Supporting Information

Computational insights into the mechanisms and origins of switchable selectivity in Gold(I)-catalyzed annulation of ynamides with Isoxazoles via 6π-electrocyclizations of azaheptatrienyl cations

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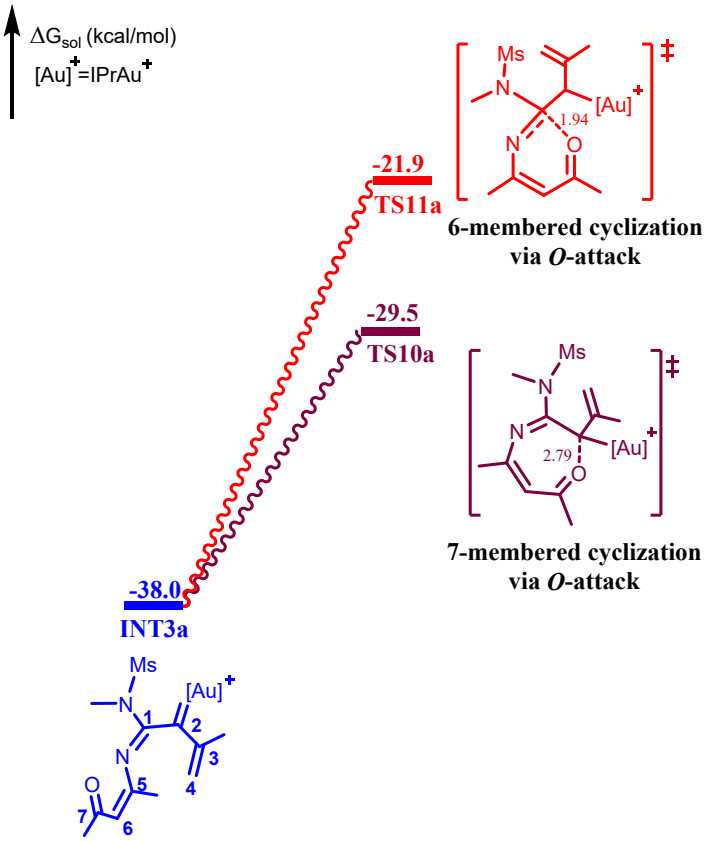


Figure S1: Energy profile showing the *O*-atom induced intramolecular seven-membered and six membered cyclization in the gold(I)-catalyzed annulation of **1a** with **2.** Bond distances are given in Å.

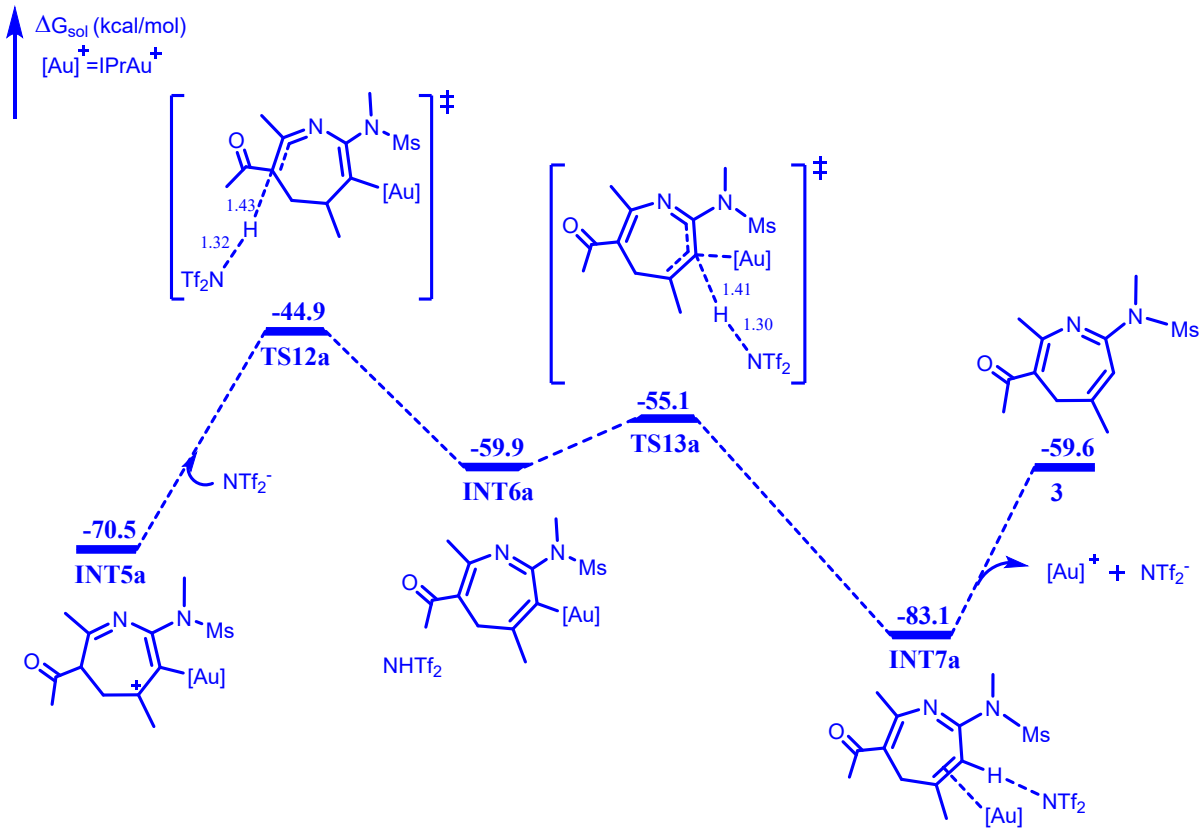


Figure S2: Energy profile showing the bis(trifluoromethane)sulfonimide ion (NTf_2 counter-ion) assisted proton transfer to afford the expected 4*H*-azepine product **3**. Bond distances are given in Å.

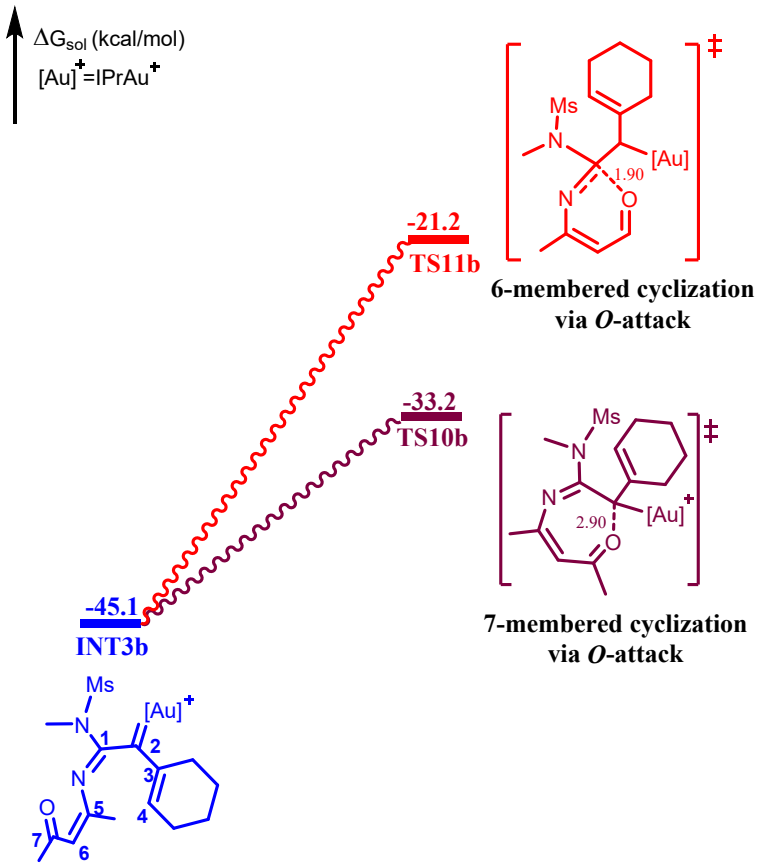
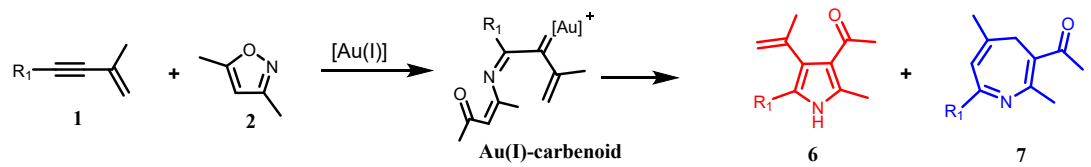
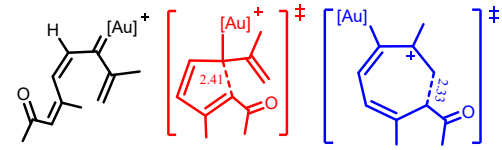
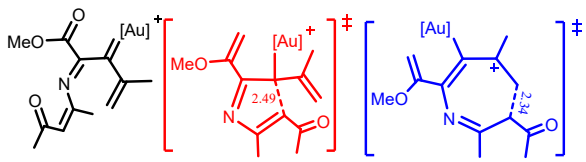
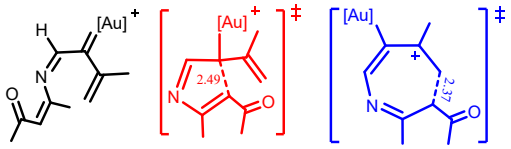


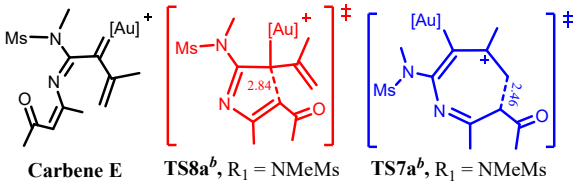
Figure S3: Energy profile showing the *O*-atom induced intramolecular seven-membered and six membered cyclization in the gold(I)-catalyzed annulation of **1b** with **2.** Bond distances are given in Å.

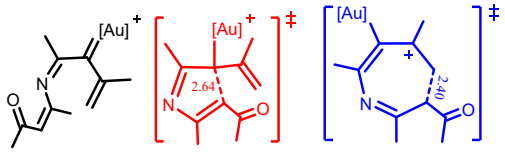


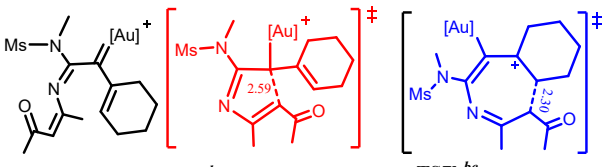






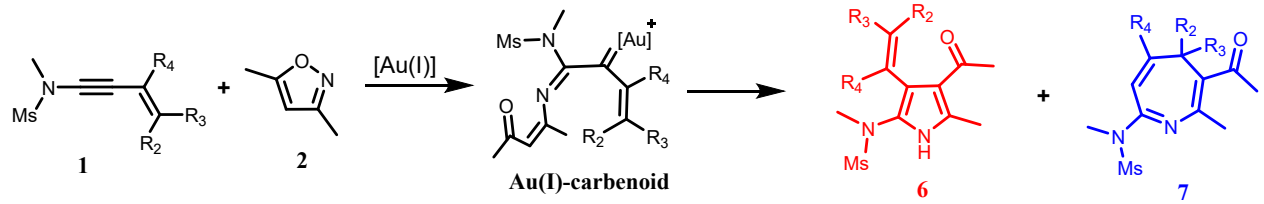


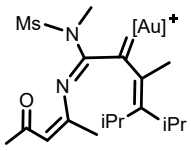




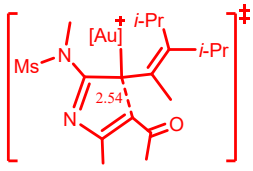
[a] the the 3,5-dimethylisoxazole is replaced with 2,4-dimethylfuran, [b]experimentally reported compound by Gir and Liu[8], [c] the propenyl unit in **1a** is replaced with cyclohexene. The Ms signifies the methanesulfonyl group.

Scheme S1a: Predictive analysis of some α-imino gold(I)-carbene intermediates. Bond distances are given in Å.





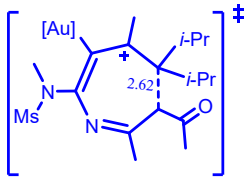
Carbene G



6g-TS

R_2=R_3= *i*-Pr, R_4 = Me

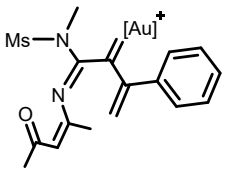
ΔΔG$^{\neq}$ = 0.0 kcal/mol



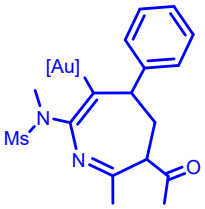
7g-TS

R_2=R_3= *i*-Pr, R_4 = Me

ΔΔG$^{\neq}$ = 11.4 kcal/mol

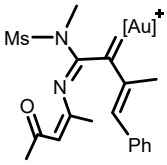


Carbene H

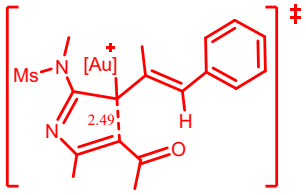


7h[c]

R_2=R_3= H, R_4 = Ph



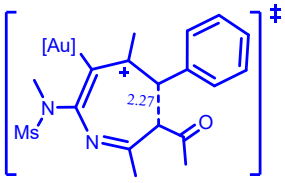
Carbene I



6i-TS[cf]

R_2= H, R_3= Ph, R_4 = Me

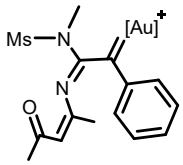
ΔΔG$^{\neq}$ = 0.0 kcal/mol



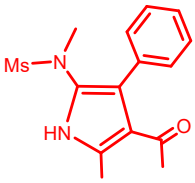
7i-TS[cf]

R_2= H, R_3 = Ph, R_4 = Me

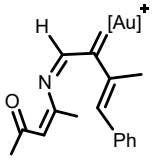
ΔΔG$^{\neq}$ = 1.3 kcal/mol



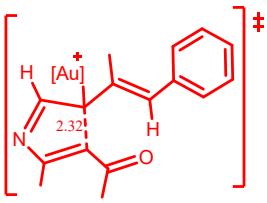
Carbene J



6j[de]



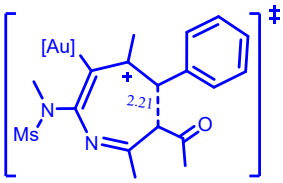
Carbene K



6k-TS

R_2= H, R_3 = Ph, R_4 = Me

ΔΔG$^{\neq}$ = 0.0 kcal/mol



7k-TS

R_2= H, R_3 = Ph, R_4 = Me

ΔΔG$^{\neq}$ = 6.2 kcal/mol

[c]experimentally reported compound by Gir and Liu[8], [d] experimentally reported by Ye's group[6a], [e] the propenyl unit in **1a** is replaced with a phenyl group, [f]both corresponding 5- and 7-membered products were obtained (43% and 48% respectively, in favor of the 7-membered **7i-TS**). The *i*-Pr signifies iso-propyl group and Ms, methanesulfonyl group.

Scheme S1b: Predictive analysis of some α-imino gold(I)-carbene intermediates. Bond distances are given in Å.

Cartesian coordinates and electronic energies for all of the calculated structure

1a

Zero-point correction= 0.173264 (Hartree/Particle)
Thermal correction to Energy= 0.186615
Thermal correction to Enthalpy= 0.187559
Thermal correction to Gibbs Free Energy= 0.132310
Sum of electronic and zero-point Energies= -876.086510
Sum of electronic and thermal Energies= -876.073158
Sum of electronic and thermal Enthalpies= -876.072214
Sum of electronic and thermal Free Energies= -876.127463
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -876.42646505

Cartesian coordinates:

C	-1.73710100	0.34241700	-0.08822200
C	-0.55176800	0.55932100	-0.23637300
N	0.75808000	0.83398600	-0.37665400
S	1.84192200	-0.45920300	-0.09463500
O	1.30817500	-1.61708800	-0.77826900
O	3.16589900	0.06782200	-0.36774300
C	1.22274500	2.20679200	-0.16723900
H	1.11636700	2.51861500	0.88196700
H	2.26906900	2.27253400	-0.47322800
H	0.62059400	2.86607500	-0.79936500
C	-3.11868200	0.01012800	0.02854100
C	-4.03596800	0.92095500	0.38122600
H	-3.76715800	1.95061500	0.60510800
H	-5.08906200	0.65339800	0.44065000
C	-3.46857700	-1.41722700	-0.28529800
H	-4.54246200	-1.59292400	-0.15618200
H	-3.19117200	-1.66976200	-1.31683600
H	-2.92049500	-2.10976000	0.36695200
C	1.68329300	-0.72708100	1.66233400
H	0.63362000	-0.94089900	1.88664700
H	2.31017300	-1.58456800	1.92388600
H	2.02695800	0.16831300	2.18942000

1b

Zero-point correction= 0.239202 (Hartree/Particle)
Thermal correction to Energy= 0.254460
Thermal correction to Enthalpy= 0.255404
Thermal correction to Gibbs Free Energy= 0.194079
Sum of electronic and zero-point Energies= -992.673281
Sum of electronic and thermal Energies= -992.658023
Sum of electronic and thermal Enthalpies= -992.657079
Sum of electronic and thermal Free Energies= -992.718404
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -993.10843995

Cartesian coordinates:

C	-0.68758000	0.31321600	-0.08914200
C	0.49365000	0.57822700	-0.18107100
N	1.81076300	0.85269800	-0.26469600
S	2.87404600	-0.48247800	-0.17021200
O	2.35380700	-1.50913800	-1.04681800
O	4.20930200	0.06679800	-0.31884900
C	2.28847400	2.16106800	0.18682900
H	2.17262900	2.28651900	1.27362000
H	3.33926400	2.26530700	-0.09205400
H	1.70194300	2.92934200	-0.32565700
C	2.66611000	-1.03092200	1.51599500
H	3.28299500	-1.92402200	1.65184300
H	2.99847700	-0.23501100	2.18969000
H	1.60989800	-1.26886100	1.67491100
C	-2.08791600	0.06901700	-0.01563700
C	-2.57987300	-1.17651400	0.10534400
C	-2.98087900	1.28640900	-0.09621700
C	-4.04265600	-1.49085600	0.12847200
H	-1.88052000	-2.01062400	0.17649400
C	-4.40844700	0.97344600	0.33129800
H	-2.55532100	2.09014400	0.52264800

C	-4.89124400	-0.31019300	-0.32882800
H	-4.24047900	-2.37310600	-0.49893800
H	-5.06769400	1.81692100	0.08572200
H	-4.80875900	-0.20435800	-1.42255100
H	-4.33796800	-1.79087000	1.14991500
H	-5.95122100	-0.49349300	-0.10739100
H	-4.44406600	0.85161000	1.42616600
H	-2.96664600	1.67014900	-1.13007500

2

Zero-point correction= 0.113467 (Hartree/Particle)
Thermal correction to Energy= 0.120398
Thermal correction to Enthalpy= 0.121343
Thermal correction to Gibbs Free Energy= 0.082526
Sum of electronic and zero-point Energies= -324.345733
Sum of electronic and thermal Energies= -324.338801
Sum of electronic and thermal Enthalpies= -324.337857
Sum of electronic and thermal Free Energies= -324.376674
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -324.54996986

Cartesian coordinates:

C	-1.07870500	-0.16613100	-0.00000100
C	0.00667500	-0.98256600	-0.00023900
C	1.10967100	-0.08487000	0.00000400
O	-0.67624700	1.11515200	-0.00013300
H	0.02420700	-2.06506400	-0.00035000
N	0.71096000	1.16573700	-0.00012700
C	2.56250600	-0.40035100	0.00011500
H	2.84001500	-0.98745200	0.88448400
H	2.84013500	-0.98752600	-0.88416600
H	3.14618400	0.52596400	0.00011800
C	-2.53952200	-0.40187300	0.00011800
H	-3.00974800	0.04680200	0.88410000
H	-3.00987500	0.04677100	-0.88381100
H	-2.75296400	-1.47529100	0.00014800

3

Zero-point correction= 0.293423 (Hartree/Particle)
Thermal correction to Energy= 0.312596
Thermal correction to Enthalpy= 0.313540
Thermal correction to Gibbs Free Energy= 0.246409
Sum of electronic and zero-point Energies= -1200.547393
Sum of electronic and thermal Energies= -1200.528221
Sum of electronic and thermal Enthalpies= -1200.527277
Sum of electronic and thermal Free Energies= -1200.594408
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -1201.0903308

Cartesian coordinates:

C	0.19699900	1.70141600	-0.69909900
C	-0.62427900	0.53920400	-0.37977000
N	-2.00380400	0.74684200	-0.30655400
S	-3.01898500	-0.46101300	0.40519500
O	-2.44837800	-0.90139100	1.66233000
O	-4.35402100	0.11570000	0.36683900
N	-0.18250200	-0.67090900	-0.24205600
C	1.12689200	-1.07985700	-0.31324300
C	3.55192800	-0.88689300	0.20953200
C	2.16748400	-0.38893500	0.26013000
C	1.28475700	-2.40010000	-1.00869400
H	0.30875600	-2.74980200	-1.36100100
H	1.97437200	-2.31891900	-1.85573800
H	1.72859200	-3.15339200	-0.34851600

O	3.86374800	-1.93698500	-0.33684800
C	4.63592200	-0.06205900	0.87602500
H	4.46691700	0.02296800	1.95823700
H	5.59415200	-0.56012100	0.70579800
H	4.68844200	0.96041400	0.47782900
C	-2.55423400	2.09416000	-0.43042800
H	-3.61954800	2.05472000	-0.19880900
H	-2.05970700	2.78475700	0.26338900
H	-2.43796600	2.46376900	-1.45640700
C	1.39345400	1.87699200	-0.10711200
C	1.83027600	0.90844900	0.95429400
H	1.01723500	0.74689900	1.67992300
C	2.31894300	2.98205400	-0.48731900
H	3.26609900	2.57400800	-0.87060800
H	1.89567700	3.63159700	-1.26189600
H	2.68108000	1.31030000	1.51392600
H	2.57614600	3.59853900	0.38588900
H	-0.15672700	2.41170500	-1.44666100
C	-2.97337000	-1.78904100	-0.77496800
H	-3.34348500	-1.41050900	-1.73150700
H	-1.94649800	-2.15297600	-0.84701300
H	-3.64507800	-2.56019800	-0.38436000

4

Zero-point correction= 0.359124 (Hartree/Particle)
Thermal correction to Energy= 0.380780
Thermal correction to Enthalpy= 0.381725
Thermal correction to Gibbs Free Energy= 0.309449
Sum of electronic and zero-point Energies= -1317.146924
Sum of electronic and thermal Energies= -1317.125268
Sum of electronic and thermal Enthalpies= -1317.124324
Sum of electronic and thermal Free Energies= -1317.196600
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -1317.78830933

Cartesian coordinates:

C	0.72782300	0.13637600	0.26853000
C	-0.20535200	1.11924200	0.52194000
N	-1.58321700	1.11821000	0.80040800
S	-2.64753300	0.80871600	-0.48481700
O	-2.32693100	-0.43296000	-1.17596200
O	-3.98357500	1.00826000	0.05421200
N	0.44169000	2.34708300	0.45696900
C	1.75571800	2.18323800	0.17614000
C	3.33258200	0.27794300	-0.16737400
C	1.98053700	0.81170100	0.04431200
C	2.67831700	3.34279300	0.08890200
H	3.51887100	3.23121800	0.78306000
H	3.12468300	3.42286200	-0.90851100
H	2.15097100	4.27836600	0.31788700
O	4.26731100	1.02930500	-0.41261600
C	3.57703900	-1.20665100	-0.05230400
H	4.61751500	-1.36194700	0.24923900
H	2.89364100	-1.70128200	0.64742100
H	3.44495500	-1.68126000	-1.03484100
C	-2.05172900	0.63627700	2.10733500
H	-2.09735200	-0.46044700	2.15471300
H	-1.34042800	0.99661200	2.85712700
H	-3.04100900	1.05316700	2.31417300
C	-2.24961800	2.14921100	-1.58827300

H	-2.45382900	3.09798000	-1.08495300
H	-1.20260600	2.07377000	-1.89516300
H	-2.90182100	2.03168700	-2.45885100
C	0.42479500	-1.30531900	0.18336200
C	0.07401200	-2.00084700	1.27375700
C	0.48092900	-1.93699100	-1.18444900
C	-0.33416700	-3.44251500	1.24997500
C	0.46976700	-3.45780300	-1.11649700
H	-0.38721800	-1.57627600	-1.75794400
C	-0.62401900	-3.92658300	-0.16617300
H	0.46159000	-4.05807200	1.70569300
H	1.44649000	-3.82314700	-0.75428400
H	-0.72348600	-5.02024800	-0.18284300
H	-1.21573600	-3.58632800	1.89352900
H	-1.58734900	-3.50946100	-0.50149500
H	0.32703800	-3.88035800	-2.12015100
H	1.36635100	-1.57176300	-1.72652800
H	0.08919800	-1.49846400	2.24413800
H	-0.01350300	3.22962200	0.65386700

5

Zero-point correction= 0.359941 (Hartree/Particle)
Thermal correction to Energy= 0.381042
Thermal correction to Enthalpy= 0.381986
Thermal correction to Gibbs Free Energy= 0.311106
Sum of electronic and zero-point Energies= -1317.124700
Sum of electronic and thermal Energies= -1317.103600
Sum of electronic and thermal Enthalpies= -1317.102655
Sum of electronic and thermal Free Energies= -1317.173535
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -1317.76011170

Cartesian coordinates:

C	0.03131900	-1.35439400	-0.66244700
C	0.99928100	-0.46414000	-0.05423500
N	2.30268500	-0.95540100	0.11001700
S	3.63725500	0.10676400	-0.06924400
O	4.80122500	-0.76574400	-0.06954900
O	3.39391300	1.01309300	-1.17584800
N	0.79582000	0.77081700	0.28372200
C	-0.34328400	1.49436800	0.00529200
C	-2.83209100	1.73904400	-0.20186500
C	-1.60935800	1.02006400	0.20687900
C	0.01108700	2.85673200	-0.52786600
H	-0.76690000	3.28485300	-1.16473300
H	0.20728900	3.56119700	0.29347300
H	0.93556200	2.78045200	-1.11135500
O	-3.76524100	1.12777600	-0.70219200
C	-2.98380700	3.22432400	0.04496700
H	-2.23934600	3.64288700	0.72916900
H	-2.94296600	3.77337700	-0.90478400
H	-3.98749800	3.38296200	0.45583100
C	2.57941700	-2.38781200	0.05232700
H	3.50822000	-2.59673700	0.58662400
H	1.75572000	-2.91603100	0.54221500
H	2.68545800	-2.75568200	-0.97713500
C	-1.28386500	-1.28774900	-0.35838000
C	-1.72471500	-0.39193300	0.76601000
H	-0.94050100	-0.43557600	1.53791000
C	-2.32381800	-2.03122400	-1.13101400
H	-2.84055900	-1.29868800	-1.77446300

H	-1.84786300	-2.76594000	-1.79495500
C	3.64802200	1.03352900	1.44861500
H	2.71312000	1.59466900	1.50813200
H	3.75000100	0.33057200	2.27998800
H	4.51675900	1.69800800	1.40193400
C	-3.36381300	-2.66585400	-0.21088000
H	-2.87363000	-3.39750500	0.45350900
H	-4.09871800	-3.22239500	-0.80753700
C	-4.04550200	-1.58205000	0.61077000
H	-4.80261900	-2.02357100	1.27411500
H	-4.56294600	-0.89154100	-0.06485600
C	-3.03150300	-0.82015000	1.46052700
H	-2.73563800	-1.48197300	2.29035900
H	-3.50231600	0.05439600	1.93081400
H	0.38036200	-2.03140300	-1.44399600

NTf2 counter-ion

Zero-point correction= 0.055863 (Hartree/Particle)
Thermal correction to Energy= 0.069904
Thermal correction to Enthalpy= 0.070848
Thermal correction to Gibbs Free Energy= 0.012497
Sum of electronic and zero-point Energies= -1826.762563
Sum of electronic and thermal Energies= -1826.748522
Sum of electronic and thermal Enthalpies= -1826.747578
Sum of electronic and thermal Free Energies= -1826.805929
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -1827.21703786

Cartesian coordinates:

N	-0.00003900	0.00011500	0.83895000
S	1.14402700	0.83778400	0.08523400
O	0.88354300	1.21144800	-1.29913300
O	1.66376800	1.84223300	1.00387200
C	2.52626300	-0.38296000	-0.03086400
S	-1.14393900	-0.83766900	0.08510600
O	-0.88336500	-1.21110600	-1.29930700
O	-1.66356700	-1.84230100	1.00360900
C	-2.52635300	0.38286300	-0.03090600
F	3.57018400	0.19872400	-0.62154400
F	2.90636100	-0.79207100	1.17403400
F	2.17725100	-1.44326900	-0.74688000
F	-2.17759700	1.44311500	-0.74712700
F	-3.57028100	-0.19905600	-0.62134500
F	-2.90632100	0.79208300	1.17399500

Au(I)-catalyst

Zero-point correction= 0.344340 (Hartree/Particle)
Thermal correction to Energy= 0.365991
Thermal correction to Enthalpy= 0.366935
Thermal correction to Gibbs Free Energy= 0.291163
Sum of electronic and zero-point Energies= -979.809924
Sum of electronic and thermal Energies= -979.788273
Sum of electronic and thermal Enthalpies= -979.787329
Sum of electronic and thermal Free Energies= -979.863101
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -980.78186308

Cartesian coordinates:

Au	0.00364900	-1.51779700	-0.08955200
C	-0.00242700	0.48535000	0.06560900
N	1.08010500	1.27957700	0.13212400
C	-0.68124300	2.59926000	0.23808500

C	0.67511200	2.59958100	0.23987000
H	-1.40423200	3.40213200	0.30270800
H	1.39711400	3.40311200	0.30754200
N	-1.08504100	1.27876400	0.12959000
C	-2.45418800	0.83064600	0.05534700
C	-3.12804200	0.56323600	1.25189900
C	-3.03158600	0.69646100	-1.21196800
C	-4.45065900	0.13457200	1.14871500
C	-4.35801900	0.26929100	-1.26061300
C	-5.05873800	-0.00995900	-0.09307900
H	-5.00751700	-0.08299100	2.05901100
H	-4.84159400	0.15906900	-2.23023200
H	-6.09391500	-0.33985900	-0.15076000
C	2.44964200	0.83124400	0.06719900
C	3.05398400	0.75456600	-1.19280600
C	3.09729300	0.50816800	1.26398200
C	4.37910600	0.32283800	-1.23295000
C	4.42222900	0.08427700	1.16983800
C	5.05530600	-0.00825400	-0.06436300
H	4.88171300	0.25133500	-2.19642900
H	4.96026900	-0.17305800	2.08110000
H	6.09067300	-0.33867200	-0.11517000
C	2.31472300	1.12828700	-2.44238000
H	2.01325000	2.18516200	-2.44068400
H	2.93894800	0.96566200	-3.32692900
H	1.39736600	0.53566400	-2.57170000
C	2.39977800	0.60478500	2.58741100
H	1.95346800	1.59520900	2.75130900
H	1.58592000	-0.13017900	2.67389400
H	3.09923100	0.41639200	3.40833600
C	-2.46190400	0.73032200	2.58434100
H	-2.12701100	1.76308500	2.75274400
H	-3.14887000	0.47163600	3.39657100
H	-1.57529500	0.08727900	2.68350400
C	-2.25782600	0.98460800	-2.46344400
H	-1.73790200	1.95153000	-2.42019400
H	-1.49087100	0.21816500	-2.65065800
H	-2.91973300	1.00125700	-3.33548400

INT1a

Zero-point correction= 0.519053 (Hartree/Particle)
Thermal correction to Energy= 0.555042
Thermal correction to Enthalpy= 0.555986
Thermal correction to Gibbs Free Energy= 0.448993
Sum of electronic and zero-point Energies= -1855.963696
Sum of electronic and thermal Energies= -1855.927706
Sum of electronic and thermal Enthalpies= -1855.926762
Sum of electronic and thermal Free Energies= -1856.033756
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1857.25676700
Cartesian coordinates:

C	-0.38156200	-2.40778200	-1.08108600
C	-1.58203900	-2.12166300	-0.83468300
N	-2.78624900	-1.73280400	-0.50393300
S	-3.15281900	-1.64686200	1.23132900
O	-1.88577200	-1.78847300	1.91860700
O	-3.99579100	-0.47817300	1.38216600
Au	0.23767300	-0.40845700	-0.45272300
C	0.97670800	1.38326200	0.16950500
N	0.32671700	2.55983200	0.26771000

C	2.36792700	2.93589400	1.00024800
C	1.17001900	3.53317200	0.78108500
H	3.30216000	3.31679200	1.39175300
H	0.83170300	4.54866700	0.94088500
N	2.22708400	1.61157200	0.61619600
C	-3.56900300	-0.84892800	-1.39358600
H	-3.40335900	-1.18044600	-2.42148200
H	-4.63103900	-0.93329900	-1.14784100
H	-3.24646600	0.19419600	-1.26961900
C	0.58847700	-3.39587800	-1.52693200
C	0.15451600	-4.53721200	-2.07825900
H	-0.90468600	-4.75124200	-2.20419100
H	0.85671200	-5.29037700	-2.43112400
C	2.04081100	-3.06726500	-1.34681600
H	2.31887200	-2.16462900	-1.91198600
H	2.27769000	-2.86486200	-0.29139600
H	2.67666700	-3.89170800	-1.68757800
C	3.22887900	0.58158400	0.69945500
C	4.09065200	0.40591500	-0.38832100
C	3.25332300	-0.22447700	1.84287900
C	5.02754400	-0.62313500	-0.30094700
C	4.20874600	-1.24068000	1.88453400
C	5.08697600	-1.43690500	0.82495200
H	5.71819600	-0.78174300	-1.12832800
H	4.26109900	-1.88046400	2.76466600
H	5.82941500	-2.23087200	0.87893000
C	-1.05709600	2.73426000	-0.08729400
C	-2.03020000	2.39409600	0.85875800
C	-1.35638700	3.20109500	-1.37193400
C	-3.36580700	2.54750700	0.48165800
C	-2.70399100	3.34126600	-1.70174700
C	-3.69814600	3.02058300	-0.78266300
H	-4.14667300	2.28716200	1.19424800
H	-2.97062000	3.71145400	-2.69101500
H	-4.74492900	3.14517100	-1.05442800
C	-4.11841500	-3.12337200	1.43629700
H	-4.43309000	-3.16125700	2.48438400
H	-4.99200700	-3.06497300	0.77991300
H	-3.49165500	-3.98621600	1.19338700
C	-1.66003800	1.87245800	2.21465900
H	-0.87519700	2.47680600	2.68980700
H	-2.53143000	1.86503700	2.87793100
H	-1.28462900	0.83846500	2.16256000
C	-0.27215200	3.52584700	-2.35454000
H	0.37738600	4.33761000	-1.99929200
H	0.37659900	2.65768900	-2.54149600
H	-0.69618100	3.83913600	-3.31439100
C	3.98852000	1.26654800	-1.61122900
H	4.03413700	2.33755900	-1.37265000
H	4.80040000	1.04660100	-2.31253500
H	3.03775900	1.09875100	-2.13968600
C	2.27455900	-0.03040900	2.96210200
H	2.15806600	1.02640500	3.23718500
H	1.27451800	-0.40209200	2.68826000
H	2.59226900	-0.57717500	3.85640800

INT2a

Zero-point correction= 0.635806 (Hartree/Particle)
Thermal correction to Energy= 0.679192
Thermal correction to Enthalpy= 0.680136
Thermal correction to Gibbs Free Energy= 0.555333
Sum of electronic and zero-point Energies= -2180.337460
Sum of electronic and thermal Energies= -2180.294075
Sum of electronic and thermal Enthalpies= -2180.293131
Sum of electronic and thermal Free Energies= -2180.417933

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.83643150

Cartesian coordinates:

C	-1.38611400	-1.00974800	-0.51896400
C	-2.45363600	-0.22583400	-0.26769200
N	-2.47530400	1.17413200	-0.06630800
S	-2.46816100	1.69364900	1.55166300
O	-2.80723600	0.52562400	2.35408700
O	-1.26749500	2.47034900	1.81972900
Au	0.55289300	-0.28749100	-0.29057800
C	2.51363000	0.32820900	-0.06041800
N	3.02636700	1.57573200	-0.12548000
C	4.74334700	0.26113200	0.27180000
C	4.39787000	1.55709400	0.07776100
H	5.69841700	-0.20976200	0.46511400
H	4.98480100	2.46629200	0.06655200
N	3.57287600	-0.47631400	0.18130300
N	-3.78104600	-0.78100900	-0.18696900
C	-5.65265200	-1.91385700	0.11102800
C	-5.82863400	-1.03102900	-0.91543200
C	-1.78166400	2.04890600	-1.01540100
H	-2.01198200	1.69284600	-2.02419100
H	-2.15456200	3.07526000	-0.91261600
H	-0.69111700	2.05936300	-0.86911000
C	-1.52017900	-2.42143200	-0.91297400
C	-2.34189200	-2.81532900	-1.89880700
H	-2.95682600	-2.10823100	-2.45562100
H	-2.36426600	-3.85158700	-2.23378000
C	-0.59571300	-3.39211300	-0.22761200
H	0.44195500	-3.25399100	-0.57025700
H	-0.57730200	-3.23996300	0.86177900
H	-0.88533200	-4.42985100	-0.43369300
C	-4.33312200	-1.72679600	0.56328200
C	-3.60001700	-2.43292400	1.63213000
H	-2.85978100	-1.77315400	2.09794500
H	-4.29982400	-2.79825200	2.38971000
H	-3.08182500	-3.29818000	1.19510900
O	-4.70002100	-0.33166900	-1.11742900
C	-6.96994700	-0.70383600	-1.79114300
H	-7.82942200	-1.33098300	-1.53949000
H	-7.25653600	0.34886200	-1.67891200
H	-6.71106400	-0.86619400	-2.84437300
H	-6.37914700	-2.60734300	0.51338900
C	3.46103800	-1.89963900	0.34467400
C	3.57804800	-2.71176300	-0.78776100
C	3.20327800	-2.39838500	1.62564300
C	3.43690500	-4.08771100	-0.60594000
C	3.07039200	-3.78035500	1.75971400
C	3.18673600	-4.61670900	0.65534900
H	3.52924900	-4.74724200	-1.46819300
H	2.87606400	-4.19965700	2.74632500
H	3.08604700	-5.69340200	0.77939800
C	2.23382700	2.75631900	-0.33650400
C	1.65950500	3.37190600	0.77922200
C	2.06529100	3.21875600	-1.64647800
C	0.88952100	4.51339500	0.55146800
C	1.29162700	4.36465900	-1.82476500
C	0.71241300	5.00732500	-0.73462000
H	0.42300000	5.00924100	1.40159600
H	1.15007600	4.75640600	-2.83164200
H	0.11883200	5.90653200	-0.89174700
C	-3.85924000	2.80512600	1.58486100
H	-3.93147900	3.20454100	2.60132700
H	-3.69490400	3.62223100	0.87630800
H	-4.76018200	2.23991700	1.32865800
C	1.83661100	2.81030400	2.15618500
H	2.88292100	2.55248500	2.36995500

H	1.49650900	3.52419400	2.91396400
H	1.23599400	1.89809800	2.28211700
C	2.67389200	2.49491400	-2.80934700
H	3.76119500	2.37935200	-2.70322200
H	2.25603000	1.48230200	-2.91229600
H	2.48553400	3.03105600	-3.74580100
C	3.81563100	-2.12436000	-2.14594700
H	4.68168800	-1.44901500	-2.16061500
H	3.99231800	-2.91164500	-2.88671000
H	2.94827800	-1.53719000	-2.48294700
C	3.05111400	-1.47920800	2.79972300
H	3.90992400	-0.80303700	2.91040600
H	2.15866600	-0.84383800	2.69664700
H	2.95066600	-2.04732900	3.73081800

INT3a

Zero-point correction= 0.633970 (Hartree/Particle)
Thermal correction to Energy= 0.678066
Thermal correction to Enthalpy= 0.679011
Thermal correction to Gibbs Free Energy= 0.554987
Sum of electronic and zero-point Energies= -2180.344309
Sum of electronic and thermal Energies= -2180.300212
Sum of electronic and thermal Enthalpies= -2180.299268
Sum of electronic and thermal Free Energies= -2180.423291

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.84446405

Cartesian coordinates:

C	-3.84911000	-2.88719600	0.87022000
C	-5.12566400	-2.55222300	0.22599100
C	-2.82165200	-2.00706000	1.06457400
O	-5.30362700	-1.51803000	-0.41169100
H	-3.78194700	-3.85099300	1.37506300
C	-1.63333300	-2.35588500	1.90451700
H	-1.42972600	-1.55002500	2.62183600
H	-1.77012200	-3.29844300	2.44339100
H	-0.73883100	-2.44219400	1.26265600
C	-6.23000500	-3.55655500	0.40998800
H	-7.10559800	-3.26301000	-0.17480000
H	-5.90156200	-4.56124000	0.11156100
H	-6.50936400	-3.62059700	1.47081700
C	-1.20327800	-0.87182700	-1.07410000
C	-2.28929000	-0.15261200	-0.40449700
Au	0.64373900	-0.20791300	-0.47350900
N	-2.85707200	-0.73687000	0.58596600
C	3.99580900	1.87192100	1.10796600
C	4.50503300	0.61376300	1.14477000
H	4.40825400	2.82350900	1.41681500
H	5.45650300	0.23209200	1.49168600
N	2.72800700	1.77069000	0.56325000
N	3.53409200	-0.22171300	0.61763100
C	2.44309000	0.48713000	0.26171100
C	-1.44607700	-2.06818700	-1.79202100
N	-2.54512400	1.15578300	-0.72336000
C	-1.87195600	1.80278600	-1.85194600
H	-0.92358300	2.27137100	-1.55273200
H	-1.68310400	1.04905000	-2.62446900
H	-2.52951700	2.57031900	-2.26629100
S	-3.28489200	2.20546800	0.45349100
O	-2.65019800	1.96703500	1.73689700
O	-3.23547700	3.51647100	-0.16718800
C	-2.73985300	-2.46630400	-2.00143200
H	-2.95827300	-3.40241900	-2.51680200
H	-3.59590300	-1.85954100	-1.70238300
C	-0.27801600	-2.89662700	-2.25062300
H	0.38863000	-2.30965900	-2.89623000
H	0.32434400	-3.23156300	-1.39358500

H	-0.60106600	-3.78137400	-2.81029600
C	3.61514200	-1.65136700	0.48463800
C	4.06265300	-2.18285000	-0.72856500
C	3.19179300	-2.43787300	1.56153800
C	4.09611800	-3.57288500	-0.84320200
C	3.23808800	-3.82204600	1.39913100
C	3.68870000	-4.38401200	0.20954000
H	4.45049200	-4.01843400	-1.77202400
H	2.92255200	-4.46241400	2.22209400
H	3.72717500	-5.46655900	0.10384300
C	1.79651600	2.84349100	0.32887800
C	1.94526800	3.59929100	-0.84007400
C	0.74749900	3.02513800	1.23711600
C	0.99018100	4.58420200	-1.08986900
C	-0.18698500	4.01854400	0.94021600
C	-0.06904900	4.78726900	-0.21104400
H	1.07898200	5.19008600	-1.99102900
H	-1.02713900	4.17029800	1.61604200
H	-0.81955100	5.54475100	-0.42808100
C	-4.96239000	1.62999600	0.47371600
H	-4.97752100	0.55297400	0.66452700
H	-5.47106700	2.18522800	1.26870800
H	-5.40740300	1.85675900	-0.49915600
C	0.58791200	2.16999200	2.45845200
H	1.55144600	1.87413500	2.89413900
H	0.00905600	2.69684200	3.22457900
H	0.02838800	1.24947500	2.22367500
C	3.07084300	3.34160400	-1.79659200
H	4.04885900	3.59392100	-1.36368000
H	3.11780300	2.28295400	-2.09312500
H	2.95292500	3.93960300	-2.70654600
C	2.69651500	-1.81505200	2.83196700
H	3.46743000	-1.20186200	3.31880500
H	1.83617600	-1.15323600	2.65052000
H	2.38487300	-2.58297600	3.54820300
C	4.46454300	-1.29660100	-1.86864300
H	3.59175000	-0.78997200	-2.30799700
H	5.16429600	-0.50959100	-1.55692200
H	4.94506200	-1.87644000	-2.66391700

INT4a

Zero-point correction= 0.634700 (Hartree/Particle)
Thermal correction to Energy= 0.678386
Thermal correction to Enthalpy= 0.679330
Thermal correction to Gibbs Free Energy= 0.556527
Sum of electronic and zero-point Energies= -2180.339594
Sum of electronic and thermal Energies= -2180.295908
Sum of electronic and thermal Enthalpies= -2180.294964
Sum of electronic and thermal Free Energies= -2180.417767
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.83661638

Cartesian coordinates:

C	-5.39991200	-1.28426500	0.46924200
C	-5.74885900	-0.39538100	-0.64366600
C	-4.19531900	-1.87230300	0.68281900
N	-3.13153900	-1.76636900	-0.19615000
O	-4.97101200	-0.07824800	-1.53886700
H	-6.20363600	-1.55096200	1.15672000
C	-7.16453700	0.11456900	-0.63867400
H	-7.86596900	-0.72208400	-0.76383500
H	-7.41036600	0.58749500	0.32162400
H	-7.30963500	0.82945900	-1.45272400
C	-3.95712000	-2.82890200	1.80702400
H	-3.70828500	-3.81920600	1.40424900
H	-3.09953100	-2.50014300	2.40873700

H	-4.84143900	-2.91638300	2.44622600
C	-1.22083000	-0.90328400	-1.24151300
C	-2.39559500	-0.74102100	-0.37435800
N	-2.55439300	0.51350700	0.27006500
S	-2.03367000	0.65656300	1.88061500
O	-1.61760700	-0.67136200	2.30610800
O	-1.12305500	1.78735600	1.95463600
Au	0.57881100	-0.24779900	-0.51284400
C	2.42440100	0.44862300	0.12558100
N	2.83206500	1.73321000	0.18653900
C	4.56208400	0.53304700	0.81718600
C	4.14769600	1.80816800	0.61300700
H	5.50769300	0.12644500	1.15129500
H	4.65430000	2.75743000	0.72801900
N	3.48752400	-0.28579200	0.50934200
C	-2.42577200	1.71374600	-0.56805300
H	-3.02508600	1.55038900	-1.46971400
H	-2.85178000	2.57029400	-0.03501600
H	-1.38234400	1.95383100	-0.82137700
C	-1.35686300	-1.50338000	-2.52080900
C	-2.58156700	-1.44772900	-3.12594800
H	-3.46511500	-1.04634800	-2.62622000
H	-2.69392700	-1.76058600	-4.16521900
C	-0.14062700	-2.02604000	-3.23162200
H	0.54217400	-1.20685800	-3.49768400
H	0.42027000	-2.71675100	-2.58822500
H	-0.41216500	-2.55611300	-4.15134600
C	3.46909400	-1.72119500	0.58812800
C	3.89440200	-2.44783900	-0.52892500
C	2.99069600	-2.31423900	1.76024400
C	3.85181800	-3.83829200	-0.44006700
C	2.97019600	-3.70866900	1.80391300
C	3.39821800	-4.46198900	0.71742100
H	4.18269200	-4.43428700	-1.28990900
H	2.61118400	-4.20340500	2.70555300
H	3.37827300	-5.54876200	0.77252000
C	1.97066200	2.84255200	-0.12036800
C	1.33760900	3.49257900	0.94305500
C	1.77234900	3.18163800	-1.46348800
C	0.45787900	4.52671700	0.62390400
C	0.88786900	4.22577700	-1.73279700
C	0.23496300	4.88930800	-0.69894600
H	-0.05894700	5.04502500	1.43069000
H	0.71874700	4.52268200	-2.76741600
H	-0.45005000	5.70363700	-0.92857300
C	-3.53134400	1.09829200	2.73243800
H	-3.27746700	1.23668500	3.78814000
H	-3.91336200	2.03395200	2.31242900
H	-4.25762300	0.29009500	2.60371500
C	1.58935700	3.08638000	2.36253700
H	2.59998700	3.36580300	2.69263700
H	0.87194300	3.56732300	3.03528900
H	1.48428700	2.00061000	2.49388400
C	2.46623100	2.44620800	-2.57140700
H	3.52828400	2.27101200	-2.35270000
H	2.01176700	1.45782900	-2.74625200
H	2.40339300	3.00730500	-3.51030700
C	4.35552400	-1.75372200	-1.77527200
H	5.22684800	-1.10971600	-1.59245100
H	4.63622800	-2.47952300	-2.54606700
H	3.56727000	-1.10736700	-2.19158300
C	2.48873300	-1.48933800	2.90713700
H	3.16321500	-0.65648600	3.14780800
H	1.50265800	-1.05255300	2.68408300
H	2.37733700	-2.10259900	3.80790000

INT5a

Zero-point correction= 0.636519 (Hartree/Particle)
Thermal correction to Energy= 0.679959
Thermal correction to Enthalpy= 0.680903
Thermal correction to Gibbs Free Energy= 0.556258
Sum of electronic and zero-point Energies= -2180.396208
Sum of electronic and thermal Energies= -2180.352768
Sum of electronic and thermal Enthalpies= -2180.351824
Sum of electronic and thermal Free Energies= -2180.476469
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.89752436

Cartesian coordinates:

C	-3.76178700	-2.63585100	-0.02096600
C	-5.29235600	-2.63661100	-0.16379200
C	-3.39533900	-1.70044100	1.10686600
O	-5.89676100	-1.59111500	-0.04913600
H	-3.41607700	-3.64414700	0.26613700
C	-3.80244400	-2.12471900	2.47550300
H	-3.42487600	-1.42518100	3.22564200
H	-4.89874000	-2.16458400	2.55054400
H	-3.43028400	-3.13561700	2.69088000
C	-5.94514400	-3.94504800	-0.47653200
H	-6.99109700	-3.79367300	-0.75562700
H	-5.41161900	-4.47805000	-1.27477100
H	-5.89985300	-4.59014900	0.41342500
C	-1.18929800	-0.96340200	-0.77096900
C	-2.18603000	-0.11661900	-0.14039800
Au	0.75217500	-0.33078100	-0.36290500
N	-2.81883300	-0.56504900	0.96833000
C	4.05066300	2.02239600	0.91068200
C	4.66605900	0.81638000	0.96167600
H	4.39559900	3.01819200	1.15642900
H	5.66532400	0.52826700	1.26124800
N	2.76465100	1.79019200	0.44921100
N	3.73956500	-0.12089400	0.52893000
C	2.56937600	0.47213500	0.21152500
C	-1.68523700	-2.06574800	-1.36840700
N	-2.42668800	1.13379400	-0.55241600
C	-1.72633200	1.68974400	-1.71824300
H	-0.73413600	2.06206200	-1.42551200
H	-1.62179600	0.90561700	-2.47189800
H	-2.31431400	2.51886000	-2.11595600
S	-3.39148600	2.28042700	0.42207900
O	-2.91164300	2.20918900	1.78419500
O	-3.32854200	3.51038600	-0.33975900
C	-3.18740100	-2.26262100	-1.40522900
H	-3.46912600	-3.04948400	-2.12018800
H	-3.69661500	-1.34543900	-1.74603200
C	-0.84647400	-3.13474300	-1.98417100
H	0.22173600	-2.95150100	-1.81949700
H	-1.10009100	-4.12032300	-1.56296500
H	-1.02369300	-3.20740900	-3.06750900
C	3.97894100	-1.53458800	0.43089200
C	4.39904400	-2.05270000	-0.79764000
C	3.76807100	-2.32161600	1.56718500
C	4.62438900	-3.42735800	-0.86788800
C	4.00586200	-3.69051300	1.44997000
C	4.43146800	-4.23761400	0.24488000
H	4.95961100	-3.86099300	-1.80940800
H	3.85581200	-4.33000900	2.31911300
H	4.61818000	-5.30747200	0.17309200
C	1.77263500	2.79860500	0.18967900
C	1.86467600	3.50732900	-1.01480600
C	0.74652900	3.00001300	1.12026600
C	0.88391100	4.46455300	-1.27568300
C	-0.21350600	3.96648800	0.81412100
C	-0.14613600	4.69200100	-0.36951600

H	0.93232400	5.03119100	-2.20504400
H	-1.02649000	4.14172600	1.51783000
H	-0.91385400	5.43138400	-0.58962600
C	-5.02711700	1.60512300	0.26762800
H	-5.07257600	0.57984200	0.64435000
H	-5.68010600	2.26244500	0.85208400
H	-5.30648600	1.64487700	-0.78963400
C	0.63836300	2.19237100	2.37856200
H	1.61440100	2.02323100	2.85252300
H	-0.01815400	2.68905500	3.10112900
H	0.20052100	1.20130200	2.17469600
C	2.96111600	3.22711500	-1.99831700
H	3.94651500	3.52854700	-1.61688500
H	3.02669900	2.15474300	-2.23502600
H	2.79277900	3.76984100	-2.93465900
C	3.29308300	-1.71578300	2.85328000
H	3.99855400	-0.96934000	3.24373800
H	2.32818700	-1.20347300	2.72428200
H	3.16520400	-2.48433400	3.62315300
C	4.58075700	-1.16867500	-1.99453300
H	3.61366300	-0.80374600	-2.37183400
H	5.18821700	-0.28208900	-1.76635900
H	5.07126500	-1.71088000	-2.81016200

INT6a

Zero-point correction= 0.697674 (Hartree/Particle)
Thermal correction to Energy= 0.754267
Thermal correction to Enthalpy= 0.755211
Thermal correction to Gibbs Free Energy= 0.607877
Sum of electronic and zero-point Energies= -4007.260670
Sum of electronic and thermal Energies= -4007.204077
Sum of electronic and thermal Enthalpies= -4007.203133
Sum of electronic and thermal Free Energies= -4007.350467
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4009.12513576

Cartesian coordinates:

H	-3.81164100	1.47905700	0.46489800
N	-3.69479900	0.48103100	0.79957200
S	-4.42636400	-0.67715600	-0.16324300
O	-4.46388600	-0.15673100	-1.51294200
O	-3.91435400	-1.98821500	0.15444400
S	-2.98350200	0.22657300	2.29762200
O	-3.03759100	1.49056600	2.99595300
O	-3.43119200	-1.02130500	2.86736500
C	-1.22927000	-0.03788600	1.77112400
C	-6.16334900	-0.58476000	0.45745100
F	-0.54932100	-0.47293500	2.81820300
F	-1.21265900	-0.94483500	0.81261400
F	-0.71718900	1.09456700	1.34668400
F	-6.89013100	-1.43681400	-0.24153900
F	-6.61186200	0.64184900	0.28708200
F	-6.19326400	-0.90532200	1.73463900
C	-2.10433900	2.76796900	-1.59344800
C	-3.55967100	2.73507700	-1.60871400
C	-1.39381900	3.28134900	-0.52159000
O	-4.24951500	2.71894300	-0.57498200
C	-2.02442400	3.92412400	0.67992000
H	-1.34208300	4.69198400	1.06204500
H	-3.00686700	4.35680000	0.47327600
H	-2.16328600	3.19796100	1.49252500
C	-4.27728500	2.70543000	-2.93187300
H	-5.32957500	2.95110900	-2.76199800
H	-3.84088300	3.39112000	-3.66827400
H	-4.23298600	1.68867700	-3.34754900
C	0.51061600	1.20428400	-1.52027400

C	0.81371800	2.53461200	-1.02350300
Au	1.53761300	-0.42679400	-0.72577100
N	-0.03589400	3.39506600	-0.52467900
C	3.94533100	-3.34387400	1.27748200
C	2.90979700	-4.14163900	0.92032100
H	4.85081200	-3.54417400	1.83492300
H	2.71156100	-5.19008700	1.09987200
N	3.66104500	-2.08185700	0.77944300
N	2.02335400	-3.34438200	0.21247100
C	2.47726700	-2.07186200	0.12456100
C	-0.57527100	1.07430400	-2.32085500
N	2.16310200	2.92960100	-0.92427500
C	3.20826700	2.27994100	-1.71324300
H	3.69792600	1.45404400	-1.17641400
H	2.73864100	1.88530600	-2.61819400
H	3.96645400	3.01970000	-1.98602900
S	2.69993700	3.75392200	0.46892000
O	2.15109600	3.11739600	1.65795100
O	4.14512600	3.86517600	0.30921400
C	-1.31047600	2.31104000	-2.78765800
H	-1.95459700	2.08322700	-3.64533000
H	-0.60150900	3.09235200	-3.10593000
C	-1.17615000	-0.23233100	-2.72940000
H	-1.09862400	-0.37910300	-3.81851400
H	-0.69805200	-1.08639500	-2.23017200
H	-2.25095900	-0.25180300	-2.48983800
C	0.77069300	-3.76732700	-0.34657800
C	0.71318600	-4.03180000	-1.71927800
C	-0.34488700	-3.83744300	0.49299400
C	-0.52573700	-4.38197900	-2.25390500
C	-1.56615200	-4.17837500	-0.08731800
C	-1.65667000	-4.44462700	-1.44737000
H	-0.60038600	-4.59084700	-3.32103600
H	-2.45923100	-4.20004700	0.53525200
H	-2.62212300	-4.69482600	-1.88356700
C	4.50065400	-0.92086900	0.87592800
C	5.55512300	-0.80195700	-0.03534900
C	4.17852400	0.06861800	1.81029700
C	6.32592200	0.35834500	0.02074600
C	4.97044700	1.21650500	1.82233900
C	6.03146100	1.36080600	0.93783000
H	7.15006300	0.48097000	-0.68194400
H	4.71883800	2.02290600	2.50934300
H	6.61351900	2.27993900	0.94702900
C	2.04272900	5.40217700	0.32480300
H	0.95369000	5.35000000	0.35709900
H	2.45689800	5.96599300	1.16731300
H	2.39134600	5.82179300	-0.62316900
C	2.99005800	-0.05485900	2.71323400
H	2.85831400	-1.07640500	3.09609600
H	3.07437100	0.63012500	3.56379300
H	2.07072800	0.21702600	2.17222500
C	5.80605500	-1.86060800	-1.06719300
H	6.09669900	-2.82180000	-0.62036100
H	4.90322300	-2.05070600	-1.66773900
H	6.60735300	-1.55667200	-1.75006100
C	-0.24657100	-3.54124100	1.95894300
H	0.08774700	-4.42191400	2.52678500
H	0.46752800	-2.73331700	2.16727700
H	-1.22351500	-3.24108600	2.35878800
C	1.92494600	-3.89852400	-2.59152600
H	2.15285200	-2.83914200	-2.78708000
H	2.82049200	-4.33690800	-2.12974600
H	1.76508600	-4.38872300	-3.55875000

INT7a

Zero-point correction= 0.696763 (Hartree/Particle)
Thermal correction to Energy= 0.754081
Thermal correction to Enthalpy= 0.755025
Thermal correction to Gibbs Free Energy= 0.602527
Sum of electronic and zero-point Energies= -4007.266531
Sum of electronic and thermal Energies= -4007.209213
Sum of electronic and thermal Enthalpies= -4007.208269
Sum of electronic and thermal Free Energies= -4007.360768
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4009.15671786

Cartesian coordinates:

H	-1.60213500	-0.06471200	0.59600300
N	-1.54252400	1.70338100	1.64766400
S	-0.61916400	2.94990900	1.27553400
O	0.18637400	2.55853100	0.11098300
O	-1.20333800	4.27822100	1.31051700
S	-2.93122300	1.74705000	2.48058800
O	-3.10844000	0.42527100	3.06364300
O	-3.16759500	2.94620500	3.26222600
C	-4.14400400	1.79846500	1.09052800
C	0.60466600	2.92053100	2.64962500
F	-5.37107700	1.81516100	1.57709500
F	-3.94468100	2.87654000	0.34771600
F	-3.99719400	0.72008200	0.31890300
F	1.49982200	3.88582200	2.47532100
F	1.25193500	1.74864600	2.65271500
F	0.00891300	3.07906800	3.81479500
C	-1.29774700	-4.02282000	0.51876700
C	-1.35198200	-5.14983200	1.46789900
C	-2.36242200	-3.68217200	-0.28216900
O	-2.31099600	-5.90275000	1.54816500
C	-3.67928300	-4.39836300	-0.29721700
H	-4.36303300	-3.87473300	-0.97370400
H	-3.56434400	-5.44314900	-0.61047600
H	-4.11048100	-4.44252800	0.70864400
C	-0.14761100	-5.38624100	2.35896500
H	-0.38930100	-6.19885100	3.04946900
H	0.73043200	-5.67663900	1.76349400
H	0.13568300	-4.49316500	2.93331300
C	-1.19551700	-0.97271600	0.13745900
C	-1.85079700	-1.47685400	-1.08218000
Au	0.94636200	-0.23835400	-0.22974800
N	-2.31132900	-2.67718500	-1.21863500
C	4.75185500	1.08139800	-1.62099600
C	5.13461200	0.05363400	-0.82461500
H	5.31878400	1.76676200	-2.23713300
H	6.10901400	-0.35560200	-0.59209200
N	3.37087100	1.15865100	-1.53913700
N	3.97528500	-0.47162200	-0.27470400
C	2.89074600	0.21028200	-0.71070800
C	-0.44496700	-1.83404400	0.92815100
N	-2.10453600	-0.57096900	-2.10770300
C	-1.66474500	0.82608000	-2.02265200
H	-2.08758400	1.33693700	-1.15006300
H	-0.56922200	0.88094400	-1.96831400
H	-1.98723300	1.34122100	-2.92889800
S	-3.46446000	-0.87987700	-3.14950400
O	-4.61690300	-1.26412700	-2.35900400
O	-3.52136500	0.27980300	-4.02505500
C	-0.05729900	-3.17818200	0.38331700
H	0.80577100	-3.57954300	0.92653300
H	0.22885600	-3.09959600	-0.67722500
C	-0.20046100	-1.53690100	2.37380600
H	-0.43515000	-0.49403100	2.61671900
H	-0.86621800	-2.16602400	2.98408300
H	0.83758400	-1.77030900	2.65605400

C	3.88920500	-1.62523300	0.57850500
C	3.69917100	-2.87373800	-0.02338900
C	3.95067300	-1.44220000	1.96333800
C	3.56148900	-3.97804300	0.81764800
C	3.80045500	-2.57413500	2.76603100
C	3.60469200	-3.82893800	2.19979900
H	3.41270500	-4.96382700	0.37637300
H	3.84020900	-2.46174900	3.84898500
H	3.48958600	-4.70058600	2.84221800
C	2.54097800	2.08017200	-2.27010900
C	1.94258000	1.63297800	-3.45316500
C	2.34345500	3.35633700	-1.73881200
C	1.11700200	2.53049700	-4.12838500
C	1.50364600	4.21583700	-2.44501100
C	0.89613800	3.80787500	-3.62529500
H	0.63450700	2.21383800	-5.05290600
H	1.30590000	5.20739800	-2.04060200
H	0.23664900	4.49097700	-4.15726900
C	-2.92819400	-2.25669100	-4.14242800
H	-2.81990400	-3.13375500	-3.50232000
H	-3.71087200	-2.40134900	-4.89465400
H	-1.98501900	-1.98524000	-4.62504700
C	2.97840200	3.76628000	-0.44697900
H	4.06899300	3.87462800	-0.53887900
H	2.57020000	4.72248600	-0.10230200
H	2.77850600	3.02876300	0.34199100
C	2.13883000	0.23529500	-3.96161300
H	3.17362700	-0.11506800	-3.84307800
H	1.49494400	-0.47836800	-3.42196800
H	1.87919800	0.16899800	-5.02438400
C	4.15335900	-0.08234800	2.55662100
H	5.08909100	0.37786700	2.21020900
H	3.34104700	0.60371400	2.28245900
H	4.19080300	-0.13439800	3.64993100
C	3.61224000	-3.01256900	-1.51293300
H	2.72346400	-2.49816800	-1.90874100
H	4.48231800	-2.57465800	-2.02150400
H	3.54682800	-4.06657900	-1.80461600

TS1a

Zero-point correction= 0.634088 (Hartree/Particle)
Thermal correction to Energy= 0.677593
Thermal correction to Enthalpy= 0.678537
Thermal correction to Gibbs Free Energy= 0.554628
Sum of electronic and zero-point Energies= -2180.312327
Sum of electronic and thermal Energies= -2180.268822
Sum of electronic and thermal Enthalpies= -2180.267878
Sum of electronic and thermal Free Energies= -2180.391787
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.80829399

Cartesian coordinates:

C	-1.38997200	-0.93631000	-0.54080800
C	-2.16818100	0.03216700	-0.16393900
N	-2.28356500	1.31579700	0.14321800
S	-2.31124600	1.74703800	1.81874700
O	-1.92950100	0.55265900	2.54697000
O	-1.58115000	2.99575200	1.93317000
Au	0.61247000	-0.28171000	-0.32275600
C	2.56948400	0.27571600	-0.06784700
N	3.08794200	1.52046300	-0.11861700
C	4.77826500	0.19646600	0.35563700
C	4.44949300	1.49394000	0.14043500
H	5.72164300	-0.27913500	0.59025100
H	5.04305200	2.39877000	0.14830500
N	3.60841900	-0.53559700	0.22191100

N	-4.07695900	-0.62427100	-0.04238600
C	-5.85287600	-1.97158600	-0.18586900
C	-5.95337000	-1.00803900	-1.14348900
C	-2.11673900	2.36823300	-0.86949000
H	-2.68847800	2.08516000	-1.75844200
H	-2.49484700	3.31825500	-0.47944500
H	-1.05325100	2.48914300	-1.11995300
C	-1.65266100	-2.30652500	-0.97952400
C	-2.56889100	-2.57685600	-1.91855800
H	-3.16150400	-1.79165100	-2.38503000
H	-2.71280000	-3.59256200	-2.28439800
C	-0.77490300	-3.36592500	-0.37484500
H	0.26876200	-3.25279600	-0.70831100
H	-0.75699300	-3.29424100	0.72260500
H	-1.11615700	-4.36937700	-0.65518000
C	-4.63648600	-1.69436100	0.48320100
C	-3.98036300	-2.41651900	1.60082300
H	-3.16690700	-1.81750500	2.02761100
H	-4.70194200	-2.65384000	2.39041900
H	-3.56263400	-3.36435200	1.23629200
O	-4.88532800	-0.18978300	-1.07216800
C	-6.95777500	-0.69925800	-2.18217000
H	-7.77005800	-1.43084800	-2.15274400
H	-7.38335300	0.30042600	-2.03186700
H	-6.50594700	-0.71894100	-3.18142500
H	-6.55189500	-2.77156400	0.02064500
C	3.47824600	-1.95895500	0.37704100
C	3.60810400	-2.76492300	-0.75821800
C	3.18756300	-2.46072400	1.64984000
C	3.44995700	-4.14030600	-0.58687400
C	3.03694500	-3.84176800	1.77258000
C	3.16826400	-4.67309400	0.66597200
H	3.55318800	-4.79625200	-1.45057800
H	2.81634500	-4.26447600	2.75210700
H	3.05380200	-5.74925800	0.78196200
C	2.30362600	2.69309900	-0.39519500
C	1.59670100	3.28253500	0.65741300
C	2.26050800	3.16023400	-1.71362500
C	0.82417100	4.40577800	0.35513400
C	1.47811700	4.28584400	-1.96708200
C	0.77003200	4.90403100	-0.94097900
H	0.25813000	4.88352600	1.15297500
H	1.42955400	4.67922200	-2.98195600
H	0.17031200	5.78714100	-1.15538300
C	-4.04028000	2.06847800	2.08453700
H	-4.15721900	2.37654800	3.12852300
H	-4.35839900	2.87468300	1.41634800
H	-4.59562400	1.14735700	1.88487900
C	1.64355200	2.71980600	2.04587700
H	2.66211900	2.43541900	2.34369600
H	1.26030400	3.44359600	2.77238900
H	1.01613400	1.81893000	2.13163000
C	3.01370100	2.46612600	-2.80810100
H	4.10052300	2.50486800	-2.65070400
H	2.73965100	1.40287900	-2.87427600
H	2.80500900	2.92787700	-3.77912000
C	3.87333900	-2.17246700	-2.10930400
H	4.70579800	-1.45618500	-2.09443200
H	4.11526000	-2.95360800	-2.83804700
H	2.99258500	-1.62955400	-2.48460600
C	3.02185600	-1.54629800	2.82589200
H	3.89163000	-0.88986400	2.96581000
H	2.14584700	-0.89166600	2.70438900
H	2.88359700	-2.11861800	3.74941100

TS2a

Zero-point correction= 0.635809 (Hartree/Particle)
Thermal correction to Energy= 0.678293
Thermal correction to Enthalpy= 0.679237
Thermal correction to Gibbs Free Energy= 0.558961
Sum of electronic and zero-point Energies= -2180.289357
Sum of electronic and thermal Energies= -2180.246873
Sum of electronic and thermal Enthalpies= -2180.245929
Sum of electronic and thermal Free Energies= -2180.366205
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.78798721

Cartesian coordinates:

C	-1.31432400	-1.02805400	-0.67678500
C	-2.14968300	-0.12099200	-0.26933100
Au	0.63612200	-0.27183200	-0.37709800
C	-5.69221000	-1.96481300	0.00816100
C	-5.84445300	-0.93228800	-0.96507000
C	-4.42704900	-1.84072300	0.47392200
N	-4.75742500	-0.20995300	-1.08870900
O	-3.85286700	-0.78363200	-0.17459900
H	-6.43297400	-2.69146100	0.31714300
C	-7.03826600	-0.61939200	-1.79160100
H	-7.31964300	-1.48298800	-2.40579900
H	-7.89818500	-0.37460600	-1.15677900
H	-6.83487200	0.22918200	-2.45159500
C	-3.60981800	-2.54690300	1.47993100
H	-2.85846100	-3.17772200	0.98510300
H	-3.07936200	-1.83636300	2.12819400
H	-4.24762400	-3.18868400	2.09486100
C	4.73411900	0.37158500	0.52049500
C	4.36004400	1.66018500	0.32713000
H	5.68424100	-0.07001900	0.79158200
H	4.91308000	2.58811700	0.39173000
C	2.54979400	0.37117100	-0.01800600
N	3.01346200	1.63789000	-0.00322700
N	3.60656300	-0.40502300	0.30241400
N	-2.35422200	1.14602100	0.04461800
S	-2.47884900	1.57463000	1.71614500
O	-2.02027800	0.41813400	2.46288500
O	-1.86364700	2.88116000	1.84695400
C	-2.27197000	2.22549800	-0.95318500
H	-2.63959300	1.83161000	-1.90397500
H	-2.90255300	3.06586200	-0.64528100
H	-1.23458400	2.57402100	-1.04859000
C	-1.50227100	-2.39041500	-1.17949300
C	-2.45523000	-2.67908300	-2.07659300
H	-3.13765100	-1.92290300	-2.46196900
H	-2.54037200	-3.68107100	-2.49478000
C	-4.23821300	1.74990100	1.92676200
H	-4.70925500	0.76697100	1.82944800
H	-4.40154600	2.15742600	2.92973300
H	-4.62212100	2.44322400	1.17180700
C	2.19009600	2.78236800	-0.28643600
C	2.19597300	3.29309800	-1.58944300
C	1.39014500	3.29471400	0.74028800
C	1.36896000	4.38420200	-1.85121600
C	0.57525800	4.38529000	0.42980300
C	0.56893100	4.92644300	-0.85029500
H	1.35672800	4.80938600	-2.85419900
H	-0.06406000	4.80080400	1.20674600
H	-0.06548200	5.78288800	-1.07224500
C	3.51799400	-1.83456400	0.43236500
C	3.18998200	-2.36305300	1.68579100
C	3.71776100	-2.62125800	-0.70651200
C	3.06898800	-3.74919000	1.78247900
C	3.59060500	-4.00301300	-0.56008700
C	3.26892400	-4.56101200	0.67182200

H	2.81973200	-4.19140800	2.74638800
H	3.74972700	-4.64311900	-1.42711900
H	3.17788200	-5.64124500	0.76873900
C	4.01964000	-2.00234300	-2.03733700
H	3.14525500	-1.46045500	-2.42851200
H	4.84399400	-1.27874500	-1.98256500
H	4.29201700	-2.76769500	-2.77192600
C	3.04027900	2.67691200	-2.66347500
H	4.11341300	2.74284300	-2.43745700
H	2.80733900	1.61003900	-2.79576500
H	2.87513200	3.17661000	-3.62403800
C	1.38741200	2.68811700	2.11125000
H	2.40041700	2.43766700	2.45469500
H	0.93594500	3.37175900	2.83759800
H	0.79802100	1.75787900	2.13788200
C	2.96167200	-1.47687700	2.87264100
H	3.83699700	-0.85193200	3.09731900
H	2.11436500	-0.79431400	2.71176400
H	2.74173800	-2.07181900	3.76559400
C	-0.51169400	-3.41226000	-0.69559600
H	-0.78178600	-4.41792600	-1.03810100
H	0.50365700	-3.18554600	-1.05782400
H	-0.44426600	-3.42294300	0.40277300

TS3a

Zero-point correction= 0.633946 (Hartree/Particle)
Thermal correction to Energy= 0.677335
Thermal correction to Enthalpy= 0.678279
Thermal correction to Gibbs Free Energy= 0.554679
Sum of electronic and zero-point Energies= -2180.293210
Sum of electronic and thermal Energies= -2180.249821
Sum of electronic and thermal Enthalpies= -2180.248876
Sum of electronic and thermal Free Energies= -2180.372477
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.79028253

Cartesian coordinates:

C	1.91414100	-1.04017500	0.44243700
C	1.51748400	0.17736400	0.50315200
Au	-0.59491600	-0.02546900	0.36380100
C	6.17105600	-0.45710900	0.10300100
C	5.77524600	-0.37785600	1.40398400
C	5.01419500	-0.87498300	-0.60293100
O	4.47873900	-0.71561800	1.49652500
N	4.01160700	-1.02865100	0.23937900
H	7.15617400	-0.26481600	-0.30279000
N	2.15086600	1.42441200	0.42420400
C	4.87221300	-1.14810900	-2.05569800
H	5.39590000	-2.07523800	-2.32194900
H	3.82009100	-1.22667800	-2.34156400
H	5.31978700	-0.33792300	-2.64383700
C	6.46139500	-0.02597800	2.66467600
H	6.47282200	-0.87999100	3.35296400
H	7.49460800	0.27178000	2.46497800
H	5.94879700	0.79953800	3.17293300
S	2.35652400	1.94450900	-1.21226600
O	2.43318200	0.75150700	-2.03839300
O	1.37969300	2.98359100	-1.50321900
C	1.54809300	2.46502800	1.27397900
H	2.15359200	3.37583800	1.21844100
H	0.51489300	2.70319500	0.97820900
H	1.56574800	2.10028700	2.30505900
C	1.62668000	-2.44842200	0.35649400
C	1.14818800	-3.07885600	1.43919200
H	1.02277800	-2.56376500	2.38962800
H	0.84079300	-4.12223600	1.38610500

C	1.81784200	-3.10106000	-0.97861800
H	1.42724700	-4.12501300	-0.97071900
H	1.30145700	-2.52955800	-1.76460400
H	2.88249400	-3.14107800	-1.24654400
C	3.97183400	2.68563800	-1.11442800
H	4.68695200	1.92023600	-0.79403700
H	4.21426500	3.05631200	-2.11572400
H	3.95063700	3.51954200	-0.40688200
C	-2.60070300	-0.06229000	-0.03125200
N	-3.35776100	-1.14098200	-0.31939500
C	-4.67791300	0.60078800	-0.57070800
C	-4.64640200	-0.75258200	-0.65595000
H	-5.47201800	1.31408500	-0.74830700
H	-5.40659900	-1.47521200	-0.92259000
N	-3.40937500	1.00526400	-0.18509900
C	-2.95723500	2.35808500	0.00932100
C	-2.22643400	2.97037700	-1.01421200
C	-3.21639700	2.96723000	1.24267200
C	-1.74934100	4.26007100	-0.77288100
C	-2.72697800	4.25776500	1.43414000
C	-1.99988500	4.89777900	0.43535300
H	-1.16857700	4.75780700	-1.54821300
H	-2.91771200	4.76089100	2.38144600
H	-1.62534300	5.90612300	0.60209100
C	-2.83810000	-2.48208600	-0.31732000
C	-2.94203500	-3.23488100	0.85656000
C	-2.20352500	-2.94573400	-1.47468900
C	-2.39845500	-4.51944100	0.84416500
C	-1.67323500	-4.23554200	-1.44016200
C	-1.77204100	-5.01597900	-0.29375500
H	-2.47478100	-5.13441400	1.74035100
H	-1.18357400	-4.62892600	-2.33096000
H	-1.36369700	-6.02545500	-0.28936000
C	-3.58659800	-2.67056300	2.08606500
H	-4.60259500	-2.30218200	1.89054400
H	-3.65168600	-3.42621400	2.87618200
H	-3.01105700	-1.82050500	2.48194800
C	-2.06975200	-2.08313600	-2.69324000
H	-3.02138000	-1.61517000	-2.97945700
H	-1.35082400	-1.26553000	-2.52649300
H	-1.71311700	-2.66782600	-3.54836000
C	-1.92283700	2.27306000	-2.30558200
H	-2.75274700	1.63995300	-2.64683300
H	-1.69762400	2.99970200	-3.09382800
H	-1.03475900	1.62962200	-2.20465500
C	-3.96787200	2.24769000	2.32182600
H	-5.00445500	2.02799700	2.03108500
H	-3.49507800	1.28516400	2.56735800
H	-4.00349200	2.84690200	3.23790400

TS4a

Zero-point correction= 0.633899 (Hartree/Particle)
Thermal correction to Energy= 0.676754
Thermal correction to Enthalpy= 0.677698
Thermal correction to Gibbs Free Energy= 0.557065
Sum of electronic and zero-point Energies= -2180.271434
Sum of electronic and thermal Energies= -2180.228579
Sum of electronic and thermal Enthalpies= -2180.227635
Sum of electronic and thermal Free Energies= -2180.348268
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.76762606

Cartesian coordinates:

C	2.18797900	0.91038600	-0.55048000
C	1.54155300	-0.15395900	-0.13618600
C	5.56684700	-0.62543100	-0.84989400

C	5.69384300	-0.16535800	0.49883000
N	2.23741600	-1.34329600	0.27409800
O	3.90028800	0.65926400	-0.44669100
C	2.12447900	-2.40745300	-0.74182000
H	1.07928300	-2.70917600	-0.91218800
H	2.56005900	-2.02391500	-1.66943600
H	2.70492700	-3.27997000	-0.42084000
S	1.72680700	-1.85473300	1.83331300
O	1.56114800	-0.63588000	2.61530000
O	0.65083500	-2.83315900	1.75265500
C	4.61769400	0.61789200	0.72832100
N	4.49380400	-0.16319100	-1.43714700
C	4.10459500	1.40735400	1.86175600
H	3.17666700	0.96868900	2.25818200
H	4.85165300	1.43177000	2.66074900
H	3.88907000	2.43754400	1.55018900
H	6.49941400	-0.38113300	1.18959100
C	6.48783300	-1.51656400	-1.60019100
H	7.48524300	-1.06682000	-1.67167800
H	6.59734400	-2.47930400	-1.08664300
H	6.11111400	-1.69448900	-2.61177500
C	3.19924900	-2.68975600	2.38593000
H	4.03217200	-1.98090500	2.37479300
H	2.99544700	-3.03116600	3.40591500
H	3.40489900	-3.55240000	1.74591200
Au	-0.55596200	-0.15364600	-0.17501100
C	-2.60839000	-0.27708400	-0.11432100
N	-3.36807100	-1.36634700	-0.35265600
C	-4.77938100	0.22519000	0.20407600
C	-4.70990300	-1.07914200	-0.15956100
H	-5.61933500	0.86006800	0.45383200
H	-5.47645400	-1.83057900	-0.29714700
N	-3.47674200	0.69969400	0.22464100
C	-3.06729100	2.02799200	0.58852000
C	-3.11446000	3.02728800	-0.38992000
C	-2.61015900	2.24909700	1.89212300
C	-2.69350200	4.30489200	-0.02304000
C	-2.20194300	3.54477300	2.21378400
C	-2.24484400	4.56196900	1.26815600
H	-2.72382900	5.10476200	-0.76231800
H	-1.85069600	3.75089200	3.22430200
H	-1.92821900	5.56719300	1.54033800
C	-2.81357900	-2.64673800	-0.70259400
C	-2.39800500	-3.48556200	0.33558200
C	-2.66902600	-2.96222200	-2.05713500
C	-1.81218300	-4.69961600	-0.02294500
C	-2.08557400	-4.18982300	-2.36716500
C	-1.65954200	-5.04877700	-1.35934400
H	-1.47021800	-5.37071500	0.76394300
H	-1.96535900	-4.46957200	-3.41325100
H	-1.20693500	-6.00386900	-1.62014800
C	-2.55045600	-3.08198600	1.76985700
H	-3.57800000	-2.77138700	2.00497800
H	-2.28264100	-3.90837200	2.43671900
H	-1.88442700	-2.24175200	2.01422400
C	-3.10030400	-2.00703900	-3.12859400
H	-4.15570500	-1.71935400	-3.02785900
H	-2.51235500	-1.07778800	-3.09589100
H	-2.96906600	-2.44915700	-4.12209100
C	-3.58407000	2.73024100	-1.78218500
H	-4.65190800	2.47266100	-1.81161100
H	-3.43771800	3.59654600	-2.43642000
H	-3.04181800	1.87932900	-2.22005000
C	-2.52546300	1.14188600	2.89950700
H	-3.37417100	0.44829500	2.83202300
H	-1.61019000	0.54546800	2.75728700
H	-2.49696300	1.54450700	3.91812600
C	2.01200500	2.25322800	-1.05777900

C	0.60973300	2.79769700	-0.97686600
C	3.01049500	2.98642400	-1.57078900
H	-0.06803600	2.25338700	-1.64934700
H	4.02775100	2.62368000	-1.67891400
H	0.19337000	2.71831700	0.03721100
H	0.60586300	3.85315100	-1.27180900
H	2.80845900	3.99400400	-1.92562300

TS5a

Zero-point correction= 0.633645 (Hartree/Particle)
Thermal correction to Energy= 0.676624
Thermal correction to Enthalpy= 0.677568
Thermal correction to Gibbs Free Energy= 0.555879
Sum of electronic and zero-point Energies= -2180.321721
Sum of electronic and thermal Energies= -2180.278742
Sum of electronic and thermal Enthalpies= -2180.277797
Sum of electronic and thermal Free Energies= -2180.399487
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.81534719

Cartesian coordinates:

C	1.43968000	0.50276000	-1.11158800
C	2.34793500	-0.36077200	-0.51116300
N	2.07872600	-1.71437700	-0.23613600
S	2.02745200	-2.19400500	1.39207000
O	1.84645700	-0.99645800	2.20457200
O	1.09695800	-3.30671400	1.47927000
Au	-0.55177100	0.24043200	-0.60856600
C	-2.47211500	0.15620200	0.14593300
N	-3.30013600	-0.89852500	0.28279200
C	-4.36514800	0.80697700	1.17614400
C	-4.47355900	-0.52002800	0.91592800
H	-5.03968600	1.50408400	1.65584800
H	-5.26322900	-1.23135300	1.12009900
N	-3.12712500	1.20265500	0.69388400
N	3.52984300	0.09759200	-0.04476500
C	5.28563700	1.46763800	0.41900000
C	5.83880900	0.49717500	-0.41461300
C	1.32759800	-2.53588600	-1.19014300
H	1.55977000	-2.16791000	-2.19408100
H	1.65298500	-3.57865700	-1.11043400
H	0.24153700	-2.49483700	-1.02628200
C	1.87089800	1.70011500	-1.81088000
C	2.98326400	1.68498900	-2.57607600
H	3.61217800	0.80080200	-2.66276000
H	3.25242600	2.54208100	-3.19216700
C	0.96410900	2.90076000	-1.77889900
H	0.03244100	2.69746900	-2.32681500
H	0.66319900	3.16664200	-0.75383400
H	1.44445600	3.77376700	-2.23591500
C	3.93813100	1.19014100	0.59851200
C	2.98442100	1.94499600	1.45732100
H	2.35550800	1.24811800	2.02483700
H	3.53015500	2.60361900	2.13944200
H	2.32660900	2.56109100	0.82858900
O	5.00936300	-0.38197700	-0.85157500
C	7.27008600	0.37024200	-0.80014800
H	7.86466300	1.18903500	-0.38475900
H	7.67040300	-0.58492600	-0.43947000
H	7.36789200	0.36976600	-1.89200200
H	5.82519600	2.27055200	0.90562800
C	-2.54057800	2.51144000	0.79130000
C	-2.84114600	3.44904000	-0.20236000
C	-1.64326300	2.75962500	1.83631300
C	-2.21825100	4.69389200	-0.12076200
C	-1.04069200	4.01840500	1.87444600

C	-1.32677300	4.97643800	0.90844700
H	-2.43778300	5.44633200	-0.87733600
H	-0.34778800	4.24698800	2.68420300
H	-0.85486400	5.95597600	0.96085300
C	-2.92790800	-2.23311400	-0.10487700
C	-2.19546800	-2.99544900	0.81079700
C	-3.26322200	-2.67547800	-1.38822000
C	-1.78846600	-4.26572200	0.40107600
C	-2.84192500	-3.95427500	-1.75057100
C	-2.11096300	-4.73993900	-0.86500600
H	-1.20129900	-4.87479300	1.08629600
H	-3.09217900	-4.33283000	-2.74104400
H	-1.79045900	-5.73566800	-1.16638900
C	3.66844100	-2.82299100	1.66947000
H	3.71901100	-3.16901300	2.70671300
H	3.83537700	-3.65721300	0.98125400
H	4.39170400	-2.02215300	1.49036400
C	-1.84292000	-2.45882600	2.16481600
H	-2.72134600	-2.05847600	2.69008000
H	-1.39414700	-3.23911800	2.78711700
H	-1.10499000	-1.64514800	2.09298600
C	-4.02914300	-1.80233700	-2.33572100
H	-5.00937600	-1.51532800	-1.93064300
H	-3.48828500	-0.86892700	-2.55080800
H	-4.20127400	-2.31580100	-3.28772100
C	-3.76873800	3.11181700	-1.32999600
H	-4.77463300	2.84907800	-0.97554200
H	-3.87034100	3.95687000	-2.01918600
H	-3.40023800	2.24917900	-1.90537800
C	-1.30634600	1.71319000	2.85637700
H	-2.18554000	1.13327700	3.16679700
H	-0.57147300	0.99084900	2.46474900
H	-0.87157000	2.17015100	3.75259000

TS6a

Zero-point correction= 0.633706 (Hartree/Particle)
Thermal correction to Energy= 0.676716
Thermal correction to Enthalpy= 0.677660
Thermal correction to Gibbs Free Energy= 0.555751
Sum of electronic and zero-point Energies= -2180.315135
Sum of electronic and thermal Energies= -2180.272126
Sum of electronic and thermal Enthalpies= -2180.271181
Sum of electronic and thermal Free Energies= -2180.393091
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.80824343
Cartesian coordinates:

C	-6.00035600	-0.97901600	0.19624300
C	-5.90814100	-0.40523700	-1.07658400
C	-4.72671300	-1.24038000	0.66164600
N	-3.73237100	-0.96875000	-0.19284500
O	-4.71727400	-0.23079700	-1.50039300
H	-6.91687000	-1.22817900	0.71691100
C	-7.04879000	-0.03386800	-1.95713500
H	-7.06557000	-0.69341900	-2.83370500
H	-8.00256800	-0.12160800	-1.42887000
H	-6.92540200	0.99089500	-2.32472400
C	-4.38959300	-1.90269500	1.95312100
H	-4.07479100	-2.93590400	1.75706600
H	-3.55053600	-1.40569900	2.45545000
H	-5.26863500	-1.92597900	2.60350700
C	-1.39603900	-1.04324900	-0.66511800
C	-2.51106700	-0.41806300	-0.10669600
N	-2.44742500	0.87393400	0.51359900
S	-1.73694300	0.98944900	2.04535000
O	-1.64448900	-0.36483200	2.57739200
O	-0.56275400	1.84830900	1.98980100

Au	0.50552300	-0.29775300	-0.35161500
C	2.44881300	0.37866300	-0.11649100
N	2.94499700	1.62857000	-0.23265900
C	4.67185900	0.35508400	0.24852200
C	4.31287100	1.63664900	-0.01042800
H	5.62997500	-0.09278700	0.47753600
H	4.89047000	2.55046300	-0.05831300
N	3.51254600	-0.40018800	0.17622400
C	-2.20446900	2.00738500	-0.38729900
H	-2.92974700	1.94405200	-1.20543300
H	-2.36352500	2.95180900	0.14527500
H	-1.18055600	2.00765200	-0.79376300
C	-1.50996000	-2.26085000	-1.44978300
C	-2.40523700	-2.35901700	-2.45249200
H	-3.12255800	-1.57220800	-2.67098200
H	-2.38389600	-3.21104700	-3.13139000
C	-0.47926700	-3.33065100	-1.20582400
H	0.52311300	-3.00056200	-1.51801400
H	-0.40534900	-3.57818900	-0.13813900
H	-0.72881300	-4.24474100	-1.75704100
C	3.40468900	-1.81792200	0.38382500
C	3.65935400	-2.66460900	-0.70008400
C	2.99542000	-2.27534400	1.64028200
C	3.50933100	-4.03494500	-0.49109000
C	2.85895700	-3.65452800	1.80226100
C	3.11478500	-4.52481500	0.74922200
H	3.70489100	-4.72111400	-1.31450300
H	2.54916000	-4.04382100	2.77148100
H	3.00749900	-5.59790000	0.89680000
C	2.12901500	2.77788500	-0.51151700
C	1.72011100	3.56896000	0.56600600
C	1.75686000	3.02567500	-1.83707000
C	0.89219100	4.65479500	0.28175300
C	0.93107600	4.12464200	-2.07310900
C	0.50175100	4.93004400	-1.02339200
H	0.55402100	5.28770400	1.10156500
H	0.63129700	4.35090600	-3.09594400
H	-0.13796100	5.78709700	-1.22755500
C	-2.99570300	1.86160800	2.95653500
H	-2.61838200	2.01038200	3.97321600
H	-3.18097500	2.83041000	2.48306600
H	-3.90699900	1.25614900	2.96798800
C	2.15305200	3.25752500	1.96539700
H	3.21749800	3.48332100	2.12170900
H	1.57789000	3.84513900	2.68868600
H	1.99814100	2.19691400	2.20440700
C	2.21351800	2.14035400	-2.95764500
H	3.28793300	1.91921300	-2.89750900
H	1.68870800	1.17273500	-2.94497400
H	2.01977100	2.60928500	-3.92864800
C	4.04638900	-2.11313800	-2.03921500
H	5.00807300	-1.58269100	-2.00692300
H	4.13641700	-2.91436000	-2.78067900
H	3.29976300	-1.39314900	-2.40760900
C	2.68301400	-1.32474700	2.75676200
H	3.43941200	-0.53394400	2.85233200
H	1.71438800	-0.82486200	2.59741700
H	2.62504300	-1.85425900	3.71402900

TS7a

Zero-point correction= 0.634137 (Hartree/Particle)
Thermal correction to Energy= 0.677416
Thermal correction to Enthalpy= 0.678360
Thermal correction to Gibbs Free Energy= 0.556095
Sum of electronic and zero-point Energies= -2180.341893
Sum of electronic and thermal Energies= -2180.298614

Sum of electronic and thermal Enthalpies= -2180.297670

Sum of electronic and thermal Free Energies= -2180.419935

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.84109712

Cartesian coordinates:

C	-3.81183600	-2.84868200	0.57068400
C	-5.13743300	-2.45018100	0.03848000
C	-2.87385400	-1.95374700	1.07213200
O	-5.41621400	-1.29965500	-0.26061300
H	-3.73806600	-3.87592900	0.93367700
C	-1.81259800	-2.39070600	2.02672500
H	-1.66292200	-1.62598400	2.79857400
H	-2.02885200	-3.35582900	2.49422000
H	-0.86087400	-2.46621100	1.47020500
C	-6.12497800	-3.57369900	-0.10986700
H	-7.02485400	-3.21672400	-0.61701900
H	-5.68432900	-4.40962500	-0.67140000
H	-6.40147700	-3.96987600	0.87694600
C	-1.25438000	-0.87153000	-1.02278300
C	-2.30582500	-0.10515900	-0.34418000
Au	0.62758000	-0.20749900	-0.48742600
N	-2.83186900	-0.67916900	0.68704800
C	4.06362100	1.82286100	0.98139100
C	4.53714600	0.55273900	1.04536400
H	4.50761700	2.77058000	1.25660200
H	5.48330800	0.15310000	1.38653200
N	2.78361900	1.74267000	0.45999400
N	3.53250800	-0.26916900	0.55916500
C	2.45534500	0.45995900	0.20000900
C	-1.53208300	-2.12389700	-1.56531300
N	-2.54544300	1.20281300	-0.65044200
C	-1.88800600	1.83911600	-1.79623700
H	-0.93703600	2.31004200	-1.51110200
H	-1.70659300	1.07559600	-2.55885100
H	-2.55229100	2.60209400	-2.20812200
S	-3.20920300	2.27683500	0.55592400
O	-2.53830500	2.00716300	1.81410900
O	-3.13592100	3.58704700	-0.06214100
C	-2.86089700	-2.53455000	-1.67627700
H	-3.10995100	-3.53060800	-2.04409700
H	-3.66233400	-1.80109900	-1.68314800
C	-0.40877600	-3.06055500	-1.92303700
H	0.28684200	-2.57711600	-2.62144000
H	0.17816300	-3.34014400	-1.03626700
H	-0.77533900	-3.97860300	-2.39637000
C	3.57249100	-1.70392600	0.47624100
C	3.99486800	-2.29199000	-0.71962100
C	3.14273800	-2.43939800	1.58622100
C	3.99642800	-3.68584800	-0.78096900
C	3.15885700	-3.82962500	1.47799200
C	3.58503800	-4.44691000	0.30693800
H	4.33056000	-4.17430300	-1.69562000
H	2.84025800	-4.43060600	2.32913500
H	3.60090100	-5.53335200	0.24334900
C	1.87437300	2.83418100	0.22880500
C	2.00002200	3.55599300	-0.96361000
C	0.86545900	3.06841900	1.16997300
C	1.06317700	4.56071500	-1.20448600
C	-0.05130300	4.08065500	0.88230700
C	0.04395400	4.81598800	-0.29284400
H	1.13469500	5.14083600	-2.12396200
H	-0.85883200	4.27785500	1.58574100
H	-0.69328000	5.58876400	-0.50167600
C	-4.90270200	1.75857900	0.63418200
H	-4.95216700	0.68363900	0.82969200
H	-5.36475900	2.33398500	1.44314500
H	-5.37281600	1.99681400	-0.32406400
C	0.73047700	2.24615700	2.41644900

H	1.70293900	1.95549600	2.83588600
H	0.17245400	2.79512800	3.18255600
H	0.16315800	1.32237700	2.21751300
C	3.08150000	3.24126200	-1.95310700
H	4.08305900	3.45380700	-1.55410500
H	3.07197300	2.17872800	-2.23891000
H	2.95989000	3.83501300	-2.86536200
C	2.66778100	-1.75713000	2.83375000
H	3.42865700	-1.08496400	3.25354500
H	1.77590900	-1.14140000	2.64140600
H	2.41033100	-2.48974300	3.60639900
C	4.40552000	-1.45902900	-1.89603700
H	3.54311300	-0.93460900	-2.33447100
H	5.13977700	-0.68900100	-1.62370200
H	4.84862600	-2.08189300	-2.68044700

TS8a

Zero-point correction= 0.634182 (Hartree/Particle)
Thermal correction to Energy= 0.677054
Thermal correction to Enthalpy= 0.677999
Thermal correction to Gibbs Free Energy= 0.558164
Sum of electronic and zero-point Energies= -2180.333640
Sum of electronic and thermal Energies= -2180.290767
Sum of electronic and thermal Enthalpies= -2180.289823
Sum of electronic and thermal Free Energies= -2180.409658

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.83636173

Cartesian coordinates:

C	-1.13559900	-1.48355800	0.12743100
C	-2.29878900	-0.61244400	-0.18260100
N	-2.76733700	-0.60424500	-1.47283500
S	-3.96484200	0.59581700	-1.94621100
O	-3.47402500	1.91450200	-1.59925700
O	-4.25325600	0.25518700	-3.32643200
Au	0.57151100	-0.34228300	0.20128800
C	2.18413000	0.91421300	-0.08308400
N	2.16189900	2.26407800	-0.13504600
C	4.19445900	1.67710900	-0.74165600
C	3.39380800	2.75320800	-0.53725000
H	5.22537000	1.59671800	-1.06115000
H	3.57680100	3.81503800	-0.63825400
N	3.43103700	0.55790200	-0.45655200
N	-2.75659500	0.21869700	0.69863300
C	-2.27529000	0.09110500	1.96971700
C	-3.15020900	-2.24037000	2.44947800
C	-2.28407200	-1.08454800	2.68974100
C	-1.76433600	1.36094600	2.56196500
H	-1.43337800	1.23641600	3.59750400
H	-0.93709300	1.76282900	1.95676600
H	-2.55920400	2.11809600	2.52166900
O	-3.95763700	-2.31358600	1.52736100
C	-2.99145900	-3.37393000	3.42762500
H	-3.71429700	-4.16352800	3.20502900
H	-1.97075700	-3.78069500	3.35945900
H	-3.12639000	-3.03571100	4.46313800
C	-2.04077800	-1.26123800	-2.56056500
H	-0.95653800	-1.16974300	-2.40151100
H	-2.30085500	-2.32416600	-2.63522900
H	-2.30573100	-0.77666100	-3.50269800
C	-1.18029600	-2.90292600	0.09288400
C	-2.33965700	-3.54266800	-0.24126100
H	-2.40414000	-4.63124900	-0.23712900
H	-3.23581900	-3.00374500	-0.53509100
C	0.05892600	-3.66245200	0.47912300
H	0.88812700	-3.43985800	-0.20838300
H	0.39341500	-3.36789600	1.48368800

H	-0.10881200	-4.74543500	0.47607600
H	-1.79748900	-1.05685200	3.66664100
C	3.84629700	-0.81346500	-0.58344200
C	4.36880700	-1.45804100	0.54156600
C	3.65691900	-1.44585800	-1.81692700
C	4.72278500	-2.80003700	0.40113600
C	4.02265000	-2.78855200	-1.90907900
C	4.55152900	-3.45846500	-0.81108400
H	5.14068800	-3.32894600	1.25686200
H	3.89547300	-3.30800600	-2.85822000
H	4.83878300	-4.50416500	-0.90321200
C	1.02120200	3.06951800	0.22021800
C	-0.04072400	3.18766500	-0.68459000
C	1.03031000	3.68697500	1.47768700
C	-1.12948800	3.97057600	-0.29492400
C	-0.06876700	4.47648600	1.81292700
C	-1.13691900	4.61874500	0.93360500
H	-1.97775800	4.06031200	-0.97146100
H	-0.08452600	4.97659900	2.78077800
H	-1.98832000	5.23684100	1.21238600
C	-5.35364600	0.14233600	-0.93753700
H	-5.65554400	-0.87151500	-1.21508000
H	-5.07388000	0.20332500	0.11603800
H	-6.14727900	0.85748600	-1.17773900
C	2.16205400	3.48047800	2.43956400
H	3.09584200	3.94578200	2.09506500
H	1.92435000	3.91269600	3.41740200
H	2.37517700	2.41069600	2.58633900
C	-0.04147900	2.49746400	-2.01571600
H	0.94082600	2.53430100	-2.50643800
H	-0.30947500	1.43304100	-1.91049600
H	-0.78219300	2.94799900	-2.68466700
C	4.52102300	-0.74231200	1.84970200
H	5.07145500	0.20232800	1.74349600
H	3.54262200	-0.49337100	2.28664200
H	5.05940800	-1.36282600	2.57394500
C	3.07139000	-0.71254500	-2.98622800
H	2.05412800	-0.35070600	-2.76993200
H	3.66663600	0.16905800	-3.26116700
H	3.01611200	-1.36155900	-3.86672700

TS9a

Zero-point correction= 0.632644 (Hartree/Particle)
Thermal correction to Energy= 0.676584
Thermal correction to Enthalpy= 0.677528
Thermal correction to Gibbs Free Energy= 0.553246
Sum of electronic and zero-point Energies= -2180.332500
Sum of electronic and thermal Energies= -2180.288559
Sum of electronic and thermal Enthalpies= -2180.287615
Sum of electronic and thermal Free Energies= -2180.411897
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.83059489
Cartesian coordinates:

C	-3.73990600	-1.76991200	2.18304300
C	-4.77290200	-2.45554900	1.38910400
C	-2.62591200	-1.21939100	1.66274900
O	-4.84218100	-2.35548000	0.17045800
H	-3.89454900	-1.68324300	3.25827000
C	-1.60909400	-0.46727000	2.45176800
H	-1.51553800	0.55316900	2.04583800
H	-1.89585400	-0.40528500	3.50641500
H	-0.61922900	-0.94277700	2.37850800
C	-5.75548200	-3.28132300	2.17026900
H	-6.46618300	-3.76283200	1.49364900
H	-5.23410700	-4.04464400	2.76356400
H	-6.30088500	-2.64818400	2.88393200

C	-0.87367300	-1.46224400	-0.80376100
C	-2.11070400	-0.74028600	-0.75819200
Au	0.78395900	-0.33705700	-0.24953300
N	-2.30715600	-1.40053200	0.31961700
C	3.41969000	2.79564300	0.87313200
C	4.34773200	1.81050600	0.77609000
H	3.50676300	3.84252000	1.13311500
H	5.41856600	1.81217200	0.93306500
N	2.20125700	2.21955600	0.55692200
N	3.67002600	0.65902400	0.40568300
C	2.35146900	0.90646400	0.27192000
C	-0.81114100	-2.80296300	-1.39750200
N	-2.65530500	0.26526500	-1.45053400
C	-2.02086300	0.72345100	-2.69234000
H	-1.49693000	1.67126300	-2.52180200
H	-1.30878900	-0.04361000	-3.01413000
H	-2.77905800	0.86209600	-3.46964800
S	-3.97338000	1.22490800	-0.81081200
O	-3.87643600	1.13299400	0.63112200
O	-3.87230700	2.48697800	-1.51437800
C	-1.76161400	-3.20049600	-2.25738400
H	-1.71074900	-4.16776800	-2.75430500
H	-2.63279600	-2.58542800	-2.48593500
C	0.36940400	-3.64963700	-1.03226300
H	1.31614800	-3.15570200	-1.29743500
H	0.39770600	-3.82037500	0.05375200
H	0.33657200	-4.62442600	-1.53082800
C	4.26058200	-0.63511000	0.19244500
C	4.77738400	-0.92553500	-1.07411500
C	4.25748800	-1.54800800	1.25139200
C	5.32475900	-2.19357300	-1.26546500
C	4.81558800	-2.80393000	1.01329900
C	5.34481500	-3.12304000	-0.23167900
H	5.73953400	-2.44944500	-2.23968500
H	4.83576600	-3.53539000	1.82036200
H	5.78034900	-4.10647100	-0.39763700
C	0.90578800	2.84366100	0.54694900
C	0.39022300	3.28394100	-0.67684200
C	0.17917300	2.87071400	1.74194600
C	-0.92455900	3.75086100	-0.68574300
C	-1.13067500	3.34812800	1.68452700
C	-1.68095500	3.77403400	0.48119600
H	-1.36366600	4.09859600	-1.62112500
H	-1.72747900	3.37152700	2.59611000
H	-2.71060600	4.12377500	0.44695100
C	-5.37400300	0.31475900	-1.40099100
H	-5.32997900	-0.69815100	-0.98013200
H	-6.26595300	0.84817200	-1.05540300
H	-5.34286600	0.30877700	-2.49516600
C	0.77667900	2.38304700	3.02742300
H	1.60310800	3.02449100	3.36376000
H	0.02629700	2.36912300	3.82598200
H	1.18573800	1.36643800	2.92840200
C	1.20494700	3.22344100	-1.93423700
H	2.19779600	3.67480000	-1.80518700
H	1.37040700	2.18446000	-2.25939700
H	0.70122700	3.75315500	-2.75076000
C	3.65976100	-1.20133500	2.58196800
H	3.98867000	-0.21700500	2.94230200
H	2.56024200	-1.17155000	2.53074400
H	3.93375400	-1.94461600	3.33852300
C	4.73129400	0.08289100	-2.18210600
H	3.70245600	0.41795400	-2.37989700
H	5.31855100	0.98142700	-1.94719000
H	5.13079400	-0.33876800	-3.11052400

TS10a

Zero-point correction= 0.633398 (Hartree/Particle)
Thermal correction to Energy= 0.676722
Thermal correction to Enthalpy= 0.677666
Thermal correction to Gibbs Free Energy= 0.554320
Sum of electronic and zero-point Energies= -2180.331672
Sum of electronic and thermal Energies= -2180.288348
Sum of electronic and thermal Enthalpies= -2180.287404
Sum of electronic and thermal Free Energies= -2180.410750
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.83028756
Cartesian coordinates:

C	-1.07262400	-1.76993800	-0.10595200
C	-2.43896100	-1.26184500	0.00419900
N	-3.06725900	-1.32275100	-1.27203600
S	-3.38373700	0.18676300	-2.02470600
O	-2.31520000	1.07646500	-1.59994500
O	-3.60876500	-0.11863700	-3.42361700
Au	0.35711200	-0.28928500	-0.02061100
C	1.89659200	1.09794800	-0.03646300
N	1.87986400	2.44289100	0.07577800
C	3.98912500	1.90779800	-0.24447700
C	3.15788500	2.96145700	-0.05156100
H	5.05996000	1.85065800	-0.39101500
H	3.34320900	4.02635000	0.00269700
N	3.19563600	0.77429400	-0.23109100
N	-2.96820700	-0.55103400	0.91458800
C	-2.34202500	-0.04974700	2.04980600
C	-1.88847300	-2.20134600	3.24810000
C	-1.90311900	-0.74446800	3.12605900
C	-2.33900000	1.44644100	2.02809800
H	-1.83905800	1.86128000	2.91038000
H	-1.82867300	1.81083300	1.12365900
H	-3.36751400	1.83137900	1.98630900
O	-1.96719500	-2.93657600	2.26934300
C	-1.76339800	-2.75582100	4.63886400
H	-2.61655000	-2.44014400	5.25452100
H	-1.71942800	-3.84768300	4.60908800
H	-0.86139600	-2.36374400	5.12823200
C	-3.78410100	-2.49877600	-1.74029400
H	-3.08618100	-3.33648400	-1.88552500
H	-4.56483900	-2.79982500	-1.02809800
H	-4.22720200	-2.27109200	-2.71412100
H	-1.61503400	-0.16617100	4.00462000
C	3.66151700	-0.57193900	-0.42732300
C	4.02116000	-1.32137000	0.69744300
C	3.70798600	-1.06985700	-1.73363000
C	4.44921800	-2.63141200	0.48155500
C	4.14512400	-2.38396200	-1.90088100
C	4.51223300	-3.15663700	-0.80467500
H	4.74213100	-3.23993600	1.33630900
H	4.19884700	-2.79964900	-2.90651800
H	4.85669400	-4.17816200	-0.95459900
C	0.69894000	3.24562000	0.24832600
C	-0.05485000	3.56999000	-0.88343400
C	0.37928700	3.67843700	1.53995500
C	-1.17231700	4.38429800	-0.68987300
C	-0.73849800	4.49852900	1.68155900
C	-1.50516700	4.85097800	0.57526400
H	-1.78039000	4.65412300	-1.55240600
H	-1.00940800	4.85843700	2.67391700
H	-2.37220900	5.49653800	0.70274000
C	-4.91998700	0.73133200	-1.30789900
H	-5.68909300	-0.01610100	-1.52848900
H	-4.77594400	0.84300100	-0.22980700
H	-5.17853400	1.68372400	-1.78194300
C	1.18455200	3.23978200	2.72588800
H	2.22932700	3.57534100	2.67219800

H	0.75879600	3.63557900	3.65466800
H	1.20789800	2.14146200	2.80567800
C	0.29120600	3.04300600	-2.24233600
H	1.37506000	3.01170800	-2.41815200
H	-0.10127900	2.02255200	-2.36909000
H	-0.16153000	3.66090300	-3.02555600
C	3.93397500	-0.74361600	2.07775100
H	4.50317600	0.19142400	2.17007300
H	2.89411300	-0.51095600	2.35144400
H	4.32527300	-1.44676200	2.82065200
C	3.27972300	-0.23255200	-2.90087700
H	2.21375000	0.03477500	-2.83633300
H	3.83814100	0.71190800	-2.95941300
H	3.43315400	-0.76809900	-3.84381300
C	-0.72466100	-3.10584600	-0.48373000
C	-1.56464700	-4.13901400	-0.20819700
H	-2.50831700	-3.99204900	0.30924900
C	0.63435400	-3.35441400	-1.08156400
H	1.43390300	-3.08660000	-0.37566900
H	0.78632700	-2.74821700	-1.98457200
H	0.76165300	-4.40827100	-1.35473500
H	-1.26816300	-5.16891400	-0.40813500

TS11a

Zero-point correction= 0.633169 (Hartree/Particle)
Thermal correction to Energy= 0.676446
Thermal correction to Enthalpy= 0.677390
Thermal correction to Gibbs Free Energy= 0.555668
Sum of electronic and zero-point Energies= -2180.324909
Sum of electronic and thermal Energies= -2180.281632
Sum of electronic and thermal Enthalpies= -2180.280688
Sum of electronic and thermal Free Energies= -2180.402409
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2181.81954018
Cartesian coordinates:

C	-1.60324400	0.44980500	0.63847300
C	-2.21523900	-0.49063500	-0.31139300
N	-1.88287800	-1.81226700	-0.28386800
S	-1.61000600	-2.72132300	-1.72019200
O	-0.67372400	-2.00912800	-2.56496400
O	-1.31079000	-4.05276700	-1.22718500
Au	0.45570700	0.25505000	0.49571200
C	2.45572100	-0.02173900	0.10357500
N	3.25512800	0.82886000	-0.57170000
C	4.45709400	-0.98225900	-0.24064800
C	4.49698800	0.25550500	-0.79477800
H	5.19854100	-1.76831700	-0.18215700
H	5.27989200	0.78181800	-1.32483700
N	3.19340900	-1.13251700	0.30674200
N	-2.09937800	0.25376000	-1.43297400
C	-2.96848200	1.22174700	-1.77498900
C	-4.82480400	0.26045800	-0.51766900
C	-4.27510500	1.29176600	-1.31841100
C	-2.43874500	2.18279100	-2.78709400
H	-1.50795000	2.63151400	-2.41020600
H	-2.17288300	1.64550800	-3.70705700
H	-3.15509500	2.97384200	-3.02847600
O	-4.11696100	-0.63567200	0.02898000
C	-6.30317500	0.16736300	-0.31400600
H	-6.52732100	0.19106400	0.76048300
H	-6.84885600	0.97264300	-0.81459900
H	-6.66438400	-0.79948800	-0.68649800
C	-1.77682200	-2.50483600	1.00241600
H	-2.05054400	-1.79181800	1.78828500
H	-2.47226400	-3.34916600	1.03850500
H	-0.75442200	-2.86333500	1.17522100

C	-2.25334700	1.52704100	1.32706600
C	-3.37733200	1.28995200	2.04280300
H	-3.90523200	0.34143200	1.99702300
C	-1.51946300	2.83542200	1.41140900
H	-1.27954700	3.20790700	0.40513700
H	-2.11872200	3.59390000	1.92740900
H	-4.94082700	2.04641500	-1.72865300
C	2.66275300	-2.31517000	0.93217500
C	2.66203500	-2.38648800	2.32879400
C	2.12161700	-3.30745300	0.10657500
C	2.08842900	-3.51787500	2.90898000
C	1.54918500	-4.41622700	0.73256900
C	1.53621300	-4.52077600	2.11931100
H	2.08069500	-3.60875700	3.99465200
H	1.10498100	-5.19678300	0.11643900
H	1.09280200	-5.39616600	2.59053400
C	2.81733600	2.12624900	-1.01162400
C	2.03504600	2.21366800	-2.16878800
C	3.15251500	3.23312500	-0.22315300
C	1.60244700	3.48682800	-2.54690900
C	2.69302300	4.48149800	-0.63890000
C	1.92784400	4.60772500	-1.79326700
H	1.01104300	3.59206200	-3.45673600
H	2.94264400	5.36175900	-0.04773700
H	1.58614900	5.59135300	-2.11030900
C	-3.21291900	-2.72208500	-2.48962200
H	-3.94163600	-3.11645000	-1.77505100
H	-3.46199300	-1.70048000	-2.79185700
H	-3.14214800	-3.37258900	-3.36755200
C	3.95494500	3.07504100	1.03302900
H	4.97269600	2.71334400	0.83190700
H	4.04381300	4.02980600	1.56213400
H	3.49031700	2.35066800	1.71851500
C	1.63421600	1.00517000	-2.96164300
H	2.41214400	0.23045700	-2.97253300
H	0.72233300	0.53781700	-2.55281100
H	1.41896300	1.27932800	-4.00110500
C	3.23927700	-1.28614900	3.16757300
H	4.24281300	-0.99359000	2.83003800
H	2.61456700	-0.38129700	3.13062700
H	3.31427000	-1.59361500	4.21622400
C	2.15939600	-3.19029300	-1.38657100
H	1.78797700	-2.21645900	-1.73504300
H	3.18164600	-3.30926400	-1.77355600
H	1.53303300	-3.95941000	-1.85118400
H	-3.73193600	2.02549600	2.76488600
H	-0.56364500	2.72288100	1.94162700

TS12a

Zero-point correction= 0.694308 (Hartree/Particle)
Thermal correction to Energy= 0.749807
Thermal correction to Enthalpy= 0.750751
Thermal correction to Gibbs Free Energy= 0.606781
Sum of electronic and zero-point Energies= -4007.233943
Sum of electronic and thermal Energies= -4007.178444
Sum of electronic and thermal Enthalpies= -4007.177499
Sum of electronic and thermal Free Energies= -4007.321469

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4009.10011511

Cartesian coordinates:

H	-2.96562500	1.19271000	-0.16207600
N	-3.44335700	0.14450800	0.48971000
S	-4.23622700	-0.91418300	-0.49521500
O	-4.20320600	-0.31189300	-1.81937000
O	-3.87233400	-2.30212900	-0.29863000
S	-3.07529300	-0.19207100	2.07263500

O	-3.33278800	0.98439500	2.87775100
O	-3.51789100	-1.50918800	2.48126500
C	-1.24309900	-0.31291600	1.95884700
C	-5.99663000	-0.72403700	0.03789100
F	-0.76591900	-0.66911200	3.13980900
F	-0.93257000	-1.23096400	1.05873100
F	-0.71917200	0.85174600	1.61321300
F	-6.72428000	-1.56975100	-0.67263700
F	-6.38824000	0.51198300	-0.20476900
F	-6.13000100	-0.99035900	1.32208800
C	-2.60994300	2.30515200	-0.98483500
C	-4.03452100	2.80925700	-1.09100100
C	-1.76005600	2.97940300	-0.05297400
O	-4.64844700	3.19783500	-0.11626200
C	-2.27358500	3.59794100	1.20631200
H	-1.42354700	3.88935700	1.83382600
H	-2.88641500	4.47908100	0.96889400
H	-2.93914000	2.92724700	1.75771300
C	-4.68218500	2.81605600	-2.45333000
H	-5.64219400	3.33314500	-2.36838100
H	-4.05629300	3.31411700	-3.20528600
H	-4.85736100	1.78750600	-2.79348200
C	0.26237000	1.06631600	-1.32101000
C	0.43227700	2.43048500	-0.87508300
Au	1.59404500	-0.39760600	-0.66901300
N	-0.45667500	3.15989200	-0.24113800
C	4.47745400	-2.96985700	1.15586800
C	3.51327800	-3.88728800	0.89570100
H	5.44102400	-3.05655700	1.64036400
H	3.45276400	-4.94662900	1.10755300
N	4.01300800	-1.75947500	0.66422600
N	2.48865400	-3.21328100	0.24967000
C	2.78955400	-1.90184300	0.10679400
C	-0.89908200	0.75983600	-1.95317500
N	1.68188000	3.03930500	-0.98195300
C	2.72373000	2.50680700	-1.86146000
H	3.39187600	1.80325400	-1.34407600
H	2.22747900	1.98847900	-2.68552100
H	3.31759000	3.33772700	-2.25195100
S	2.24848700	4.02606700	0.31222700
O	1.94543300	3.37905000	1.57846700
O	3.62786100	4.33150400	-0.04014700
C	-1.92179800	1.83545100	-2.26154200
H	-2.66560600	1.43988600	-2.95842900
H	-1.43577600	2.69337000	-2.75936700
C	-1.20702100	-0.65577700	-2.35435800
H	-0.32896300	-1.12208000	-2.82079900
H	-1.44776500	-1.27515900	-1.47355400
H	-2.05601600	-0.72718900	-3.04128500
C	1.22546100	-3.75278500	-0.17487400
C	1.03750300	-4.01796400	-1.53486500
C	0.20896500	-3.88047800	0.77690700
C	-0.23558600	-4.41828500	-1.93941200
C	-1.05366400	-4.26145600	0.32406200
C	-1.27565100	-4.52191500	-1.02256500
H	-0.41279200	-4.62655800	-2.99455900
H	-1.87952700	-4.31087100	1.03341100
H	-2.27417300	-4.79305100	-1.35939500
C	4.70249300	-0.49933900	0.65753800
C	5.65566900	-0.28552400	-0.34434000
C	4.31325000	0.48864400	1.56852900
C	6.24912500	0.97403800	-0.41106100
C	4.92549100	1.73757200	1.45539500
C	5.87992800	1.97944600	0.47579300
H	6.99081700	1.16945300	-1.18541400
H	4.61766600	2.53690600	2.12793000
H	6.32067300	2.97068500	0.39158300
C	1.33229100	5.54705700	0.18095900

H	0.28734600	5.36228800	0.43342100
H	1.80511400	6.23846900	0.88657700
H	1.43600000	5.92051200	-0.84176200
C	3.24070000	0.25433700	2.58898200
H	3.27874600	-0.75997400	3.00863000
H	3.32426700	0.97431000	3.41045700
H	2.24182400	0.39120800	2.14429200
C	5.97968900	-1.35648100	-1.34248800
H	6.44740600	-2.23551500	-0.87746400
H	5.07102100	-1.71317100	-1.85124900
H	6.66861400	-0.98048400	-2.10709500
C	0.45384100	-3.57385100	2.22329700
H	1.06060400	-4.35157100	2.70874000
H	0.98742400	-2.62103000	2.35117400
H	-0.49463600	-3.50153200	2.76805700
C	2.14473200	-3.83282900	-2.52861500
H	2.32072600	-2.76480400	-2.73177100
H	3.09663400	-4.25025100	-2.17240700
H	1.89734300	-4.31558400	-3.48104900

TS13a

Zero-point correction= 0.692360 (Hartree/Particle)
Thermal correction to Energy= 0.748621
Thermal correction to Enthalpy= 0.749565
Thermal correction to Gibbs Free Energy= 0.602626
Sum of electronic and zero-point Energies= -4007.236264
Sum of electronic and thermal Energies= -4007.180003
Sum of electronic and thermal Enthalpies= -4007.179059
Sum of electronic and thermal Free Energies= -4007.325998
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4009.11216323
Cartesian coordinates:

H	-1.20589600	0.16639400	-0.05676700
N	-1.72977100	0.36164900	-1.22679400
S	-0.87541100	-0.23401100	-2.48877800
O	0.07515600	-1.17477300	-1.91429200
O	-1.69839900	-0.56088100	-3.63211300
S	-2.98061400	1.42347900	-1.38625200
O	-3.33600600	1.80494900	-0.03044000
O	-2.72520700	2.41570600	-2.41365700
C	-4.40031300	0.38622100	-2.00031500
C	0.18320200	1.20928800	-3.02352200
F	-5.51496100	0.97423700	-1.58862700
F	-4.39730700	0.32906900	-3.31316100
F	-4.32197600	-0.82271100	-1.48892500
F	1.32094700	0.72528900	-3.51628200
F	0.46924900	1.97742900	-1.97646700
F	-0.40853800	1.92791100	-3.94830200
C	-3.38811100	0.42156700	2.87645200
C	-4.39061400	1.43517200	3.25266500
C	-3.69586400	-0.62596100	2.03450900
O	-5.56948900	1.34795300	2.94175600
C	-5.06058600	-0.87746000	1.46918400
H	-5.02116500	-1.76177200	0.82372800
H	-5.80699900	-1.01703200	2.25938200
H	-5.40231200	-0.01106300	0.89098100
C	-3.94047100	2.61937400	4.08696700
H	-4.79183100	3.29649300	4.19704200
H	-3.61258400	2.29941100	5.08617600
H	-3.10380100	3.16551500	3.63110400
C	-0.85295200	-0.17030500	1.26118900
C	-1.53489900	-1.45652200	1.42913400
Au	1.20037300	0.08714200	0.62757100
N	-2.79582900	-1.60158900	1.70645000
C	5.41143100	0.00878000	-0.07122800
C	5.22841800	1.34577400	0.04193900

H	6.29810300	-0.58728100	-0.24287200
H	5.92018300	2.17611900	-0.01011500
N	4.16257900	-0.57653500	0.07196700
N	3.87284300	1.54147300	0.25479400
C	3.20793600	0.36149100	0.26837200
C	-1.18115400	0.83554900	2.14663200
N	-0.88180400	-2.63939600	1.04385900
C	0.51942400	-2.90821900	1.33387100
H	1.17356700	-2.71997900	0.47210000
H	0.82302700	-2.27783800	2.17754600
H	0.63957600	-3.95744700	1.62922800
S	-1.66249900	-3.72732200	-0.00935700
O	-2.48436500	-2.98557700	-0.94587000
O	-0.60465600	-4.61621900	-0.46880900
C	-1.96756000	0.51212500	3.37835900
H	-1.84858300	1.28030300	4.14983200
H	-1.64274200	-0.45102000	3.80217200
C	-0.87315100	2.27270800	1.88561400
H	-0.38068200	2.42705700	0.91631100
H	-1.80468500	2.85631100	1.88553000
H	-0.22500700	2.68460500	2.67541900
C	3.22206300	2.81363600	0.38851400
C	2.89469900	3.26722000	1.67032400
C	2.90707900	3.51650000	-0.77831800
C	2.21684900	4.48191800	1.76553500
C	2.21785100	4.72058300	-0.63514600
C	1.87488800	5.19811500	0.62390800
H	1.94951900	4.86226100	2.75151500
H	1.94337200	5.28182100	-1.52767200
H	1.33451300	6.13843400	0.71645600
C	3.90374900	-1.98920200	0.02401900
C	4.02961900	-2.72135000	1.20986600
C	3.51215200	-2.55538900	-1.19219100
C	3.75428500	-4.08619300	1.15302500
C	3.23107800	-3.92312100	-1.19735300
C	3.35213900	-4.67999400	-0.03952800
H	3.84332900	-4.68299100	2.06074500
H	2.89990000	-4.38919000	-2.12406900
H	3.12028600	-5.74306100	-0.06445200
C	-2.73344500	-4.66799500	1.05993500
H	-3.44826100	-3.97596500	1.51250300
H	-3.23343900	-5.41610900	0.43627600
H	-2.11702500	-5.15703700	1.82088300
C	3.35327400	-1.72752400	-2.42900300
H	4.12879600	-0.95441000	-2.51794900
H	3.39372100	-2.35707200	-3.32492400
H	2.37670600	-1.22410200	-2.42893400
C	4.40931800	-2.04937500	2.49527800
H	5.39249500	-1.56173300	2.43489400
H	3.68488600	-1.26555500	2.76515900
H	4.44534900	-2.77197900	3.31819300
C	3.29978800	2.99836700	-2.12854800
H	4.36004800	3.19850600	-2.34145700
H	3.15200300	1.91384300	-2.21282200
H	2.71006800	3.47901600	-2.91731900
C	3.22620500	2.46546200	2.89266300
H	2.55308600	1.59912000	2.99028000
H	4.25016800	2.06806300	2.86406100
H	3.12216100	3.07387100	3.79843400

INT1b

Zero-point correction= 0.584952 (Hartree/Particle)
Thermal correction to Energy= 0.622824
Thermal correction to Enthalpy= 0.623768
Thermal correction to Gibbs Free Energy= 0.512863
Sum of electronic and zero-point Energies= -1972.551857
Sum of electronic and thermal Energies= -1972.513985

Sum of electronic and thermal Enthalpies= -1972.513041
Sum of electronic and thermal Free Energies= -1972.623946
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1973.94130091
Cartesian coordinates:

C	-0.83142700	2.10046800	-0.64567700
C	0.35462600	2.50323300	-0.51822800
N	1.60686300	2.82331600	-0.30247700
S	2.15779900	2.79513500	1.38181400
O	1.13412200	2.09788400	2.13422700
O	3.53183300	2.33664500	1.32936400
Au	-0.14628600	0.04867800	-0.29106500
C	0.31187800	-1.89673400	0.09475900
N	1.51174700	-2.50233800	-0.00333800
C	0.12068800	-4.03937900	0.73622100
C	1.41511100	-3.82831000	0.39001300
H	-0.39343000	-4.91909100	1.10068400
H	2.27570200	-4.48445000	0.38613000
N	-0.54128800	-2.83663300	0.54649400
C	2.63506300	2.62068400	-1.34440400
H	2.20018600	2.91906300	-2.30138300
H	3.50403200	3.24687400	-1.12492700
H	2.94426000	1.56636500	-1.37628400
C	-1.92940100	-2.56512300	0.80922900
C	-2.85472900	-2.80273000	-0.21257400
C	-2.27163000	-2.01982700	2.05094200
C	-4.18741200	-2.48527200	0.04669300
C	-3.61781600	-1.72100000	2.26528900
C	-4.56515400	-1.95138900	1.27425900
H	-4.93403700	-2.66278500	-0.72664200
H	-3.91971700	-1.30364200	3.22517500
H	-5.61123100	-1.71589700	1.46184900
C	2.70279900	-1.83102800	-0.45172900
C	3.43139500	-1.08042900	0.47724600
C	3.04556900	-1.93358200	-1.80436000
C	4.56673200	-0.41661800	0.00804700
C	4.18992200	-1.25712900	-2.22541400
C	4.94454600	-0.50959300	-1.32678700
H	5.15118600	0.18134800	0.70531100
H	4.48962200	-1.32381500	-3.27067500
H	5.83942100	0.00572500	-1.67147000
C	2.11195500	4.52737500	1.77285600
H	2.45905500	4.63672600	2.80549100
H	2.78080400	5.05818500	1.08859400
H	1.08048800	4.87852200	1.67665200
C	3.00558700	-0.97787800	1.91091700
H	2.77907700	-1.96147500	2.34526100
H	3.78978600	-0.50927200	2.51484600
H	2.10076400	-0.36024600	2.02158000
C	2.20978100	-2.73036200	-2.76020500
H	2.20992400	-3.80120300	-2.51376800
H	1.16004000	-2.40192000	-2.75101200
H	2.58408600	-2.62881000	-3.78438200
C	-2.42374800	-3.35058800	-1.53950500
H	-1.94399200	-4.33438100	-1.44532400
H	-3.28026500	-3.46321600	-2.21259400
H	-1.69531700	-2.68800500	-2.03099600
C	-1.23398800	-1.73084800	3.09396800
H	-0.50768300	-2.54779700	3.19967100
H	-0.66074200	-0.82393300	2.84507000

H	-1.69923900	-1.56509600	4.07164000
C	-2.23457100	2.38056300	-0.85213600
C	-2.63793600	3.65664600	-1.00934600
C	-3.20096100	1.22114300	-0.85374400
C	-4.06817800	4.05791300	-1.15246700
H	-1.88544000	4.44751000	-1.02794200
C	-4.57753200	1.62047800	-1.36955400
H	-2.78838000	0.40100600	-1.46490700
C	-5.02316100	2.93905000	-0.75279200
H	-4.25080000	4.96559500	-0.55861800
H	-5.29985600	0.82136100	-1.15753800
H	-5.03305600	2.84326500	0.34460400
H	-4.24648900	4.36019300	-2.19933500
H	-6.04679800	3.19016700	-1.05714200
H	-4.53960300	1.72932700	-2.46543000
H	-3.27752500	0.81106400	0.17032900

INT2b

Zero-point correction= 0.701745 (Hartree/Particle)
Thermal correction to Energy= 0.746992
Thermal correction to Enthalpy= 0.747936
Thermal correction to Gibbs Free Energy= 0.619199
Sum of electronic and zero-point Energies= -2296.923982
Sum of electronic and thermal Energies= -2296.878735
Sum of electronic and thermal Enthalpies= -2296.877791
Sum of electronic and thermal Free Energies= -2297.006529
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.51942953
Cartesian coordinates:

C	5.81479500	0.34928900	0.36845900
C	5.80816100	-0.45725400	-0.73330600
C	4.48444000	0.39210300	0.82702300
N	3.75187100	-0.35337500	0.00910500
O	4.56123100	-0.89144600	-0.97620400
H	6.66717400	0.84211500	0.81704400
C	6.86044200	-0.93306800	-1.65161000
H	6.63476800	-0.64502200	-2.68537700
H	7.82713000	-0.50682700	-1.37017800
H	6.93565500	-2.02687900	-1.62136700
C	3.90564600	1.13234900	1.96554000
H	3.54007600	2.10556200	1.60668500
H	3.06484500	0.57982000	2.40035900
H	4.67008800	1.31038000	2.72764200
C	1.46752200	0.40524800	-0.29096900
C	2.34019200	-0.60660500	-0.10579400
N	2.05438900	-1.99121000	0.00891800
S	1.68975200	-2.52158100	1.58323100
O	2.32038900	-1.56517900	2.48390700
O	0.27302500	-2.83833100	1.70141300
Au	-0.58836800	0.11202900	-0.16642700
C	-2.64926500	0.00181300	-0.04965700
N	-3.46993300	-1.05164100	-0.24583100
C	-4.79558200	0.63840800	0.22534300
C	-4.79631400	-0.68189600	-0.08146000
H	-5.60098900	1.33052500	0.43392000
H	-5.60261100	-1.39438800	-0.19776300
N	-3.46792600	1.03870600	0.23923700
C	1.28878200	-2.63786400	-1.06043600
H	1.70696000	-2.30393800	-2.01508500
H	1.40411000	-3.72674100	-0.99431400

H	0.21644900	-2.39713800	-1.02237200
C	1.88796800	1.78932700	-0.54392300
C	2.78572700	2.11252900	-1.49449400
H	3.26028400	1.31083900	-2.06753700
C	1.15970400	2.85814000	0.24227900
H	0.12061500	2.92801000	-0.12952700
H	1.06031400	2.54647300	1.29591000
C	-2.98912600	2.37053300	0.49036400
C	-2.76417800	3.21154700	-0.60440900
C	-2.72541500	2.74488200	1.81202700
C	-2.26623500	4.48859800	-0.34142500
C	-2.23133100	4.03129300	2.02795600
C	-2.00713100	4.89604000	0.96252700
H	-2.08753900	5.16873300	-1.17417100
H	-2.02390700	4.35336500	3.04782500
H	-1.62984900	5.89996700	1.15073600
C	-3.00027100	-2.36227000	-0.60364900
C	-2.68270800	-3.25746300	0.42118300
C	-2.85297100	-2.65982200	-1.96291300
C	-2.20149900	-4.51182200	0.04412400
C	-2.37322100	-3.92672300	-2.29201800
C	-2.05148300	-4.84414400	-1.29650200
H	-1.94100900	-5.22893200	0.82172900
H	-2.25676200	-4.19280900	-3.34220500
H	-1.68485900	-5.83187000	-1.57140900
C	2.59523200	-4.05234800	1.67948800
H	2.41490400	-4.46291000	2.67798200
H	2.22615900	-4.75115700	0.92341100
H	3.65832500	-3.84199300	1.53726300
C	-2.82678700	-2.87239900	1.86070900
H	-3.82913500	-2.48391000	2.08682400
H	-2.63859500	-3.73157200	2.51338200
H	-2.09663900	-2.09611300	2.12904200
C	-3.17494100	-1.64528500	-3.01833600
H	-4.19642800	-1.25301800	-2.91870400
H	-2.49609100	-0.78106100	-2.96065200
H	-3.07996100	-2.07869000	-4.01988000
C	-3.00013200	2.74537900	-2.00914000
H	-3.95164800	2.20777400	-2.11772800
H	-3.00739800	3.59034800	-2.70644400
H	-2.20542300	2.05439300	-2.33076500
C	-2.93419300	1.78706100	2.94533000
H	-3.95568800	1.38400900	2.96559300
H	-2.25409400	0.92578300	2.86733100
H	-2.74754100	2.27397200	3.90851700
C	1.82566000	4.22201100	0.13154100
H	1.17142200	4.98773000	0.57039000
H	2.76324600	4.23985800	0.71479200
C	3.13134200	3.51907500	-1.88020700
H	4.14708500	3.75643800	-1.51405500
C	2.13531900	4.53135400	-1.32541500
H	1.19812500	4.47784600	-1.90419300
H	2.52339000	5.55125600	-1.44352200
H	3.19523600	3.59895300	-2.97542600

INT3b

Zero-point correction= 0.699852 (Hartree/Particle)
Thermal correction to Energy= 0.745897

Thermal correction to Enthalpy= 0.746841
Thermal correction to Gibbs Free Energy= 0.617831
Sum of electronic and zero-point Energies= -2296.940108
Sum of electronic and thermal Energies= -2296.894064
Sum of electronic and thermal Enthalpies= -2296.893120
Sum of electronic and thermal Free Energies= -2297.022129
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.53879502
Cartesian coordinates:

C	-4.06401100	-1.56829100	1.70731800
C	-5.29965200	-1.10323400	1.07426800
C	-2.87145800	-0.91161700	1.65944600
O	-5.34166200	-0.18745600	0.25489000
H	-4.13287400	-2.43696900	2.36223400
C	-1.68178400	-1.38474700	2.43655700
H	-1.23659300	-0.54785000	2.99098100
H	-1.94120300	-2.18635600	3.13537100
H	-0.90526200	-1.75991600	1.74695400
C	-6.55501200	-1.82044000	1.49637400
H	-7.40909500	-1.45434400	0.92044800
H	-6.45121100	-2.90586400	1.35942400
H	-6.74449900	-1.65877000	2.56643300
C	-1.28024000	-0.47407700	-0.74208900
C	-2.10431700	0.55438300	-0.09256700
Au	0.71669200	-0.20679500	-0.34027600
N	-2.71988800	0.27257300	0.99413700
C	4.56182600	1.23279600	0.76424000
C	4.76784700	-0.08819700	1.00043400
H	5.20272700	2.09486900	0.89496500
H	5.62646500	-0.62639500	1.38047100
N	3.27088900	1.35246100	0.28052900
N	3.59629600	-0.73968700	0.65046200
C	2.67699400	0.14339600	0.20968300
C	-1.86741300	-1.59842300	-1.34203200
N	-2.08959800	1.83582300	-0.59699800
C	-1.39229100	2.15089800	-1.84546900
H	-0.32546600	2.36468500	-1.68431300
H	-1.49774100	1.30137000	-2.52949100
H	-1.86032200	3.02678900	-2.30039700
S	-2.45383800	3.17010800	0.45492200
O	-1.74355200	2.97539700	1.70658300
O	-2.20142800	4.34359500	-0.36268500
C	-3.23605700	-1.60526600	-1.53997100
C	3.33273600	-2.14891200	0.75768000
C	3.57916700	-2.95792100	-0.35541300
C	2.78850900	-2.62808200	1.95405300
C	3.27360500	-4.31422200	-0.23948000
C	2.49424400	-3.98948300	2.02195500
C	2.73680900	-4.82465800	0.93677600
H	3.46446300	-4.97353600	-1.08554400
H	2.07638800	-4.39537400	2.94261100
H	2.50979600	-5.88654800	1.01096700
C	2.59611500	2.56559900	-0.10200300
C	2.81180100	3.05603400	-1.39563100
C	1.70112600	3.14508600	0.80388800
C	2.08846500	4.18419700	-1.78010800
C	0.99610200	4.26982200	0.37106900
C	1.18391700	4.78062400	-0.90695400
H	2.23418200	4.59027600	-2.78060200
H	0.27582000	4.73116600	1.04492800

H	0.60904500	5.64792800	-1.22595900
C	-4.20375600	2.99939800	0.69851500
H	-4.42394800	1.99070100	1.05947800
H	-4.48974300	3.75949800	1.43301300
H	-4.69498600	3.18753700	-0.26018800
C	1.45624200	2.57013200	2.16658300
H	2.34877700	2.09042900	2.58933900
H	1.12060900	3.34940300	2.85936700
H	0.65026000	1.81958800	2.13295400
C	3.76294100	2.37876000	-2.33626600
H	4.80429900	2.44613200	-1.99175600
H	3.53301300	1.30829400	-2.44579100
H	3.71777000	2.83497500	-3.33095600
C	2.51888300	-1.70951000	3.10762500
H	3.42991300	-1.20114600	3.45226200
H	1.80105800	-0.92044500	2.83684100
H	2.10546000	-2.26156800	3.95866300
C	4.12062800	-2.38600800	-1.63070600
H	3.37336000	-1.75250100	-2.13236400
H	5.00641700	-1.75895300	-1.46256100
H	4.40134600	-3.18233700	-2.32836900
C	-3.96093600	-2.69782100	-2.21475800
C	-3.05404400	-3.72323900	-2.88367000
C	-1.85856100	-4.03082000	-1.99163500
C	-1.02154100	-2.77667200	-1.76681500
H	-4.69820300	-2.26172800	-2.90741300
H	-3.62345600	-4.63137600	-3.11394500
H	-2.21617900	-4.41197400	-1.02096700
H	-0.24709400	-2.95242400	-1.00306400
H	-4.58982500	-3.16815700	-1.43279700
H	-2.69960600	-3.32367300	-3.84636300
H	-1.23792300	-4.82182200	-2.42933200
H	-0.47621600	-2.51543000	-2.68917400
H	-3.83900400	-0.77045400	-1.16594100

INT4b

Zero-point correction= 0.699734 (Hartree/Particle)
Thermal correction to Energy= 0.745870
Thermal correction to Enthalpy= 0.746814
Thermal correction to Gibbs Free Energy= 0.615720
Sum of electronic and zero-point Energies= -2296.936652
Sum of electronic and thermal Energies= -2296.890515
Sum of electronic and thermal Enthalpies= -2296.889571
Sum of electronic and thermal Free Energies= -2297.020666
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.52984529
Cartesian coordinates:

C	5.21280300	0.21557100	1.59372000
C	5.66748200	-0.15923700	0.25287500
C	4.01590500	0.76898200	1.91996700
N	3.06483300	1.14000700	0.98755600
O	5.01313600	0.01088100	-0.77270700
H	5.92959300	0.08758600	2.40602100
C	7.03957800	-0.77632300	0.19135100
H	7.26497000	-1.09086000	-0.83101300
H	7.79560400	-0.05027500	0.52130600
H	7.11518700	-1.63628200	0.87044500
C	3.68198800	1.17495900	3.31981600
H	3.52031100	2.25985800	3.36152300

H	2.74595300	0.69754400	3.63890500
H	4.48505000	0.90782000	4.01425100
C	1.27427500	0.97784100	-0.52943500
C	2.31805300	0.36450000	0.30874700
N	2.33633700	-1.05549700	0.36289300
S	1.64552600	-1.82335900	1.70936500
O	1.22901700	-0.77518600	2.62924800
O	0.69704400	-2.80940600	1.21761300
Au	-0.64061500	0.28991900	-0.23253500
C	-2.58294300	-0.40721500	-0.03029800
N	-3.09762500	-1.53969000	-0.55387100
C	-4.76607500	-0.56061100	0.48920500
C	-4.44257900	-1.65527400	-0.24294300
H	-5.69751700	-0.24343700	0.93965500
H	-5.03132900	-2.50161900	-0.57156300
N	-3.60885500	0.19305500	0.60571200
C	2.24309500	-1.77125700	-0.91639300
H	2.96388400	-1.31416800	-1.60252000
H	2.53942700	-2.81458500	-0.76614800
H	1.22783600	-1.76301500	-1.34108700
C	1.59085500	1.97401500	-1.46507500
C	2.90087100	2.08136200	-1.89792400
H	3.66900400	1.45772800	-1.43133300
C	0.50319000	2.82294500	-2.08248600
H	-0.08463900	2.20164700	-2.77996200
H	-0.19841100	3.13230800	-1.29308700
C	-3.47932800	1.43687100	1.31449300
C	-3.78089100	2.61944500	0.63081100
C	-3.02147200	1.40312200	2.63498300
C	-3.63329500	3.81677500	1.32884100
C	-2.89210900	2.62647200	3.29377200
C	-3.19703800	3.81912000	2.64946300
H	-3.86680900	4.75528500	0.82721100
H	-2.54590500	2.63535700	4.32662500
H	-3.09350200	4.76260400	3.18212400
C	-2.30087900	-2.49346000	-1.27618200
C	-1.80219400	-3.59376000	-0.57285800
C	-2.01872900	-2.24424600	-2.62373700
C	-0.96988300	-4.47054200	-1.26851000
C	-1.18647300	-3.15139200	-3.27883600
C	-0.66358400	-4.25110900	-2.60596300
H	-0.55604000	-5.33051500	-0.74334400
H	-0.95473300	-2.99224400	-4.33157700
H	-0.01663900	-4.94924200	-3.13435400
C	3.02788700	-2.69537800	2.41294300
H	2.65626300	-3.24955100	3.28063200
H	3.42293700	-3.38974700	1.66475300
H	3.79003600	-1.96661100	2.70595800
C	-2.14696100	-3.81635500	0.86757700
H	-3.19811900	-4.11334400	0.99192100
H	-1.52248200	-4.60599700	1.29748700
H	-1.98524500	-2.90852600	1.46486800
C	-2.57280900	-1.04473500	-3.33317700
H	-3.63900800	-0.89198100	-3.11786600
H	-2.05357200	-0.12147400	-3.03071800
H	-2.45935500	-1.14732700	-4.41810000
C	-4.22305100	2.59505400	-0.80161200
H	-5.15262000	2.02560800	-0.93908400
H	-4.39871100	3.61027000	-1.17351500

H	-3.46617200	2.12480500	-1.44846600
C	-2.65002400	0.11454000	3.30537300
H	-3.37932600	-0.68303100	3.10943500
H	-1.67062300	-0.24958000	2.95695100
H	-2.58031100	0.24752300	4.39056700
C	3.32423300	2.97241000	-2.99393100
H	3.94752100	3.75150200	-2.51119100
H	4.03604200	2.43732600	-3.64133700
C	1.06932100	4.03305000	-2.81560700
C	2.17498800	3.60448800	-3.76994800
H	1.47335400	4.75203400	-2.08470700
H	0.26704900	4.55234900	-3.35371300
H	2.54465300	4.45184500	-4.35941800
H	1.77491800	2.87334000	-4.48950300

INT5b

Zero-point correction= 0.703192 (Hartree/Particle)
Thermal correction to Energy= 0.748161
Thermal correction to Enthalpy= 0.749105
Thermal correction to Gibbs Free Energy= 0.622305
Sum of electronic and zero-point Energies= -2296.970130
Sum of electronic and thermal Energies= -2296.925162
Sum of electronic and thermal Enthalpies= -2296.924218
Sum of electronic and thermal Free Energies= -2297.051018

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.56841891

Cartesian coordinates:

C	-4.02086000	-1.73534300	0.49037400
C	-5.47742600	-1.24393900	0.28308100
C	-3.46007300	-0.82621600	1.55516300
O	-5.65305200	-0.11742100	-0.12718600
H	-4.04019600	-2.75250800	0.91595000
C	-3.98140800	-1.03459200	2.93828100
H	-3.42773000	-0.41958900	3.65338900
H	-5.04450200	-0.75120100	2.99033000
H	-3.91899400	-2.09042600	3.23261200
C	-6.58663500	-2.19394500	0.60429400
H	-7.55717900	-1.71809200	0.44045200
H	-6.50296200	-3.09185200	-0.02411900
H	-6.50835200	-2.53965100	1.64476300
C	-1.21534900	-0.68369900	-0.37656800
C	-2.02472000	0.36746500	0.17885100
Au	0.82041500	-0.27261100	-0.16257500
N	-2.66962100	0.16318400	1.35928100
C	4.62531500	1.58521000	0.24062700
C	5.00645100	0.31502600	0.52091300
H	5.18162300	2.51270400	0.20451400
H	5.96767800	-0.10830600	0.78171500
N	3.26547600	1.54041500	-0.02273900
N	3.86885700	-0.47169700	0.41997400
C	2.79647000	0.27701600	0.08714200
C	-1.83082900	-1.78714700	-0.84968300
N	-2.08287700	1.59310100	-0.35261700
C	-1.43962000	1.88597200	-1.63791200
H	-0.36921700	2.09392300	-1.49828600
H	-1.56486000	1.01973400	-2.29253600
H	-1.92281800	2.76155100	-2.07576300
S	-2.58794000	3.00535200	0.61344800
O	-1.75413100	3.02749700	1.79634500

O	-2.56510700	4.08725500	-0.34978100
C	-3.35481700	-1.77942100	-0.91645300
C	3.80523800	-1.88559600	0.66698400
C	3.88604700	-2.75849800	-0.42176800
C	3.63383300	-2.31385200	1.98710300
C	3.80648800	-4.12473200	-0.15178000
C	3.55999600	-3.68824300	2.20924300
C	3.64801000	-4.58488000	1.15034300
H	3.87577100	-4.83188200	-0.97773600
H	3.43156700	-4.05393000	3.22739100
H	3.59440000	-5.65487600	1.34244200
C	2.43412500	2.65744500	-0.38109700
C	2.41560500	3.05811900	-1.72253900
C	1.64733400	3.25404700	0.61022900
C	1.56989300	4.11274800	-2.06595000
C	0.81172000	4.30175400	0.21777700
C	0.77266100	4.72646500	-1.10488200
H	1.53570100	4.44746300	-3.10232100
H	0.17611500	4.77663600	0.96399800
H	0.10292500	5.53652400	-1.38809000
C	-4.28373600	2.65082600	1.03328800
H	-4.30251200	2.07263200	1.95993600
H	-4.75586100	3.62975100	1.16935700
H	-4.76331100	2.10036800	0.21692700
C	1.66048600	2.76996800	2.02880600
H	2.67012200	2.50400600	2.36949000
H	1.25780700	3.53353900	2.70279800
H	1.02968500	1.87448500	2.14513900
C	3.25044100	2.35743500	-2.75195300
H	4.32629400	2.49654100	-2.57727700
H	3.06614200	1.27256100	-2.74906200
H	3.02960600	2.73460200	-3.75628400
C	3.51713100	-1.32906300	3.11120800
H	4.43686400	-0.74219800	3.24289000
H	2.70401900	-0.60949500	2.93301500
H	3.31358600	-1.83987100	4.05843100
C	4.02771600	-2.24680600	-1.82365700
H	3.09382100	-1.78118300	-2.17455800
H	4.81398200	-1.48450900	-1.91011700
H	4.27173700	-3.06142100	-2.51425800
C	-4.00047400	-2.92680000	-1.71874000
C	-3.04824400	-3.57425500	-2.71110600
C	-1.83731000	-4.09662100	-1.95274600
C	-1.01986500	-2.93063600	-1.41335000
H	-4.90772100	-2.55540800	-2.21775600
H	-3.56519200	-4.38357400	-3.24219700
H	-2.18392100	-4.74258400	-1.12907900
H	-0.28800700	-3.26075600	-0.65832300
H	-4.33115400	-3.72049900	-1.02657500
H	-2.72910100	-2.84709900	-3.47621900
H	-1.20351500	-4.72454400	-2.59134200
H	-0.41341900	-2.52044000	-2.23774600
H	-3.64077700	-0.83546500	-1.41109100

INT6b

Zero-point correction= 0.705024 (Hartree/Particle)
Thermal correction to Energy= 0.748908
Thermal correction to Enthalpy= 0.749852
Thermal correction to Gibbs Free Energy= 0.628715

Sum of electronic and zero-point Energies= -2296.986929
Sum of electronic and thermal Energies= -2296.943045
Sum of electronic and thermal Enthalpies= -2296.942100
Sum of electronic and thermal Free Energies= -2297.063237
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.59164396
Cartesian coordinates:

C	1.66798800	-0.87540000	0.51948700
C	1.26002900	-1.79658900	-0.49876700
N	1.37335800	-1.69060800	-1.84580200
S	0.22573700	-2.60445300	-2.85831100
O	-1.09772100	-2.46968500	-2.27896200
O	0.49518400	-2.12756400	-4.20067200
Au	-0.23762600	0.25685400	0.26081200
C	-1.94267300	1.37860100	0.14612900
N	-3.20517300	0.96697500	0.37658500
C	-3.35034200	3.10299100	-0.13511200
C	-4.09192000	2.01786200	0.20587900
H	-3.63163000	4.12323700	-0.36146800
H	-5.15836500	1.89090300	0.33912900
N	-2.02779200	2.68758500	-0.16475500
N	0.62797800	-2.93731600	0.00502500
C	0.68638400	-2.87321100	1.29348300
C	2.84105400	-2.20271400	2.30131000
C	1.45809500	-1.69941400	1.80512200
C	0.07782300	-3.88753900	2.17781000
H	0.82877300	-4.30405100	2.86367800
H	-0.70372300	-3.42086500	2.79440600
H	-0.36915200	-4.69647100	1.59340300
O	3.41264500	-3.07710900	1.69519300
C	3.39474800	-1.51982500	3.51172000
H	4.39360400	-1.90335600	3.73627700
H	3.44111200	-0.43471700	3.34038900
H	2.73289700	-1.67770700	4.37470300
C	1.90498600	-0.47260600	-2.45857800
H	1.41941200	0.41561500	-2.02070500
H	2.98315500	-0.40469700	-2.29165200
H	1.70161600	-0.50741900	-3.53003100
H	0.94108300	-1.16552000	2.61732500
C	-0.85994700	3.46642300	-0.48512300
C	-0.19115600	4.11904100	0.55550000
C	-0.39851500	3.45042900	-1.80605700
C	0.99432800	4.78281600	0.23813100
C	0.79486700	4.12255500	-2.07442500
C	1.48618000	4.77928400	-1.06232900
H	1.53300100	5.30670600	1.02721100
H	1.17619400	4.13373800	-3.09486000
H	2.41223600	5.30362800	-1.29181200
C	-3.48852200	-0.40372200	0.71708500
C	-3.66424500	-1.31429900	-0.32932600
C	-3.43373400	-0.77489200	2.06487800
C	-3.76380400	-2.66374700	0.01058200
C	-3.55652800	-2.13269400	2.35685900
C	-3.70540900	-3.06879900	1.33777100
H	-3.88579600	-3.39763200	-0.78471100
H	-3.53687700	-2.45340200	3.39854800
H	-3.79076700	-4.12588700	1.58453300
C	0.82204600	-4.26985800	-2.72294100
H	1.85749000	-4.28598100	-3.07388700
H	0.73362600	-4.59541700	-1.68480200

H	0.18789400	-4.86785700	-3.38612000
C	-3.22456400	0.23999700	3.14818600
H	-3.96204000	1.05250100	3.10242400
H	-3.30450000	-0.22370300	4.13753200
H	-2.23133400	0.70898700	3.07689800
C	-3.71704300	-0.86752300	-1.75738100
H	-4.36786400	0.00585500	-1.89493500
H	-2.71599700	-0.60708400	-2.12623100
H	-4.08615200	-1.67357900	-2.40026700
C	-0.70949500	4.08399100	1.96109400
H	-1.73752200	4.46390500	2.03338200
H	-0.72092300	3.05915700	2.36164300
H	-0.08365000	4.69302500	2.62220500
C	-1.13971400	2.72083900	-2.88537800
H	-1.09407200	1.63048600	-2.74204200
H	-2.20377500	2.99122100	-2.91237400
H	-0.71337100	2.94185400	-3.86974100
C	2.84313500	0.04887500	0.45107700
C	4.02726100	-0.38215400	-0.01230400
C	2.66182300	1.45853800	0.96181000
C	5.23938800	0.48646100	-0.14943800
C	3.98548000	2.17773300	1.18619500
H	2.05132100	2.03225800	0.23697900
C	4.89856300	1.96510800	-0.01233900
H	5.98423200	0.19335100	0.61010800
H	4.47764300	1.78404000	2.09139700
H	5.81439700	2.56342600	0.07142700
H	5.72474400	0.28597200	-1.11667700
H	4.37536700	2.30781900	-0.92233900
H	3.80554500	3.24620500	1.36616800
H	2.05945700	1.44710400	1.88910000
H	4.12454300	-1.42679700	-0.32086600

TS1b

Zero-point correction= 0.699321 (Hartree/Particle)
Thermal correction to Energy= 0.745061
Thermal correction to Enthalpy= 0.746005
Thermal correction to Gibbs Free Energy= 0.616052
Sum of electronic and zero-point Energies= -2296.900019
Sum of electronic and thermal Energies= -2296.854280
Sum of electronic and thermal Enthalpies= -2296.853335
Sum of electronic and thermal Free Energies= -2296.983289
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.49198979
Cartesian coordinates:

C	1.40643000	0.41153700	-0.36940800
C	1.97221700	-0.72684900	-0.10248100
N	1.82819600	-2.04128400	0.01277800
S	1.71575600	-2.69108500	1.61445900
O	1.67470500	-1.55405100	2.51354900
O	0.66437900	-3.69185000	1.58207800
Au	-0.68965900	0.15005100	-0.23015500
C	-2.72878300	0.03691400	-0.03593300
N	-3.53321000	-1.03509800	-0.18747100
C	-4.86222400	0.62410900	0.37686900
C	-4.85369900	-0.69485000	0.06252700
H	-5.66777900	1.29694300	0.64051100
H	-5.65024200	-1.42419100	-0.00561100
N	-3.54610000	1.05479800	0.30927400
N	3.94509900	-0.47091200	0.19939600

C	5.90775500	0.59530400	0.26143200
C	5.92713800	-0.30230500	-0.76339900
C	1.34441700	-2.86306300	-1.10625200
H	1.82297300	-2.50035300	-2.02005700
H	1.61796000	-3.91094700	-0.94567900
H	0.25092500	-2.78938100	-1.19410300
C	4.62200400	0.46152400	0.83859300
C	4.01348000	1.20139000	1.97102500
H	3.10652800	0.69752700	2.32418800
H	4.72080400	1.29168300	2.80280100
H	3.74726400	2.21712700	1.64607400
O	4.74707500	-0.94866100	-0.81794800
C	6.94363000	-0.69049600	-1.76308900
H	7.84671900	-0.08624700	-1.63949600
H	7.21497400	-1.74788200	-1.65580600
H	6.56432600	-0.54920600	-2.78241200
H	6.70391500	1.25951100	0.57200200
C	-3.06972100	2.38709500	0.56431000
C	-2.92071300	3.25795000	-0.51940000
C	-2.72774100	2.72648400	1.87758500
C	-2.41391100	4.53055000	-0.25250400
C	-2.22584000	4.00900000	2.09680600
C	-2.07085700	4.90233800	1.04247600
H	-2.29360400	5.23501000	-1.07507900
H	-1.95550900	4.30495000	3.10977800
H	-1.68402300	5.90192500	1.23342500
C	-3.04864300	-2.33386900	-0.56856300
C	-2.51322000	-3.16259900	0.42179000
C	-3.09643900	-2.67964300	-1.92397700
C	-2.01614000	-4.40230000	0.01422000
C	-2.59308700	-3.92891900	-2.28280500
C	-2.06004200	-4.78239000	-1.32147100
H	-1.58356000	-5.06466700	0.76217800
H	-2.62225700	-4.23097200	-3.32923600
H	-1.67576100	-5.75675600	-1.61859100
C	3.28707700	-3.50901300	1.77256200
H	3.32136200	-3.96177700	2.76865000
H	3.36389700	-4.28437700	1.00431700
H	4.07494200	-2.75887200	1.65751800
C	-2.44524300	-2.73303600	1.85604200
H	-3.36046700	-2.21901000	2.17949300
H	-2.28322300	-3.59457300	2.51228600
H	-1.60415500	-2.04268900	2.02426600
C	-3.65180300	-1.73433700	-2.94636800
H	-4.72641600	-1.55489800	-2.80245200
H	-3.15649700	-0.75314900	-2.89961500
H	-3.51772000	-2.13115200	-3.95842500
C	-3.25056900	2.83060100	-1.91773400
H	-4.20842400	2.29681000	-1.97706000
H	-3.30391600	3.69492500	-2.58867300
H	-2.48110500	2.15041600	-2.31449500
C	-2.87165400	1.73850500	2.99531800
H	-3.90385800	1.37591300	3.09584300
H	-2.23833200	0.85367600	2.83202400
H	-2.58135000	2.18537600	3.95211300
C	1.92566400	1.74875600	-0.62833200
C	2.95256600	1.95860100	-1.47076700
C	1.19654600	2.88625700	0.04897200
C	3.47396900	3.31759100	-1.81990900

C	1.96544200	4.19832500	-0.02964600
H	0.19980400	3.00571200	-0.41676000
C	2.49768700	4.42412800	-1.43741400
H	4.43932200	3.47179000	-1.30184300
H	2.81287600	4.17929200	0.67771800
H	2.98163600	5.40538500	-1.52430800
H	0.99018500	2.61647100	1.09817400
H	1.31622400	5.02558100	0.28763700
H	1.65346500	4.42283400	-2.14562000
H	3.71239800	3.36249700	-2.89255200
H	3.42529700	1.09728000	-1.94793800

TS2b

Zero-point correction= 0.702144 (Hartree/Particle)
Thermal correction to Energy= 0.744789
Thermal correction to Enthalpy= 0.745733
Thermal correction to Gibbs Free Energy= 0.627064
Sum of electronic and zero-point Energies= -2296.876153
Sum of electronic and thermal Energies= -2296.833508
Sum of electronic and thermal Enthalpies= -2296.832563
Sum of electronic and thermal Free Energies= -2296.951232
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.47196195
Cartesian coordinates:

C	1.35116200	0.60379600	-0.40855900
C	2.01359600	-0.48281700	-0.14738100
Au	-0.70480400	0.14313000	-0.25065900
C	5.76638900	0.76397200	0.43600000
C	5.79834200	-0.09578600	-0.70244600
C	4.49091600	0.71888300	0.88883300
N	4.63022000	-0.64295600	-0.93760000
O	3.79556800	-0.13001400	0.07398700
H	6.58986400	1.32469000	0.86007300
C	6.95406800	-0.40967100	-1.58111500
H	7.36662000	0.50722100	-2.01845000
H	7.75748500	-0.89042600	-1.01015800
H	6.64938100	-1.07942200	-2.39082100
C	3.76173600	1.33384700	2.01508800
H	3.09931600	2.13150900	1.65138900
H	3.13855600	0.59283500	2.53324500
H	4.47165800	1.76966000	2.72422000
C	-4.88255700	0.15921800	0.48349200
C	-4.73525500	-1.15439500	0.18131600
H	-5.74946200	0.73983900	0.77099500
H	-5.44570000	-1.96994600	0.14859500
C	-2.71282400	-0.18794900	-0.00273400
N	-3.39412700	-1.34623300	-0.11519700
N	-3.62730200	0.73542900	0.36402500
N	2.00528400	-1.80154100	-0.05679200
S	2.02556000	-2.51984200	1.51479400
O	1.77167300	-1.44332000	2.45424600
O	1.18202700	-3.69680100	1.43580700
C	1.76173500	-2.67361500	-1.21712100
H	2.07261100	-2.12379800	-2.10870300
H	2.35813900	-3.58870800	-1.13579400
H	0.69741200	-2.93920100	-1.27453200
C	1.75408300	1.98134000	-0.67142000
C	2.81190000	2.27463300	-1.44981700
H	3.40643400	1.45732900	-1.86411100
C	3.72229100	-3.03631900	1.66613400

H	4.36182400	-2.14815200	1.67039100
H	3.81076200	-3.58025000	2.61214100
H	3.97427900	-3.69399500	0.82851900
C	-2.78011800	-2.58722200	-0.50304100
C	-2.86141800	-2.96570300	-1.84835200
C	-2.09533400	-3.32654000	0.46606400
C	-2.23833000	-4.15660600	-2.21667000
C	-1.48628700	-4.51233900	0.04981100
C	-1.56041300	-4.92471300	-1.27480800
H	-2.28885700	-4.48053400	-3.25559400
H	-0.93815600	-5.10214400	0.78231900
H	-1.08492500	-5.85574400	-1.57838100
C	-3.29014800	2.11261400	0.60399400
C	-2.89848700	2.48128600	1.89517100
C	-3.31455200	3.00079000	-0.47603900
C	-2.52932600	3.81138800	2.09579900
C	-2.93657800	4.32079600	-0.22769200
C	-2.54897600	4.72241600	1.04558600
H	-2.22656700	4.13044600	3.09242800
H	-2.95274700	5.03770000	-1.04788500
H	-2.26436600	5.75813500	1.22296300
C	-3.70206300	2.54600600	-1.85002500
H	-2.96846000	1.83365800	-2.25786700
H	-4.67723000	2.04014900	-1.86016800
H	-3.75950500	3.39483600	-2.54002900
C	-3.57565700	-2.11283800	-2.85268500
H	-4.65699700	-2.06679800	-2.66207200
H	-3.20610100	-1.07668900	-2.83723100
H	-3.43752900	-2.50593800	-3.86568700
C	-1.98517800	-2.86253100	1.88684300
H	-2.92714600	-2.43979100	2.26188800
H	-1.69479900	-3.69128000	2.54150000
H	-1.21115900	-2.08503900	1.99410300
C	-2.85501100	1.48258500	3.01162200
H	-3.82406900	0.98702500	3.16147300
H	-2.11814100	0.68894900	2.81534500
H	-2.58005600	1.96595500	3.95533400
C	0.86318800	3.05664600	-0.09294200
H	-0.09441900	3.06101200	-0.64637600
H	0.59003000	2.79726400	0.94423300
C	1.50177000	4.43733600	-0.15585100
H	0.75015900	5.19982100	0.09011100
H	2.29435900	4.52036700	0.60761900
C	2.10448500	4.68119400	-1.53181300
H	2.49556000	5.70300200	-1.61752300
H	1.31559800	4.57892400	-2.29436100
C	3.20884800	3.66956000	-1.81634200
H	3.50746800	3.70505700	-2.87429400
H	4.12076800	3.93527600	-1.25022200

TS3b

Zero-point correction= 0.700295 (Hartree/Particle)
Thermal correction to Energy= 0.745385
Thermal correction to Enthalpy= 0.746329
Thermal correction to Gibbs Free Energy= 0.619480
Sum of electronic and zero-point Energies= -2296.885135
Sum of electronic and thermal Energies= -2296.840045
Sum of electronic and thermal Enthalpies= -2296.839101
Sum of electronic and thermal Free Energies= -2296.965950

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.47677132
Cartesian coordinates:

C	2.06260300	0.26891100	-0.38793500
C	1.28903300	-0.76213900	-0.41056500
Au	-0.72323300	-0.10003100	-0.39604800
C	6.23153100	-0.19635800	-0.24444600
C	5.83109400	-0.79207500	-1.40309500
C	5.03961400	-0.01684800	0.49838600
O	4.49751800	-0.96766600	-1.37957100
N	4.01289800	-0.49479600	-0.17774700
H	7.23905700	0.07062300	0.04753000
N	1.55985200	-2.11629800	-0.19629700
C	4.83414400	0.62682900	1.81986900
H	4.78400200	1.71895400	1.70149700
H	3.89841700	0.28029700	2.27315200
H	5.66528000	0.40639100	2.49831700
C	6.54303800	-1.27187300	-2.60610300
H	6.13705400	-0.80792800	-3.51305900
H	7.60821100	-1.03352200	-2.53718100
H	6.43640300	-2.35803100	-2.71708600
S	1.77567400	-2.52439700	1.46386100
O	2.09798200	-1.30440800	2.18644600
O	0.64891200	-3.34972200	1.87710800
C	0.71123100	-3.07086700	-0.92349700
H	1.10965000	-4.08308500	-0.79448400
H	-0.33387500	-3.05646600	-0.58090500
H	0.76099600	-2.81269800	-1.98536100
C	2.21749600	1.68391400	-0.23366600
C	3.05779800	2.36225100	-1.04235200
H	3.62304300	1.80499800	-1.79337600
C	1.43711900	2.36284200	0.87389700
H	0.38138200	2.45881300	0.55739400
H	1.42744800	1.70572500	1.75739800
C	3.22852300	-3.54791600	1.38105800
H	4.05493500	-2.93731300	1.00573400
H	3.42985100	-3.90499300	2.39611100
H	3.03580000	-4.39701200	0.71876300
C	-2.72455000	0.26188100	-0.09918400
N	-3.36774700	1.42429000	0.13871000
C	-4.90131000	-0.14372600	0.30414100
C	-4.71352300	1.19580900	0.38865900
H	-5.78435800	-0.75651300	0.42944100
H	-5.39608400	2.00814700	0.60204800
N	-3.66767400	-0.69902300	0.00423800
C	-3.38545900	-2.10300800	-0.13873000
C	-2.83623200	-2.78737000	0.95135600
C	-3.63710200	-2.70224000	-1.37841000
C	-2.54461500	-4.14121000	0.77251700
C	-3.33507200	-4.05678100	-1.50735700
C	-2.79679900	-4.76974900	-0.44070200
H	-2.10824400	-4.69774500	1.60073900
H	-3.52544500	-4.55317800	-2.45828000
H	-2.57004800	-5.82788300	-0.55835900
C	-2.71674600	2.70438300	0.19131900
C	-2.57704900	3.43263700	-0.99406400
C	-2.23838200	3.14855300	1.42890500
C	-1.93499000	4.66882200	-0.91351200
C	-1.61516400	4.39635100	1.46347200
C	-1.46531400	5.14924600	0.30404000

H	-1.81689400	5.26313200	-1.81895300
H	-1.24787200	4.77733000	2.41639600
H	-0.97921700	6.12277400	0.35060200
C	-3.09017200	2.90021400	-2.29759100
H	-4.15352500	2.63034100	-2.24015600
H	-2.97584900	3.64203000	-3.09518000
H	-2.54795700	1.99350100	-2.60315500
C	-2.35548600	2.30136900	2.65953000
H	-3.38596400	1.96736300	2.84158700
H	-1.73807500	1.39369300	2.57623900
H	-2.02054300	2.85057100	3.54605100
C	-2.52756000	-2.10280400	2.24847300
H	-3.28712300	-1.35766000	2.52092100
H	-2.45119800	-2.83176400	3.06243300
H	-1.55672100	-1.58492300	2.19752500
C	-4.18985400	-1.91062000	-2.52517900
H	-5.20536800	-1.54254800	-2.32332000
H	-3.56901100	-1.02870000	-2.74211800
H	-4.23580800	-2.52052200	-3.43371400
C	3.28669200	3.83180100	-0.94654100
H	3.31451000	4.26159900	-1.95878600
H	4.30143200	3.99914100	-0.54109900
C	2.24537100	4.52926000	-0.07875600
H	1.29764500	4.60622600	-0.63690400
H	2.56714500	5.55452500	0.14428600
C	1.99924900	3.73955100	1.19973800
H	1.30436700	4.27502000	1.86084300
H	2.94566100	3.63499200	1.75623800

TS4b

Zero-point correction= 0.699250 (Hartree/Particle)
Thermal correction to Energy= 0.744260
Thermal correction to Enthalpy= 0.745204
Thermal correction to Gibbs Free Energy= 0.618534
Sum of electronic and zero-point Energies= -2296.860025
Sum of electronic and thermal Energies= -2296.815015
Sum of electronic and thermal Enthalpies= -2296.814071
Sum of electronic and thermal Free Energies= -2296.940741
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.45236939
Cartesian coordinates:

C	2.20767100	0.85580600	-0.43218200
C	1.54226700	-0.22959100	-0.08766000
C	5.48949000	-0.62081000	-1.01716000
C	5.72681000	-0.10625200	0.29826000
N	2.25086700	-1.45611800	0.19238100
O	3.82587600	0.62476500	-0.50066300
C	1.94288300	-2.49408100	-0.80705500
H	0.87365000	-2.75773100	-0.82051700
H	2.24025500	-2.10427400	-1.78525400
H	2.53615500	-3.39205800	-0.60001600
S	1.92901900	-1.96479900	1.79720500
O	2.03960600	-0.76641300	2.61910400
O	0.73809300	-2.80186200	1.87186700
C	4.65600300	0.65290500	0.60884100
N	4.35099700	-0.22266300	-1.51813500
C	4.22725100	1.47634400	1.75196600
H	3.33404500	1.04243400	2.22424900
H	5.03100400	1.51910200	2.49275400

H	3.98958100	2.49793500	1.42607700
H	6.60170000	-0.27311700	0.91413300
C	6.37260400	-1.50493200	-1.81932000
H	7.33865900	-1.01943400	-2.00168400
H	6.57033000	-2.44051600	-1.28264800
H	5.91041300	-1.73892400	-2.78281400
C	3.35036800	-2.99268200	2.10689900
H	4.25471200	-2.40126800	1.93951000
H	3.28068000	-3.30051400	3.15516100
H	3.32672200	-3.87731800	1.46489300
Au	-0.54400000	-0.17283300	-0.09174200
C	-2.60516900	-0.25489600	-0.11564800
N	-3.33720100	-1.36223200	-0.36617700
C	-4.80208800	0.23329000	0.00079300
C	-4.69257500	-1.08389300	-0.29853000
H	-5.66398000	0.87033200	0.15104100
H	-5.43894900	-1.84930000	-0.46632100
N	-3.50836800	0.72398400	0.10706800
C	-3.16448600	2.07747000	0.44351500
C	-3.00226900	3.00353100	-0.59206100
C	-3.00006300	2.39847600	1.79494200
C	-2.69375700	4.31641100	-0.23423000
C	-2.68536300	3.72165700	2.10530000
C	-2.54543300	4.67328300	1.10169800
H	-2.57633700	5.06532300	-1.01745200
H	-2.56034000	4.00437800	3.14985100
H	-2.31886900	5.70588300	1.36338100
C	-2.74764100	-2.64329500	-0.64720300
C	-2.33883600	-3.43449500	0.43015200
C	-2.56608500	-3.00638300	-1.98616000
C	-1.72327500	-4.65018000	0.12881000
C	-1.95287300	-4.23227900	-2.23833600
C	-1.53477600	-5.04571800	-1.18967700
H	-1.38847300	-5.28623100	0.94724000
H	-1.80304700	-4.54734400	-3.27050500
H	-1.06004400	-6.00156700	-1.40465000
C	-2.51838800	-2.98314900	1.84697700
H	-3.51359600	-2.55305100	2.02425600
H	-2.37797300	-3.81884700	2.54109600
H	-1.77170100	-2.21914800	2.10874000
C	-2.99491400	-2.09992400	-3.10029600
H	-4.07904200	-1.92096400	-3.09432800
H	-2.50969800	-1.11520100	-3.02610700
H	-2.73622700	-2.52880900	-4.07440800
C	-3.11741300	2.59451100	-2.02936700
H	-4.03620700	2.02746400	-2.23069500
H	-3.11195100	3.47048200	-2.68739100
H	-2.27590300	1.94903000	-2.32481400
C	-3.13778700	1.35561400	2.86228000
H	-4.09355700	0.81801400	2.79529200
H	-2.34169100	0.60020700	2.78538800
H	-3.07506000	1.80506000	3.85903800
C	1.94589900	2.25925300	-0.69117900
C	0.86519400	2.91095000	0.14734600
C	2.66685800	2.95573600	-1.58945500
C	1.02102600	4.42503600	0.16276800
H	-0.13289400	2.64862000	-0.24840600
C	2.45129900	4.40386400	-1.88475500
H	3.46020600	2.44979800	-2.14312900

C	1.17256700	4.94726500	-1.25807800
H	0.15310800	4.87615400	0.66143400
H	2.45139800	4.55192200	-2.97486100
H	0.30369700	4.61757300	-1.85236200
H	1.17597700	6.04434700	-1.28303600
H	3.32590200	4.97201200	-1.52166400
H	1.91092200	4.70106600	0.75373200
H	0.89545500	2.49330700	1.16652200

TS5b

Zero-point correction= 0.699498 (Hartree/Particle)
Thermal correction to Energy= 0.744525
Thermal correction to Enthalpy= 0.745469
Thermal correction to Gibbs Free Energy= 0.619445
Sum of electronic and zero-point Energies= -2296.911089
Sum of electronic and thermal Energies= -2296.866063
Sum of electronic and thermal Enthalpies= -2296.865118
Sum of electronic and thermal Free Energies= -2296.991143
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.50217198
Cartesian coordinates:

C	-5.36857400	-0.22125600	0.91908900
C	-5.73854900	0.67535200	-0.07776000
C	-3.98883600	-0.16113200	1.07876000
N	-3.40209400	0.71062400	0.26313000
O	-4.75658000	1.29041100	-0.64128400
H	-6.04147400	-0.81080000	1.52924400
C	-7.12091600	1.01375400	-0.50939200
H	-7.22877200	0.86359500	-1.58984700
H	-7.85867600	0.40052900	0.01619800
H	-7.32543000	2.07232900	-0.30821900
C	-3.17798100	-0.92608200	2.06408100
H	-2.75456600	-1.81256300	1.57100100
H	-2.35100800	-0.31229000	2.44008300
H	-3.80856500	-1.26176600	2.89296700
C	-1.42424000	-0.23856400	-0.67606200
C	-2.15849300	0.86118200	-0.25108000
N	-1.65469700	2.17724900	-0.20623800
S	-1.43023200	2.87925600	1.31873700
O	-1.46350000	1.80993800	2.30913600
O	-0.29094500	3.77648800	1.22010300
Au	0.62591400	-0.20331700	-0.37704200
C	2.63341700	-0.29674100	0.10417900
N	3.59163600	0.64510000	-0.01073600
C	4.58026000	-1.08812800	0.91520900
C	4.79946500	0.17889100	0.48402700
H	5.23658000	-1.81772100	1.37134200
H	5.68896700	0.79537800	0.48265100
N	3.24313000	-1.36098100	0.67103300
C	-0.85630300	2.71597700	-1.30996900
H	-1.21133900	2.24565500	-2.23195000
H	-1.01207200	3.79826200	-1.38360900
H	0.21969500	2.52585600	-1.19142500
C	-2.05744000	-1.47129600	-1.08798600
C	-3.19241000	-1.46078400	-1.83126400
H	-3.65301700	-0.50007600	-2.07075000
C	-1.35461800	-2.77266600	-0.76436800
H	-0.46710200	-2.87469000	-1.41414200
H	-0.95039500	-2.73692400	0.26169000
C	2.54568800	-2.57524800	0.99514100

C	2.57463200	-3.62352100	0.06895900
C	1.82541800	-2.62907700	2.19315100
C	1.85744300	-4.77760700	0.38181000
C	1.12468500	-3.80543100	2.46516500
C	1.14129800	-4.86906900	1.57039100
H	1.86687100	-5.61268700	-0.31804600
H	0.56565500	-3.88259300	3.39742600
H	0.59488100	-5.78130100	1.80378600
C	3.33747200	1.96365400	-0.52642500
C	2.83849300	2.92714600	0.35556400
C	3.55722900	2.19999900	-1.88741100
C	2.55700800	4.18847900	-0.17146100
C	3.26787900	3.47643100	-2.36732800
C	2.77280200	4.46019800	-1.51700100
H	2.15442400	4.95509500	0.48824200
H	3.43461700	3.69587400	-3.42142300
H	2.55415700	5.45183100	-1.90932800
C	-2.89647100	3.86994700	1.51159200
H	-2.83472400	4.37228900	2.48210800
H	-2.92156200	4.60705900	0.70306100
H	-3.77271900	3.21621100	1.46667100
C	2.59059700	2.60842100	1.79850300
H	3.44482600	2.09380000	2.26006100
H	2.38807100	3.51997400	2.36948100
H	1.71127500	1.95668500	1.91518500
C	4.06313100	1.11769700	-2.79260000
H	5.03432800	0.72314500	-2.46364100
H	3.36825300	0.26554300	-2.82649400
H	4.18549600	1.48967200	-3.81551500
C	3.31721600	-3.49365800	-1.22613400
H	4.38220300	-3.27212700	-1.07467400
H	3.24961400	-4.41764900	-1.81036200
H	2.90746800	-2.67683200	-1.83923700
C	1.76604700	-1.46099600	3.13119700
H	2.73342000	-0.95117400	3.22926500
H	1.04426600	-0.70626300	2.77911900
H	1.44842000	-1.77876200	4.13058300
C	-2.27118100	-3.97542800	-0.94121500
H	-1.69530700	-4.90294700	-0.82480500
H	-3.03695900	-3.97908400	-0.14604300
C	-3.84145000	-2.68112800	-2.39275800
H	-4.78481100	-2.84483300	-1.83856900
C	-2.95765600	-3.91975500	-2.29814000
H	-2.19076700	-3.88129600	-3.08777200
H	-3.55255900	-4.82314700	-2.48164500
H	-4.15313500	-2.49330100	-3.43086200

TS6b

Zero-point correction= 0.699328 (Hartree/Particle)
Thermal correction to Energy= 0.743607
Thermal correction to Enthalpy= 0.744551
Thermal correction to Gibbs Free Energy= 0.619314
Sum of electronic and zero-point Energies= -2296.910165
Sum of electronic and thermal Energies= -2296.865887
Sum of electronic and thermal Enthalpies= -2296.864942
Sum of electronic and thermal Free Energies= -2296.990179
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.49952571
Cartesian coordinates:

C	5.89309300	0.09581500	0.99386300
C	5.93918000	0.06440500	-0.43004000
C	4.64752600	0.42988200	1.43870200
N	3.68755200	0.73181700	0.52031400
O	4.86187800	0.30532500	-1.01574000
H	6.74770600	-0.04848200	1.64617400
C	7.18579000	-0.22236200	-1.20251800
H	7.26139500	0.45762800	-2.05740800
H	8.08232000	-0.14142300	-0.58012500
H	7.13367800	-1.24296600	-1.60365300
C	4.29271900	0.66362600	2.87073500
H	4.18187300	1.74198500	3.04428200
H	3.33211600	0.20264800	3.13209300
H	5.08729300	0.28939200	3.52363400
C	1.42477700	0.90437500	-0.22585600
C	2.53242700	0.16369100	0.29396200
N	2.42988600	-1.25891600	0.49974200
S	1.57398800	-1.82770700	1.83915300
O	1.35451500	-0.68635300	2.71932400
O	0.46065600	-2.65971100	1.40527700
Au	-0.46289800	0.06918100	-0.27622400
C	-2.40311800	-0.64590100	-0.41406200
N	-2.87248900	-1.82031600	-0.88365000
C	-4.65246500	-0.67412700	-0.28606400
C	-4.25616500	-1.85934600	-0.81268800
H	-5.63363800	-0.28107300	-0.05413500
H	-4.81713000	-2.72398600	-1.14243000
N	-3.49895100	0.05587100	-0.05065600
C	2.32848500	-2.06932500	-0.71977200
H	3.09521300	-1.71258100	-1.41611600
H	2.53236800	-3.12079800	-0.48714300
H	1.33331700	-2.00632800	-1.18781100
C	1.55013500	2.24526200	-0.70489100
C	2.64467300	2.63196400	-1.42736400
H	3.47640200	1.93914900	-1.54132200
C	0.36192000	3.17424700	-0.55425900
H	-0.44667100	2.84770000	-1.23214700
H	-0.05325700	3.07533900	0.46045300
C	-3.41582600	1.38525900	0.48887300
C	-3.55180200	2.46340200	-0.39233800
C	-3.13221200	1.53377800	1.85012200
C	-3.40451900	3.74536300	0.13588900
C	-2.99430800	2.83563100	2.33386200
C	-3.12837400	3.92943600	1.48657400
H	-3.51041200	4.60573400	-0.52453200
H	-2.77965000	2.98530300	3.39137400
H	-3.02133600	4.93711500	1.88415700
C	-2.02282800	-2.87297500	-1.36887600
C	-1.70594100	-3.91739300	-0.49609500
C	-1.52974500	-2.78131900	-2.67484100
C	-0.84578900	-4.90688200	-0.97160900
C	-0.67724900	-3.79637400	-3.10813600
C	-0.33698800	-4.84776200	-2.26338100
H	-0.57491700	-5.73024800	-0.31164800
H	-0.28446200	-3.75978200	-4.12385900
H	0.32665400	-5.63367600	-2.62011300
C	2.77083400	-2.90793900	2.59901900
H	2.29904500	-3.34397900	3.48529500
H	3.03763900	-3.69991800	1.89271900
H	3.65419800	-2.32620500	2.87814100
C	-2.26094400	-3.96129000	0.89414000
H	-3.33496500	-4.19576900	0.89752600
H	-1.75078300	-4.72504200	1.49053500
H	-2.12719000	-2.99900900	1.40646200
C	-1.88580300	-1.63203800	-3.56950000
H	-2.95866100	-1.39796800	-3.53680300
H	-1.35000400	-0.71604900	-3.27632800
H	-1.62041600	-1.85124100	-4.60966900

C	-3.81902200	2.24464500	-1.85107400
H	-4.79493000	1.77124400	-2.02657000
H	-3.81203300	3.19507100	-2.39587700
H	-3.06222700	1.58785400	-2.30578700
C	-2.95034600	0.34605600	2.74669700
H	-3.72540100	-0.41565600	2.58743500
H	-1.97883100	-0.14266600	2.57219400
H	-2.98158300	0.64514100	3.80003700
C	2.74919000	3.93099400	-2.14226300
H	3.52531200	4.51876900	-1.61663300
H	3.16576600	3.76507700	-3.14718700
C	0.72725900	4.62144800	-0.85315100
C	1.44162500	4.71243500	-2.19300400
H	1.38308400	5.01314000	-0.05862100
H	-0.17986000	5.23983000	-0.84385800
H	1.63769300	5.75437200	-2.47436300
H	0.79389000	4.29085300	-2.97788600

TS7b

Zero-point correction= 0.700942 (Hartree/Particle)
Thermal correction to Energy= 0.745683
Thermal correction to Enthalpy= 0.746627
Thermal correction to Gibbs Free Energy= 0.621695
Sum of electronic and zero-point Energies= -2296.928838
Sum of electronic and thermal Energies= -2296.884097
Sum of electronic and thermal Enthalpies= -2296.883153
Sum of electronic and thermal Free Energies= -2297.008085
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.52473468
Cartesian coordinates:

C	-2.79582100	-1.88163500	1.24958600
C	-4.00025700	-1.79128500	0.37635700
C	-2.00777500	-0.76082900	1.53486800
O	-4.09690900	-0.99088600	-0.53863500
H	-2.86568800	-2.62175700	2.05277700
C	-1.28251000	-0.63364400	2.83130800
H	-1.24952600	0.41490800	3.14824400
H	-1.70417900	-1.25494600	3.62708900
H	-0.23528800	-0.94283500	2.65554800
C	-5.10202500	-2.75797200	0.71130400
H	-5.90327700	-2.68176300	-0.02826100
H	-4.72348500	-3.78958800	0.74435900
H	-5.50736600	-2.54336100	1.70958000
C	-0.00384100	-0.79391500	-0.47594900
C	-1.12860300	0.14392900	-0.47693700
Au	1.77856500	0.20819400	-0.12744700
N	-1.79643500	0.19293700	0.63769000
C	5.02390300	2.90540400	0.42885100
C	5.43538700	1.91034700	1.25466600
H	5.45915400	3.86666200	0.18894300
H	6.30705600	1.81523500	1.88898600
N	3.82955400	2.48588500	-0.13316500
N	4.48013800	0.90864000	1.17258000
C	3.49379100	1.26118000	0.32173000
C	-0.19808100	-2.14778000	-0.30177700
N	-1.28961100	1.07251200	-1.45997300
C	-0.44813700	1.04632500	-2.66124400
H	0.44386200	1.67818100	-2.54676700
H	-0.14518300	0.01143900	-2.84424800
H	-1.03217100	1.40550800	-3.51143500
S	-2.06847800	2.59824200	-1.11723000
O	-1.53645800	3.10405600	0.13467600
O	-1.91803400	3.35046400	-2.34827000
C	-1.49836900	-2.69720900	-0.46885900
C	4.46806800	-0.32940100	1.90266100
C	5.01245500	-1.46659600	1.29871600

C	3.85477700	-0.34510700	3.16016800
C	4.94574000	-2.66394600	2.01224900
C	3.80966600	-1.56421900	3.83567700
C	4.35202300	-2.71223200	3.26808000
H	5.37140900	-3.56546000	1.57270500
H	3.34777700	-1.60644400	4.82159200
H	4.31664100	-3.65359100	3.81344500
C	3.00449700	3.21339300	-1.06090800
C	3.32082200	3.13800300	-2.42213800
C	1.88357800	3.88866900	-0.56571500
C	2.46342100	3.78048500	-3.31469700
C	1.05204900	4.51178600	-1.49782400
C	1.33610700	4.45515600	-2.85674200
H	2.68300700	3.74028900	-4.38114800
H	0.16190400	5.03138900	-1.14631700
H	0.66346800	4.93538600	-3.56489100
C	-3.77017600	2.13869400	-0.92322200
H	-3.86785400	1.43908900	-0.09071200
H	-4.31441700	3.06915600	-0.73045000
H	-4.10986300	1.67456000	-1.85303400
C	1.54761100	3.90972200	0.89496400
H	2.44152300	3.94239900	1.53202700
H	0.91941300	4.77456100	1.13423400
H	0.96836300	3.01559700	1.17423600
C	4.51733800	2.37177500	-2.90052200
H	5.46023600	2.81719600	-2.55408700
H	4.50393300	1.33325900	-2.53704600
H	4.55053000	2.34397100	-3.99494300
C	3.24838700	0.89537300	3.74368800
H	3.97349700	1.71735100	3.81648200
H	2.41556400	1.26336000	3.12520800
H	2.86073200	0.70482700	4.75035800
C	5.61276500	-1.40985900	-0.07336400
H	4.83612900	-1.27242000	-0.84120200
H	6.31953600	-0.57675100	-0.18447700
H	6.14757400	-2.33728300	-0.30509300
C	-1.76105600	-4.17796200	-0.43745200
C	-0.48555400	-5.01281300	-0.35732100
C	0.47879900	-4.38982900	0.64014300
C	0.95127700	-3.03900800	0.12231600
H	-2.36301700	-4.44059000	-1.32009400
H	-0.74008100	-6.04423000	-0.08482200
H	-0.02936300	-4.25980500	1.61213600
H	1.56150700	-2.51853300	0.87650000
H	-2.39800100	-4.42218400	0.42601600
H	-0.00451000	-5.05844700	-1.34672600
H	1.34054000	-5.04370100	0.82229600
H	1.61848200	-3.19129700	-0.74323400
H	-2.19008800	-2.09198600	-1.05246000

TS8b

Zero-point correction= 0.699479 (Hartree/Particle)
Thermal correction to Energy= 0.744422
Thermal correction to Enthalpy= 0.745366
Thermal correction to Gibbs Free Energy= 0.620262
Sum of electronic and zero-point Energies= -2296.929204
Sum of electronic and thermal Energies= -2296.884261
Sum of electronic and thermal Enthalpies= -2296.883317
Sum of electronic and thermal Free Energies= -2297.008421
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.52776123
Cartesian coordinates:

C	1.33013500	0.91332700	0.23371200
C	2.25944600	-0.19108000	-0.10550700
N	2.74828000	-0.26949400	-1.38181900
S	3.67423500	-1.68878200	-1.87660100

O	2.87466200	-2.87904800	-1.66519300
O	4.12979300	-1.33598600	-3.20805900
Au	-0.60149800	0.16278300	0.22622600
C	-2.43985900	-0.69674500	-0.13783700
N	-2.71580900	-2.01605400	-0.23064000
C	-4.54656500	-0.97932600	-0.87609700
C	-4.01136000	-2.21040600	-0.68250200
H	-5.52281100	-0.66422700	-1.22097500
H	-4.42083800	-3.20245300	-0.82133400
N	-3.56389100	-0.06416900	-0.53524200
N	2.47463400	-1.17546600	0.72957900
C	2.00156000	-0.96671600	1.97884600
C	3.20058800	1.21331700	2.48458100
C	2.09137700	0.25776200	2.62421200
C	1.32596100	-2.13732600	2.60615200
H	1.09221100	-1.97364300	3.66231800
H	0.39832700	-2.37426100	2.06043900
H	1.96704400	-3.02221200	2.50229300
O	4.13770200	1.07758600	1.70853800
C	3.11831500	2.40180500	3.40655800
H	3.91532600	3.11382900	3.17206800
H	2.13536600	2.88861300	3.31805200
H	3.22046900	2.08821900	4.45444300
C	2.21607800	0.54815000	-2.47294600
H	1.14100200	0.71849800	-2.32378300
H	2.72495800	1.51797600	-2.53600800
H	2.37110800	0.02038400	-3.41638600
H	1.50234500	0.36898500	3.53806100
C	-3.66311300	1.36730300	-0.62856300
C	-4.05442400	2.08291000	0.50659100
C	-3.31412800	1.97345400	-1.84008800
C	-4.10437500	3.47288900	0.39956700
C	-3.37832200	3.36525800	-1.90017600
C	-3.77078800	4.10736600	-0.79137200
H	-4.41447600	4.05891000	1.26398500
H	-3.12238500	3.86732600	-2.83261900
H	-3.82336000	5.19245700	-0.85845300
C	-1.79255400	-3.06002300	0.13247600
C	-0.74945300	-3.38501900	-0.74290800
C	-1.97980400	-3.68883300	1.37015800
C	0.13423400	-4.38920000	-0.34114300
C	-1.08878800	-4.70376800	1.71581400
C	-0.04240800	-5.05079000	0.86743000
H	0.96945800	-4.64119700	-0.99257400
H	-1.21648000	-5.21771600	2.66802800
H	0.64742400	-5.84205900	1.15530300
C	5.06143900	-1.63519400	-0.76885400
H	5.56309300	-0.67218000	-0.90011600
H	4.71596800	-1.77106500	0.25733300
H	5.71912300	-2.45368800	-1.07993600
C	-3.07654600	-3.26625000	2.30147700
H	-4.07454600	-3.51028200	1.91217700
H	-2.97496000	-3.76342900	3.27207000
H	-3.06015300	-2.17966800	2.47549500
C	-0.56061500	-2.68834700	-2.05722500
H	-1.51462400	-2.49168800	-2.56539400
H	-0.06051200	-1.71515500	-1.92221300
H	0.07345100	-3.28307700	-2.72312200
C	-4.38380000	1.38504800	1.79152000

H	-5.10765600	0.57160600	1.64687100
H	-3.48692200	0.93594700	2.24353400
H	-4.80750600	2.08510300	2.51948800
C	-2.87330500	1.15758100	-3.01804400
H	-1.96872300	0.57283300	-2.78864900
H	-3.64130600	0.43752400	-3.33253500
H	-2.65012600	1.79931000	-3.87714600
C	1.63948900	2.29098100	0.13607300
C	2.90188900	2.70407300	-0.21305700
C	0.55679200	3.30065500	0.44991800
C	3.30160400	4.12317500	-0.34715100
C	1.11549400	4.69217500	0.72233100
H	-0.15952800	3.33340800	-0.39067300
C	2.12164500	5.08757100	-0.34919500
H	3.98162600	4.33297500	0.50136000
H	1.61359300	4.70455500	1.70646600
H	2.47741700	6.11420100	-0.20119200
H	3.93934900	4.24340300	-1.23624400
H	1.63321600	5.06379300	-1.33602200
H	0.29620400	5.41940700	0.77931100
H	-0.02395500	2.93855000	1.31305500
H	3.66858700	1.95206300	-0.39700400

TS9b

Zero-point correction= 0.699036 (Hartree/Particle)
Thermal correction to Energy= 0.744650
Thermal correction to Enthalpy= 0.745594
Thermal correction to Gibbs Free Energy= 0.618291
Sum of electronic and zero-point Energies= -2296.919829
Sum of electronic and thermal Energies= -2296.874214
Sum of electronic and thermal Enthalpies= -2296.873270
Sum of electronic and thermal Free Energies= -2297.000573
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.51479111
Cartesian coordinates:

C	3.78539600	0.78506500	2.54332700
C	4.85935900	1.49760900	1.83506700
C	2.60070000	0.46328100	1.98986600
O	4.85045700	1.66278500	0.62057400
H	3.96870400	0.47193900	3.57087900
C	1.53894600	-0.33654600	2.66192000
H	1.36669700	-1.25895100	2.08209200
H	1.83273200	-0.60742600	3.68099000
H	0.58543100	0.21134300	2.69589500
C	5.98698800	1.99971200	2.69187500
H	6.72213800	2.52765000	2.07892300
H	5.60822500	2.67110300	3.47439900
H	6.47496800	1.16121900	3.20796100
C	0.87809200	1.28889600	-0.31344500
C	2.11171200	0.57899900	-0.49455200
Au	-0.80278600	0.08273300	-0.08119300
N	2.25522500	0.93351500	0.72518900
C	-3.53406300	-3.14033800	0.35424900
C	-4.43923500	-2.13136500	0.41516500
H	-3.64960000	-4.21456500	0.41532900
H	-5.51411000	-2.13548400	0.54114900
N	-2.29560800	-2.54601300	0.18179100
N	-3.72781900	-0.94851000	0.27995600
C	-2.41075000	-1.19994900	0.13776200

N	2.66789200	-0.19830200	-1.42646900
C	2.01501200	-0.31397900	-2.73699600
H	1.43477300	-1.24208200	-2.79102600
H	1.35427400	0.54945900	-2.86434900
H	2.76999600	-0.31070300	-3.52940300
S	3.90557500	-1.37768900	-1.04359800
O	3.85449100	-1.55776200	0.39197200
O	3.66634000	-2.46774100	-1.96824900
C	-4.28648700	0.37653300	0.28076500
C	-4.79873300	0.87663100	-0.92075900
C	-4.25892700	1.11074100	1.47027700
C	-5.32044900	2.16939300	-0.90515400
C	-4.79270200	2.39919000	1.43825400
C	-5.32022900	2.92229300	0.26371700
H	-5.73092300	2.58550800	-1.82443100
H	-4.79516900	2.99312000	2.35159100
H	-5.73728900	3.92754100	0.25910700
C	-1.01064400	-3.18280900	0.08117300
C	-0.46431000	-3.37059600	-1.19292200
C	-0.31673700	-3.45810600	1.26384100
C	0.84828900	-3.83687800	-1.26366200
C	0.99093000	-3.93015600	1.14369800
C	1.57170900	-4.10588800	-0.10689700
H	1.31286500	-3.98430900	-2.23836100
H	1.56126400	-4.14738800	2.04665400
H	2.60063600	-4.45069100	-0.18562900
C	5.37809800	-0.51636700	-1.52399500
H	5.46644300	0.38909200	-0.91360500
H	6.21259700	-1.20242900	-1.34375000
H	5.30865000	-0.28887000	-2.59234000
C	-0.94265300	-3.22272300	2.60564600
H	-1.79616100	-3.89135600	2.78411200
H	-0.21772900	-3.39381400	3.40958000
H	-1.32056100	-2.19372100	2.70354900
C	-1.24141500	-3.04265400	-2.43279500
H	-2.25654100	-3.46108300	-2.40895000
H	-1.35147300	-1.95464500	-2.56314100
H	-0.73765200	-3.43614200	-3.32296400
C	-3.65807200	0.55022400	2.72422600
H	-3.96143200	-0.49029600	2.90298900
H	-2.55756000	0.55887800	2.67511200
H	-3.95291300	1.14242100	3.59742600
C	-4.77335300	0.05816300	-2.17626000
H	-3.75787800	-0.29747200	-2.40472900
H	-5.41295600	-0.83232600	-2.10245600
H	-5.12441600	0.64500900	-3.03172400
C	0.78964400	2.73086600	-0.55490300
C	-0.42450100	3.44016400	-0.01218000
C	1.74121100	3.37320400	-1.25941400
C	-0.26625200	4.95496100	-0.04629200
H	-1.31659200	3.13327400	-0.58837000
C	1.67004000	4.81911000	-1.62373000
H	2.63316200	2.82338500	-1.57670200
C	0.28019400	5.40273700	-1.39513600
H	-1.22692900	5.43900900	0.17072000
H	1.98893400	4.95433600	-2.66785300
H	-0.39676300	5.05770000	-2.19318600
H	-0.61111600	3.09000200	1.01716600
H	0.43169400	5.26693200	0.74739100

H	0.31498400	6.49724400	-1.46344300
H	2.41848800	5.36512200	-1.02284000

TS10b

Zero-point correction= 0.698870 (Hartree/Particle)
Thermal correction to Energy= 0.744238
Thermal correction to Enthalpy= 0.745183
Thermal correction to Gibbs Free Energy= 0.617733
Sum of electronic and zero-point Energies= -2296.926737
Sum of electronic and thermal Energies= -2296.881369
Sum of electronic and thermal Enthalpies= -2296.880425
Sum of electronic and thermal Free Energies= -2297.007874
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.51977186
Cartesian coordinates:

C	0.90696100	-1.60480200	0.17948900
C	-0.14943600	-2.62213900	0.22711600
N	-0.25696800	-3.36530500	-0.97410700
S	-1.73549600	-3.19758400	-1.83615300
O	-2.21533600	-1.84846100	-1.58607700
O	-1.44540400	-3.65441500	-3.18225900
Au	0.14712400	0.32001800	0.06297500
C	-0.46409900	2.28328900	-0.19319000
N	-1.69661200	2.83119100	-0.24205500
C	-0.30411900	4.49101800	-0.62383700
C	-1.62039000	4.18924500	-0.50839800
H	0.20765800	5.42266600	-0.82747800
H	-2.51054500	4.79891100	-0.59311100
N	0.38808700	3.30835200	-0.42652600
N	-1.13131400	-2.69607300	1.04084200
C	-1.50540400	-1.79998400	2.02730900
C	0.55604100	-1.82338500	3.43224000
C	-0.81382900	-1.43865000	3.13856800
C	-2.91820400	-1.35258200	1.82231100
H	-3.20257400	-0.56680700	2.53113300
H	-3.04692000	-0.97760800	0.79611700
H	-3.60523700	-2.20300600	1.93710500
O	1.33574000	-2.18082900	2.54814700
C	0.99287200	-1.75930300	4.86743900
H	0.39117400	-2.44292600	5.48110000
H	2.05020600	-2.02218700	4.95706900
H	0.82942200	-0.75002500	5.26918300
C	0.69130500	-4.37834500	-1.41713400
H	1.68172600	-3.93686900	-1.58840800
H	0.77439300	-5.18980100	-0.68194600
H	0.34197000	-4.78206200	-2.37107000
H	-1.35680700	-0.88956000	3.90857700
C	1.81561300	3.15327400	-0.49758400
C	2.55897900	3.28274200	0.67979600
C	2.38451200	2.84889700	-1.73860500
C	3.93879100	3.09794300	0.58866000
C	3.76787300	2.67401000	-1.78206900
C	4.53722600	2.79786400	-0.63031300
H	4.54661000	3.19906500	1.48708100
H	4.24201400	2.44149600	-2.73541000
H	5.61669400	2.66629700	-0.68440400
C	-2.93201700	2.10910400	-0.09709400
C	-3.43380500	1.42046100	-1.20572900
C	-3.58061500	2.15436900	1.14159800
C	-4.65770000	0.76732800	-1.04782200

C	-4.80806500	1.50265900	1.24571900
C	-5.34340100	0.81851600	0.15923200
H	-5.07131200	0.21797500	-1.89253800
H	-5.34324100	1.52912100	2.19474200
H	-6.30449800	0.31692900	0.25689600
C	-2.83907300	-4.36802200	-1.07505500
H	-2.39637100	-5.36533200	-1.16562900
H	-2.96944700	-4.08740200	-0.02683400
H	-3.78394000	-4.32677500	-1.62656800
C	-2.95601600	2.83953800	2.31965400
H	-2.81633000	3.91692600	2.15557600
H	-3.57684300	2.72061900	3.21455600
H	-1.96101600	2.42157300	2.53965200
C	-2.68578000	1.35809000	-2.50197900
H	-2.22027100	2.31851200	-2.76300600
H	-1.88904400	0.60090300	-2.45236600
H	-3.35227200	1.06877600	-3.32169700
C	1.89440900	3.59112000	1.98723600
H	1.30041000	4.51399500	1.93921300
H	1.20691700	2.78645400	2.28754100
H	2.63620800	3.71291200	2.78375900
C	1.53732600	2.68864500	-2.96462900
H	0.84406000	1.83932900	-2.86587000
H	0.92144000	3.57689700	-3.16145100
H	2.15843400	2.51174400	-3.84926000
C	2.28614400	-1.83462900	-0.07744700
C	2.87890800	-2.99079200	0.35075700
H	2.25182600	-3.75605200	0.81030500
C	3.12440700	-0.72413200	-0.67416300
H	3.23870000	0.08570300	0.06832600
H	2.58489100	-0.27455800	-1.52154100
C	4.33761900	-3.25127200	0.31498200
H	4.50703200	-4.04099900	-0.44163900
H	4.64270200	-3.71387200	1.26551600
C	4.49487300	-1.21555600	-1.12133100
H	5.11217200	-0.35780800	-1.41866400
C	5.16267500	-2.01158400	-0.01030800
H	6.18384000	-2.30338600	-0.28368700
H	5.24278900	-1.38319700	0.89014600
H	4.38868500	-1.85179700	-2.01567500

TS11b

Zero-point correction= 0.699498 (Hartree/Particle)
Thermal correction to Energy= 0.744803
Thermal correction to Enthalpy= 0.745747
Thermal correction to Gibbs Free Energy= 0.617877
Sum of electronic and zero-point Energies= -2296.909197
Sum of electronic and thermal Energies= -2296.863892
Sum of electronic and thermal Enthalpies= -2296.862948
Sum of electronic and thermal Free Energies= -2296.990817
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2298.50077968
Cartesian coordinates:

C	-1.60432400	0.49199900	0.55625300
C	-2.31386700	-0.44500500	-0.33611000
N	-1.95414900	-1.77296500	-0.33005900
S	-1.51321200	-2.59811700	-1.77062500
O	-0.52629500	-1.82227200	-2.49791600
O	-1.20076700	-3.94376900	-1.32080900

Au	0.44257400	0.27216500	0.28050100
C	2.45624800	-0.03849700	-0.02150500
N	3.32523200	0.79964600	-0.62103900
C	4.47983800	-1.00931700	-0.14456000
C	4.58127600	0.21986500	-0.70931000
H	5.20768700	-1.79667700	0.00165800
H	5.41527200	0.73702100	-1.16540800
N	3.16610500	-1.14723500	0.27311900
N	-2.36632100	0.24889100	-1.49525500
C	-3.27828500	1.20027800	-1.72540500
C	-4.93189600	0.22433600	-0.23511600
C	-4.51245200	1.26821900	-1.08434200
C	-2.92364200	2.15752000	-2.81515900
H	-2.07366600	2.77430200	-2.48863600
H	-2.58670400	1.60990600	-3.70353500
H	-3.75628200	2.81450500	-3.08432600
O	-4.13482900	-0.64618800	0.23342400
C	-6.37615800	0.06623300	0.12126800
H	-6.48700300	-0.01004500	1.21049500
H	-6.99106300	0.89111300	-0.25141800
H	-6.75329200	-0.87554800	-0.29760700
C	-1.67877800	-2.42040600	0.95387200
H	-2.32608500	-1.95830800	1.70693700
H	-1.92651900	-3.48170800	0.88233500
H	-0.62390100	-2.32100200	1.24854600
C	-2.14019000	1.52866000	1.35193400
C	-3.22964400	1.32615600	2.16093900
H	-3.82589800	0.42069500	2.06798900
C	-1.34966600	2.78356100	1.61973200
H	-0.45571600	2.83167500	0.98259700
H	-1.97684000	3.64650200	1.34251900
H	-5.24524700	1.99673900	-1.42091200
C	2.58599900	-2.30148000	0.90626900
C	2.49315400	-2.31491100	2.30215600
C	2.09860800	-3.32772100	0.08900900
C	1.88391800	-3.42333300	2.89037100
C	1.48373700	-4.40901400	0.72226700
C	1.38169100	-4.45774800	2.10779300
H	1.80623400	-3.46999600	3.97620700
H	1.07515800	-5.21226100	0.11088900
H	0.90708300	-5.31373800	2.58440000
C	2.94294300	2.09299600	-1.11864800
C	2.37297500	2.17188600	-2.39318500
C	3.10603600	3.19823300	-0.27652100
C	1.98266300	3.43620700	-2.83766400
C	2.70023000	4.43976600	-0.76312700
C	2.14724800	4.55772400	-2.03393500
H	1.54697000	3.53394100	-3.83160000
H	2.82343400	5.32140500	-0.13502000
H	1.84407600	5.53614100	-2.40222700
C	-3.04124800	-2.62441800	-2.67943300
H	-3.80379500	-3.09586900	-2.05259800
H	-3.31390200	-1.59790800	-2.94011600
H	-2.86303700	-3.21749700	-3.58242000
C	3.65711800	3.04351300	1.10893700
H	4.63521300	2.54392800	1.11682900
H	3.77675400	4.01848900	1.59358600
H	2.98634800	2.43655900	1.73714400
C	2.14381700	0.95077300	-3.23217700

H	2.98019700	0.24132100	-3.17830600
H	1.24223200	0.40711500	-2.90738400
H	2.00030600	1.22279700	-4.28381400
C	3.00149100	-1.17422300	3.13223000
H	4.00443000	-0.84922300	2.82427600
H	2.34334400	-0.29523900	3.05041200
H	3.04896300	-1.45329100	4.19058600
C	2.23237100	-3.27116600	-1.40195800
H	1.85464700	-2.32508800	-1.81329700
H	3.28095200	-3.37389200	-1.71631200
H	1.65815800	-4.07764100	-1.87018400
C	-3.46679900	2.27744400	3.27435400
H	-3.83617400	3.22453400	2.84330400
H	-4.24521200	1.91951500	3.95665500
C	-2.15267300	2.56134700	4.03659900
H	-2.33446600	3.38356600	4.73854700
C	-0.96951100	2.87874800	3.10376500
H	-0.14635800	2.17210900	3.28932400
H	-0.56872800	3.87947300	3.30777000
H	-1.92382000	1.68057800	4.65003900

TS12b

Zero-point correction= 0.758646 (Hartree/Particle)
Thermal correction to Energy= 0.816445
Thermal correction to Enthalpy= 0.817389
Thermal correction to Gibbs Free Energy= 0.669285
Sum of electronic and zero-point Energies= -4123.828451
Sum of electronic and thermal Energies= -4123.770652
Sum of electronic and thermal Enthalpies= -4123.769708
Sum of electronic and thermal Free Energies= -4123.917812
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4125.79080371
Cartesian coordinates:

C	1.03690400	1.87519600	0.70318500
C	1.59877300	1.31318700	1.90517300
N	2.90149700	0.86764000	2.13412900
S	3.15365600	-0.32837400	3.36446200
O	2.18537600	-1.40478100	3.21747100
O	4.57559500	-0.64251600	3.30576800
Au	0.70852700	-0.31509700	0.07745600
C	0.67841600	-2.25141300	-0.66063300
N	-0.15560200	-3.30976800	-0.52666700
C	1.53161500	-4.05710500	-1.72871100
C	0.35698700	-4.42565100	-1.17195600
H	2.25891400	-4.60035300	-2.31757300
H	-0.17834800	-5.36558200	-1.16787200
N	1.71206500	-2.72260000	-1.40574200
N	0.71838900	1.28740900	2.93743300
C	-0.38886700	1.90608600	2.52856800
C	-0.99471800	3.66183600	0.86939100
C	-0.32179400	2.34687500	1.15916700
C	-1.50892500	2.06823600	3.48619500
H	-1.98083500	3.05134200	3.38743400
H	-2.29034200	1.32631300	3.27987300
H	-1.14367000	1.90428300	4.50565300
O	-2.12350500	3.85396900	1.29259500
C	-0.29984600	4.74397800	0.08647900
H	0.59419500	5.09810300	0.61555500
H	0.02144900	4.38781300	-0.89768600

H	-1.01003400	5.56712800	-0.03714300
C	3.88942300	0.84263000	1.05512300
H	3.45133200	0.42939600	0.13354800
H	4.25961800	1.85067600	0.85046100
H	4.72540000	0.21336000	1.36622200
C	2.87445300	-1.96802500	-1.77916800
C	2.83580600	-1.21850000	-2.95985400
C	3.99793700	-2.03638100	-0.94786700
C	3.98258000	-0.49993400	-3.30006200
C	5.12682800	-1.31466600	-1.33800200
C	5.11737000	-0.54824800	-2.49778600
H	3.97920300	0.10120900	-4.20950400
H	6.01621500	-1.34770000	-0.70861200
H	6.00480500	0.01477600	-2.78266700
C	-1.41692900	-3.37959500	0.16687900
C	-1.41926800	-3.41994000	1.56703300
C	-2.57633400	-3.51608100	-0.60197000
C	-2.64307000	-3.63323700	2.19627600
C	-3.77733900	-3.72725600	0.07615700
C	-3.81100300	-3.79342100	1.46037200
H	-2.67223500	-3.66523400	3.28501500
H	-4.69678300	-3.81107400	-0.50285700
H	-4.75726300	-3.95757700	1.97330200
C	2.86270300	0.55154100	4.87955600
H	3.56703300	1.38671400	4.92344400
H	1.82531400	0.89144600	4.88216400
H	3.06635900	-0.16542900	5.68164700
C	-2.57893100	-3.42348000	-2.09945800
H	-2.71419300	-4.40989300	-2.56637900
H	-3.41116300	-2.78622100	-2.42489800
H	-1.65431200	-2.98998400	-2.49910400
C	-0.17984500	-3.20223500	2.37282700
H	0.71830700	-3.63405100	1.91024200
H	0.02104000	-2.12835600	2.49939200
H	-0.28373000	-3.63079300	3.37646900
C	1.60416200	-1.16386400	-3.81171600
H	1.81283400	-0.66622000	-4.76572300
H	1.20837400	-2.16562500	-4.03016000
H	0.79628100	-0.60691000	-3.31675000
C	3.97069200	-2.81710200	0.33104700
H	3.20136600	-2.43734500	1.02229200
H	3.74400200	-3.87917500	0.16162500
H	4.93328200	-2.75517900	0.85076300
C	1.82886100	2.57030500	-0.35757800
C	2.69494400	3.53418300	-0.01814600
C	1.63410100	2.16519300	-1.79596200
C	3.56482300	4.26855700	-0.99243900
C	2.24736600	3.14619600	-2.78512700
H	2.09847100	1.17088000	-1.93899200
C	3.64443600	3.54153300	-2.32897400
H	3.16775000	5.28944700	-1.14327300
H	1.61643700	4.04790000	-2.85778400
H	4.15063100	4.16560800	-3.07803600
H	4.57048100	4.40688500	-0.56482000
H	4.25136400	2.62588700	-2.20708400
H	2.26680200	2.69853300	-3.78970700
H	0.56031000	2.02748900	-1.99978000
H	2.78329800	3.81131400	1.03758600
H	-1.42278200	1.65292200	0.43368700

N	-2.38786400	1.22827700	-0.22440800
S	-2.66311800	1.84771200	-1.72862400
O	-4.05759800	2.12246600	-1.99024600
O	-1.63007400	2.84926500	-1.92020900
S	-3.32035200	0.05227800	0.44378200
O	-3.90040000	-0.77983800	-0.59451500
O	-2.55351900	-0.48146700	1.55467100
C	-4.74315400	0.94382000	1.22824100
C	-2.19725600	0.44461400	-2.88796800
F	-1.49553500	0.96121800	-3.88587200
F	-3.27065800	-0.14321900	-3.36647900
F	-1.44216400	-0.45105100	-2.26319700
F	-5.37536400	0.05808300	1.98546800
F	-4.29268300	1.92882900	1.97763200
F	-5.56466400	1.40943400	0.31465500

TS13b

Zero-point correction= 0.758339 (Hartree/Particle)
Thermal correction to Energy= 0.817495
Thermal correction to Enthalpy= 0.818439
Thermal correction to Gibbs Free Energy= 0.662284
Sum of electronic and zero-point Energies= -4123.850936
Sum of electronic and thermal Energies= -4123.791781
Sum of electronic and thermal Enthalpies= -4123.790836
Sum of electronic and thermal Free Energies= -4123.946991

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4125.81820062

Cartesian coordinates:

C	-0.18531400	1.19296500	0.62167600
C	0.69056800	0.55714800	-0.33932400
N	0.82797600	0.78918700	-1.71563800
S	0.52677700	-0.54688600	-2.74573900
O	-0.52455700	-1.39612100	-2.18739300
O	0.35535700	0.00988100	-4.08031100
Au	-1.91894300	-0.10021500	0.16500800
C	-3.60583800	-1.21695400	-0.06410100
N	-4.76946300	-0.83848100	-0.63372000
C	-5.10065100	-2.89016600	0.08613300
C	-5.70696000	-1.85799100	-0.55205300
H	-5.45545500	-3.87604600	0.35616300
H	-6.70424500	-1.74878200	-0.95724900
N	-3.81067000	-2.47469900	0.37909900
N	1.42857500	-0.41876700	0.21172300
C	1.10199500	-0.49344800	1.54018900
C	-0.42950400	0.59348400	3.20551800
C	0.15794600	0.46675600	1.87071200
C	1.76774300	-1.50265100	2.40502000
H	2.29220600	-1.02608100	3.24344500
H	1.03004200	-2.17549500	2.85941600
H	2.47828300	-2.09737100	1.81673600
O	-0.17814800	-0.21876000	4.08987900
C	-1.37991800	1.73532400	3.48516000
H	-1.65450400	1.71114700	4.54421400
H	-0.92839100	2.70416200	3.23361700
H	-2.29184600	1.64258000	2.87619700
C	0.46872400	2.09228000	-2.27137000
H	-0.61495200	2.28629500	-2.21636500
H	1.01212800	2.85628700	-1.70970900
H	0.77666600	2.12391500	-3.31776300

C	-2.76722600	-3.22740700	1.02351100
C	-1.98327500	-4.06872200	0.22781000
C	-2.51187300	-2.99107600	2.37820100
C	-0.91555500	-4.71895700	0.84501500
C	-1.42670700	-3.65472600	2.95026600
C	-0.63852500	-4.51167000	2.19119100
H	-0.28475700	-5.37951600	0.25115500
H	-1.19058500	-3.47122700	3.99829300
H	0.21042800	-5.01445600	2.65176900
C	-4.93711900	0.46854900	-1.20492800
C	-5.47154700	1.47575300	-0.39467000
C	-4.45706900	0.69625700	-2.49850300
C	-5.54208800	2.76152900	-0.92836700
C	-4.54889700	1.99911000	-2.99165700
C	-5.08378800	3.02048400	-2.21578500
H	-5.95103500	3.56697700	-0.31850500
H	-4.18420800	2.20754700	-3.99710700
H	-5.14176700	4.03100600	-2.61714900
C	2.04627100	-1.46378700	-2.70603600
H	2.86214000	-0.78426800	-2.96552300
H	2.18214900	-1.89260800	-1.70905500
H	1.94619800	-2.25202700	-3.45949700
C	-3.82132900	-0.39550600	-3.30379800
H	-4.37572500	-1.34114200	-3.23118500
H	-3.76041900	-0.11515200	-4.36128000
H	-2.79541300	-0.60015700	-2.95758700
C	-5.90547900	1.18757400	1.01078200
H	-6.71465600	0.44534400	1.05276800
H	-5.07439900	0.78305500	1.60868300
H	-6.26190100	2.09854900	1.50429000
C	-2.24767100	-4.21733100	-1.23947200
H	-3.28776700	-4.50080200	-1.45154200
H	-2.04716900	-3.27343500	-1.76798200
H	-1.59608100	-4.98312000	-1.67465200
C	-3.32840500	-2.02220300	3.17807300
H	-3.06527100	-0.98548300	2.91732400
H	-4.40694800	-2.13678400	3.00114900
H	-3.13650500	-2.14269900	4.24971800
C	-0.52104700	2.66192400	0.59737900
C	0.46453200	3.53449600	0.85550300
C	-1.92164300	3.13044400	0.28968800
C	0.31349400	5.02458200	0.79638500
C	-2.13397000	4.60782300	0.59376100
H	-2.15921800	2.92562300	-0.77171500
C	-0.96494600	5.43233300	0.07540100
H	0.31784000	5.44079100	1.81973400
H	-2.21484500	4.74860600	1.68543600
H	-1.15088000	6.50822200	0.19650100
H	1.19477500	5.46067700	0.30193500
H	-0.84696600	5.24900800	-1.00631000
H	-3.08663200	4.94434600	0.16003300
H	-2.65030200	2.52090400	0.85089500
H	1.45762300	3.14161000	1.09210400
H	2.92375200	-0.38187200	-0.09104800
N	4.02629700	-0.16031200	-0.14826900
S	5.05009200	-1.47499100	-0.08091100
O	6.03048200	-1.36582400	0.97436200
O	4.15922900	-2.61226600	-0.21194600
S	4.47735800	1.43252300	-0.05310400

O	5.85255700	1.57066900	-0.47842300
O	3.39116300	2.21396200	-0.60700100
C	4.42968200	1.78874700	1.75994300
C	6.00601100	-1.38828600	-1.68566400
F	6.25872300	-2.63486500	-2.04254900
F	7.13117500	-0.73777100	-1.52025600
F	5.27841100	-0.80278800	-2.62359700
F	4.65395300	3.08195700	1.91537600
F	3.22618600	1.49157100	2.22420400
F	5.34112000	1.09052300	2.39735700

TS14b

Zero-point correction= 0.757976 (Hartree/Particle)
Thermal correction to Energy= 0.816204
Thermal correction to Enthalpy= 0.817148
Thermal correction to Gibbs Free Energy= 0.666892
Sum of electronic and zero-point Energies= -4123.794981
Sum of electronic and thermal Energies= -4123.736753
Sum of electronic and thermal Enthalpies= -4123.735809
Sum of electronic and thermal Free Energies= -4123.886065

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4125.75867705

Cartesian coordinates:

H	2.88292000	1.05761500	0.08242200
N	3.33297700	0.10552000	-0.76225900
S	4.14517400	-1.23663300	-0.19561000
O	4.23133500	-1.11923500	1.24500600
O	3.69271800	-2.47728200	-0.79575900
S	2.80466800	0.13068600	-2.34183200
O	2.91399800	1.48896800	-2.83648100
O	3.28075400	-0.98950400	-3.12310300
C	0.99351300	-0.16108300	-2.11588500
C	5.87185200	-0.96914800	-0.81160400
F	0.46433700	-0.52867000	-3.27060800
F	0.80849500	-1.11994100	-1.22274200
F	0.41227300	0.95331900	-1.70604700
F	6.57500200	-2.03534800	-0.46236900
F	6.39270600	0.10499100	-0.26185500
F	5.88196100	-0.84364600	-2.12552700
C	2.52878300	2.19037300	0.96845600
C	3.95206800	2.65658700	1.24669500
C	1.73213700	2.93740000	0.04840500
O	4.88288800	1.88602600	1.31074400
C	2.37261100	3.67898800	-1.08526200
H	1.78042000	3.55850200	-1.99854200
H	2.38259800	4.75005900	-0.82964000
H	3.39599000	3.35056600	-1.29087500
C	4.13648700	4.12459000	1.56707200
H	4.28372700	4.69459200	0.64031500
H	3.25937400	4.54518200	2.07755900
H	5.03280900	4.24748900	2.18382100
C	-0.34687600	1.06812400	1.27079500
C	-0.49853200	2.40863700	0.76298400
Au	-1.68611900	-0.39689200	0.62225700
N	0.41800900	3.11602400	0.11814800
C	-4.58889900	-3.05017700	-1.06215400
C	-3.60194000	-3.94091100	-0.79349500
H	-5.56219000	-3.17083600	-1.51919200
H	-3.52718400	-5.00584000	-0.96970000

N	-4.13512600	-1.81444200	-0.62582800
N	-2.57553700	-3.22632800	-0.19700800
C	-2.89611500	-1.91586800	-0.09546900
C	0.80045100	0.77468200	1.93816200
N	-1.75044600	3.02106500	0.79072000
C	-2.81404500	2.53777700	1.67265000
H	-3.46811500	1.80307500	1.18097000
H	-2.33822500	2.06937400	2.53767600
H	-3.41872800	3.38893200	1.99731700
S	-2.30390800	3.89107000	-0.59057800
O	-2.01361600	3.11646600	-1.78576400
O	-3.67703800	4.25277300	-0.26836600
C	1.76436700	1.89202800	2.27841900
H	1.16743200	2.80129600	2.47058900
C	1.21765300	-0.62551400	2.27598300
H	0.34249300	-1.29059400	2.23470800
H	1.89236700	-0.97601900	1.47642600
C	-1.28659400	-3.71361800	0.21403300
C	-1.06126700	-3.93309600	1.57653900
C	-0.28240000	-3.81211600	-0.75414000
C	0.24032600	-4.24645700	1.96831900
C	1.00695000	-4.10893100	-0.31534700
C	1.26882500	-4.31015300	1.03459700
H	0.44791800	-4.41058700	3.02609600
H	1.82440400	-4.12666600	-1.03416500
H	2.29085100	-4.50323300	1.35724200
C	-4.84579200	-0.56658000	-0.65214800
C	-5.76373300	-0.31805200	0.37400800
C	-4.50985900	0.37946500	-1.62612800
C	-6.37652100	0.93382400	0.40072500
C	-5.13878300	1.62290900	-1.55212500
C	-6.05981600	1.89836200	-0.54953300
H	-7.09220300	1.15624700	1.19207600
H	-4.87304400	2.39128000	-2.27671600
H	-6.51649400	2.88485400	-0.49860000
C	-1.36519900	5.40434700	-0.61302400
H	-0.33126800	5.18049100	-0.87751900
H	-1.85251100	6.03936500	-1.36058600
H	-1.43301200	5.86393400	0.37702300
C	-3.47045700	0.10646700	-2.66994500
H	-3.52790300	-0.91962300	-3.05750500
H	-3.57046500	0.80313300	-3.50930800
H	-2.46015200	0.24870000	-2.25563800
C	-6.03135000	-1.34361400	1.43442600
H	-6.48447700	-2.25818600	1.02719200
H	-5.10001400	-1.64809400	1.93610700
H	-6.71125600	-0.94755400	2.19697800
C	-0.56944300	-3.55825600	-2.20316100
H	-1.15615600	-4.37287900	-2.65152300
H	-1.14230400	-2.63113300	-2.34832000
H	0.36287700	-3.46528000	-2.77164400
C	-2.15697900	-3.77296800	2.58747700
H	-2.35413100	-2.70844700	2.79029500
H	-3.10444200	-4.21416900	2.24913700
H	-1.88185100	-4.24510000	3.53767600
C	1.95398600	-0.76746100	3.60645300
C	2.55245500	1.65251400	3.57211800
H	3.36122600	2.39162200	3.67459000
H	1.85104800	1.86218900	4.39796300

C	3.08629300	0.24219900	3.74247600
H	1.23908700	-0.62707100	4.43612100
H	2.34133800	-1.79319600	3.68788800
H	3.86364400	0.04247100	2.99687700
H	3.55670700	0.14947800	4.73189600

TS15b

Zero-point correction= 0.758062 (Hartree/Particle)
Thermal correction to Energy= 0.815696
Thermal correction to Enthalpy= 0.816640
Thermal correction to Gibbs Free Energy= 0.667468
Sum of electronic and zero-point Energies= -4123.811775
Sum of electronic and thermal Energies= -4123.754141
Sum of electronic and thermal Enthalpies= -4123.753197
Sum of electronic and thermal Free Energies= -4123.902369
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -4125.78029737
Cartesian coordinates:

H	-1.20575500	-0.01795600	0.26985700
N	-1.69594000	0.16134600	1.40510100
S	-0.80728100	1.08311600	2.43728700
O	0.17062000	1.77845300	1.61821500
O	-1.62927000	1.75827100	3.41725400
S	-2.99908900	-0.72782500	1.89904600
O	-3.44230000	-1.45511300	0.72372500
O	-2.74784500	-1.39562500	3.16121600
C	-4.33802500	0.52929800	2.24091500
C	0.19623100	-0.16899200	3.39523300
F	-5.49526300	-0.06774500	1.97393700
F	-4.32179800	0.89251500	3.50217600
F	-4.19374000	1.57487300	1.45800900
F	1.35167700	0.40375700	3.72373300
F	0.44449100	-1.22928900	2.63709600
F	-0.41843200	-0.54294400	4.49267900
C	-3.41759600	-1.08525000	-2.40511300
C	-4.35009100	-2.21804500	-2.24833500
C	-3.66844900	0.18954800	-1.94492700
O	-3.91595600	-3.35317200	-2.10445700
C	-4.98582800	0.68163200	-1.40236200
H	-4.84277400	1.69742100	-1.01987400
H	-5.77369600	0.70989000	-2.16567700
H	-5.34128700	0.05703200	-0.57506800
C	-5.84792500	-2.02849400	-2.28730100
H	-6.28736600	-2.98068500	-2.60104900
H	-6.22884900	-1.80287700	-1.28289200
H	-6.17068600	-1.22820500	-2.96213800
C	-0.81342100	-0.10116600	-1.14746900
C	-1.47490500	1.09381500	-1.66218700
Au	1.24110700	-0.18021900	-0.49583100
N	-2.73916200	1.19174100	-1.96146500
C	5.45313100	0.19479000	0.16609500
C	5.30550400	-1.12201700	0.44181500
H	6.32108800	0.84111500	0.16441300
H	6.01565700	-1.88334200	0.73669700
N	4.19244400	0.67712500	-0.15067200
N	3.95887000	-1.40905000	0.28382600
C	3.26146900	-0.30429000	-0.07640900
C	-1.20469800	-1.31263200	-1.69072800
N	-0.79438700	2.32578300	-1.63084000
C	0.58041100	2.49213800	-2.07899200

H	1.27873900	2.61602400	-1.24309600
H	0.85755100	1.61090100	-2.66823500
H	0.65975700	3.37671400	-2.72480700
S	-1.53915000	3.68768900	-0.94897400
O	-2.39571500	3.27129600	0.14571900
O	-0.45865900	4.64245100	-0.74469400
C	-2.01783100	-1.34158900	-2.94996600
H	-1.77116700	-0.43647100	-3.52621000
C	-0.90675700	-2.63479100	-1.06532600
H	-0.26904500	-2.51208900	-0.17567700
H	-1.86736500	-3.06653400	-0.73567600
C	3.36403200	-2.69428300	0.51354400
C	3.14167500	-3.53139700	-0.58359400
C	3.02722300	-3.04003400	1.82521800
C	2.54507700	-4.76664200	-0.33480300
C	2.41536000	-4.27755700	2.02442800
C	2.17634000	-5.13225000	0.95503200
H	2.36233600	-5.44258200	-1.17014100
H	2.12432000	-4.56705600	3.03365300
H	1.69847500	-6.09473700	1.12853600
C	3.91211100	2.03865600	-0.51304700
C	4.04343900	2.40459100	-1.85641000
C	3.51028200	2.92471300	0.49088900
C	3.75609700	3.72699700	-2.19131400
C	3.21095700	4.23183400	0.10510500
C	3.33398000	4.62908400	-1.22045200
H	3.84774000	4.04195100	-3.23082000
H	2.86240000	4.93751700	0.85743200
H	3.08450100	5.65062200	-1.50093300
C	-2.57234000	4.31895900	-2.25786200
H	-3.30452800	3.54629300	-2.50647500
H	-3.05338100	5.22782600	-1.88228600
H	-1.93651700	4.55412300	-3.11757800
C	3.38073100	2.47880600	1.91374600
H	4.26805200	1.92735600	2.25529700
H	3.23590000	3.33784100	2.57774400
H	2.50972900	1.82196100	2.03865900
C	4.44126800	1.39975900	-2.89558300
H	5.42512500	0.95540800	-2.68890300
H	3.72331800	0.56678300	-2.94102200
H	4.48515400	1.86091700	-3.88862600
C	3.32633600	-2.12088900	2.97022800
H	4.38544300	-2.17714000	3.26156200
H	3.11473000	-1.07287300	2.72191500
H	2.72807900	-2.38407200	3.84988200
C	3.51608700	-3.10724300	-1.97120000
H	2.88878700	-2.26909900	-2.31174800
H	4.55991300	-2.76778500	-2.03151400
H	3.38419600	-3.93216600	-2.68074900
C	-0.28154600	-3.57584000	-2.09694900
H	0.65149400	-3.12336800	-2.48201400
H	0.00313600	-4.51860200	-1.60905400
C	-1.25838800	-3.83645700	-3.23449000
C	-1.74002500	-2.53718400	-3.88082400
H	-2.62106600	-2.72728000	-4.50949900
H	-0.94780100	-2.19577200	-4.56730100
H	-0.78213700	-4.45851300	-4.00691000
H	-2.11309200	-4.39589800	-2.84246700

6a-TS

Zero-point correction= 0.561508 (Hartree/Particle)
Thermal correction to Energy= 0.597608
Thermal correction to Enthalpy= 0.598552
Thermal correction to Gibbs Free Energy= 0.491566
Sum of electronic and zero-point Energies= -1481.995634
Sum of electronic and thermal Energies= -1481.959535
Sum of electronic and thermal Enthalpies= -1481.958590
Sum of electronic and thermal Free Energies= -1482.065576
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1483.31180705
Cartesian coordinates:

C	-1.13168500	2.02762300	-1.10264300
C	-0.39568000	3.15693500	-1.49677700
Au	-0.15086700	0.29101100	-0.40349600
C	0.69002400	-1.51443100	0.13541000
N	1.98717600	-1.86227100	0.27332000
C	0.83972800	-3.67250500	0.76801600
C	2.10113900	-3.18882400	0.66296500
H	0.46237700	-4.64929900	1.04156600
H	3.06673200	-3.65092300	0.82273700
N	-0.01149200	-2.62896500	0.44050800
C	0.70980500	3.26319900	0.59343300
C	-1.78742000	3.14653500	1.24703900
C	-0.39701500	2.57676100	1.12456400
C	2.01521600	3.30290100	1.32188400
H	1.89022000	3.32025200	2.40994300
H	2.61640600	2.41504100	1.06110400
H	2.60118800	4.17992200	1.02206200
O	-2.07448600	4.26551200	0.88332700
C	-2.76411900	2.25165500	1.96185300
H	-3.78026600	2.62928700	1.81738600
H	-2.69209700	1.21110000	1.61555100
H	-2.54391500	2.25286800	3.03898000
C	-2.54177100	1.90632200	-1.45094900
C	-3.27576600	3.02775000	-1.62172200
H	-4.33714600	2.97867300	-1.86360100
H	-2.85156700	4.02152500	-1.49051300
C	-3.16271700	0.54131800	-1.55600300
H	-2.63888400	-0.07771600	-2.29818100
H	-3.11196800	-0.00443400	-0.60124300
H	-4.21721100	0.60356700	-1.84889500
C	-1.44799800	-2.68604500	0.42510400
C	-2.13956700	-2.28375900	1.57286100
C	-2.08259200	-3.10607300	-0.74805400
C	-3.53345400	-2.31181700	1.52334700
C	-3.47758800	-3.12090000	-0.75039800
C	-4.19574700	-2.72777700	0.37322500
H	-4.10110200	-2.01094200	2.40337900
H	-4.00157700	-3.44677400	-1.64816300
H	-5.28366200	-2.75002500	0.35434200
C	3.09221800	-0.97049300	0.05147000
C	3.61797300	-0.87066800	-1.24018000
C	3.58429200	-0.24475000	1.14119600
C	4.69515100	-0.00338300	-1.42631400
C	4.66326200	0.60835400	0.90799100
C	5.21420500	0.72645700	-0.36373200
H	5.13127100	0.09182500	-2.41990400
H	5.07584600	1.17998400	1.73934000
H	6.06029900	1.39121700	-0.52668800

C	2.96439600	-0.36671100	2.50082800
H	3.05348200	-1.38365000	2.90747800
H	3.44313100	0.31638200	3.21156900
H	1.88915000	-0.13135200	2.47604400
C	3.03663900	-1.64994200	-2.38096800
H	2.92856500	-2.71676800	-2.14265200
H	2.03576100	-1.27940200	-2.64783200
H	3.66771100	-1.56781300	-3.27222500
C	-1.41169600	-1.81884600	2.79839600
H	-0.63984000	-2.53177500	3.11884700
H	-0.90019900	-0.85995900	2.62005000
H	-2.10469700	-1.67652200	3.63480500
C	-1.29336200	-3.50114300	-1.95930500
H	-0.65048500	-2.67869000	-2.30697000
H	-0.63325900	-4.35667300	-1.76059800
H	-1.95695400	-3.78019900	-2.78459500
H	-0.17911200	1.87841100	1.94398100
H	-0.61734000	3.58444500	-2.47768800
C	0.59763800	3.73118900	-0.71373400
H	1.30264000	4.44953400	-1.12947800

7a-TS

Zero-point correction= 0.561853 (Hartree/Particle)
Thermal correction to Energy= 0.598228
Thermal correction to Enthalpy= 0.599173
Thermal correction to Gibbs Free Energy= 0.488581
Sum of electronic and zero-point Energies= -1481.971887
Sum of electronic and thermal Energies= -1481.935511
Sum of electronic and thermal Enthalpies= -1481.934567
Sum of electronic and thermal Free Energies= -1482.045159

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1483.28735339

Cartesian coordinates:

C	5.39674400	-0.21568600	0.36035500
C	5.85017900	-0.87105900	-0.92829400
C	4.65983400	-0.93244400	1.28565200
O	5.33689900	-1.87501300	-1.36733200
H	6.09451400	0.53164000	0.75123400
C	4.94636500	-0.81349300	2.75444800
H	5.00116200	-1.80965800	3.21468300
H	5.88678400	-0.29155500	2.95677100
H	4.13583600	-0.27748900	3.26947100
C	7.03072400	-0.20391900	-1.57583800
H	7.22537200	-0.65440900	-2.55234300
H	6.86690600	0.87741300	-1.68219700
H	7.92119500	-0.32684500	-0.94367500
C	1.96827500	-0.25687800	-0.12879300
C	2.51223000	-1.54069300	0.08290400
Au	-0.10784300	-0.09664200	-0.05031600
C	-4.39394900	-0.07888800	0.06528100
C	-4.14167900	1.25256000	0.09196800
H	-5.32052500	-0.63810100	0.07648600
H	-4.79944900	2.11098600	0.13411400
N	-3.16399600	-0.71591600	0.01178000
N	-2.76372500	1.39232500	0.05475200
C	-2.15790500	0.18407800	0.00463100
C	2.71308200	0.93788700	-0.21262600
C	3.88269900	0.96437800	-0.95421300
C	2.20671600	2.19350400	0.44131700

H	1.38851500	2.64126300	-0.14316800
H	1.80538200	1.99359000	1.44371800
H	3.00337700	2.94263700	0.52318300
C	-2.04873400	2.63908600	0.04151700
C	-1.80179800	3.24246500	-1.19651700
C	-1.61074700	3.17146900	1.25795600
C	-1.08526600	4.43916300	-1.19380100
C	-0.90051100	4.37166200	1.21216000
C	-0.64104200	4.99948400	-0.00080200
H	-0.88184800	4.93624600	-2.14157300
H	-0.55375900	4.81676400	2.14425400
H	-0.09183700	5.93908500	-0.01668900
C	-2.97908700	-2.14037800	-0.05509300
C	-2.87122800	-2.73411500	-1.31615500
C	-2.91340400	-2.85725900	1.14354500
C	-2.70003400	-4.11769600	-1.35730200
C	-2.73912300	-4.23766500	1.05308100
C	-2.63572100	-4.86170000	-0.18506300
H	-2.61922700	-4.61212800	-2.32463800
H	-2.68809800	-4.82583600	1.96862800
H	-2.50643100	-5.94107900	-0.23688900
C	-3.01808000	-2.16437200	2.46865000
H	-3.98323000	-1.65342300	2.59132400
H	-2.91549400	-2.87897800	3.29226900
H	-2.23661900	-1.39930600	2.58670000
C	-2.91469200	-1.91554800	-2.57130600
H	-3.75092900	-1.20300000	-2.57573600
H	-1.99361100	-1.32643200	-2.69478400
H	-3.01571100	-2.55757300	-3.45294400
C	-1.86421800	2.46585700	2.55581400
H	-2.90959800	2.14554400	2.65878000
H	-1.24553200	1.55937600	2.64334800
H	-1.62606200	3.11386400	3.40629600
C	-2.27722300	2.61630300	-2.47255400
H	-1.85487600	1.60975400	-2.60851100
H	-3.37027200	2.50706000	-2.49511300
H	-1.98655900	3.22166600	-3.33764000
H	4.40034800	1.91114000	-1.12337100
H	4.04219600	0.19364800	-1.70096800
H	1.83791000	-2.38464900	-0.07048400
C	3.61588700	-1.80973100	0.89614700
H	3.52884700	-2.72952900	1.48492000

6b-TS

Zero-point correction= 0.550164 (Hartree/Particle)
Thermal correction to Energy= 0.585821
Thermal correction to Enthalpy= 0.586766
Thermal correction to Gibbs Free Energy= 0.481373
Sum of electronic and zero-point Energies= -1498.043617
Sum of electronic and thermal Energies= -1498.007959
Sum of electronic and thermal Enthalpies= -1498.007015
Sum of electronic and thermal Free Energies= -1498.112408
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1499.35331680
Cartesian coordinates:

C	-1.29030700	1.92108500	-1.05511800
C	-0.62712500	3.12658400	-1.45395400
Au	-0.18066800	0.25146300	-0.45556000
C	0.77877100	-1.48800600	0.10733900

N	2.09242600	-1.75642900	0.26212000
C	1.04903800	-3.63161900	0.74695200
C	2.28047700	-3.07318300	0.65481700
H	0.72775200	-4.62872300	1.01881100
H	3.27004500	-3.47661200	0.82636200
N	0.14122000	-2.64148000	0.40713100
N	0.36556000	3.69774600	-0.82464300
C	0.55555900	3.22387800	0.41970900
C	-1.88367500	3.26802500	1.30074300
C	-0.50340400	2.70874600	1.17435700
C	1.96822500	3.15924100	0.88835900
H	2.05557500	2.85580500	1.93660500
H	2.53709300	2.45318000	0.26285300
H	2.43575700	4.14265700	0.75331100
O	-2.22488900	4.31975600	0.80006800
C	-2.80180600	2.44567600	2.16446700
H	-3.83151700	2.79398400	2.04472700
H	-2.72950600	1.37609100	1.91611200
H	-2.51816700	2.55215700	3.22096000
C	-2.71117600	1.76834400	-1.28533900
C	-3.47895700	2.87116000	-1.46969100
H	-4.55370100	2.78967900	-1.63115500
H	-3.07123400	3.87984100	-1.44253800
C	-3.31715700	0.39245900	-1.27103000
H	-2.84391000	-0.25344400	-2.02395000
H	-3.17702000	-0.10392300	-0.29859300
H	-4.39316100	0.42472500	-1.47766700
C	-1.29017300	-2.77790700	0.40181200
C	-1.99592200	-2.38490300	1.54462100
C	-1.90788000	-3.26664100	-0.75365000
C	-3.38583200	-2.50068200	1.51001200
C	-3.29918900	-3.36921600	-0.74065500
C	-4.03072700	-2.99131900	0.37951800
H	-3.96349700	-2.21216900	2.38769200
H	-3.80946300	-3.75212500	-1.62362600
H	-5.11508100	-3.08413500	0.37345000
C	3.14614100	-0.79482300	0.08302500
C	3.64905400	-0.58464600	-1.20464900
C	3.61560400	-0.11813800	1.21376300
C	4.67832700	0.34750800	-1.34261300
C	4.65188800	0.79683200	1.02895100
C	5.17940500	1.02600400	-0.23743500
H	5.09570300	0.53105000	-2.33180300
H	5.04367700	1.33538600	1.89160000
H	5.99016900	1.74070600	-0.36443100
C	3.00827500	-0.35019700	2.56454100
H	3.15356600	-1.38117500	2.91568400
H	3.45070500	0.31712900	3.31247200
H	1.92148900	-0.17282500	2.55097900
C	3.10145000	-1.32528500	-2.38716200
H	3.06279200	-2.40919400	-2.21229300
H	2.07643200	-1.00360900	-2.62396100
H	3.71661600	-1.15073100	-3.27618900
C	-1.29082400	-1.83953100	2.75056000
H	-0.43996300	-2.46452400	3.05414700
H	-0.88891800	-0.83202300	2.55767900
H	-1.97459900	-1.76675200	3.60335800
C	-1.10680100	-3.63847900	-1.96444100
H	-0.52216800	-2.78381000	-2.33707900

H	-0.39087400	-4.44503500	-1.75534300
H	-1.75897400	-3.97772600	-2.77609600
H	-0.21194600	2.09535400	2.03441000
H	-0.91378700	3.56250700	-2.41690800

7b-TS

Zero-point correction= 0.550521 (Hartree/Particle)
Thermal correction to Energy= 0.586607
Thermal correction to Enthalpy= 0.587551
Thermal correction to Gibbs Free Energy= 0.478201
Sum of electronic and zero-point Energies= -1498.035050
Sum of electronic and thermal Energies= -1497.998964
Sum of electronic and thermal Enthalpies= -1497.998020
Sum of electronic and thermal Free Energies= -1498.107370
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1499.34341766
Cartesian coordinates:

C	5.26818100	-0.36231200	0.54237100
C	6.10373600	-1.46375300	-0.02698900
C	4.04790700	-0.58145800	1.16657100
O	5.61567800	-2.47791400	-0.48758400
H	5.81361200	0.52322800	0.87586400
C	3.48321100	0.39159800	2.14534700
H	3.13840200	-0.13057400	3.04560100
H	4.19911600	1.16970700	2.42405700
H	2.59255700	0.86268100	1.69085200
C	7.58550200	-1.22479200	0.02489600
H	8.11126900	-2.04052200	-0.47772400
H	7.84267000	-0.26703100	-0.44832400
H	7.92558500	-1.16216000	1.06774000
C	1.84503900	-0.62363400	-0.67186500
C	2.35794600	-1.78799700	0.03116800
Au	-0.14178300	-0.21354500	-0.27500000
N	3.28425500	-1.65487300	0.91331200
C	-4.30862400	0.48188600	0.49421700
C	-3.82705300	1.74872900	0.53328900
H	-5.30781100	0.08580300	0.62158200
H	-4.31343000	2.70029400	0.70444900
N	-3.22849400	-0.34764800	0.23709400
N	-2.46503600	1.65784300	0.29873700
C	-2.09269500	0.37037500	0.11646400
C	2.70347700	0.29069300	-1.26874200
C	4.04623900	-0.07595100	-1.46655600
C	2.22997100	1.66724800	-1.65506000
H	1.42739100	1.60198200	-2.40211600
H	1.81839300	2.21412100	-0.79372800
H	3.03686300	2.26887900	-2.08973600
C	-1.53848800	2.75599600	0.25632500
C	-1.33570400	3.40512500	-0.96589700
C	-0.85440600	3.09244500	1.42929300
C	-0.40464300	4.44350500	-0.99259600
C	0.06795800	4.13657800	1.35461700
C	0.28913600	4.80678500	0.15636300
H	-0.22874900	4.97243300	-1.92864100
H	0.60855800	4.43018000	2.25395700
H	1.00546500	5.62544500	0.11890100
C	-3.29916000	-1.77970200	0.12009600
C	-3.48681500	-2.33452700	-1.14910400
C	-3.16995200	-2.54225800	1.28503200

C	-3.55668300	-3.72508600	-1.23259000
C	-3.24449600	-3.92804600	1.15232200
C	-3.43795000	-4.51324700	-0.09397600
H	-3.70827000	-4.18943700	-2.20625200
H	-3.15138300	-4.55095200	2.04110800
H	-3.49900700	-5.59651400	-0.17829400
C	-2.94987500	-1.89221300	2.61779500
H	-3.77269900	-1.21571400	2.88793900
H	-2.86550800	-2.64382800	3.40986800
H	-2.02876100	-1.29078700	2.62545900
C	-3.58770200	-1.47228300	-2.37126400
H	-4.30514700	-0.65028000	-2.24296200
H	-2.61805200	-1.01445400	-2.61809200
H	-3.90397600	-2.06066400	-3.23921400
C	-1.08338700	2.34502900	2.70858000
H	-2.15110300	2.23867400	2.94271800
H	-0.66837500	1.32664400	2.65676200
H	-0.60542900	2.85678000	3.55101400
C	-2.07479600	2.98471500	-2.20010500
H	-1.87992100	1.93044800	-2.44749800
H	-3.16259200	3.08533000	-2.08353100
H	-1.77678000	3.59270300	-3.06093300
H	4.74738500	0.63216700	-1.90987600
H	4.31838700	-1.12743200	-1.51957000
H	1.84648000	-2.75173100	-0.02974000

6c-TS

Zero-point correction= 0.577525 (Hartree/Particle)
Thermal correction to Energy= 0.615013
Thermal correction to Enthalpy= 0.615957
Thermal correction to Gibbs Free Energy= 0.506018
Sum of electronic and zero-point Energies= -1537.305996
Sum of electronic and thermal Energies= -1537.268509
Sum of electronic and thermal Enthalpies= -1537.267564
Sum of electronic and thermal Free Energies= -1537.377504
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1538.65252571
Cartesian coordinates:

C	1.84447800	-1.32300500	-0.85777000
C	1.59186600	-2.70030300	-1.25555000
Au	0.22276600	-0.10258100	-0.38793600
C	-1.28234000	1.23866900	0.07382100
N	-2.61384800	1.06287100	0.21427300
C	-2.26401400	3.20123400	0.59155900
C	-3.23697900	2.26011500	0.53187700
H	-2.29756500	4.26133900	0.80691100
H	-4.30739900	2.31797900	0.68129500
N	-1.07256400	2.55404100	0.30781000
N	0.79954600	-3.49372200	-0.58889000
C	0.45357000	-3.08665500	0.65017300
C	2.79618600	-2.56364400	1.57937200
C	1.32458200	-2.40842800	1.49168200
C	-0.96027900	-3.36370200	1.03577800
H	-1.19607700	-3.01825000	2.04784400
H	-1.64975800	-2.88909300	0.32167300
H	-1.14124800	-4.44489100	0.97399400
O	3.42523900	-3.40839600	0.96716200
C	3.46061800	-1.61167700	2.53829800
H	4.54748800	-1.67928200	2.43811800
H	3.12494600	-0.57958400	2.35481800

H	3.18581100	-1.85772300	3.57334100
C	3.14902000	-0.71631300	-0.95985400
C	4.26111700	-1.49134800	-1.05139400
H	5.25505200	-1.04397300	-1.07064900
H	4.22236400	-2.57627700	-1.07809400
C	3.26930600	0.78140900	-0.87503600
H	2.66868300	1.27298500	-1.65292600
H	2.90291400	1.16304300	0.08995800
H	4.30930600	1.10841000	-0.99066100
C	0.22418000	3.17458300	0.28822900
C	1.00780500	3.11112000	1.44537400
C	0.64332800	3.79842000	-0.89146400
C	2.26229600	3.72081500	1.40286900
C	1.90552200	4.39238500	-0.88779800
C	2.70540200	4.35775800	0.24897600
H	2.89150300	3.69954900	2.29216900
H	2.25803400	4.89099700	-1.78990100
H	3.68312400	4.83568500	0.23665700
C	-3.29517700	-0.19630200	0.08440300
C	-3.68535600	-0.61719000	-1.19073000
C	-3.54626800	-0.92983200	1.24851200
C	-4.36644000	-1.83178800	-1.28045600
C	-4.23943300	-2.13218800	1.11116900
C	-4.64734000	-2.57785700	-0.14136400
H	-4.68837000	-2.18598500	-2.25890600
H	-4.45487900	-2.72416800	2.00043100
H	-5.18993500	-3.51691800	-0.23096900
C	-3.05990000	-0.45458700	2.58461000
H	-3.50670800	0.50666300	2.87386100
H	-3.30223400	-1.17959400	3.36961000
H	-1.96834400	-0.30694700	2.58352300
C	-3.38020400	0.20060700	-2.40924700
H	-3.69460900	1.24681600	-2.29191400
H	-2.30148900	0.21441400	-2.62466600
H	-3.88900900	-0.20570100	-3.28978000
C	0.53693600	2.39012000	2.67307600
H	-0.50214800	2.63632700	2.93049400
H	0.57908000	1.29748000	2.53276400
H	1.16450600	2.63733700	3.53631300
C	-0.22243900	3.80663500	-2.11484000
H	-0.47401700	2.78466100	-2.43598300
H	-1.17407200	4.32850800	-1.94447100
H	0.28297900	4.30550300	-2.94844900
H	0.87168900	-1.94466000	2.37400800
C	2.12276900	-3.21525100	-2.56145800
H	2.92656700	-3.93805700	-2.36260600
H	1.32535300	-3.76366000	-3.07384800
H	2.50919200	-2.42699800	-3.21362200

7c-TS

Zero-point correction= 0.578218 (Hartree/Particle)
Thermal correction to Energy= 0.615981
Thermal correction to Enthalpy= 0.616925
Thermal correction to Gibbs Free Energy= 0.504534
Sum of electronic and zero-point Energies= -1537.302814
Sum of electronic and thermal Energies= -1537.265051
Sum of electronic and thermal Enthalpies= -1537.264107
Sum of electronic and thermal Free Energies= -1537.376499

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1538.64851749
Cartesian coordinates:

C	5.26650900	0.65461300	0.78542900
C	6.21568700	0.09653500	-0.22133700
C	4.14883200	-0.03677100	1.23498200
O	5.86803600	-0.68717700	-1.08612300
H	5.68875300	1.37772700	1.48633800
C	3.52484400	0.25778200	2.55760000
H	3.38342700	-0.66901500	3.12620200
H	4.11347000	0.96228700	3.15177000
H	2.51954600	0.67767600	2.38197700
C	7.63611700	0.56553000	-0.07951500
H	8.24090200	0.17450200	-0.90166900
H	7.68508400	1.66316200	-0.06890800
H	8.05766200	0.22251000	0.87532100
C	1.86550200	0.31454800	-0.47963300
C	2.63323400	-0.92525400	-0.38631600
Au	-0.15674900	0.07245100	-0.13940400
N	3.55835500	-0.98956600	0.50791500
C	-4.23724500	-1.11420400	0.25739800
C	-4.40539300	0.23151800	0.25366400
H	-4.94694900	-1.92874100	0.32200100
H	-5.29362400	0.84691800	0.31498800
N	-2.87476200	-1.34313400	0.15180600
N	-3.14094400	0.78817100	0.14705900
C	-2.19787600	-0.17629300	0.08421100
C	2.49132100	1.55146900	-0.58705800
C	3.85475500	1.59505100	-0.91106800
C	1.73547000	2.82448300	-0.30827800
H	0.81780500	2.87267200	-0.91036700
H	1.42458400	2.88070100	0.74471500
H	2.33269100	3.71514600	-0.53544100
C	-2.84346700	2.19344200	0.07188200
C	-2.79443700	2.78949400	-1.19259800
C	-2.59022900	2.88583500	1.25987000
C	-2.48373300	4.14816000	-1.24732100
C	-2.28480600	4.24290400	1.15606000
C	-2.23263500	4.86781900	-0.08454900
H	-2.44496900	4.64325700	-2.21692700
H	-2.09093400	4.81225700	2.06441400
H	-1.99925100	5.92910800	-0.14575300
C	-2.24022700	-2.63253900	0.09238200
C	-1.94513600	-3.17037100	-1.16460500
C	-1.92079300	-3.26957900	1.29605400
C	-1.31209500	-4.41357100	-1.19543000
C	-1.28442200	-4.50766400	1.21588900
C	-0.98569300	-5.07580400	-0.01768900
H	-1.07817200	-4.86389300	-2.15955100
H	-1.02597800	-5.03028700	2.13605600
H	-0.49627900	-6.04691100	-0.06118000
C	-2.23876700	-2.63767800	2.61740600
H	-3.31943800	-2.49831600	2.75852800
H	-1.87552400	-3.25750100	3.44403300
H	-1.77548200	-1.64468700	2.71127400
C	-2.26183600	-2.43031900	-2.42916400
H	-3.26625800	-1.98602600	-2.41376200
H	-1.55079100	-1.60556600	-2.59411500
H	-2.20126100	-3.09578000	-3.29715400
C	-2.62732700	2.19271700	2.58830600

H	-3.57213500	1.65635000	2.74993500
H	-1.82117000	1.44903400	2.67447900
H	-2.50732700	2.91043700	3.40692300
C	-3.04923600	1.99478400	-2.43773800
H	-2.28383100	1.21750400	-2.58170000
H	-4.02055300	1.48209500	-2.40974600
H	-3.03874000	2.64011700	-3.32253000
H	4.37491300	2.55146200	-0.97517800
H	4.31720900	0.75373600	-1.42027700
C	2.22388200	-2.15418100	-1.12260900
H	1.39208700	-2.65179700	-0.60126600
H	1.86935900	-1.89963200	-2.12952700
H	3.06674700	-2.84975300	-1.18683300

6d-TS

Zero-point correction= 0.592823 (Hartree/Particle)
Thermal correction to Energy= 0.633311
Thermal correction to Enthalpy= 0.634255
Thermal correction to Gibbs Free Energy= 0.516156
Sum of electronic and zero-point Energies= -1725.749870
Sum of electronic and thermal Energies= -1725.709382
Sum of electronic and thermal Enthalpies= -1725.708438
Sum of electronic and thermal Free Energies= -1725.826537

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1727.16892638

Cartesian coordinates:

C	2.09675900	0.36127200	-0.10618000
C	2.94648300	-0.79349300	-0.18544200
Au	0.01929600	0.10447600	-0.12921900
C	-2.04010300	0.00664700	-0.20142400
N	-2.86752800	-1.05961200	-0.22000300
C	-4.18135500	0.70436800	-0.26814900
C	-4.19207900	-0.65072100	-0.26251100
H	-4.98214700	1.43192100	-0.29525700
H	-5.00434800	-1.36563500	-0.28590500
N	-2.85035600	1.08801100	-0.22983000
N	2.82829000	-1.87354700	0.54325900
C	1.97514900	-1.73988600	1.57468700
C	2.78317900	0.50253900	2.58713400
C	1.75492300	-0.50676500	2.19574500
C	1.17828300	-2.95112700	1.91595400
H	0.56132000	-2.81632400	2.81019700
H	0.52832600	-3.22156300	1.06859500
H	1.86117800	-3.79673000	2.06737700
O	3.97596500	0.31800200	2.46159300
C	2.21491000	1.74537300	3.21899100
H	2.99194500	2.51153900	3.29128600
H	1.35531000	2.12587100	2.64698100
H	1.85422900	1.51848800	4.23208600
C	2.63694500	1.69373400	-0.25637200
C	3.95277100	1.91739900	-0.00496300
H	4.37235200	2.92057200	-0.08201100
H	4.63851000	1.13054500	0.30424400
C	1.71247600	2.82090600	-0.62511800
H	1.20482600	2.61651500	-1.57820600
H	0.92257000	2.96155500	0.12848400
H	2.25397400	3.76891500	-0.72318800
C	-2.36546400	2.44103500	-0.18728100
C	-2.07866800	3.00238600	1.06213300

C	-2.17490400	3.11705400	-1.39648000
C	-1.58476600	4.30712200	1.07937700
C	-1.68406300	4.42125400	-1.32987300
C	-1.39266700	5.01071000	-0.10492000
H	-1.36106100	4.77614700	2.03709900
H	-1.53121100	4.97673700	-2.25438300
H	-1.01625200	6.03134900	-0.07213000
C	-2.43226200	-2.42849800	-0.15859900
C	-2.06342200	-3.06824300	-1.34600400
C	-2.40248600	-3.05105200	1.09377600
C	-1.65478900	-4.39932100	-1.25231100
C	-1.99754000	-4.38498700	1.13696300
C	-1.62852500	-5.05307700	-0.02569400
H	-1.36515000	-4.92805500	-2.15947500
H	-1.96939400	-4.89959900	2.09720400
H	-1.31745600	-6.09469300	0.02449600
C	-2.76658100	-2.30341300	2.34110000
H	-3.81922400	-1.98828900	2.34611000
H	-2.60527700	-2.92328700	3.23002600
H	-2.16382400	-1.38830600	2.45054200
C	-2.10227300	-2.35285700	-2.66268800
H	-3.06765200	-1.85674200	-2.83279600
H	-1.32836000	-1.57326800	-2.72094600
H	-1.93310300	-3.04978600	-3.49032900
C	-2.27007600	2.22680200	2.33120300
H	-3.24713800	1.72630100	2.37099100
H	-1.50736600	1.43873800	2.43631000
H	-2.19263000	2.88226700	3.20552500
C	-2.45901200	2.45359000	-2.70994200
H	-1.83437200	1.55823300	-2.84990100
H	-3.50438400	2.12629100	-2.79159800
H	-2.25896100	3.13473800	-3.54375700
H	0.84271100	-0.44308800	2.79964400
C	4.00137600	-0.84939200	-1.27157600
O	5.16994400	-1.01179900	-1.04425600
O	3.44520400	-0.69026000	-2.46962200
C	4.36175500	-0.74621300	-3.57350000
H	3.75385200	-0.61690100	-4.46920300
H	5.10347400	0.05398100	-3.48615300
H	4.87477200	-1.71245000	-3.58757000

7d-TS

Zero-point correction= 0.594141 (Hartree/Particle)
Thermal correction to Energy= 0.634447
Thermal correction to Enthalpy= 0.635391
Thermal correction to Gibbs Free Energy= 0.517581
Sum of electronic and zero-point Energies= -1725.749656
Sum of electronic and thermal Energies= -1725.709351
Sum of electronic and thermal Enthalpies= -1725.708406
Sum of electronic and thermal Free Energies= -1725.826217
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1727.16468421
Cartesian coordinates:

C	-4.98869800	-1.47522700	0.88950200
C	-6.02101400	-0.93736500	-0.05129400
C	-3.97291300	-0.68788300	1.41565600
O	-5.78257800	-0.02828700	-0.82249300
H	-5.30549700	-2.31211100	1.51559700
C	-3.29407500	-1.02738600	2.69869900

H	-3.25373600	-0.14822400	3.35248200
H	-3.78291100	-1.85242700	3.22372900
H	-2.24905900	-1.30309900	2.47398500
C	-7.36521900	-1.59991800	0.03874500
H	-8.02985600	-1.19929000	-0.73078600
H	-7.27071900	-2.68838400	-0.07895800
H	-7.81009500	-1.42788400	1.02848100
C	-1.67193700	-0.63723800	-0.31839200
C	-2.56616500	0.48506600	-0.08626000
Au	0.32768100	-0.21700300	-0.02221400
N	-3.50364100	0.39718600	0.78870000
C	4.35391900	1.19368200	0.07496200
C	4.58449600	-0.14054300	-0.00435500
H	5.02746600	2.04042300	0.09661700
H	5.50235200	-0.71084300	-0.06455000
N	2.97891700	1.35701300	0.12442700
N	3.34331300	-0.75626900	-0.00108100
C	2.35480600	0.16086800	0.07720400
C	-2.16708300	-1.91838500	-0.51598000
C	-3.52889800	-2.07867700	-0.83310500
C	3.09801300	-2.16934600	-0.10559600
C	2.90188900	-2.71372700	-1.37916000
C	3.02769700	-2.92064900	1.07152300
C	2.63355000	-4.08078200	-1.45569900
C	2.75578700	-4.28294500	0.94610200
C	2.56133600	-4.85748500	-0.30484000
H	2.48580700	-4.53647600	-2.43424400
H	2.70220900	-4.89650400	1.84476100
H	2.35804100	-5.92380900	-0.38427100
C	2.28348700	2.61476800	0.18370400
C	1.75284400	3.13964200	-0.99808700
C	2.14532200	3.23281300	1.43244000
C	1.06581800	4.35135200	-0.90373800
C	1.45494800	4.44205700	1.47642100
C	0.92281100	4.99809800	0.31724800
H	0.64503700	4.78647600	-1.81035900
H	1.33607500	4.95003200	2.43270600
H	0.39508000	5.94948100	0.36809900
C	2.70209600	2.60563800	2.67480000
H	3.79930900	2.55034300	2.65614000
H	2.41726400	3.18000300	3.56276200
H	2.33405900	1.57740500	2.80529400
C	1.87039000	2.42801200	-2.31113600
H	2.82229500	1.89070000	-2.41574900
H	1.05598900	1.69604600	-2.42505300
H	1.78682100	3.13506800	-3.14406700
C	3.21659500	-2.28151800	2.41391600
H	4.17251700	-1.74525600	2.48603900
H	2.42438000	-1.54757100	2.62276700
H	3.19541500	-3.03253200	3.21087900
C	2.95119200	-1.85793200	-2.60885100
H	2.10613600	-1.15312200	-2.64053800
H	3.86809600	-1.25486000	-2.65806400
H	2.90599500	-2.47197800	-3.51467500
H	-4.06785300	-1.25890000	-1.30086600
H	-3.94226800	-3.07759100	-0.97808100
C	-1.27649800	-3.12313800	-0.36284700
H	-0.44910100	-3.08721700	-1.08551500
H	-0.81706300	-3.16050600	0.63480000

H	-1.82165400	-4.05987100	-0.52783500
C	-2.26643300	1.81961600	-0.72917400
O	-1.45295300	1.93052500	-1.61732100
O	-3.01224300	2.78755600	-0.23171600
C	-2.82241400	4.07678400	-0.82446900
H	-3.02660100	4.03096200	-1.89887500
H	-3.53064800	4.73811200	-0.32447700
H	-1.79193700	4.41324700	-0.66296300

6g-TS

Zero-point correction= 0.804065 (Hartree/Particle)
Thermal correction to Energy= 0.854967
Thermal correction to Enthalpy= 0.855911
Thermal correction to Gibbs Free Energy= 0.719008
Sum of electronic and zero-point Energies= -2415.845401
Sum of electronic and thermal Energies= -2415.794499
Sum of electronic and thermal Enthalpies= -2415.793555
Sum of electronic and thermal Free Energies= -2415.930458
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2417.58324421
Cartesian coordinates:

C	1.41395300	0.25290400	0.10720000
C	1.73658900	-1.11720200	-0.15520700
N	2.07118700	-1.47531800	-1.43840400
S	1.95538600	-3.17247700	-1.91751700
O	0.66409000	-3.69871900	-1.51812000
O	2.33937600	-3.14999200	-3.31687300
Au	-0.69866100	0.33679000	0.08614900
C	-2.72495700	0.42306800	-0.21467700
N	-3.63046000	-0.57439200	-0.13615900
C	-4.75387900	1.19378900	-0.81193600
C	-4.88873900	-0.11885100	-0.50236600
H	-5.47068700	1.93325700	-1.14433700
H	-5.74912200	-0.77513400	-0.50825300
N	-3.41602500	1.50670700	-0.62786200
N	1.56233600	-2.11386300	0.72277100
C	0.90475400	-1.85909000	1.84835300
C	1.66331500	0.37727800	2.87149600
C	0.65610000	-0.57174600	2.38893800
O	2.87144900	0.20851100	2.77832500
C	1.09516800	1.58280900	3.58386500
H	1.87471800	2.33964100	3.71480000
H	0.24059000	2.00916100	3.04009400
H	0.73364600	1.29242800	4.58009900
C	1.90484100	-0.50933700	-2.52406800
H	0.87647300	-0.11009600	-2.52517200
H	2.60172000	0.32637000	-2.40394500
H	2.11071100	-1.01083100	-3.47176900
C	2.26144400	1.37766700	0.11325200
C	3.66878400	1.31288700	0.13410700
C	1.56796100	2.72939100	0.12666300
H	1.59321600	3.21324100	-0.86117800
H	0.50740700	2.61567900	0.38361000
H	2.00063900	3.43095900	0.84977400
C	-2.80005900	2.78644700	-0.84502800
C	-2.64306100	3.64125500	0.25043700
C	-2.34208200	3.09027800	-2.13115900
C	-2.00757200	4.86224000	0.02316300
C	-1.71248100	4.32164800	-2.31108700

C	-1.54886400	5.19960500	-1.24520900
H	-1.87906000	5.55500500	0.85414600
H	-1.35148100	4.59144800	-3.30296800
H	-1.06219600	6.15982100	-1.40588100
C	-3.32338200	-1.91026100	0.29903100
C	-2.69219900	-2.78396500	-0.59276400
C	-3.67113900	-2.26458800	1.60836600
C	-2.42274800	-4.07633700	-0.13708000
C	-3.40249700	-3.57232300	2.01106600
C	-2.78833300	-4.47056700	1.14355500
H	-1.92117600	-4.77378600	-0.80628900
H	-3.67647000	-3.88316600	3.01897200
H	-2.58478500	-5.48748000	1.47445100
C	3.27095700	-3.93160100	-0.99763400
H	4.20566500	-3.44078700	-1.28461500
H	3.06210900	-3.83958300	0.06955800
H	3.28530200	-4.98044700	-1.31295800
C	-4.29278300	-1.27127900	2.54437100
H	-5.31936600	-1.00860700	2.25335400
H	-4.33602900	-1.67079100	3.56340400
H	-3.72112500	-0.33106100	2.57197800
C	-2.30721400	-2.35999900	-1.97801300
H	-3.07738400	-1.73424600	-2.44956300
H	-1.37238000	-1.77673200	-1.96520000
H	-2.12665200	-3.23124000	-2.61599800
C	-3.11347200	3.24847800	1.61879200
H	-4.15331800	2.89417800	1.61442700
H	-2.50253200	2.43037900	2.03207200
H	-3.05011100	4.09401200	2.31224600
C	-2.50797000	2.12022300	-3.26174600
H	-2.03687700	1.15166200	-3.03419200
H	-3.56574000	1.91401700	-3.47611900
H	-2.05496800	2.50846100	-4.18025500
C	4.40169900	2.63322700	0.04391100
H	3.71093700	3.34402700	-0.42619100
C	4.45518700	0.03194400	0.29080200
H	3.75680600	-0.74004000	0.63499400
H	-0.28506200	-0.50064600	2.94956400
C	0.24406100	-3.04005000	2.48341800
H	-0.84670000	-2.88258200	2.48125400
H	0.45287600	-3.95171600	1.91546500
H	0.55073400	-3.16547200	3.52963200
C	4.69450700	3.18557200	1.45435500
H	5.56116800	2.69058000	1.90401200
H	4.91840200	4.25706300	1.38027600
H	3.84895700	3.05238400	2.14071700
C	5.66272800	2.67498100	-0.81781600
H	6.00243800	3.71705700	-0.87532300
H	6.49295300	2.09107500	-0.40661400
H	5.47246500	2.33661600	-1.84391900
C	5.53361100	0.09517700	1.38105400
H	5.92422900	-0.92051100	1.52511100
H	6.38538600	0.72749300	1.10518400
H	5.11956100	0.42841300	2.33582800
C	5.10501900	-0.47358900	-1.01002200
H	4.41035800	-0.56099100	-1.85243900
H	5.94270300	0.15701800	-1.32355900
H	5.51703700	-1.47315000	-0.81513900

7g-TS

Zero-point correction= 0.805855 (Hartree/Particle)
Thermal correction to Energy= 0.855664
Thermal correction to Enthalpy= 0.856608
Thermal correction to Gibbs Free Energy= 0.724240
Sum of electronic and zero-point Energies= -2415.831282
Sum of electronic and thermal Energies= -2415.781473
Sum of electronic and thermal Enthalpies= -2415.780529
Sum of electronic and thermal Free Energies= -2415.912897
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2417.57036125
Cartesian coordinates:

C	4.13670800	-0.52046100	-1.24834300
C	4.98225100	0.61383300	-0.81568400
C	2.84639400	-0.29552400	-1.72646600
O	4.55133400	1.61971400	-0.27256900
H	4.68059600	-1.33870700	-1.72447700
C	2.22268300	-1.14364700	-2.78679700
H	1.91286000	-0.50278200	-3.62192300
H	2.89125000	-1.92464400	-3.16142100
H	1.30211500	-1.60362600	-2.39274200
C	6.43831700	0.50189500	-1.19793100
H	7.03373500	1.21902000	-0.62486600
H	6.83489500	-0.51233600	-1.06185300
H	6.54565300	0.74242600	-2.26526600
C	1.16228500	-0.20162700	0.63504700
C	1.63941700	0.95720100	-0.13346100
Au	-0.92523600	-0.28039100	0.33998100
N	2.12848900	0.74566700	-1.31389400
C	-5.11115400	0.16236100	-0.33792100
C	-4.99439400	-1.16888800	-0.56947800
H	-5.96355000	0.82795800	-0.37738200
H	-5.72230600	-1.91771500	-0.85348100
N	-3.84571000	0.62075000	-0.00928100
N	-3.65861300	-1.48708500	-0.37621400
C	-2.95053200	-0.38852000	-0.03523700
C	1.87455700	-1.29178200	1.04928100
N	1.29551700	2.22618200	0.25526500
C	0.58051600	2.49140300	1.50831400
H	-0.50152200	2.59993200	1.34556000
H	0.75792800	1.65646100	2.18961500
H	0.96837800	3.41118000	1.95304200
S	1.13514800	3.49347600	-0.93246000
O	0.27826300	3.01432700	-2.00299900
O	0.75430500	4.65251200	-0.14541800
C	3.33606300	-1.44795600	1.06912700
C	1.10363500	-2.47265400	1.62408400
H	0.07917700	-2.15368500	1.84511500
H	1.03534500	-3.33925500	0.95396500
H	1.54737100	-2.81932000	2.57029800
C	-3.05578400	-2.77899900	-0.55413200
C	-3.01364500	-3.65204200	0.53708300
C	-2.49307100	-3.07707400	-1.79948400
C	-2.38343900	-4.88214400	0.34959500
C	-1.87125500	-4.31755700	-1.94049200
C	-1.81812300	-5.21191700	-0.87707800
H	-2.34279500	-5.58755700	1.17894100
H	-1.43297500	-4.58325400	-2.90211600
H	-1.33819700	-6.18015300	-1.00824500
C	-3.47101400	1.98189600	0.26782300

C	-3.59992300	2.45583600	1.57715800
C	-2.93009500	2.73683800	-0.77824700
C	-3.15993400	3.75498900	1.83098400
C	-2.49652000	4.02765100	-0.47475000
C	-2.60707500	4.52972800	0.81648000
H	-3.24655300	4.15485700	2.84086100
H	-2.04551200	4.63157900	-1.26039500
H	-2.24769600	5.53366100	1.03391800
C	2.78288700	3.75109500	-1.54077300
H	3.05781300	2.92679900	-2.19987400
H	2.73851800	4.70107700	-2.08423900
H	3.47023100	3.81292000	-0.69362700
C	-2.78034000	2.16529100	-2.15516900
H	-3.69798300	1.66743000	-2.49869600
H	-2.51988100	2.94758800	-2.87505300
H	-1.96935800	1.42166700	-2.18316300
C	-4.16046600	1.59160200	2.66611000
H	-5.19977300	1.29577800	2.46699100
H	-3.58210600	0.66282400	2.78100500
H	-4.14576700	2.11651200	3.62736200
C	-2.53249100	-2.09102600	-2.92787900
H	-3.54206100	-1.69243200	-3.09656200
H	-1.88228500	-1.22613000	-2.72539000
H	-2.19409200	-2.55217000	-3.86224400
C	-3.60316000	-3.26859600	1.86046900
H	-3.10155000	-2.38457300	2.28159600
H	-4.66960000	-3.01786800	1.78052100
H	-3.50681100	-4.08546100	2.58374600
C	4.09917900	-0.62128900	2.08598600
H	4.04544000	-1.39833800	2.88759800
C	3.81796300	-2.86616300	0.79719700
H	3.35152300	-3.40427700	1.64582800
C	3.39756200	0.60647900	2.65383200
H	3.33463400	1.40240900	1.90134500
H	2.39750600	0.38359900	3.04124800
H	3.99929400	0.99277600	3.48570500
C	5.59076600	-0.29058200	1.92064800
H	5.70614700	0.76511700	1.65729100
H	6.10657200	-0.44648600	2.87596000
H	6.10864700	-0.88454700	1.16761400
C	5.30516600	-3.18467900	0.89654100
H	5.74841600	-2.92558100	1.86374900
H	5.42929300	-4.26688300	0.76477300
H	5.88543600	-2.69998900	0.10047300
C	3.26428700	-3.50992700	-0.47732100
H	3.22686100	-4.59917300	-0.35387800
H	2.26073900	-3.16585800	-0.74840800
H	3.92893000	-3.30679500	-1.32590000

6i-TS

Zero-point correction= 0.716391 (Hartree/Particle)
Thermal correction to Energy= 0.763544
Thermal correction to Enthalpy= 0.764488
Thermal correction to Gibbs Free Energy= 0.633874
Sum of electronic and zero-point Energies= -2411.136539
Sum of electronic and thermal Energies= -2411.089387
Sum of electronic and thermal Enthalpies= -2411.088443
Sum of electronic and thermal Free Energies= -2411.219057

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2412.78025121
Cartesian coordinates:

C	1.23717700	-0.08812500	0.36049700
C	1.33409900	-1.50828100	-0.04479600
N	1.72536900	-1.81667800	-1.31793100
S	1.62645200	-3.48710200	-1.88386300
O	0.26542100	-3.96234600	-1.73714200
O	2.24746300	-3.43192000	-3.19400300
Au	-0.78248800	0.42518900	0.26632100
C	-2.75792100	0.82314900	-0.16101400
N	-3.76072900	-0.06938200	-0.31155500
C	-4.59814600	1.87152600	-0.92380000
C	-4.90412400	0.55839800	-0.78064500
H	-5.18515100	2.71587600	-1.26111500
H	-5.81699800	0.00786100	-0.96673100
N	-3.27497900	2.01225800	-0.53737300
N	0.86984500	-2.46902900	0.72778100
C	0.57513700	-2.06661900	1.97723300
C	2.79903100	-1.01663200	2.58466200
C	1.32805300	-1.09796700	2.63556000
O	3.50167500	-1.74256800	1.89364300
C	3.39929400	0.03034000	3.48422800
H	4.47217900	0.12148900	3.29074100
H	2.90436400	1.00069100	3.33206700
H	3.24896000	-0.23955900	4.53863100
C	1.86799000	-0.80045000	-2.36117800
H	1.09268100	-0.03150000	-2.24091300
H	2.85480300	-0.32338400	-2.32479800
H	1.75469900	-1.28162700	-3.33479300
C	2.28475600	0.86441600	0.29631700
C	3.56950100	0.42471300	0.03354300
C	1.94394900	2.29711500	0.60984600
H	1.62121500	2.85022100	-0.28594800
H	1.10673400	2.33817700	1.31949500
H	2.78986700	2.83545900	1.05400100
C	-2.50601500	3.22671900	-0.57039800
C	-2.45693800	4.01533700	0.58280900
C	-1.80986800	3.53400200	-1.74426300
C	-1.67582900	5.16994400	0.53469300
C	-1.04218600	4.69844800	-1.74618000
C	-0.97678800	5.50870300	-0.61800200
H	-1.62304300	5.80977800	1.41479500
H	-0.49672000	4.97123000	-2.64907500
H	-0.37911400	6.41810500	-0.63948700
C	-3.64974100	-1.47235800	-0.00664000
C	-2.98607000	-2.31513600	-0.90559600
C	-4.20707000	-1.92162700	1.19775700
C	-2.89683000	-3.66773100	-0.56854200
C	-4.11005400	-3.28281600	1.48176000
C	-3.46310100	-4.14777800	0.60481900
H	-2.36462600	-4.33980300	-1.24001700
H	-4.54250100	-3.66199100	2.40720200
H	-3.39462100	-5.20767000	0.84309100
C	2.73200500	-4.31893700	-0.76953200
H	3.72855600	-3.88927300	-0.90519900
H	2.37898900	-4.19968600	0.25645500
H	2.72494900	-5.37109000	-1.07278900
C	-4.85174900	-0.96942600	2.16028100
H	-5.77538900	-0.52893900	1.76036800

H	-5.11050400	-1.47765100	3.09537000
H	-4.18101900	-0.13195500	2.40580000
C	-2.36618300	-1.80815300	-2.17315400
H	-2.95790700	-1.00845000	-2.63880200
H	-1.35865600	-1.40247100	-1.98178000
H	-2.24643100	-2.62049900	-2.89780500
C	-3.19716500	3.62287300	1.82546600
H	-4.26254500	3.43883600	1.63121700
H	-2.78874500	2.69816500	2.25915500
H	-3.12687300	4.40718000	2.58667300
C	-1.87141000	2.63522300	-2.94246400
H	-1.44010600	1.64560200	-2.72467800
H	-2.90302700	2.46101500	-3.27783900
H	-1.31686800	3.06527800	-3.78345500
H	0.87484600	-0.64053200	3.51934400
C	-0.65755100	-2.65114800	2.57427600
H	-1.54385200	-2.21622400	2.08319400
H	-0.69311600	-3.72622300	2.36021800
H	-0.72812900	-2.48159700	3.65280800
H	3.69115300	-0.65443700	-0.06351900
C	4.80985200	1.14980200	-0.06535500
C	5.98629300	0.41758800	0.19737400
C	4.92389400	2.50785200	-0.42163700
C	7.22681900	1.03083500	0.15422700
H	5.89628000	-0.63381700	0.47227600
C	6.17070300	3.10770600	-0.49373600
H	4.03855800	3.07864400	-0.69051200
C	7.32041500	2.37730700	-0.19414700
H	8.12489700	0.46037400	0.38027100
H	6.25187100	4.15144700	-0.78947800
H	8.29529600	2.85828000	-0.24406000

7i-TS

Zero-point correction= 0.716466 (Hartree/Particle)
Thermal correction to Energy= 0.763704
Thermal correction to Enthalpy= 0.764648
Thermal correction to Gibbs Free Energy= 0.634215
Sum of electronic and zero-point Energies= -2411.141577
Sum of electronic and thermal Energies= -2411.094339
Sum of electronic and thermal Enthalpies= -2411.093395
Sum of electronic and thermal Free Energies= -2411.223828
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2412.78261763
Cartesian coordinates:

C	-3.84543500	-0.00950200	1.51848800
C	-4.84716800	1.03453800	1.16133700
C	-2.53141400	0.29979200	1.89221000
O	-4.54561000	2.10309200	0.65738000
H	-4.27240800	-0.89437500	1.99992000
C	-1.78976500	-0.53710700	2.87867300
H	-1.10397200	0.08577900	3.46446700
H	-2.44523100	-1.10714200	3.54402300
H	-1.16169400	-1.24442600	2.30555400
C	-6.27026500	0.66637400	1.47438700
H	-6.95126100	1.40297400	1.03907100
H	-6.50840800	-0.33811000	1.09600200
H	-6.41776300	0.63967400	2.56322800
C	-1.07535600	0.03780500	-0.51694300
C	-1.37433700	1.33278400	0.10901600

Au	0.94961300	-0.38448500	-0.33282100
N	-1.85269900	1.28317200	1.31579300
C	5.15364700	-0.42266200	0.32593200
C	4.89463900	-1.72950100	0.58216300
H	6.07173500	0.14897900	0.36213500
H	5.53730700	-2.54478200	0.88797700
N	3.94720600	0.15882400	-0.02715600
N	3.53524600	-1.91017200	0.37709100
C	2.95177200	-0.75171200	0.00361400
C	-2.07475300	-0.87490300	-0.76195300
N	-0.96303800	2.50591500	-0.45247900
C	-0.31481900	2.52338100	-1.76850500
H	0.77628200	2.41736300	-1.68480700
H	-0.71839200	1.69775000	-2.36123600
H	-0.54409900	3.46939100	-2.26343800
S	-0.70031300	3.91600800	0.54517300
O	0.02541800	3.50584100	1.73330100
O	-0.13911400	4.89267700	-0.36908600
C	-3.43454700	-0.42290800	-0.67558100
C	-1.73847300	-2.30782900	-1.06966200
H	-0.71708300	-2.38006900	-1.46248700
H	-1.77007200	-2.93076200	-0.16167800
H	-2.42409900	-2.75260500	-1.80097500
C	2.79710300	-3.12951600	0.55918600
C	2.60952100	-3.96567400	-0.54516900
C	2.25346300	-3.38887000	1.82163900
C	1.85268200	-5.12155400	-0.35160500
C	1.50177400	-4.55430100	1.96790000
C	1.30510000	-5.41339300	0.89215100
H	1.69709600	-5.79846600	-1.19095700
H	1.07392400	-4.78949400	2.94203800
H	0.72366000	-6.32374200	1.02650100
C	3.72203400	1.53725600	-0.37254300
C	3.97513200	1.93464900	-1.69078500
C	3.19050100	2.38998500	0.60091200
C	3.68072700	3.25481400	-2.02910400
C	2.91156400	3.70207100	0.21468700
C	3.14872600	4.12857700	-1.08607100
H	3.86527600	3.59344600	-3.04814100
H	2.48336500	4.38597600	0.94572900
H	2.90295700	5.15087400	-1.36712700
C	-2.35142500	4.40221500	0.97095000
H	-2.85759100	3.58144000	1.48412700
H	-2.25230600	5.27947300	1.61875700
H	-2.88008900	4.66031700	0.04920700
C	2.87801300	1.91969400	1.98994800
H	3.58858200	1.16267100	2.34771800
H	2.88297800	2.76016400	2.69245700
H	1.86793300	1.47991900	2.03498800
C	4.51181400	0.96888300	-2.70422000
H	5.52879000	0.63252400	-2.45906000
H	3.88630600	0.06631700	-2.77317900
H	4.54929400	1.42787700	-3.69800000
C	2.45231300	-2.43680900	2.96234500
H	3.51546200	-2.24492700	3.16170100
H	1.98971900	-1.45979400	2.75405000
H	2.00753700	-2.83064700	3.88279900
C	3.17187300	-3.61756100	-1.89013000
H	2.65201400	-2.75104200	-2.32614900

H	4.23728000	-3.35571200	-1.84037400
H	3.06401500	-4.45475600	-2.58811200
H	-3.54781600	0.65569200	-0.79788200
C	-4.63604200	-1.17153800	-1.02225400
C	-5.65238900	-0.48638100	-1.70849000
C	-4.84617400	-2.51265200	-0.66215800
C	-6.82784200	-1.13435300	-2.06253500
H	-5.50756300	0.56347500	-1.96557100
C	-6.03211400	-3.14908700	-0.99497500
H	-4.09021000	-3.04411700	-0.08645700
C	-7.02022500	-2.46543700	-1.70356300
H	-7.59989600	-0.59731300	-2.60917600
H	-6.19140000	-4.18427500	-0.70056500
H	-7.94627100	-2.97176900	-1.96821300

6k-TS

Zero-point correction= 0.632158 (Hartree/Particle)
Thermal correction to Energy= 0.672296
Thermal correction to Enthalpy= 0.673240
Thermal correction to Gibbs Free Energy= 0.557276
Sum of electronic and zero-point Energies= -1728.843436
Sum of electronic and thermal Energies= -1728.803298
Sum of electronic and thermal Enthalpies= -1728.802354
Sum of electronic and thermal Free Energies= -1728.918318

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1730.29526614

Cartesian coordinates:

C	1.35228400	-1.03975100	-0.57469700
C	1.28930000	-2.29539700	-1.27351200
Au	-0.49555200	-0.06020600	-0.28392000
C	-2.22858500	1.01310800	0.01310900
N	-3.51829000	0.61356400	0.01444400
C	-3.57229900	2.76772700	0.45683100
C	-4.36244100	1.68070600	0.28507100
H	-3.80471400	3.80027400	0.68285800
H	-5.43668600	1.55520700	0.32619700
N	-2.26642900	2.33650600	0.28656600
N	0.58982400	-3.33197400	-0.88136500
C	0.11470700	-3.16293900	0.36617600
C	2.23965700	-2.36853400	1.59746300
C	0.78219100	-2.32097200	1.26857300
C	-1.21610400	-3.75856700	0.65798600
H	-1.53995300	-3.59037700	1.69043700
H	-1.97144800	-3.34667500	-0.02912400
H	-1.17529700	-4.83831600	0.46291900
O	3.00741500	-3.17282500	1.10952900
C	2.67384000	-1.37245000	2.63863100
H	3.74915100	-1.18717500	2.54420800
H	2.11430000	-0.43013200	2.56266100
H	2.48701700	-1.78782400	3.63905000
C	2.57693500	-0.29847300	-0.49267200
C	3.75050500	-0.99015700	-0.69609600
H	3.65796900	-2.07053800	-0.82685700
C	2.54051900	1.15235600	-0.09460000
H	2.39142200	1.81484200	-0.96051900
H	1.70305800	1.35126400	0.58915200
H	3.46405800	1.46153300	0.41047100
C	-1.09462200	3.16177900	0.39858300
C	-0.41626500	3.19293300	1.62147400
C	-0.67971300	3.87700800	-0.72976100

C	0.72149800	3.99677500	1.70168100
C	0.46410700	4.66467800	-0.60321600
C	1.15610600	4.72671300	0.60132000
H	1.26603300	4.05033300	2.64389600
H	0.80871100	5.23829900	-1.46284500
H	2.04122000	5.35455100	0.68462600
C	-3.96183000	-0.73586400	-0.20736200
C	-4.19746500	-1.15385100	-1.52085100
C	-4.15127200	-1.55806200	0.90817200
C	-4.65869600	-2.45824900	-1.70241800
C	-4.62349900	-2.85020400	0.67897500
C	-4.87828700	-3.29484600	-0.61396200
H	-4.85636600	-2.81287800	-2.71313800
H	-4.78874200	-3.51245800	1.52860600
H	-5.25056700	-4.30468200	-0.77526300
C	-3.82878900	-1.07638000	2.29060900
H	-4.40941600	-0.18587800	2.56856200
H	-4.03730300	-1.85322400	3.03452000
H	-2.76658700	-0.79879000	2.37866200
C	-3.95594300	-0.24096000	-2.68481400
H	-4.45268400	0.73066200	-2.55767700
H	-2.88348500	-0.03585600	-2.81769400
H	-4.32530200	-0.68712700	-3.61421900
C	-0.86544900	2.36762200	2.79012600
H	-1.95293300	2.40743200	2.93895000
H	-0.60264600	1.30599400	2.64930700
H	-0.38624500	2.70614200	3.71529300
C	-1.42937800	3.78647900	-2.02434100
H	-1.50022800	2.74685000	-2.37667700
H	-2.45794300	4.16161500	-1.93211600
H	-0.93321600	4.37223400	-2.80532800
H	0.17458000	-1.94369900	2.09969900
H	1.78331500	-2.36731000	-2.24773400
C	5.12043200	-0.53574000	-0.66407400
C	5.53608300	0.76604000	-0.99909100
C	6.09224600	-1.48302000	-0.28744200
C	6.87849100	1.10620200	-0.94189200
H	4.81060800	1.49512900	-1.35279500
C	7.42895000	-1.12873100	-0.20271100
H	5.77046300	-2.49408000	-0.03573000
C	7.82363700	0.16636600	-0.53253800
H	7.19493300	2.10831700	-1.22348800
H	8.16818500	-1.86383900	0.10774700
H	8.87517900	0.44230800	-0.48305600

7k-TS

Zero-point correction= 0.632770 (Hartree/Particle)
Thermal correction to Energy= 0.672966
Thermal correction to Enthalpy= 0.673910
Thermal correction to Gibbs Free Energy= 0.556482
Sum of electronic and zero-point Energies= -1728.834371
Sum of electronic and thermal Energies= -1728.794175
Sum of electronic and thermal Enthalpies= -1728.793230
Sum of electronic and thermal Free Energies= -1728.910658
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1730.28457426
Cartesian coordinates:

C	4.15772300	-1.56194300	1.31026800
C	5.02878800	-2.48367800	0.50812700

C	2.85605000	-1.88515400	1.69422400
O	4.58261500	-3.24006500	-0.32990800
H	4.70281900	-0.93031600	2.01788600
C	2.25455400	-1.34464600	2.94464700
H	1.69747900	-2.12835900	3.47074500
H	2.99693800	-0.90468400	3.61628100
H	1.51898300	-0.57193200	2.65743400
C	6.49421700	-2.37276900	0.81884300
H	7.06979600	-2.99368000	0.12713200
H	6.82239700	-1.32499600	0.74526600
H	6.69099700	-2.69725100	1.84997100
C	1.14871500	-0.74168600	-0.26647100
C	1.33854900	-2.16910400	-0.06583800
Au	-0.84572000	-0.17884900	-0.11750000
N	2.04441200	-2.60823700	0.91845100
C	-5.04521800	0.69386000	0.03477300
C	-4.53048800	1.93788800	0.18929900
H	-6.06556000	0.33520100	-0.00695800
H	-5.00240000	2.90419400	0.31106600
N	-3.96794200	-0.17125900	-0.07936400
N	-3.15200600	1.79880000	0.16436000
C	-2.80038700	0.50294500	-0.00120700
C	2.20984400	0.13448700	-0.29573400
C	3.53616400	-0.41098900	-0.47911200
C	1.99697500	1.61785400	-0.16566500
H	0.97061600	1.88523500	-0.44680600
H	2.13672100	1.95241600	0.87452000
H	2.68617300	2.19757500	-0.79142100
C	-2.20149300	2.87218100	0.26430500
C	-1.71295400	3.43730200	-0.91829500
C	-1.79339900	3.28225000	1.53786500
C	-0.77794000	4.46615200	-0.79741500
C	-0.85565000	4.31177000	1.60963600
C	-0.35420500	4.89949200	0.45344500
H	-0.38550800	4.93216700	-1.70062900
H	-0.52350600	4.65727300	2.58807400
H	0.37002900	5.70858700	0.52842600
C	-4.07411200	-1.58917800	-0.29526000
C	-4.12429800	-2.05095000	-1.61422400
C	-4.11975000	-2.43233400	0.81873200
C	-4.23350400	-3.42778500	-1.80531500
C	-4.22924600	-3.80182600	0.57891000
C	-4.28681300	-4.29426800	-0.71963800
H	-4.27929500	-3.81916400	-2.82089100
H	-4.27215800	-4.48549200	1.42597200
H	-4.37680700	-5.36577800	-0.88753500
C	-4.03923800	-1.88515500	2.21186400
H	-4.80243200	-1.11748900	2.39955600
H	-4.17679300	-2.68043400	2.95233400
H	-3.06280200	-1.41572500	2.40215000
C	-4.05001700	-1.10298500	-2.77299700
H	-4.83502100	-0.33517300	-2.73013100
H	-3.08668000	-0.57232300	-2.79651700
H	-4.15887200	-1.63756400	-3.72266200
C	-2.33776600	2.63132400	2.77330300
H	-3.42560100	2.75861900	2.86003000
H	-2.14458500	1.54862400	2.77736200
H	-1.88268200	3.05865200	3.67331500
C	-2.14951900	2.93828400	-2.26270000

H	-1.68780000	1.96602800	-2.49354800
H	-3.23697800	2.79571900	-2.32190200
H	-1.85762000	3.63811700	-3.05321500
H	0.74610900	-2.89718700	-0.62597400
H	3.54065600	-1.38567100	-0.96944800
C	4.76053700	0.35301800	-0.69986800
C	5.64194100	-0.10230300	-1.69373400
C	5.12064500	1.47258100	0.06696300
C	6.83124000	0.56978900	-1.94348400
H	5.38125000	-0.98851600	-2.27295200
C	6.32154400	2.12450400	-0.16699200
H	4.47017000	1.80818500	0.87347300
C	7.17398200	1.68082000	-1.17835300
H	7.49746000	0.21842000	-2.72831700
H	6.59906800	2.98286700	0.44119000
H	8.11231000	2.19983300	-1.36308700