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Supporting Information

Exploring the Role of Ligands in Gold(I)-Catalyzed Cyclizations: Insights from Density Functional Theory

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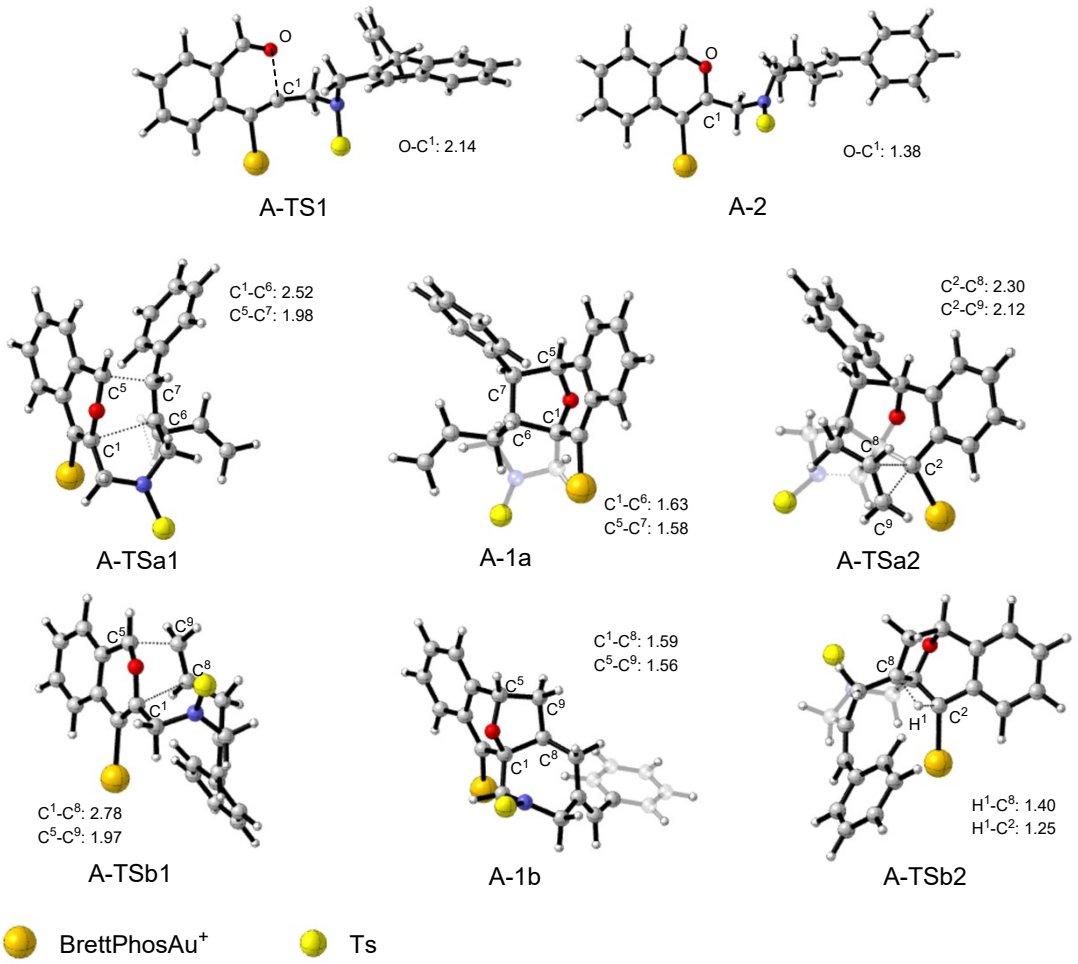

Figure S1. The stereostructures of key transition states and intermediates in the A series, representative bond lengths are in Å.

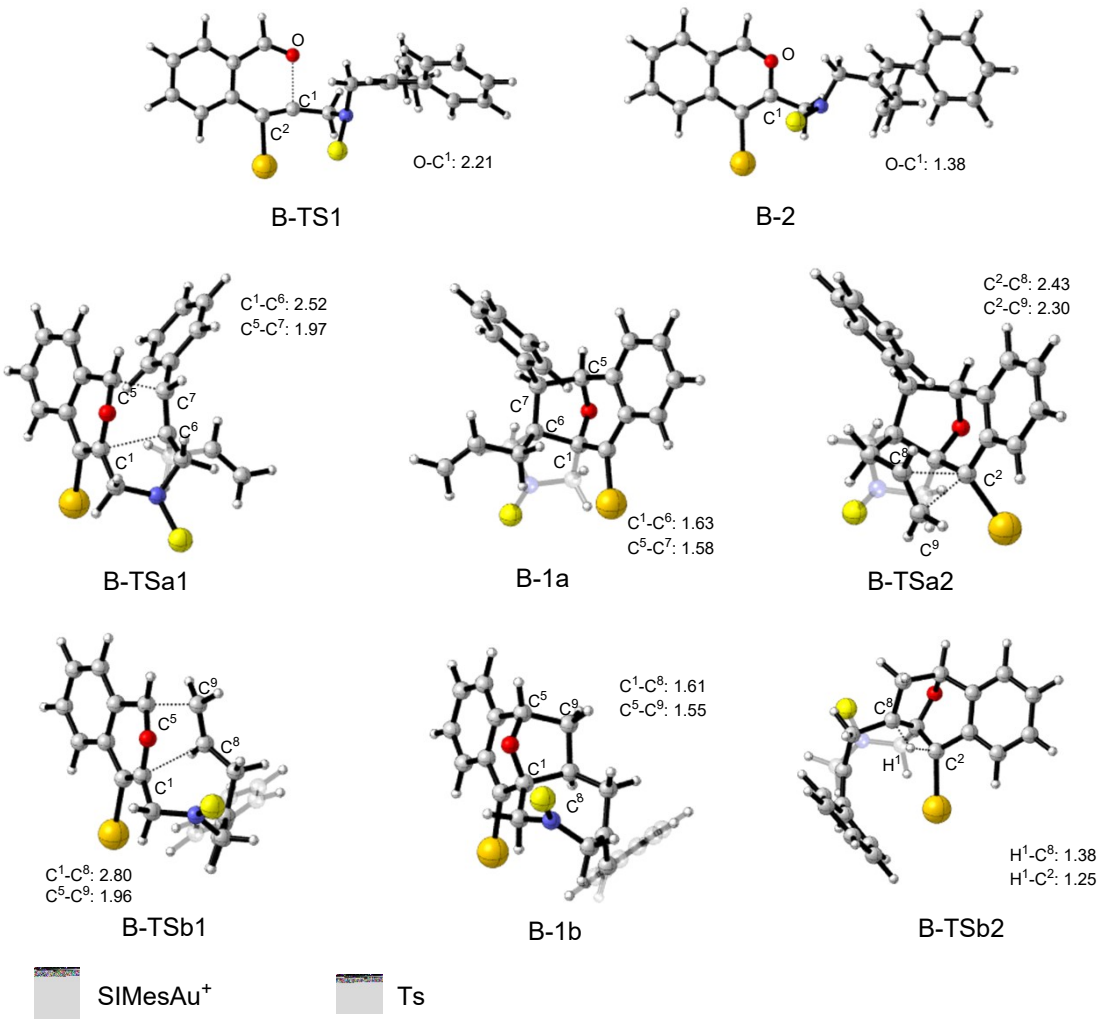

Figure S2. The stereostructures of key transition states and intermediates in the B series, representative bond lengths are in Å.

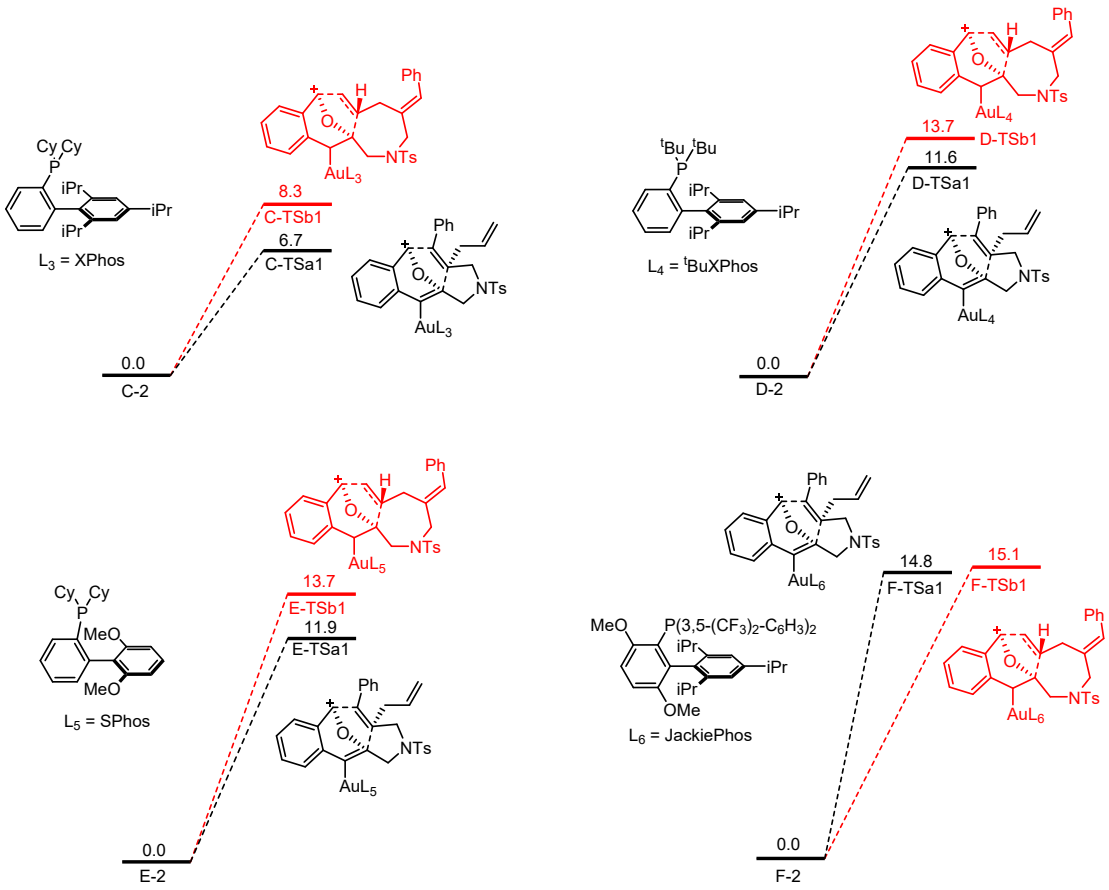

Figure S3. Calculated energy distributions for the [3+2] cycloaddition pathway with different phosphine ligands. Free energies are given in kcal/mol.

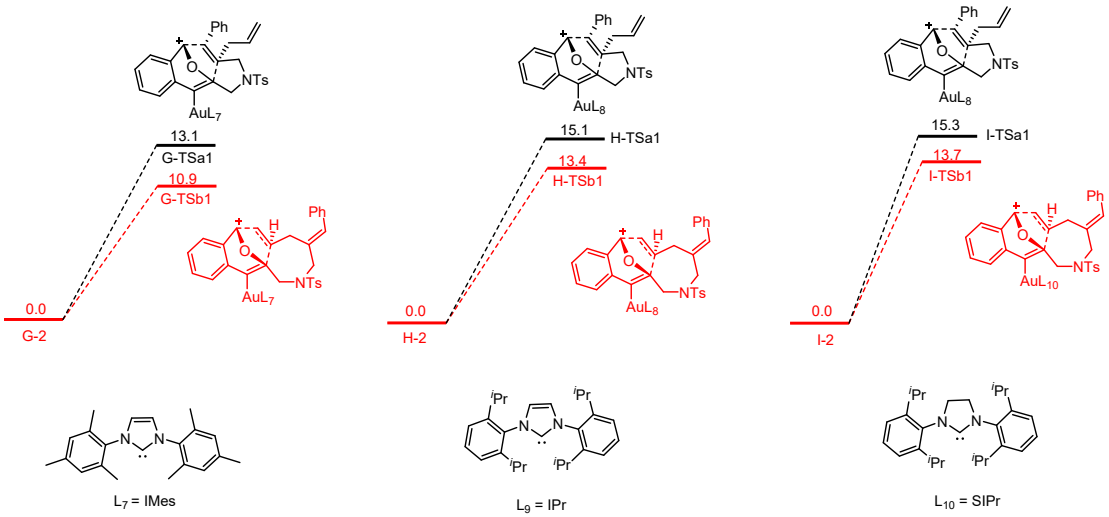

Figure S4. Calculated energy distributions for the [3+2] cycloaddition pathway with different NHC ligands. Free energies are given in kcal/mol.

The Cartesian coordinates of the stationary points

1a

C	-7.45505500	-0.48608800	0.68059700
C	-6.30349600	0.23988500	0.96802300
C	-5.08719500	-1.03309600	-0.71192500
C	-6.25539900	-1.75746900	-0.98035300
C	-7.43457500	-1.48994200	-0.29452700
H	-8.37258200	-0.27004300	1.22001700
H	-6.31618900	1.01479100	1.72729900
H	-6.20361300	-2.52856200	-1.74240500
H	-8.33509700	-2.05529900	-0.51401500
C	-3.85358300	-1.35072500	-1.48313100
O	-3.79439400	-2.27126800	-2.28065200
H	-2.98084600	-0.69722600	-1.30150200
C	-5.10395800	-0.02038800	0.27859000
C	-3.93015900	0.72454200	0.60364100
C	-2.94215200	1.36342600	0.89538300
C	-1.66719700	2.02713800	1.18232900
H	-1.65660000	3.03571800	0.76315800
H	-1.50816100	2.11579000	2.26287900
N	-0.48754100	1.29735500	0.66153700
C	-0.36281200	-0.09693100	1.16824500
H	-0.86581500	-0.09604400	2.13933800
H	-0.89956900	-0.79854300	0.52209100
C	1.56423900	-1.54139100	0.64598500
H	0.85175700	-2.07689800	0.01846400
C	1.08395100	-0.49374700	1.34114400
C	1.88042700	0.36718300	2.30567900
H	2.81072300	-0.14669000	2.56832900
H	2.15850300	1.30159500	1.80326900
C	1.13247900	0.69134300	3.57507700
C	0.78694500	1.91844200	3.96593800
H	0.87162600	-0.16261600	4.20135200
H	0.26514000	2.09659500	4.90160200
H	1.02754900	2.79153300	3.36390000
O	-0.78613700	0.25345800	-1.72732000
O	-0.79210700	2.78429600	-1.38050500
S	-0.28174500	1.45139500	-1.03691000
C	2.93466300	-2.07917200	0.59849000
C	3.11613500	-3.46495800	0.43736800
C	4.08102400	-1.26403300	0.64053700
C	4.39112000	-4.02110500	0.36288100
H	2.24236000	-4.10863900	0.37753100

C	5.35737500	-1.82040500	0.56442400
H	3.97073600	-0.18788500	0.68718600
C	5.51944500	-3.20052000	0.43157400
H	4.50492600	-5.09505000	0.24729100
H	6.22764100	-1.17081700	0.60180900
H	6.51415700	-3.63196500	0.37062600
C	1.49899700	1.46273800	-1.22334800
C	2.10404200	0.47787500	-2.00373400
C	2.24677700	2.48395500	-0.63881000
C	3.48326800	0.50994400	-2.17919500
H	1.49611400	-0.30293700	-2.44534400
C	3.62954600	2.49527100	-0.81845700
H	1.75478000	3.25064300	-0.05007800
C	4.26692300	1.50952500	-1.58448600
H	3.96370200	-0.26538200	-2.76876800
H	4.22136100	3.28050600	-0.35657900
C	5.76584100	1.49000300	-1.75083900
H	6.04737400	1.53157900	-2.80868900
H	6.24287400	2.33054500	-1.24036300
H	6.18325000	0.56183500	-1.34339600

Zero-point correction= 0.489965 (Hartree/Particle)

Thermal correction to Energy= 0.521846

Thermal correction to Enthalpy= 0.522790

Thermal correction to Gibbs Free Energy= 0.422551

Sum of electronic and zero-point Energies= -1799.412419

Sum of electronic and thermal Energies= -1799.380537

Sum of electronic and thermal Enthalpies= -1799.379593

Sum of electronic and thermal Free Energies= -1799.479832

BrettPhosAu

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C	3.12131400	-0.74936400	0.94920400
C	2.26033800	0.33391900	1.17071500
H	3.16926700	-0.80879900	-2.43575700
H	3.54614000	-1.26673800	1.80185900
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C	2.69963500	2.48147200	-2.80808200
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H	2.14440700	0.10323600	-4.12957100
H	2.92874500	3.10167200	-1.93906300
H	3.62204200	1.98159700	-3.12330700
H	2.36902400	3.12884300	-3.62666500
C	4.22541400	-2.47909500	-0.55902800
C	3.39720900	-3.71609700	-0.15627800
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H	4.43213400	-2.55177400	-1.63438800
H	2.45513600	-3.75899500	-0.71921400
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C	3.08194600	1.71567800	3.09811400
C	1.75212400	-0.38764600	3.57379200
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H	3.20613200	2.56851000	2.42773000
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C	-4.32643300	-1.04052300	-3.37561300
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H	-4.70628900	0.95814700	-2.63584200
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H	-5.36514200	-1.33781800	-1.49942100
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C	-1.70653500	-0.70019600	1.89174800
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C	-3.33629700	-0.71599600	3.83196000
H	-3.86508800	-0.86365300	1.74295500
H	-3.31359300	0.73975600	2.21785200
C	-1.65098700	-2.58137200	3.59421700
H	-2.07513700	-2.80520800	1.48141500
H	-0.39163800	-2.43837500	1.82708600
C	-3.06244000	-2.20667300	4.06431700
H	-4.35733100	-0.45871900	4.13454200
H	-2.66183800	-0.11670900	4.45924700
H	-1.47152900	-3.65415400	3.72299500
H	-0.91162300	-2.06129000	4.21831500
H	-3.18705500	-2.45709300	5.12302200
H	-3.80121400	-2.80218000	3.51024700
P	-1.33938400	-0.13987600	0.14371500
Au	0.29881200	-1.45197900	-0.84968800

Zero-point correction=	0.817851 (Hartree/Particle)
Thermal correction to Energy=	0.860834
Thermal correction to Enthalpy=	0.861778
Thermal correction to Gibbs Free Energy=	0.740775
Sum of electronic and zero-point Energies=	-1992.140616
Sum of electronic and thermal Energies=	-1992.097632
Sum of electronic and thermal Enthalpies=	-1992.096688
Sum of electronic and thermal Free Energies=	-1992.217691

A-1

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C	-0.41784000	4.97727800	-3.28411200
C	0.46858700	4.64205700	-4.30462900
H	1.76491500	3.11351200	-5.10629200
H	1.28784800	1.49435400	-3.29155200
H	-0.92492900	5.93675000	-3.26515300
H	0.67363700	5.34996000	-5.10125400
C	-1.66206000	4.46295300	-1.19254000
O	-2.28363600	5.50916400	-1.19035200
H	-1.80965200	3.73066600	-0.37970100
C	-0.04539200	2.81120100	-2.24009000
C	-0.32791600	1.89589300	-1.17482400
C	-0.75603900	1.30811100	-0.17497300
C	-1.75678500	0.87314800	0.83480900
H	-1.29129500	0.31115000	1.64058900
H	-2.19695100	1.78132700	1.25807200
N	-2.84532300	0.09393300	0.24756000
C	-3.74734000	0.80097500	-0.71131500
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H	-3.79859500	0.23575300	-1.64491500
C	-6.14330500	0.27081200	-0.60552800
H	-5.92812100	-0.33975400	-1.48112900
C	-5.12015400	0.98861100	-0.10599600
C	-5.20924300	1.96873100	1.04945900
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H	-4.76231300	1.53168000	1.95403700
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H	-3.29146300	4.90641400	1.27930800
H	-3.42064000	3.54005600	2.53219800
O	-1.99225600	-1.56857400	-1.60071500
O	-1.47984500	-1.93655600	0.85280100
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C	-7.85425000	0.08809800	1.24525100
C	-9.87714900	-0.24827700	-0.64627300
H	-8.32118600	-0.04890800	-2.11877900
C	-9.17099300	-0.11171500	1.65910600
H	-7.06574200	0.16315600	1.98602000
C	-10.18880100	-0.27323900	0.71605900

H	-10.66016100	-0.38365600	-1.38645900
H	-9.40125200	-0.15163000	2.71978300
H	-11.21353400	-0.42883700	1.03931900
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C	-5.92441400	-2.79005800	1.30076700
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H	-8.24377800	-4.22138200	1.20653900
C	3.02353900	0.79176800	1.67432400
C	1.94203700	0.67935700	2.58299200
C	1.05273300	1.75190700	2.69902200
C	1.21159600	2.94572100	1.98339400
C	2.30109300	3.03774100	1.11798400
C	3.20843600	1.98442200	0.94558600
H	0.22002700	1.66482500	3.39054800
H	2.46485400	3.95095300	0.55890700
C	1.78180000	-0.53663000	3.49037300
C	0.33173000	-1.02918000	3.61596900
C	2.36371300	-0.23034300	4.88628100
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H	-0.12077400	-1.22806100	2.64303200
H	0.30234300	-1.96007000	4.19154900
H	-0.29707900	-0.30672700	4.14833900
H	3.40079000	0.10335400	4.81809700
H	1.78796700	0.56543300	5.37192700
H	2.31924700	-1.11876500	5.52519100
C	0.20919400	4.08098900	2.17744400
C	0.43407500	5.28021000	1.24809500
C	0.18150600	4.55564600	3.64461800
H	-0.78586000	3.66818500	1.94916800
H	0.50041200	4.98255100	0.19793500
H	-0.38977500	5.99344000	1.33964000
H	1.36061100	5.80704500	1.50178800
H	-0.04272000	3.73990400	4.33743500
H	1.15327000	4.97461700	3.92671900

H	-0.57680300	5.33326800	3.78224600
C	4.39081900	2.17690400	0.00373300
C	5.40595500	3.16594600	0.60677000
C	3.94654000	2.61503700	-1.40212700
H	4.89835300	1.21361100	-0.10159500
H	5.72230500	2.83142500	1.59834000
H	6.28976300	3.25402400	-0.03399200
H	4.96482900	4.16309100	0.71204600
H	3.21662200	1.91365100	-1.81726400
H	3.48057100	3.60538500	-1.39502300
H	4.80535100	2.66058100	-2.08044800
C	4.05670600	-0.29689300	1.59318000
C	4.03582700	-1.38073200	0.69037500
C	5.13731100	-0.18482900	2.50312300
C	5.07704300	-2.34535300	0.73676300
C	6.13833000	-1.15156600	2.54470800
C	6.10687700	-2.23309200	1.66449600
H	6.95597000	-1.07626200	3.25048000
H	6.89825500	-2.97017400	1.70788100
O	5.11517100	0.92107000	3.30472300
O	5.00905600	-3.34947300	-0.19031300
C	6.15935400	1.09492500	4.25665400
H	7.13891500	1.17469400	3.76884400
H	5.93617000	2.02932000	4.77208100
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C	6.04096500	-4.33116900	-0.22768300
H	7.01687400	-3.87575300	-0.43451900
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H	5.77707200	-5.00742200	-1.04129200
C	1.99553400	-3.30689700	-0.31101400
C	1.51044000	-3.44889500	1.14244700
C	0.86781200	-3.60176100	-1.32068500
H	2.81907700	-4.00705000	-0.48018300
C	0.88289700	-4.83042900	1.38401700
H	0.76507300	-2.67561500	1.34512200
H	2.34676900	-3.29336600	1.83241500
C	0.24414100	-4.98294500	-1.05515500
H	0.09090400	-2.83417100	-1.24828500
H	1.25666000	-3.57289300	-2.34455500
C	-0.25204400	-5.11509800	0.39084100
H	0.51448300	-4.88477200	2.41470800
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H	-0.57864200	-5.14452300	-1.76077100
H	0.99102500	-5.76386300	-1.25752800

H	-0.66054200	-6.11790700	0.55950500
H	-1.06326500	-4.39882800	0.56383800
C	3.57218900	-1.70288900	-2.27051100
C	2.62932300	-1.21237100	-3.38991600
C	4.91458100	-0.95093800	-2.35538200
H	3.76827200	-2.77280200	-2.41051600
C	3.26182500	-1.42122300	-4.77360000
H	2.45409200	-0.13952700	-3.23827600
H	1.65014300	-1.69676400	-3.33315400
C	5.55532300	-1.15156700	-3.73913900
H	4.74264200	0.11853200	-2.18858200
H	5.60066400	-1.29035500	-1.57731600
C	4.61874500	-0.71071200	-4.87234200
H	2.57781300	-1.05826300	-5.54915600
H	3.39466400	-2.49713400	-4.95177200
H	6.50123300	-0.60051600	-3.78701200
H	5.80417900	-2.21447700	-3.86595400
H	5.08165600	-0.90185300	-5.84649100
H	4.46135500	0.37556200	-4.80564600
P	2.73286800	-1.61648600	-0.59133600
Au	1.03994600	0.01165700	-0.57321100

Zero-point correction=	1.311717 (Hartree/Particle)
Thermal correction to Energy=	1.387328
Thermal correction to Enthalpy=	1.388272
Thermal correction to Gibbs Free Energy=	1.196451
Sum of electronic and zero-point Energies=	-3791.604030
Sum of electronic and thermal Energies=	-3791.528419
Sum of electronic and thermal Enthalpies=	-3791.527475
Sum of electronic and thermal Free Energies=	-3791.719296

A-TS1

C	1.66481800	3.86602200	-3.95847900
C	1.33782900	2.88902800	-3.02013900
C	-0.28907600	4.38640700	-2.03308600
C	0.05714500	5.36437500	-2.98183500
C	1.03029100	5.11284800	-3.94093300
H	2.42164900	3.65350600	-4.70735300
H	1.83075900	1.92548900	-3.04365400
H	-0.45097100	6.32534700	-2.95843900
H	1.29093200	5.87257200	-4.67014700
C	-1.33120100	4.73184400	-1.07543200
O	-1.78141900	3.99482500	-0.19419900
H	-1.74349000	5.75294300	-1.16390100
C	0.36804100	3.12545900	-2.03790900

C	0.03485500	2.11534600	-1.04346700
C	-0.83135900	2.07546600	-0.11654700
C	-1.71200800	1.50927300	0.91516400
H	-1.11191900	0.83354200	1.52570100
H	-2.07777800	2.30384400	1.56817700
N	-2.89443100	0.79544000	0.40716300
C	-3.92591000	1.62401900	-0.27697800
H	-3.72419800	2.65181600	0.03255300
H	-3.79691800	1.57861300	-1.36384400
C	-6.21785200	0.87782600	-0.80329500
H	-5.88922800	0.95305200	-1.84065300
C	-5.32102900	1.21943400	0.14033900
C	-5.57798400	1.24787900	1.63677700
H	-6.65758500	1.22390700	1.81717000
H	-5.15553000	0.34450300	2.09426600
C	-5.00053000	2.46413400	2.31865200
C	-4.09467900	2.43510600	3.29803500
H	-5.38302000	3.42546000	1.97383000
H	-3.73812800	3.34310500	3.77568500
H	-3.69520100	1.49440700	3.67143700
O	-2.45080700	-0.55914300	-1.79049800
O	-1.37888100	-1.21164600	0.42175400
S	-2.53911700	-0.69920300	-0.32993700
C	-7.60360600	0.40523000	-0.64186500
C	-8.56625200	0.77388900	-1.59911600
C	-7.99871500	-0.45638400	0.39863700
C	-9.88471200	0.33420300	-1.49937900
H	-8.27414200	1.42040200	-2.42281500
C	-9.31826800	-0.89739700	0.49777200
H	-7.26064500	-0.81501900	1.10611800
C	-10.26785000	-0.49974300	-0.44591400
H	-10.61330400	0.63973000	-2.24447000
H	-9.60388700	-1.55708400	1.31248600
H	-11.29452700	-0.84439000	-0.36752700
C	-3.93954600	-1.72852000	0.05483700
C	-4.78647200	-2.13701100	-0.97623300
C	-4.13484000	-2.14754000	1.37176500
C	-5.86065700	-2.96525700	-0.67117100
H	-4.60293500	-1.79999100	-1.98979600
C	-5.21989000	-2.97476200	1.65674200
H	-3.44785000	-1.83799900	2.15230900
C	-6.09993400	-3.38856500	0.64559500
H	-6.53578200	-3.27712400	-1.46252100
H	-5.38578400	-3.30413600	2.67833600

C	-7.30536500	-4.23868500	0.95431300
H	-8.22278200	-3.66669800	0.77225100
H	-7.34299100	-5.12244300	0.30904700
H	-7.31336700	-4.57406500	1.99427800
C	3.07234900	0.47487700	1.72288900
C	1.94593800	0.47239400	2.58266400
C	1.22911100	1.66122000	2.74333600
C	1.59787200	2.85705200	2.11438600
C	2.73105600	2.83875600	1.30338800
C	3.47730800	1.67130100	1.09576500
H	0.36579700	1.66785500	3.40315300
H	3.05553600	3.75003900	0.81478100
C	1.56311300	-0.75785200	3.40092100
C	0.04734700	-1.00162200	3.49123300
C	2.16430000	-0.65192400	4.81813300
H	2.00691200	-1.63231100	2.91630400
H	-0.42128100	-1.04415000	2.50662000
H	-0.14490300	-1.95437000	3.99584500
H	-0.45251700	-0.22397600	4.08010800
H	3.24383700	-0.49874700	4.77947500
H	1.72533900	0.19762100	5.35340000
H	1.95533100	-1.56012100	5.39373000
C	0.77765300	4.11731000	2.36825000
C	1.09416100	5.27329100	1.41156400
C	0.93292900	4.58065800	3.83127900
H	-0.27747700	3.84835900	2.21578800
H	1.04667200	4.96053100	0.36472200
H	0.38111000	6.09034600	1.55907700
H	2.09569600	5.67837800	1.59317400
H	0.65808300	3.79106600	4.53647300
H	1.97244500	4.86045000	4.03350700
H	0.30040800	5.45176200	4.03228800
C	4.73306100	1.74206800	0.23493800
C	5.84777700	2.50630300	0.97436800
C	4.46078700	2.35326000	-1.14961100
H	5.09040700	0.72089200	0.07302800
H	6.04464700	2.04871000	1.94736500
H	6.77413200	2.50382700	0.38981500
H	5.55870200	3.54925600	1.14431900
H	3.66020600	1.81165900	-1.66057700
H	4.15705400	3.40293000	-1.08237200
H	5.36108000	2.31040600	-1.77206100
C	3.91800700	-0.75890700	1.57785600
C	3.75495300	-1.74523600	0.58210000

C	4.96844300	-0.90211900	2.51888000
C	4.61737400	-2.87384000	0.57626500
C	5.79451500	-2.02214600	2.50181200
C	5.61611300	-3.01044000	1.53406800
H	6.58775900	-2.14129700	3.22894900
H	6.27181600	-3.87171800	1.53676800
O	5.10326300	0.12565800	3.41016200
O	4.41657600	-3.78181300	-0.42782800
C	6.13383100	0.04803200	4.38836200
H	7.12693600	0.00399000	3.92364700
H	6.05155000	0.96198600	4.97720900
H	5.99964600	-0.81974200	5.04663900
C	5.29244400	-4.89849800	-0.53873700
H	6.33077800	-4.57805000	-0.68731200
H	5.23177000	-5.54596800	0.34419400
H	4.95600400	-5.45337800	-1.41517400
C	1.46726200	-3.20575200	-0.63205000
C	0.96876200	-3.40248300	0.81188300
C	0.31137200	-3.20061800	-1.65476700
H	2.15463400	-4.02066300	-0.87820300
C	0.07574400	-4.64672700	0.93270900
H	0.39998800	-2.52155100	1.11548500
H	1.82434500	-3.49435100	1.48965400
C	-0.58243200	-4.44296500	-1.49404500
H	-0.29555700	-2.30103800	-1.52242000
H	0.71153300	-3.17610100	-2.67415400
C	-1.09615800	-4.59597100	-0.05650000
H	-0.29140500	-4.73014500	1.96232200
H	0.67738200	-5.54627100	0.73874900
H	-1.42052800	-4.37277500	-2.19691900
H	-0.01206100	-5.34081500	-1.77159500
H	-1.70837000	-5.50083200	0.03155600
H	-1.73858100	-3.74444300	0.19376300
C	3.39182400	-1.78697900	-2.40321300
C	2.59933700	-1.10795700	-3.54140700
C	4.83825600	-1.25370100	-2.38880800
H	3.43014100	-2.86586000	-2.59425800
C	3.26505700	-1.36390300	-4.90172900
H	2.58064000	-0.02682100	-3.35314400
H	1.55535800	-1.43388500	-3.55433200
C	5.51417400	-1.49853400	-3.74842900
H	4.82763200	-0.17796500	-2.17803500
H	5.42078000	-1.72771800	-1.59644100
C	4.71959800	-0.87414600	-4.90372700

H	2.68994700	-0.86916700	-5.69271900
H	3.23830100	-2.44020200	-5.12093600
H	6.53557200	-1.10185900	-3.72745500
H	5.60129300	-2.58190900	-3.91187300
H	5.19924200	-1.09955100	-5.86253200
H	4.72974900	0.22025100	-4.79589400
P	2.48793700	-1.64270100	-0.75936100
Au	1.12104000	0.26622800	-0.74662200

Zero-point correction=	1.311574 (Hartree/Particle)
Thermal correction to Energy=	1.386071
Thermal correction to Enthalpy=	1.387015
Thermal correction to Gibbs Free Energy=	1.196970
Sum of electronic and zero-point Energies=	-3791.603937
Sum of electronic and thermal Energies=	-3791.529441
Sum of electronic and thermal Enthalpies=	-3791.528496
Sum of electronic and thermal Free Energies=	-3791.718542

A-TS11

C	-1.27917200	3.78005500	3.78472700
C	-0.86452700	2.89138100	2.79597200
C	0.52354300	4.66348700	1.88749800
C	0.10231000	5.55136300	2.88691200
C	-0.80891600	5.10440100	3.83498300
H	-1.98391500	3.43593200	4.53563100
H	-1.22533700	1.87158700	2.77066200
H	0.48975600	6.56532600	2.91438200
H	-1.15218100	5.77017400	4.61939000
C	1.46228000	4.91403600	0.82968200
O	1.71786300	3.97154600	0.05499300
H	1.94402100	5.88821600	0.68247100
C	0.03530800	3.33500300	1.81727200
C	0.53014100	2.55250400	0.73431500
C	0.59681800	1.48421000	0.02153900
C	1.59625700	1.14968300	-1.07276000
H	1.13295900	0.52261100	-1.82959600
H	1.96031300	2.06490500	-1.54255900
N	2.78255600	0.46053600	-0.54067600
C	3.67274500	1.26200100	0.34287700
H	3.37893600	2.30177500	0.18432000
H	3.48495800	1.02473500	1.39529000
C	5.99919100	0.70395800	0.94048800
H	5.59368000	0.57058200	1.94442600
C	5.13179200	1.08435900	-0.01524500
C	5.48388000	1.39009500	-1.45931600

H	6.57173600	1.45462000	-1.56099900
H	5.14803900	0.56282400	-2.09691800
C	4.87613200	2.67941700	-1.95634000
C	4.05626400	2.78681000	-3.00302200
H	5.15755400	3.57653700	-1.40361300
H	3.66967200	3.74683600	-3.33237500
H	3.75778000	1.91413200	-3.57997300
O	2.28896400	-1.19294300	1.42543400
O	1.47666900	-1.66856100	-0.93877800
S	2.50981500	-1.14310300	-0.02934700
C	7.44467800	0.43681200	0.83329100
C	8.28575300	0.79429500	1.90246100
C	8.01838400	-0.21856000	-0.27186000
C	9.65607200	0.54558200	1.85365800
H	7.85669800	1.28093400	2.77482700
C	9.38997600	-0.46834500	-0.32045500
H	7.38083300	-0.56949100	-1.07486800
C	10.21528700	-0.08258600	0.73811900
H	10.28785500	0.83917600	2.68680100
H	9.81356900	-0.97092300	-1.18559400
H	11.28252700	-0.27873500	0.69921700
C	4.04760700	-1.96665100	-0.38546600
C	4.83324300	-2.42919200	0.67104200
C	4.42593000	-2.15567800	-1.71522300
C	6.03128400	-3.07318100	0.38208300
H	4.50754900	-2.27225400	1.69272300
C	5.63127700	-2.80194000	-1.98328800
H	3.78765800	-1.80731100	-2.52033800
C	6.45346300	-3.26099200	-0.94318600
H	6.65893500	-3.42375100	1.19615800
H	5.93886200	-2.95138600	-3.01422500
C	7.78508500	-3.90866500	-1.22344100
H	8.59703900	-3.25498900	-0.88349100
H	7.88592900	-4.85651500	-0.68501900
H	7.92816500	-4.10359000	-2.28914100
C	-3.26768600	0.57654400	-1.53124800
C	-2.25377200	0.51081900	-2.51795500
C	-1.48068900	1.65002900	-2.75918300
C	-1.69657100	2.86189700	-2.09234700
C	-2.72315100	2.90711900	-1.15009900
C	-3.51370500	1.78862200	-0.85550000
H	-0.69361900	1.59964900	-3.50581200
H	-2.93148200	3.83427200	-0.62941900
C	-2.04359100	-0.73694300	-3.36885700

C	-0.56455100	-1.08866800	-3.59223500
C	-2.76539400	-0.57840100	-4.72334600
H	-2.50447100	-1.57924100	-2.84549400
H	-0.01507600	-1.15646000	-2.65217400
H	-0.48380400	-2.05600200	-4.09887500
H	-0.06579400	-0.35154500	-4.23157600
H	-3.82410300	-0.35248200	-4.58331600
H	-2.32075000	0.24278800	-5.29674600
H	-2.67382300	-1.49436900	-5.31681200
C	-0.82581600	4.06749600	-2.43403500
C	-1.04829800	5.27833700	-1.51924200
C	-1.01560500	4.48386400	-3.90723400
H	0.22021500	3.75095600	-2.30935900
H	-0.95741100	5.01550700	-0.46174200
H	-0.31548600	6.06001400	-1.74378100
H	-2.04345100	5.71160400	-1.66809000
H	-0.80678100	3.65894200	-4.59373200
H	-2.04716400	4.80839700	-4.08142800
H	-0.34941800	5.31418300	-4.16452400
C	-4.65255100	1.93285500	0.14742500
C	-5.80959500	2.74462200	-0.46590900
C	-4.18720400	2.54532500	1.47853300
H	-5.03698600	0.93303400	0.36879700
H	-6.14656800	2.28609200	-1.39896300
H	-6.65642500	2.79896600	0.22679000
H	-5.49004900	3.76832600	-0.69031900
H	-3.35347700	1.97407200	1.89528100
H	-3.85149100	3.58030800	1.35891600
H	-5.00450100	2.54682900	2.20778500
C	-4.16963400	-0.60076700	-1.28940500
C	-3.95911700	-1.60084400	-0.31580900
C	-5.33298800	-0.66139200	-2.09613600
C	-4.91336500	-2.64373500	-0.17770900
C	-6.24084200	-1.70770900	-1.96193200
C	-6.03156800	-2.69830300	-1.00280200
H	-7.12368000	-1.76431000	-2.58624800
H	-6.75580600	-3.49706300	-0.90737100
O	-5.48889100	0.36903100	-2.98120300
O	-4.67589800	-3.55217400	0.81822800
C	-6.62115400	0.36054600	-3.84280600
H	-7.55968500	0.39966800	-3.27542500
H	-6.53307700	1.25830300	-4.45530300
H	-6.62466200	-0.52288400	-4.49387000
C	-5.61130200	-4.60292000	1.03649900

H	-6.60192300	-4.20892700	1.29421300
H	-5.69400400	-5.25559000	0.15919200
H	-5.22078500	-5.17717400	1.87727000
C	-1.68732000	-3.30576000	0.53572700
C	-1.35693400	-3.49982600	-0.95583400
C	-0.43825000	-3.47411500	1.42509400
H	-2.43724500	-4.04602200	0.82974400
C	-0.65438100	-4.84312900	-1.20247000
H	-0.70052800	-2.69051200	-1.28521600
H	-2.27570400	-3.44494400	-1.54956300
C	0.26304800	-4.81474800	1.14724900
H	0.26402400	-2.65619400	1.24059500
H	-0.71745200	-3.42724800	2.48349400
C	0.60682300	-4.97968200	-0.33912200
H	-0.40508000	-4.93178100	-2.26619700
H	-1.34710500	-5.66500300	-0.97088800
H	1.16841800	-4.87813800	1.76175200
H	-0.39103700	-5.64029800	1.46258500
H	1.08330600	-5.95159000	-0.51157600
H	1.32609000	-4.20618300	-0.63384300
C	-3.12537700	-1.68026900	2.57736200
C	-2.09065900	-1.06813700	3.54624900
C	-4.49465900	-1.00150900	2.77571700
H	-3.23692500	-2.74772200	2.80222800
C	-2.54995300	-1.20606900	5.00548300
H	-1.98405300	-0.00204200	3.30713600
H	-1.10047400	-1.51133600	3.40656100
C	-4.95781200	-1.12531700	4.23693500
H	-4.41549400	0.05909400	2.51249900
H	-5.24444000	-1.43894900	2.11385100
C	-3.92244900	-0.55230000	5.21403900
H	-1.80289400	-0.75882400	5.67126000
H	-2.60669500	-2.27122000	5.26859400
H	-5.92274700	-0.62032500	4.35992300
H	-5.12689100	-2.18611500	4.46937400
H	-4.25818800	-0.68413400	6.24850200
H	-3.83301300	0.53143600	5.04683200
P	-2.49115800	-1.63911300	0.80782600
Au	-0.89135700	0.05684100	0.47151800

Zero-point correction= 1.311915 (Hartree/Particle)

Thermal correction to Energy= 1.386370

Thermal correction to Enthalpy= 1.387314

Thermal correction to Gibbs Free Energy= 1.197221

Sum of electronic and zero-point Energies= -3791.601039

Sum of electronic and thermal Energies= -3791.526584

Sum of electronic and thermal Enthalpies= -3791.525640

Sum of electronic and thermal Free Energies= -3791.715734

A-2

C	2.52677600	4.31621100	-3.49015800
C	2.10780100	3.27398200	-2.69138800
C	0.03720600	4.48509800	-2.26859600
C	0.48521800	5.55191000	-3.10358300
C	1.71492400	5.46406000	-3.70247400
H	3.49811900	4.26236700	-3.97262400
H	2.73336000	2.40221800	-2.54327000
H	-0.15275400	6.41830000	-3.25161700
H	2.07378900	6.26519900	-4.33996900
C	-1.19166200	4.54485300	-1.63130200
O	-1.60921200	3.57957400	-0.85224200
H	-1.89193400	5.37000500	-1.70874700
C	0.84577300	3.31311400	-2.04540300
C	0.37013600	2.25107800	-1.20261000
C	-0.86716200	2.43707900	-0.63098100
C	-1.63005800	1.50142000	0.26743900
H	-0.97507400	0.67630600	0.52614700
H	-1.90276400	2.01020100	1.19461500
N	-2.88493800	0.97918400	-0.29164600
C	-4.09836100	1.84159100	-0.26031800
H	-3.80128400	2.77093100	0.23250100
H	-4.40069100	2.10231200	-1.27929400
C	-6.36690300	0.87677500	-0.14418300
H	-6.43984800	1.19302000	-1.18520100
C	-5.22423500	1.17574000	0.49977200
C	-4.94172400	0.90542300	1.96520900
H	-5.86093700	0.56937500	2.45556900
H	-4.21010000	0.09185200	2.05947100
C	-4.43483900	2.12573300	2.69847300
C	-3.37707400	2.15255100	3.51182700
H	-5.02134300	3.03451700	2.55753800
H	-3.08491100	3.05075600	4.04778100
H	-2.78755200	1.25888900	3.70064200
O	-3.03019900	0.72734800	-2.87579700
O	-1.39239000	-0.65348300	-1.49659500
S	-2.71275700	-0.02166800	-1.65072900
C	-7.55610300	0.16079400	0.35262700
C	-8.83178100	0.57073400	-0.07382100
C	-7.46512400	-0.96689400	1.18827000

C	-9.97943500	-0.09625700	0.35070800
H	-8.91952100	1.42666200	-0.73819300
C	-8.61340200	-1.63640500	1.61173100
H	-6.48837700	-1.34570200	1.46679400
C	-9.87508800	-1.20054500	1.20021000
H	-10.95544600	0.24289600	0.01643200
H	-8.52130700	-2.50543100	2.25723700
H	-10.76823000	-1.72284200	1.52957200
C	-3.96547400	-1.26326700	-1.40278400
C	-5.03249000	-1.35036100	-2.29458100
C	-3.84198700	-2.14056500	-0.32282000
C	-6.00635600	-2.32340100	-2.08184700
H	-5.09337200	-0.66206800	-3.13015000
C	-4.82311300	-3.10810400	-0.13079000
H	-2.99401300	-2.06622400	0.34930000
C	-5.92476400	-3.20687300	-0.99666600
H	-6.84898500	-2.39210800	-2.76366400
H	-4.73796100	-3.79559500	0.70621600
C	-7.02422200	-4.20382000	-0.73768300
H	-6.66799400	-5.05894200	-0.15678500
H	-7.82964000	-3.72360000	-0.16874200
H	-7.45712400	-4.57635400	-1.67033400
C	2.43448200	0.10601900	2.17266600
C	1.10783800	0.09131500	2.65995700
C	0.43602600	1.30804600	2.80490200
C	1.02008800	2.53423400	2.47839700
C	2.33935500	2.52475100	2.02361900
C	3.06206400	1.33495300	1.87389900
H	-0.57906200	1.30575000	3.18948200
H	2.82876700	3.46283800	1.78498200
C	0.41718300	-1.19670600	3.09909900
C	-1.00427400	-1.35176800	2.52836100
C	0.38821700	-1.28912500	4.63777400
H	1.01000100	-2.03786400	2.72837200
H	-1.01439100	-1.25481300	1.44116500
H	-1.40598500	-2.33792300	2.78460600
H	-1.69178800	-0.60554900	2.93928200
H	1.39559700	-1.20517700	5.05015500
H	-0.21572700	-0.47787400	5.05980700
H	-0.04947500	-2.23980800	4.96100500
C	0.23064400	3.81990100	2.68465900
C	0.58118900	4.92775500	1.67992400
C	0.39460100	4.32309800	4.13251800
H	-0.83146200	3.57191600	2.54665400

H	0.55566100	4.55663600	0.65113100
H	-0.12285400	5.76126900	1.76994700
H	1.58316200	5.33156900	1.85847300
H	0.08984700	3.55629100	4.85119400
H	1.44219000	4.57202200	4.33402400
H	-0.20920100	5.22012400	4.30839600
C	4.52680600	1.39938800	1.45830400
C	5.38741400	1.89875000	2.63533700
C	4.75699500	2.25260700	0.19957300
H	4.85383700	0.38200000	1.22571800
H	5.23146600	1.27293900	3.51823100
H	6.45122400	1.88132500	2.37483300
H	5.12073100	2.92764000	2.90134300
H	4.13919800	1.89692800	-0.63048000
H	4.51410600	3.30649500	0.37026800
H	5.80780600	2.20503100	-0.10587200
C	3.21780400	-1.17451200	2.10575800
C	3.36194800	-1.97976100	0.95658300
C	3.85041700	-1.57043800	3.31039200
C	4.10752900	-3.18577300	1.04925400
C	4.56509400	-2.76252900	3.38142400
C	4.68864000	-3.57251800	2.25255000
H	5.03797500	-3.07577300	4.30369500
H	5.25286300	-4.49324900	2.32755900
O	3.70688000	-0.70667400	4.36127500
O	4.23671200	-3.90909500	-0.10559700
C	4.32238800	-1.03604400	5.60083900
H	5.41193600	-1.12007000	5.50014200
H	4.08573300	-0.21347400	6.27642700
H	3.92170500	-1.97039300	6.01457600
C	5.04152500	-5.08258200	-0.10304800
H	6.07780900	-4.85582600	0.17615200
H	4.63898500	-5.84540500	0.57432400
H	5.01659600	-5.46110500	-1.12548500
C	1.57610500	-2.94207600	-1.19461100
C	0.43010700	-3.09377600	-0.17880700
C	1.02912900	-2.77103100	-2.62732100
H	2.20846600	-3.83406700	-1.16047200
C	-0.52084700	-4.23838500	-0.56041800
H	-0.13487400	-2.15839400	-0.15717400
H	0.83502000	-3.26047800	0.82520000
C	0.08461300	-3.93049400	-2.99196300
H	0.48113700	-1.82429600	-2.70208300
H	1.85291000	-2.73613400	-3.34850200

C	-1.06436200	-4.06168400	-1.98422900
H	-1.34587500	-4.28267600	0.16160900
H	0.01251700	-5.19670800	-0.48631300
H	-0.30865900	-3.77281500	-4.00268700
H	0.65681700	-4.86906500	-3.01928500
H	-1.71175200	-4.90474900	-2.25165700
H	-1.67912600	-3.15570300	-2.02252200
C	4.10876200	-1.54547300	-1.90835300
C	3.83989300	-0.61401100	-3.11115600
C	5.48083700	-1.20110000	-1.29592500
H	4.14501700	-2.58277000	-2.26135200
C	4.93757500	-0.76404000	-4.17547100
H	3.83141900	0.42317400	-2.74971100
H	2.85256700	-0.79435600	-3.54575100
C	6.59219100	-1.34444800	-2.34920800
H	5.46428800	-0.16772900	-0.92981900
H	5.70094100	-1.83967200	-0.43836100
C	6.32365900	-0.47266400	-3.58362700
H	4.73057500	-0.09514200	-5.01889300
H	4.91571700	-1.78763300	-4.57435300
H	7.55898500	-1.08645300	-1.90192100
H	6.65899800	-2.39808200	-2.65512100
H	7.10328600	-0.62713800	-4.33781600
H	6.37316300	0.58631100	-3.29153300
P	2.67184500	-1.51029200	-0.69368400
Au	1.45284900	0.50819400	-0.86390300

Zero-point correction=	1.314866 (Hartree/Particle)
Thermal correction to Energy=	1.388936
Thermal correction to Enthalpy=	1.389881
Thermal correction to Gibbs Free Energy=	1.201454
Sum of electronic and zero-point Energies=	-3791.634298
Sum of electronic and thermal Energies=	-3791.560228
Sum of electronic and thermal Enthalpies=	-3791.559283
Sum of electronic and thermal Free Energies=	-3791.747710

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C	-1.40428400	3.85396100	3.67558000
C	-0.96473900	2.95737000	2.71620100
C	0.45993300	4.74955800	1.84956500
C	0.00210400	5.65639000	2.83610600
C	-0.93328200	5.19449000	3.73611400
H	-2.13283600	3.52397500	4.41007500
H	-1.31985900	1.93622800	2.68640800
H	0.37982900	6.67254900	2.87842900

H	-1.31399200	5.85302800	4.50962100
C	1.38962900	4.86854200	0.81428100
O	1.51309600	3.75290600	0.13346400
H	1.99533000	5.70642600	0.49157100
C	-0.03015900	3.40763200	1.77223000
C	0.62224900	2.76639100	0.67180700
C	0.55806000	1.52941800	0.09820100
C	1.58047300	1.17960800	-0.97518700
H	1.13434000	0.52042600	-1.71617600
H	1.98389600	2.05528300	-1.48728600
N	2.74660100	0.49179000	-0.37699000
C	3.65838800	1.29158800	0.48232100
H	3.37542400	2.33260100	0.31883300
H	3.49036000	1.06171600	1.53944600
C	5.98255300	0.67402900	1.03073400
H	5.58774800	0.52065700	2.03604700
C	5.11003200	1.10047200	0.09924900
C	5.44736600	1.43830500	-1.34109200
H	6.53466300	1.46718900	-1.46124400
H	5.07076200	0.64421700	-1.99802300
C	4.88402000	2.76569500	-1.78775700
C	4.06848300	2.94349800	-2.82849400
H	5.20365800	3.63082000	-1.20492600
H	3.72095600	3.92921700	-3.12418600
H	3.73845800	2.10574700	-3.43909500
O	2.39582000	-1.21462200	1.56532400
O	1.44264700	-1.63887500	-0.76044900
S	2.51802900	-1.12407300	0.10242200
C	7.41968700	0.37740200	0.89445700
C	8.28193000	0.67642900	1.96472500
C	7.96420400	-0.25131000	-0.24079000
C	9.64535500	0.39835200	1.88885600
H	7.87525800	1.14035600	2.85986200
C	9.32873000	-0.53036500	-0.31641800
H	7.30915300	-0.56080100	-1.04649900
C	10.17584100	-0.20165900	0.74415400
H	10.29406200	0.64674400	2.72365000
H	9.72960400	-1.01139500	-1.20431300
H	11.23764000	-0.42069800	0.68419800
C	4.03361400	-1.93319600	-0.37502100
C	4.87282800	-2.44906600	0.61315600
C	4.33171500	-2.07243700	-1.73098300
C	6.04215500	-3.09632800	0.22888300
H	4.60927700	-2.33034300	1.65766000

C	5.51054700	-2.72095100	-2.09542900
H	3.65203900	-1.68657400	-2.48345200
C	6.38400900	-3.23463100	-1.12533100
H	6.71056900	-3.48714900	0.99046100
H	5.75553100	-2.83075100	-3.14794400
C	7.68475600	-3.89216300	-1.50937700
H	8.52918000	-3.29742400	-1.14184300
H	7.77238300	-4.88782100	-1.06211600
H	7.78577400	-3.99518600	-2.59259700
C	-3.17902600	0.46429700	-1.65148800
C	-2.13213200	0.32524800	-2.59550200
C	-1.34194500	1.44120900	-2.88431500
C	-1.56930100	2.69501700	-2.30387100
C	-2.62697700	2.81027600	-1.40306500
C	-3.43806300	1.71897700	-1.06569500
H	-0.53200600	1.33952500	-3.60081900
H	-2.84466000	3.77104200	-0.95141900
C	-1.90956800	-0.97845900	-3.35504200
C	-0.42822400	-1.34155000	-3.54209800
C	-2.61901500	-0.91794600	-4.72393500
H	-2.37266300	-1.78257700	-2.77600300
H	0.11508600	-1.33800000	-2.59652400
H	-0.34358200	-2.34322800	-3.97612500
H	0.07238900	-0.65273600	-4.23212600
H	-3.67961100	-0.68657900	-4.61240100
H	-2.17071300	-0.13689600	-5.34841500
H	-2.51806200	-1.87274000	-5.25110100
C	-0.68543400	3.87271200	-2.70323300
C	-0.87951200	5.12257700	-1.83505400
C	-0.89028600	4.22969900	-4.18995000
H	0.35840600	3.54553700	-2.58439400
H	-0.80381900	4.89666100	-0.76765500
H	-0.12606800	5.87696900	-2.08339700
H	-1.86204500	5.57590800	-2.00531500
H	-0.70043100	3.37238800	-4.84150900
H	-1.92086900	4.55767600	-4.36314200
H	-0.21896600	5.04072600	-4.49211300
C	-4.60780900	1.93447500	-0.11264600
C	-5.72795300	2.73468900	-0.80393300
C	-4.17399000	2.60425200	1.20140500
H	-5.01744400	0.95310700	0.14325200
H	-6.04725700	2.23257800	-1.72058000
H	-6.59340700	2.84301700	-0.14127000
H	-5.38039800	3.73834100	-1.07274400

H	-3.36799900	2.03800700	1.67478800
H	-3.81040300	3.62425400	1.04022300
H	-5.01523900	2.66145600	1.90064800
C	-4.09635300	-0.69098900	-1.36602600
C	-3.91704000	-1.63416600	-0.33215900
C	-5.23399800	-0.79516000	-2.20432200
C	-4.86816800	-2.67766200	-0.17809900
C	-6.14108800	-1.83878500	-2.04905700
C	-5.95613900	-2.78209600	-1.03837400
H	-7.00324300	-1.93117000	-2.69759000
H	-6.67749900	-3.58165600	-0.92924100
O	-5.36519900	0.19177500	-3.14230100
O	-4.66171300	-3.53464100	0.86884000
C	-6.47253200	0.13915400	-4.03366400
H	-7.42672100	0.20059100	-3.49503100
H	-6.36989700	1.00792000	-4.68458100
H	-6.45575000	-0.77340900	-4.64308400
C	-5.59960000	-4.57838400	1.10632700
H	-6.60044700	-4.17836200	1.31011800
H	-5.64947000	-5.27417300	0.26016000
H	-5.23613800	-5.10846600	1.98733300
C	-1.67303500	-3.24251100	0.76371600
C	-1.27936100	-3.55497400	-0.69270100
C	-0.45790300	-3.30791300	1.71254200
H	-2.41975100	-3.97200800	1.09004700
C	-0.53190600	-4.89401100	-0.79618200
H	-0.63204000	-2.75859100	-1.06777200
H	-2.17510000	-3.57962100	-1.32308500
C	0.28683600	-4.64679000	1.57625300
H	0.23701200	-2.49333000	1.48932600
H	-0.78127800	-3.18079400	2.75177300
C	0.69570800	-4.92171600	0.12329400
H	-0.23754000	-5.06464200	-1.83825000
H	-1.21177600	-5.71349600	-0.52176300
H	1.16747800	-4.63305200	2.22860800
H	-0.35861200	-5.46275600	1.93181500
H	1.20484100	-5.88962700	0.04966600
H	1.40558800	-4.15424400	-0.20736800
C	-3.26268800	-1.52145500	2.59398300
C	-2.30769600	-0.82446400	3.58685800
C	-4.65509400	-0.86472700	2.66897300
H	-3.36738100	-2.57479200	2.87998500
C	-2.85091500	-0.89644800	5.02145500
H	-2.21999500	0.22985100	3.29457500

H	-1.29808100	-1.24156800	3.53280100
C	-5.20748700	-0.92182000	4.10309000
H	-4.57931900	0.18195900	2.35329500
H	-5.35372300	-1.35284300	1.98700600
C	-4.25012600	-0.27232100	5.11145100
H	-2.15797900	-0.39254700	5.70529500
H	-2.89620500	-1.94706400	5.33950200
H	-6.18917800	-0.43568300	4.13819400
H	-5.36756900	-1.97292400	4.38156900
H	-4.64682900	-0.36230800	6.12875900
H	-4.17774800	0.80401100	4.89539800
P	-2.51007900	-1.57117200	0.86927400
Au	-0.88134200	0.12857800	0.52276100

Zero-point correction= 1.314275 (Hartree/Particle)
Thermal correction to Energy= 1.388452
Thermal correction to Enthalpy= 1.389396
Thermal correction to Gibbs Free Energy= 1.199866
Sum of electronic and zero-point Energies= -3791.615124
Sum of electronic and thermal Energies= -3791.540948
Sum of electronic and thermal Enthalpies= -3791.540003
Sum of electronic and thermal Free Energies= -3791.729533

A-TSa1

C	0.02128700	-4.74485600	1.40344700
C	0.06535100	-3.38041400	1.16649400
C	-2.31085600	-3.24240100	1.64239000
C	-2.35514100	-4.62964500	1.85616100
C	-1.19013500	-5.37384200	1.74927300
H	0.93062500	-5.33287100	1.32321500
H	0.99694700	-2.88805300	0.92459300
H	-3.29725100	-5.10723600	2.10687800
H	-1.21306300	-6.44402700	1.92798300
C	-3.49505100	-2.41320800	1.68693000
O	-3.30315900	-1.11556200	2.07347800
H	-4.38128700	-2.82651300	2.16121700
C	-1.09966800	-2.59474900	1.28431600
C	-1.11587700	-1.16853400	1.03389800
C	-2.24095900	-0.49276900	1.46592500
C	-2.45820700	0.98664300	1.36184000
H	-3.22306800	1.29910100	2.08705500
H	-1.53567400	1.53544300	1.53617600
N	-2.90058700	1.22818200	-0.02932300
C	-3.96058000	0.30854100	-0.44428400
H	-4.77781900	0.28241700	0.28916100

H	-4.36411800	0.65890800	-1.40001800
C	-4.12201000	-2.18902300	-0.15641200
H	-5.11329000	-1.88173500	0.18247100
C	-3.39880500	-1.08050200	-0.69026300
C	-2.41427100	-1.14902100	-1.83090500
H	-1.82201900	-0.23380200	-1.82493200
H	-1.72310800	-1.98296300	-1.71806500
C	-3.17973800	-1.25252300	-3.13757300
C	-3.39509900	-0.20289900	-3.93374600
H	-3.57683200	-2.23404000	-3.38682900
H	-3.94845300	-0.30376300	-4.86285100
H	-3.03168800	0.79058600	-3.67988900
O	-1.77025700	3.46713400	-0.05246700
O	-3.33389700	2.77523900	-1.96499500
S	-3.00308000	2.84111500	-0.53768400
C	-4.16620500	-3.53393300	-0.81280200
C	-5.42738100	-4.11331600	-1.02683600
C	-3.02745500	-4.25286200	-1.21294500
C	-5.55236600	-5.35857500	-1.64207000
H	-6.32202800	-3.57795000	-0.71819400
C	-3.15213700	-5.49669000	-1.83054100
H	-2.03642100	-3.85863000	-1.02450900
C	-4.41306800	-6.05346400	-2.05134100
H	-6.53877000	-5.78301300	-1.80207200
H	-2.25808000	-6.03404000	-2.13215500
H	-4.50683000	-7.02180300	-2.53303500
C	-4.38137900	3.55051500	0.34271300
C	-4.17103000	4.08776700	1.61607900
C	-5.65884800	3.49561000	-0.22112600
C	-5.26453000	4.57150300	2.33030500
H	-3.16655700	4.14486200	2.02158200
C	-6.73746300	3.98699400	0.51002900
H	-5.79332000	3.09864000	-1.22157300
C	-6.56007900	4.52934200	1.79250900
H	-5.10972300	4.99663000	3.31798600
H	-7.73295300	3.95730700	0.07596500
C	-7.73099900	5.09134500	2.55920700
H	-7.57737600	5.01668700	3.63928400
H	-7.87093100	6.15266300	2.32102900
H	-8.66142800	4.57511500	2.30690100
C	3.14117500	0.32394200	1.56466400
C	3.25318900	-1.04605300	1.89994800
C	2.50252200	-1.54102000	2.97190400
C	1.67090800	-0.71978900	3.74114100

C	1.57622200	0.62611600	3.38592800
C	2.29685400	1.16997900	2.31520000
H	2.60274300	-2.58814600	3.24215100
H	0.94796200	1.28068900	3.98421300
C	4.26232600	-1.95654800	1.20338700
C	3.67939800	-3.31004600	0.76440500
C	5.48964700	-2.16921500	2.11269100
H	4.60809600	-1.44631000	0.29953900
H	2.84172800	-3.18204400	0.07227800
H	4.44472000	-3.90265500	0.25266100
H	3.32766700	-3.89984200	1.61757400
H	5.91823900	-1.21009900	2.41134000
H	5.20497700	-2.70819100	3.02318700
H	6.25843400	-2.75533000	1.59747000
C	0.93924500	-1.25040400	4.96695200
C	1.91618500	-1.87980700	5.97705600
C	-0.18081700	-2.23923300	4.59972800
H	0.46862400	-0.38845800	5.45815600
H	2.71131100	-1.17851900	6.24702200
H	1.38936000	-2.17166800	6.89150000
H	2.38794900	-2.77892700	5.56605000
H	-0.93021000	-1.76655300	3.95902900
H	0.21773400	-3.10600100	4.06227200
H	-0.68422500	-2.60404200	5.50142600
C	2.21750400	2.66707400	2.04201700
C	3.01320400	3.44765000	3.10642900
C	0.77257100	3.17737800	1.94525200
H	2.68932800	2.85705300	1.07345800
H	4.04691400	3.09629200	3.15282700
H	3.01401700	4.51912000	2.87931600
H	2.56774000	3.31247400	4.09834500
H	0.21315000	2.63706600	1.17906000
H	0.23876300	3.07593000	2.89690900
H	0.75530900	4.23748100	1.67346000
C	4.03380300	0.90950800	0.50696200
C	3.70495000	1.02287400	-0.85878100
C	5.30029700	1.36670800	0.94971600
C	4.66335400	1.55403400	-1.76106300
C	6.21516100	1.90920800	0.05197600
C	5.89998900	1.99697100	-1.30462600
H	7.18203800	2.26300700	0.38693000
H	6.63131400	2.40879500	-1.98826300
O	5.53788600	1.23467500	2.28999600
O	4.29814400	1.57849300	-3.07938000

C	6.78348000	1.68644600	2.80788200
H	6.92096400	2.76277000	2.64354900
H	6.74776400	1.48765600	3.87939100
H	7.62622300	1.13953200	2.36607200
C	5.17748900	2.16723500	-4.03113700
H	6.12490800	1.61839000	-4.09572600
H	4.66060700	2.10688200	-4.98950500
H	5.37920200	3.21844700	-3.79232800
C	2.33711000	-0.74377300	-2.86357400
C	3.60451100	-1.58978500	-2.63944300
C	1.11037100	-1.66856200	-3.02874600
H	2.47264100	-0.16709500	-3.78628200
C	3.80685000	-2.59424200	-3.78545700
H	3.51086600	-2.13400700	-1.69325400
H	4.48462900	-0.94930800	-2.55326900
C	1.31264500	-2.66009700	-4.18390100
H	0.96222500	-2.22904400	-2.09510400
H	0.19712100	-1.08766700	-3.18683500
C	2.58155800	-3.49791300	-3.97791400
H	4.70139700	-3.19679800	-3.59053400
H	3.99833300	-2.04041800	-4.71524200
H	0.43162300	-3.30685700	-4.27160100
H	1.38873300	-2.10489400	-5.12895500
H	2.73571700	-4.17678000	-4.82393900
H	2.45531700	-4.12801300	-3.08552300
C	1.42764200	2.04598800	-2.47093500
C	-0.04416300	1.87390000	-2.89533700
C	1.60445400	3.36426700	-1.69546400
H	2.05084800	2.09142500	-3.36886600
C	-0.50630300	3.06443500	-3.75282300
H	-0.66764100	1.80821600	-1.99754400
H	-0.18767800	0.94447900	-3.45710000
C	1.17044200	4.55451300	-2.56692300
H	0.98723300	3.33894200	-0.79109000
H	2.64532100	3.49052600	-1.38039300
C	-0.28251700	4.40426400	-3.03816800
H	-1.56743700	2.94342000	-3.99345400
H	0.04694200	3.05506100	-4.70270300
H	1.29379200	5.48624000	-2.00297800
H	1.83875000	4.62215300	-3.43773500
H	-0.55405400	5.23292200	-3.70211400
H	-0.94521500	4.45772700	-2.16866800
P	2.04886300	0.55336600	-1.52399200
Au	0.42659600	-0.24385600	0.00992100

Zero-point correction=	1.315750 (Hartree/Particle)
Thermal correction to Energy=	1.388361
Thermal correction to Enthalpy=	1.389305
Thermal correction to Gibbs Free Energy=	1.205417
Sum of electronic and zero-point Energies=	-3791.613723
Sum of electronic and thermal Energies=	-3791.541112
Sum of electronic and thermal Enthalpies=	-3791.540168
Sum of electronic and thermal Free Energies=	-3791.724055

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C	-0.04708200	4.57864600	2.09868400
C	-0.09915300	3.28673200	1.60355700
C	2.33863500	3.10845200	1.81695400
C	2.37951500	4.41226700	2.29221400
C	1.19372900	5.13963700	2.43972900
H	-0.95919500	5.15319100	2.22193800
H	-1.04439800	2.82776300	1.34610300
H	3.33166000	4.86426500	2.55218500
H	1.23590000	6.15375700	2.82638600
C	3.56766400	2.25880300	1.64760700
O	3.21368800	0.92302400	1.98720400
H	4.36325900	2.58913400	2.31871300
C	1.08640100	2.52181700	1.45409000
C	1.05430700	1.20252900	0.91483600
C	2.37014300	0.49954900	0.91249800
C	2.34890000	-1.03965400	0.90304500
H	2.97560500	-1.38695800	1.73703800
H	1.35509100	-1.47073400	0.99552600
N	2.93701600	-1.35549700	-0.40082600
C	3.98843400	-0.36797600	-0.65100500
H	4.81922700	-0.47815100	0.06181200
H	4.36267400	-0.45432400	-1.67015500
C	4.09678700	2.11039700	0.16897600
H	5.09956900	1.69592600	0.30558400
C	3.21803500	0.95331400	-0.40976500
C	2.35658800	1.25749400	-1.66333500
H	1.69559100	0.40111300	-1.80139200
H	1.71504800	2.12160900	-1.47235600
C	3.13177300	1.46994100	-2.93913600
C	3.22662800	0.54349400	-3.89655000
H	3.62271300	2.43112200	-3.06777300
H	3.78307700	0.72663600	-4.81100300
H	2.76456000	-0.43601700	-3.79347600
O	1.87902500	-3.61707300	-0.49961500

O	3.63486700	-2.91266400	-2.23519000
S	3.14032000	-2.95731400	-0.85686200
C	4.25811600	3.38892500	-0.62802600
C	5.53322700	3.70919800	-1.11709700
C	3.20028100	4.26440500	-0.92486600
C	5.74951400	4.85459200	-1.88364100
H	6.36787200	3.04634500	-0.90315900
C	3.41181500	5.40969600	-1.69232200
H	2.19784000	4.05518800	-0.57121200
C	4.68637000	5.70949200	-2.17664600
H	6.74650600	5.07569100	-2.25238900
H	2.57616000	6.06687400	-1.91436000
H	4.84841900	6.59979100	-2.77640600
C	4.42939900	-3.59475600	0.19808600
C	4.09055700	-4.14220300	1.43863200
C	5.76366900	-3.45867400	-0.19457500
C	5.11015500	-4.55797200	2.29185200
H	3.04721500	-4.25857700	1.71160600
C	6.76723600	-3.88152300	0.67357400
H	6.00120800	-3.05064000	-1.17120600
C	6.45910000	-4.43531000	1.92573700
H	4.85569400	-4.99131000	3.25511800
H	7.80690200	-3.78760100	0.37248400
C	7.55338900	-4.92415900	2.84175200
H	7.26003500	-4.85169100	3.89279500
H	7.78278500	-5.97703200	2.63779800
H	8.47755600	-4.35628000	2.70252200
C	-3.12402800	-0.43534400	1.55281500
C	-3.20814500	0.85127600	2.14011500
C	-2.36663900	1.15749500	3.21668700
C	-1.46702300	0.22817900	3.75223000
C	-1.40620600	-1.03203000	3.15727900
C	-2.22357100	-1.39191900	2.07664100
H	-2.44860900	2.13581900	3.68053800
H	-0.73569700	-1.77649300	3.57833500
C	-4.28085600	1.85670400	1.72187900
C	-3.74970300	3.28134500	1.49105900
C	-5.41149900	1.88184100	2.77175100
H	-4.71414300	1.51323900	0.77704500
H	-2.98658900	3.30781700	0.71028200
H	-4.56564700	3.93998300	1.17675400
H	-3.32400000	3.70854400	2.40561000
H	-5.80900500	0.87955400	2.93881900
H	-5.03633000	2.25893900	3.72954500

H	-6.22679200	2.53667300	2.44603300
C	-0.62459500	0.53801700	4.98331700
C	-1.48471900	1.06406300	6.14651500
C	0.53309300	1.50588800	4.67906600
H	-0.17809400	-0.41059600	5.30904300
H	-2.30955000	0.38118300	6.37049800
H	-0.87717500	1.17738900	7.05009100
H	-1.91435800	2.04474900	5.91506100
H	1.20986500	1.10362800	3.91998800
H	0.15415000	2.46876200	4.31957100
H	1.11958000	1.69463700	5.58457600
C	-2.20056500	-2.83092500	1.57637100
C	-2.87839900	-3.75540800	2.60750500
C	-0.78709900	-3.32018500	1.23017700
H	-2.79683300	-2.87893500	0.66089000
H	-3.88797400	-3.40360800	2.83617200
H	-2.94035100	-4.77904100	2.22337700
H	-2.30923000	-3.77973200	3.54320300
H	-0.32252500	-2.69690500	0.46303200
H	-0.12779500	-3.32279900	2.10479800
H	-0.81292800	-4.34329400	0.84297800
C	-4.09526700	-0.84273600	0.47941400
C	-3.83448100	-0.79755900	-0.90632300
C	-5.34770900	-1.33251000	0.92428700
C	-4.84526000	-1.19445400	-1.81975300
C	-6.33001200	-1.70835900	0.01128200
C	-6.08292400	-1.63230000	-1.35960000
H	-7.29294400	-2.07085600	0.34831800
H	-6.86016500	-1.93146300	-2.05121300
O	-5.49871800	-1.41585000	2.28044000
O	-4.51286500	-1.14015400	-3.14586300
C	-6.72018800	-1.93073800	2.79942400
H	-6.89773400	-2.95925300	2.46114600
H	-6.60725700	-1.92212500	3.88384000
H	-7.57429000	-1.30114800	2.51948600
C	-5.41128200	-1.68590200	-4.10725400
H	-6.35161900	-1.12296000	-4.14415100
H	-4.90341800	-1.60154400	-5.06845200
H	-5.62356300	-2.74120900	-3.89799800
C	-2.50228100	1.11480400	-2.73416300
C	-3.01357100	2.32182700	-1.92685900
C	-1.24112700	1.49164300	-3.53874000
H	-3.28351600	0.79012300	-3.42772900
C	-3.26875200	3.53848200	-2.82812400

H	-2.25264800	2.58679100	-1.18002700
H	-3.92179300	2.05683500	-1.37541100
C	-1.49666700	2.71822900	-4.43035800
H	-0.41877300	1.71395100	-2.84478600
H	-0.91264800	0.65359700	-4.16101000
C	-2.00704600	3.91447700	-3.61636600
H	-3.61126400	4.38253700	-2.21829200
H	-4.08174500	3.30619200	-3.52946300
H	-0.57526000	2.97771100	-4.96356100
H	-2.24113800	2.45822800	-5.19536200
H	-2.20561700	4.76766300	-4.27421100
H	-1.22380600	4.23319300	-2.91266700
C	-1.58671300	-1.73065100	-2.68862200
C	-0.04298500	-1.72912100	-2.75740100
C	-2.09107500	-3.12801000	-2.27805500
H	-1.99518700	-1.49954800	-3.68006200
C	0.47486900	-2.79409300	-3.73586500
H	0.36064200	-1.94310700	-1.76131200
H	0.33419500	-0.74378100	-3.04465800
C	-1.58009600	-4.19290800	-3.26346400
H	-1.72112400	-3.36647300	-1.27609100
H	-3.18259900	-3.15166500	-2.23456700
C	-0.04838300	-4.18638700	-3.36094100
H	1.56945800	-2.78863000	-3.72445800
H	0.15531700	-2.53681600	-4.75608200
H	-1.94189600	-5.17943900	-2.95129500
H	-2.01349700	-3.99835800	-4.25527900
H	0.28850500	-4.92846500	-4.09328000
H	0.38202400	-4.47118400	-2.39316800
P	-2.19124800	-0.33099500	-1.59049500
Au	-0.54617700	0.38981600	-0.02917300

Zero-point correction=	1.318007 (Hartree/Particle)
Thermal correction to Energy=	1.390283
Thermal correction to Enthalpy=	1.391227
Thermal correction to Gibbs Free Energy=	1.208187
Sum of electronic and zero-point Energies=	-3791.632674
Sum of electronic and thermal Energies=	-3791.560399
Sum of electronic and thermal Enthalpies=	-3791.559454
Sum of electronic and thermal Free Energies=	-3791.742494

A-TSa2

C	-1.16383600	-5.04153300	0.34335500
C	-0.89221800	-3.81228900	-0.24874100
C	-2.71434800	-2.80433300	0.99351700

C	-2.95902600	-4.03252000	1.60917900
C	-2.19588500	-5.15300300	1.28142600
H	-0.55937800	-5.90734200	0.09209100
H	-0.07669600	-3.71708000	-0.96034700
H	-3.75411800	-4.10955700	2.34514300
H	-2.39536300	-6.10494900	1.76298300
C	-3.50095100	-1.56189800	1.33331500
O	-2.62255500	-0.43002900	1.23827300
H	-3.86478700	-1.60996500	2.36171000
C	-1.66764000	-2.68070400	0.05594900
C	-1.39030700	-1.35368800	-0.55320900
C	-2.41271300	-0.25987000	-0.16668400
C	-1.97601900	1.19241500	-0.43884000
H	-1.95390700	1.73681800	0.51512600
H	-1.00289500	1.27624700	-0.91476100
N	-3.01882900	1.67555200	-1.34540400
C	-4.28456200	1.09394400	-0.90268800
H	-4.59725400	1.50069000	0.07109800
H	-5.07199200	1.27056000	-1.63707200
C	-4.64858600	-1.16761700	0.34317100
H	-5.21523900	-0.40933500	0.89179600
C	-3.86688100	-0.39026100	-0.77487700
C	-3.83027500	-0.99939300	-2.20420200
H	-4.75525900	-1.54554100	-2.40005900
H	-3.75522900	-0.16994200	-2.91267000
C	-2.65017400	-1.88767500	-2.39942800
C	-1.39728900	-1.40464100	-2.67277200
H	-2.77984300	-2.96001500	-2.29720500
H	-0.58597600	-2.07642500	-2.92358900
H	-1.24760400	-0.35384900	-2.90285200
O	-1.51570200	3.35540900	-2.41282000
O	-4.03679900	3.32360600	-2.92515800
S	-2.91619000	3.22142300	-1.99109500
C	-5.64749600	-2.22845900	-0.06694500
C	-7.01157400	-1.97570500	0.14339700
C	-5.28986800	-3.44731300	-0.66719700
C	-7.98661400	-2.90176200	-0.22819000
H	-7.31464500	-1.03922200	0.60516700
C	-6.26158600	-4.37654500	-1.03993400
H	-4.24702400	-3.68954600	-0.82959700
C	-7.61390700	-4.10808600	-0.82213600
H	-9.03486600	-2.68021500	-0.05217500
H	-5.95887900	-5.31339300	-1.49831800
H	-8.36893200	-4.83239000	-1.11177500

C	-3.19998000	4.33041100	-0.62304300
C	-2.11022700	4.86709500	0.06348800
C	-4.51217800	4.58469600	-0.21142800
C	-2.34239200	5.66146500	1.18469100
H	-1.10496600	4.67630300	-0.29122700
C	-4.72292700	5.38059800	0.91114400
H	-5.34654100	4.18486400	-0.77794300
C	-3.64603100	5.92867200	1.62676300
H	-1.49746300	6.08507200	1.72056000
H	-5.73920800	5.58858200	1.23428700
C	-3.89202700	6.81787300	2.82014400
H	-4.77093700	6.49538200	3.38599900
H	-3.03321900	6.83094200	3.49676700
H	-4.07312300	7.85061300	2.49873900
C	2.33261800	0.00265600	2.01847900
C	1.97106200	-1.28656500	2.46198600
C	0.75532400	-1.45848900	3.13841200
C	-0.11323200	-0.39566700	3.38498200
C	0.24753900	0.86349600	2.89322600
C	1.45894700	1.09323000	2.23912900
H	0.50201400	-2.44948700	3.49645200
H	-0.42211200	1.70048000	3.07151600
C	2.90062400	-2.48176200	2.29055500
C	2.17901300	-3.71266800	1.71744600
C	3.59529200	-2.82854700	3.62197800
H	3.67954600	-2.19651500	1.57741200
H	1.62004300	-3.45811000	0.81375900
H	2.90196300	-4.49758200	1.47055600
H	1.46569700	-4.13597200	2.43190000
H	4.13546300	-1.96487100	4.01621400
H	2.85694600	-3.13298600	4.37189500
H	4.30108000	-3.65539000	3.48740200
C	-1.38477700	-0.52737700	4.21460000
C	-1.23685500	0.24725700	5.54163000
C	-1.80059800	-1.97476500	4.50346400
H	-2.18572200	-0.05115400	3.63475500
H	-0.99664100	1.30091700	5.37277400
H	-2.16399300	0.19962800	6.12280500
H	-0.43324000	-0.18442400	6.14832800
H	-1.86793600	-2.57144600	3.59087100
H	-1.08630900	-2.46760800	5.17260100
H	-2.77558000	-1.99574700	5.00164000
C	1.85521800	2.52145700	1.88376800
C	2.26166800	3.28777300	3.15818600

C	0.75502100	3.27201800	1.12004800
H	2.73386900	2.47949900	1.23440400
H	3.05122500	2.75457600	3.69383200
H	2.61933400	4.29350800	2.91170200
H	1.40615200	3.38621400	3.83551800
H	0.45869200	2.73296100	0.21562500
H	-0.14175800	3.41530700	1.73055900
H	1.10806900	4.26570400	0.82200400
C	3.70872700	0.26180800	1.47355500
C	4.05107300	0.29706600	0.10661100
C	4.71221800	0.53645900	2.43621300
C	5.37970300	0.62126300	-0.27522000
C	6.01687000	0.82278700	2.04280000
C	6.35065500	0.86907600	0.68885300
H	6.78726400	1.02556300	2.77601700
H	7.36780700	1.10912100	0.40682800
O	4.30147400	0.50909000	3.73891400
O	5.62193300	0.69552200	-1.62111500
C	5.25531200	0.77657700	4.76038000
H	5.67537900	1.78591400	4.66466400
H	4.70942700	0.70120800	5.70117100
H	6.06919500	0.04046400	4.75421700
C	6.91031300	1.10437000	-2.07033400
H	7.68726300	0.39472500	-1.76165700
H	6.85199800	1.12451800	-3.15901700
H	7.16129200	2.10590300	-1.70102300
C	3.60157000	-1.44344200	-2.23449200
C	3.85069100	-2.68554900	-1.35948600
C	2.74160900	-1.79574100	-3.46396100
H	4.56315200	-1.05524900	-2.58090300
C	4.46689400	-3.83348200	-2.17373100
H	2.89659600	-3.01863700	-0.93156500
H	4.50273800	-2.42980500	-0.51791900
C	3.36642800	-2.94830600	-4.26786900
H	1.73863500	-2.09666900	-3.12926500
H	2.61251000	-0.92203800	-4.11080900
C	3.59918600	-4.18416500	-3.38885900
H	4.60154500	-4.70943700	-1.52917600
H	5.46805000	-3.53786800	-2.51642800
H	2.72148600	-3.19392000	-5.11930400
H	4.32561000	-2.61532400	-4.68726100
H	4.06351500	-4.98580500	-3.97331800
H	2.62887700	-4.56938900	-3.04161500
C	2.75939400	1.41251200	-2.38548600

C	1.37116700	1.52735300	-3.05548500
C	3.12876300	2.75397500	-1.72333400
H	3.51328500	1.19256600	-3.15187200
C	1.33127000	2.66482100	-4.08640500
H	0.62108200	1.74395500	-2.28573500
H	1.07969700	0.57958200	-3.52136000
C	3.09115100	3.89696700	-2.75168300
H	2.41056100	2.97063600	-0.92667700
H	4.11647600	2.69822000	-1.26094200
C	1.72394000	3.99929700	-3.44080100
H	0.32227700	2.73259200	-4.50494500
H	2.01665800	2.43435900	-4.91440900
H	3.34346100	4.84067100	-2.25426000
H	3.87037900	3.72342800	-3.50758200
H	1.73513600	4.79662000	-4.19191800
H	0.95516800	4.26810700	-2.70491500
P	2.83399000	-0.06828500	-1.22095500
Au	0.65542400	-0.77251100	-0.64330100

Zero-point correction=	1.318538 (Hartree/Particle)
Thermal correction to Energy=	1.389686
Thermal correction to Enthalpy=	1.390630
Thermal correction to Gibbs Free Energy=	1.210640
Sum of electronic and zero-point Energies=	-3791.610119
Sum of electronic and thermal Energies=	-3791.538972
Sum of electronic and thermal Enthalpies=	-3791.538028
Sum of electronic and thermal Free Energies=	-3791.718017

A-2a

C	-0.99663500	-4.11781400	-2.94845200
C	-1.54264800	-2.85896200	-3.22174100
C	-1.90943100	-2.52326100	-0.84777600
C	-1.34298300	-3.76771300	-0.58242300
C	-0.90234000	-4.57644300	-1.63409500
H	-0.64436600	-4.73925300	-3.76610400
H	-1.61232500	-2.50774900	-4.24673400
H	-1.23393200	-4.10078300	0.44471300
H	-0.47168900	-5.55011700	-1.42408400
C	-2.26207300	-1.54988200	0.25561200
O	-1.71222100	-0.26449900	-0.18432200
H	-1.72418000	-1.81372900	1.16172900
C	-2.01904800	-2.06175500	-2.18050400
C	-2.78669800	-0.80131000	-2.35151600
C	-2.68096300	0.19629000	-1.16861100
C	-2.43770900	1.69304800	-1.40080600

H	-1.55955600	2.01257200	-0.81947200
H	-2.28032000	1.96951500	-2.44187100
N	-3.67918600	2.29177300	-0.89361200
C	-4.22646900	1.45903800	0.18777500
H	-3.64915800	1.57028100	1.11913800
H	-5.26660900	1.72907100	0.37358900
C	-3.72461600	-1.10797900	0.59474200
H	-3.61283700	-0.61896300	1.56755600
C	-4.03638100	0.06010100	-0.42529100
C	-5.06761200	-0.23518100	-1.53967100
H	-5.89672300	-0.83749500	-1.16348100
H	-5.47934600	0.70588300	-1.91639400
C	-4.28901700	-0.98496900	-2.61445200
C	-3.41530300	-0.28353000	-3.61836600
H	-4.62591200	-1.98014700	-2.88587300
H	-3.21059300	-0.80549500	-4.54831100
H	-3.51432000	0.79220900	-3.73389300
O	-3.31606100	4.40184700	-2.18054000
O	-5.20194200	4.22198800	-0.43400800
S	-3.83568300	3.96182900	-0.88398100
C	-4.74148000	-2.21014000	0.78294800
C	-5.54968400	-2.18680600	1.92940400
C	-4.91873400	-3.25675300	-0.13455900
C	-6.50920300	-3.17353900	2.15573300
H	-5.42399500	-1.38525500	2.65359900
C	-5.87583000	-4.24704800	0.09092900
H	-4.30382100	-3.31048500	-1.02431200
C	-6.67461300	-4.20944500	1.23486700
H	-7.12360900	-3.13394100	3.05015700
H	-5.99536300	-5.05019500	-0.63021900
H	-7.41841700	-4.98116600	1.40780000
C	-2.71219900	4.55216100	0.37898000
C	-1.46453600	5.06221700	0.01337000
C	-3.10584300	4.50295800	1.71986400
C	-0.60827800	5.53070600	1.00869200
H	-1.19551600	5.12391300	-1.03568500
C	-2.22913200	4.96001900	2.70033400
H	-4.09822600	4.15059300	1.98031800
C	-0.97028400	5.48037800	2.36236500
H	0.35338700	5.95248700	0.72906300
H	-2.53360500	4.93434200	3.74309300
C	-0.01913300	5.94422200	3.43678400
H	0.55867800	5.09702500	3.82800100
H	0.69351300	6.68028000	3.05472900

H	-0.55326400	6.39089700	4.28015200
C	2.15447100	-0.92609000	1.93057100
C	1.75746100	-2.27914900	2.00433500
C	0.52902400	-2.59364300	2.60437900
C	-0.31076500	-1.61550300	3.14050000
C	0.10504400	-0.28131700	3.05087100
C	1.32574200	0.08305100	2.47719700
H	0.24119900	-3.63672900	2.67374500
H	-0.53082500	0.49230400	3.47345700
C	2.66343900	-3.41493200	1.53843600
C	1.94010100	-4.43274100	0.64203200
C	3.30182500	-4.12427100	2.74978300
H	3.47492900	-2.97604800	0.94935700
H	1.42744100	-3.94483600	-0.18777400
H	2.65701800	-5.15168600	0.23178000
H	1.19424400	-5.00608800	1.20355500
H	3.83524900	-3.41378800	3.38387200
H	2.53161500	-4.60735400	3.36088000
H	4.00257900	-4.89763000	2.41774500
C	-1.60889100	-1.93858900	3.87665200
C	-1.39469300	-1.78929300	5.39788300
C	-2.20872400	-3.31621000	3.56052400
H	-2.34503900	-1.17846300	3.57493000
H	-1.01460100	-0.79553000	5.65224000
H	-2.33265500	-1.94756800	5.93998900
H	-0.66691200	-2.52697400	5.75269400
H	-2.37824200	-3.46698200	2.49033600
H	-1.56373400	-4.12489100	3.92034500
H	-3.17732800	-3.42535200	4.05625200
C	1.77847400	1.53542900	2.53160800
C	2.23079800	1.89163800	3.96167800
C	0.71977100	2.52553500	2.02840100
H	2.65318700	1.63665700	1.88329800
H	2.99900500	1.19535300	4.30821300
H	2.63556000	2.90911900	3.99807100
H	1.38755100	1.83618200	4.65897300
H	0.37617600	2.27616900	1.01950300
H	-0.16136200	2.56207800	2.67631600
H	1.13456800	3.53640200	1.99654000
C	3.52742500	-0.57409100	1.42437900
C	3.84569500	-0.15785600	0.11264700
C	4.57294600	-0.67186300	2.37676900
C	5.19860500	0.10325100	-0.23050600
C	5.89540200	-0.42409000	2.01579800

C	6.21038000	-0.04419500	0.71177700
H	6.69530600	-0.51740000	2.73943600
H	7.24447200	0.14461500	0.45344500
O	4.18510700	-1.01115400	3.64114200
O	5.42107100	0.52369000	-1.51392000
C	5.18062800	-1.13135100	4.65270400
H	5.71251000	-0.18433400	4.80719900
H	4.64412900	-1.39676400	5.56385400
H	5.90216900	-1.92259600	4.41372400
C	6.74053100	0.89981800	-1.90205800
H	7.43015200	0.04918200	-1.85141200
H	6.66019400	1.23762200	-2.93559200
H	7.12003400	1.71809100	-1.27867700
C	3.00628400	-0.98823600	-2.61813900
C	2.79485100	-2.45289000	-2.19056100
C	2.18517300	-0.66292000	-3.88102800
H	4.06721400	-0.82069900	-2.82829200
C	3.14153600	-3.42099900	-3.33140700
H	1.74196300	-2.59291700	-1.91275700
H	3.39396900	-2.68153400	-1.30358500
C	2.53395900	-1.63725400	-5.01955000
H	1.11431000	-0.74161700	-3.64557400
H	2.37100800	0.36402900	-4.21166800
C	2.33483200	-3.09826900	-4.59610900
H	2.95024400	-4.44929200	-3.00444800
H	4.21554100	-3.35430800	-3.55303200
H	1.92245900	-1.40385700	-5.89833000
H	3.58061400	-1.48202800	-5.31558100
H	2.61713300	-3.77222100	-5.41227000
H	1.27001600	-3.26965500	-4.39249200
C	2.79412400	1.91903900	-1.81259500
C	1.46886100	2.46390900	-2.39526900
C	3.32016700	2.88938600	-0.73692100
H	3.54030200	1.85044300	-2.61296000
C	1.66630700	3.86364500	-2.99679700
H	0.73276800	2.53116400	-1.58338200
H	1.04866200	1.78146100	-3.13962400
C	3.51297400	4.29784400	-1.32424200
H	2.59523600	2.93956500	0.08324100
H	4.26128800	2.53225200	-0.31320600
C	2.21834200	4.83693400	-1.94751400
H	0.71256500	4.22673800	-3.39594000
H	2.36065900	3.80236000	-3.84601100
H	3.87257200	4.97308000	-0.53951600

H	4.29907600	4.26167200	-2.09136400
H	2.38801500	5.82416900	-2.39013600
H	1.46714000	4.96777900	-1.15586600
P	2.59719800	0.15152100	-1.20265000
Au	0.43026700	-0.18566000	-0.59203800

Zero-point correction= 1.322062 (Hartree/Particle)
Thermal correction to Energy= 1.392651
Thermal correction to Enthalpy= 1.393595
Thermal correction to Gibbs Free Energy= 1.216061
Sum of electronic and zero-point Energies= -3791.662368
Sum of electronic and thermal Energies= -3791.591779
Sum of electronic and thermal Enthalpies= -3791.590834
Sum of electronic and thermal Free Energies= -3791.768368

2a

C	-6.30640644	-3.17721008	-6.84567375
C	-6.85241944	-1.91835808	-7.11896275
C	-7.21920244	-1.58265708	-4.74499775
C	-6.65275444	-2.82710908	-4.47964475
C	-6.21211144	-3.63583908	-5.53131675
H	-5.95413744	-3.79864908	-7.66332575
H	-6.92209644	-1.56714508	-8.14395575
H	-6.54370344	-3.16017908	-3.45250875
H	-5.78146044	-4.60951308	-5.32130575
C	-7.57184444	-0.60927808	-3.64160975
O	-7.02199244	0.67610492	-4.08154375
H	-7.03395144	-0.87312508	-2.73549275
C	-7.32881944	-1.12115108	-6.07772575
C	-8.09646944	0.13929392	-6.24873775
C	-7.99073444	1.13689392	-5.06583275
C	-7.74748044	2.63365192	-5.29802775
H	-6.86932744	2.95317592	-4.71669375
H	-7.59009144	2.91011892	-6.33909275
N	-8.98895744	3.23237692	-4.79083375
C	-9.53624044	2.39964192	-3.70944675
H	-8.95892944	2.51088492	-2.77808375
H	-10.57638044	2.66967492	-3.52363275
C	-9.03438744	-0.16737508	-3.30247975
H	-8.92260844	0.32164092	-2.32966575
C	-9.34615244	1.00070492	-4.32251275
C	-10.37738344	0.70542292	-5.43689275
H	-11.20649444	0.10310892	-5.06070275
H	-10.78911744	1.64648692	-5.81361575
C	-9.59878844	-0.04436508	-6.51167375

C	-8.72507444	0.65707392	-7.51558775
H	-9.93568344	-1.03954308	-6.78309475
H	-8.52036444	0.13510892	-8.44553275
H	-8.82409144	1.73281292	-7.63111475
O	-8.62583244	5.34245092	-6.07776175
O	-10.51171344	5.16259192	-4.33122975
S	-9.14545444	4.90243292	-4.78120275
C	-10.05125144	-1.26953608	-3.11427375
C	-10.85945544	-1.24620208	-1.96781775
C	-10.22850544	-2.31614908	-4.03178075
C	-11.81897444	-2.23293508	-1.74148875
H	-10.73376644	-0.44465108	-1.24362275
C	-11.18560144	-3.30644408	-3.80629275
H	-9.61359244	-2.36988108	-4.92153375
C	-11.98438444	-3.26884108	-2.66235475
H	-12.43338044	-2.19333708	-0.84706475
H	-11.30513444	-4.10959108	-4.52744075
H	-12.72818844	-4.04056208	-2.48942175
C	-8.02197044	5.49276492	-3.51824175
C	-6.77430744	6.00282092	-3.88385175
C	-8.41561444	5.44356192	-2.17735775
C	-5.91804944	6.47130992	-2.88852975
H	-6.50528744	6.06451692	-4.93290675
C	-7.53890344	5.90062292	-1.19688775
H	-9.40799744	5.09119692	-1.91690375
C	-6.28005544	6.42098192	-1.53485675
H	-4.95638444	6.89309092	-3.16815875
H	-7.84337644	5.87494592	-0.15412875
C	-5.32890444	6.88482592	-0.46043775
H	-4.75109344	6.03762892	-0.06922075
H	-4.61625844	7.62088392	-0.84249275
H	-5.86303544	7.33150092	0.38293025

Zero-point correction=	0.499814 (Hartree/Particle)
Thermal correction to Energy=	0.526597
Thermal correction to Enthalpy=	0.527541
Thermal correction to Gibbs Free Energy=	0.441799
Sum of electronic and zero-point Energies=	-1799.470324
Sum of electronic and thermal Energies=	-1799.443541
Sum of electronic and thermal Enthalpies=	-1799.442597
Sum of electronic and thermal Free Energies=	-1799.528340

A-TSb1

C	1.31188500	-0.43488700	4.99421300
C	0.87202700	-0.20061300	3.70213300

C	3.13055600	-0.54004100	2.89170200
C	3.57717200	-0.75606300	4.20675600
C	2.66782200	-0.71991400	5.25121700
H	0.60683800	-0.39377600	5.81876200
H	-0.16598300	0.03311600	3.50536300
H	4.62758500	-0.96303600	4.39369000
H	2.99904800	-0.90566800	6.26790700
C	4.04703600	-0.47948800	1.77551400
O	3.54571400	-0.77466300	0.55795800
H	5.05285700	-0.87672600	1.88178500
C	1.76568300	-0.26267800	2.61131100
C	1.35562200	-0.03046400	1.23968600
C	2.29504900	-0.32230500	0.26721700
C	2.08463800	-0.36425400	-1.21762400
H	2.13151600	-1.39829900	-1.55641600
H	1.08334000	0.00131100	-1.44350400
N	3.06757400	0.44018200	-1.93768900
C	2.61697900	1.77103100	-2.36694200
H	3.44598000	2.25395700	-2.89191000
H	1.79235400	1.68191000	-3.08684400
C	0.95527700	3.13469600	-1.16866300
H	0.33879000	2.91021000	-2.03683400
C	2.19011700	2.60409700	-1.17821000
C	3.29176500	2.86347700	-0.16228600
H	4.25573400	2.75529400	-0.66908500
H	3.20731900	3.91561100	0.15579400
C	3.35293400	2.09521900	1.13016500
C	4.49369800	1.43160000	1.58728400
H	2.56750300	2.29493000	1.84816100
H	4.73838900	1.52791400	2.64193600
H	5.35202800	1.38773000	0.91918800
O	3.99640700	-1.77006500	-2.79279800
O	4.53042000	0.42979500	-4.01322600
S	4.30981500	-0.33614100	-2.78454400
C	0.31815200	4.04988600	-0.20579300
C	-0.44083100	5.12397200	-0.71012500
C	0.38436500	3.88317400	1.18687800
C	-1.06721800	6.02513800	0.14812400
H	-0.51892900	5.25924900	-1.78548900
C	-0.23666100	4.78872400	2.04749200
H	0.85851000	3.00002600	1.59201100
C	-0.95684200	5.86739700	1.53307800
H	-1.63875600	6.85216200	-0.26216900
H	-0.17648600	4.63704100	3.12133700

H	-1.44264200	6.57030700	2.20278400
C	5.74752400	-0.10355900	-1.74067900
C	6.14730100	-1.12193200	-0.87568500
C	6.42808800	1.11551900	-1.78190800
C	7.22822600	-0.89962400	-0.02299100
H	5.61726100	-2.06739400	-0.87749100
C	7.50218900	1.32299800	-0.91809900
H	6.13317600	1.87865900	-2.49456700
C	7.91744800	0.32342900	-0.02374300
H	7.55411400	-1.69490500	0.64285500
H	8.03655400	2.26852300	-0.94814400
C	9.10788900	0.54167500	0.87690000
H	9.21037600	1.59285600	1.16117400
H	9.03874500	-0.05711700	1.78960700
H	10.03357800	0.25080700	0.36622000
Au	-0.60259700	0.32197800	0.62923800
P	-2.79432100	0.69109800	-0.21640400
C	-3.77280800	-0.81194600	-0.69951500
C	-5.13285600	-0.64208500	-1.07772300
C	-5.93438400	-1.73558000	-1.38877600
H	-6.96758100	-1.60060800	-1.68114600
C	-5.41646800	-3.02621900	-1.31429100
H	-6.06136600	-3.86407700	-1.54699200
C	-4.09296000	-3.22265800	-0.93401700
C	-3.24491900	-2.12402600	-0.64140000
C	-1.84410000	-2.49328500	-0.23440200
C	-0.85642000	-2.75907900	-1.20881800
C	-1.14392600	-2.67329100	-2.70882300
H	-2.05853800	-2.08630300	-2.84233800
C	-1.40172400	-4.08494300	-3.27817300
H	-0.49738900	-4.69759200	-3.19413300
H	-1.67351000	-4.02877600	-4.33770500
H	-2.20025400	-4.58998900	-2.73426400
C	-0.03163300	-1.99483600	-3.52966700
H	0.18107800	-0.98200800	-3.18351000
H	-0.33519200	-1.92714600	-4.57924800
H	0.90714700	-2.55692800	-3.50253500
C	0.39829600	-3.22582700	-0.78822000
C	0.71324900	-3.41841300	0.55715800
C	2.07197900	-3.92669100	1.03566900
H	2.42906100	-3.20533100	1.78661500
C	3.14014700	-4.02689400	-0.06236600
H	4.09732800	-4.32470500	0.37873000
H	3.29648500	-3.08658800	-0.59483700

H	2.87653900	-4.78938900	-0.80303100
C	1.92357500	-5.29196000	1.73970600
H	1.21254900	-5.25080000	2.56925800
H	2.88695100	-5.62937900	2.13646400
H	1.56577000	-6.04624100	1.03069700
C	-0.29112100	-3.16581400	1.49905400
C	-1.56977600	-2.74098500	1.13367800
C	-2.66445200	-2.66478700	2.19538800
H	-3.51935500	-2.13364900	1.76708700
C	-3.13576000	-4.08846700	2.55578700
H	-2.32158000	-4.65504800	3.02119700
H	-3.45134000	-4.62938000	1.66117900
H	-3.97210100	-4.05259700	3.26231100
C	-2.24833000	-1.89939100	3.45912500
H	-1.41410500	-2.38096800	3.97904000
H	-3.08695800	-1.84363800	4.16094200
H	-1.94527100	-0.87995800	3.20965000
H	1.13688200	-3.46323400	-1.54530700
H	-0.07387000	-3.33092700	2.55024200
C	-2.55447000	1.79969400	-1.71337900
C	-2.00755500	0.96808200	-2.88679200
C	-3.70532200	2.71344400	-2.17071100
H	-1.74882200	2.45058700	-1.35181700
C	-1.58245000	1.85279900	-4.06789900
H	-2.78333300	0.26608400	-3.21934000
H	-1.16371300	0.36040500	-2.54931500
C	-3.23058800	3.62100300	-3.31786300
H	-4.54397500	2.10393400	-2.51392000
H	-4.07052200	3.32234100	-1.33700100
C	-2.71251300	2.79494200	-4.50421700
H	-1.25797100	1.22109700	-4.90251400
H	-0.70947900	2.45469700	-3.77809200
H	-4.05266300	4.27213500	-3.63598100
H	-2.43175000	4.28184000	-2.95276400
H	-2.36940300	3.45285800	-5.31027600
H	-3.53995100	2.19923400	-4.91438400
C	-3.82618100	1.67653000	0.98342800
C	-4.38880800	0.81135200	2.12329300
C	-3.00605800	2.85638000	1.53924400
H	-4.66919500	2.07265100	0.41354900
C	-5.23871400	1.66273800	3.07965400
H	-3.55880700	0.36242700	2.67994900
H	-4.98540900	-0.01316800	1.71916300
C	-3.86077800	3.70589600	2.49142100

H	-2.13373400	2.47057700	2.08171000
H	-2.60978400	3.48130700	0.73217700
C	-4.44259600	2.85567500	3.62952800
H	-5.61113100	1.03850300	3.89988600
H	-6.12165600	2.03358000	2.54054300
H	-3.25335400	4.52553700	2.89029600
H	-4.68073800	4.16994000	1.92557700
H	-5.07552200	3.46861000	4.28085900
H	-3.61875100	2.48003800	4.25369000
O	-5.60275000	0.64018500	-1.10487100
O	-3.52613500	-4.45899100	-0.79458300
C	-4.31905200	-5.60880800	-1.06693400
H	-4.66130800	-5.62445500	-2.10944000
H	-3.66727200	-6.46480000	-0.89001100
H	-5.18566400	-5.66825200	-0.39640400
C	-6.97023700	0.87994100	-1.41620700
H	-7.10128900	1.96082800	-1.35247700
H	-7.21665900	0.54547400	-2.43117700
H	-7.63672400	0.38856000	-0.69719300

Zero-point correction=	1.316531 (Hartree/Particle)
Thermal correction to Energy=	1.388598
Thermal correction to Enthalpy=	1.389542
Thermal correction to Gibbs Free Energy=	1.209331
Sum of electronic and zero-point Energies=	-3791.608213
Sum of electronic and thermal Energies=	-3791.536146
Sum of electronic and thermal Enthalpies=	-3791.535202
Sum of electronic and thermal Free Energies=	-3791.715413

A-1b

C	1.50946600	-2.22516300	4.58541600
C	1.01963900	-1.62588500	3.43774200
C	3.25667600	-0.73258000	2.95416200
C	3.72496800	-1.30516400	4.12773200
C	2.85942800	-2.05709300	4.93121400
H	0.85457700	-2.81347900	5.21949100
H	-0.01719300	-1.73850300	3.15214600
H	4.76674000	-1.18794600	4.41160800
H	3.24179600	-2.52156500	5.83576300
C	4.11541600	0.08137500	2.02412800
O	3.73244100	-0.25613100	0.69688400
H	5.17601600	-0.15194800	2.13850200
C	1.87840400	-0.87502300	2.59230100
C	1.39934800	-0.24847200	1.40902100
C	2.45638000	0.35261800	0.51860500

C	2.08327000	0.17621200	-0.96205500
H	2.01332300	-0.89237900	-1.15716900
H	1.08917600	0.59640300	-1.12446300
N	3.00517600	0.79558100	-1.88749600
C	2.66878600	2.14333400	-2.36951200
H	3.56812800	2.58207800	-2.81160200
H	1.90704600	2.10176900	-3.15852500
C	1.11533200	3.76290300	-1.32171200
H	0.61924000	3.79152400	-2.29206700
C	2.19712700	2.97731900	-1.19922500
C	3.06975800	2.88051000	0.02959200
H	4.09184600	2.65529000	-0.29416100
H	3.08885900	3.84375300	0.55064500
C	2.66586900	1.82105400	1.09000900
C	3.79913500	1.60166700	2.12682200
H	1.75189900	2.16462900	1.57412700
H	3.51958800	1.90008900	3.13952900
H	4.68943500	2.16622200	1.83981400
O	3.61850200	-1.52505600	-2.74025500
O	4.41525100	0.59102500	-3.95691100
S	4.12491100	-0.14517400	-2.72457500
C	0.53785600	4.65412100	-0.28858400
C	0.00477900	4.14722000	0.90783900
C	0.45503700	6.03679900	-0.52509600
C	-0.56419800	5.00138800	1.85510100
H	0.00014500	3.07460600	1.07512800
C	-0.11687200	6.88908400	0.41873100
H	0.84875700	6.44180700	-1.45322400
C	-0.62425800	6.37478700	1.61485100
H	-0.96731100	4.59257600	2.77728800
H	-0.16587400	7.95571400	0.22113300
H	-1.06877500	7.03919000	2.34952400
C	5.58930800	-0.11374900	-1.69669000
C	5.96020200	-1.24681400	-0.97770900
C	6.30253500	1.08184000	-1.58069300
C	7.05407300	-1.17166500	-0.11599100
H	5.39004700	-2.16144000	-1.08311800
C	7.38610400	1.14227000	-0.70902200
H	6.02146900	1.94661800	-2.17286100
C	7.77849600	0.01889000	0.03749800
H	7.35181600	-2.05455300	0.44356300
H	7.94598300	2.06889800	-0.61501800
C	8.98021200	0.08458500	0.94813200
H	9.90332000	-0.08570100	0.38130000

H	9.07051400	1.06541100	1.42482700
H	8.93460000	-0.67663100	1.73216600
Au	-0.54919000	0.00082300	0.85142100
P	-2.71525100	0.64046200	0.06097300
C	-3.69765500	-0.66125700	-0.80264000
C	-5.00335300	-0.32227200	-1.24153900
C	-5.80934600	-1.26358700	-1.87134700
H	-6.80648000	-1.00892700	-2.20693900
C	-5.33511400	-2.55961200	-2.07780700
H	-5.97954500	-3.27958500	-2.56623900
C	-4.05488800	-2.91250500	-1.66020500
C	-3.21298500	-1.96622200	-1.02336500
C	-1.85524200	-2.46455700	-0.61718400
C	-0.79299700	-2.47649000	-1.55166200
C	-0.98081200	-2.01148700	-2.99341800
H	-1.95862300	-1.52443800	-3.06551700
C	-1.01015500	-3.23481800	-3.93355000
H	-0.03874300	-3.74035700	-3.94248900
H	-1.23707600	-2.92523700	-4.95920600
H	-1.76478900	-3.95426200	-3.60735500
C	0.07936500	-0.99989200	-3.46284100
H	0.06560100	-0.09531600	-2.84884600
H	-0.12087900	-0.70145500	-4.49704200
H	1.09233900	-1.41146800	-3.42967400
C	0.43414300	-3.03958100	-1.17307700
C	0.62865600	-3.62052200	0.08328400
C	1.92129100	-4.33682500	0.44861900
H	1.93745900	-4.43503100	1.54322100
C	3.18991200	-3.57921000	0.02866300
H	4.07845600	-4.13123100	0.35486100
H	3.23475800	-2.57982900	0.46642700
H	3.25631800	-3.46195700	-1.05707000
C	1.91022500	-5.75818700	-0.15032100
H	1.02604200	-6.31743700	0.17104600
H	2.80169700	-6.31690900	0.15396000
H	1.89780700	-5.70975100	-1.24466500
C	-0.44761400	-3.62363200	0.97528600
C	-1.68776200	-3.06189500	0.65382500
C	-2.85214000	-3.19282100	1.63070600
H	-3.65535300	-2.53439300	1.28818200
C	-3.39638800	-4.63486100	1.61009200
H	-2.63977200	-5.33842500	1.97456400
H	-3.66421100	-4.92915800	0.59249000
H	-4.28126700	-4.72607600	2.24919400

C	-2.49728600	-2.76123200	3.06236100
H	-1.73703600	-3.41188400	3.50810500
H	-3.38133600	-2.81017900	3.70639400
H	-2.12436300	-1.73113500	3.08229000
H	1.24272800	-3.05767800	-1.89732900
H	-0.31981600	-4.10682900	1.94059800
C	-2.42179600	2.06063800	-1.16423800
C	-2.55235300	1.57900800	-2.62300400
C	-3.24235200	3.34535100	-0.93373800
H	-1.36811600	2.31172100	-0.99083200
C	-2.11882600	2.67639000	-3.60522900
H	-3.59698200	1.31654500	-2.82068900
H	-1.96180700	0.67432900	-2.78335900
C	-2.82333200	4.44042000	-1.93156700
H	-4.30599100	3.12200200	-1.05977800
H	-3.10168200	3.72083200	0.08424800
C	-2.92516700	3.96350200	-3.38649600
H	-2.23745300	2.31597000	-4.63325300
H	-1.04809800	2.88178400	-3.46936800
H	-3.44620100	5.32834300	-1.77455000
H	-1.79285100	4.74504200	-1.71445600
H	-2.58402600	4.74999000	-4.06887400
H	-3.97873400	3.76908200	-3.63251600
C	-3.77531000	1.29893400	1.45496900
C	-4.60338800	0.21045800	2.16113200
C	-2.90751200	2.06394800	2.47420800
H	-4.47156900	2.00014700	0.98911500
C	-5.47817400	0.83434700	3.26142600
H	-3.93150700	-0.52704700	2.61383200
H	-5.22984400	-0.32562100	1.44295600
C	-3.78261200	2.69183600	3.57034400
H	-2.19357900	1.36604800	2.93390100
H	-2.31211800	2.83318500	1.97381600
C	-4.63727400	1.62701300	4.27246600
H	-6.04638800	0.04745200	3.77023500
H	-6.21555800	1.50339700	2.79635800
H	-3.14946500	3.21618700	4.29569900
H	-4.43739800	3.44969900	3.11862000
H	-5.28376500	2.09157000	5.02494200
H	-3.97520100	0.93372000	4.81066400
O	-3.52191800	-4.16081500	-1.81490900
O	-5.39458500	0.96722300	-1.00684800
C	-4.30323300	-5.16033900	-2.46091300
H	-4.55313200	-4.87251300	-3.48979600

H	-3.68150000	-6.05577200	-2.47837700
H	-5.22601100	-5.37041500	-1.90541500
C	-6.69699800	1.38028100	-1.40794400
H	-6.82787500	1.29202000	-2.49309600
H	-7.47484900	0.80144400	-0.89593500
H	-6.77772100	2.42899200	-1.11973200

Zero-point correction= 1.320006 (Hartree/Particle)

Thermal correction to Energy= 1.391638

Thermal correction to Enthalpy= 1.392583

Thermal correction to Gibbs Free Energy= 1.210808

Sum of electronic and zero-point Energies= -3791.627046

Sum of electronic and thermal Energies= -3791.555414

Sum of electronic and thermal Enthalpies= -3791.554470

Sum of electronic and thermal Free Energies= -3791.736244

A-TSb2

S	1.82434700	2.76919100	-0.49737500
O	3.28403700	-1.86199300	-1.91764600
O	0.52024900	2.35093500	-1.01858100
O	1.93584800	3.47867000	0.78242800
N	2.73798400	1.34653700	-0.30977300
C	1.38657700	-1.69091900	-0.31217500
C	3.13993000	-1.50985800	0.40674000
C	3.95144700	-2.75680800	0.14355200
H	5.00221400	-2.45083200	0.16691300
H	3.80583300	-3.55079200	0.87940700
C	3.51217500	-3.14256400	-1.29086100
C	2.65879100	-1.06153700	-0.93671000
C	2.68372400	0.38876200	-1.41830600
H	1.77957700	0.56769100	-1.99971600
H	3.55553500	0.49763500	-2.07568300
C	4.06201000	1.56449200	0.30378900
H	4.79419700	1.90700000	-0.44206100
H	3.93328900	2.36285900	1.04003000
C	4.56553900	0.33213100	1.02654900
C	3.47371100	-0.57453400	1.55934100
H	3.78984500	-1.16853500	2.41522400
H	2.59247600	0.01166100	1.83664000
C	5.88439600	0.07921200	1.09018800
H	6.54266400	0.74494900	0.53036100
C	2.65605700	3.72848200	-1.74913600
C	3.61087300	4.67284200	-1.36319700
H	3.78618300	4.86835300	-0.31095600
C	4.30348900	5.37034500	-2.35041800

H	5.04233400	6.11157500	-2.05929100
C	4.05817300	5.13848900	-3.71216400
C	3.09158500	4.18411900	-4.06701600
H	2.88428200	3.99868200	-5.11718200
C	2.38622300	3.47648800	-3.09782700
H	1.62496600	2.75816600	-3.37843300
C	4.78809400	5.92300900	-4.77331500
H	5.76015700	6.27430400	-4.41704900
H	4.94703900	5.32529100	-5.67534200
H	4.20661400	6.80583900	-5.06527800
C	6.56557700	-1.02285900	1.79970000
C	7.56183400	-1.75269700	1.12615700
C	6.27063800	-1.36222400	3.13135000
C	8.20920400	-2.81888300	1.74931900
H	7.82098600	-1.48355000	0.10524700
C	6.92379900	-2.42409200	3.75637200
H	5.55517000	-0.76538100	3.68896200
C	7.88746200	-3.16173500	3.06479900
H	8.97037100	-3.37633700	1.21175800
H	6.69074900	-2.66641000	4.78893900
H	8.39676100	-3.98673700	3.55325400
C	2.03385200	-5.21606300	-1.56128900
H	2.86640100	-5.78561200	-1.96511600
C	0.78893100	-5.82111600	-1.36519700
H	0.64767000	-6.86570600	-1.62464200
C	1.13932800	-3.12079200	-0.70739100
C	-0.09871900	-3.73504200	-0.51080400
H	-0.92689200	-3.15501700	-0.12727700
C	-0.27146900	-5.08058600	-0.83878600
C	2.20622300	-3.87645900	-1.22674400
H	-1.23919900	-5.54655400	-0.68573900
H	4.27891900	-3.66705600	-1.86256300
H	1.82017900	-1.82311900	0.82933100
Au	-0.22071200	-0.44137000	0.35430800
P	-1.84942100	0.80874900	1.52816800
C	-3.57104400	0.87881700	0.86455900
C	-4.53080300	1.60471400	1.62079600
C	-5.83419600	1.76036000	1.16663100
H	-6.56243800	2.31766500	1.74136600
C	-6.21792100	1.19535500	-0.04898800
H	-7.23517100	1.33267900	-0.39306600
C	-5.30414900	0.45919400	-0.79405300
C	-3.96808100	0.27141900	-0.34345700
C	-3.15624100	-0.65259800	-1.21248400

C	-2.41325900	-0.16133500	-2.31781800
C	-2.18808300	1.33346400	-2.54003200
H	-1.95419300	1.76840700	-1.56420200
C	-3.43635100	2.04754600	-3.10074300
H	-3.75262900	1.58008000	-4.03904100
H	-3.20409800	3.09853400	-3.30421200
H	-4.27736400	2.01913200	-2.40977200
C	-0.99810600	1.64165600	-3.46235800
H	-0.10638800	1.08459100	-3.16524800
H	-0.76392500	2.70774700	-3.40693700
H	-1.22549700	1.40265600	-4.50693100
C	-1.91142300	-1.07977100	-3.24102900
C	-2.13041900	-2.45819000	-3.14030100
C	-1.59409900	-3.36610000	-4.24249500
H	-1.92648500	-2.92184800	-5.19194000
C	-2.13391700	-4.80083700	-4.19400000
H	-1.78488800	-5.36379100	-5.06496400
H	-3.22820300	-4.82440400	-4.19350600
H	-1.77877200	-5.32697700	-3.30134200
C	-0.05166200	-3.37495600	-4.25802700
H	0.35981300	-2.36288700	-4.31611300
H	0.32005900	-3.94065500	-5.11913400
H	0.33769600	-3.84252800	-3.35173100
C	-2.84918800	-2.91605800	-2.03906200
C	-3.36544900	-2.04288400	-1.07088400
C	-4.22154300	-2.62638700	0.05368300
H	-4.40070500	-1.83586900	0.78739800
C	-5.59269800	-3.08657900	-0.48123200
H	-5.47094500	-3.90470500	-1.19968600
H	-6.10931500	-2.27202800	-0.99093000
H	-6.22436100	-3.44851100	0.33730000
C	-3.53583300	-3.78760500	0.79517200
H	-3.40392700	-4.65949600	0.14588300
H	-4.14814700	-4.10763300	1.64464000
H	-2.55243800	-3.50466200	1.18048100
H	-1.35902400	-0.71654900	-4.10055100
H	-3.04108500	-3.97731400	-1.93123900
C	-1.21881100	2.58288400	1.73854300
C	-1.91717600	3.56948600	0.77992500
C	-1.17039900	3.14369700	3.17443800
H	-0.18560200	2.48702800	1.40448200
C	-1.24689600	4.95217800	0.82046800
H	-2.96996500	3.66976900	1.06550500
H	-1.89240800	3.18519200	-0.24243400

C	-0.47390200	4.51660200	3.18208400
H	-2.18360500	3.24823400	3.56959700
H	-0.63129700	2.46593500	3.84305100
C	-1.18265000	5.50668300	2.24897200
H	-1.79523000	5.63811200	0.16408300
H	-0.22952600	4.87042000	0.42255700
H	-0.44815100	4.90410700	4.20746500
H	0.56627300	4.39451400	2.85513800
H	-0.66866700	6.47458900	2.25914400
H	-2.20290800	5.68724600	2.61787600
C	-1.96641500	0.06419900	3.24594000
C	-2.93304200	-1.13097400	3.30307000
C	-0.57886700	-0.34519200	3.78437500
H	-2.36978900	0.85732000	3.88027100
C	-3.03715700	-1.68255000	4.73422300
H	-2.57188400	-1.91989200	2.63280200
H	-3.92456500	-0.83808900	2.94561300
C	-0.69082900	-0.86497800	5.22619600
H	-0.16900300	-1.14325800	3.15030600
H	0.12880800	0.48983300	3.72603800
C	-1.66080100	-2.05270100	5.30463300
H	-3.70348000	-2.55265700	4.74605100
H	-3.50230600	-0.92152000	5.37619300
H	0.30017200	-1.15310700	5.59597300
H	-1.04683000	-0.05563700	5.87836000
H	-1.75779500	-2.39955200	6.33933900
H	-1.24620700	-2.89228500	4.72816800
O	-4.09102300	2.12301700	2.80755200
O	-5.60597600	-0.12517600	-1.99106700
C	-6.88712900	0.10678100	-2.56075000
H	-7.06682000	1.17710300	-2.72453100
H	-6.88109300	-0.40960100	-3.52110800
H	-7.68980300	-0.30551700	-1.93552600
C	-4.99300100	2.87529000	3.61098200
H	-4.42384400	3.18311300	4.48896100
H	-5.35241400	3.76679000	3.08287700
H	-5.84838000	2.26699600	3.92855100

Zero-point correction= 1.316377 (Hartree/Particle)

Thermal correction to Energy= 1.387439

Thermal correction to Enthalpy= 1.388384

Thermal correction to Gibbs Free Energy= 1.209300

Sum of electronic and zero-point Energies= -3791.601199

Sum of electronic and thermal Energies= -3791.530136

Sum of electronic and thermal Enthalpies= -3791.529192

Sum of electronic and thermal Free Energies= -3791.708276

A-2b

C	-0.84291400	-0.30845700	4.97716700
C	-0.75425500	-0.81578200	3.67752100
C	-2.93329600	0.12954100	3.18440100
C	-3.01275500	0.64492400	4.47412600
C	-1.96166500	0.42845700	5.37238600
H	-0.03462500	-0.48567100	5.68008100
H	0.11784100	-1.38853600	3.36888800
H	-3.89235100	1.20444500	4.78138500
H	-2.02173600	0.82428900	6.38134400
C	-3.98847800	0.22966000	2.11591800
O	-3.36995400	0.84798600	0.95124400
H	-4.84793700	0.84002100	2.39505500
C	-1.79208000	-0.58498300	2.77360800
C	-1.79546200	-1.01881200	1.35719800
C	-2.61044900	-0.16246000	0.34393300
C	-2.11755200	0.21722600	-1.04059200
H	-2.15217500	1.29928000	-1.13369700
H	-1.06920700	-0.07178000	-1.16508800
N	-2.86482100	-0.39545600	-2.12118200
C	-2.52746400	-1.77307400	-2.51695400
H	-3.39349200	-2.20007300	-3.03144700
H	-1.70510500	-1.75453100	-3.24310600
C	-0.95056200	-3.23604300	-1.32095500
H	-0.35567500	-3.07301200	-2.21835300
C	-2.15245400	-2.62406500	-1.31845700
C	-3.19512200	-2.68332000	-0.22533200
H	-4.18809500	-2.66617800	-0.69157600
H	-3.12564000	-3.62007100	0.33523100
C	-3.14427500	-1.49415400	0.72636000
C	-4.33985600	-1.19168200	1.61916300
H	-0.95288700	-1.62842600	0.99929100
H	-4.46689900	-1.89398100	2.44740800
H	-5.24560800	-1.18146300	1.00750900
O	-3.84045200	1.84941400	-2.71207600
O	-4.40517400	-0.24847900	-4.09270200
S	-4.15712500	0.42020800	-2.81426900
C	-0.28860100	-4.14599800	-0.37181000
C	0.75590100	-4.94394700	-0.88534700
C	-0.58596900	-4.26991300	1.00053900
C	1.45785000	-5.83657500	-0.07913500
H	1.00173600	-4.87210500	-1.94175000

C	0.12475100	-5.15552100	1.81060700
H	-1.36435600	-3.67087500	1.45346000
C	1.14556100	-5.94565500	1.27802600
H	2.24737600	-6.44555100	-0.50920600
H	-0.12573100	-5.22984100	2.86480300
H	1.68875400	-6.63952500	1.91199100
C	-5.56849800	0.10566400	-1.75505600
C	-5.94217300	1.04613600	-0.79502900
C	-6.25944000	-1.10272500	-1.88705900
C	-7.01692900	0.76246700	0.04691100
H	-5.40459800	1.98211200	-0.71707400
C	-7.32159800	-1.37453600	-1.02802500
H	-5.98458800	-1.80306100	-2.66871700
C	-7.71857800	-0.44809600	-0.04963700
H	-7.31959200	1.49739500	0.78815900
H	-7.86327200	-2.31109100	-1.12814200
C	-8.89833100	-0.73386700	0.84604200
H	-8.98371300	-1.80128900	1.06949800
H	-8.82745300	-0.18890200	1.79155900
H	-9.83276800	-0.42729000	0.36095000
Au	0.72227900	-0.35133500	0.54356500
P	2.83835900	-0.58644400	-0.33407200
C	3.65181800	1.03184200	-0.66501300
C	5.02278600	0.99832800	-1.03488300
C	5.72506600	2.17541800	-1.26776200
H	6.76771000	2.15323500	-1.55739400
C	5.08999800	3.40539200	-1.11399000
H	5.65722100	4.31111400	-1.28668500
C	3.75216500	3.46348300	-0.73081200
C	2.99974200	2.27992200	-0.51675400
C	1.57253800	2.50332300	-0.09173700
C	0.58542700	2.83812000	-1.04592600
C	0.85708000	2.83892100	-2.54969800
H	1.80195000	2.31137300	-2.71972700
C	1.02331700	4.28094700	-3.07263700
H	0.09062600	4.84117000	-2.94788200
H	1.27070000	4.27525700	-4.13938700
H	1.80799900	4.81103100	-2.53141600
C	-0.23664500	2.12196300	-3.36560100
H	-0.39293600	1.09198300	-3.03918400
H	0.04572900	2.09567500	-4.42311800
H	-1.20487100	2.62624100	-3.30019800
C	-0.67315600	3.26298600	-0.59402600
C	-1.00592400	3.32043700	0.75907800

C	-2.34637700	3.83494700	1.26997400
H	-2.71373400	3.08261500	1.97853900
C	-3.40864200	4.01083300	0.17857100
H	-4.36987100	4.26972800	0.63437300
H	-3.54428000	3.10318700	-0.41177300
H	-3.14705200	4.82476900	-0.50680200
C	-2.14956200	5.16003200	2.03649900
H	-1.43836400	5.05422700	2.86102600
H	-3.10077700	5.50754600	2.45319200
H	-1.77015900	5.93821100	1.36514100
C	-0.02748600	2.93283700	1.68381800
C	1.26698400	2.57343900	1.29609300
C	2.34969700	2.41090700	2.35949100
H	3.19142600	1.87981400	1.90732000
C	2.85993300	3.80177600	2.79184400
H	2.05837400	4.36388600	3.28328200
H	3.19465200	4.38413600	1.93096900
H	3.69110800	3.70530100	3.49866700
C	1.90322600	1.60337000	3.58635400
H	1.11800100	2.11238700	4.15292900
H	2.74964200	1.45232100	4.26460100
H	1.51083000	0.62346100	3.30387000
H	-1.40783000	3.56197900	-1.33274100
H	-0.27133500	2.96267300	2.74132400
C	2.60875500	-1.58250200	-1.89959000
C	1.89211100	-0.73397900	-2.96431000
C	3.84933900	-2.28089500	-2.48694000
H	1.91546200	-2.36219700	-1.55685400
C	1.51784200	-1.57581600	-4.19316300
H	2.55050300	0.08860500	-3.27128300
H	0.99683700	-0.27443300	-2.53720700
C	3.43777400	-3.14664600	-3.69026400
H	4.57340500	-1.52863300	-2.80942000
H	4.34286400	-2.89754500	-1.72852000
C	2.73677100	-2.30888800	-4.76906900
H	1.05661500	-0.93155200	-4.94950700
H	0.75619800	-2.31451600	-3.90767100
H	4.32397300	-3.64046000	-4.10385500
H	2.76472200	-3.94641700	-3.35031300
H	2.43644700	-2.94276300	-5.61013900
H	3.44610800	-1.57077700	-5.16814000
C	3.86600100	-1.59730000	0.84073200
C	4.30718800	-0.78262200	2.06903300
C	3.11559000	-2.87664900	1.25870000

H	4.75780600	-1.87763400	0.27405000
C	5.17114300	-1.64313600	3.00456700
H	3.41828700	-0.43980300	2.61109100
H	4.85942900	0.11016500	1.75776800
C	3.98869700	-3.72899000	2.19202700
H	2.18926200	-2.60423900	1.78177000
H	2.81360900	-3.46439700	0.38733500
C	4.44140900	-2.92833500	3.42045900
H	5.45148100	-1.05641800	3.88633500
H	6.10650700	-1.90515400	2.49063800
H	3.42660600	-4.61883300	2.49300200
H	4.87026100	-4.08376300	1.63992000
H	5.08533500	-3.54134900	4.06018300
H	3.55974500	-2.66373600	4.02181900
O	3.08327300	4.63229300	-0.51548200
O	5.59140300	-0.23996800	-1.13047800
C	3.77589200	5.86440300	-0.69174400
H	4.12075500	5.98721500	-1.72600100
H	3.05041800	6.64408900	-0.45941800
H	4.62934100	5.94635300	-0.00718100
C	6.96672300	-0.35330200	-1.48640100
H	7.18186500	-1.42223000	-1.49558200
H	7.15708900	0.06355800	-2.48232200
H	7.61047100	0.14241800	-0.75054200

Zero-point correction=	1.319394 (Hartree/Particle)
Thermal correction to Energy=	1.391127
Thermal correction to Enthalpy=	1.392071
Thermal correction to Gibbs Free Energy=	1.211118
Sum of electronic and zero-point Energies=	-3791.640086
Sum of electronic and thermal Energies=	-3791.568352
Sum of electronic and thermal Enthalpies=	-3791.567408
Sum of electronic and thermal Free Energies=	-3791.748361

3a

S	2.51614400	-0.52696100	-1.34882500
O	-1.28561700	-1.17308900	1.77739900
O	2.33434100	-1.97595400	-1.22756700
O	2.61927100	0.13807700	-2.65142500
N	1.21378600	0.17781700	-0.56344700
C	-1.13065600	-1.78081300	-0.62755300
H	-0.41531400	-1.90189200	-1.43553900
C	-1.69229900	-0.35330000	-0.42865300
C	-2.97382800	-0.30232500	0.39160100
H	-3.07238800	0.68795200	0.84642000

H	-3.87661200	-0.52230800	-0.18591600
C	-2.69218400	-1.38113200	1.46168600
C	-0.67786600	-0.89953800	0.53439300
C	0.74343100	-0.41641700	0.69000700
H	1.38871100	-1.24919700	0.97674500
H	0.77941600	0.33107700	1.49258200
C	0.91578700	1.59879100	-0.78683700
H	1.43739400	2.23221100	-0.05397200
H	1.29293300	1.84670800	-1.78332600
C	-0.57935100	1.84906600	-0.74954600
C	-1.40435100	0.77213500	-1.42466800
H	-2.35394700	1.16041600	-1.79428700
H	-0.85456800	0.37893800	-2.28508200
C	-1.06189900	2.90275300	-0.07043700
H	-0.35180400	3.50021800	0.50286200
C	3.95902700	-0.07737700	-0.38581200
C	4.56429300	1.16291100	-0.60202200
H	4.20785300	1.80543000	-1.39975700
C	5.63729200	1.54108500	0.20028800
H	6.11456000	2.50317100	0.03435300
C	6.11774400	0.69847800	1.21383000
C	5.49482800	-0.54260000	1.40363700
H	5.85972100	-1.21083100	2.17881600
C	4.41899100	-0.93854700	0.61129900
H	3.94913000	-1.90679500	0.74375600
C	7.30379500	1.10544000	2.05359900
H	8.24260900	0.82182200	1.56244500
H	7.33203100	2.18803800	2.20844600
H	7.28769100	0.62001600	3.03342600
C	-2.47265800	3.33238700	0.04208500
C	-3.00706900	3.60985100	1.31205800
C	-3.30269000	3.49738700	-1.07878000
C	-4.33756200	3.99790300	1.46081000
H	-2.37286000	3.50141400	2.18800900
C	-4.63320000	3.88824300	-0.93138600
H	-2.89206200	3.33758000	-2.07075600
C	-5.15813900	4.13309400	0.33871200
H	-4.73391700	4.19553700	2.45263100
H	-5.25815500	4.01052100	-1.81136200
H	-6.19440100	4.43701500	0.45268500
C	-3.65907400	-3.76900100	1.27955500
H	-4.29904100	-3.61276800	2.14469300
C	-3.66909700	-4.99206000	0.60199400
H	-4.32255600	-5.79251800	0.93626900

C	-1.98479200	-2.93541400	-0.27372100
C	-1.98838200	-4.16251300	-0.93858100
H	-1.33334400	-4.31589600	-1.79193200
C	-2.83383000	-5.18548500	-0.50102600
C	-2.82304300	-2.74717500	0.84201600
H	-2.83874800	-6.13855000	-1.02226500
H	-3.26039800	-1.26790300	2.38684100

Zero-point correction= 0.498017 (Hartree/Particle)
Thermal correction to Energy= 0.525794
Thermal correction to Enthalpy= 0.526738
Thermal correction to Gibbs Free Energy= 0.436869
Sum of electronic and zero-point Energies= -1799.468964
Sum of electronic and thermal Energies= -1799.441187
Sum of electronic and thermal Enthalpies= -1799.440243
Sum of electronic and thermal Free Energies= -1799.530112

A-TSc1

C	1.31791600	3.52393200	3.83743900
C	0.71287600	2.55430600	3.05073000
C	2.83364500	1.37489700	2.92048100
C	3.44470300	2.37284800	3.69981500
C	2.68462400	3.43653200	4.16272300
H	0.73304200	4.36171100	4.20458500
H	-0.33667700	2.62971100	2.78643600
H	4.50048100	2.29825000	3.94028700
H	3.14369900	4.20301200	4.77882300
C	3.56798100	0.24760900	2.39004900
O	2.85816900	-0.89031000	2.17195400
H	4.55044000	0.02726100	2.79865200
C	1.45482500	1.45209400	2.57985900
C	0.91082200	0.44244300	1.68946700
C	1.65956300	-0.70633000	1.54176800
C	1.41437300	-1.82546900	0.58512100
H	1.62483600	-2.79253000	1.03913200
H	0.38031400	-1.81371500	0.23920700
N	2.38907000	-1.60926700	-0.50575500
C	2.34905200	-0.29235400	-1.12475700
H	2.97557900	-0.30651300	-2.02423800
H	1.33730400	-0.03518500	-1.45411800
C	4.09143200	0.59957100	0.49374300
H	4.46029300	-0.41510500	0.34419500
C	2.89032900	0.81189600	-0.23140600
C	2.32520500	2.17714100	-0.53499900
H	1.25279800	2.09333900	-0.72627000

H	2.43979000	2.84334600	0.32272800
C	3.02158400	2.73759900	-1.76077400
C	2.42427500	2.87595300	-2.94511100
H	4.06898800	3.00276400	-1.63776200
H	2.95433700	3.27239000	-3.80566000
H	1.38072300	2.60960400	-3.09574400
O	2.48900800	-4.11893400	-0.72222500
O	2.15789900	-2.72161300	-2.84066600
S	2.76496900	-2.92053000	-1.51845500
C	5.22346000	1.57586300	0.61398100
C	5.10273500	2.92864400	0.97113300
C	6.51101300	1.06333400	0.37322900
C	6.23280600	3.74320900	1.06217600
H	4.13462100	3.35593500	1.19497800
C	7.63778700	1.87866800	0.46455300
H	6.62430100	0.01770100	0.10082400
C	7.50336600	3.22536700	0.80755000
H	6.11560100	4.78713900	1.33723600
H	8.62095100	1.45956800	0.27092200
H	8.37876900	3.86316900	0.87969200
C	4.52938200	-2.67047200	-1.66877000
C	5.34572900	-2.98420700	-0.57923300
C	5.05039600	-2.08819300	-2.82423700
C	6.70456600	-2.68938900	-0.65143300
H	4.91964800	-3.45429300	0.30094300
C	6.41258600	-1.79380800	-2.87388900
H	4.39618400	-1.87941000	-3.66405400
C	7.25564800	-2.07685100	-1.78992000
H	7.35010100	-2.93825200	0.18629800
H	6.82726000	-1.33873600	-3.76894100
C	8.71611200	-1.70149400	-1.83608200
H	8.84530200	-0.63800300	-1.59808200
H	9.30438900	-2.27617000	-1.11604700
H	9.13951800	-1.86299600	-2.83151100
C	-3.13227800	-1.51431100	0.79659100
C	-3.11477700	-0.99587500	2.11357100
C	-2.29497200	-1.60431200	3.07078400
C	-1.51524000	-2.72422200	2.77994000
C	-1.54135700	-3.21318300	1.47049500
C	-2.33211200	-2.63689800	0.46916800
H	-2.29656300	-1.22125400	4.08725900
H	-0.95592200	-4.09432600	1.22643400
C	-4.04009500	0.13864700	2.54278100
C	-3.34294300	1.19920900	3.41163900

C	-5.27321900	-0.43144000	3.27242900
H	-4.39820500	0.64309200	1.64172200
H	-2.43674000	1.57617100	2.92720400
H	-4.01695300	2.04415100	3.58752800
H	-3.05624300	0.80243900	4.39059800
H	-5.78718200	-1.16842200	2.65142800
H	-4.97153400	-0.92900000	4.20062400
H	-5.97715600	0.36786300	3.52843300
C	-0.76195100	-3.44672600	3.88842700
C	0.73100900	-3.65311300	3.58626600
C	-1.44539200	-4.79277200	4.20122200
H	-0.83152500	-2.82162000	4.78831300
H	1.24362800	-2.69869600	3.43538500
H	1.22098500	-4.16757900	4.41926200
H	0.87754000	-4.27090700	2.69317200
H	-2.50101600	-4.64921300	4.45069900
H	-1.39441600	-5.46475200	3.33743000
H	-0.95652300	-5.29102700	5.04504900
C	-2.38770900	-3.30796700	-0.90356500
C	-3.25767800	-4.58123700	-0.84096200
C	-1.00485400	-3.66199700	-1.48038100
H	-2.86979800	-2.61046200	-1.59659400
H	-4.25450800	-4.36164700	-0.45697600
H	-3.35124700	-5.03100400	-1.83510200
H	-2.79840700	-5.32250300	-0.17778500
H	-0.34944500	-2.79524400	-1.57053800
H	-0.47978900	-4.40766600	-0.87634900
H	-1.11412400	-4.08357100	-2.48444400
C	-4.15613400	-0.99924500	-0.18087700
C	-4.00373100	0.10844500	-1.04749100
C	-5.39217100	-1.69475200	-0.17209700
C	-5.08160300	0.47577400	-1.89645200
C	-6.42793900	-1.32575800	-1.02566600
C	-6.27229800	-0.24347800	-1.88914100
H	-7.36722400	-1.86414200	-1.02625900
H	-7.09217800	0.03173600	-2.53996900
O	-5.48811100	-2.71672200	0.72994800
O	-4.88207000	1.56650800	-2.69425200
C	-6.70409700	-3.45195700	0.80383100
H	-6.92630100	-3.95937400	-0.14352300
H	-6.55018600	-4.19822800	1.58362500
H	-7.54815000	-2.80731000	1.08010500
C	-5.90424700	1.96678900	-3.59938200
H	-6.81983800	2.25600400	-3.06950400

H	-5.50605400	2.83197600	-4.13079200
H	-6.13432000	1.17334700	-4.32071000
C	-2.97145300	2.93702200	-0.92079800
C	-3.90486600	3.17024400	0.28114300
C	-1.72371700	3.84159600	-0.83132100
H	-3.51668000	3.18166400	-1.83478500
C	-4.29944100	4.65056200	0.39544500
H	-3.39038300	2.86041200	1.19945700
H	-4.80137100	2.54762900	0.19011800
C	-2.12998100	5.32042000	-0.72169000
H	-1.13354700	3.56318500	0.05283900
H	-1.07446000	3.69774100	-1.70267200
C	-3.06247000	5.55528800	0.47489600
H	-4.93916700	4.79567500	1.27322400
H	-4.89925200	4.93185400	-0.48129400
H	-1.23209200	5.94350000	-0.63918900
H	-2.64007000	5.62467600	-1.64609100
H	-3.36116300	6.60814400	0.52400600
H	-2.51663300	5.33882000	1.40485000
C	-1.56030700	0.98528200	-2.67325000
C	-1.09042700	-0.46183100	-2.89794000
C	-2.20108900	1.55111800	-3.95195200
H	-0.66386200	1.58479200	-2.45418800
C	-0.10187600	-0.54699000	-4.06968000
H	-1.96137200	-1.09740600	-3.10117800
H	-0.63030800	-0.85246700	-1.98648400
C	-1.20564000	1.47366900	-5.12323300
H	-3.09440400	0.96793700	-4.19454400
H	-2.53073900	2.58415000	-3.80130100
C	-0.71175500	0.03695200	-5.35051400
H	0.21686100	-1.58373800	-4.21019900
H	0.80537600	0.01841200	-3.81226200
H	-1.67737200	1.86583100	-6.03141200
H	-0.34518800	2.12595300	-4.91392100
H	0.01728500	0.00954600	-6.16787100
H	-1.55920600	-0.58836700	-5.66422400
P	-2.47515300	1.14181400	-1.04468600
Au	-0.82240800	0.67476200	0.58308900

Zero-point correction= 1.314865 (Hartree/Particle)

Thermal correction to Energy= 1.387796

Thermal correction to Enthalpy= 1.388740

Thermal correction to Gibbs Free Energy= 1.204300

Sum of electronic and zero-point Energies= -3791.601665

Sum of electronic and thermal Energies= -3791.528734

Sum of electronic and thermal Enthalpies= -3791.527790

Sum of electronic and thermal Free Energies= -3791.712230

A-TSd1

C	-0.87854900	-3.99507700	3.34185500
C	-0.64348700	-2.94860200	2.46538400
C	1.70431100	-3.53837000	2.41732100
C	1.46705600	-4.58734700	3.32193300
C	0.17816800	-4.82010100	3.77477800
H	-1.88811700	-4.18280100	3.69429100
H	-1.45726700	-2.32392200	2.12348300
H	2.29036600	-5.21803800	3.64636100
H	-0.01851500	-5.63972400	4.45836000
C	3.03630700	-3.20562200	1.96138600
O	3.13467800	-2.58473100	0.76846900
H	3.83983600	-3.92673200	2.08523300
C	0.65488000	-2.69246000	1.97539300
C	0.95564500	-1.60286500	1.06028500
C	2.20236900	-1.63779500	0.46745200
C	2.70089200	-0.79392900	-0.67755500
H	2.95282100	-1.45644700	-1.51081200
H	1.90453000	-0.12552500	-0.99887100
N	3.86541600	0.02685200	-0.35722700
C	3.65092100	1.36511800	0.20179300
H	4.63888800	1.80582300	0.37672800
H	3.16563800	1.98032200	-0.56653600
C	1.79967500	2.26805500	1.54923700
H	1.59131100	2.84930600	0.65116200
C	2.84310000	1.42267300	1.48427900
C	3.43056900	0.65211300	2.65418300
H	4.50738000	0.55552300	2.49744400
H	3.27869500	1.26308600	3.55917000
C	2.88521200	-0.69463900	3.03629900
C	3.67461000	-1.82845100	3.22553100
H	1.87245100	-0.71529900	3.42070400
H	3.44283000	-2.46075100	4.07899100
H	4.72709900	-1.75253500	2.96017500
O	5.90340600	-0.73051100	1.05405800
O	5.29328200	-1.88764900	-1.13584800
S	5.40077800	-0.66856000	-0.33071200
C	0.91719900	2.58333700	2.68909600
C	0.61167000	3.93068000	2.95938800
C	0.31853100	1.59608500	3.48999500
C	-0.23890100	4.27816600	4.00722400

H	1.05224700	4.70915500	2.34315600
C	-0.52604200	1.94342500	4.54557400
H	0.46037800	0.55324600	3.24053600
C	-0.80766000	3.28458800	4.81005800
H	-0.45643300	5.32441200	4.19987000
H	-0.97433800	1.16236400	5.15221400
H	-1.46839600	3.55434800	5.62817000
C	6.38396900	0.54535100	-1.19757200
C	7.37663600	1.25001200	-0.51747200
C	6.14967500	0.75124800	-2.56049100
C	8.13969900	2.18373700	-1.21870800
H	7.54563200	1.06009300	0.53664500
C	6.92198100	1.68522400	-3.24155900
H	5.38097400	0.18338000	-3.07420700
C	7.92818600	2.41419900	-2.58445300
H	8.91473600	2.73751900	-0.69650600
H	6.74838800	1.85141400	-4.30114500
C	8.78121400	3.39745400	-3.34645600
H	8.20188200	3.92015100	-4.11331000
H	9.22652400	4.14391900	-2.68341500
H	9.60169000	2.87847100	-3.85650800
Au	-0.48178400	-0.22405700	0.47593900
P	-2.16152100	1.39466700	-0.04959800
C	-3.41476000	0.93304700	-1.33447600
C	-4.37395600	1.90866100	-1.71134800
C	-5.32838200	1.63824600	-2.68620500
H	-6.06866800	2.37880800	-2.96091200
C	-5.32111200	0.41004000	-3.34599300
H	-6.05851800	0.22522400	-4.11679200
C	-4.36105600	-0.54648000	-3.02839800
C	-3.41329500	-0.31437500	-2.00040700
C	-2.43662800	-1.42784100	-1.74568900
C	-1.22291000	-1.45959900	-2.47167300
C	-0.90656200	-0.42674800	-3.54799300
H	-1.66213600	0.36135700	-3.48827400
C	-1.03436800	-1.06860900	-4.94326200
H	-0.28633200	-1.85690700	-5.08065500
H	-0.88832000	-0.32148500	-5.73093200
H	-2.02347500	-1.51828300	-5.06376400
C	0.46653900	0.23965500	-3.36601600
H	0.53773300	0.72656100	-2.38765400
H	0.62828000	1.00185500	-4.13576000
H	1.28343600	-0.48466900	-3.44438000
C	-0.33401000	-2.51468700	-2.25658400

C	-0.61650100	-3.56429600	-1.37575500
C	0.39532200	-4.69657600	-1.21941900
H	1.36005300	-4.22733200	-0.97295300
C	0.57366300	-5.45243100	-2.55261200
H	1.34025100	-6.22839600	-2.45760400
H	0.86959000	-4.78456800	-3.36629400
H	-0.36608800	-5.93491800	-2.84255100
C	0.06508000	-5.69048300	-0.09876900
H	-0.08343500	-5.19424300	0.86230300
H	0.88067600	-6.41105200	0.01527100
H	-0.84226500	-6.25971000	-0.33040600
C	-1.84159100	-3.53408900	-0.70810700
C	-2.76486100	-2.49206800	-0.87750000
C	-4.14081300	-2.59985000	-0.22062300
H	-4.61097200	-1.61130800	-0.26080200
C	-5.02655100	-3.57323200	-1.02808100
H	-4.61674200	-4.58823400	-0.97831100
H	-5.07198300	-3.28163700	-2.07799600
H	-6.04350500	-3.59843300	-0.62165300
C	-4.11310500	-3.03924900	1.25342500
H	-3.69913400	-4.04594900	1.37057700
H	-5.13211500	-3.06068200	1.65326500
H	-3.52886200	-2.35862100	1.87432400
H	0.60196100	-2.53300600	-2.80913600
H	-2.10141200	-4.34841500	-0.04283900
C	-1.24489000	2.94256100	-0.64389600
C	-1.31766800	3.17242200	-2.16662100
C	-1.51726100	4.25791900	0.10758900
H	-0.21152400	2.65362700	-0.41894700
C	-0.29148600	4.23466500	-2.59150800
H	-2.32259800	3.51389500	-2.42975800
H	-1.14464900	2.24418900	-2.71251400
C	-0.49720300	5.32868800	-0.31640600
H	-2.52584700	4.60456400	-0.13448500
H	-1.46601300	4.11198200	1.18997500
C	-0.50841200	5.55322800	-1.83481600
H	-0.35550900	4.39864200	-3.67326700
H	0.72290200	3.85952500	-2.39136200
H	-0.70451100	6.26579900	0.21315400
H	0.50934100	5.01252000	-0.00671400
H	0.25300900	6.28831500	-2.11851600
H	-1.47935300	5.97678100	-2.12728900
C	-3.02050700	1.70964300	1.59736800
C	-4.13541100	2.76385900	1.73789600

C	-3.52611200	0.35689400	2.14581000
H	-2.16826500	2.02207200	2.21704400
C	-4.55758000	2.89779100	3.21145800
H	-5.00034800	2.45424900	1.14188900
H	-3.81751100	3.73215400	1.35387900
C	-4.00519300	0.46926600	3.60062300
H	-4.34828900	-0.00001600	1.51200300
H	-2.73198700	-0.39192900	2.08145000
C	-5.06567200	1.56327900	3.77073700
H	-5.33070200	3.66971200	3.30054300
H	-3.69707300	3.24082300	3.80265600
H	-4.39209700	-0.50141000	3.93294500
H	-3.14190800	0.70235800	4.23708100
H	-5.34223700	1.66595900	4.82610100
H	-5.97807600	1.27152300	3.23210100
O	-4.26947300	3.12116700	-1.09042200
O	-4.24363800	-1.74470200	-3.67696500
C	-5.15430600	-2.04241900	-4.72914200
H	-5.07625600	-1.31467100	-5.54678300
H	-4.86921300	-3.02885600	-5.09592400
H	-6.19020000	-2.07647500	-4.36836300
C	-5.25042700	4.11953800	-1.33924400
H	-4.98392300	4.96308000	-0.70122900
H	-5.23900600	4.44147400	-2.38760500
H	-6.25517200	3.76887500	-1.07435000

Zero-point correction= 1.316384 (Hartree/Particle)

Thermal correction to Energy= 1.388497

Thermal correction to Enthalpy= 1.389441

Thermal correction to Gibbs Free Energy= 1.207959

Sum of electronic and zero-point Energies= -3791.599815

Sum of electronic and thermal Energies= -3791.527702

Sum of electronic and thermal Enthalpies= -3791.526758

Sum of electronic and thermal Free Energies= -3791.708241

SIMesAu

C	-0.00000100	0.59816700	-0.00010300
C	-0.77452000	2.77942800	-0.00010000
C	0.77451800	2.77942900	-0.00079800
N	1.10535800	1.33175900	-0.00023800
N	-1.10535900	1.33175800	-0.00020700
C	2.45106600	0.82245000	-0.00012200
C	3.07891500	0.57824900	1.23186800
C	3.07901800	0.57777600	-1.23200900
C	4.38510800	0.08397600	1.20458500

C	4.38516300	0.08349900	-1.20443000
C	5.05620100	-0.16260600	0.00016400
H	4.89094500	-0.11547500	2.14549400
H	4.89106800	-0.11636500	-2.14522300
C	-2.45106600	0.82244800	-0.00009000
C	-3.07897400	0.57784800	-1.23200500
C	-3.07896000	0.57817500	1.23187100
C	-4.38512800	0.08357700	-1.20451500
C	-4.38514400	0.08389600	1.20450000
C	-5.05620100	-0.16260700	0.00003600
H	-4.89100100	-0.11621200	-2.14534000
H	-4.89101400	-0.11563100	2.14537800
C	-2.35568300	0.81678400	-2.53544200
H	-1.44218500	0.21437100	-2.60253200
C	-2.35573300	0.81749000	2.53527400
H	-2.05919300	1.86610700	2.65136300
Au	0.00000100	-1.38611000	0.00019700
H	-1.20268000	3.25241800	-0.88693100
H	1.20184600	3.25177400	-0.88838300
H	1.20268000	3.25269600	0.88588400
H	-1.20185100	3.25205000	0.88733600
H	-2.98826200	0.55889900	3.38663300
H	-1.44170900	0.21586700	2.60218300
H	-2.05821300	1.86515300	-2.65136600
H	-2.98851300	0.55887900	-3.38678600
C	-6.48062300	-0.65969600	-0.00001500
H	-6.69671200	-1.26016400	0.88781600
H	-7.18131000	0.18381300	-0.00317100
H	-6.69484200	-1.26509700	-0.88496800
C	2.35558900	0.81757600	2.53521500
H	2.05804400	1.86596100	2.65078700
H	1.44213200	0.21512200	2.60248800
H	2.98842000	0.55999400	3.38665500
C	2.35582600	0.81670300	-2.53550200
H	1.44176900	0.21510900	-2.60223500
H	2.05934700	1.86529900	-2.65193400
H	2.98835900	0.55780300	-3.38676400
C	6.48062100	-0.65969700	0.00013400
H	7.18130800	0.18380500	-0.00443000
H	6.69710600	-1.25904600	0.88861900
H	6.69444300	-1.26621300	-0.88415500

Zero-point correction= 0.423562 (Hartree/Particle)

Thermal correction to Energy= 0.449925

Thermal correction to Enthalpy= 0.450869

Thermal correction to Gibbs Free Energy=	0.361395
Sum of electronic and zero-point Energies=	-1060.346515
Sum of electronic and thermal Energies=	-1060.320152
Sum of electronic and thermal Enthalpies=	-1060.319208
Sum of electronic and thermal Free Energies=	-1060.408682

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C	-3.35601600	-3.96349700	3.19932500
C	-2.69967400	-2.73698400	3.13064600
C	-1.46699000	-3.51637900	1.16894800
C	-2.12312900	-4.74661900	1.27117200
C	-3.06404200	-4.97091500	2.27320300
H	-4.09019000	-4.13604000	3.97987200
H	-2.90988100	-1.95470400	3.85247200
H	-1.88280300	-5.51250100	0.54269100
H	-3.57176200	-5.92831100	2.33578100
C	-0.50391700	-3.29835500	0.05259600
O	-0.13722200	-4.19382900	-0.68571200
H	-0.14269200	-2.26203400	-0.08867700
C	-1.74910700	-2.50756800	2.12127800
C	-1.05175900	-1.25457600	2.08753800
C	-0.38503000	-0.21436200	2.14246700
C	0.78892200	0.68048300	2.34829200
H	0.49788000	1.72626100	2.25703100
H	1.19374300	0.51763000	3.35240200
N	1.87619900	0.39424200	1.40196200
C	2.46165700	-0.97505500	1.50048100
H	2.22620100	-1.31380400	2.51381500
H	1.97093300	-1.65876800	0.80062600
C	4.49016700	-1.70614300	0.31432400
H	3.79497200	-2.31986300	-0.26006700
C	3.95801800	-0.95799200	1.29895500
C	4.72689400	-0.07787900	2.26778700
H	5.79097800	-0.32802600	2.21697300
H	4.62622900	0.97124800	1.96292400
C	4.26222100	-0.22543500	3.69656900
C	3.73001700	0.75282300	4.43180800
H	4.39245200	-1.21526300	4.13549600
H	3.44008800	0.59907400	5.46714800
H	3.59525400	1.75389900	4.02752300
O	0.98392900	-0.18509200	-0.98738900
O	0.74455500	2.15379600	-0.01973300
S	1.54067500	0.92803900	-0.19146200
C	5.89370800	-1.82792200	-0.11353600

C	6.34589300	-3.06562200	-0.60661500
C	6.79350600	-0.74549000	-0.11211400
C	7.65904900	-3.22973800	-1.04249400
H	5.65868600	-3.90739300	-0.63692000
C	8.10747300	-0.90958900	-0.54999300
H	6.45150000	0.23668400	0.19173200
C	8.54776300	-2.15228900	-1.01100800
H	7.98875500	-4.19713700	-1.40942300
H	8.78795800	-0.06276400	-0.53450100
H	9.57099700	-2.27780900	-1.35177400
C	3.13479900	1.34526000	-0.85587900
C	3.64286300	0.60381900	-1.92434200
C	3.83308500	2.42595800	-0.31510600
C	4.88522100	0.94835400	-2.44414300
H	3.07689000	-0.23082500	-2.32107800
C	5.07882400	2.75093900	-0.84878200
H	3.41048400	2.99846800	0.50369300
C	5.62465000	2.01680500	-1.91232100
H	5.30000400	0.36895100	-3.26349500
H	5.63586000	3.58545900	-0.43307300
C	6.99148800	2.33093800	-2.46333600
H	6.95348500	2.49214000	-3.54576300
H	7.42413600	3.22126900	-2.00079000
H	7.66971000	1.48828300	-2.28614300
C	-3.14410300	1.00016500	-0.88176900
C	-4.65250300	1.00302200	-2.66374200
C	-4.40187000	2.45759900	-2.19919700
N	-3.42006700	2.28337100	-1.10516400
N	-3.82339600	0.21748800	-1.72234400
C	-2.79199700	3.37640100	-0.41722400
C	-3.34655600	3.82978700	0.78921800
C	-1.61814600	3.92259800	-0.95856900
C	-2.69909800	4.87627100	1.45064700
C	-1.00808600	4.96730200	-0.26123800
C	-1.53419400	5.46059600	0.93776600
H	-3.11217000	5.24246200	2.38726600
H	-0.09049800	5.39424500	-0.65668800
C	-3.62864700	-1.20124400	-1.83387200
C	-2.56206600	-1.67682700	-2.61742900
C	-4.48100000	-2.06141300	-1.12712200
C	-2.38848300	-3.05882900	-2.70440500
C	-4.26337800	-3.43793100	-1.24315500
C	-3.22866700	-3.95362000	-2.03021000
H	-1.55823500	-3.44940400	-3.28612200

H	-4.90728800	-4.12017600	-0.69450300
C	-1.58894600	-0.73097300	-3.27843500
H	-0.88489300	-0.32686400	-2.54165000
C	-5.55765100	-1.50881200	-0.22582000
H	-6.26141600	-0.86967700	-0.77032000
Au	-1.91537600	0.28393000	0.54905400
H	-4.32352800	0.81915000	-3.69059100
H	-3.98190800	3.09142900	-2.98405500
H	-5.30369200	2.94050200	-1.81229100
H	-5.70064600	0.70441500	-2.58032000
H	-6.13078500	-2.31350400	0.23994100
H	-5.11958900	-0.89689700	0.57165600
H	-2.08857700	0.11777900	-3.75541200
H	-1.00412400	-1.24847300	-4.04230300
C	-2.98301000	-5.43771800	-2.14012000
H	-3.62227900	-6.00602600	-1.45895300
H	-3.17916100	-5.79482700	-3.15729500
H	-1.93659100	-5.66406200	-1.90989600
C	-4.57880500	3.17620400	1.36654700
H	-5.41912900	3.19662700	0.66359500
H	-4.38856200	2.12336000	1.60694600
H	-4.89751600	3.67989600	2.28171200
C	-1.02001500	3.36805700	-2.22690500
H	-0.83010900	2.29596000	-2.12683000
H	-1.68119400	3.51570900	-3.08896800
H	-0.06730500	3.85153100	-2.45032100
C	-0.87232700	6.61440500	1.65165800
H	-1.26321600	7.57200600	1.28693200
H	-1.05373000	6.57840000	2.72968400
H	0.20891400	6.62043700	1.48589100

Zero-point correction=	0.916252 (Hartree/Particle)
Thermal correction to Energy=	0.975193
Thermal correction to Enthalpy=	0.976137
Thermal correction to Gibbs Free Energy=	0.815919
Sum of electronic and zero-point Energies=	-2859.826036
Sum of electronic and thermal Energies=	-2859.767096
Sum of electronic and thermal Enthalpies=	-2859.766152
Sum of electronic and thermal Free Energies=	-2859.926370

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C	4.19257400	-4.22046700	0.00917000
C	3.47471500	-3.03544900	-0.14954300
C	1.69425800	-4.27315100	-1.24605200
C	2.43340300	-5.45532600	-1.07767300

C	3.67631900	-5.43509100	-0.45308800
H	5.16070900	-4.19039300	0.49848800
H	3.88838200	-2.10224000	0.21748900
H	2.02134000	-6.39303700	-1.44254100
H	4.23859100	-6.35434800	-0.32634900
C	0.39920700	-4.38328600	-1.91892700
O	-0.38427300	-3.46302900	-2.15367800
H	0.12392800	-5.40433000	-2.24258800
C	2.22109200	-3.04118000	-0.77548200
C	1.45633200	-1.81522300	-0.93770800
C	0.33162400	-1.49896100	-1.42260800
C	-0.89250900	-0.74602400	-1.74616600
H	-0.61057700	0.30583400	-1.85392100
H	-1.28644100	-1.07938600	-2.70910200
N	-1.98818500	-0.85471300	-0.77763500
C	-2.80222400	-2.10263900	-0.77861400
H	-2.57718600	-2.60171700	-1.72226900
H	-2.47994000	-2.76878500	0.02737600
C	-4.97160500	-2.21337100	0.38650200
H	-4.43020500	-2.83489100	1.10023400
C	-4.27434000	-1.77882600	-0.68031300
C	-4.83184900	-0.93497900	-1.81371300
H	-5.92187200	-1.04167300	-1.83634600
H	-4.62111500	0.12359400	-1.61513900
C	-4.28233300	-1.29698700	-3.17066700
C	-3.61860300	-0.46136500	-3.97201600
H	-4.47097300	-2.31798200	-3.50425100
H	-3.27401900	-0.76156600	-4.95721300
H	-3.42010500	0.56712300	-3.67563000
O	-1.55153900	-1.21386000	1.76594600
O	-0.62236500	0.81515100	0.53405400
S	-1.70278200	-0.16302100	0.75245200
C	-6.37864100	-1.96756500	0.74356100
C	-7.09078300	-2.97061800	1.42694300
C	-7.03291100	-0.74742700	0.48929600
C	-8.41813400	-2.78062000	1.80488500
H	-6.59527900	-3.91134900	1.65324900
C	-8.36074100	-0.55606600	0.87047800
H	-6.48826500	0.06949600	0.03214900
C	-9.06124100	-1.57258400	1.52308900
H	-8.95077800	-3.57320300	2.32203200
H	-8.84776700	0.39220600	0.66007200
H	-10.09519800	-1.42208600	1.81859800
C	-3.20112000	0.74211400	1.09656400

C	-3.93149100	0.44288600	2.24646800
C	-3.58782000	1.76867500	0.23450700
C	-5.07780700	1.18124400	2.52310700
H	-3.60993800	-0.36506900	2.89349300
C	-4.74091000	2.49509000	0.52723800
H	-2.99885600	1.99130900	-0.64742700
C	-5.50410100	2.21042000	1.66950600
H	-5.66511900	0.94230700	3.40480600
H	-5.05654400	3.28806400	-0.14512900
C	-6.77818600	2.95821800	1.96985300
H	-6.97831100	3.73735200	1.23013300
H	-7.62925700	2.26767500	1.97769300
H	-6.73678800	3.42896500	2.95791700
C	3.03447900	1.84485600	0.21379300
C	4.63471000	3.24324400	1.19137700
C	3.55575700	4.10452000	0.49405800
N	2.58812500	3.08747200	0.02248500
N	4.21333000	1.86867800	0.84381800
C	1.34937600	3.40329600	-0.63337400
C	1.28917900	3.36965000	-2.03711700
C	0.22533300	3.68367500	0.15536200
C	0.05535100	3.61906800	-2.64382700
C	-0.98008600	3.95441100	-0.49779000
C	-1.08910500	3.91240800	-1.89027600
H	-0.01169900	3.59595600	-3.72894700
H	-1.86079000	4.16944600	0.10062300
C	4.91541700	0.68179700	1.24363100
C	4.53685600	0.03081200	2.43059500
C	5.91242800	0.17130400	0.39834700
C	5.20694500	-1.14719800	2.77126100
C	6.55744300	-1.00866200	0.78283100
C	6.22486300	-1.67596100	1.96747100
H	4.92468900	-1.66643700	3.68367100
H	7.33237100	-1.41754800	0.13948200
C	3.40229300	0.55644900	3.27620000
H	2.44443600	0.45074700	2.75297200
C	6.23472900	0.85217300	-0.90874300
H	6.60055800	1.87381900	-0.75686700
Au	2.12809200	0.13079400	-0.36388500
H	4.63908900	3.36821800	2.27888200
H	3.06979400	4.81022300	1.17111000
H	3.94842400	4.66333700	-0.36144000
H	5.64290200	3.43962700	0.81891200
H	7.00233400	0.30416100	-1.45942400

H	5.34249900	0.92084100	-1.54130300
H	3.52391500	1.61906200	3.51047600
H	3.33138500	0.01068100	4.21936500
C	6.95477400	-2.93061200	2.38404200
H	7.45229500	-3.40945800	1.53550900
H	7.72756000	-2.70204800	3.12731500
H	6.27464200	-3.65636000	2.84122700
C	2.51079000	3.04294300	-2.86224600
H	3.37980100	3.63434600	-2.55531300
H	2.78916400	1.98800900	-2.75470400
H	2.33067700	3.23648600	-3.92208500
C	0.29483800	3.61548200	1.65919700
H	0.56931700	2.60343800	1.97165100
H	1.03037300	4.31211900	2.07606900
H	-0.67490200	3.84876600	2.10374200
C	-2.41759400	4.14418800	-2.57130600
H	-3.12263800	4.65859400	-1.91230900
H	-2.30458600	4.74273900	-3.48020000
H	-2.87799600	3.19307800	-2.87031700

Zero-point correction=	0.915696 (Hartree/Particle)
Thermal correction to Energy=	0.973812
Thermal correction to Enthalpy=	0.974756
Thermal correction to Gibbs Free Energy=	0.815700
Sum of electronic and zero-point Energies=	-2859.819661
Sum of electronic and thermal Energies=	-2859.761546
Sum of electronic and thermal Enthalpies=	-2859.760601
Sum of electronic and thermal Free Energies=	-2859.919658

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C	-4.02698300	4.06543500	-0.89791000
C	-3.18232200	2.95708300	-0.95121000
C	-1.83064900	4.16375000	-2.56955400
C	-2.68385500	5.27091900	-2.50354500
C	-3.79148100	5.21656300	-1.66505300
H	-4.88415800	4.02566300	-0.23511900
H	-3.37926800	2.08680000	-0.33598700
H	-2.47400300	6.15411100	-3.09960300
H	-4.46936500	6.06076500	-1.59865200
C	-0.63153600	4.05474700	-3.36430200
O	0.02845800	3.00820700	-3.28875100
H	-0.30081400	4.87140800	-4.02112100
C	-2.07131600	2.99258600	-1.80726500
C	-1.13178900	1.93004900	-1.97237100
C	-0.61074200	0.77500200	-1.79317300

C	0.71588000	0.21521600	-2.27932000
H	0.58608100	-0.81352700	-2.61067300
H	1.08724600	0.82538800	-3.10462100
N	1.74625300	0.24887000	-1.23391000
C	2.05945100	1.59161100	-0.67446800
H	1.71655700	2.30222000	-1.43103700
H	1.48122100	1.77052600	0.23812000
C	3.97790800	2.00424700	0.81493100
H	3.21321400	2.10948000	1.58562300
C	3.54102500	1.76299200	-0.43563000
C	4.41522400	1.63246900	-1.67038900
H	5.40132600	2.05891800	-1.45923000
H	4.56744100	0.56929000	-1.89529600
C	3.83628200	2.31647300	-2.88418100
C	3.51354000	1.70531800	-4.02458000
H	3.68641300	3.39305600	-2.79390600
H	3.11480300	2.25109600	-4.87435000
H	3.65270000	0.63385900	-4.15156600
O	1.10960100	-0.54012900	1.17487900
O	1.03946000	-2.14373700	-0.80160700
S	1.68033500	-1.02323400	-0.09852000
C	5.35688900	2.14318200	1.31211700
C	5.60700200	3.01980100	2.38402000
C	6.43381500	1.38973000	0.80784200
C	6.88958300	3.17084800	2.90672600
H	4.78361800	3.59359000	2.80213400
C	7.71720200	1.53882900	1.33291100
H	6.25780400	0.65345400	0.03325800
C	7.95257200	2.43340400	2.37902200
H	7.06033800	3.86100500	3.72767200
H	8.53480800	0.95017900	0.92603000
H	8.95248800	2.54789100	2.78655300
C	3.38899100	-1.43513400	0.19589500
C	3.91248500	-1.29842400	1.48229200
C	4.15844500	-1.93517700	-0.85527500
C	5.23776200	-1.65366100	1.70811200
H	3.29042100	-0.90453800	2.27723600
C	5.48701000	-2.27877900	-0.60984900
H	3.72727600	-2.04906400	-1.84422000
C	6.04662800	-2.13929500	0.66882900
H	5.66062200	-1.53125100	2.70085700
H	6.09827600	-2.65909600	-1.42315500
C	7.49341300	-2.46971500	0.93403100
H	8.02591200	-1.58167600	1.29339400

H	7.58693700	-3.23672400	1.71040000
H	8.00023500	-2.83195700	0.03636300
C	-2.76226700	-1.46431000	0.94298000
C	-3.98619400	-1.99829000	2.86867200
C	-3.55419800	-3.29779800	2.15928400
N	-2.72018100	-2.79296600	1.04540300
N	-3.51352600	-0.95652900	1.93025400
C	-2.08321000	-3.67555400	0.10831800
C	-2.74096700	-3.97767000	-1.09509200
C	-0.82413400	-4.20258800	0.42804200
C	-2.10422900	-4.84600300	-1.98478500
C	-0.23088200	-5.07012800	-0.49107900
C	-0.85376700	-5.40615800	-1.69693900
H	-2.59473200	-5.09143700	-2.92344700
H	0.75337800	-5.47361000	-0.26915900
C	-3.74392400	0.44127200	2.14435000
C	-2.75148100	1.21778200	2.76856700
C	-4.96564200	0.99179500	1.72246600
C	-3.01160300	2.57871200	2.95573300
C	-5.18630900	2.35404100	1.95202100
C	-4.21957300	3.16375800	2.55901700
H	-2.25536500	3.19546500	3.43497400
H	-6.13568200	2.79034600	1.64950200
C	-1.44113100	0.60935600	3.20497200
H	-0.79792700	0.37238200	2.35119700
C	-5.99956600	0.14221400	1.02438500
H	-6.47458500	-0.56708800	1.71223700
Au	-1.76885300	-0.34338000	-0.44189800
H	-3.50177200	-1.86463000	3.84149300
H	-2.97008900	-3.96174700	2.79985900
H	-4.39968400	-3.86466300	1.75592700
H	-5.06682400	-1.92610000	3.01039900
H	-6.79218800	0.76103100	0.59748800
H	-5.54864100	-0.44402900	0.21733000
H	-1.59213700	-0.32621400	3.75324000
H	-0.89446200	1.29462000	3.85712800
C	-4.45431800	4.64270300	2.74900700
H	-3.98175000	5.21588800	1.94119800
H	-5.52051700	4.88603700	2.74731800
H	-4.02579500	4.99869200	3.69032300
C	-4.07666800	-3.35798600	-1.43027800
H	-4.80314800	-3.48441200	-0.61985400
H	-3.97734000	-2.27996000	-1.60524200
H	-4.50108300	-3.80630900	-2.33146300

C	-0.11832800	-3.80584000	1.69992900
H	-0.06155100	-2.71776300	1.79259500
H	-0.63004000	-4.19290300	2.58956900
H	0.90178600	-4.19579900	1.71228500
C	-0.20013500	-6.36877700	-2.65880100
H	-0.50917400	-6.17789600	-3.69053900
H	0.89067300	-6.30216200	-2.61077200
H	-0.47488300	-7.40378700	-2.42134600

Zero-point correction= 0.916186 (Hartree/Particle)

Thermal correction to Energy= 0.974087

Thermal correction to Enthalpy= 0.975031

Thermal correction to Gibbs Free Energy= 0.816725

Sum of electronic and zero-point Energies= -2859.820403

Sum of electronic and thermal Energies= -2859.762502

Sum of electronic and thermal Enthalpies= -2859.761558

Sum of electronic and thermal Free Energies= -2859.919864

B-2

C	4.28923500	-4.13243000	0.02904700
C	3.62688200	-2.94402800	-0.19413900
C	1.67319800	-4.22297700	-0.91081600
C	2.37672300	-5.44075900	-0.66995000
C	3.66602100	-5.38914400	-0.20584400
H	5.31128000	-4.10879100	0.39532200
H	4.11957400	-1.99706900	-0.00084700
H	1.88320000	-6.39010700	-0.85620900
H	4.21637800	-6.30474000	-0.01597000
C	0.37231700	-4.22705700	-1.39121700
O	-0.28397600	-3.11832100	-1.62690400
H	-0.19765800	-5.12039900	-1.62443500
C	2.29021000	-2.94367000	-0.67039100
C	1.54260000	-1.73850500	-0.88694700
C	0.26171000	-1.88242400	-1.36118300
C	-0.75838300	-0.79402000	-1.57459500
H	-0.27561900	0.16982000	-1.41422500
H	-1.13837400	-0.80822200	-2.59869800
N	-1.93751000	-0.89071400	-0.69380700
C	-3.06413600	-1.76204500	-1.13076200
H	-2.81106400	-2.10485200	-2.13838600
H	-3.12928700	-2.65741800	-0.50324900
C	-5.44290600	-1.52762300	-0.51451500
H	-5.29248800	-2.49129500	-0.02744700
C	-4.37929200	-1.00761600	-1.15394900
C	-4.36316400	0.28901700	-1.94049200

H	-5.37837400	0.68968300	-2.00414500
H	-3.75216000	1.02534000	-1.40538100
C	-3.83496500	0.13205000	-3.34650500
C	-2.77834200	0.77755600	-3.84564400
H	-4.39707400	-0.55002200	-3.98522000
H	-2.46774700	0.65184700	-4.87893800
H	-2.19265000	1.46156100	-3.23568900
O	-1.19277000	-2.38785100	1.30832900
O	-0.50989300	0.05889500	1.16918100
S	-1.51572200	-0.99248400	0.95647100
C	-6.81162000	-0.99939300	-0.36437800
C	-7.88464200	-1.90887000	-0.33474800
C	-7.09856400	0.36563400	-0.17948800
C	-9.19667200	-1.47121100	-0.16527800
H	-7.68245600	-2.97038000	-0.45334800
C	-8.41138100	0.80481200	-0.00693900
H	-6.28590900	1.07989400	-0.12290600
C	-9.46681900	-0.10999100	-0.00492600
H	-10.00859500	-2.19232900	-0.15438600
H	-8.60858000	1.86327200	0.13764600
H	-10.48796300	0.23295600	0.13101900
C	-3.03601000	-0.54536500	1.75850700
C	-3.74304600	-1.50550700	2.47849100
C	-3.49828200	0.76655400	1.63528500
C	-4.95594000	-1.14427400	3.06272600
H	-3.34938600	-2.51198500	2.56703300
C	-4.70663900	1.10739300	2.23089400
H	-2.91912800	1.49219600	1.07639400
C	-5.46269000	0.15643200	2.93797000
H	-5.52266600	-1.88636000	3.61747000
H	-5.08103800	2.12362600	2.14088800
C	-6.81175500	0.51840500	3.50157100
H	-6.83403400	1.55204000	3.85928200
H	-7.57502600	0.42364600	2.71961500
H	-7.09514600	-0.13869500	4.32785000
C	2.96724600	1.95091700	0.17392200
C	4.48745300	3.53340500	1.00333800
C	3.18780600	4.24876500	0.56544500
N	2.31769300	3.11811900	0.16892400
N	4.21957000	2.13412000	0.61107800
C	0.95343500	3.28786600	-0.24499800
C	0.66043600	3.39196600	-1.61546900
C	-0.05132900	3.32912300	0.73366600
C	-0.67580300	3.56038500	-1.99250600

C	-1.36840000	3.53004200	0.30893200
C	-1.70299000	3.64537600	-1.04387400
H	-0.91726300	3.64746400	-3.04906300
H	-2.15218800	3.59896900	1.05919900
C	5.13475900	1.04302300	0.79224800
C	5.05837400	0.27596100	1.96583300
C	6.01074700	0.71615900	-0.25527300
C	5.90337800	-0.83294900	2.07956400
C	6.83544400	-0.40061000	-0.09768700
C	6.79852600	-1.18410900	1.06285400
H	5.85343000	-1.44067800	2.97959000
H	7.51459300	-0.67136700	-0.90235900
C	4.04236100	0.59451400	3.03518200
H	3.02533500	0.41205600	2.66823200
C	6.00525500	1.51464700	-1.53508900
H	6.23969700	2.57015000	-1.35818300
Au	2.24368400	0.13003600	-0.38398800
H	4.66086300	3.59532000	2.08267400
H	2.72456600	4.82544000	1.36954000
H	3.34044200	4.91551400	-0.28955700
H	5.37529500	3.91327600	0.49161700
H	6.73788400	1.12568400	-2.24570600
H	5.01684100	1.47919200	-2.00715500
H	4.08795100	1.64328700	3.34617100
H	4.19805500	-0.02464700	3.92137300
C	7.71796800	-2.37243900	1.21677800
H	7.32485200	-3.09549800	1.93801000
H	7.87433500	-2.88490000	0.26214200
H	8.70453400	-2.05899000	1.57828800
C	1.75319100	3.28568400	-2.65108000
H	2.58368100	3.96759200	-2.43985300
H	2.17122700	2.27231800	-2.67297500
H	1.37325500	3.51835000	-3.64847500
C	0.25837100	3.08390000	2.18833300
H	0.42797000	2.01348600	2.34505200
H	1.14914200	3.61978400	2.52825900
H	-0.57893800	3.38484900	2.82261100
C	-3.13124500	3.89340100	-1.46787000
H	-3.84088000	3.49407600	-0.73649100
H	-3.32793600	4.96819100	-1.55996600
H	-3.35122400	3.43647300	-2.43695800

Zero-point correction= 0.919957 (Hartree/Particle)

Thermal correction to Energy= 0.977076

Thermal correction to Enthalpy= 0.978021

Thermal correction to Gibbs Free Energy=	0.823012
Sum of electronic and zero-point Energies=	-2859.854059
Sum of electronic and thermal Energies=	-2859.796939
Sum of electronic and thermal Enthalpies=	-2859.795995
Sum of electronic and thermal Free Energies=	-2859.951004

B-21

C	5.79507700	-2.10844000	0.88935500
C	4.46957500	-1.70730700	0.82825700
C	3.87865000	-3.99500800	1.47036600
C	5.23657900	-4.38996400	1.51956200
C	6.18309700	-3.43174200	1.23161800
H	6.56517800	-1.38109100	0.65846400
H	4.21011200	-0.69419800	0.54405200
H	5.51249500	-5.40760400	1.77530400
H	7.23827100	-3.68252200	1.25983100
C	2.69169200	-4.69388900	1.69659200
O	1.63558500	-3.93221000	1.54150800
H	2.51297400	-5.72731800	1.96815900
C	3.48383600	-2.66031600	1.13339700
C	2.05075700	-2.61522000	1.18469700
C	1.09999900	-1.65908200	0.97338400
C	-0.35367400	-2.05110200	1.13157900
H	-0.49928000	-3.12910400	1.04560200
H	-0.66272700	-1.75598300	2.14191300
N	-1.27498200	-1.37718300	0.21272900
C	-1.91865200	-0.09933600	0.59857700
H	-1.32627400	0.35429000	1.39937200
H	-1.85884700	0.59031100	-0.24156900
C	-4.33394700	0.12565200	0.19732300
H	-4.01475800	0.66918100	-0.68955400
C	-3.35869700	-0.30544400	1.01809100
C	-3.57648600	-0.99744900	2.34925200
H	-4.63323500	-0.92157500	2.62734300
H	-3.35106700	-2.07000300	2.26245000
C	-2.74816400	-0.39935900	3.46221300
C	-2.00262900	-1.09432400	4.32382600
H	-2.79795900	0.68587500	3.55196100
H	-1.45506300	-0.61031000	5.12691300
H	-1.93870400	-2.17967700	4.27389900
O	-0.41813600	-0.40553100	-2.05998500
O	-0.26626300	-2.88734900	-1.51939000
S	-0.99447900	-1.61446800	-1.43490000
C	-5.79388800	-0.03615900	0.29530000

C	-6.62307100	0.99630000	-0.18037000
C	-6.40533600	-1.21367400	0.76292800
C	-8.01126900	0.87713400	-0.15126500
H	-6.16773400	1.90158400	-0.57451100
C	-7.79431600	-1.33699000	0.78735000
H	-5.78764800	-2.05211800	1.06525800
C	-8.60340800	-0.29039700	0.33794700
H	-8.63151400	1.69083800	-0.51537800
H	-8.24597300	-2.25709500	1.14658000
H	-9.68447800	-0.38868100	0.35615200
C	-2.66579500	-1.76352200	-2.03941800
C	-3.16275200	-0.81791200	-2.93360100
C	-3.48274300	-2.77133700	-1.51990100
C	-4.51444700	-0.86188000	-3.27728400
H	-2.50526600	-0.05048400	-3.32638400
C	-4.82416500	-2.80115800	-1.87793500
H	-3.07578500	-3.49978300	-0.82669700
C	-5.36871500	-1.83174500	-2.73748500
H	-4.91517000	-0.11762400	-3.95966700
H	-5.47171900	-3.56910200	-1.46495800
C	-6.84941800	-1.80629400	-3.01301700
H	-7.08219000	-1.25567500	-3.92817400
H	-7.25817200	-2.81689000	-3.10549700
H	-7.37100700	-1.31560600	-2.18219600
C	1.89953500	2.18238200	-0.21578000
C	1.67940300	4.48255500	-0.60406400
C	2.97605700	3.98311200	-1.26398600
N	3.04213300	2.58216800	-0.79199800
N	1.05707800	3.21987800	-0.14397100
C	4.11961200	1.70970800	-1.15583100
C	5.29865000	1.74873900	-0.39323700
C	3.97729900	0.85951700	-2.26800200
C	6.35608900	0.91698400	-0.77521800
C	5.05554400	0.03139600	-2.59462900
C	6.25032200	0.04731500	-1.86669800
H	7.28213500	0.95017400	-0.20571400
H	4.96225600	-0.63537700	-3.44820000
C	-0.25012000	3.20135800	0.44579000
C	-1.36775000	3.17662800	-0.40866400
C	-0.38285100	3.23219900	1.84154900
C	-2.63565600	3.21696400	0.17309500
C	-1.67727700	3.24086800	2.37715900
C	-2.81330800	3.24321300	1.56284400
H	-3.51059800	3.20209100	-0.47161000

H	-1.79698300	3.26191800	3.45747400
C	-1.19834800	3.01990600	-1.90057500
H	-0.71961100	2.06109100	-2.12996600
C	0.82669100	3.22401700	2.74442000
H	1.59168600	3.93197700	2.40962400
Au	1.52475700	0.25885800	0.41265800
H	1.01853700	5.01079600	-1.29389900
H	2.92845700	3.99883900	-2.35857900
H	3.86072000	4.53997900	-0.94942400
H	1.86575800	5.13223900	0.25844700
H	0.55178900	3.48335100	3.76938800
H	1.29530900	2.23295800	2.75982700
H	-0.57880800	3.80972400	-2.33813100
H	-2.16715300	3.04560900	-2.40572000
C	-4.20272700	3.25433700	2.15005900
H	-4.76862600	4.12734900	1.80703600
H	-4.75933900	2.36366300	1.83965500
H	-4.17989200	3.27794300	3.24275800
C	5.41391000	2.65121100	0.81099100
H	5.51410200	3.70405100	0.52127400
H	4.52710900	2.57448100	1.44824700
H	6.29114400	2.39595200	1.41009400
C	2.70407200	0.82029400	-3.07887600
H	1.92438800	0.22864800	-2.58671200
H	2.28803600	1.82075000	-3.23354600
H	2.88645600	0.37643400	-4.06034600
C	7.38112200	-0.88385300	-2.23052800
H	7.19374400	-1.89036100	-1.83530200
H	7.48806100	-0.97919300	-3.31496400
H	8.33588700	-0.53962000	-1.82332700

Zero-point correction= 0.918903 (Hartree/Particle)
Thermal correction to Energy= 0.976325
Thermal correction to Enthalpy= 0.977270
Thermal correction to Gibbs Free Energy= 0.821658
Sum of electronic and zero-point Energies= -2859.847308
Sum of electronic and thermal Energies= -2859.789886
Sum of electronic and thermal Enthalpies= -2859.788942
Sum of electronic and thermal Free Energies= -2859.944553

B-TSa1

C	3.25544200	3.70208500	-0.93895100
C	2.61128800	2.47486600	-0.93992200
C	0.49841100	3.62080600	-1.31280600
C	1.15546900	4.86142300	-1.27474900

C	2.53009700	4.89830900	-1.10067700
H	4.33276600	3.74086000	-0.80912000
H	3.17773100	1.55771100	-0.81453300
H	0.58555700	5.77854200	-1.38744300
H	3.04864800	5.85156800	-1.08650700
C	-0.93696300	3.51013200	-1.45076600
O	-1.39670700	2.37681200	-2.06136400
H	-1.47600700	4.38314900	-1.80883800
C	1.21221900	2.40641300	-1.12951600
C	0.46512000	1.16415500	-1.10601100
C	-0.82039900	1.21627200	-1.60708600
C	-1.74481000	0.04547300	-1.76353800
H	-2.47932700	0.26529900	-2.55167800
H	-1.19880900	-0.86434400	-2.00850700
N	-2.40086800	-0.14282700	-0.45032800
C	-2.86491800	1.11461500	0.13327600
H	-3.46667100	1.69381400	-0.58012800
H	-3.49131700	0.88078300	0.99989400
C	-1.68868300	3.32446700	0.36029300
H	-2.66995200	3.64963700	0.00913600
C	-1.69008200	1.92767500	0.64890900
C	-0.93083800	1.26324200	1.77367400
H	-0.93251500	0.18321400	1.60931900
H	0.10733600	1.59116400	1.81223800
C	-1.65130700	1.59826000	3.06977000
C	-2.55402200	0.78989300	3.62918800
H	-1.42419600	2.56834500	3.50530500
H	-3.06327900	1.06398400	4.54870500
H	-2.80653500	-0.17095100	3.18909700
O	-2.60023100	-2.61866900	-0.83637300
O	-3.84681600	-1.48720000	1.10859800
S	-3.38483200	-1.51320200	-0.28315800
C	-1.06043000	4.35004300	1.24924700
C	-1.83734000	5.46006500	1.61802700
C	0.26043500	4.27489300	1.72132000
C	-1.32287200	6.45273700	2.45158200
H	-2.86000100	5.54134500	1.25774300
C	0.77420000	5.26551900	2.55702000
H	0.90301600	3.45671000	1.41943000
C	-0.01478100	6.35560000	2.92895200
H	-1.94450400	7.29877200	2.72818100
H	1.79785400	5.18751100	2.91065200
H	0.38789800	7.12526500	3.58008300
C	-4.79227600	-1.23594400	-1.34542600

C	-4.73009500	-1.63582900	-2.68333600
C	-5.90862300	-0.56246900	-0.84171700
C	-5.80443000	-1.34945400	-3.52248000
H	-3.86561700	-2.18144100	-3.04580100
C	-6.97227200	-0.28756300	-1.69752800
H	-5.94759800	-0.28621800	0.20642600
C	-6.93817600	-0.67322500	-3.04664900
H	-5.76667500	-1.66279200	-4.56201400
H	-7.84769400	0.22702600	-1.31132900
C	-8.11127800	-0.40300700	-3.95527500
H	-8.81418500	-1.24455000	-3.93400900
H	-8.66187500	0.48992300	-3.64659800
H	-7.79331200	-0.26998600	-4.99310600
C	2.27883100	-2.17457800	0.43433400
C	4.06230400	-3.65386000	0.81149400
C	2.85862000	-4.06255100	1.69143500
N	1.82407000	-3.07578700	1.30473900
N	3.55525500	-2.44498800	0.12866700
C	0.54486500	-3.01722000	1.95400600
C	0.39823500	-2.20113400	3.08587900
C	-0.51473700	-3.78282200	1.44256600
C	-0.83918300	-2.20302600	3.73720900
C	-1.73203100	-3.74742300	2.12324400
C	-1.91008300	-2.97539800	3.27722700
H	-0.97042200	-1.57908100	4.61681900
H	-2.56938600	-4.31653700	1.73085900
C	4.35000400	-1.61788800	-0.73271500
C	4.36095500	-1.87696400	-2.11187000
C	5.04045100	-0.52930900	-0.17518600
C	5.10552700	-1.02640000	-2.93372600
C	5.77249300	0.29422100	-1.03561600
C	5.82143700	0.05896000	-2.41505100
H	5.12082500	-1.21038700	-4.00502100
H	6.31593800	1.13975600	-0.62010200
C	3.54084300	-3.00577400	-2.68510300
H	2.47608300	-2.85422400	-2.47331400
C	4.93543100	-0.22289700	1.29871900
H	5.21882300	-1.07937000	1.91943700
Au	1.29442100	-0.55510900	-0.34187800
H	4.32740700	-4.41938200	0.07602500
H	2.50697800	-5.07712900	1.48812900
H	3.06553600	-3.98136300	2.76289400
H	4.95705900	-3.41546100	1.39331400
H	5.57966100	0.61564500	1.57307900

H	3.90425300	0.03610100	1.56645700
H	3.81908800	-3.97328200	-2.25329000
H	3.66738500	-3.07452500	-3.76772700
C	6.64614600	0.94145000	-3.32034200
H	6.19864500	1.02522200	-4.31491500
H	6.75592500	1.94899600	-2.90878200
H	7.65436900	0.52995400	-3.44994500
C	1.52359800	-1.31333100	3.55993400
H	2.45326100	-1.86922200	3.72420400
H	1.74398100	-0.53877600	2.81539200
H	1.26062100	-0.81535400	4.49580600
C	-0.35151300	-4.56446300	0.16414500
H	-0.18892100	-3.88054400	-0.67539400
H	0.50092500	-5.25149600	0.20529900
H	-1.24939900	-5.14403100	-0.05582900
C	-3.24564200	-2.95813500	3.97737900
H	-3.21448100	-2.36379300	4.89476300
H	-4.00929300	-2.53733700	3.31566900
H	-3.56453200	-3.97165200	4.24331600

Zero-point correction=	0.919614 (Hartree/Particle)
Thermal correction to Energy=	0.975881
Thermal correction to Enthalpy=	0.976825
Thermal correction to Gibbs Free Energy=	0.823241
Sum of electronic and zero-point Energies=	-2859.834091
Sum of electronic and thermal Energies=	-2859.777824
Sum of electronic and thermal Enthalpies=	-2859.776880
Sum of electronic and thermal Free Energies=	-2859.930464

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C	2.69869300	4.07211300	-1.21590500
C	2.22857600	2.77608300	-1.10261000
C	-0.07587200	3.63461600	-1.00234300
C	0.41685500	4.93062500	-1.07703200
C	1.79283000	5.14639900	-1.19532600
H	3.76314200	4.25916700	-1.31061500
H	2.92117800	1.93938800	-1.09932800
H	-0.26712100	5.77316600	-1.05003100
H	2.16704900	6.16322900	-1.27196400
C	-1.53997600	3.31546200	-0.88073000
O	-1.77817900	2.12500800	-1.62140900
H	-2.14768200	4.11689200	-1.30571100
C	0.83011500	2.52677000	-0.99822500
C	0.31401200	1.21689800	-0.78842700
C	-1.16841100	1.09667400	-0.83566000

C	-1.75684100	-0.25143200	-1.28950700
H	-2.30721200	-0.07107900	-2.22321400
H	-1.01413300	-1.03078100	-1.45374000
N	-2.63616900	-0.62758100	-0.17563800
C	-3.11116000	0.59447100	0.47354100
H	-3.82120900	1.14152400	-0.16275900
H	-3.57782400	0.36251900	1.43013400
C	-2.02610600	2.94324300	0.57713300
H	-3.10841500	3.09012500	0.53264900
C	-1.79580400	1.39669200	0.64068500
C	-0.99835100	0.81786700	1.83903000
H	-0.86441200	-0.25246300	1.65293500
H	-0.00035500	1.26266700	1.87411500
C	-1.67804100	1.01114100	3.17273800
C	-2.38539800	0.06064100	3.78725700
H	-1.57680200	1.99038800	3.63335600
H	-2.86226400	0.23891400	4.74671700
H	-2.51294200	-0.92459200	3.34934200
O	-2.89727400	-2.94434900	-1.09081000
O	-4.28890600	-2.16376700	0.92303900
S	-3.68344000	-1.92399900	-0.38923900
C	-1.51676000	3.83097600	1.69485600
C	-2.45055900	4.59147600	2.41402400
C	-0.16360000	3.93543400	2.05774900
C	-2.05581200	5.42303100	3.46247400
H	-3.50426700	4.52471300	2.15510600
C	0.23486000	4.76242300	3.10784700
H	0.59254100	3.36493800	1.53175700
C	-0.70864400	5.50954700	3.81533200
H	-2.80084000	5.99822400	4.00368100
H	1.28612200	4.82008800	3.37435200
H	-0.39685600	6.15092600	4.63387000
C	-4.95202500	-1.33242700	-1.49597400
C	-4.77565700	-1.46469100	-2.87614000
C	-6.06603500	-0.67342700	-0.96814700
C	-5.73315400	-0.92561900	-3.73255200
H	-3.91651800	-2.00253900	-3.26202900
C	-7.01112200	-0.14198000	-1.84205600
H	-6.19485300	-0.60493300	0.10670000
C	-6.86124500	-0.25796500	-3.23266900
H	-5.60723800	-1.03087300	-4.80651400
H	-7.88443700	0.36380800	-1.43959300
C	-7.91086200	0.28835700	-4.16824600
H	-8.67723000	-0.46975300	-4.37005400

H	-8.41742300	1.15780600	-3.73992600
H	-7.47945100	0.58022100	-5.12982600
C	2.69144700	-1.93806600	0.22023900
C	4.60899700	-3.27483600	0.33224300
C	3.43574000	-3.99009500	1.04564600
N	2.35017600	-2.98621500	0.96366200
N	3.95703700	-2.05652500	-0.19780000
C	1.06634600	-3.14376800	1.59105500
C	0.90904900	-2.68281000	2.90700800
C	0.00686400	-3.71551400	0.86663600
C	-0.33489500	-2.86271900	3.51849900
C	-1.22069800	-3.86409600	1.51647400
C	-1.40434700	-3.46477200	2.84635300
H	-0.47488700	-2.51386600	4.53797100
H	-2.05659800	-4.28154100	0.96563800
C	4.62322000	-1.02203000	-0.93729400
C	4.66109700	-1.10711200	-2.33856100
C	5.13500700	0.08802500	-0.24552900
C	5.24192800	-0.05091500	-3.04511600
C	5.70438200	1.12282300	-0.99535600
C	5.77005700	1.07020300	-2.39262700
H	5.27481100	-0.09889900	-4.13063200
H	6.10849300	1.98801400	-0.47503900
C	4.04052400	-2.28264800	-3.05187100
H	2.97633500	-2.37024300	-2.80533200
C	5.01675900	0.19064500	1.25594000
H	5.38154200	-0.70984200	1.75993400
Au	1.47599400	-0.36123900	-0.27454000
H	5.03641400	-3.86643800	-0.48079100
H	3.12598300	-4.90711500	0.53508800
H	3.65168800	-4.23317100	2.08865200
H	5.41674400	-2.99831700	1.01764900
H	5.58559900	1.04156600	1.63742200
H	3.96990500	0.32017600	1.55668900
H	4.51462900	-3.22790800	-2.76561800
H	4.13229900	-2.17950300	-4.13514600
C	6.41735700	2.18324700	-3.18077700
H	5.89794400	2.35815800	-4.12771200
H	6.43119500	3.12141900	-2.61825800
H	7.45721700	1.93345200	-3.42265600
C	2.03363700	-1.97049700	3.61882500
H	2.94808100	-2.57271700	3.66073300
H	2.29013900	-1.03683600	3.10378000
H	1.75204900	-1.72170900	4.64429600

C	0.17796500	-4.13123300	-0.57421900
H	0.62702700	-3.32623400	-1.16714400
H	0.83336100	-5.00582500	-0.66860000
H	-0.78819600	-4.37172700	-1.01920400
C	-2.73606100	-3.67822300	3.52275200
H	-2.76987100	-3.20101300	4.50604100
H	-3.54750400	-3.27896700	2.90743100
H	-2.92913700	-4.74767100	3.66517700

Zero-point correction= 0.922773 (Hartree/Particle)

Thermal correction to Energy= 0.978476

Thermal correction to Enthalpy= 0.979420

Thermal correction to Gibbs Free Energy= 0.828089

Sum of electronic and zero-point Energies= -2859.851423

Sum of electronic and thermal Energies= -2859.795720

Sum of electronic and thermal Enthalpies= -2859.794776

Sum of electronic and thermal Free Energies= -2859.946107

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C	-2.13976300	4.29311800	-0.00326000
C	-1.73169100	3.03827700	-0.43964200
C	0.35798100	3.29749600	0.77028700
C	-0.07616400	4.53551300	1.23933400
C	-1.31506400	5.04212000	0.84443800
H	-3.11137400	4.67594100	-0.29703500
H	-2.39127100	2.44263500	-1.06319100
H	0.56197800	5.10923000	1.90517400
H	-1.64387000	6.01134500	1.20659000
C	1.68640700	2.70553900	1.15782600
O	1.53323700	1.28008500	1.28512900
H	2.01466100	3.08754500	2.12681000
C	-0.46942800	2.52658500	-0.07869900
C	-0.03665200	1.17066800	-0.46499000
C	1.40736100	0.81307400	-0.07038300
C	1.75074200	-0.68801200	-0.12390700
H	1.78833300	-1.06746900	0.90601300
H	1.03167000	-1.28340600	-0.68656600
N	3.05934500	-0.72986900	-0.80017100
C	3.73900600	0.54791900	-0.58325700
H	4.13063400	0.62761400	0.44150800
H	4.56126800	0.66914500	-1.29048200
C	2.81369400	2.84456000	0.07557800
H	3.73789700	2.67013600	0.63269600
C	2.58844900	1.55526400	-0.79281800
C	2.31349300	1.71643500	-2.31154700

H	2.89692300	2.55433500	-2.70157500
H	2.64957500	0.79791100	-2.80150100
C	0.86064700	1.91265700	-2.59937900
C	-0.01586400	0.88334500	-2.74401300
H	0.48095800	2.92737700	-2.65494300
H	-1.05661600	1.05900400	-2.98991000
H	0.32434100	-0.14776700	-2.77610000
O	3.03063900	-3.22530300	-1.06785300
O	5.18958000	-1.88460800	-1.45440400
S	3.96179300	-2.15182900	-0.70686800
C	3.01080400	4.17089300	-0.63226000
C	4.30100000	4.72465100	-0.63102900
C	2.00249500	4.86515200	-1.32131400
C	4.57967800	5.92322300	-1.28815800
H	5.10145700	4.20819400	-0.10695600
C	2.27644900	6.06471200	-1.97951300
H	0.98788200	4.48937200	-1.33359800
C	3.56544000	6.59936400	-1.96670800
H	5.58742600	6.32676800	-1.26766200
H	1.47687800	6.58293600	-2.50069600
H	3.77623900	7.53309000	-2.47880500
C	4.36762600	-2.33403400	1.02228500
C	3.48480600	-3.00892400	1.87026000
C	5.52847400	-1.73454400	1.51920900
C	3.77258000	-3.07615400	3.23157500
H	2.60237200	-3.48788700	1.46013300
C	5.79827900	-1.81373800	2.88332100
H	6.21470300	-1.24139600	0.83909100
C	4.92843300	-2.48150200	3.75911300
H	3.09385100	-3.60486800	3.89520200
H	6.70350300	-1.35792900	3.27485500
C	5.25241900	-2.59128300	5.22826500
H	5.89565800	-3.45946800	5.41585400
H	5.78665200	-1.70733300	5.58814600
H	4.34913300	-2.71652000	5.83168000
C	-3.00972300	-1.59759800	0.10855400
C	-5.03060900	-2.42763600	0.94804600
C	-4.21497700	-3.58814800	0.32350100
N	-3.00709900	-2.89766900	-0.18178400
N	-4.12969100	-1.26938200	0.75974600
C	-1.94211700	-3.53676700	-0.90383400
C	-2.04769000	-3.65380100	-2.29730900
C	-0.79536700	-3.95174200	-0.20531700
C	-0.97269700	-4.22125600	-2.98973500

C	0.25183800	-4.50986500	-0.93862300
C	0.18312600	-4.65346600	-2.33139600
H	-1.03665500	-4.31847700	-4.07054900
H	1.15820200	-4.81309700	-0.42496000
C	-4.41936400	0.07773100	1.16512200
C	-3.93391900	0.53246700	2.40266700
C	-5.09622300	0.92475000	0.27484600
C	-4.15831800	1.86743500	2.74362300
C	-5.29792400	2.25441600	0.65997300
C	-4.83574700	2.74318800	1.88608800
H	-3.78596000	2.23739800	3.69571300
H	-5.82275500	2.92374800	-0.01722800
C	-3.13754900	-0.38221200	3.29989800
H	-2.16669900	-0.61411700	2.84572900
C	-5.54519900	0.42642500	-1.07722200
H	-6.28370000	-0.37868600	-0.99359900
Au	-1.52149300	-0.26243200	-0.29722900
H	-5.23788100	-2.57759500	2.01109300
H	-3.92932600	-4.34815800	1.05678200
H	-4.73975700	-4.08371200	-0.49696700
H	-5.98099200	-2.25381100	0.43512300
H	-6.00041900	1.22952700	-1.66120500
H	-4.69938400	0.02637700	-1.64857200
H	-3.64747400	-1.33576400	3.47177200
H	-2.95316000	0.08215300	4.27106500
C	-5.02630000	4.18900000	2.27459800
H	-5.68929400	4.71159300	1.57994800
H	-5.45125800	4.27835300	3.27947000
H	-4.06363300	4.71376800	2.28194600
C	-3.26685900	-3.14472000	-3.02774800
H	-4.16967300	-3.70646300	-2.76125400
H	-3.46099000	-2.09293800	-2.78753400
H	-3.13835100	-3.22742300	-4.10924400
C	-0.67483200	-3.73870800	1.28460600
H	-0.54690000	-2.67431600	1.51867800
H	-1.56466600	-4.07803800	1.82495600
H	0.18641500	-4.27818200	1.68634600
C	1.34402200	-5.24888100	-3.08726600
H	1.17459900	-5.23207400	-4.16705500
H	2.26211300	-4.69754100	-2.86433100
H	1.50922100	-6.29056900	-2.78954400

Zero-point correction= 0.922757 (Hartree/Particle)

Thermal correction to Energy= 0.977527

Thermal correction to Enthalpy= 0.978471

Thermal correction to Gibbs Free Energy=	0.828894
Sum of electronic and zero-point Energies=	-2859.831104
Sum of electronic and thermal Energies=	-2859.776334
Sum of electronic and thermal Enthalpies=	-2859.775390
Sum of electronic and thermal Free Energies=	-2859.924967

B-2a

C	-3.47029700	3.23757900	-0.53330700
C	-2.59084200	2.29084000	-1.06128400
C	-0.87889100	3.01982700	0.49422400
C	-1.76877400	3.95554600	1.02060400
C	-3.05928100	4.07582500	0.50346100
H	-4.47713900	3.31289900	-0.93066800
H	-2.92059500	1.64844300	-1.87329900
H	-1.44144300	4.60477200	1.82821100
H	-3.74220400	4.81314500	0.91188000
C	0.52547700	2.84653200	1.02229300
O	0.78133800	1.42788800	1.06525000
H	0.58975400	3.22344400	2.04538900
C	-1.29196400	2.17614900	-0.55464300
C	-0.20021600	1.33899700	-1.18061300
C	1.07057000	1.09697000	-0.28217900
C	1.82215700	-0.25150300	-0.29782900
H	1.87483400	-0.60754000	0.73992800
H	1.38391100	-1.04128600	-0.90793200
N	3.14523500	0.11050100	-0.84037800
C	3.44212700	1.51098400	-0.49829100
H	3.72399200	1.61784800	0.55989300
H	4.25444000	1.88279000	-1.12467100
C	1.73681100	3.38455900	0.16508800
H	2.55596800	3.43472900	0.88805300
C	2.08399000	2.16835500	-0.77606200
C	1.81367800	2.29998500	-2.29074100
H	2.03157500	3.30425400	-2.65824100
H	2.44299200	1.59194200	-2.83713300
C	0.33225700	1.98314700	-2.47102600
C	-0.20933700	0.61274300	-2.62954000
H	-0.29905000	2.76786500	-2.87447700
H	-1.13556300	0.51422100	-3.18911700
H	0.49456100	-0.20459600	-2.75851200
O	3.77620600	-2.29724800	-1.14433800
O	5.51713300	-0.43235000	-1.46563600
S	4.38838100	-1.02324700	-0.74992000
C	1.63656400	4.76104800	-0.45764900

C	2.69490100	5.65967800	-0.25254500
C	0.56310700	5.18126800	-1.26004800
C	2.68827300	6.93174600	-0.82480200
H	3.53763900	5.35774700	0.36476500
C	0.55187900	6.45413500	-1.83209600
H	-0.28060900	4.52597200	-1.43254600
C	1.61346200	7.33443600	-1.61840200
H	3.52044600	7.60649900	-0.64814400
H	-0.29185100	6.75725700	-2.44516800
H	1.60244300	8.32411400	-2.06460300
C	4.80419800	-1.11612900	0.98483200
C	4.10940400	-2.00077500	1.81231000
C	5.76661600	-0.24662400	1.50651800
C	4.38315300	-2.00988700	3.17821000
H	3.38579300	-2.68111200	1.38020300
C	6.02705200	-0.27096800	2.87434700
H	6.31263200	0.41457300	0.84231000
C	5.34233100	-1.14819500	3.73009900
H	3.85166000	-2.70189800	3.82585400
H	6.78037200	0.39533000	3.28550700
C	5.66277800	-1.18699700	5.20368000
H	6.54236800	-1.81497100	5.38934100
H	5.88984100	-0.18906000	5.59010600
H	4.83498200	-1.60081900	5.78593000
C	-2.37725500	-2.18011100	0.19391900
C	-3.80934400	-3.29169000	1.64937300
C	-2.95159700	-4.32606200	0.88726300
N	-2.01998200	-3.46217300	0.12886200
N	-3.43684800	-2.01740400	0.98961600
C	-0.87128600	-3.92552800	-0.59948700
C	-1.00367100	-4.26062100	-1.95381900
C	0.36903500	-3.94304500	0.06122300
C	0.15590200	-4.61766300	-2.65100200
C	1.49483600	-4.31241800	-0.67340400
C	1.41084700	-4.64306500	-2.03337200
H	0.07685400	-4.87326800	-3.70447000
H	2.46896700	-4.31043400	-0.19593900
C	-3.98077800	-0.74758200	1.38557300
C	-3.27229700	0.06434400	2.28773000
C	-5.21706900	-0.35539200	0.84132800
C	-3.84762700	1.28721300	2.64925000
C	-5.74793300	0.87241900	1.23709200
C	-5.08129500	1.70388800	2.14596400
H	-3.30879500	1.93261700	3.33780100

H	-6.70127700	1.19154700	0.82311200
C	-1.91588600	-0.31127700	2.83723000
H	-1.11601500	0.16664200	2.25756800
C	-5.93668200	-1.22722200	-0.15915200
H	-6.36530900	-2.12002700	0.31183900
Au	-1.41627000	-0.70666000	-0.73580200
H	-3.55690400	-3.23114500	2.71366900
H	-2.39803900	-4.99788300	1.54647600
H	-3.54087000	-4.93086400	0.19083400
H	-4.88136600	-3.47324300	1.55697500
H	-6.75943400	-0.68414800	-0.62927000
H	-5.25952800	-1.57195300	-0.94765800
H	-1.73734700	-1.38928000	2.81768500
H	-1.81465300	0.02822900	3.87187300
C	-5.69547300	3.01111300	2.58165900
H	-6.43747400	2.84749500	3.37205800
H	-4.94050400	3.69686400	2.97477900
H	-6.21069000	3.50667000	1.75294600
C	-2.34617000	-4.19549300	-2.64044600
H	-3.06386400	-4.89583000	-2.19815600
H	-2.78356900	-3.19314000	-2.56181800
H	-2.25671900	-4.44242900	-3.70048400
C	0.48111300	-3.50764900	1.50303900
H	0.33924700	-2.42381200	1.59839300
H	-0.26972300	-3.98459000	2.14151500
H	1.46294300	-3.75619700	1.91082800
C	2.66093600	-4.99765100	-2.79762500
H	2.45420000	-5.16355100	-3.85791700
H	3.39831600	-4.19478000	-2.70232400
H	3.11786500	-5.90943400	-2.39669300

Zero-point correction=	0.925515 (Hartree/Particle)
Thermal correction to Energy=	0.979877
Thermal correction to Enthalpy=	0.980821
Thermal correction to Gibbs Free Energy=	0.833083
Sum of electronic and zero-point Energies=	-2859.856299
Sum of electronic and thermal Energies=	-2859.801938
Sum of electronic and thermal Enthalpies=	-2859.800994
Sum of electronic and thermal Free Energies=	-2859.948731

2a

S	3.17136700	0.37703000	-1.81587700
O	-0.24612400	-1.13833500	0.92160700
N	1.54645300	0.19533000	-1.44991000
O	3.51661100	-0.74986700	-2.68611800

O	3.34349200	1.77330100	-2.22414100
C	-1.61196000	-1.46797100	-1.11283200
C	-2.56609400	-2.05087000	-0.13370100
C	-0.32176400	-0.86772900	-0.47420800
C	-0.55061400	0.66754200	-0.56944400
C	-2.18282900	-0.37805900	-2.03303800
H	-3.26118700	-0.25951500	-2.05764900
C	-2.56773600	-1.43855400	1.13896700
C	-1.32614800	0.93634900	0.77981500
H	-0.61832600	1.46532900	1.42558500
C	-2.56098800	1.80885200	0.70461800
C	-1.42011000	-0.49590700	1.44457400
H	-1.29866500	-0.40850300	2.52748200
C	1.05987300	-1.15378400	-1.07641400
H	1.68002900	-1.62117400	-0.30148700
H	1.05357800	-1.79533900	-1.95581700
C	-1.33025100	0.87775600	-1.88426200
H	-1.95062700	1.77591600	-1.84887700
H	-0.62204500	0.99023000	-2.71179000
C	4.03218700	0.15250400	-0.26027100
C	-2.41766000	3.18139200	0.96247200
H	-1.44043400	3.56892600	1.24098400
C	-3.83345700	1.33807600	0.34758200
H	-3.98576700	0.28580600	0.14915100
C	-1.63425800	-1.65714700	-2.60526800
H	-2.34757900	-2.35902300	-3.02760100
H	-0.68793500	-1.62584500	-3.13798400
C	0.87947900	1.21931800	-0.62244500
H	0.97005400	2.19432100	-1.10358900
H	1.31760900	1.26982000	0.38570300
C	-4.91945900	2.21022900	0.25646500
H	-5.89540700	1.81909900	-0.01663600
C	-3.51520900	-3.03119800	-0.42269800
H	-3.51160600	-3.51690800	-1.39400500
C	-3.51752900	-1.80709800	2.08795600
H	-3.50451400	-1.33890300	3.06909000
C	-3.49849800	4.05660600	0.86542500
H	-3.35654100	5.11391000	1.06985300
C	-4.75858100	3.57207300	0.51190200
H	-5.60530700	4.24808700	0.43819500
C	4.43989100	-1.12685500	0.12505600
H	4.31301100	-1.95863600	-0.55897300
C	-4.48302700	-2.77061400	1.78236500
H	-5.22665500	-3.04835900	2.52314000

C	-4.47510100	-3.38522200	0.53024200
H	-5.21303500	-4.14609700	0.29323200
C	5.03658500	-1.30164100	1.37143900
H	5.36475600	-2.29323200	1.67119600
C	4.22116700	1.24966100	0.58313000
H	3.92756800	2.23903600	0.24992600
C	5.22909800	-0.21943700	2.24193800
C	4.81972600	1.05528700	1.82595600
H	4.97936300	1.90782300	2.48053400
C	5.84616100	-0.42831400	3.60320700
H	5.08228800	-0.71709400	4.33558600
H	6.32532000	0.48309300	3.97162200
H	6.59581600	-1.22482800	3.58457600

Zero-point correction= 0.499814 (Hartree/Particle)
Thermal correction to Energy= 0.526597
Thermal correction to Enthalpy= 0.527541
Thermal correction to Gibbs Free Energy= 0.441799
Sum of electronic and zero-point Energies= -1799.470324
Sum of electronic and thermal Energies= -1799.443541
Sum of electronic and thermal Enthalpies= -1799.442597
Sum of electronic and thermal Free Energies= -1799.528340

B-TSb1

C	1.59247500	4.58559800	-1.21592900
C	1.41317200	3.22642200	-1.01924300
C	-0.98496100	3.53890800	-1.24316900
C	-0.79743700	4.91998000	-1.42268700
C	0.48813600	5.43756600	-1.41941200
H	2.59655800	4.99890800	-1.20930500
H	2.26990200	2.57938800	-0.86036600
H	-1.65561300	5.56907600	-1.57529900
H	0.64553900	6.50024300	-1.57428700
C	-2.30198900	2.94499400	-1.14783800
O	-2.42235800	1.64560100	-1.51777500
H	-3.16094000	3.51475800	-1.49243400
C	0.11386500	2.66821800	-1.03127900
C	-0.14125400	1.25147600	-0.84749800
C	-1.40712500	0.79951000	-1.17350500
C	-1.79498900	-0.63774600	-1.43302900
H	-2.11385300	-0.71974800	-2.47613200
H	-0.91509600	-1.27364300	-1.30520700
N	-2.86271400	-1.14130300	-0.57754400
C	-2.48469800	-1.69462800	0.73152400
H	-3.38842700	-2.12108200	1.17745800

H	-1.77867400	-2.51873000	0.59644500
C	-0.74062500	-0.88845500	2.29010000
H	-0.21276000	-1.80063100	2.01852000
C	-1.90068300	-0.64984000	1.65473000
C	-2.71069000	0.62763400	1.74695100
H	-3.62366300	0.53627300	1.15345600
H	-3.05495400	0.79823200	2.77846100
C	-1.99899500	1.87936600	1.34510900
C	-2.68689000	2.94996700	0.76978500
H	-0.96781500	1.99743800	1.66204600
H	-2.31919200	3.95397800	0.96067500
H	-3.77209000	2.85717500	0.72364000
O	-4.24257700	-1.38862600	-2.68836600
O	-4.83048600	-2.74864900	-0.59086000
S	-4.37198200	-1.51191200	-1.23412500
C	-0.05621900	-0.03175300	3.28031900
C	1.33671200	0.14339200	3.19568500
C	-0.73908900	0.60043900	4.33377000
C	2.01383800	0.96020600	4.09974400
H	1.88114200	-0.35398900	2.39914700
C	-0.06194300	1.41064300	5.24446800
H	-1.80253700	0.42735800	4.46285600
C	1.31615900	1.60292100	5.12486200
H	3.08754900	1.08871200	4.00913700
H	-0.60918400	1.88241200	6.05524600
H	1.84345300	2.23409200	5.83362300
C	-5.42477100	-0.18383100	-0.65639700
C	-5.46946100	1.01109600	-1.37763100
C	-6.11332900	-0.32605900	0.54994300
C	-6.19777100	2.08199100	-0.86401700
H	-4.94359000	1.08915700	-2.32185900
C	-6.83426300	0.75781700	1.04926400
H	-6.08934400	-1.27395900	1.07665500
C	-6.88512700	1.97676200	0.35678000
H	-6.25236000	3.01048100	-1.42694200
H	-7.37446400	0.65293700	1.98603500
C	-7.70104500	3.13054100	0.88526300
H	-7.29826000	4.09338500	0.55785700
H	-8.73341300	3.06874000	0.52090700
H	-7.74139100	3.12764200	1.97817800
C	2.89055600	-1.45186600	-0.25559900
C	4.07496600	-3.47782300	-0.20221000
C	5.08003500	-2.30320300	-0.25583800
N	4.18873000	-1.12368700	-0.29226000

N	2.76756300	-2.78302200	-0.18235600
C	4.64952400	0.22918600	-0.42833900
C	5.06855500	0.92831400	0.71659700
C	4.61214400	0.83618100	-1.69465500
C	5.42186300	2.27202100	0.57428600
C	4.97687800	2.18375600	-1.78746300
C	5.37577900	2.91909900	-0.66689100
H	5.73441900	2.82983800	1.45365600
H	4.94500000	2.66958800	-2.75947700
C	1.51174900	-3.47784600	-0.20883600
C	0.99327700	-4.00194800	0.98593800
C	0.82747000	-3.60984300	-1.43236800
C	-0.24397400	-4.65549700	0.93708800
C	-0.41137800	-4.25649600	-1.42695400
C	-0.96759000	-4.78429600	-0.25419600
H	-0.65996600	-5.05823000	1.85706200
H	-0.95705600	-4.35633800	-2.36206200
C	1.73506400	-3.85494900	2.29305600
H	2.17588400	-2.85879200	2.39590400
C	1.39582500	-3.05315900	-2.71611700
H	2.47057800	-3.24084500	-2.80176900
Au	1.35527200	-0.09838600	-0.44081200
H	4.19168700	-4.09373200	0.69298500
H	5.72875400	-2.26258300	0.62345600
H	5.71297600	-2.32273600	-1.14788000
H	4.13452200	-4.13073300	-1.07818600
H	0.90278300	-3.49712000	-3.58382000
H	1.26010500	-1.96654400	-2.77124000
H	2.55007900	-4.58398000	2.37701100
H	1.06722200	-4.01830500	3.14212300
C	-2.33300100	-5.42637300	-0.27971400
H	-2.53017000	-5.98924600	0.63638700
H	-3.11889700	-4.66808400	-0.38532300
H	-2.43122800	-6.11106100	-1.12785900
C	5.13011600	0.25066800	2.06317800
H	4.23485200	-0.34783900	2.25509400
H	5.99172500	-0.42434700	2.13106700
H	5.23359000	0.98438800	2.86580200
C	4.14804500	0.08102600	-2.91652700
H	4.53594900	-0.94188600	-2.93752400
H	3.05430900	0.00773900	-2.93843000
H	4.46918300	0.58484600	-3.83114800
C	5.77541500	4.36996700	-0.79081500
H	5.42207300	4.95559700	0.06378000

H	6.86644200	4.47352000	-0.82345400
H	5.37827400	4.82049600	-1.70508800

Zero-point correction= 0.920440 (Hartree/Particle)

Thermal correction to Energy= 0.976176

Thermal correction to Enthalpy= 0.977120

Thermal correction to Gibbs Free Energy= 0.826486

Sum of electronic and zero-point Energies= -2859.838076

Sum of electronic and thermal Energies= -2859.782340

Sum of electronic and thermal Enthalpies= -2859.781396

Sum of electronic and thermal Free Energies= -2859.932030

B-1b

C	-1.53391100	-4.62152100	-1.37051200
C	-1.37450600	-3.27311500	-1.10079700
C	1.05824700	-3.59767400	-0.95122300
C	0.87925700	-4.95179400	-1.19804100
C	-0.40749800	-5.45800100	-1.41489400
H	-2.52430800	-5.03112300	-1.53899200
H	-2.24045400	-2.61937300	-1.05144100
H	1.73808700	-5.61569700	-1.23714500
H	-0.53431200	-6.51614200	-1.62560100
C	2.40259100	-2.97897300	-0.66961300
O	2.42190700	-1.66911100	-1.22558400
H	3.21824700	-3.55278200	-1.11479400
C	-0.07694400	-2.72990700	-0.88650300
C	0.11285900	-1.35631900	-0.55379300
C	1.53999600	-0.90224200	-0.40130800
C	1.73255600	0.58088700	-0.80488800
H	1.75626200	0.60772900	-1.89599700
H	0.86651700	1.16357300	-0.48580500
N	2.90936400	1.24183500	-0.28181900
C	2.78622300	1.90940400	1.02663900
H	3.79210400	2.14904200	1.38261700
H	2.23801600	2.85000900	0.92496500
C	0.94326300	1.31980900	2.58225700
H	0.53808500	2.30521200	2.35458200
C	2.09083800	0.96804600	1.97549500
C	2.69034700	-0.41672800	1.96447300
H	3.71079300	-0.37221500	1.57570600
H	2.74543000	-0.86048800	2.96019800
C	1.85998200	-1.38975900	1.09608100
C	2.59555300	-2.72466100	0.84623800
H	0.91648200	-1.55070000	1.62769400
H	2.23037300	-3.54489400	1.46792700

H	3.66672400	-2.59609900	1.02627800
O	3.90252900	1.24082300	-2.60643700
O	4.93858700	2.65344200	-0.72793400
S	4.29758600	1.42319100	-1.20755200
C	0.11887600	0.47682400	3.47369400
C	-1.27154300	0.41138900	3.27072300
C	0.66915700	-0.26573400	4.53189300
C	-2.07391600	-0.41041700	4.06092900
H	-1.71770300	1.00375000	2.47657100
C	-0.13379000	-1.08208200	5.32876300
H	1.72818000	-0.17566500	4.75096500
C	-1.50674400	-1.16688500	5.08939800
H	-3.14289900	-0.45538700	3.88086100
H	0.31212500	-1.64260500	6.14510300
H	-2.13176500	-1.80184700	5.70989600
C	5.35089500	0.05425300	-0.73826700
C	5.31329600	-1.12809900	-1.47774000
C	6.13633700	0.16202100	0.41260500
C	6.05585900	-2.22231200	-1.03744200
H	4.70477500	-1.18206800	-2.37167500
C	6.86552700	-0.94530400	0.84117600
H	6.18619300	1.10348400	0.94912000
C	6.83376500	-2.15404000	0.12866000
H	6.04245800	-3.14282600	-1.61566400
H	7.47833400	-0.86725500	1.73502900
C	7.65798000	-3.33472300	0.57956700
H	7.22550900	-4.28096600	0.24195800
H	8.67298500	-3.27500300	0.16882200
H	7.75034900	-3.36785300	1.66903800
C	-2.87409600	1.40889600	-0.41944000
C	-3.94257000	3.46619400	-0.74809500
C	-5.00758500	2.34609800	-0.68288200
N	-4.17867700	1.13172800	-0.51809900
N	-2.67933300	2.72759700	-0.51292000
C	-4.69374500	-0.20855500	-0.51344600
C	-5.17821700	-0.75305400	0.68717100
C	-4.63602900	-0.95847000	-1.70004600
C	-5.59825300	-2.08548900	0.68124300
C	-5.06696700	-2.28869500	-1.65662400
C	-5.54847300	-2.86960800	-0.47788100
H	-5.96766200	-2.52459100	1.60463600
H	-5.02886300	-2.88240100	-2.56678900
C	-1.39003900	3.36183500	-0.56021500
C	-0.93634600	4.06727800	0.56568700

C	-0.61881700	3.26940500	-1.73592700
C	0.31943600	4.68138500	0.49472100
C	0.63628300	3.88267700	-1.74946400
C	1.12308100	4.59907400	-0.64855900
H	0.68089700	5.23374400	1.35855000
H	1.25152800	3.80247400	-2.64203000
C	-1.77272800	4.17457300	1.81848300
H	-2.31964200	3.24972700	2.02275100
C	-1.10515800	2.51193600	-2.94851500
H	-2.17869700	2.64254300	-3.11393000
Au	-1.39193100	-0.02179800	-0.31321600
H	-4.08262700	4.23096500	0.01934300
H	-5.68569400	2.45758600	0.16785200
H	-5.60821900	2.27205500	-1.59353600
H	-3.90156800	3.96059800	-1.72355000
H	-0.57878400	2.84135300	-3.84699500
H	-0.92939400	1.43506200	-2.83771800
H	-2.51189000	4.98118900	1.73746900
H	-1.14922000	4.39763100	2.68775500
C	2.48861700	5.23851900	-0.69945400
H	2.66605900	5.87664900	0.17017300
H	3.27906900	4.47950300	-0.73158400
H	2.59813400	5.85294300	-1.59892200
C	-5.22837500	0.07490400	1.94711100
H	-4.29438300	0.62427700	2.09992900
H	-6.03770900	0.81378500	1.90959600
H	-5.40576900	-0.55356700	2.82277500
C	-4.08237200	-0.36517300	-2.97274500
H	-4.50331600	0.62401600	-3.17900600
H	-2.99518300	-0.24058100	-2.90696000
H	-4.29626600	-1.00755300	-3.82981100
C	-6.03269200	-4.29932800	-0.45888200
H	-5.76745800	-4.79926400	0.47757000
H	-7.12450900	-4.34085700	-0.55038000
H	-5.61496800	-4.87794900	-1.28790500

Zero-point correction= 0.924474 (Hartree/Particle)

Thermal correction to Energy= 0.979543

Thermal correction to Enthalpy= 0.980487

Thermal correction to Gibbs Free Energy= 0.830693

Sum of electronic and zero-point Energies= -2859.864290

Sum of electronic and thermal Energies= -2859.809221

Sum of electronic and thermal Enthalpies= -2859.808277

Sum of electronic and thermal Free Energies= -2859.958072

B-TSb2

C	-1.60963900	-4.55131600	-1.27955000
C	-1.35154600	-3.25966000	-0.81912900
C	1.02347400	-3.65225200	-1.11320400
C	0.76357300	-4.94116800	-1.56940300
C	-0.55732000	-5.39050800	-1.65498900
H	-2.63610900	-4.89876400	-1.34536100
H	-2.17470600	-2.61270200	-0.53345300
H	1.58555900	-5.59116700	-1.85675100
H	-0.76374900	-6.39403800	-2.01419600
C	2.39332500	-3.06095600	-0.93780000
O	2.40445700	-1.76911300	-1.58338100
H	3.18987200	-3.66335300	-1.37637800
C	-0.03181100	-2.79799100	-0.74324900
C	0.29784100	-1.40412100	-0.29713500
C	1.70691500	-0.90108000	-0.71551200
C	1.91897600	0.55528900	-1.13966100
H	2.27561500	0.55771100	-2.17064100
H	0.97259600	1.09856100	-1.11722000
N	2.86005900	1.27128400	-0.29637100
C	2.37283600	1.86771000	0.95354300
H	3.24540400	2.24539200	1.49435700
H	1.73811900	2.72887200	0.72940500
C	0.49487400	1.27413300	2.45591700
H	0.11550700	2.26599200	2.21375800
C	1.61876300	0.88665100	1.82473300
C	2.21118600	-0.49780600	1.90605300
H	3.30724900	-0.43394300	1.93426900
H	1.89862600	-1.03461200	2.80171600
C	1.92803400	-1.37587300	0.68980900
C	2.63248100	-2.70888600	0.55034700
H	0.57278200	-1.55066600	0.91531200
H	2.29042200	-3.47854500	1.24596300
H	3.69603600	-2.51300300	0.72748500
O	4.40062300	1.57163000	-2.28210700
O	4.97107500	2.60511300	-0.00158900
S	4.43820900	1.51051100	-0.81967000
C	-0.31193000	0.50435400	3.42722800
C	-1.70949400	0.45175700	3.28098900
C	0.26593600	-0.15136800	4.52805900
C	-2.49610900	-0.27715800	4.17101200
H	-2.17383100	0.97742700	2.45215300
C	-0.52128700	-0.87649700	5.42306000
H	1.33372500	-0.05984600	4.70357500

C	-1.90361400	-0.95143100	5.24144200
H	-3.57202000	-0.31246500	4.03379600
H	-0.05591400	-1.37061600	6.27066500
H	-2.51607600	-1.51449600	5.93890900
C	5.29956500	0.00693500	-0.36267700
C	5.39445000	-1.03599400	-1.28440700
C	5.80531000	-0.12543300	0.93374600
C	5.99724700	-2.23084200	-0.89190400
H	5.00242900	-0.90851400	-2.28596000
C	6.39271700	-1.33130500	1.31161300
H	5.75743200	0.71245900	1.62171000
C	6.49961600	-2.40144700	0.40706100
H	6.08729600	-3.04154600	-1.61004800
H	6.79282700	-1.43891800	2.31608500
C	7.18160700	-3.68483800	0.81189200
H	7.03133800	-3.90323600	1.87314400
H	6.81824200	-4.53618600	0.22954300
H	8.26291600	-3.61309100	0.64483800
C	-2.72218800	1.40219900	-0.52425400
C	-3.83847100	3.39807000	-1.04439500
C	-4.85894400	2.23720900	-1.01559800
N	-4.01324600	1.07618600	-0.66025500
N	-2.56345800	2.71632200	-0.72249600
C	-4.50445000	-0.27237700	-0.61492300
C	-5.13701600	-0.73048900	0.55340500
C	-4.32184900	-1.10277000	-1.73382800
C	-5.55749500	-2.06185700	0.59396000
C	-4.76564300	-2.42661600	-1.64689600
C	-5.37238400	-2.92776900	-0.49094100
H	-6.04027000	-2.43346900	1.49433700
H	-4.62857600	-3.08152900	-2.50369500
C	-1.29631900	3.39197300	-0.74586700
C	-0.91179900	4.16797600	0.35930200
C	-0.47600600	3.26700800	-1.88334600
C	0.33062200	4.81080500	0.31159000
C	0.76640200	3.90772300	-1.87273700
C	1.19119600	4.68241100	-0.78596200
H	0.64251100	5.41136200	1.16247400
H	1.42211100	3.79930200	-2.73278900
C	-1.80332000	4.30618600	1.57033500
H	-2.30205400	3.36349000	1.81438700
C	-0.90814300	2.45135700	-3.07908500
H	-1.94596400	2.65894500	-3.35882100
Au	-1.22728500	0.04831100	-0.21326400

H	-4.05252200	4.16791900	-0.29861600
H	-5.64208200	2.37942300	-0.26643000
H	-5.33828500	2.06509900	-1.98398500
H	-3.76450800	3.87951300	-2.02367300
H	-0.27542400	2.66542400	-3.94306200
H	-0.84592700	1.37580600	-2.87661900
H	-2.58548200	5.05801500	1.40935000
H	-1.23005300	4.62303400	2.44504400
C	2.56433100	5.30680500	-0.77955000
H	2.62233600	6.14388500	-0.07873100
H	3.32354400	4.57112500	-0.48525500
H	2.83992900	5.67124200	-1.77328800
C	-5.36589300	0.18880100	1.72786400
H	-4.48674700	0.80539300	1.93585600
H	-6.20404500	0.87129800	1.54165400
H	-5.60935700	-0.37998100	2.62815000
C	-3.62836100	-0.61094100	-2.98124200
H	-3.89659900	0.42147900	-3.22357800
H	-2.53890800	-0.63712200	-2.85702200
H	-3.88037700	-1.23807500	-3.83942200
C	-5.79357400	-4.37467500	-0.40139100
H	-5.01988200	-4.97312900	0.09573200
H	-6.71286600	-4.48978700	0.18009800
H	-5.96063400	-4.80729900	-1.39168400

Zero-point correction=	0.920117 (Hartree/Particle)
Thermal correction to Energy=	0.974735
Thermal correction to Enthalpy=	0.975679
Thermal correction to Gibbs Free Energy=	0.829054
Sum of electronic and zero-point Energies=	-2859.837661
Sum of electronic and thermal Energies=	-2859.783044
Sum of electronic and thermal Enthalpies=	-2859.782099
Sum of electronic and thermal Free Energies=	-2859.928725

B-2b

C	-6.35890300	1.24769200	-3.10039800
C	-5.53207700	1.37984100	-1.98066400
C	-4.75568800	-0.89164000	-2.32030600
C	-5.57321100	-1.01856500	-3.43861300
C	-6.37826100	0.05628000	-3.83012300
H	-6.99247900	2.07648600	-3.40222000
H	-5.52651400	2.30119000	-1.40469900
H	-5.58843300	-1.95019200	-3.99873000
H	-7.02229200	-0.03763700	-4.69910600
C	-3.85852800	-1.95583200	-1.74776600

O	-2.51025800	-1.40611000	-1.67247000
H	-3.81028000	-2.86456700	-2.34979800
C	-4.72470500	0.31037600	-1.58894700
C	-3.79309900	0.32942100	-0.43942700
C	-2.53252200	-0.53884800	-0.55717900
C	-1.15588400	-0.07246500	-0.14942800
H	-0.46790300	-0.25270600	-0.97655200
H	-1.14332700	0.99917000	0.04653500
N	-0.63357800	-0.70928500	1.07815600
C	-1.08834600	-0.16809900	2.38521900
H	-0.87924400	-0.92159500	3.14870500
H	-0.47494100	0.70888700	2.62203800
C	-2.90796900	1.45734500	2.68578700
H	-2.09597500	2.15938300	2.88086800
C	-2.55589300	0.19560600	2.37461500
C	-3.49436600	-0.89817700	1.90710100
H	-3.12069800	-1.86955200	2.25746500
H	-4.49284500	-0.77479200	2.32661400
C	-3.61720800	-0.95713200	0.38842000
C	-4.23234700	-2.18713500	-0.26381600
H	-3.68884900	1.26099400	0.10536800
H	-5.31466600	-2.26558700	-0.12816500
H	-3.75266700	-3.08852000	0.12678500
O	1.17555600	-1.97043200	-0.13976500
O	0.74547900	-2.37810000	2.35501500
S	0.20958400	-2.12716400	1.01914800
C	-4.25686400	2.05777900	2.72357500
C	-4.44151400	3.32215500	2.13535300
C	-5.36433700	1.43746000	3.32472300
C	-5.70055200	3.91871900	2.09113600
H	-3.58667400	3.83981300	1.70810900
C	-6.62253000	2.03784500	3.29097500
H	-5.23319000	0.49613300	3.84808600
C	-6.79911100	3.27246000	2.66260900
H	-5.82206400	4.89050200	1.62168900
H	-7.46542100	1.54429000	3.76537600
H	-7.78055600	3.73558400	2.63485100
C	-0.81448800	-3.49422600	0.52836800
C	-1.00656500	-3.79391300	-0.82119400
C	-1.43872600	-4.23019200	1.54135100
C	-1.83965100	-4.85986400	-1.15242500
H	-0.52295600	-3.20671200	-1.58987700
C	-2.27553100	-5.28282300	1.18404900
H	-1.25092300	-3.99608800	2.58348500

C	-2.48781300	-5.61562700	-0.16429700
H	-1.98875800	-5.10771400	-2.19931000
H	-2.76259800	-5.86307200	1.96225600
C	-3.36810600	-6.78167100	-0.53575900
H	-4.20569400	-6.88793900	0.15947600
H	-3.76998500	-6.67667100	-1.54692000
H	-2.79724500	-7.71742700	-0.50386500
C	3.40868500	1.48331000	-0.36387900
C	5.17140100	3.01229000	-0.34040700
C	3.85778700	3.75500500	-0.67702300
N	2.84813300	2.67606600	-0.59349300
N	4.72871700	1.60453800	-0.23083500
C	1.44880200	2.89847100	-0.82536600
C	0.93544900	2.73268800	-2.12320000
C	0.63375800	3.26446400	0.25628800
C	-0.42587200	2.97309600	-2.32376300
C	-0.71934800	3.51495400	0.00209900
C	-1.26595400	3.38223000	-1.28012300
H	-0.84283600	2.84036900	-3.31867000
H	-1.36149800	3.80724600	0.82838800
C	5.62523600	0.52097300	0.06339500
C	5.83040200	0.15362700	1.40219300
C	6.24692800	-0.14649500	-1.00291000
C	6.70853500	-0.90232200	1.65913300
C	7.11665400	-1.19532000	-0.69564500
C	7.36586700	-1.58217700	0.62694300
H	6.87903200	-1.20530700	2.68892500
H	7.60615100	-1.72779300	-1.50702700
C	5.08746400	0.84464600	2.51989500
H	4.01068300	0.64772000	2.45323400
C	5.94357000	0.23182000	-2.43217900
H	6.18933100	1.27916900	-2.64116900
Au	2.38377500	-0.20038500	-0.22669700
H	5.61221100	3.33580600	0.60700400
H	3.62177400	4.54975000	0.03489600
H	3.85843100	4.18489900	-1.68310200
H	5.92927900	3.10820300	-1.12151600
H	6.51087500	-0.38689700	-3.13056100
H	4.87771400	0.10137500	-2.65311000
H	5.21833100	1.93201500	2.49195300
H	5.43153000	0.49283000	3.49470600
C	8.33890200	-2.69455400	0.93281200
H	8.35612500	-3.44207800	0.13473000
H	9.35734200	-2.30026800	1.03370100

H	8.08953400	-3.19982600	1.86998300
C	1.82241600	2.26615500	-3.25148500
H	2.70918600	2.89910200	-3.36333200
H	2.17915600	1.24524200	-3.07100900
H	1.28472200	2.27194800	-4.20172800
C	1.19452100	3.32932900	1.65549200
H	1.62922400	2.36479200	1.94331100
H	1.98929900	4.07773600	1.74809400
H	0.41678800	3.58392000	2.37937200
C	-2.72379300	3.66285500	-1.54628500
H	-2.84601700	4.62015800	-2.06619900
H	-3.16701500	2.88833800	-2.17859600
H	-3.30254000	3.71191100	-0.62062600

Zero-point correction= 0.498425 (Hartree/Particle)
Thermal correction to Energy= 0.525968
Thermal correction to Enthalpy= 0.526912
Thermal correction to Gibbs Free Energy= 0.439742
Sum of electronic and zero-point Energies= -1799.472541
Sum of electronic and thermal Energies= -1799.444998
Sum of electronic and thermal Enthalpies= -1799.444053
Sum of electronic and thermal Free Energies= -1799.531224

3a

C	3.48371700	3.85192800	-1.01028700
C	3.17830000	2.48828000	-1.01502600
C	0.88503200	3.02698700	-0.44578400
C	1.18902100	4.38387800	-0.45054700
C	2.49486100	4.79852900	-0.73097700
H	4.49737200	4.17707500	-1.22649700
H	3.94712300	1.75022200	-1.22864600
H	0.41343800	5.11449100	-0.23395700
H	2.73973300	5.85652900	-0.73149300
C	-0.45611100	2.41311300	-0.14201900
O	-0.82231700	1.56873300	-1.26880900
H	-1.25511700	3.14358900	-0.00324500
C	1.87814100	2.07005900	-0.72891200
C	1.42486800	0.66301400	-0.72104500
C	-0.03312300	0.40351500	-1.12706800
C	-0.45540900	-0.72102300	-2.05261900
H	-1.08531100	-0.30995500	-2.84291500
H	0.41974500	-1.17208800	-2.52880300
N	-1.18171800	-1.80008500	-1.37792500
C	-0.40549400	-2.83087900	-0.66740400
H	-1.08689200	-3.34934000	0.01265300

H	-0.05153200	-3.57805700	-1.38937700
C	2.00588100	-2.70823600	-0.15343000
H	2.11520300	-3.45368200	-0.94197400
C	0.76621700	-2.25156200	0.09793200
C	0.43985900	-1.10422500	1.02892000
H	-0.53310100	-1.28853600	1.50164700
H	1.17663600	-1.01967800	1.82989900
C	0.35853600	0.23649900	0.30885500
C	-0.29148700	1.41052800	1.02420500
H	2.14635500	-0.09736400	-1.00017700
H	0.31804200	1.82810400	1.83126900
H	-1.26067400	1.10515200	1.42440300
O	-3.33123800	-1.17433900	-2.53766200
O	-3.26087100	-3.09204200	-0.82879600
S	-2.85005000	-1.75833100	-1.28260300
C	3.27486400	-2.26786300	0.46814000
C	4.34138800	-1.88135300	-0.36140400
C	3.46659200	-2.23420200	1.85814000
C	5.54567700	-1.43526100	0.18057200
H	4.21498500	-1.92132600	-1.44040200
C	4.67324600	-1.79392700	2.40166200
H	2.67029800	-2.57572300	2.51217100
C	5.71399700	-1.38535500	1.56604600
H	6.35371900	-1.13051300	-0.47818700
H	4.80270900	-1.77696700	3.47992100
H	6.65216900	-1.04059100	1.99029600
C	-3.29758000	-0.60743500	0.02288100
C	-3.58375600	0.72003600	-0.29581400
C	-3.34942100	-1.05677000	1.34411400
C	-3.91979000	1.60370200	0.72791400
H	-3.53629900	1.04754400	-1.32635500
C	-3.67698000	-0.15702400	2.35599000
H	-3.15794300	-2.10096900	1.56592200
C	-3.96801100	1.18424500	2.06476700
H	-4.14710600	2.63807000	0.48426000
H	-3.71830600	-0.50207700	3.38554700
C	-4.35721000	2.14480300	3.16167100
H	-3.89872900	1.87082800	4.11624600
H	-4.05922100	3.16938500	2.92079400
H	-5.44403200	2.14693800	3.30942200

Zero-point correction= 0.929615 (Hartree/Particle)

Thermal correction to Energy= 0.978867

Thermal correction to Enthalpy= 0.980821

Thermal correction to Gibbs Free Energy= 0.828556

Sum of electronic and zero-point Energies=	-2859.866399
Sum of electronic and thermal Energies=	-2859.831838
Sum of electronic and thermal Enthalpies=	-2859.850994
Sum of electronic and thermal Free Energies=	-2859.974846

B-TSc1

C	1.05314500	4.40552900	-1.55333900
C	1.23283200	3.03375200	-1.44827000
C	-1.16678600	2.73094200	-1.71054300
C	-1.34114600	4.12283100	-1.79825000
C	-0.23149500	4.95286900	-1.73101300
H	1.91424600	5.06430200	-1.49345800
H	2.22413300	2.61872100	-1.29422900
H	-2.33719500	4.53548100	-1.92245100
H	-0.35473400	6.02805100	-1.81329700
C	-2.27758300	1.80374700	-1.73102700
O	-2.02238900	0.55609600	-2.20997600
H	-3.24779900	2.16021200	-2.06642700
C	0.12518900	2.16443200	-1.53693800
C	0.22243100	0.72548300	-1.36249400
C	-0.87824000	-0.01829500	-1.73353400
C	-1.10365100	-1.48508700	-1.52299900
H	-1.56661700	-1.95059000	-2.39453800
H	-0.16904700	-2.00641300	-1.29301200
N	-2.05104800	-1.55564300	-0.39468000
C	-1.62937400	-0.87440600	0.81732500
H	-2.30742600	-1.15079400	1.63281600
H	-0.63148000	-1.21743000	1.11378000
C	-2.76128300	1.30210600	0.13187500
H	-3.50590300	0.58061000	-0.20044000
C	-1.63908700	0.64628900	0.70638400
C	-0.64244900	1.33242700	1.60770700
H	0.28464900	0.75510800	1.62610900
H	-0.38781900	2.32227800	1.22168900
C	-1.20929200	1.41982900	3.01258700
C	-0.72918100	0.71798500	4.03972600
H	-2.06239100	2.07994200	3.14707200
H	-1.15969400	0.80058400	5.03296300
H	0.11839800	0.04594500	3.92831200
O	-3.10407800	-3.50649200	-1.57342700
O	-3.07506700	-3.45834400	0.99287500
S	-3.20356300	-2.78224400	-0.30396000
C	-3.41432400	2.54109800	0.67091100
C	-2.74888600	3.72319000	1.03450700

C	-4.81525700	2.50540000	0.78378500
C	-3.46311200	4.82363700	1.51135300
H	-1.67472800	3.80331400	0.93888700
C	-5.52667600	3.60481200	1.26120300
H	-5.34790200	1.60126800	0.50625200
C	-4.85268400	4.77074800	1.62883500
H	-2.92697000	5.72612600	1.78926400
H	-6.60794400	3.54802500	1.34565300
H	-5.40342100	5.62885200	2.00125800
C	-4.73565100	-1.85840200	-0.27776500
C	-5.16258800	-1.22928200	-1.45316600
C	-5.44880300	-1.73192000	0.91193100
C	-6.31937200	-0.45933800	-1.42083900
H	-4.59620100	-1.34714700	-2.37077100
C	-6.60938200	-0.95476500	0.92338200
H	-5.10362000	-2.24083700	1.80516300
C	-7.06049400	-0.30820400	-0.23403800
H	-6.66138100	0.03025600	-2.32867700
H	-7.17134700	-0.85244500	1.84717600
C	-8.31326700	0.53225400	-0.22412500
H	-8.68801500	0.68694000	0.79066900
H	-8.13305500	1.51345000	-0.67646600
H	-9.10891400	0.05185100	-0.80474100
C	3.44032100	-1.09274000	0.39877900
C	5.47925100	-1.38973200	1.51129400
C	4.68623600	-2.72315200	1.52424700
N	3.45309900	-2.36948900	0.78728400
N	4.56426500	-0.48275900	0.78449200
C	2.35095600	-3.25648200	0.53466500
C	1.29208900	-3.30959900	1.45475500
C	2.31718300	-3.96690600	-0.67642400
C	0.19082000	-4.11726100	1.14922700
C	1.20261200	-4.76776900	-0.93539300
C	0.13388700	-4.86548400	-0.03317300
H	-0.65029400	-4.15345000	1.83472800
H	1.16286800	-5.32908100	-1.86574700
C	4.79299600	0.91163500	0.52819100
C	5.40249400	1.28813300	-0.67861200
C	4.28891800	1.85845600	1.43467000
C	5.51658300	2.65331200	-0.95780700
C	4.42429900	3.21161600	1.11349400
C	5.03574100	3.62800400	-0.07529400
H	5.98112000	2.96244600	-1.89074100
H	4.03365400	3.95759200	1.80126800

C	5.85506700	0.24420200	-1.66940700
H	6.57360300	-0.45434700	-1.22723000
C	3.55762900	1.42178500	2.68025100
H	4.15820200	0.74203400	3.29381800
Au	1.87321000	-0.18773100	-0.54999600
H	6.43303100	-1.47055900	0.98245200
H	5.21352300	-3.53431100	1.01463300
H	4.43822400	-3.05823900	2.53541500
H	5.67719700	-1.00425700	2.51552800
H	3.28587200	2.27967800	3.29920800
H	2.63638500	0.88803400	2.41862500
H	6.32961800	0.70502600	-2.53841000
H	5.00335500	-0.34960700	-2.02124900
C	5.18867000	5.09687000	-0.38961400
H	4.37557800	5.68686800	0.04467200
H	6.12699700	5.48778300	0.02172900
H	5.20763100	5.27705300	-1.46844100
C	1.32936700	-2.48947900	2.72229800
H	0.38171900	-2.55977900	3.26148200
H	2.12176400	-2.82485500	3.40142100
H	1.52337200	-1.43307900	2.50333000
C	3.43016400	-3.81766000	-1.68429400
H	3.48496600	-2.78511700	-2.04940200
H	4.40808800	-4.05785400	-1.25304700
H	3.27357300	-4.47334800	-2.54350300
C	-1.03897800	-5.76520900	-0.33563400
H	-1.81506000	-5.67777200	0.42626000
H	-1.49492500	-5.50706400	-1.29586500
H	-0.71540900	-6.81088000	-0.38819200

Zero-point correction= 0.919352 (Hartree/Particle)

Thermal correction to Energy= 0.975759

Thermal correction to Enthalpy= 0.976704

Thermal correction to Gibbs Free Energy= 0.823240

Sum of electronic and zero-point Energies= -2859.832378

Sum of electronic and thermal Energies= -2859.775970

Sum of electronic and thermal Enthalpies= -2859.775026

Sum of electronic and thermal Free Energies= -2859.928489

B-TSd1

C	-3.83555400	-3.69583600	-1.11685400
C	-2.96568100	-2.61866700	-1.05063600
C	-1.10004500	-4.16785100	-0.92794400
C	-1.98827700	-5.25471100	-0.97929000
C	-3.35083200	-5.01767800	-1.08171400

H	-4.90393400	-3.51609700	-1.19079900
H	-3.35037200	-1.60401500	-1.06852300
H	-1.60403200	-6.27098800	-0.95025300
H	-4.04403800	-5.85108700	-1.13548500
C	0.32742300	-4.34691800	-0.74059100
O	1.13726900	-3.36328700	-1.18973100
H	0.76593000	-5.32071600	-0.94400400
C	-1.57205300	-2.83039800	-0.95564800
C	-0.61042100	-1.74324500	-0.85175700
C	0.71669200	-2.07866900	-1.02720900
C	1.89395000	-1.14195400	-1.15328200
H	2.46292700	-1.42232800	-2.04377800
H	1.54649200	-0.11259400	-1.26858000
N	2.76532900	-1.21277500	0.01655500
C	2.50738300	-0.31480100	1.14524700
H	3.36242500	-0.39440500	1.82531200
H	2.47293000	0.71852400	0.78425000
C	0.40084700	0.35074200	2.24266600
H	0.66806400	1.34595900	1.89519300
C	1.24241500	-0.64329400	1.91464600
C	1.14165000	-2.08544200	2.37900800
H	2.14651600	-2.51274700	2.42633800
H	0.73196700	-2.07679400	3.40328600
C	0.24215100	-3.03158100	1.64385500
C	0.62208700	-4.29579700	1.19413500
H	-0.81706900	-2.80434700	1.66378300
H	-0.08138800	-5.11063900	1.35118500
H	1.67291100	-4.56505300	1.29102600
O	4.21418200	-2.82290600	1.32672400
O	4.10334700	-2.93649600	-1.23273300
S	4.14736400	-2.16813400	0.01285300
C	-0.82267800	0.28561600	3.07022700
C	-0.96062800	1.17488700	4.15179500
C	-1.88067600	-0.59931700	2.80194400
C	-2.08891000	1.13893300	4.96968700
H	-0.16310300	1.88269900	4.36134700
C	-3.01073200	-0.63657400	3.61996500
H	-1.84425100	-1.21641700	1.91327900
C	-3.11352000	0.22281700	4.71434800
H	-2.16764900	1.82261700	5.80970100
H	-3.81706500	-1.32632400	3.38817200
H	-3.98988300	0.19223600	5.35475600
C	5.51232200	-1.01561700	-0.08031300
C	6.17306800	-0.62020100	1.08359600

C	5.89307300	-0.52124400	-1.33159400
C	7.21932700	0.29783000	0.98792900
H	5.88950100	-1.05020900	2.03803900
C	6.94214300	0.38932100	-1.40604600
H	5.39375800	-0.87237300	-2.22832300
C	7.61622300	0.81929200	-0.25102600
H	7.74336000	0.60294000	1.88924400
H	7.25326700	0.76653100	-2.37646100
C	8.72701700	1.83496800	-0.34806800
H	8.31601500	2.84881100	-0.42957500
H	9.37381500	1.81157500	0.53271300
H	9.34708400	1.66437300	-1.23302700
C	-1.76210200	2.19994900	-0.73260100
C	-1.73406600	4.53016400	-1.01769800
C	-3.20044900	4.03897700	-0.98795700
N	-3.04030600	2.57679100	-0.84744400
N	-0.97190100	3.28130700	-0.79032700
C	-4.12818700	1.65010200	-0.70492200
C	-4.62378500	1.38771400	0.58358400
C	-4.59751600	0.97184600	-1.83868900
C	-5.61345800	0.41104900	0.71558100
C	-5.59282900	0.00495700	-1.65769400
C	-6.10831800	-0.29138900	-0.39113300
H	-6.00098900	0.18667500	1.70632900
H	-5.96537600	-0.53414100	-2.52511700
C	0.45387700	3.23727400	-0.64611000
C	1.02029600	3.59360200	0.59080700
C	1.24615800	2.81145600	-1.72603600
C	2.40799900	3.49987400	0.73115900
C	2.62897900	2.71805800	-1.53088500
C	3.22856100	3.05517000	-0.31268500
H	2.85873900	3.76692500	1.68392500
H	3.25395800	2.38230900	-2.35469800
C	0.15917600	4.04127400	1.74816300
H	-0.73788700	3.42223700	1.84594500
C	0.63004800	2.44539100	-3.05466400
H	-0.13758400	3.16476100	-3.35599300
Au	-1.17401900	0.23239100	-0.68677700
H	-1.51673700	5.26219600	-0.23655900
H	-3.76551500	4.44242200	-0.14278400
H	-3.74508500	4.27367400	-1.90648100
H	-1.45274500	4.96396300	-1.98226700
H	1.38911500	2.40889100	-3.83955300
H	0.14284300	1.46439000	-3.00769200

H	-0.16921700	5.08048700	1.62880700
H	0.71276800	3.98630800	2.68864700
C	4.71496500	2.90183700	-0.10801700
H	4.94593900	1.95087300	0.38526100
H	5.25487400	2.90785300	-1.05779200
H	5.11639400	3.70182500	0.52128000
C	-4.06152800	2.10459500	1.78545500
H	-2.99560000	1.88569500	1.90706500
H	-4.17036800	3.19115300	1.69935900
H	-4.56302400	1.79045700	2.70130800
C	-3.99507100	1.23057100	-3.19739100
H	-3.98732800	2.29764400	-3.44338900
H	-2.95437400	0.88596600	-3.22911200
H	-4.54998400	0.70857800	-3.98012300
C	-7.18708200	-1.33341700	-0.21565000
H	-7.26189800	-1.98739800	-1.08923800
H	-6.99914300	-1.95663500	0.66455100
H	-8.16712400	-0.86276700	-0.07444600

Zero-point correction=	0.920781 (Hartree/Particle)
Thermal correction to Energy=	0.976411
Thermal correction to Enthalpy=	0.977355
Thermal correction to Gibbs Free Energy=	0.827311
Sum of electronic and zero-point Energies=	-2859.838011
Sum of electronic and thermal Energies=	-2859.782381
Sum of electronic and thermal Enthalpies=	-2859.781437
Sum of electronic and thermal Free Energies=	-2859.931481

B-1d

C	3.70550500	3.69228100	-1.32153800
C	2.83213100	2.66749500	-0.94544100
C	1.13917100	4.32612700	-0.52921800
C	1.99413100	5.35346900	-0.92020300
C	3.29272700	5.02758700	-1.31804300
H	4.71739100	3.43765800	-1.62260700
H	3.17170400	1.63851400	-0.95360800
H	1.65823500	6.38655900	-0.90581400
H	3.97864400	5.81139300	-1.62346500
C	-0.24209700	4.48752700	0.00244700
O	-1.13338800	3.57583700	-0.79135800
H	-0.68694400	5.47307600	-0.12260600
C	1.53201000	2.98269700	-0.54547700
C	0.47743000	1.97412500	-0.06207000
C	-0.80003000	2.33737400	-0.70369300
C	-1.92076700	1.38473300	-1.06587500

H	-2.57686800	1.85512900	-1.80027000
H	-1.53688200	0.43710200	-1.44345900
N	-2.62893500	1.15765300	0.19141600
C	-2.30212400	0.00943500	1.05121800
H	-3.15284800	-0.11747800	1.72930700
H	-2.24976800	-0.88944600	0.43118300
C	-0.39875800	-0.97166000	2.25014000
H	-0.83462300	-1.90291800	1.89392400
C	-1.03545600	0.16042300	1.88625800
C	-0.71651300	1.55141400	2.36884600
H	-1.67221700	2.05597000	2.52881900
H	-0.23285300	1.48388800	3.34797600
C	0.18509400	2.46257000	1.47401300
C	-0.34590000	3.92693000	1.43652900
H	1.19455600	2.46687300	1.88866300
H	0.22894400	4.58222500	2.09616600
H	-1.39358700	3.97443600	1.74691800
O	-3.93793700	2.37899000	1.99234100
O	-4.01653200	3.16035500	-0.44896300
S	-4.00101600	2.09592000	0.55595900
C	0.79511700	-1.15155400	3.08887800
C	0.92385800	-2.34694400	3.82334000
C	1.84424800	-0.21562200	3.16896300
C	2.02769800	-2.57614100	4.64191400
H	0.13614700	-3.09322700	3.76175400
C	2.94819600	-0.44384300	3.98904900
H	1.81974100	0.67332400	2.55322300
C	3.04133800	-1.61887600	4.73718400
H	2.09635000	-3.50021200	5.20814800
H	3.74483500	0.29328000	4.02997900
H	3.90076100	-1.79448800	5.37707300
C	-5.39407100	1.01676100	0.27309000
C	-5.96571200	0.32909700	1.34582600
C	-5.90573900	0.89566500	-1.02232500
C	-7.05681400	-0.50509900	1.10602300
H	-5.58213500	0.47617000	2.34955600
C	-6.99709200	0.06012100	-1.23884000
H	-5.47738000	1.47461600	-1.83339700
C	-7.58490000	-0.65753200	-0.18438300
H	-7.51404900	-1.03449200	1.93702600
H	-7.41043800	-0.02781500	-2.23972500
C	-8.74282100	-1.58854300	-0.44094500
H	-8.37875600	-2.57753700	-0.74589800
H	-9.35498800	-1.72590900	0.45415900

H	-9.38629000	-1.21691900	-1.24329200
C	1.69164000	-1.88965000	-1.05007600
C	1.67285700	-4.03811000	-2.00830500
C	3.13486600	-3.56816200	-1.83917000
N	2.97046500	-2.21938100	-1.25676200
N	0.90635700	-2.90436000	-1.44496300
C	4.07891700	-1.38690900	-0.88674800
C	4.61064000	-1.50744500	0.40666600
C	4.57070700	-0.45592400	-1.81456700
C	5.66249700	-0.65773100	0.76098000
C	5.63032400	0.36512600	-1.41777900
C	6.18734500	0.28030500	-0.13600800
H	6.08058300	-0.73011300	1.76182700
H	6.02561900	1.09177500	-2.12364900
C	-0.52169500	-2.90266900	-1.34121300
C	-1.12590100	-3.57955000	-0.26677000
C	-1.28117200	-2.21868900	-2.30467900
C	-2.51925300	-3.54212700	-0.16559000
C	-2.67306300	-2.19771900	-2.15321300
C	-3.30987500	-2.85164200	-1.09306400
H	-3.00034500	-4.05610400	0.66313100
H	-3.27399300	-1.66811400	-2.88837100
C	-0.29537200	-4.31665000	0.75611100
H	0.57869200	-3.73393500	1.06134800
C	-0.61631500	-1.51794200	-3.46555600
H	0.07861500	-2.18241200	-3.98932200
Au	1.05880400	-0.04120300	-0.41765400
H	1.45726500	-4.95729800	-1.45800900
H	3.71086300	-4.20497300	-1.16192300
H	3.67371200	-3.50504800	-2.78867400
H	1.39412200	-4.19253200	-3.05522300
H	-1.35734800	-1.16946100	-4.18877000
H	-0.03049500	-0.65440000	-3.12928100
H	0.06739100	-5.27385600	0.36339400
H	-0.88424900	-4.53993700	1.64922900
C	-4.80731400	-2.79338000	-0.92334500
H	-5.07888700	-2.16912600	-0.06509000
H	-5.29755100	-2.36762000	-1.80160500
H	-5.22506900	-3.78975500	-0.74599100
C	4.03652000	-2.49950800	1.38684600
H	2.98351900	-2.28488500	1.59371100
H	4.09722000	-3.52554900	1.00696400
H	4.56725500	-2.46431500	2.33885900
C	3.92317300	-0.30202200	-3.16830100

H	3.87706000	-1.25150900	-3.71221000
H	2.89295000	0.05749800	-3.05933300
H	4.46941500	0.41314900	-3.78729900
C	7.34650100	1.16253500	0.25969100
H	7.31728700	2.12275300	-0.26369400
H	7.35120200	1.36012400	1.33534800
H	8.30154800	0.68445300	0.01076400

Zero-point correction= 0.924704 (Hartree/Particle)

Thermal correction to Energy= 0.979619

Thermal correction to Enthalpy= 0.980563

Thermal correction to Gibbs Free Energy= 0.832815

Sum of electronic and zero-point Energies= -2859.862024

Sum of electronic and thermal Energies= -2859.807109

Sum of electronic and thermal Enthalpies= -2859.806165

Sum of electronic and thermal Free Energies= -2859.953913

C-2

C	2.57524400	4.17057100	-3.02777400
C	2.21857200	3.01557000	-2.36836300
C	-0.08817000	3.80491800	-2.31479800
C	0.30360100	4.99867000	-2.99311300
C	1.61621400	5.17320100	-3.34421600
H	3.61178600	4.32390500	-3.31282600
H	2.95845100	2.26173700	-2.13469600
H	-0.44618000	5.74896800	-3.22547500
H	1.93090200	6.07249000	-3.86292700
C	-1.40493100	3.59006200	-1.94499400
O	-1.76954500	2.47978800	-1.35301800
H	-2.23035000	4.27470800	-2.10602300
C	0.87241300	2.77971700	-1.98451400
C	0.44964800	1.58300000	-1.32191900
C	-0.89779000	1.46789800	-1.08078200
C	-1.62125300	0.23485200	-0.57495000
H	-1.32508700	-0.59177900	-1.22573000
H	-1.26104300	-0.01421600	0.42533700
N	-3.07042500	0.32256200	-0.50885700
C	-3.67384800	1.00864200	0.65600300
H	-2.91530600	0.95329200	1.44464500
H	-3.85032000	2.06646600	0.43553600
C	-6.07498400	1.07817400	1.17252300
H	-5.97486200	2.12360900	0.88127300
C	-4.94786900	0.34031200	1.12347300
C	-4.84862700	-1.13206900	1.48698500
H	-5.61969600	-1.35966500	2.23263900

H	-5.07911900	-1.73987000	0.60336000
C	-3.51232300	-1.56514700	2.03291000
C	-2.73406900	-2.49052900	1.47056200
H	-3.19538800	-1.09560600	2.96463700
H	-1.79635600	-2.79859500	1.91967700
H	-3.02217600	-2.98213600	0.54415200
O	-4.63297900	1.75397800	-2.00137500
O	-2.85169400	0.22391800	-3.01719600
S	-3.88113800	0.49271600	-2.00135000
C	-7.44123800	0.70816700	1.57391300
C	-8.27509800	1.72164500	2.08685900
C	-7.98596300	-0.58345800	1.43456300
C	-9.58263600	1.45188000	2.48124500
H	-7.88278400	2.73103600	2.18201500
C	-9.29897000	-0.85111000	1.82175600
H	-7.40032000	-1.37290100	0.98296800
C	-10.10026800	0.16014300	2.35407500
H	-10.20083600	2.24957300	2.88236500
H	-9.69878500	-1.85386900	1.69946700
H	-11.12147700	-0.05198400	2.65593900
C	-5.04608200	-0.85605500	-2.00272700
C	-6.40310800	-0.59711200	-1.82428000
C	-4.56546100	-2.16005100	-2.14988400
C	-7.29136300	-1.67069200	-1.78096900
H	-6.74779900	0.42273900	-1.70446300
C	-5.46719100	-3.21858000	-2.09806500
H	-3.50680100	-2.33685000	-2.30724100
C	-6.84092900	-2.99205500	-1.90967600
H	-8.34873500	-1.47607000	-1.62814600
H	-5.10396500	-4.23661000	-2.20789300
C	-7.81525600	-4.14301500	-1.87722800
H	-8.66843200	-3.92623800	-1.22796200
H	-8.21129600	-4.34096800	-2.88056800
H	-7.34023700	-5.06308700	-1.52541200
Au	1.74210500	0.09995900	-0.67211300
C	4.05788400	-1.54473600	1.60054700
C	3.95525400	-0.41408100	2.44750800
C	4.64800500	-0.42253100	3.66916600
H	4.57954700	0.45549300	4.30367500
C	5.40731100	-1.51605900	4.07684800
H	5.92781400	-1.49123700	5.02932300
C	5.49368500	-2.63750200	3.25290200
H	6.08014200	-3.50022000	3.55295900
C	4.83175600	-2.64181300	2.02817200

H	4.93643600	-3.50952800	1.39063300
C	3.14093600	0.80709800	2.14058100
C	1.81178600	0.89528000	2.62045800
C	1.08543700	2.05907400	2.36281400
H	0.06143800	2.13121500	2.71845200
C	1.63313600	3.15011300	1.67582700
C	2.95023100	3.04338300	1.22931000
H	3.40525400	3.87475600	0.70371400
C	3.71595400	1.88714600	1.44276900
C	0.77914600	4.39933200	1.47412400
H	-0.16612300	4.06379700	1.01826300
C	0.43359800	5.04676800	2.83134400
H	-0.22369500	5.91133500	2.69192900
H	-0.06787400	4.34524900	3.50365200
H	1.34652600	5.39059000	3.32918400
C	1.40026900	5.44637400	0.54202600
H	1.68341000	5.02368900	-0.42419500
H	0.69033700	6.25922300	0.36175100
H	2.29594700	5.89046900	0.99022500
C	1.19726800	-0.22212900	3.45777200
H	1.77393100	-1.13460100	3.27526100
C	-0.25883300	-0.53175300	3.08778800
H	-0.61882200	-1.39693500	3.65346500
H	-0.93096000	0.30277600	3.31436600
H	-0.35502200	-0.76357800	2.02527600
C	1.31107900	0.11262900	4.95827400
H	0.89355100	-0.69499600	5.56873600
H	2.35255900	0.25919700	5.25613700
H	0.76360600	1.03302900	5.18890600
C	5.16430600	1.84450500	0.96403100
H	5.52454200	0.81658300	1.07142100
C	6.05137300	2.73547200	1.85402000
H	7.09786700	2.68553400	1.53562300
H	5.73001300	3.78139200	1.80249900
H	5.99759500	2.42017400	2.90045900
C	5.31436600	2.22169900	-0.51864200
H	4.69645800	1.57381400	-1.14821100
H	5.01654700	3.25760600	-0.70981400
H	6.35613400	2.11344900	-0.83749600
P	3.26603900	-1.61811700	-0.05986000
C	4.64637100	-1.56959900	-1.32423400
C	2.33165100	-3.23424400	-0.20341200
H	4.92250200	-0.50668100	-1.30626000
C	4.08355600	-1.87543400	-2.73120500

C	5.93065000	-2.37184400	-1.04125100
H	3.19161800	-1.26819800	-2.92711100
H	3.76863000	-2.92573600	-2.78128800
C	5.14661900	-1.61842400	-3.81085900
H	6.34182400	-2.09863400	-0.06536100
C	6.97835100	-2.10890200	-2.13712700
H	5.70825100	-3.44467100	-1.00608200
H	5.38356400	-0.54520900	-3.83122800
H	4.73849900	-1.86957900	-4.79607600
H	7.28531700	-1.05438000	-2.09160400
C	6.42774600	-2.41689200	-3.53609900
H	7.87532600	-2.70472300	-1.93546100
H	6.20672300	-3.49098000	-3.61027100
H	7.18323000	-2.19892000	-4.29872200
C	1.29650100	-3.32752200	0.93845400
C	3.10522600	-4.55878200	-0.35136500
H	1.77841100	-3.07221900	-1.13979200
H	3.66808000	-4.77056700	0.56414600
H	3.82755300	-4.50074600	-1.17011300
C	2.12691100	-5.72101200	-0.59788300
H	1.82681600	-3.45180600	1.89183400
C	0.33778100	-4.50907500	0.72132000
H	0.73000600	-2.39269200	1.01094100
H	2.68740000	-6.65685200	-0.69884000
H	1.60827800	-5.55964900	-1.55323500
C	1.09607900	-5.83002700	0.53341300
H	-0.27666100	-4.31017200	-0.16806200
H	-0.35274700	-4.58550800	1.56834500
H	0.39321800	-6.64556800	0.33160400
H	1.61333900	-6.08507400	1.46885000

Zero-point correction=	1.249034 (Hartree/Particle)
Thermal correction to Energy=	1.318049
Thermal correction to Enthalpy=	1.318993
Thermal correction to Gibbs Free Energy=	1.139467
Sum of electronic and zero-point Energies=	-3562.619186
Sum of electronic and thermal Energies=	-3562.550171
Sum of electronic and thermal Enthalpies=	-3562.549227
Sum of electronic and thermal Free Energies=	-3562.728753

C-TSa1

C	1.25110600	-4.39879900	-1.72368200
C	1.01764600	-3.07103600	-1.40069900
C	-1.34851500	-3.40970200	-1.82333400
C	-1.11012600	-4.76145800	-2.11859900

C	0.18775800	-5.24842400	-2.08400600
H	2.26501300	-4.78649000	-1.69596300
H	1.83455000	-2.41301600	-1.13843700
H	-1.94015300	-5.41143400	-2.37772900
H	0.38347900	-6.28731300	-2.32908100
C	-2.68043500	-2.84452500	-1.79983800
O	-2.76743300	-1.52144300	-2.13897700
H	-3.47410100	-3.41251800	-2.27794200
C	-0.28851400	-2.54151600	-1.45099100
C	-0.59684800	-1.16326700	-1.12702100
C	-1.84023800	-0.71582500	-1.52851400
C	-2.35447600	0.68259000	-1.36562100
H	-1.56561500	1.41591300	-1.51824000
H	-3.17422800	0.86112500	-2.07582800
N	-2.82275100	0.76755100	0.03337600
C	-3.67156800	-0.36220900	0.40942600
H	-4.16254700	-0.12146400	1.35788100
H	-4.45450800	-0.54053100	-0.34004400
C	-3.29374500	-2.83043700	0.05826000
H	-4.33648200	-2.74176900	-0.25404000
C	-2.83057400	-1.60799000	0.63098200
C	-1.84193000	-1.49911100	1.76274000
H	-1.05418600	-2.24366900	1.68299800
H	-1.37234300	-0.51476700	1.70751600
C	-2.56742600	-1.62448400	3.09101200
C	-2.51201800	-2.69784500	3.88011200
H	-3.14634900	-0.75211200	3.39099800
H	-3.03093500	-2.72198200	4.83369500
H	-1.95118300	-3.58553200	3.60170600
O	-3.45241200	2.07354400	2.08044100
O	-2.08386800	3.15405500	0.19710500
S	-3.18112700	2.29799600	0.65661300
C	-3.02406800	-4.16706000	0.67889300
C	-4.12860700	-4.97940300	0.97843100
C	-1.74058500	-4.65266900	0.97856100
C	-3.96331400	-6.22590600	1.58183700
H	-5.13110400	-4.62617300	0.74953400
C	-1.57400500	-5.89924500	1.58099600
H	-0.86129100	-4.06996900	0.73219700
C	-2.68323900	-6.68899700	1.88979200
H	-4.83410800	-6.83253300	1.81065700
H	-0.57222800	-6.25498300	1.80263700
H	-2.55066100	-7.65848700	2.35990600
C	-4.68339200	2.82517200	-0.14348800

C	-5.91549900	2.53655900	0.44886100
C	-4.60502300	3.46054300	-1.38669000
C	-7.08317000	2.88932600	-0.22335900
H	-5.95153700	2.07020600	1.42751000
C	-5.78523400	3.80211800	-2.04184600
H	-3.63727900	3.70267300	-1.81267300
C	-7.03865200	3.52355800	-1.47451400
H	-8.04556100	2.67767600	0.23396700
H	-5.73416700	4.30193700	-3.00506000
C	-8.30845700	3.93532200	-2.17630100
H	-9.14799000	3.29152100	-1.90029100
H	-8.57985700	4.96252200	-1.90449200
H	-8.19406300	3.90550800	-3.26351800
C	3.36629600	1.13755800	-1.50434500
C	2.37974700	1.80317700	-2.27058800
C	1.80450000	1.13290500	-3.35285300
C	2.16585500	-0.17155200	-3.70890500
C	3.14577700	-0.80205800	-2.94077200
C	3.75923400	-0.17301100	-1.84722200
H	1.06797900	1.65291300	-3.95927300
H	3.46781300	-1.80183800	-3.20671000
C	1.98624400	3.24793600	-1.98303500
C	0.46469800	3.45947600	-1.95918800
C	2.66513200	4.19623100	-2.98962200
H	2.36011600	3.50795700	-0.98901000
H	-0.01374200	2.78930300	-1.24160100
H	0.22531100	4.48428000	-1.65894800
H	0.01272300	3.29267700	-2.94305600
H	3.75428600	4.09664100	-2.95152100
H	2.34326800	3.97232700	-4.01257600
H	2.40981300	5.23879100	-2.77274600
C	1.51341900	-0.81470900	-4.93071600
C	-0.00791200	-0.98614600	-4.74114800
C	2.14118100	-2.15054400	-5.34860500
H	1.65690700	-0.10791200	-5.76074400
H	-0.48631700	-0.05721700	-4.41658500
H	-0.47802800	-1.29941700	-5.67907200
H	-0.21500000	-1.75117400	-3.98837200
H	3.21514900	-2.05564200	-5.53577800
H	1.99373000	-2.91549400	-4.57687100
H	1.67233600	-2.51625400	-6.26699700
C	4.89782900	-0.88156100	-1.11699500
C	6.18815200	-0.81669600	-1.95786200
C	4.57549800	-2.33746000	-0.73970200

H	5.08936400	-0.34039200	-0.18567500
H	6.46790400	0.21911300	-2.16995000
H	7.02102400	-1.29334600	-1.43009800
H	6.05281000	-1.33005000	-2.91598400
H	3.67294400	-2.40239000	-0.12413900
H	4.42793200	-2.96656100	-1.62426500
H	5.40154400	-2.77152000	-0.16726200
C	4.07274700	1.86998700	-0.40100400
C	3.64069400	1.90927100	0.94381500
C	5.24535400	2.56417800	-0.74585900
C	4.40088500	2.62369700	1.88946100
C	5.98563400	3.27022100	0.19831600
C	5.56336300	3.29748300	1.52841600
H	6.88686100	3.79591100	-0.10207900
H	6.13136300	3.84028500	2.27741200
C	1.24184100	2.41702300	2.52915700
C	1.01248500	3.70803000	1.72142700
C	-0.08779800	1.91423400	3.12607300
H	1.92474300	2.64545600	3.36042300
C	0.39169100	4.79365600	2.61639600
H	0.33123400	3.49627200	0.89127100
H	1.95548000	4.06798000	1.29722900
C	-0.74437900	2.99612600	4.00072700
H	-0.76580800	1.64801000	2.30775300
H	0.06668000	1.01167800	3.72667500
C	-0.92555400	4.31911200	3.24469900
H	0.22626300	5.70166600	2.02567100
H	1.10741900	5.05910700	3.40789200
H	-1.71385300	2.62861500	4.35293900
H	-0.11919100	3.16223500	4.88958600
H	-1.32062700	5.08504600	3.92166000
H	-1.66599600	4.17736700	2.45230100
C	2.64199200	-0.14601100	2.86153100
C	1.62215900	-1.29997200	2.99657900
C	4.05616400	-0.72276500	2.65360100
H	2.64019100	0.42656200	3.80038900
C	1.99709100	-2.24907600	4.14400800
H	1.60649800	-1.86468900	2.05363800
H	0.60932900	-0.91622700	3.14179300
C	4.43459800	-1.68247300	3.79443300
H	4.08273200	-1.26684400	1.70321600
H	4.79688400	0.07748800	2.57891400
C	3.41042500	-2.81403300	3.95271800
H	1.25944800	-3.05795800	4.20547600

H	1.94396300	-1.70495200	5.09709100
H	5.43409500	-2.09198100	3.60960200
H	4.49741500	-1.11583400	4.73390800
H	3.68306400	-3.46062700	4.79398000
H	3.42708900	-3.44406400	3.05150600
P	2.10587300	1.08969900	1.53729200
Au	0.71100600	0.02083200	-0.04352100
H	5.57002300	2.54200900	-1.78149300
H	4.08233100	2.65203800	2.92738500

Zero-point correction= 1.250068 (Hartree/Particle)
Thermal correction to Energy= 1.317498
Thermal correction to Enthalpy= 1.318442
Thermal correction to Gibbs Free Energy= 1.144899
Sum of electronic and zero-point Energies= -3562.614147
Sum of electronic and thermal Energies= -3562.546717
Sum of electronic and thermal Enthalpies= -3562.545772
Sum of electronic and thermal Free Energies= -3562.719316

C-TSb1

C	1.84705500	-2.76933200	4.50405900
C	1.62914400	-2.03193100	3.35267700
C	-0.61831100	-2.93308300	3.22995300
C	-0.40310000	-3.65930100	4.41245900
C	0.83120700	-3.58764100	5.03802500
H	2.80988000	-2.71702100	5.00288500
H	2.41495900	-1.41104300	2.94149700
H	-1.19508300	-4.28288000	4.81782500
H	1.01777000	-4.16266500	5.93937900
C	-1.91015600	-2.88338700	2.57715900
O	-1.89571800	-2.72150200	1.22521300
H	-2.65471400	-3.62511300	2.85331300
C	0.38815100	-2.09887700	2.67956000
C	0.11425500	-1.39389500	1.44425900
C	-0.99225100	-1.82151500	0.72558900
C	-1.19254100	-1.59658600	-0.74569600
H	-0.26331800	-1.21296900	-1.16728400
H	-1.38712700	-2.56178800	-1.21696100
N	-2.32267500	-0.71026200	-1.02340800
C	-2.21430000	0.68685000	-0.56330300
H	-1.27646500	0.75751500	-0.00310600
H	-2.13567000	1.36741900	-1.41433500
C	-4.18643400	2.07533200	-0.00722500
H	-3.89197400	2.67015800	-0.87157900
C	-3.38699700	1.04172100	0.31337700

C	-3.63627400	0.09974500	1.46430800
H	-4.43018500	0.51192300	2.10520500
H	-4.04314500	-0.85140800	1.08864400
C	-2.51423300	-0.20932800	2.40663400
C	-2.67462300	-1.26466500	3.31800000
H	-1.67998900	0.47903300	2.50532800
H	-2.12491000	-1.20962300	4.25113000
H	-3.69704000	-1.62519900	3.42904500
O	-3.14945700	0.23179200	-3.27940300
O	-2.78689700	-2.28022900	-2.95237300
S	-3.21659300	-0.97224800	-2.44229300
C	-5.42712100	2.52191900	0.65362800
C	-5.65716200	3.89856100	0.82303800
C	-6.42423800	1.62091200	1.07047900
C	-6.82543100	4.35892900	1.42706900
H	-4.90689100	4.60815000	0.48358100
C	-7.59624400	2.08335400	1.66993700
H	-6.30448600	0.56110300	0.87723100
C	-7.79800100	3.45193000	1.85733300
H	-6.98131600	5.42566600	1.55729000
H	-8.35724000	1.37260600	1.97997700
H	-8.71109900	3.81136600	2.32196000
C	-4.89126600	-1.10836500	-1.82812900
C	-5.84583400	-0.17300900	-2.22661800
C	-5.21391300	-2.14793300	-0.95367700
C	-7.14224500	-0.28058700	-1.73007800
H	-5.56395500	0.62597500	-2.90243500
C	-6.51518700	-2.23460800	-0.46110200
H	-4.45765600	-2.86942600	-0.66066100
C	-7.49621600	-1.30466300	-0.83899900
H	-7.88835500	0.45166900	-2.02483100
H	-6.77631900	-3.03814900	0.22206400
C	-8.90363200	-1.38721700	-0.30229400
H	-8.98982300	-2.12204800	0.50224900
H	-9.23110000	-0.41552100	0.08307200
H	-9.60684700	-1.67331300	-1.09260800
C	3.27059700	-0.80802900	-1.83326500
C	2.16694100	-1.20832300	-2.62061500
C	1.58551000	-2.45926100	-2.37311700
C	2.04598000	-3.31314300	-1.36994600
C	3.14077500	-2.89451600	-0.60757700
C	3.77291500	-1.66691500	-0.82766300
H	0.74867200	-2.78124900	-2.98727200
H	3.53732500	-3.55839700	0.15494600

C	1.63703900	-0.35924400	-3.77447700
C	0.11213700	-0.16355100	-3.73254000
C	2.06389100	-0.96756800	-5.12512400
H	2.09781900	0.63087900	-3.70462700
H	-0.20908100	0.29637800	-2.79554000
H	-0.21335700	0.49325900	-4.54451100
H	-0.43309200	-1.10468900	-3.84593300
H	3.15166100	-1.06077600	-5.19534500
H	1.63299200	-1.96591100	-5.25556700
H	1.72060400	-0.34124900	-5.95495700
C	1.43055900	-4.69159100	-1.17475800
C	0.96304600	-4.93928800	0.27026000
C	2.41506000	-5.78824500	-1.62576800
H	0.54718800	-4.75071100	-1.82442700
H	0.19295500	-4.22480300	0.56958700
H	0.54621000	-5.94684200	0.36917700
H	1.79143600	-4.85223000	0.98136300
H	2.73230300	-5.63108200	-2.66087700
H	3.31237300	-5.78902100	-0.99698800
H	1.95334200	-6.77851000	-1.55419600
C	5.04445100	-1.33390100	-0.05348300
C	6.21286000	-2.20397200	-0.55615100
C	4.87354500	-1.46390700	1.46851900
H	5.30654500	-0.29301200	-0.26214400
H	6.36763300	-2.06714800	-1.63080500
H	7.14271600	-1.94153900	-0.04053600
H	6.01402000	-3.26646100	-0.37973800
H	4.08916400	-0.79012900	1.82706100
H	4.60435900	-2.48180400	1.76689400
H	5.80515300	-1.20487600	1.98275900
C	3.98396100	0.47304400	-2.15344200
C	3.79930600	1.69710100	-1.47159000
C	4.89528400	0.43940600	-3.22392500
C	4.50666600	2.83737100	-1.90054700
C	5.59196500	1.57215900	-3.63427300
C	5.39261200	2.78432900	-2.97158600
H	6.28551100	1.50987100	-4.46724200
H	5.92548900	3.67795500	-3.28084900
C	1.56468900	3.30757100	-0.56415100
C	0.72750900	2.85904400	-1.77635600
C	0.66176600	3.81601200	0.57770000
H	2.22316600	4.13089900	-0.87333000
C	-0.23522400	3.95703000	-2.25109700
H	0.15153600	1.97257900	-1.48882800

H	1.38293900	2.55205300	-2.59709900
C	-0.27586100	4.93027700	0.08381700
H	0.06268400	2.97931200	0.96524100
H	1.26426500	4.18921500	1.41210600
C	-1.12307600	4.46359600	-1.10605500
H	-0.84779000	3.57098500	-3.07368700
H	0.34544000	4.79645200	-2.65716500
H	-0.91705000	5.26129300	0.90861900
H	0.32602100	5.79951000	-0.21513500
H	-1.76941200	5.27598100	-1.45659300
H	-1.78687500	3.65558900	-0.77140300
C	3.72312000	2.66678200	1.35105900
C	3.10127100	2.34680600	2.73029700
C	5.21424300	2.27103700	1.34772500
H	3.66337500	3.75283200	1.18742100
C	3.84950100	3.07517300	3.85691000
H	3.16425100	1.26265000	2.89654900
H	2.03538800	2.59470800	2.75007300
C	5.96784200	2.99612700	2.47565700
H	5.30322800	1.18956900	1.49573600
H	5.67914800	2.49689800	0.38516000
C	5.34228500	2.71848700	3.84922500
H	3.39736000	2.82310500	4.82285000
H	3.73094400	4.15998700	3.72754700
H	7.02039100	2.69204500	2.46487900
H	5.95233900	4.07754700	2.28044600
H	5.87230600	3.27542300	4.62942100
H	5.45816000	1.65191400	4.08898700
P	2.68534300	1.91198200	-0.02506000
Au	1.36744100	0.08236600	0.70208800
H	4.37308500	3.78251100	-1.38167700
H	5.04649400	-0.50406400	-3.73870800

Zero-point correction=	1.249440 (Hartree/Particle)
Thermal correction to Energy=	1.316898
Thermal correction to Enthalpy=	1.317842
Thermal correction to Gibbs Free Energy=	1.144307
Sum of electronic and zero-point Energies=	-3562.607455
Sum of electronic and thermal Energies=	-3562.539997
Sum of electronic and thermal Enthalpies=	-3562.539053
Sum of electronic and thermal Free Energies=	-3562.712588

D-2

C	2.79465900	4.26167000	-2.82435100
C	2.46379200	3.02263700	-2.32276600

C	0.15129700	3.76553100	-2.11767900
C	0.51320600	5.04217600	-2.64373200
C	1.81715400	5.28288000	-2.98803700
H	3.82377600	4.46763100	-3.10299200
H	3.21608100	2.25362800	-2.20777300
H	-0.25066900	5.80508800	-2.75990000
H	2.11089800	6.24820600	-3.38638500
C	-1.14941600	3.49347600	-1.73055000
O	-1.47907500	2.32040700	-1.25163100
H	-1.98727900	4.17998300	-1.78232800
C	1.13051900	2.71939700	-1.94437500
C	0.74211300	1.44526500	-1.41979300
C	-0.59229100	1.29362300	-1.12811900
C	-1.29350100	0.01282500	-0.71295400
H	-1.07101700	-0.73165900	-1.48154000
H	-0.85015300	-0.34994300	0.21746700
N	-2.73235500	0.09871300	-0.50861400
C	-3.19791800	0.68726600	0.76936100
H	-2.41704900	0.43509200	1.49543100
H	-3.24993100	1.77929500	0.69849300
C	-5.54889600	0.98096700	1.40670000
H	-5.33535400	2.02827300	1.19510100
C	-4.52212100	0.12374800	1.23472300
C	-4.59213900	-1.37701500	1.47303900
H	-5.33471500	-1.56658800	2.25740200
H	-4.96406700	-1.87286500	0.56865200
C	-3.29435200	-2.02471000	1.87998300
C	-2.65478000	-2.94877600	1.16204500
H	-2.88513200	-1.71855500	2.84240000
H	-1.74046200	-3.41507800	1.51556800
H	-3.03882700	-3.27825000	0.19956800
O	-4.33026100	1.76079800	-1.71840700
O	-2.73340700	0.25128900	-3.02628800
S	-3.65731900	0.46839600	-1.90223500
C	-6.92998400	0.74637900	1.85502400
C	-7.60869400	1.81666500	2.47176500
C	-7.63512800	-0.45966000	1.67171600
C	-8.91879400	1.68071900	2.92191800
H	-7.09131100	2.76366400	2.60376500
C	-8.95096800	-0.59225600	2.11506700
H	-7.17385200	-1.28474300	1.14605700
C	-9.59622000	0.47094800	2.74850900
H	-9.41425200	2.51906100	3.40259800
H	-9.47595300	-1.53041400	1.95844600

H	-10.61999800	0.36278900	3.09367400
C	-4.89793600	-0.80987400	-1.93122000
C	-6.22157300	-0.49293900	-1.63559800
C	-4.50919400	-2.11914100	-2.22756300
C	-7.16981100	-1.51511300	-1.62561800
H	-6.49224300	0.52816800	-1.39615000
C	-5.46918900	-3.12580900	-2.20737800
H	-3.47548600	-2.33931200	-2.47157300
C	-6.81162900	-2.84143800	-1.90396700
H	-8.20103900	-1.27646700	-1.38282500
H	-5.17776500	-4.14796600	-2.43238300
C	-7.84949800	-3.93578500	-1.90920100
H	-8.67921300	-3.70475100	-1.23535600
H	-8.26981500	-4.06239500	-2.91422800
H	-7.42143700	-4.89716000	-1.61114800
Au	2.04053900	-0.11459500	-1.00078400
P	3.41820600	-1.99907100	-0.52548200
C	4.23988000	-1.99326100	1.13597500
C	4.09531600	-0.95705000	2.09691700
C	4.84143200	-1.04113300	3.28597900
H	4.73954400	-0.23860300	4.00904600
C	5.70194200	-2.10119300	3.55368000
H	6.26101000	-2.12630400	4.48395500
C	5.84071500	-3.12106500	2.61423500
H	6.50847300	-3.95714700	2.79653700
C	5.12025400	-3.05566200	1.42577000
H	5.25832100	-3.84854700	0.70380000
C	3.21561400	0.25391800	1.95903200
C	1.89183200	0.23281000	2.46433900
C	1.10224100	1.37677900	2.32565700
H	0.07952900	1.35404500	2.68917500
C	1.59176500	2.56693400	1.77328100
C	2.92351700	2.58648600	1.36195100
H	3.34856200	3.50285100	0.97186400
C	3.74664600	1.45392600	1.44010700
C	4.83095200	-2.12028400	-1.83021800
C	5.98706300	-1.22217800	-1.35099000
H	6.74402200	-1.16946200	-2.14151600
H	6.46817300	-1.60723500	-0.44929200
H	5.64817000	-0.20507300	-1.15154800
C	5.37470200	-3.53787000	-2.09007200
H	6.18744800	-3.46559600	-2.82169200
H	4.62243600	-4.20621600	-2.51293300
H	5.79539700	-4.00354200	-1.19708200

C	4.29562100	-1.55015000	-3.16463700
H	5.07916300	-1.64019300	-3.92562000
H	4.03609500	-0.49120000	-3.07790400
H	3.41487400	-2.08122800	-3.53036400
C	2.27846400	-3.53780400	-0.58534400
C	2.91616100	-4.86765000	-0.14021800
H	2.16652600	-5.65992400	-0.24851800
H	3.20916400	-4.84318900	0.91161800
H	3.77967100	-5.15950100	-0.73811900
C	1.72123700	-3.67410500	-2.01750400
H	0.94401900	-4.44679000	-2.01999300
H	2.48254000	-3.98052300	-2.73801300
H	1.26600100	-2.74250300	-2.36924300
C	1.10311800	-3.24656400	0.36955400
H	0.42085500	-4.10409100	0.36412400
H	0.53173400	-2.36745000	0.06295300
H	1.44129900	-3.09886200	1.39711100
C	0.67439800	3.78402300	1.67756700
H	-0.20206200	3.47186400	1.08733600
C	0.16381800	4.20626000	3.07091400
H	-0.52993300	5.04929400	2.98870500
H	-0.35603900	3.39309300	3.58434200
H	1.00273300	4.51708600	3.70252300
C	1.30674000	4.99224900	0.97423200
H	1.69784800	4.74285200	-0.01504900
H	0.56600400	5.78842700	0.85262900
H	2.13149200	5.40145500	1.56771900
C	1.36777400	-0.95383800	3.26774100
H	1.94492900	-1.83857400	2.98193000
C	-0.11610900	-1.25965100	3.03115500
H	-0.39586800	-2.19270700	3.53061700
H	-0.76117500	-0.47422100	3.43903400
H	-0.34825300	-1.36771200	1.97146200
C	1.61487600	-0.71290200	4.77228000
H	1.25548800	-1.56254000	5.36230600
H	2.67644900	-0.57506600	4.98919500
H	1.08377000	0.18487600	5.10625100
C	5.21836800	1.58006800	1.05830600
H	5.63548000	0.57252300	0.97725300
C	5.99172200	2.30517300	2.17783000
H	7.05629500	2.37553200	1.93115500
H	5.60686400	3.32070400	2.32039800
H	5.89762100	1.77512300	3.12994600
C	5.44024200	2.28132200	-0.29137700

H	4.89293200	1.77377900	-1.09065200
H	5.11104200	3.32503800	-0.27141500
H	6.50340300	2.27704800	-0.55175000

Zero-point correction= 1.172663 (Hartree/Particle)
Thermal correction to Energy= 1.240268
Thermal correction to Enthalpy= 1.241213
Thermal correction to Gibbs Free Energy= 1.068443
Sum of electronic and zero-point Energies= -3407.826072
Sum of electronic and thermal Energies= -3407.758467
Sum of electronic and thermal Enthalpies= -3407.757522
Sum of electronic and thermal Free Energies= -3407.930292

D-TSa1

C	0.93282000	-4.57343900	0.52258500
C	0.80994700	-3.19601000	0.43428000
C	-1.47480700	-3.36865000	1.23451800
C	-1.35386400	-4.76615800	1.29776300
C	-0.14870100	-5.36262800	0.95842300
H	1.87365800	-5.04567400	0.25685200
H	1.64259500	-2.58254400	0.11761600
H	-2.19980500	-5.36750900	1.61568100
H	-0.04134000	-6.44064900	1.02231000
C	-2.71606400	-2.68498600	1.52286600
O	-2.60309100	-1.41963700	2.02910100
H	-3.48689100	-3.24098300	2.05003000
C	-0.39275500	-2.55821500	0.80140400
C	-0.57442000	-1.12347500	0.73975300
C	-1.69299100	-0.62618200	1.38058400
C	-2.07166300	0.82308100	1.44839300
H	-2.82202000	0.97704100	2.23671300
H	-1.20525000	1.45366300	1.63400900
N	-2.61309300	1.13779300	0.11018100
C	-3.64296800	0.18455500	-0.30622900
H	-4.40017700	0.05201600	0.47851400
H	-4.14027700	0.58115700	-1.19759500
C	-3.61217700	-2.33613400	-0.18061800
H	-4.55859300	-2.11861800	0.31773400
C	-3.02746600	-1.14494600	-0.70646200
C	-2.16915300	-1.07075800	-1.94411700
H	-1.62262200	-0.12728200	-1.92428900
H	-1.43198600	-1.87202100	-1.96900200
C	-3.06073800	-1.11992500	-3.17141600
C	-3.39451400	-0.03015200	-3.86615900
H	-3.44416400	-2.09935200	-3.44838300

H	-4.03618000	-0.09423200	-4.74013200
H	-3.04287300	0.95913100	-3.58093200
O	-1.69069400	3.46416600	0.29855800
O	-3.09592300	2.77292000	-1.73594200
S	-2.83616400	2.76790300	-0.29277000
C	-3.68720200	-3.62708300	-0.93733600
C	-4.93989900	-4.25678700	-1.02021000
C	-2.58805500	-4.24955100	-1.55179100
C	-5.09841300	-5.45620500	-1.71348700
H	-5.80293100	-3.79645100	-0.54530700
C	-2.74682900	-5.44765700	-2.24758500
H	-1.59829100	-3.81725100	-1.47339900
C	-4.00090400	-6.05425000	-2.33490700
H	-6.07821500	-5.92058800	-1.76818500
H	-1.88352400	-5.91037700	-2.71619000
H	-4.12072000	-6.98662900	-2.87780500
C	-4.31710000	3.28264100	0.55635100
C	-4.22235200	3.72449100	1.87927400
C	-5.55346900	3.16663900	-0.08462900
C	-5.39071100	4.04905300	2.56425300
H	-3.24960700	3.83366700	2.34672300
C	-6.70874900	3.49797200	0.61889900
H	-5.59900400	2.84617300	-1.11996800
C	-6.64761300	3.94145800	1.94916000
H	-5.32692400	4.40032900	3.59024000
H	-7.67376700	3.41981200	0.12608600
C	-7.90286800	4.33309600	2.68796900
H	-8.13070500	5.39269500	2.52053700
H	-8.76684300	3.75622600	2.34636100
H	-7.79644900	4.18843100	3.76658700
C	3.55177200	0.45824100	1.18331400
C	3.80099600	-0.92983700	1.34082600
C	3.16997000	-1.61448600	2.38597300
C	2.33706800	-0.97272300	3.30757000
C	2.12675400	0.39668600	3.14566300
C	2.72384000	1.13025400	2.11283800
H	3.37148200	-2.67308100	2.51226200
H	1.51210700	0.91789800	3.87405500
C	4.31904000	1.23944000	0.14795000
C	3.89440700	1.55163700	-1.17148900
C	5.60196200	1.65790900	0.54577100
C	4.80471000	2.19269300	-2.03602500
C	6.47558900	2.31609700	-0.31432200
C	6.08004800	2.56913400	-1.62589400

H	7.45847300	2.61675100	0.03534500
H	6.75024500	3.06092200	-2.32391900
P	2.20615100	1.17963500	-1.83192900
Au	0.75300400	0.07605100	-0.30174800
C	2.44720500	-0.04195100	-3.29789800
C	3.48376000	-1.07652800	-2.82657400
H	4.47979000	-0.64245900	-2.71378100
H	3.18954600	-1.51503800	-1.87060100
H	3.54725100	-1.88706200	-3.56151300
C	2.91916800	0.59448500	-4.61651400
H	3.85880800	1.14092900	-4.51235200
H	3.09507500	-0.20521600	-5.34535400
H	2.16815300	1.26189000	-5.04459700
C	1.11614400	-0.78388700	-3.55744400
H	0.82696500	-1.39131400	-2.69584700
H	0.28724700	-0.11287900	-3.78811000
H	1.24914100	-1.45520500	-4.41369900
C	1.43105700	2.83460200	-2.39461900
C	1.21047400	3.65747200	-1.11200100
H	0.57871300	3.13956600	-0.39285400
H	2.15936900	3.92316700	-0.63827600
H	0.69583300	4.58876300	-1.37206000
C	2.25325800	3.70187800	-3.36845800
H	1.64212200	4.57019600	-3.63942200
H	3.16282600	4.08531000	-2.90203800
H	2.51942300	3.19364400	-4.29553700
C	0.06157500	2.51297300	-3.02882200
H	0.16200100	2.04087100	-4.00986200
H	-0.55290900	1.87463300	-2.38980900
H	-0.49529200	3.44523800	-3.16655400
H	5.91404600	1.44330000	1.56236800
H	4.51456500	2.40641700	-3.05521400
C	1.73258700	-1.71331500	4.49375100
H	1.32384200	-0.95122600	5.17026200
C	2.57046200	2.64643500	2.09017100
H	2.85474500	2.99400600	1.09449400
C	4.85689700	-1.66090500	0.50856100
H	5.04936000	-1.07199600	-0.39227300
C	1.13576500	3.12506200	2.35599100
H	1.06117100	4.20588700	2.20245700
H	0.42416400	2.65049900	1.67827400
H	0.82164500	2.92032600	3.38501400
C	3.54671500	3.29031000	3.09559500
H	3.46244300	4.38184700	3.06940700

H	3.32691300	2.95579900	4.11524700
H	4.58332500	3.02474000	2.87056800
C	6.17811800	-1.74101100	1.30360500
H	6.03590700	-2.31773900	2.22368900
H	6.95742100	-2.23095400	0.71027800
H	6.54023100	-0.74956900	1.58385400
C	4.45416900	-3.07724200	0.06042300
H	4.31152300	-3.74892300	0.91319400
H	3.53468900	-3.08297300	-0.52986700
H	5.24541700	-3.50811700	-0.56094300
C	0.56870100	-2.62901900	4.07535100
H	0.15738300	-3.15163400	4.94546400
H	-0.23795400	-2.05466700	3.61177300
H	0.90103300	-3.38258000	3.35383200
C	2.79436900	-2.50361600	5.27979800
H	2.35880700	-2.92864300	6.18983300
H	3.19354900	-3.33499700	4.68886500
H	3.63328900	-1.86315500	5.56777700

Zero-point correction=	1.173225 (Hartree/Particle)
Thermal correction to Energy=	1.239626
Thermal correction to Enthalpy=	1.240570
Thermal correction to Gibbs Free Energy=	1.071425
Sum of electronic and zero-point Energies=	-3407.814188
Sum of electronic and thermal Energies=	-3407.747788
Sum of electronic and thermal Enthalpies=	-3407.746843
Sum of electronic and thermal Free Energies=	-3407.915989

D-TSb1

C	0.20363000	-0.45381300	4.72963100
C	-0.05065300	-0.10545000	3.41486700
C	2.21845300	-0.71338900	2.82916500
C	2.48052000	-1.04809600	4.16844000
C	1.47224700	-0.93428200	5.11149000
H	-0.58051900	-0.35594400	5.47390700
H	-1.02243900	0.27189500	3.12354700
H	3.46643800	-1.40632600	4.45249400
H	1.65884600	-1.21064200	6.14426600
C	3.25803000	-0.73636500	1.82094900
O	2.85604000	-0.92710200	0.54128500
H	4.16211600	-1.30823000	2.01401500
C	0.94400300	-0.23954100	2.42115600
C	0.71241400	0.06784600	1.02414100
C	1.70927500	-0.30523000	0.14165600
C	1.57898300	-0.36657400	-1.35624600

H	1.35771200	-1.39768100	-1.63565000
H	0.71686000	0.23382900	-1.65205100
N	2.75100600	0.09716200	-2.08450100
C	2.73913400	1.48919900	-2.55578700
H	3.67235300	1.66621100	-3.09777500
H	1.92220400	1.64222200	-3.27372600
C	1.62455700	3.35257200	-1.34196200
H	0.89362600	3.36751800	-2.14815000
C	2.60817700	2.44627600	-1.39489000
C	3.66064500	2.28835800	-0.31279100
H	4.45406500	1.61593300	-0.64908400
H	4.13972300	3.26776900	-0.14323400
C	3.19955900	1.86508200	1.04575000
C	3.99785500	1.03999800	1.84801900
H	2.32913000	2.36203100	1.46113900
H	3.95772200	1.19093700	2.92281600
H	4.99119800	0.81668400	1.45798000
O	3.16345100	-2.33249200	-2.67315200
O	4.26788900	-0.45371200	-4.04016200
S	3.81625300	-1.02141900	-2.76841500
C	1.43521600	4.34022900	-0.24773300
C	2.29972900	5.43413600	-0.09826400
C	0.38237000	4.17954700	0.66707800
C	2.11846200	6.34415800	0.94548700
H	3.10801200	5.57600800	-0.81054800
C	0.20303400	5.08713700	1.71129300
H	-0.27578700	3.32322500	0.56421200
C	1.07134100	6.17277100	1.85324100
H	2.79281600	7.18934900	1.04640400
H	-0.61465400	4.94683000	2.41303200
H	0.93129500	6.88168000	2.66360500
C	5.22517900	-1.03011500	-1.65931200
C	5.32313500	-2.00752900	-0.66917200
C	6.18120500	-0.01745800	-1.76739200
C	6.37413900	-1.94261700	0.24462000
H	4.58542900	-2.79913500	-0.62157700
C	7.22024000	0.03804900	-0.83963000
H	6.11910900	0.70455000	-2.57492700
C	7.33116200	-0.91685900	0.18319800
H	6.46423100	-2.71127300	1.00832800
H	7.96591300	0.82418900	-0.92003600
C	8.48419600	-0.87480500	1.15538300
H	8.21997100	-1.32717100	2.11557300
H	9.34095200	-1.43206700	0.75827900

H	8.81989400	0.15001300	1.33776000
Au	-1.16361900	0.60176200	0.30157000
P	-3.35068500	1.15988900	-0.48961700
C	-4.45804900	-0.28066500	-0.85504100
C	-5.73857900	0.00772400	-1.37155800
C	-6.64322100	-0.98984200	-1.71993400
H	-7.61824100	-0.72175800	-2.11446100
C	-6.28022400	-2.32551400	-1.56050300
H	-6.96874800	-3.12192700	-1.82556900
C	-5.01726300	-2.63228100	-1.06525500
C	-4.08218700	-1.64266300	-0.70968500
C	-2.75396600	-2.15468800	-0.22292000
C	-1.75946800	-2.52545400	-1.15663800
C	-2.00181000	-2.45614300	-2.66368900
H	-2.86842400	-1.81181500	-2.83748400
C	-2.35671300	-3.85881500	-3.19886600
H	-1.52502100	-4.55341200	-3.04079300
H	-2.56771600	-3.82044300	-4.27260200
H	-3.23542600	-4.26856200	-2.69373900
C	-0.82506700	-1.87245700	-3.46400600
H	-0.56083800	-0.87066200	-3.11679900
H	-1.09357400	-1.79823400	-4.52250900
H	0.07371500	-2.49412900	-3.40214400
C	-0.56370800	-3.08936200	-0.68628100
C	-0.31890500	-3.28922100	0.67259100
C	0.96411900	-3.92275900	1.20510600
H	1.36385800	-3.23235800	1.96248200
C	2.05115200	-4.13949500	0.14428700
H	2.96684500	-4.50529300	0.62118500
H	2.29648400	-3.22806400	-0.40295400
H	1.74709600	-4.89455300	-0.58832700
C	0.65829500	-5.25952800	1.91349600
H	-0.06628200	-5.14086800	2.72369100
H	1.57183000	-5.68804300	2.33904300
H	0.24646300	-5.98096300	1.19971400
C	-1.33340300	-2.94110700	1.57343900
C	-2.55879100	-2.41707600	1.15701700
C	-3.70751600	-2.29215700	2.15541800
H	-4.44351200	-1.59956100	1.73616700
C	-4.40368400	-3.66158500	2.30912500
H	-3.70138400	-4.40344600	2.70402400
H	-4.77916900	-4.03198500	1.35242100
H	-5.24975100	-3.58893800	3.00063200
C	-3.30064800	-1.76409200	3.53847600

H	-2.64234400	-2.46304800	4.06410200
H	-4.18988000	-1.62625200	4.16167900
H	-2.78458500	-0.80663000	3.46731800
H	-6.04036800	1.03527300	-1.51537600
H	-4.72567900	-3.67112200	-0.95289900
C	-3.19806700	2.13809000	-2.13921100
C	-4.21519400	2.20147700	0.86962600
H	0.17716600	-3.40497200	-1.41189100
H	-1.16982400	-3.11798900	2.63173700
C	-5.70702800	2.51216100	0.64328800
H	-5.90100600	3.06534000	-0.27612200
H	-6.31431500	1.60491600	0.64366700
H	-6.05610200	3.13561500	1.47431100
C	-4.10179300	1.38911200	2.17454600
H	-4.60313000	0.42225700	2.09743200
H	-3.05994400	1.21719000	2.45510200
H	-4.57940700	1.94766700	2.98748600
C	-3.43201200	3.51793300	1.04538400
H	-2.37072500	3.33620700	1.23317000
H	-3.52178600	4.18242700	0.18361300
H	-3.83487200	4.05410100	1.91210900
C	-4.37211500	3.07450600	-2.47809000
H	-5.32138100	2.54613700	-2.58265300
H	-4.49491900	3.87559300	-1.74658500
H	-4.16619200	3.54895200	-3.44440800
C	-3.03481900	1.09822800	-3.26399100
H	-2.21921700	0.40533500	-3.04930300
H	-3.94440700	0.51692500	-3.42854400
H	-2.79168400	1.61819500	-4.19727600
C	-1.90306400	2.97549100	-2.07562600
H	-1.89680700	3.70401100	-1.26289000
H	-1.02804600	2.33264500	-1.95470700
H	-1.79003300	3.52700100	-3.01639500

Zero-point correction=	1.173067 (Hartree/Particle)
Thermal correction to Energy=	1.239295
Thermal correction to Enthalpy=	1.240239
Thermal correction to Gibbs Free Energy=	1.072036
Sum of electronic and zero-point Energies=	-3407.812035
Sum of electronic and thermal Energies=	-3407.745807
Sum of electronic and thermal Enthalpies=	-3407.744863
Sum of electronic and thermal Free Energies=	-3407.913066

E-2

C	3.00929400	5.45404000	-0.05314700
C	2.63424400	4.13163600	-0.13662400
C	0.31656300	4.80937900	0.23438700
C	0.72838700	6.17446300	0.31469200
C	2.05502500	6.48587300	0.17457500
H	4.05515900	5.72269900	-0.16839900
H	3.36884300	3.35567700	-0.32507300
H	-0.01651200	6.94659300	0.48285900
H	2.38540700	7.51765500	0.23125700
C	-1.01358100	4.45064500	0.37834000
O	-1.39432600	3.19801400	0.29896400
H	-1.83691300	5.13309500	0.55849700
C	1.27190100	3.75178900	0.00573300
C	0.82913600	2.39635100	-0.08027000
C	-0.52301900	2.18249300	0.04409800
C	-1.23109900	0.85290800	-0.12583400
H	-0.87614100	0.42835500	-1.06836100
H	-0.91161700	0.16724900	0.66504000
N	-2.68328900	0.89147800	-0.11639000
C	-3.38385000	0.90818500	1.18752900
H	-2.64839200	0.53920700	1.91039400
H	-3.64847900	1.93131000	1.47276700
C	-5.80031000	0.55712900	1.50321900
H	-5.79476800	1.61608200	1.76189300
C	-4.60672500	0.01644600	1.18884200
C	-4.37394100	-1.43771100	0.81014700
H	-5.18145200	-2.04662200	1.23094700
H	-4.43218100	-1.54233300	-0.28020400
C	-3.05245800	-1.98843600	1.28073700
C	-2.06252700	-2.38019900	0.47754100
H	-2.93114800	-2.05918200	2.36263500
H	-1.12245100	-2.76869600	0.85438800
H	-2.16498500	-2.31246700	-0.60289100
O	-4.23952400	2.82575500	-0.84422700
O	-2.32679500	2.01762700	-2.33989500
S	-3.42129400	1.73989700	-1.39745500
C	-7.13382200	-0.06244500	1.57060600
C	-8.06884300	0.47045300	2.47936400
C	-7.54884300	-1.12598200	0.74591000
C	-9.35098800	-0.06090900	2.59113200
H	-7.77695200	1.30711900	3.10916000
C	-8.83624600	-1.65218700	0.85234200
H	-6.88152600	-1.51494200	-0.01212600

C	-9.73962900	-1.12987500	1.77928900
H	-10.04986000	0.36192900	3.30678100
H	-9.13602900	-2.46894000	0.20163300
H	-10.74072100	-1.54240700	1.86062700
C	-4.50972200	0.53466200	-2.13263600
C	-5.88608600	0.64487100	-1.94984600
C	-3.95241200	-0.52352600	-2.85637800
C	-6.71689000	-0.33175900	-2.49759300
H	-6.29034200	1.47103100	-1.37752000
C	-4.79739500	-1.49284800	-3.38760100
H	-2.87888900	-0.57889700	-3.00316200
C	-6.18979700	-1.41443500	-3.21491100
H	-7.78984600	-0.25797700	-2.34795800
H	-4.37469800	-2.32232600	-3.94772400
C	-7.09975500	-2.45756800	-3.81427300
H	-8.02634000	-2.55673800	-3.24184900
H	-7.37657300	-2.18448600	-4.83969500
H	-6.61500000	-3.43714500	-3.85713700
Au	2.05863100	0.74568200	-0.28052300
P	3.43818200	-1.14832500	-0.56971100
C	4.13835800	1.97784700	2.71474700
H	3.52832200	2.64508300	2.09360500
H	5.18604100	2.07415700	2.42737500
H	4.02420400	2.25523800	3.76969100
C	2.52710300	-2.36201700	-1.65055500
H	2.23289100	-1.75129400	-2.51590100
C	1.23943800	-2.82780600	-0.93673600
H	1.50102300	-3.36194000	-0.01469100
H	0.64551200	-1.95938000	-0.62934900
C	0.40595200	-3.74260100	-1.84703800
H	-0.48072200	-4.09097900	-1.30608100
H	0.04404100	-3.16054800	-2.70708700
C	1.22873800	-4.93520500	-2.35360800
H	0.62721700	-5.55427100	-3.02830000
H	1.50236800	-5.57178500	-1.50065900
C	2.50695600	-4.46383400	-3.06131000
H	2.23780200	-3.90684700	-3.96966200
H	3.10513500	-5.32256500	-3.38564000
C	3.35261200	-3.56166400	-2.14663000
H	4.24844000	-3.22251900	-2.68007300
H	3.69286400	-4.14549600	-1.28289600
C	4.97247100	-0.61708000	-1.47510500
H	5.58665500	-1.50422100	-1.67102800
C	5.78213400	0.35426500	-0.58853200

H	5.14150600	1.21010300	-0.32950700
H	6.04990400	-0.12940800	0.35672200
C	7.03727900	0.85680800	-1.31693900
H	7.57634400	1.56565100	-0.67802000
H	7.71753700	0.01129500	-1.48881500
C	6.68070700	1.50339200	-2.66250900
H	7.58768800	1.83356600	-3.18030400
H	6.07526700	2.40373400	-2.48150900
C	5.88593900	0.53269600	-3.54661700
H	5.60567200	1.01283400	-4.49063800
H	6.52200000	-0.32452800	-3.80746400
C	4.62161700	0.02631200	-2.83304900
H	4.09395700	-0.68867400	-3.47404800
H	3.93624500	0.86938100	-2.66734700
O	3.80156600	0.61382400	2.49472900
O	0.81551000	-2.99883900	2.50498100
C	4.02976300	-2.11340700	0.87723900
C	2.52598600	0.20639800	2.75027700
C	1.51165000	1.04666000	3.22881300
H	1.70163300	2.09391900	3.42414200
C	0.24256600	0.51416700	3.45668600
H	-0.54472400	1.16078300	3.83371600
C	5.58258000	-3.80490300	1.71152200
H	6.42891600	-4.46196200	1.53731200
C	5.12280900	-2.98080800	0.68840700
H	5.62485200	-3.02265100	-0.27143300
C	4.94726900	-3.77905800	2.95290900
H	5.29201700	-4.41788900	3.76023700
C	3.40118900	-2.07398500	2.14010300
C	3.87190700	-2.92017500	3.15628900
H	3.38210000	-2.88478600	4.12422000
C	2.27764100	-1.15958300	2.50145100
C	-0.03263900	-0.83153000	3.22378200
H	-1.02179300	-1.22817300	3.41054000
C	-0.14361100	-3.71020400	3.29157100
H	-0.04312400	-3.45947800	4.35358500
H	0.07423800	-4.76843500	3.14088600
H	-1.17038500	-3.51204400	2.96646600
C	0.99172600	-1.66553900	2.75375400

Zero-point correction= 1.058675 (Hartree/Particle)

Thermal correction to Energy= 1.120390

Thermal correction to Enthalpy= 1.121334

Thermal correction to Gibbs Free Energy= 0.956039

Sum of electronic and zero-point Energies= -3437.987180

Sum of electronic and thermal Energies= -3437.925465

Sum of electronic and thermal Enthalpies= -3437.924521

Sum of electronic and thermal Free Energies= -3438.089816

E-TSa1

C	-4.06953600	-2.79623100	-1.96079900
C	-2.87170500	-2.17799100	-1.63434100
C	-3.85807400	-0.02948000	-2.18932700
C	-5.07409400	-0.66005200	-2.49763100
C	-5.17232400	-2.03983900	-2.39982700
H	-4.15970800	-3.87465700	-1.87184300
H	-2.02684700	-2.76058200	-1.28413700
H	-5.92730100	-0.06461100	-2.80759100
H	-6.10463300	-2.53611900	-2.64890600
C	-3.71299900	1.41247700	-2.18984300
O	-2.46481500	1.88504800	-2.49870700
H	-4.47521600	1.98867700	-2.70805000
C	-2.73130500	-0.77774400	-1.75604200
C	-1.51360900	-0.06480200	-1.42245900
C	-1.43926200	1.24435600	-1.85058200
C	-0.25813100	2.14979700	-1.64659300
H	0.67850600	1.60340600	-1.74807100
H	-0.28976400	2.97360600	-2.37167600
N	-0.38195300	2.65538300	-0.27156700
C	-1.71519800	3.11284400	0.08767200
H	-1.66028500	3.65910600	1.03400600
H	-2.08888000	3.80468600	-0.67678000
C	-3.95370000	2.04127200	-0.36490600
H	-4.14005400	3.06360900	-0.70131000
C	-2.67990400	1.94755800	0.27571100
C	-2.35182900	1.03204100	1.42447500
H	-2.88224600	0.08594100	1.34989900
H	-1.28328000	0.81440800	1.40579400
C	-2.68326400	1.73867500	2.73056200
C	-3.78525100	1.51710600	3.44788800
H	-1.93781200	2.45766600	3.06462700
H	-3.95751100	2.03803400	4.38513700
H	-4.54644400	0.81021800	3.13049500
O	0.41734900	3.01171300	2.07210000
O	1.90382000	1.83562000	0.34568500
S	0.94913800	2.88926900	0.70839400
C	-5.19609000	1.43086500	0.20994800
C	-6.28707000	2.28212100	0.44503700
C	-5.33227600	0.07058400	0.53180800

C	-7.46836000	1.79988900	1.00796600
H	-6.20584100	3.33782600	0.19816800
C	-6.51353900	-0.41297000	1.09388400
H	-4.52492300	-0.62429400	0.33564000
C	-7.58397000	0.44903900	1.33940000
H	-8.29539100	2.47980100	1.18775700
H	-6.59649300	-1.46844200	1.33500800
H	-8.50139000	0.07033300	1.77915100
C	1.66478000	4.45439300	0.24049300
C	1.46832600	5.57484800	1.04793300
C	2.37909100	4.53809300	-0.95909700
C	2.00313300	6.79676800	0.64234000
H	0.92148300	5.48074100	1.97964000
C	2.90015200	5.76831500	-1.34741600
H	2.52939300	3.65259300	-1.56756300
C	2.72394100	6.91461700	-0.55471300
H	1.86138000	7.67288800	1.26872700
H	3.45725900	5.84286600	-2.27722300
C	3.32698700	8.23400100	-0.96728600
H	2.76604300	9.07806200	-0.55721300
H	4.35752500	8.31624700	-0.60121700
H	3.35846700	8.33804400	-2.05555100
C	3.05154300	-1.39192900	-1.69934400
C	3.56452100	-0.08203700	-1.67975500
C	3.14428400	0.86346200	-2.62745000
C	2.19444300	0.49358500	-3.57875800
C	1.63447200	-0.78315300	-3.59524200
C	2.07043000	-1.72466200	-2.65042300
H	3.56692500	1.85969700	-2.63986300
H	0.88888900	-1.03836000	-4.33669400
C	3.63264600	-2.42870000	-0.79498100
C	3.04733500	-2.85336900	0.41237100
C	4.85943600	-2.99023800	-1.18342000
C	3.71152300	-3.81254400	1.19918600
C	5.50242000	-3.94630400	-0.40354800
C	4.92693800	-4.35871700	0.79956900
H	6.45015300	-4.36396000	-0.72947800
H	5.42132600	-5.09702600	1.42333100
C	1.91869300	-1.29294200	2.63860400
C	3.25932100	-0.53564800	2.50398800
C	0.80208900	-0.31285800	3.05858800
H	2.02577100	-2.07517300	3.40513000
C	3.60368100	0.20175700	3.80823200
H	3.18056900	0.18338200	1.68106900

H	4.06565100	-1.22627900	2.24367800
C	1.14747200	0.41761600	4.36392600
H	0.69567500	0.43280100	2.26647500
H	-0.16334100	-0.81937700	3.15068900
C	2.48487900	1.15878800	4.24045900
H	4.54554600	0.74740300	3.67738400
H	3.77896600	-0.53629900	4.60414500
H	0.34174700	1.12002900	4.60477600
H	1.19830500	-0.30699400	5.18900000
H	2.74217900	1.64122400	5.19034900
H	2.37502900	1.95569500	3.49492100
C	0.51342000	-3.71822000	1.52033200
C	-0.81911900	-3.38759000	2.22482800
C	0.28550000	-4.58014800	0.25804200
H	1.13625400	-4.28778200	2.22249000
C	-1.64157100	-4.65509300	2.50743800
H	-1.40592400	-2.70959100	1.58892000
H	-0.63085500	-2.85700900	3.16321000
C	-0.54752400	-5.83274700	0.56414300
H	-0.23657800	-3.97375200	-0.49430100
H	1.24556600	-4.85536000	-0.18863100
C	-1.88112700	-5.46806800	1.22909000
H	-2.59323800	-4.37630100	2.97435000
H	-1.10657800	-5.27948600	3.23613500
H	-0.71635800	-6.39621600	-0.36096800
H	0.02079300	-6.49385300	1.23264300
H	-2.45918000	-6.37143800	1.45266000
H	-2.48533000	-4.87069300	0.52907800
P	1.46764400	-2.17785200	1.05139100
Au	0.02527400	-0.94586100	-0.35976200
H	5.30776600	-2.65780100	-2.11442100
H	3.28281600	-4.13043000	2.14480200
H	1.87930100	1.21850200	-4.32416900
O	1.59448200	-3.00014700	-2.56601700
O	4.47676200	0.16307000	-0.70449700
C	0.50167000	-3.37152800	-3.39617600
H	0.24779700	-4.39400600	-3.11337400
H	-0.36452300	-2.71947200	-3.22539900
H	0.77287600	-3.34911300	-4.45863800
C	5.01889400	1.47433400	-0.57986500
H	4.23227500	2.20490300	-0.36740500
H	5.70688600	1.42728000	0.26509400
H	5.57503000	1.76561200	-1.47995000

Zero-point correction= 1.059134 (Hartree/Particle)

Thermal correction to Energy=	1.119484
Thermal correction to Enthalpy=	1.120428
Thermal correction to Gibbs Free Energy=	0.959644
Sum of electronic and zero-point Energies=	-3437.977006
Sum of electronic and thermal Energies=	-3437.916656
Sum of electronic and thermal Enthalpies=	-3437.915712
Sum of electronic and thermal Free Energies=	-3438.076497

E-TSb1

C	-2.27664400	5.52528700	-0.00571300
C	-1.95792000	4.17840200	-0.05359700
C	0.04080300	4.71985000	-1.31975200
C	-0.27723700	6.08663500	-1.25399300
C	-1.43950800	6.48389200	-0.61210700
H	-3.17691000	5.84973000	0.50694200
H	-2.59462000	3.43946100	0.42231700
H	0.38059800	6.82003300	-1.71230800
H	-1.70480000	7.53546200	-0.57113100
C	1.29694800	4.24467900	-1.86410000
O	1.30531700	2.99632000	-2.39844000
H	1.87920300	4.92130900	-2.48410600
C	-0.79259600	3.74022600	-0.72423900
C	-0.42476800	2.34590400	-0.84288200
C	0.58133700	2.03808200	-1.74598400
C	0.84302100	0.66535400	-2.30425300
H	-0.05665800	0.05707700	-2.17903200
H	1.04091500	0.76340400	-3.37385100
N	2.02570500	0.02466800	-1.69055900
C	1.94385100	-0.21609600	-0.22836800
H	0.99316400	0.19858600	0.12153100
H	1.89889200	-1.28468100	-0.00942200
C	3.76781400	-0.24644600	1.43915400
H	3.42001200	-1.25680500	1.65564300
C	3.09326500	0.43601900	0.49804200
C	3.39153900	1.85380000	0.08195800
H	4.25448200	2.23180800	0.64839100
H	3.69172800	1.88234100	-0.97492100
C	2.31584000	2.87659900	0.30263500
C	2.43215100	4.14188300	-0.28871800
H	1.57052900	2.69945100	1.07283300
H	2.01691800	4.98829700	0.24836000
H	3.39015600	4.34435200	-0.76694700
O	1.70664200	-2.51340300	-2.23465200
O	2.62575300	-0.90303800	-3.97788700

S	2.53689200	-1.34434000	-2.58314900
C	4.93521900	0.18344800	2.23536300
C	6.05588600	0.79625000	1.64718200
C	4.96510700	-0.07832800	3.61560700
C	7.15628100	1.16561200	2.42232600
H	6.08125700	0.93403800	0.57120600
C	6.06239100	0.29388300	4.39055700
H	4.11611300	-0.57189700	4.08167400
C	7.16076400	0.92173200	3.79729800
H	8.01552100	1.63215100	1.94905600
H	6.06362600	0.08971600	5.45712600
H	8.01805600	1.20607800	4.39968500
C	4.15605100	-1.58831100	-1.88573000
C	4.36721800	-2.63703000	-0.99193900
C	5.17107800	-0.68279100	-2.20259800
C	5.61467300	-2.75869900	-0.38287100
H	3.56357200	-3.33281300	-0.77735500
C	6.41148800	-0.82643900	-1.58920000
H	4.98853100	0.10759000	-2.92312100
C	6.64826600	-1.85239100	-0.65839200
H	5.78784400	-3.56775900	0.32093200
H	7.21210200	-0.13339500	-1.83307600
C	7.97079900	-1.94776300	0.05723700
H	7.95344600	-1.31932600	0.95637200
H	8.18618800	-2.97208700	0.37244600
H	8.79481900	-1.60085300	-0.57271400
C	-3.31070800	-1.23413800	-1.82615500
C	-2.40015700	-1.86839600	-2.69512400
C	-1.80833700	-1.16011300	-3.75202200
C	-2.15431700	0.17582600	-3.94869500
C	-3.05357000	0.83162900	-3.10908600
C	-3.62740800	0.11950600	-2.04560300
H	-1.09507900	-1.63664000	-4.41165500
H	-3.30146400	1.87015700	-3.28519000
C	-4.04371200	-2.02048300	-0.78885600
C	-3.79395100	-1.95035400	0.59864400
C	-5.06624000	-2.86562100	-1.24674000
C	-4.58964100	-2.71068000	1.47648500
C	-5.84216100	-3.61669300	-0.36904800
C	-5.60683800	-3.53460900	1.00324400
H	-6.62895600	-4.25828800	-0.75388200
H	-6.20707100	-4.10860900	1.70233500
C	-1.05539400	-2.20704600	1.66773900
C	-1.40630500	-3.28652600	2.70698200

C	-0.56616500	-2.84591300	0.35163300
H	-0.24488700	-1.58066400	2.06873500
C	-0.20796400	-4.22077500	2.94924500
H	-2.25395400	-3.87704300	2.33856900
H	-1.71859900	-2.82928500	3.65294500
C	0.62534700	-3.78083700	0.60168600
H	-1.38431200	-3.41530700	-0.10231700
H	-0.29517200	-2.07897100	-0.38055000
C	0.28373300	-4.85647100	1.64106000
H	-0.48529400	-4.99455200	3.67367000
H	0.61070700	-3.64390000	3.40326300
H	0.94020800	-4.22591900	-0.34704200
H	1.48075500	-3.19223100	0.96778500
H	1.15318100	-5.49523700	1.83318900
H	-0.50355100	-5.50860800	1.23846500
C	-3.02531900	-0.32697100	2.93923100
C	-1.88192100	0.34605400	3.72778900
C	-4.19448600	0.65409500	2.70443900
H	-3.39255000	-1.17206300	3.53415200
C	-2.39773300	0.94175600	5.04782500
H	-1.44532100	1.14644000	3.11363800
H	-1.07853500	-0.37144600	3.93075000
C	-4.69381600	1.24820300	4.03001000
H	-3.84780800	1.46455600	2.04685500
H	-5.00996800	0.15060800	2.17491100
C	-3.55410700	1.92212100	4.80661800
H	-1.57446500	1.43780900	5.57418200
H	-2.74242300	0.12770300	5.70028800
H	-5.50167600	1.96214300	3.83369200
H	-5.12714800	0.44681100	4.64424300
H	-3.92263500	2.31703600	5.75961300
H	-3.18331200	2.78251500	4.23062100
P	-2.41215500	-0.97543400	1.30834200
Au	-1.44147100	0.81327300	0.11155000
H	-4.41644700	-2.66696000	2.54580300
H	-5.24832200	-2.92046800	-2.31518000
H	-1.70826200	0.72057400	-4.77578900
O	-4.50712600	0.65812300	-1.15073700
O	-2.16919300	-3.18079800	-2.43469800
C	-4.93339500	2.00102400	-1.34100600
H	-5.63270800	2.20840700	-0.52989400
H	-4.09273800	2.70335800	-1.28401000
H	-5.44542200	2.12781000	-2.30261400
C	-1.22549000	-3.88808500	-3.24378600

H	-0.22702000	-3.44767100	-3.16387000
H	-1.20977600	-4.90453900	-2.84860700
H	-1.54582700	-3.91519200	-4.29220400

Zero-point correction= 1.059478 (Hartree/Particle)

Thermal correction to Energy= 1.119352

Thermal correction to Enthalpy= 1.120296

Thermal correction to Gibbs Free Energy= 0.961489

Sum of electronic and zero-point Energies= -3437.969720

Sum of electronic and thermal Energies= -3437.909846

Sum of electronic and thermal Enthalpies= -3437.908902

Sum of electronic and thermal Free Energies= -3438.067709

F-2

C	-1.80045800	-5.23391300	-2.43864200
C	-1.48481700	-4.03360300	-1.84194200
C	0.88248400	-4.58625800	-2.06851100
C	0.53304900	-5.83019900	-2.67704000
C	-0.78909000	-6.14622600	-2.85115300
H	-2.84466200	-5.48061800	-2.60243300
H	-2.27287300	-3.34676700	-1.55968200
H	1.32057100	-6.50371900	-3.00175300
H	-1.07142700	-7.08546400	-3.31491500
C	2.20595400	-4.21036200	-1.90837100
O	2.53113100	-3.05840000	-1.37169400
H	3.06874100	-4.79491700	-2.20822100
C	-0.13281200	-3.66434000	-1.61836500
C	0.25467100	-2.43304600	-1.00240200
C	1.59868400	-2.16511100	-0.93505700
C	2.22985000	-0.88521000	-0.42094800
H	1.73577900	-0.05693900	-0.93537200
H	1.98899900	-0.78471900	0.64300600
N	3.67008400	-0.76419300	-0.57633700
C	4.54373800	-1.51360300	0.36027800
H	3.95264100	-1.63381000	1.27321500
H	4.76611400	-2.51176400	-0.02852500
C	6.99254000	-1.34502500	0.34601700
H	6.92672200	-2.33263300	-0.10934000
C	5.81940600	-0.76672600	0.67179400
C	5.67768700	0.59434000	1.33606600
H	6.55540000	0.77801500	1.96321000
H	5.68138100	1.36791600	0.55364700
C	4.42770900	0.77405800	2.16043300
C	4.40452800	0.86419400	3.49099300
H	3.49753300	0.85648000	1.60145100

H	3.48186600	1.02740300	4.04119800
H	5.31414000	0.79496300	4.08281000
O	5.12226600	-1.79057500	-2.46974600
O	3.00742500	-0.45380900	-2.99502400
S	4.22600800	-0.66055100	-2.19770700
C	8.37352400	-0.86626600	0.51149800
C	9.39624800	-1.83016500	0.61580400
C	8.74791700	0.49194600	0.51908900
C	10.73013900	-1.45825300	0.75812500
H	9.13260600	-2.88452000	0.59011700
C	10.08564800	0.86384100	0.65223500
H	8.00138600	1.26174000	0.37696400
C	11.08126600	-0.10593400	0.78023600
H	11.49718400	-2.22210800	0.84510600
H	10.35052600	1.91748300	0.64877300
H	12.12140900	0.18761000	0.88485400
C	5.17880400	0.84443700	-2.20704300
C	6.56848800	0.79000700	-2.27935600
C	4.49746400	2.06111900	-2.12201000
C	7.28627500	1.98556100	-2.25468200
H	7.07232300	-0.16715900	-2.33457200
C	5.23105300	3.24166500	-2.09778500
H	3.41646500	2.08208500	-2.09229100
C	6.63483400	3.22340700	-2.16090600
H	8.37082400	1.95045700	-2.29670700
H	4.70464900	4.19003500	-2.03646600
C	7.41920900	4.51183200	-2.15986200
H	8.44604400	4.35755000	-1.81729600
H	7.47011100	4.93248900	-3.17140200
H	6.95168800	5.26469300	-1.51828400
C	-3.47169000	0.85864600	1.79448700
C	-4.65349200	1.63486500	1.89601300
C	-5.26799100	1.80379200	3.13351800
H	-6.17430100	2.38960900	3.22557600
C	-4.69676400	1.24350500	4.27702400
H	-5.18417300	1.40109900	5.23107300
C	-3.50928500	0.51374200	4.19601400
C	-2.88656000	0.29877500	2.94570300
C	-3.42598700	0.17024000	6.56806500
H	-3.48423200	1.23608500	6.82146400
H	-2.74716700	-0.32873600	7.25982900
H	-4.42291300	-0.28065700	6.65016900
C	-1.61967700	-0.50088800	2.92418000
C	-1.68400800	-1.91323200	2.89430400

C	-0.49445800	-2.64282800	2.97859500
H	-0.54613300	-3.72726900	2.98059600
C	0.75210800	-2.01630200	3.08105400
C	0.78833500	-0.61960000	3.07041400
H	1.75112600	-0.12535400	3.15185200
C	-0.37488400	0.15756700	2.99824100
C	-3.01801200	-2.64628800	2.79674500
H	-3.78175900	-1.91129800	2.52091700
C	-3.02032900	-3.73282800	1.70621700
H	-2.63252700	-3.34462700	0.75998300
H	-4.03585500	-4.10437900	1.53488600
H	-2.39692500	-4.58933000	1.98324700
C	-3.41704000	-3.23831200	4.16208200
H	-2.69006100	-3.99404100	4.47948900
H	-4.40014000	-3.71745400	4.10540300
H	-3.44750000	-2.46007900	4.92825100
C	2.03210600	-2.81717900	3.27045400
H	2.87191300	-2.11744300	3.16475000
C	2.20617200	-3.93079700	2.22424100
H	1.42604400	-4.69354500	2.31778700
H	3.17212900	-4.42960500	2.35262700
H	2.16020100	-3.53203000	1.20776700
C	2.09492100	-3.39578800	4.69749300
H	2.01955500	-2.60179500	5.44618400
H	3.03550500	-3.93279100	4.85868500
H	1.27026400	-4.09659800	4.86788700
C	-0.27679100	1.67714100	3.07162600
H	-1.24226100	2.09344900	2.77139800
C	-0.03104500	2.12891600	4.52389100
H	-0.79649000	1.72058300	5.19013500
H	-0.04791900	3.22167600	4.59333300
H	0.94458300	1.77936100	4.87992500
C	0.77811600	2.26394200	2.11967800
H	1.79516600	2.01067700	2.43093400
H	0.70144100	3.35434000	2.11050000
H	0.63426900	1.90186300	1.09625900
C	-1.97634100	2.23645300	-0.31837000
C	-1.02649700	2.24700500	-1.35207700
H	-0.85310800	1.35683100	-1.94771600
C	-0.24849300	3.37896500	-1.57966600
C	-0.40208500	4.51746200	-0.78560900
H	0.23175300	5.38341300	-0.93518500
C	-1.36070500	4.51219200	0.22337500
C	-2.15157600	3.38545900	0.45608800

H	-2.87254300	3.40632900	1.26286700
C	-1.46745500	5.66646200	1.18668300
C	-4.05980900	0.19148800	-1.00319700
C	-4.45331000	-1.15020500	-1.01825800
H	-3.99463200	-1.86452300	-0.34223400
C	-5.43090000	-1.58800500	-1.90906100
C	-6.05141500	-0.68929900	-2.77594600
H	-6.81656700	-1.02536100	-3.46489000
C	-5.66746500	0.65275300	-2.74364900
C	-4.66536400	1.09390800	-1.87821400
H	-4.37597800	2.13880000	-1.87507700
C	-5.72383300	-3.06408400	-1.95111900
C	-6.36984400	1.68127900	-3.59313400
F	1.87964900	4.08637600	-2.32077400
F	0.32458600	3.85990900	-3.82583600
F	1.21450600	2.09371200	-2.91605700
F	-0.94107200	6.79750300	0.68605700
F	-2.75094700	5.90844200	1.52421700
F	-0.80473500	5.38003400	2.33615600
F	-4.67357400	-3.73756700	-2.50489500
F	-5.88597400	-3.57213700	-0.70996900
F	-6.81502700	-3.35564000	-2.67390500
F	-7.13398400	1.12183400	-4.54622900
F	-7.17794900	2.45569800	-2.82238400
F	-5.48819100	2.50997300	-4.18755300
O	-5.08704300	2.21555700	0.74211700
O	-2.86880900	-0.02699900	5.27172200
P	-2.70355300	0.61906800	0.15696900
C	-6.40399600	2.76648000	0.68194200
H	-6.46750800	3.70309200	1.24734600
H	-7.14538500	2.05444700	1.06175800
H	-6.59795500	2.95778600	-0.37403000
C	0.79253600	3.35686000	-2.67085800
Au	-1.07597400	-1.04772400	-0.27469500

Zero-point correction=	1.191379 (Hartree/Particle)
Thermal correction to Energy=	1.278397
Thermal correction to Enthalpy=	1.279341
Thermal correction to Gibbs Free Energy=	1.056756
Sum of electronic and zero-point Energies=	-5132.606260
Sum of electronic and thermal Energies=	-5132.519242
Sum of electronic and thermal Enthalpies=	-5132.518298
Sum of electronic and thermal Free Energies=	-5132.740883

F-TSa1

C	-4.70726300	-0.09038500	-2.75868100
C	-3.34215900	-0.15512800	-2.53417900
C	-3.15953200	2.19975100	-3.09473000
C	-4.54963700	2.26863700	-3.28165200
C	-5.31690200	1.12491300	-3.12378400
H	-5.31334300	-0.98221100	-2.63469900
H	-2.86885900	-1.08826700	-2.25664700
H	-5.01068900	3.21258900	-3.55529600
H	-6.39001000	1.16679000	-3.27942200
C	-2.29861400	3.35552600	-3.22918600
O	-1.01810900	3.08606000	-3.63324300
H	-2.69528900	4.20864500	-3.77326200
C	-2.53511600	0.99075100	-2.69169500
C	-1.10961500	0.99739800	-2.42234200
C	-0.40401800	2.06908100	-2.93515000
C	1.08485400	2.25653800	-2.92598900
H	1.58427200	1.29336500	-2.82448200
H	1.39310400	2.72861000	-3.86534800
N	1.46582300	3.13225600	-1.79174400
C	0.45472600	4.10283900	-1.38879000
H	0.86006200	4.69724800	-0.56370900
H	0.28718700	4.77986200	-2.23218600
C	-2.04792100	4.12577200	-1.45352700
H	-1.80769100	5.10120000	-1.88316000
C	-0.87242600	3.50885200	-0.92917400
C	-0.83651000	2.64682100	0.30534000
H	-1.69972900	1.98666900	0.34770700
H	0.04952300	2.00888600	0.26013600
C	-0.75618700	3.47293800	1.57386700
C	-1.67034900	3.41628400	2.54286000
H	0.14637400	4.06490600	1.69597100
H	-1.54380300	3.96213700	3.47216500
H	-2.57284500	2.81955300	2.44300600
O	2.42751400	3.40838300	0.51021400
O	2.44579200	1.09791700	-0.55290600
S	2.58885200	2.55596800	-0.67608100
C	-3.35029300	4.17360900	-0.71656500
C	-3.93111400	5.43664500	-0.52083100
C	-4.02139100	3.04637300	-0.21442300
C	-5.12892200	5.57827000	0.17861800
H	-3.43245400	6.32165800	-0.90879900
C	-5.21979500	3.18694300	0.48480800
H	-3.63000200	2.04970400	-0.37560200
C	-5.77438500	4.45160300	0.68922900

H	-5.55383800	6.56668200	0.32417500
H	-5.72097600	2.30463100	0.86447000
H	-6.70645300	4.55674600	1.23600700
C	4.16276600	2.85005200	-1.45293200
C	4.43707800	4.08682600	-2.04274800
C	5.12974300	1.84627800	-1.38013200
C	5.70097100	4.30805900	-2.57864400
H	3.67258500	4.85540500	-2.08854500
C	6.39101900	2.09130900	-1.91990600
H	4.90055700	0.89889100	-0.90890100
C	6.69624000	3.31693000	-2.52742700
H	5.92372800	5.26465300	-3.04293700
H	7.14864700	1.31496900	-1.86351700
C	8.05249000	3.56491600	-3.13847400
H	8.37885400	4.59692800	-2.97963300
H	8.81018600	2.89709500	-2.72067400
H	8.02379200	3.39582700	-4.22173600
C	-0.04671000	-3.62817300	-1.18440700
C	0.95606200	-3.27179100	-2.11247000
C	0.57398400	-2.92456400	-3.41126500
C	-0.76149800	-2.93368700	-3.82563700
C	-1.73020500	-3.31917500	-2.89466100
C	-1.40465200	-3.66236200	-1.57550400
H	1.34304200	-2.64941600	-4.12860800
H	-2.76841300	-3.36473600	-3.20017900
C	2.43494300	-3.28773400	-1.74422100
C	3.11297200	-1.92543400	-1.97278300
C	3.16858000	-4.41648600	-2.49249200
H	2.51082900	-3.51624300	-0.67615700
H	2.60445600	-1.12316700	-1.43182600
H	4.15100600	-1.95324200	-1.62742700
H	3.12240600	-1.65921200	-3.03549400
H	2.69410700	-5.38117900	-2.29242700
H	3.15100200	-4.24685400	-3.57441300
H	4.21612200	-4.46834000	-2.17749400
C	-1.09603600	-2.51173700	-5.25258800
C	-0.81886400	-1.00643800	-5.45150500
C	-2.52808800	-2.84486100	-5.68915200
H	-0.40963700	-3.06123100	-5.91212000
H	0.20265400	-0.74139400	-5.16205300
H	-0.96256600	-0.72247100	-6.49930900
H	-1.50326800	-0.41165500	-4.83991700
H	-2.75799800	-3.90656100	-5.55633000
H	-3.26180000	-2.26127300	-5.12046200

H	-2.66641400	-2.59982700	-6.74628000
C	-2.49535700	-4.13861400	-0.61595300
C	-2.68166100	-5.66558900	-0.74218300
C	-3.85391500	-3.44002300	-0.79628300
H	-2.15599400	-3.92928600	0.40491700
H	-1.73841500	-6.19512800	-0.60085400
H	-3.40652400	-6.02908600	-0.00606000
H	-3.05615900	-5.91614800	-1.74092300
H	-3.77303300	-2.35098000	-0.78313700
H	-4.33390900	-3.72653900	-1.73804100
H	-4.53215400	-3.72490700	0.01261900
C	0.33707900	-4.02977300	0.20745200
C	0.36911300	-3.13194200	1.29164300
C	0.67483400	-5.38336700	0.43668300
C	0.66132800	-3.60099600	2.59840700
C	0.97831000	-5.82821500	1.72314800
C	0.96147300	-4.94426900	2.80360600
H	1.22967100	-6.86569100	1.90500100
H	1.19583600	-5.31571500	3.79332600
O	0.67972300	-6.18114000	-0.67090500
O	0.63501900	-2.66553600	3.58708600
C	1.01024400	-7.55775900	-0.51819600
H	0.29687700	-8.07183300	0.13831900
H	0.95333400	-7.98795000	-1.51827900
H	2.02676600	-7.68565400	-0.12555600
C	0.81082100	-3.06797600	4.94353700
H	0.09070200	-3.84572600	5.22322400
H	1.83077100	-3.42710900	5.12300500
H	0.62408300	-2.17569500	5.54265600
P	0.14593700	-1.33128800	1.04597100
Au	-0.32586300	-0.35167100	-1.07274600
C	-1.26685500	-0.80608800	2.11039600
C	-2.53578500	-0.79842000	1.52128600
C	-1.13856800	-0.38553300	3.43861000
C	-3.65455700	-0.39094300	2.24872000
H	-2.65644900	-1.09532000	0.48658000
C	-2.25504200	0.05496300	4.14607200
H	-0.17379100	-0.38857700	3.92484500
C	-3.52325500	0.04969700	3.56418800
H	-4.38768800	0.38641200	4.12387700
C	1.66695800	-0.58618300	1.75050400
C	1.67768300	0.67997300	2.34889800
C	2.87849800	-1.23721200	1.50358900
C	2.88781900	1.26147600	2.72135400

H	0.76320900	1.23780500	2.51316100
C	4.08392700	-0.62497900	1.84018000
H	2.89723900	-2.21670500	1.04126900
C	4.09913500	0.62269800	2.45822700
H	5.03734400	1.09330400	2.72778300
C	-5.00441100	-0.46736500	1.58781700
C	-2.05946000	0.62361100	5.52819800
C	2.91296100	2.56976600	3.47168100
C	5.37251800	-1.29773000	1.45090000
F	-4.93870000	-0.04133900	0.29651900
F	-5.92382600	0.29398100	2.21673900
F	-5.47516700	-1.73044200	1.55392800
F	-1.02796400	0.02359300	6.16687100
F	-3.16007600	0.48205400	6.28987000
F	-1.77496800	1.94361800	5.46427800
F	1.75013700	3.24545000	3.36241900
F	3.90823900	3.36790500	3.04456400
F	3.11917100	2.34802300	4.79178900
F	6.40865800	-0.89223800	2.20601600
F	5.69482900	-1.01921800	0.15395900
F	5.28297300	-2.64052800	1.54030000

Zero-point correction= 1.192928 (Hartree/Particle)

Thermal correction to Energy= 1.277703

Thermal correction to Enthalpy= 1.278647

Thermal correction to Gibbs Free Energy= 1.066751

Sum of electronic and zero-point Energies= -5132.596751

Sum of electronic and thermal Energies= -5132.511976

Sum of electronic and thermal Enthalpies= -5132.511032

Sum of electronic and thermal Free Energies= -5132.722929

F-TSb1

C	2.36141000	0.63800400	5.32525500
C	1.88964000	0.08291300	4.14809200
C	-0.36420500	0.13216000	5.05289200
C	0.11656200	0.71411400	6.23763300
C	1.47504400	0.95407100	6.37503400
H	3.42365100	0.83045500	5.43286100
H	2.57968900	-0.15799300	3.34774500
H	-0.57328300	0.96015800	7.04018800
H	1.85889100	1.38543700	7.29402400
C	-1.77969800	-0.04552300	4.79218200
O	-2.12374200	-1.07696800	3.97345700
H	-2.46533300	0.00531200	5.63385000
C	0.51124000	-0.18532600	3.98386100

C	-0.05287500	-0.76726600	2.78464700
C	-1.33927000	-1.26907500	2.87173300
C	-1.93171400	-2.25543500	1.91034600
H	-1.12796500	-2.66179600	1.29207000
H	-2.37426200	-3.07261800	2.48315500
N	-2.98900400	-1.64988400	1.08698000
C	-2.53839300	-0.62971000	0.11174600
H	-1.47732400	-0.44420100	0.30812300
H	-2.59651400	-1.02010200	-0.90329300
C	-3.95918600	1.14976000	-0.82396200
H	-3.76670500	0.63988400	-1.76704700
C	-3.33436900	0.64051200	0.25557600
C	-3.43013900	1.18389300	1.65985100
H	-3.86259500	2.19424600	1.62296300
H	-4.13111100	0.57887600	2.25190300
C	-2.17398500	1.38575700	2.45101600
C	-2.25430800	1.57658700	3.83947000
H	-1.25077800	1.60852900	1.92801400
H	-1.52275300	2.24048700	4.28795600
H	-3.26451000	1.70389200	4.22811000
O	-3.83546900	-3.10312800	-0.91781400
O	-4.25992300	-3.80657200	1.49398300
S	-4.14614700	-2.75315500	0.47873800
C	-4.86282800	2.30450400	-0.94806900
C	-4.88431500	3.01343100	-2.16483000
C	-5.75955400	2.70178400	0.06159200
C	-5.71179600	4.12111600	-2.33875400
H	-4.25553500	2.68166800	-2.98436400
C	-6.59027100	3.80839200	-0.11430200
H	-5.85270900	2.10944100	0.96418800
C	-6.55989200	4.53271700	-1.30804800
H	-5.70303100	4.65588400	-3.28390700
H	-7.27349800	4.09684500	0.67946700
H	-7.20694300	5.39403800	-1.44216400
C	-5.61762600	-1.74505800	0.47581200
C	-6.19574200	-1.37567100	-0.73841800
C	-6.14952400	-1.32096800	1.69465300
C	-7.31478800	-0.54796800	-0.72525000
H	-5.76394100	-1.72719000	-1.66852700
C	-7.26988800	-0.49253000	1.68672700
H	-5.69594400	-1.64064300	2.62728300
C	-7.86256600	-0.08629700	0.48087700
H	-7.76548000	-0.24542100	-1.66602200
H	-7.69531600	-0.15972100	2.62946700

C	-9.03981000	0.85500700	0.46694200
H	-8.72242900	1.84764600	0.12568800
H	-9.81728300	0.50851700	-0.22085200
H	-9.48536200	0.96415800	1.45906500
C	1.67733100	-2.79024600	-1.62666900
C	0.34117800	-3.00423500	-2.03223100
C	-0.48439100	-3.79855300	-1.22939400
C	-0.01385500	-4.41883800	-0.06616000
C	1.31416900	-4.19290500	0.31038200
C	2.17302300	-3.38431100	-0.44489700
H	-1.51948700	-3.95636700	-1.51899000
H	1.69707100	-4.66028500	1.20988600
C	-0.18823100	-2.48112500	-3.36581300
C	-1.47251500	-1.65025500	-3.22923700
C	-0.39051600	-3.65262700	-4.34679300
H	0.57272300	-1.82515600	-3.80084200
H	-1.31256400	-0.79466100	-2.56752700
H	-1.78063100	-1.25822200	-4.20320300
H	-2.30071200	-2.24100100	-2.82609500
H	0.53254700	-4.22823600	-4.45357700
H	-1.17278300	-4.32930900	-3.98735100
H	-0.69149400	-3.28256900	-5.33282600
C	-0.93741600	-5.35659500	0.70259400
C	-0.55125300	-5.55013000	2.17579800
C	-1.01408500	-6.71886400	-0.01763200
H	-1.94480100	-4.92344700	0.67507000
H	-0.39476400	-4.59523200	2.68945800
H	-1.34127100	-6.09413000	2.70148000
H	0.36980500	-6.13470000	2.27723300
H	-1.34830100	-6.59922700	-1.05234000
H	-0.03024000	-7.20104300	-0.03352900
H	-1.71553100	-7.38634200	0.49329200
C	3.63070800	-3.21395600	-0.02560300
C	4.48986500	-4.35577000	-0.60666800
C	3.83458800	-3.11492000	1.49740200
H	3.99726300	-2.27984600	-0.46794700
H	4.38043000	-4.41744000	-1.69161900
H	5.54766900	-4.20741000	-0.36440600
H	4.17524500	-5.31646300	-0.18468400
H	3.12943900	-2.41536500	1.96047000
H	3.69678000	-4.08325800	1.98853900
H	4.85179200	-2.77880300	1.72277400
C	2.56688300	-1.96125800	-2.50251400
C	2.72891500	-0.57137900	-2.33626800

C	3.20861500	-2.58986800	-3.59336400
C	3.47944500	0.18361400	-3.27253200
C	3.97197100	-1.84106900	-4.49093100
C	4.10066600	-0.45949200	-4.33927100
H	4.46241900	-2.31833600	-5.33007400
H	4.67683700	0.10132500	-5.06463800
O	3.00836700	-3.93423500	-3.69593800
O	3.52092400	1.52927700	-3.06285700
C	3.59152800	-4.63131200	-4.79297300
H	4.68644200	-4.56319500	-4.77664500
H	3.29395800	-5.67293600	-4.67180400
H	3.21437300	-4.25467800	-5.75198200
C	4.47418300	2.31545400	-3.78073100
H	5.47695600	1.87916000	-3.70961100
H	4.18955000	2.41822800	-4.83390600
H	4.47757000	3.29451500	-3.30138100
P	2.05438900	0.27243000	-0.87091800
Au	0.97008200	-0.68536600	1.00472200
C	3.42986300	1.23283000	-0.11132600
C	3.69308500	2.57480700	-0.39826400
C	4.19686100	0.58189600	0.86108800
C	4.71824000	3.24438900	0.27017800
H	3.10482900	3.09958700	-1.14082400
C	5.20523000	1.26524400	1.53931700
H	3.99936500	-0.45422800	1.11053600
C	5.47848600	2.60065300	1.24710400
H	6.26257300	3.13157000	1.77244900
C	4.97950400	4.68027900	-0.10741400
C	5.93815100	0.52854100	2.62945200
F	3.86833700	5.43117600	0.04713900
F	5.33368200	4.77337800	-1.41469000
F	5.96298000	5.23096300	0.62343700
F	6.94089500	1.24921400	3.15453700
F	6.44500400	-0.63905800	2.17914500
F	5.08594000	0.20960000	3.64454100
C	0.82881900	1.51923200	-1.42572600
C	0.21118500	1.45284100	-2.67411500
C	0.35486000	2.43004700	-0.46780700
C	-0.88382800	2.27921700	-2.94902900
H	0.55827200	0.75275600	-3.42553700
C	-0.72545800	3.25452600	-0.75756500
H	0.81529100	2.47720500	0.51289300
C	-1.35472700	3.18522000	-2.00291800
H	-2.21491100	3.80822800	-2.21679800

C	-1.63745800	2.10472200	-4.24223000
C	-1.26413600	4.20519300	0.28055600
F	-2.19840600	3.25728200	-4.65684200
F	-2.65399100	1.21189100	-4.08270700
F	-0.85202400	1.63356600	-5.22751400
F	-0.67185300	4.01681900	1.48667800
F	-2.59411600	4.02220700	0.45988100
F	-1.08259900	5.48900100	-0.06950500

Zero-point correction= 1.193149 (Hartree/Particle)
Thermal correction to Energy= 1.277751
Thermal correction to Enthalpy= 1.278696
Thermal correction to Gibbs Free Energy= 1.066962
Sum of electronic and zero-point Energies= -5132.590395
Sum of electronic and thermal Energies= -5132.505793
Sum of electronic and thermal Enthalpies= -5132.504849
Sum of electronic and thermal Free Energies= -5132.716582

G-2

C	-4.30330900	4.14121700	0.04217800
C	-3.64242200	2.95323500	-0.18715500
C	-1.68611300	4.23281500	-0.89489400
C	-2.38811000	5.45025200	-0.64783300
C	-3.67795600	5.39822700	-0.18534500
H	-5.32580600	4.11771300	0.40748500
H	-4.13572900	2.00525000	0.00048600
H	-1.89293000	6.39988300	-0.82816400
H	-4.22704500	6.31363300	0.00902800
C	-0.38424400	4.23790200	-1.37294000
O	0.27048000	3.12921400	-1.61381000
H	0.18776000	5.13155500	-1.59971200
C	-2.30537900	2.95323800	-0.66277900
C	-1.56026700	1.74766200	-0.88626100
C	-0.27781000	1.89307500	-1.35766700
C	0.73957500	0.80334700	-1.57905900
H	0.25328200	-0.16018600	-1.42757600
H	1.12045900	0.82489700	-2.60268100
N	1.91862800	0.88630300	-0.69664200
C	3.04569600	1.76252800	-1.12211600
H	2.79517800	2.11347700	-2.12759200
H	3.10817100	2.65292800	-0.48720000
C	5.42535400	1.53114300	-0.50845400
H	5.27290800	2.49288500	-0.01819000
C	4.36226800	1.01040800	-1.14823500
C	4.34885900	-0.28440800	-1.93794600

H	5.36605700	-0.67906100	-2.00764600
H	3.74505100	-1.02545500	-1.40118000
C	3.81225600	-0.12866600	-3.34083200
C	2.75585300	-0.77864200	-3.83460100
H	4.36797700	0.55592800	-3.98241900
H	2.43911500	-0.65405000	-4.86615500
H	2.17581800	-1.46483600	-3.22160200
O	1.16053800	2.35606200	1.32090700
O	0.49787800	-0.09513500	1.15562100
S	1.49474000	0.96710200	0.95467100
C	6.79586400	1.00665400	-0.36187500
C	7.86576200	1.91972300	-0.32868700
C	7.08782600	-0.35826000	-0.18404800
C	9.17946900	1.48584400	-0.16266200
H	7.65977900	2.98110300	-0.44179000
C	8.40234500	-0.79367600	-0.01493000
H	6.27777700	-1.07564700	-0.13010700
C	9.45457000	0.12479600	-0.00940200
H	9.98885700	2.20975300	-0.14892000
H	8.60339200	-1.85213400	0.12425200
H	10.47704200	-0.21522500	0.12385300
C	3.01763000	0.52407600	1.75424500
C	3.71936300	1.48434100	2.47929500
C	3.48667400	-0.78485100	1.62553200
C	4.93374600	1.12658600	3.06250800
H	3.32033700	2.48824900	2.57277400
C	4.69635400	-1.12247300	2.22032800
H	2.91121000	-1.51086200	1.06342100
C	5.44719200	-0.17096400	2.93216900
H	5.49627100	1.86890600	3.62119400
H	5.07580200	-2.13646000	2.12617100
C	6.79757200	-0.52879800	3.49523400
H	6.82452000	-1.56375700	3.84876500
H	7.56089700	-0.42721900	2.71419600
H	7.07724500	0.12627200	4.32437500
C	-2.95861200	-1.94292600	0.16783900
C	-4.36084700	-3.53162700	0.95829400
C	-3.18364800	-4.13872400	0.64843000
N	-2.33518500	-3.14561900	0.16773100
N	-4.20082200	-2.18493900	0.65631800
C	-0.96406800	-3.33098400	-0.24158800
C	-0.67881200	-3.43163600	-1.61207000
C	0.03384600	-3.36100400	0.74214500
C	0.65903100	-3.59031600	-1.98719700

C	1.35184100	-3.55191600	0.31517200
C	1.68652900	-3.66450600	-1.03773800
H	0.90106300	-3.67785800	-3.04340100
H	2.13583300	-3.61451100	1.06545500
C	-5.16052800	-1.12241400	0.82651900
C	-5.08767700	-0.33781500	1.98598400
C	-6.03718200	-0.83668000	-0.23005200
C	-5.95020800	0.75951700	2.07761700
C	-6.87894800	0.26966600	-0.09062900
C	-6.84960700	1.07754000	1.05358900
H	-5.91053000	1.38381900	2.96654100
H	-7.56457100	0.51304100	-0.89829500
C	-4.06971800	-0.62978200	3.06027500
H	-3.05810200	-0.40481800	2.70168200
C	-6.02042900	-1.66469800	-1.49058700
H	-6.19382700	-2.72541300	-1.28126300
Au	-2.25790500	-0.12193900	-0.39490300
H	-6.78578700	-1.32796000	-2.19294000
H	-5.04469500	-1.59140800	-1.98497400
H	-4.07911200	-1.68457300	3.35254900
H	-4.25630200	-0.02662500	3.95135200
C	-7.78456400	2.25641400	1.18400200
H	-7.39919700	3.00017900	1.88808000
H	-7.94974000	2.74548800	0.21881900
H	-8.76564800	1.93724400	1.55521500
C	-1.77618800	-3.34351800	-2.64394800
H	-2.60482800	-4.01999600	-2.41041400
H	-2.19239900	-2.32990600	-2.68171100
H	-1.40039000	-3.59539700	-3.63805400
C	-0.28028000	-3.12271000	2.19688800
H	-0.44088500	-2.05130600	2.35845000
H	-1.17724200	-3.65469200	2.52554100
H	0.55293800	-3.43401500	2.83128200
C	3.11686000	-3.90000800	-1.46160400
H	3.82294000	-3.49564700	-0.72964900
H	3.32197900	-4.97309200	-1.55467300
H	3.33310300	-3.44039000	-2.43019700
H	-2.86979000	-5.16730200	0.72414100
H	-5.28154500	-3.92341100	1.35973100

Zero-point correction= 0.896676 (Hartree/Particle)

Thermal correction to Energy= 0.953034

Thermal correction to Enthalpy= 0.953978

Thermal correction to Gibbs Free Energy= 0.800898

Sum of electronic and zero-point Energies= -2858.668293

Sum of electronic and thermal Energies=	-2858.611935
Sum of electronic and thermal Enthalpies=	-2858.610991
Sum of electronic and thermal Free Energies=	-2858.764071

G-TSa1

C	2.75114700	3.83379800	-1.62411100
C	2.26748000	2.54820100	-1.43946300
C	0.00468700	3.39215600	-1.72496300
C	0.50195500	4.69683000	-1.87507300
C	1.87045900	4.91230300	-1.83595700
H	3.82165000	4.01337500	-1.60057700
H	2.95032600	1.72014400	-1.27497200
H	-0.18601600	5.52290900	-2.02691300
H	2.26495000	5.91479900	-1.96680900
C	-1.41220700	3.09998600	-1.71890500
O	-1.76479500	1.85776000	-2.16760100
H	-2.08005900	3.85537200	-2.12425600
C	0.87688700	2.29748200	-1.48546500
C	0.29664300	0.99031900	-1.24833500
C	-1.02170600	0.83161600	-1.63049500
C	-1.80230100	-0.44760500	-1.61229200
H	-2.52930100	-0.42817100	-2.43708700
H	-1.15055300	-1.31320900	-1.71664400
N	-2.48466700	-0.53500500	-0.29667600
C	-3.01685400	0.74889700	0.15691800
H	-3.65522200	1.21965900	-0.60302000
H	-3.63127600	0.56284800	1.04382700
C	-1.99561100	3.04060700	0.16608400
H	-3.02016500	3.27812500	-0.12865300
C	-1.88770900	1.67637100	0.56960900
C	-1.04113800	1.17222200	1.71334500
H	-0.84364200	0.10665500	1.57382800
H	-0.08568300	1.68829400	1.76892500
C	-1.83020500	1.37140900	2.99788900
C	-1.60809300	2.34875000	3.87763300
H	-2.62269500	0.64693700	3.17537400
H	-2.20090300	2.43319000	4.78374500
H	-0.83061600	3.09199400	3.72682800
O	-2.62876100	-3.04208600	-0.47043700
O	-4.01236300	-1.77428900	1.28426200
S	-3.46167000	-1.90716600	-0.06830700
C	-1.37326700	4.16068200	0.93680700
C	-2.21198000	5.19528900	1.37941100
C	-0.00608800	4.23139200	1.25117900

C	-1.71077700	6.25397700	2.13643700
H	-3.27258600	5.16322100	1.14242000
C	0.49651200	5.29018900	2.00647400
H	0.67772600	3.46884500	0.89812600
C	-0.35329100	6.30234200	2.45743800
H	-2.38094100	7.03802300	2.47526400
H	1.55703200	5.32544400	2.23717200
H	0.04005500	7.12436500	3.04743600
C	-4.80191000	-1.74848800	-1.23609600
C	-4.66707000	-2.29845500	-2.51399100
C	-5.93937400	-1.01926100	-0.87736100
C	-5.68912700	-2.10695000	-3.44106300
H	-3.78753100	-2.88328200	-2.76043700
C	-6.94902200	-0.83997400	-1.81936200
H	-6.03849000	-0.62819200	0.12946300
C	-6.84137800	-1.37720100	-3.11178400
H	-5.59477400	-2.53716800	-4.43413700
H	-7.84066200	-0.28294300	-1.54549300
C	-7.95778900	-1.20853000	-4.11164800
H	-8.51411600	-0.28271100	-3.94102000
H	-7.57982000	-1.19954500	-5.13774700
H	-8.67093200	-2.03797400	-4.03309400
C	2.51502400	-1.85853500	0.66856600
C	4.28439400	-3.11208200	1.30560400
C	3.25929800	-3.38243700	2.15829100
N	2.18469400	-2.60140300	1.75071400
N	3.80697900	-2.17204500	0.39997600
C	0.91229700	-2.48887400	2.42202000
C	0.79028100	-1.54095900	3.44667000
C	-0.15914900	-3.28042600	1.98442200
C	-0.45101200	-1.43240400	4.08006700
C	-1.38301400	-3.12291500	2.63848100
C	-1.54441800	-2.21422700	3.69288100
H	-0.57170200	-0.70231100	4.87471100
H	-2.23494600	-3.70387000	2.30177700
C	4.55287000	-1.53173800	-0.65394300
C	4.59356900	-2.13867500	-1.91619400
C	5.13501700	-0.28228500	-0.39389000
C	5.26772600	-1.46316600	-2.93708900
C	5.79395300	0.35530900	-1.44916800
C	5.87499800	-0.21988600	-2.72325000
H	5.31304300	-1.91523500	-3.92450200
H	6.25846400	1.32213800	-1.27071200
C	3.89190400	-3.45096200	-2.16240800

H	2.81408000	-3.34966900	-1.98993900
C	5.00978400	0.37010300	0.96144600
H	5.24924100	-0.32465800	1.77232600
Au	1.37287600	-0.48873300	-0.32014700
H	5.67490800	1.23273500	1.04397700
H	3.98218600	0.71433800	1.13130100
H	4.25030600	-4.23501400	-1.48716100
H	4.04353300	-3.79157300	-3.18866600
C	6.62623700	0.47115100	-3.83520100
H	6.19140700	0.24602700	-4.81318100
H	6.62973000	1.55698600	-3.70382200
H	7.67187100	0.14141000	-3.85911000
C	1.93947500	-0.63316700	3.81040400
H	2.83888000	-1.19507100	4.08384500
H	2.20856900	0.00461000	2.95926300
H	1.67536200	0.01427200	4.64930500
C	0.00495200	-4.23538200	0.82925000
H	0.26751800	-3.69123400	-0.08463800
H	0.80368900	-4.96103700	1.01884000
H	-0.92342600	-4.77193000	0.63418100
C	-2.88078100	-2.07790500	4.37887900
H	-2.88442000	-1.24836400	5.09171000
H	-3.67132100	-1.91568300	3.64102800
H	-3.13191700	-2.99110200	4.93028000
H	5.29211200	-3.49210100	1.25631000
H	3.19126300	-4.04535600	3.00576500

Zero-point correction= 0.896366 (Hartree/Particle)

Thermal correction to Energy= 0.951822

Thermal correction to Enthalpy= 0.952766

Thermal correction to Gibbs Free Energy= 0.801734

Sum of electronic and zero-point Energies= -2858.647002

Sum of electronic and thermal Energies= -2858.591546

Sum of electronic and thermal Enthalpies= -2858.590602

Sum of electronic and thermal Free Energies= -2858.741634

G-TSb1

C	-2.60454300	-4.52909300	-0.48660600
C	-2.15502900	-3.21976500	-0.46628900
C	0.12538900	-4.02985000	-0.68304000
C	-0.33611200	-5.35755500	-0.68079300
C	-1.69682800	-5.60285800	-0.59292900
H	-3.66915400	-4.73015700	-0.41677900
H	-2.86146300	-2.40031800	-0.38198800
H	0.37120000	-6.17843600	-0.76281700
H	-2.06584400	-6.62348900	-0.60870000

C	1.53467200	-3.70342500	-0.68953200
O	1.89476600	-2.51157600	-1.22937000
H	2.24658600	-4.47583700	-0.96803000
C	-0.77182500	-2.93829300	-0.56481200
C	-0.23466900	-1.59184600	-0.56116900
C	1.08209100	-1.44658700	-0.97191900
C	1.69871700	-0.15582700	-1.45333500
H	1.88568800	-0.26834900	-2.52609100
H	0.97718000	0.65352300	-1.31604300
N	2.96366300	0.16704800	-0.79156100
C	2.84970600	0.99083700	0.42894700
H	3.87060900	1.17672000	0.78607600
H	2.39540300	1.96099000	0.20743500
C	1.02292000	0.87926500	2.07767000
H	0.75062400	1.84515400	1.65550200
C	2.07304800	0.26640300	1.50059400
C	2.58075200	-1.13321600	1.78111600
H	3.44272700	-1.34209000	1.13854700
H	2.96571500	-1.20751200	2.81094400
C	1.57769800	-2.23358700	1.61566900
C	1.96954000	-3.51399600	1.21723100
H	0.57045800	-2.05853300	1.97723800
H	1.38871800	-4.36175800	1.56761400
H	3.04304100	-3.69217500	1.16122500
O	4.04488100	-0.09863200	-3.07251700
O	4.43610600	2.07203200	-1.79251100
S	4.25886300	0.61134000	-1.80781000
C	0.14687900	0.45162400	3.18181900
C	0.53517600	-0.42111800	4.21547300
C	-1.14909900	1.00000700	3.24071200
C	-0.34224500	-0.74691500	5.24880700
H	1.54026400	-0.82456600	4.23942300
C	-2.02429000	0.68077700	4.27676200
H	-1.46338400	1.67977200	2.45660800
C	-1.62711200	-0.20080900	5.28420800
H	-0.01462100	-1.41665400	6.03843200
H	-3.01310300	1.12851400	4.30505900
H	-2.30480100	-0.44779100	6.09556600
C	5.61759000	-0.12773400	-0.91633900
C	5.63327700	-1.51696500	-0.75375600
C	6.63221900	0.67643300	-0.40241700
C	6.68531300	-2.09826500	-0.05492500
H	4.82923400	-2.11790100	-1.16644900
C	7.68034900	0.07285500	0.29412000

H	6.59430700	1.75043600	-0.54836700
C	7.72536200	-1.31524500	0.47697900
H	6.71071100	-3.17667900	0.07747100
H	8.47543100	0.69168900	0.70017600
C	8.87924800	-1.96398300	1.20025200
H	9.64442300	-2.29046300	0.48574000
H	9.35729800	-1.27188500	1.89855700
H	8.55767700	-2.84831700	1.75831300
C	-2.68235600	1.68031400	-0.35632900
C	-4.59132700	2.86104500	-0.64639200
C	-3.56266500	3.74964100	-0.60385800
N	-2.39930600	3.00725300	-0.42575000
N	-4.03042400	1.59881100	-0.49450400
C	-1.05456700	3.52844400	-0.38461400
C	-0.23687800	3.35785300	-1.51920600
C	-0.59390500	4.14915700	0.78433400
C	1.08926800	3.78568500	-1.43461800
C	0.74309400	4.56956700	0.81260000
C	1.60022600	4.39026800	-0.27615300
H	1.74813900	3.64135500	-2.28696900
H	1.12059300	5.04356300	1.71516300
C	-4.71224800	0.32919700	-0.58014200
C	-4.86653200	-0.25647600	-1.84658800
C	-5.09021900	-0.31765900	0.60268700
C	-5.44044700	-1.52858800	-1.90506800
C	-5.65985900	-1.59046900	0.49189200
C	-5.84359700	-2.20964000	-0.74922300
H	-5.56500200	-2.00388300	-2.87460600
H	-5.95747000	-2.11170900	1.39803300
C	-4.37282100	0.44249100	-3.08868400
H	-3.28546500	0.57566100	-3.04759300
C	-4.81840900	0.30615900	1.94679700
H	-5.13771100	1.35265100	1.98354600
Au	-1.42740200	0.06493800	-0.31757900
H	-5.33030200	-0.23708500	2.74421800
H	-3.74430000	0.28516200	2.15811200
H	-4.81408700	1.43861700	-3.19794600
H	-4.61172500	-0.13406900	-3.98459300
C	-6.47650500	-3.57707000	-0.84711700
H	-6.37677900	-4.13461200	0.08873600
H	-7.54779900	-3.49625600	-1.06600800
H	-6.02730900	-4.16823300	-1.65131800
C	-0.76315800	2.74059100	-2.79354800
H	-0.81411700	1.64822500	-2.72166800

H	-1.77418500	3.09092800	-3.02231600
H	-0.11509600	2.99061800	-3.63638000
C	-1.48357200	4.39609900	1.98046700
H	-1.83558900	5.43437900	1.98996800
H	-2.36642100	3.75357100	1.98805600
H	-0.93615600	4.23035500	2.91222200
C	3.03967600	4.84040600	-0.22894700
H	3.36233200	5.04517900	0.79556300
H	3.69918300	4.08362400	-0.66364800
H	3.17354300	5.76112300	-0.80881000
H	-3.54531500	4.82476000	-0.68048600
H	-5.65285300	3.00459000	-0.76907300

Zero-point correction= 0.896893 (Hartree/Particle)
Thermal correction to Energy= 0.951970
Thermal correction to Enthalpy= 0.952914
Thermal correction to Gibbs Free Energy= 0.802989
Sum of electronic and zero-point Energies= -2858.651100
Sum of electronic and thermal Energies= -2858.596023
Sum of electronic and thermal Enthalpies= -2858.595079
Sum of electronic and thermal Free Energies= -2858.745004

H-2

C	3.85735900	4.48246200	-0.68387900
C	3.20862900	3.31812000	-0.33428900
C	1.24190400	4.64593200	0.24828300
C	1.93253100	5.83856300	-0.12336100
C	3.22156800	5.75103500	-0.58207600
H	4.87825100	4.42768600	-1.04963100
H	3.71269900	2.36223500	-0.42657400
H	1.42876800	6.79697600	-0.03885400
H	3.76204300	6.64668200	-0.87003400
C	-0.05890500	4.68688600	0.72576400
O	-0.70213600	3.59938900	1.07728000
H	-0.64388500	5.59124200	0.85627000
C	1.87266600	3.35385800	0.14421500
C	1.14201300	2.17106200	0.49596900
C	-0.13892300	2.34954600	0.95748000
C	-1.13077600	1.28006000	1.33628100
H	-0.65465000	0.31142800	1.18568500
H	-1.39451800	1.35128600	2.39548500
N	-2.39500400	1.33070200	0.59576800
C	-3.49680300	2.19348200	1.09421100
H	-3.18663500	2.52677200	2.08833900
H	-3.60108500	3.08222400	0.46471500

C	-5.85005300	1.83662600	0.44894000
H	-5.72144700	2.76061600	-0.11617600
C	-4.79494000	1.42138200	1.17440300
C	-4.76647500	0.19378100	2.06731800
H	-5.79155300	-0.14867600	2.24122900
H	-4.24025600	-0.61772500	1.54881400
C	-4.10857000	0.43444400	3.40386300
C	-3.02574500	-0.20812900	3.84653100
H	-4.58506000	1.18271400	4.03827000
H	-2.61000000	-0.01851500	4.83225000
H	-2.52680800	-0.95897400	3.23814100
O	-2.61315300	2.43750000	-1.73612300
O	-0.95425900	0.54497900	-1.31807800
S	-2.26972600	1.16258600	-1.09053600
C	-7.17698900	1.21437900	0.29806000
C	-8.30899800	2.03965900	0.17158700
C	-7.35751500	-0.17841500	0.21003400
C	-9.58069200	1.49464400	0.00578200
H	-8.18596500	3.11892200	0.21375300
C	-8.63005900	-0.72379400	0.04124400
H	-6.49342400	-0.83168300	0.23007400
C	-9.74711800	0.10875200	-0.05512300
H	-10.44196300	2.15062000	-0.07937900
H	-8.74830700	-1.80221800	-0.01956900
H	-10.73719900	-0.31722700	-0.18678500
C	-3.53157300	-0.02976500	-1.50006700
C	-4.56729600	0.32998700	-2.36199300
C	-3.43293400	-1.31898800	-0.97730300
C	-5.52590600	-0.62317400	-2.69226900
H	-4.61808200	1.34116200	-2.74906700
C	-4.40433900	-2.25842400	-1.31797900
H	-2.61584000	-1.58226200	-0.31532500
C	-5.46475900	-1.92603800	-2.17423100
H	-6.34591400	-0.34878900	-3.34940100
H	-4.34357200	-3.26268800	-0.90703600
C	-6.54566700	-2.92164400	-2.50993100
H	-7.51216200	-2.57288200	-2.12829900
H	-6.65116600	-3.04126100	-3.59334500
H	-6.34333300	-3.90465700	-2.07720900
C	2.78211900	-1.55070300	-0.00943900
C	4.44450400	-3.09994800	-0.57159000
C	3.30505400	-3.81936800	0.17633200
N	2.27220800	-2.76057000	0.25292000
N	4.04665600	-1.68468500	-0.42916200

C	0.97084900	-2.97580100	0.82135600
C	0.75785700	-2.70279700	2.18617400
C	-0.04977800	-3.45256900	-0.02844200
C	-0.53038100	-2.91780200	2.69637200
C	-1.31116300	-3.66766300	0.53598100
C	-1.55298400	-3.39692700	1.88332200
H	-0.72718100	-2.72282700	3.74582900
H	-2.11511800	-4.05091500	-0.08163100
C	4.83799800	-0.57450900	-0.88246800
C	4.65366400	-0.09190600	-2.19339700
C	5.72106500	0.03029600	0.03274200
C	5.40459000	1.02491000	-2.58188400
C	6.44523900	1.14648800	-0.40283800
C	6.29357600	1.63570900	-1.69956000
H	5.28762000	1.42191400	-3.58542500
H	7.12951300	1.63963100	0.28025900
C	3.66298800	-0.72078000	-3.16544100
C	5.84401400	-0.45604900	1.47109500
H	5.30183700	-1.40355600	1.55307500
Au	1.90925200	0.27719100	0.24347200
H	3.17400100	-1.56084300	-2.66334200
C	1.86677600	-2.22228300	3.11527100
H	2.75740600	-2.01502600	2.51508200
C	0.20516900	-3.66770300	-1.51735300
H	1.24085200	-4.00799800	-1.63217700
H	2.92870600	-4.69904500	-0.34888400
H	5.42823600	-3.27243800	-0.12918200
C	2.23707800	-3.31846700	4.13302300
H	2.53220500	-4.24582000	3.63109500
H	3.06894500	-2.99091600	4.76510600
H	1.39063800	-3.55262200	4.78702100
C	1.49513300	-0.90798500	3.82577100
H	1.25864900	-0.12425000	3.09986300
H	0.63084700	-1.03572800	4.48554100
H	2.33276800	-0.56085700	4.43916700
C	-0.69617600	-4.74201700	-2.14519100
H	-0.36804700	-4.94976900	-3.16796400
H	-0.66948900	-5.67898000	-1.58016400
H	-1.73735900	-4.40750200	-2.20600500
C	0.07224600	-2.33787300	-2.28731100
H	-0.95216800	-1.96077100	-2.24091000
H	0.71276600	-1.55669700	-1.87456200
H	0.33609200	-2.48277800	-3.34071600
C	5.16500300	0.53791800	2.43400000

H	5.66150500	1.51384800	2.40003600
H	4.11267800	0.68515500	2.17057500
H	5.21526000	0.16999700	3.46436300
C	7.30422200	-0.72024600	1.87723300
H	7.34621000	-1.14006000	2.88725300
H	7.78791000	-1.42421400	1.19282000
H	7.89572200	0.20082300	1.88114000
C	2.55126500	0.27099700	-3.55818800
H	2.00547100	0.62994300	-2.68047700
H	2.96112700	1.13948500	-4.08438700
H	1.83057600	-0.21377900	-4.22398300
C	4.37880900	-1.27954100	-4.40941800
H	5.15551800	-2.00048100	-4.13393200
H	3.66219200	-1.78152100	-5.06722700
H	4.85659900	-0.48147400	-4.98684000
H	6.87247100	2.49592500	-2.02441700
H	-2.54116600	-3.56715800	2.30106200
H	3.59272100	-4.11555800	1.19218300
H	4.48636000	-3.36668200	-1.63428900

Zero-point correction= 1.093944 (Hartree/Particle)

Thermal correction to Energy= 1.157696

Thermal correction to Enthalpy= 1.158640

Thermal correction to Gibbs Free Energy= 0.990425

Sum of electronic and zero-point Energies= -3095.592597

Sum of electronic and thermal Energies= -3095.528844

Sum of electronic and thermal Enthalpies= -3095.527900

Sum of electronic and thermal Free Energies= -3095.696116

H-TSa1

C	2.08259600	3.94803700	-2.08744900
C	1.66156200	2.65332300	-1.83360000
C	-0.63662500	3.44338500	-1.77969600
C	-0.19721700	4.75964400	-1.99630700
C	1.15670300	5.00706300	-2.15709200
H	3.14140600	4.14405400	-2.22391100
H	2.38612100	1.84948500	-1.76994200
H	-0.91953500	5.56871100	-2.04563000
H	1.50421700	6.01869800	-2.34077300
C	-2.02974700	3.11235600	-1.58626800
O	-2.39964400	1.85679300	-1.97873600
H	-2.76860800	3.84420200	-1.90123300
C	0.28669300	2.37044500	-1.66336500
C	-0.21874400	1.05411500	-1.31766800
C	-1.57282300	0.85420500	-1.52005900

C	-2.32000700	-0.44121200	-1.41511900
H	-3.11009100	-0.44481500	-2.17979100
H	-1.66381800	-1.29504900	-1.56439700
N	-2.89362100	-0.52561100	-0.04746200
C	-3.35780600	0.76228800	0.46801200
H	-4.08926600	1.23378300	-0.20135600
H	-3.84294300	0.58286400	1.43309800
C	-2.34143600	3.05248400	0.36818300
H	-3.39489800	3.30042600	0.22182500
C	-2.18408100	1.68349400	0.73550800
C	-1.21325500	1.16105800	1.76590900
H	-1.10465800	0.08177900	1.63922600
H	-0.22886000	1.61069900	1.66024800
C	-1.79269200	1.47316600	3.13527100
C	-2.47569200	0.58446700	3.86083600
H	-1.65244400	2.49248800	3.48888300
H	-2.88544800	0.84541500	4.83232300
H	-2.64825900	-0.42852700	3.50520200
O	-3.29451900	-2.98220300	-0.45049400
O	-4.15222700	-1.85271800	1.69377400
S	-3.91444200	-1.85325000	0.24718000
C	-1.59940100	4.16305600	1.03899000
C	-2.33776300	5.25832500	1.51482100
C	-0.20426600	4.17788100	1.20621900
C	-1.70858800	6.32426200	2.15791900
H	-3.41778600	5.27145700	1.38935300
C	0.42488500	5.24111400	1.85098300
H	0.40164500	3.37259300	0.81103500
C	-0.32360600	6.31679200	2.33282400
H	-2.30084500	7.15790400	2.52262500
H	1.50438500	5.22864200	1.96862200
H	0.16791400	7.14428400	2.83505000
C	-5.44947000	-1.46784500	-0.57932300
C	-5.61002100	-1.82480900	-1.92167700
C	-6.44177600	-0.76089300	0.10535600
C	-6.78108100	-1.45810000	-2.58071900
H	-4.84160500	-2.40220700	-2.42411900
C	-7.60548800	-0.40562900	-0.57220300
H	-6.30978100	-0.52160500	1.15504500
C	-7.79372300	-0.74521500	-1.92097100
H	-6.91625100	-1.73814100	-3.62165200
H	-8.38571000	0.13511800	-0.04379800
C	-9.07427400	-0.38945500	-2.63395500
H	-8.90979500	-0.24070700	-3.70480100

H	-9.80976900	-1.19560900	-2.52512400
H	-9.52378400	0.51954600	-2.22466700
N	3.83432700	-1.42158000	-0.05905400
N	2.40120700	-2.52435300	1.16516900
C	2.54322700	-1.53144500	0.28375800
C	4.69844600	-2.35860400	0.68963700
C	3.66200000	-3.26388700	1.39041100
C	4.35142100	-0.37347500	-0.89309300
C	4.65830500	0.87402900	-0.31344000
C	5.15812000	1.87499200	-1.15620400
C	5.32388000	1.64852800	-2.52117900
C	4.98908100	0.41351400	-3.07288800
C	4.50231400	-0.62516300	-2.27044000
C	4.43359800	1.16815000	1.16498200
H	5.71195300	2.43798200	-3.15829600
C	4.09734800	-1.95511900	-2.89154600
C	1.13149400	-2.86395100	1.74723000
C	0.24138700	-3.67056200	1.01639800
C	-1.04471800	-3.84679400	1.54034700
C	-1.41491200	-3.25314000	2.74419700
C	-0.49462000	-2.49977500	3.47240200
C	0.80259900	-2.29208300	2.99166300
C	0.64226400	-4.34551700	-0.29064000
H	-2.43021700	-3.37037200	3.10714500
C	1.80381000	-1.44318000	3.76918700
H	5.35325900	-2.90427400	0.00604400
H	3.59054300	-4.25639100	0.93213600
H	5.41340800	2.84428000	-0.73865400
H	5.10591700	0.25421400	-4.14008900
H	3.99992800	0.27849800	1.63071500
H	3.85862900	-2.64677600	-2.07748400
H	-1.77507900	-4.42289700	0.98528400
H	-0.79416300	-2.05610400	4.41584100
H	1.70126200	-4.13457100	-0.47408300
H	2.80571800	-1.66757700	3.38859100
C	1.56210400	0.05757200	3.52840800
H	0.57513700	0.35320500	3.89595800
H	2.31538100	0.65867200	4.04970400
H	1.61274300	0.29476900	2.46245700
C	1.81087400	-1.76365200	5.27327900
H	2.62113700	-1.22031600	5.76998900
H	0.87569100	-1.46203500	5.75526400
H	1.95260100	-2.83336400	5.45398700
C	0.48979400	-5.87510400	-0.18703100

H	-0.55878300	-6.16210600	-0.06088700
H	0.85858800	-6.35737100	-1.09820500
H	1.04979300	-6.27450400	0.66450700
C	-0.14149700	-3.79401500	-1.49566500
H	0.13815900	-4.33111000	-2.40860200
H	-1.21984100	-3.89462600	-1.34953800
H	0.08345200	-2.73335600	-1.64939100
C	5.23364300	-2.58409200	-3.71632600
H	4.93118600	-3.56842900	-4.08736900
H	5.49008600	-1.97081500	-4.58610300
H	6.14110500	-2.70818700	-3.11685400
C	2.81762600	-1.78825300	-3.73386700
H	2.99044300	-1.11254700	-4.57847500
H	2.49349200	-2.75439600	-4.13448700
H	2.00251300	-1.37390500	-3.13170300
C	5.75709100	1.47526600	1.88881800
H	6.22664200	2.38142200	1.49262100
H	5.58144900	1.63060400	2.95824700
H	6.47293600	0.65486600	1.77462600
C	3.41505500	2.30873100	1.35504200
H	3.22155100	2.47389600	2.41934500
H	3.78035800	3.24827900	0.92752000
H	2.46669800	2.06589300	0.86701600
H	5.32222400	-1.79997100	1.39698400
H	3.85084800	-3.39147800	2.45848400
Au	1.08322800	-0.31811900	-0.50542000

Zero-point correction=	1.095078 (Hartree/Particle)
Thermal correction to Energy=	1.157291
Thermal correction to Enthalpy=	1.158236
Thermal correction to Gibbs Free Energy=	0.995948
Sum of electronic and zero-point Energies=	-3095.572884
Sum of electronic and thermal Energies=	-3095.510671
Sum of electronic and thermal Enthalpies=	-3095.509727
Sum of electronic and thermal Free Energies=	-3095.672014

H-TSb1

C	-0.31630400	-4.84757300	0.16584700
C	-0.41091400	-3.47231100	0.03470600
C	1.99211800	-3.36367600	-0.29344800
C	2.08347500	-4.75694800	-0.13604000
C	0.93215300	-5.49590700	0.08546600
H	-1.21784100	-5.42915600	0.33133900
H	-1.37871500	-2.98578900	0.09794400
H	3.05084500	-5.24758200	-0.20579500

H	0.99071000	-6.57456400	0.19076400
C	3.16740800	-2.53535700	-0.47949700
O	2.98700000	-1.35837900	-1.12353300
H	4.09304100	-3.00277300	-0.80613800
C	0.74615800	-2.69150400	-0.19614400
C	0.70933700	-1.24622000	-0.34488400
C	1.85258000	-0.65116800	-0.83992800
C	1.99128800	0.75952900	-1.34734600
H	2.16146400	0.72932200	-2.42721000
H	1.05696900	1.29790500	-1.17713800
N	3.07903600	1.49721800	-0.71240900
C	2.71956500	2.30204000	0.46233800
H	3.60119900	2.88248500	0.74819500
H	1.93211500	3.01872500	0.19951400
C	1.11855400	1.66830300	2.25238300
H	0.46588600	2.45108800	1.86670300
C	2.27429600	1.43897400	1.61818100
C	3.25655000	0.35746900	2.03290100
H	4.23750400	0.54069200	1.58859800
H	3.38357900	0.41714600	3.12813300
C	2.85756100	-1.06305400	1.79025800
C	3.74156300	-2.02931800	1.30421400
H	1.89903000	-1.37423000	2.19057300
H	3.65134300	-3.03504600	1.70645900
H	4.76271200	-1.70625900	1.10409800
O	4.19970800	1.55227100	-2.99057200
O	4.95993200	3.14748100	-1.12444600
S	4.48732200	1.83829100	-1.58179800
C	0.67437600	0.96791700	3.48884100
C	0.95411500	1.52984300	4.74422400
C	-0.04435800	-0.23556200	3.43715900
C	0.53347600	0.89924400	5.91679000
H	1.50402000	2.46547400	4.79796500
C	-0.46391600	-0.86740400	4.60913500
H	-0.28239100	-0.66764500	2.47038000
C	-0.17559100	-0.30219100	5.85272000
H	0.76052700	1.34673300	6.87991100
H	-1.02168000	-1.79708400	4.54732300
H	-0.50252500	-0.79199500	6.76493900
C	5.67001000	0.61645300	-1.01394400
C	5.80851900	-0.58406000	-1.71068300
C	6.40923100	0.86550900	0.14453100
C	6.67695400	-1.55699900	-1.21749800
H	5.24462700	-0.74244900	-2.62230200

C	7.26758200	-0.12093300	0.62791300
H	6.32355500	1.82425400	0.64516000
C	7.41298800	-1.34692800	-0.04019900
H	6.80169700	-2.48780900	-1.76523800
H	7.84598100	0.06890300	1.52785000
C	8.37847900	-2.38979500	0.46646000
H	8.44275100	-2.38152100	1.55842100
H	8.09251300	-3.39541000	0.14536500
H	9.38674000	-2.19865700	0.08029700
N	-3.20750000	1.94305200	-0.63344200
N	-4.04455100	-0.07397400	-0.66561800
C	-2.93274600	0.64325700	-0.46657400
C	-4.59783800	2.17820600	-1.08290700
C	-5.21508900	0.76234800	-1.00384200
C	-2.18214100	2.94936800	-0.61977800
C	-1.38815400	3.12609000	-1.76986100
C	-0.31847200	4.02710700	-1.68197600
C	-0.07495500	4.73512100	-0.50662500
C	-0.90710400	4.57351000	0.60268600
C	-1.98373000	3.67998000	0.56809400
C	-1.71001800	2.43991800	-3.09485300
H	0.75735500	5.43139600	-0.46010000
C	-2.89993700	3.47620800	1.77104800
C	-4.09126300	-1.50744900	-0.58828500
C	-4.40127600	-2.10557800	0.64766000
C	-4.40237200	-3.50433600	0.71114300
C	-4.11466700	-4.27218600	-0.41576600
C	-3.80814400	-3.65479100	-1.62676400
C	-3.78552000	-2.25954900	-1.73992100
C	-4.66387100	-1.27822300	1.89877000
H	-4.13097700	-5.35643500	-0.35044500
C	-3.42489400	-1.60629600	-3.06803400
H	-5.09781600	2.89973900	-0.43209500
H	-5.97753500	0.67393300	-0.22312300
H	0.31974700	4.18619300	-2.54573900
H	-0.71734300	5.15285900	1.49979000
H	-2.54506500	1.75275500	-2.93057500
H	-3.85859600	3.10794000	1.39130100
H	-4.62840900	-3.99615100	1.65199000
H	-3.57908800	-4.26376800	-2.49557100
H	-4.71734800	-0.22503100	1.60577000
H	-3.39423100	-0.52314900	-2.91550500
C	-2.02465800	-2.03074700	-3.54848700
H	-1.98252800	-3.10378800	-3.76147000

H	-1.76348000	-1.49839200	-4.46874100
H	-1.26491000	-1.80499000	-2.79462500
C	-4.49343600	-1.89726600	-4.13835200
H	-4.25116100	-1.38073000	-5.07272900
H	-4.55449000	-2.96870400	-4.35512400
H	-5.48597500	-1.56921000	-3.81229400
C	-5.99870700	-1.64058600	2.57200300
H	-5.99688400	-2.66958800	2.94547700
H	-6.18211900	-0.98186300	3.42673100
H	-6.83718300	-1.54040100	1.87561700
C	-3.48286100	-1.40883100	2.87722900
H	-3.62530900	-0.76607900	3.75150000
H	-3.37686300	-2.44156500	3.22782900
H	-2.54755600	-1.11717000	2.39352100
C	-3.18711600	4.77819200	2.53577200
H	-3.94445400	4.59942600	3.30519700
H	-2.29436900	5.15474300	3.04552300
H	-3.55353000	5.56490200	1.86949200
C	-2.35070200	2.39397300	2.71862300
H	-1.44069000	2.73656400	3.21868400
H	-3.08362000	2.15662300	3.49691100
H	-2.10884300	1.47163300	2.18431500
C	-2.16736400	3.48663900	-4.13057600
H	-1.35667500	4.18090600	-4.37335500
H	-2.47811300	2.99672300	-5.05896900
H	-3.00843500	4.07883100	-3.75542700
C	-0.55117600	1.59038900	-3.64356700
H	-0.81836500	1.18088200	-4.62304700
H	0.36408700	2.17767500	-3.76898800
H	-0.33574600	0.74959000	-2.97956600
H	-4.59214600	2.58215700	-2.10050100
H	-5.65097200	0.43146600	-1.95055700
Au	-1.07923300	-0.21682800	-0.24148900

Zero-point correction= 1.094654 (Hartree/Particle)

Thermal correction to Energy= 1.156956

Thermal correction to Enthalpy= 1.157900

Thermal correction to Gibbs Free Energy= 0.994551

Sum of electronic and zero-point Energies= -3095.571042

Sum of electronic and thermal Energies= -3095.508740

Sum of electronic and thermal Enthalpies= -3095.507796

Sum of electronic and thermal Free Energies= -3095.671145

I-2

C	-3.87764800	4.50064100	0.67019900

C	-3.23036900	3.33657500	0.31685200
C	-1.26036500	4.66303800	-0.25735400
C	-1.94956600	5.85535100	0.11774300
C	-3.23955100	5.76844300	0.57391700
H	-4.89912900	4.44752800	1.03467300
H	-3.73519000	2.38042600	0.40518400
H	-1.44393600	6.81319400	0.03807600
H	-3.77892300	6.66393600	0.86439300
C	0.04224900	4.70371700	-0.73047800
O	0.68449400	3.61624800	-1.08377600
H	0.62938900	5.60744400	-0.85526400
C	-1.89381300	3.37191900	-0.16033000
C	-1.16560200	2.18881400	-0.51668200
C	0.11817800	2.36739200	-0.97217100
C	1.10871600	1.29708000	-1.35280200
H	0.62693000	0.32920900	-1.21620900
H	1.38219900	1.37765700	-2.40880700
N	2.36739700	1.33257200	-0.60120000
C	3.47522700	2.19843800	-1.08089400
H	3.17429500	2.54259200	-2.07418300
H	3.57570600	3.08075700	-0.44170100
C	5.82511800	1.83597800	-0.42636300
H	5.69441100	2.75694800	0.14318800
C	4.77292800	1.42520200	-1.15857200
C	4.74805500	0.20232400	-2.05809900
H	5.77393800	-0.13885600	-2.22980600
H	4.22018600	-0.61202400	-1.54578100
C	4.09526800	0.44899800	-3.39603900
C	3.01511300	-0.19268700	-3.84646600
H	4.57368800	1.20057700	-4.02504400
H	2.60333100	0.00099600	-4.83303200
H	2.51418100	-0.94670800	-3.24359300
O	2.55275300	2.42125100	1.74260900
O	0.91364800	0.51861200	1.29191600
S	2.22588100	1.14929100	1.08260800
C	7.15127700	1.21267500	-0.27311800
C	8.28270700	2.03712900	-0.13638900
C	7.33143400	-0.18063500	-0.19266400
C	9.55361300	1.49109200	0.03207700
H	8.15990800	3.11663100	-0.17265200
C	8.60319100	-0.72706500	-0.02131000
H	6.46742300	-0.83371700	-0.22059200
C	9.71978500	0.10486200	0.08533500
H	10.41446500	2.14652300	0.12522800

H	8.72119800	-1.80583900	0.03341400
H	10.70924100	-0.32193000	0.21900200
C	3.49194800	-0.03718000	1.49623800
C	4.52133200	0.32588500	2.36431100
C	3.40114400	-1.32644700	0.97227000
C	5.48162200	-0.62384300	2.69958700
H	4.56563200	1.33684100	2.75275700
C	4.37414700	-2.26243800	1.31785300
H	2.58815000	-1.59189700	0.30620500
C	5.42832800	-1.92664400	2.18050900
H	6.29657500	-0.34690600	3.36189900
H	4.31977900	-3.26678900	0.90620000
C	6.51099700	-2.91839600	2.52169900
H	7.47687700	-2.56938800	2.13868200
H	6.61630500	-3.03234600	3.60570100
H	6.31096100	-3.90394800	2.09370500
C	-2.75995000	-1.54108300	0.00850400
C	-4.31122700	-3.10382000	0.52828200
C	-3.22774000	-3.75244400	0.02298200
N	-2.28352700	-2.77701600	-0.28170000
N	-4.00289600	-1.74988400	0.50843600
C	-0.97432000	-3.00648200	-0.84495700
C	-0.77332300	-2.71946500	-2.20676400
C	0.04615600	-3.47766000	0.00700000
C	0.51539200	-2.92322400	-2.72043000
C	1.30613100	-3.68037800	-0.56614500
C	1.54254600	-3.39962100	-1.91217500
H	0.70752400	-2.72195100	-3.76928200
H	2.11425400	-4.06233300	0.04619000
C	-4.84347500	-0.65538600	0.93161900
C	-4.67632900	-0.15269800	2.23451300
C	-5.70702000	-0.07798900	-0.01634000
C	-5.44390100	0.96385600	2.58971900
C	-6.44917300	1.03764800	0.39067500
C	-6.32291700	1.55016400	1.68101500
H	-5.34654700	1.38033400	3.58725600
H	-7.12689000	1.51213300	-0.31188500
C	-3.68757500	-0.75378100	3.22556000
C	-5.80592100	-0.58936200	-1.44831100
H	-5.21303700	-1.50561700	-1.52729200
Au	-1.92650900	0.29457100	-0.27081400
H	-3.21444900	-1.62120900	2.75626000
C	-1.88957900	-2.24641000	-3.13132000
H	-2.77828500	-2.04233900	-2.52858400

C	-0.19735700	-3.70564700	1.49708800
H	-1.21643800	-4.09092400	1.61457200
H	-3.03840300	-4.80018600	-0.14536400
H	-5.25714100	-3.47008800	0.89290800
C	-2.25936900	-3.35119100	-4.13952300
H	-2.56028200	-4.27046400	-3.62712400
H	-3.08962400	-3.02657900	-4.77512200
H	-1.41275200	-3.59362400	-4.79036200
C	-1.52557400	-0.93377900	-3.84834400
H	-1.28832200	-0.14615600	-3.12668400
H	-0.66530100	-1.05954100	-4.51376100
H	-2.36865600	-0.59265400	-4.45749200
C	0.74988900	-4.74289600	2.11969700
H	0.43168500	-4.96509100	3.14240600
H	0.75997700	-5.67997000	1.55428300
H	1.77652400	-4.36554100	2.17937000
C	-0.11213300	-2.37334400	2.27146700
H	0.89750000	-1.95851100	2.22405800
H	-0.78215400	-1.61364500	1.86600400
H	-0.36790000	-2.53397400	3.32435600
C	-5.20155600	0.43213500	-2.43161000
H	-5.76466100	1.37151200	-2.41646000
H	-4.16073600	0.65635100	-2.17733200
H	-5.23032700	0.04024400	-3.45378700
C	-7.25286800	-0.94751400	-1.83148900
H	-7.28334800	-1.37106300	-2.84030100
H	-7.67819100	-1.68096600	-1.13951700
H	-7.90193700	-0.06587300	-1.82475700
C	-2.56564100	0.24562300	3.56788500
H	-2.02088400	0.56134300	2.67305400
H	-2.96755300	1.13985900	4.05607400
H	-1.84612900	-0.21447000	4.25229000
C	-4.39969600	-1.25224900	4.49657200
H	-5.18614000	-1.97466300	4.25632200
H	-3.68223900	-1.73689500	5.16613500
H	-4.86096300	-0.42644600	5.04793900
H	-6.91420800	2.41113700	1.98036700
H	2.53100500	-3.56072000	-2.33271400

Zero-point correction= 1.070555 (Hartree/Particle)

Thermal correction to Energy= 1.133739

Thermal correction to Enthalpy= 1.134683

Thermal correction to Gibbs Free Energy= 0.967537

Sum of electronic and zero-point Energies= -3094.405720

Sum of electronic and thermal Energies= -3094.342536

Sum of electronic and thermal Enthalpies=	-3094.341592
Sum of electronic and thermal Free Energies=	-3094.508738

I-TSa1

C	2.14043800	3.92217800	-2.11577000
C	1.70109900	2.63336500	-1.86282900
C	-0.58485700	3.45766600	-1.79670300
C	-0.12663100	4.76765300	-2.01262200
C	1.23004200	4.99496700	-2.17970200
H	3.20140700	4.10388000	-2.25586000
H	2.41353600	1.81834000	-1.80141600
H	-0.83668700	5.58784000	-2.05594400
H	1.59189500	6.00163800	-2.36293500
C	-1.98162200	3.14778500	-1.59283800
O	-2.37475000	1.89946100	-1.98580100
H	-2.71159300	3.89228500	-1.89873900
C	0.32263300	2.37072400	-1.68879400
C	-0.20110600	1.06115700	-1.34454900
C	-1.55968100	0.88317400	-1.53812700
C	-2.32329200	-0.40232500	-1.43084400
H	-3.12384200	-0.39166100	-2.18450500
H	-1.68036900	-1.26421300	-1.59286100
N	-2.87867400	-0.48515000	-0.05585500
C	-3.32391100	0.80616500	0.46821800
H	-4.05580100	1.28797300	-0.19326000
H	-3.80214900	0.62902700	1.43713000
C	-2.27592200	3.08381700	0.36491500
H	-3.32678500	3.34820600	0.22899600
C	-2.13551400	1.71148200	0.72724500
C	-1.16703500	1.17202600	1.75199400
H	-1.08322000	0.09036400	1.62675800
H	-0.17330600	1.59894000	1.63821000
C	-1.72859200	1.49752600	3.12544400
C	-2.41518500	0.62050300	3.86177700
H	-1.57125300	2.51617000	3.47376300
H	-2.81133400	0.89054000	4.83642600
H	-2.60466300	-0.39160700	3.51209200
O	-3.29134400	-2.94095900	-0.44625100
O	-4.12823700	-1.80038200	1.70020000
S	-3.90217500	-1.80704800	0.25160300
C	-1.51020300	4.18110300	1.03086100
C	-2.22576100	5.29011500	1.50971600
C	-0.11386700	4.17126400	1.18909100
C	-1.57354000	6.34574500	2.14683800

H	-3.30616800	5.32236200	1.39114600
C	0.53819500	5.22421600	1.82793000
H	0.47554500	3.35501200	0.79131800
C	-0.18780100	6.31391500	2.31271100
H	-2.14847700	7.19039000	2.51394100
H	1.61805600	5.19269100	1.93855400
H	0.32166600	7.13335500	2.81023800
C	-5.44199300	-1.41850600	-0.56405600
C	-5.61464200	-1.77948100	-1.90383500
C	-6.42536100	-0.70389300	0.12559000
C	-6.78875100	-1.40899200	-2.55529700
H	-4.85301300	-2.36249900	-2.41011400
C	-7.59232200	-0.34501100	-0.54443100
H	-6.28428100	-0.46144500	1.17336300
C	-7.79258700	-0.68839200	-1.89050800
H	-6.93323900	-1.69199600	-3.59417300
H	-8.36562400	0.20178900	-0.01210300
C	-9.07661100	-0.32844000	-2.59506500
H	-9.51811500	0.58455400	-2.18593700
H	-8.91954700	-0.18473100	-3.66770600
H	-9.81556600	-1.13018700	-2.47745800
C	2.50090600	-1.53902100	0.29807200
C	4.53734400	-2.42475600	0.72899100
C	3.62270800	-3.12052500	1.45797300
N	2.38352700	-2.55631600	1.18537400
N	3.82844000	-1.45838300	0.02731700
C	1.11083500	-2.90065400	1.77658800
C	0.78499400	-2.32714700	3.02047300
C	0.22498500	-3.69343200	1.02904800
C	-0.51767300	-2.53063900	3.48839500
C	-1.06611500	-3.86121700	1.54405800
C	-1.43902000	-3.27114700	2.74822300
H	-0.82017900	-2.09468700	4.43396500
H	-1.79640800	-4.42940500	0.98115100
C	4.38380000	-0.46058500	-0.85465800
C	4.49463400	-0.76646300	-2.22263500
C	4.72008300	0.79431800	-0.31485000
C	4.99565800	0.23452100	-3.06391200
C	5.22540400	1.75579500	-1.19929600
C	5.36530400	1.47913900	-2.55797900
H	5.09278200	0.03744100	-4.12669900
H	5.50610800	2.73279500	-0.81821700
C	4.04517100	-2.10376700	-2.79711900
C	4.51429300	1.14013300	1.15514000

H	4.11905700	0.25741800	1.66561100
Au	1.07325500	-0.32739000	-0.52757500
H	3.74889300	-2.75202500	-1.96707200
C	1.78862400	-1.49130500	3.81057800
H	2.79512600	-1.77542200	3.48606000
C	0.63234400	-4.37045700	-0.27490500
H	1.69612200	-4.17437900	-0.44580500
H	5.60714000	-2.52384300	0.64153100
H	3.73334700	-3.94999200	2.13755900
C	1.61833000	0.00965200	3.50985500
H	1.70492100	0.21100100	2.43916100
H	0.63629800	0.35796500	3.84316300
H	2.38352300	0.59509000	4.03141100
C	1.71948700	-1.75327400	5.32433300
H	1.79799400	-2.82067100	5.55097100
H	2.53882000	-1.23360800	5.83095300
H	0.78511000	-1.38356500	5.75830800
C	3.46597400	2.25926400	1.31120800
H	3.79761800	3.18698100	0.83301200
H	2.51628800	1.96845100	0.85252900
H	3.28654000	2.46808300	2.37047600
C	5.83909400	1.51345200	1.84344000
H	5.67241200	1.70779400	2.90777500
H	6.57287000	0.70645100	1.75449500
H	6.27987100	2.41514400	1.40591300
C	2.80489100	-1.91809800	-3.69247900
H	1.99234500	-1.43431500	-3.14099500
H	3.03671500	-1.29922800	-4.56577600
H	2.44695400	-2.88814300	-4.05239100
C	5.18253800	-2.81473900	-3.55176300
H	6.05479000	-2.96520300	-2.90799700
H	4.84627300	-3.79400300	-3.90642400
H	5.50654900	-2.24054700	-4.42567900
C	0.46186200	-5.89845300	-0.17251400
H	0.83333200	-6.38293000	-1.08130100
H	1.01221400	-6.30420400	0.68205400
H	-0.59056600	-6.17507700	-0.05528900
C	-0.13891700	-3.81070200	-1.48427300
H	-1.21906600	-3.90650500	-1.34729400
H	0.09145500	-2.75080200	-1.63350900
H	0.14549000	-4.34739800	-2.39587800
H	-2.45751000	-3.38169600	3.10401300
H	5.75997600	2.23816400	-3.22709900

Zero-point correction= 1.071735 (Hartree/Particle)

Thermal correction to Energy=	1.133277
Thermal correction to Enthalpy=	1.134221
Thermal correction to Gibbs Free Energy=	0.973425
Sum of electronic and zero-point Energies=	-3094.387057
Sum of electronic and thermal Energies=	-3094.325515
Sum of electronic and thermal Enthalpies=	-3094.324571
Sum of electronic and thermal Free Energies=	-3094.485367

I-TSb1

C	1.89551900	-4.54689800	1.76092000
C	1.57149300	-3.28728300	1.28757000
C	-0.77192800	-3.75493700	1.72192600
C	-0.43791000	-5.04086600	2.18055200
C	0.89142900	-5.43008000	2.20750400
H	2.93580400	-4.85628000	1.78760000
H	2.35216100	-2.61351800	0.94921900
H	-1.21866300	-5.71364200	2.52541400
H	1.16139500	-6.41435500	2.57673500
C	-2.14693600	-3.31296900	1.61077400
O	-2.37804600	-1.97791500	1.69809500
H	-2.90775600	-3.86288600	2.15870900
C	0.22294600	-2.85805400	1.25583200
C	-0.17762200	-1.54236100	0.79833100
C	-1.47667600	-1.15309600	1.08714600
C	-1.95343200	0.27578100	1.08289000
H	-2.05655600	0.57623900	2.12894900
H	-1.18594200	0.90787100	0.62999400
N	-3.24512000	0.47243700	0.42169700
C	-3.15746300	0.78038400	-1.02153300
H	-4.18488700	0.91101400	-1.38485300
H	-2.62352300	1.72091700	-1.19041800
C	-1.44098600	-0.10617600	-2.56643300
H	-1.00625200	0.89175800	-2.54927200
C	-2.50318300	-0.34042200	-1.78319800
C	-3.12207000	-1.71142000	-1.58038200
H	-4.00419300	-1.63549600	-0.93639200
H	-3.47924100	-2.10445400	-2.54658800
C	-2.19813900	-2.76100200	-1.04717900
C	-2.65531800	-3.78016900	-0.20774200
H	-1.19762600	-2.80647800	-1.46326500
H	-2.15154100	-4.74117600	-0.25099100
H	-3.73491200	-3.84264300	-0.07424200
O	-4.06177900	1.30337700	2.68437400
O	-4.28600000	2.86087700	0.68296600

S	-4.32793200	1.50521800	1.25519400
C	-0.80179000	-1.10784000	-3.45527100
C	-1.51339400	-1.67359500	-4.52505900
C	0.52498100	-1.51287200	-3.24244200
C	-0.91840700	-2.62799600	-5.35142800
H	-2.53237700	-1.34811100	-4.71604500
C	1.11878900	-2.47107900	-4.06369600
H	1.07697500	-1.08597000	-2.41280200
C	0.39831000	-3.03241600	-5.12085700
H	-1.48127400	-3.05119700	-6.17815400
H	2.14422900	-2.77612100	-3.87816000
H	0.86095600	-3.77525000	-5.76359300
C	-5.88050200	0.75046300	0.80397900
C	-6.85053700	1.50554600	0.14812500
C	-6.09883000	-0.59026700	1.13694300
C	-8.06278800	0.89922500	-0.18309900
H	-6.65163400	2.54318800	-0.09659800
C	-7.31292000	-1.17576900	0.79562000
H	-5.32350800	-1.15443900	1.64506900
C	-8.31405100	-0.44176300	0.13531900
H	-8.82468500	1.47882100	-0.69649800
H	-7.49566600	-2.21684600	1.04802800
C	-9.64094600	-1.07916900	-0.19367300
H	-10.11850400	-0.59606400	-1.05037500
H	-9.53124300	-2.14448300	-0.41669700
H	-10.32840800	-0.99333000	0.65648700
C	2.62859600	1.34344800	0.04198200
C	3.62070800	3.37684900	0.00989000
C	4.58091000	2.45787600	0.30033100
N	3.95221400	1.21935700	0.31480500
N	2.43221100	2.67426000	-0.14599400
C	4.56275600	-0.04653400	0.64495800
C	5.16754700	-0.78492800	-0.38656100
C	4.46086100	-0.51049000	1.96992100
C	5.69908200	-2.03651900	-0.05306300
C	5.01190000	-1.76728000	2.24931700
C	5.62419500	-2.52227800	1.25081400
H	6.17047800	-2.63845800	-0.82331500
H	4.96003200	-2.15691800	3.26097600
C	1.11153300	3.22414700	-0.35109400
C	0.67847800	3.45322800	-1.67086800
C	0.29911000	3.42200100	0.78082400
C	-0.65737500	3.83729800	-1.84027500
C	-1.03346000	3.79037200	0.55161200

C	-1.50874200	3.98256200	-0.74296200
H	-1.03921800	4.02509200	-2.83774900
H	-1.71236000	3.92685200	1.38687300
C	1.62984300	3.28627700	-2.85454600
C	0.83748600	3.32650600	2.20560800
H	1.88553800	3.01726600	2.15890700
Au	1.21339700	-0.12631300	0.23003600
H	2.64099800	3.50407700	-2.49214300
C	5.19085200	-0.29491200	-1.82864500
H	4.83461300	0.73943600	-1.84636000
C	3.79623800	0.29834500	3.07721500
H	3.33097200	1.17963700	2.62756000
H	5.63632900	2.56388300	0.49237000
H	3.66771500	4.44864700	-0.09597000
C	6.60682100	-0.30269400	-2.42885300
H	6.58912400	0.11168300	-3.44172600
H	7.29799100	0.29501200	-1.82672700
H	7.01275800	-1.31692900	-2.49620300
C	4.21165800	-1.12698000	-2.67706700
H	4.53088300	-2.17374700	-2.72831000
H	3.21045900	-1.10055900	-2.23983200
H	4.15158900	-0.73852100	-3.69862800
C	4.84348200	0.79482800	4.09199400
H	5.61606300	1.39741700	3.60383300
H	4.36769500	1.40866400	4.86356700
H	5.33999900	-0.04503400	4.58908700
C	2.67448800	-0.49232100	3.77448800
H	1.92762300	-0.83649300	3.05354800
H	3.06494100	-1.36754300	4.30347400
H	2.17154300	0.14239600	4.51057600
C	0.80267500	4.71736300	2.87030500
H	1.25805200	4.67553200	3.86494000
H	1.34716100	5.45637200	2.27414200
H	-0.22562000	5.07388000	2.98629600
C	0.09964600	2.28716700	3.06625100
H	-0.97334100	2.49570200	3.12532700
H	0.23769500	1.27842600	2.66777200
H	0.49515300	2.29942200	4.08701700
C	1.64186200	1.83651900	-3.37552800
H	1.84836200	1.12478000	-2.57365000
H	0.67875200	1.57179600	-3.82204300
H	2.40821200	1.71301400	-4.14785300
C	1.34304200	4.27108900	-3.99883100
H	1.29021800	5.30312600	-3.63973400

H	2.13702700	4.20949300	-4.74914300
H	0.40150500	4.03971700	-4.50755500
H	-2.55107500	4.24811700	-0.88612100
H	6.04805200	-3.49320500	1.49058500

Zero-point correction= 1.071158 (Hartree/Particle)

Thermal correction to Energy= 1.132817

Thermal correction to Enthalpy= 1.133761

Thermal correction to Gibbs Free Energy= 0.971099

Sum of electronic and zero-point Energies= -3094.384164

Sum of electronic and thermal Energies= -3094.322505

Sum of electronic and thermal Enthalpies= -3094.321561

Sum of electronic and thermal Free Energies= -3094.485065