.26479500 1.38561900 1.51037800
O -0.01963000 2.04276300 -2.09182500
O 1.13449900 2.36646500 1.84618000
C -0.64204600 3.05635400 -2.90288100
H -0.36518500 2.81969200 -3.92983900
H -1.72690500 3.02840200 -2.77840200
H -0.27734900 4.04711700 -2.62333600
C 0.99089100 2.87929400 3.18013700
H 1.13577000 2.08587100 3.91720300
H 1.75857500 3.64584900 3.28394200
H -0.00346200 3.31149400 3.31398700
C 1.93738600 0.90816300 -0.33652700
H 2.46933100 1.81426500 -0.04272000
H 2.02985600 0.79609800 -1.41938500
H 7.79071500 -0.57029500 -1.11714200
O -5.93049900 -0.57208000 -0.53573500
C -6.72438100 -0.81014200 0.62578200
H -6.46321800 -1.78302600 1.06592800
H -6.52503100 -0.03696200 1.38096600
C -8.18071400 -0.78503000 0.19714000
H -8.83028400 -0.96465100 1.05925600
H -8.43810400 0.18571100 -0.23540400

H -8.37555400 -1.55785100 -0.55158400

H 3.19859100 -3.10393100 0.23161500

H 2.46296700 -2.50859000 1.73845000

H 1.27297000 -4.48015200 -0.19908900

H 0.83575400 -4.15478700 1.48097400

H -0.19615700 -2.87180800 -1.05257100

H -1.01261400 -2.95380500 0.52512500

Thermal Correction to Free Energy: 0.455065 Hartree

Entropy: 200.391 cal/mol-kelvin

Single Point Energy with Solvent Effect: -1456.879663 Hartree

Thermal Free Energy with Correction: -1456.424598 Hartree