Supporting Information

Theoretical study on the mechanism, chemo- and enantioselectivity of the Ag- vs. Rh-catalyzed intramolecular carbene transfer reaction of diazoacetamides

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Table of Contents

I. Intramolecular 1° / 3° C-H insertion reaction of Ag-carbene

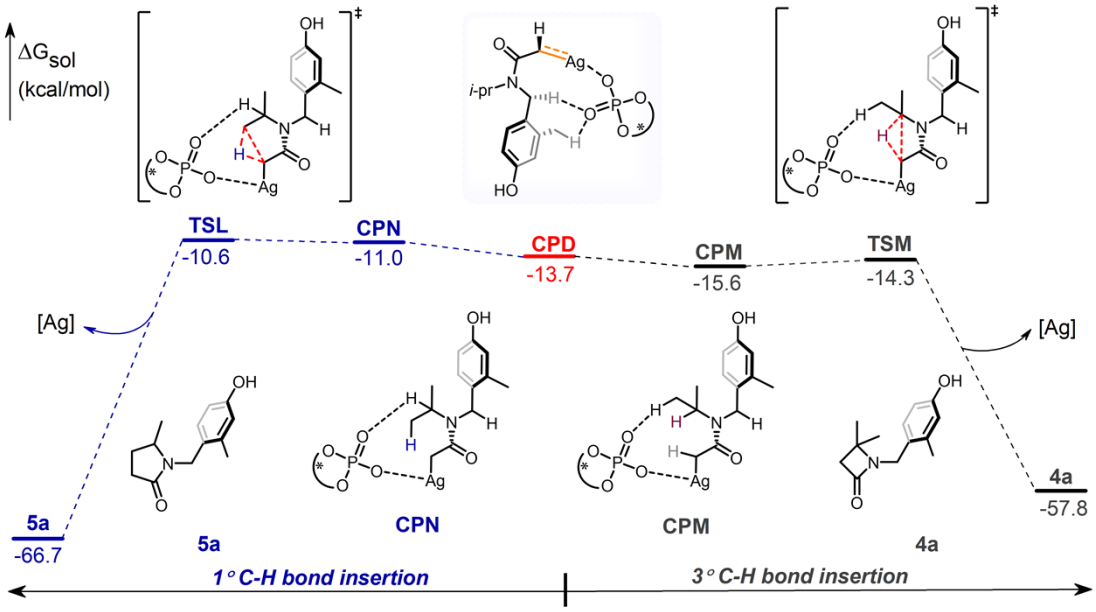


Figure S1. Gibbs free energy profile (in kcal/mol) for the pathways of intramolecular 1° / 3° C-H insertion reaction of Ag-carbene.

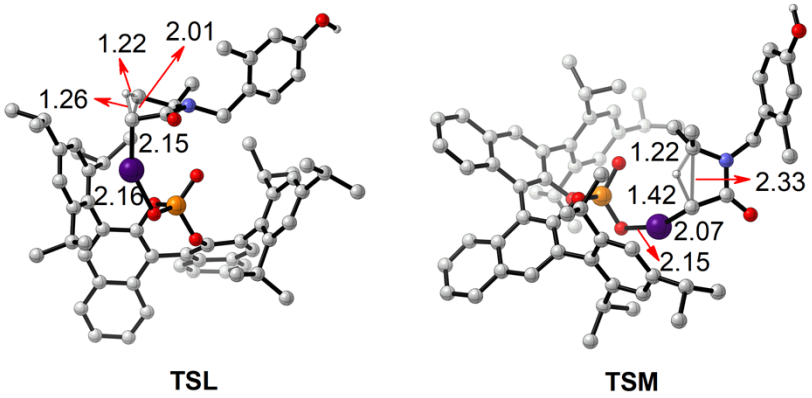


Figure S2. TSL and **TSM** transition state structures involved in silver catalyzed C-H insertion reaction.

II. Intramolecular 1° / 3° C-H insertion reaction of Rh-carbene

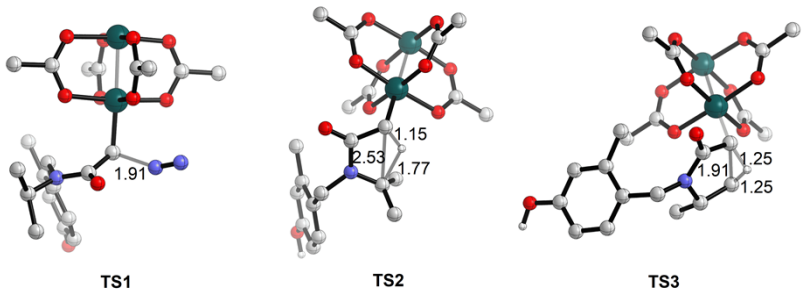


Figure S3. TS1, **TS2** and **TS3** transition state structures involved in rhodium catalyzed C-H

insertion reaction.

III. The Büchner reaction mechanism catalyzed by $Rh_2(OAc)_4$

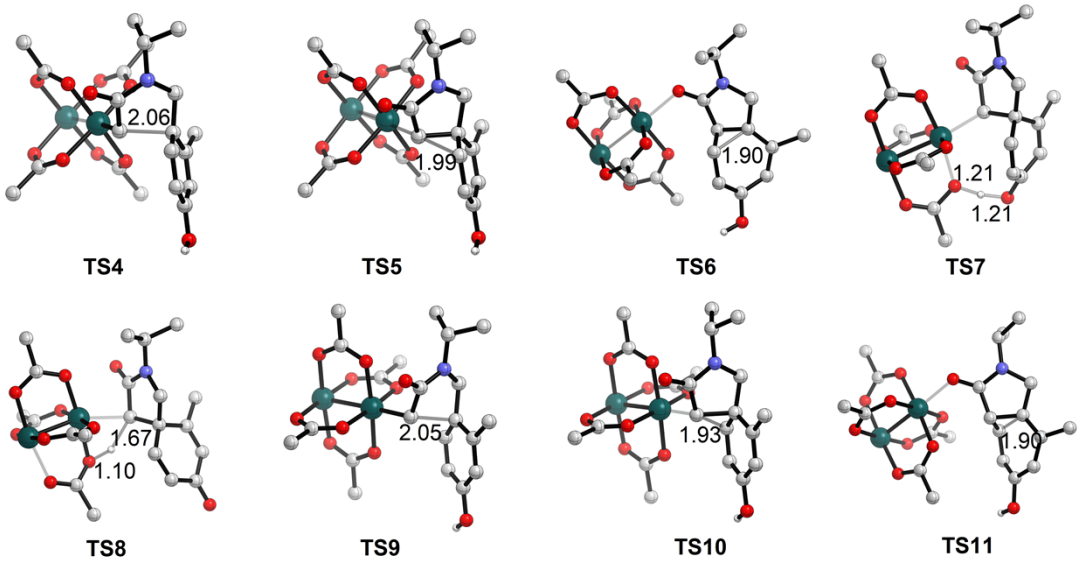
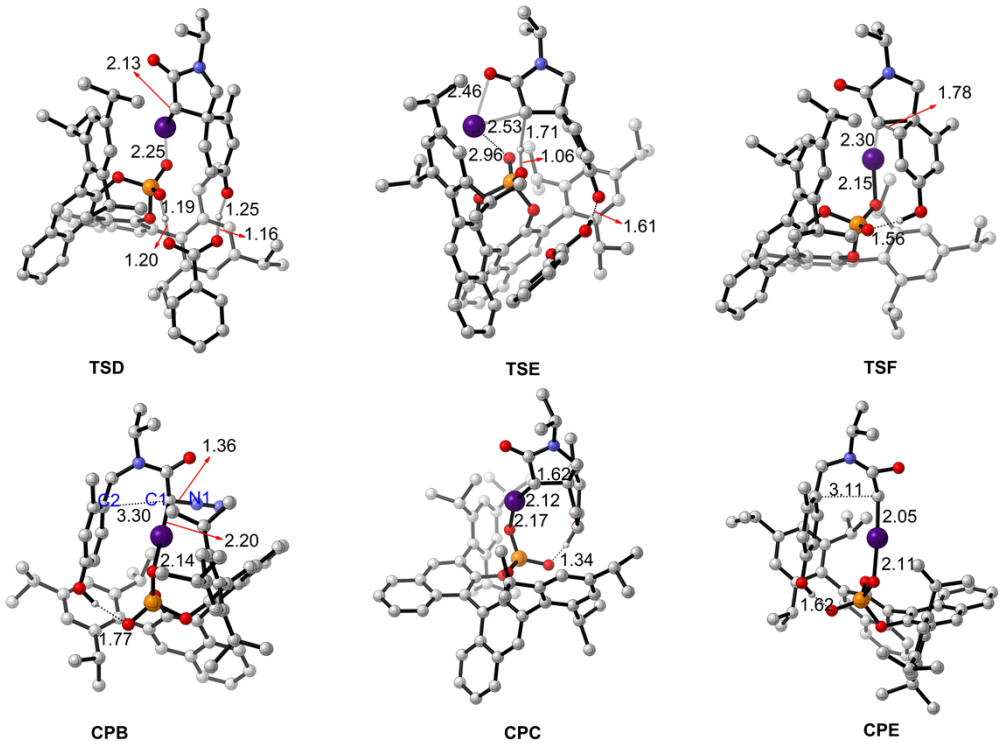


Figure S4. Key transition state structures involved in the Büchner reaction mechanism catalyzed by $Rh_2(OAc)_4$.

IV. Electrophilic addition of R configuration catalyzed by chiral silver phosphate



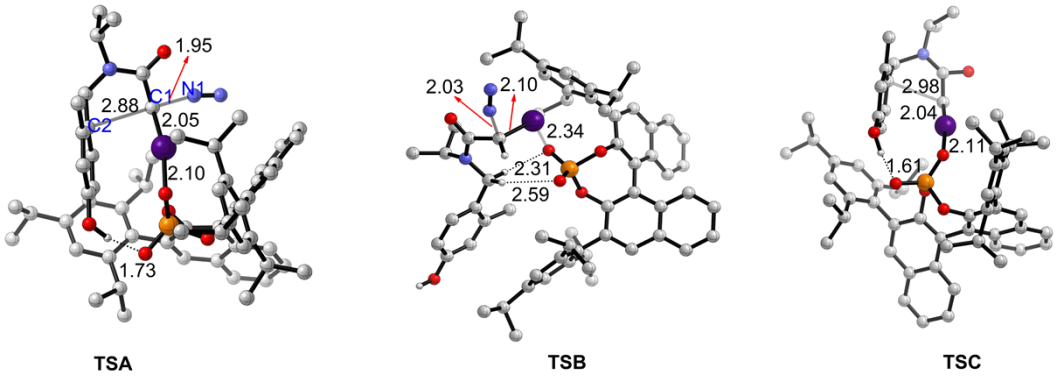


Figure S5. The 3D structures of key transition states and intermediates involved in the Ag-catalyzed asymmetric R-configuration de-aromatization reaction.

V. Proto-demetalation process without Benzoic acid and Büchner reaction of R configuration

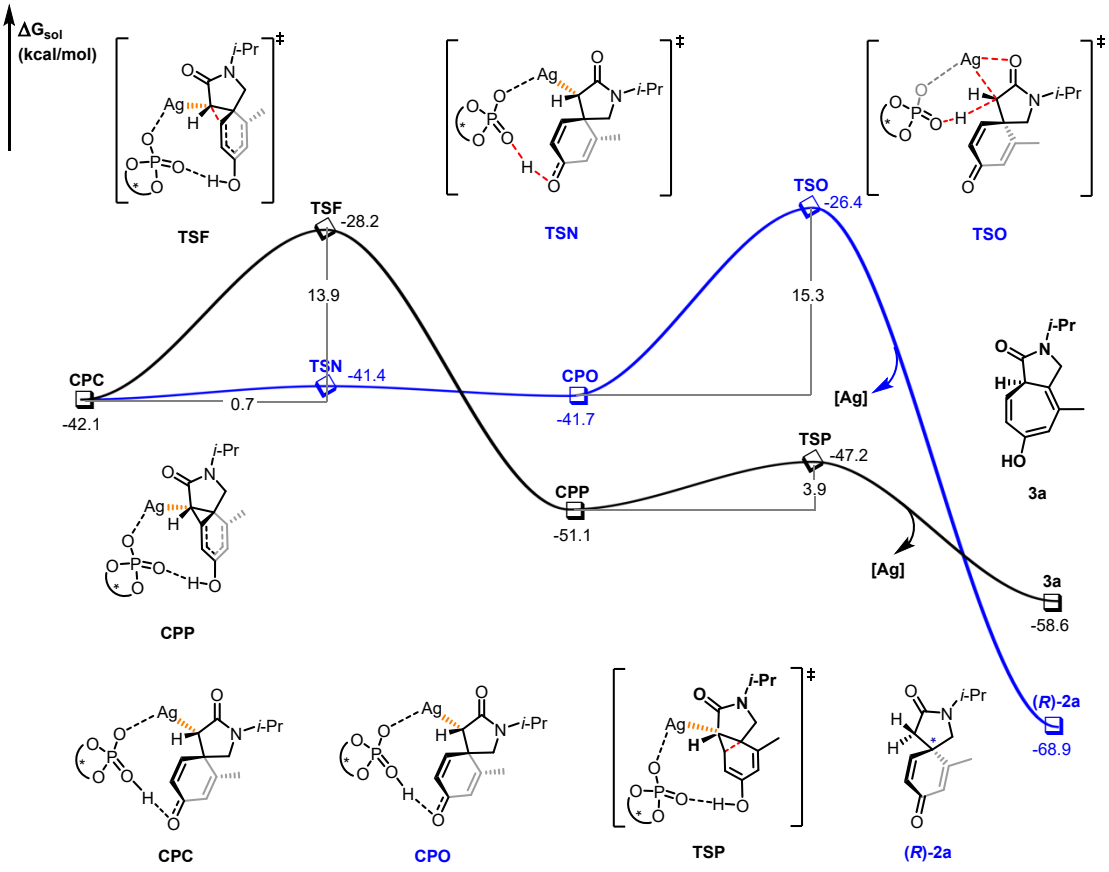


Figure S6. Gibbs free energy profile (in kcal/mol) for the proto-demetalation process without the assistance of benzoic acid and Büchner reaction mechanism of R configuration catalyzed by chiral silver phosphate.

VI. Electrophilic addition of S configuration catalyzed by chiral silver phosphate

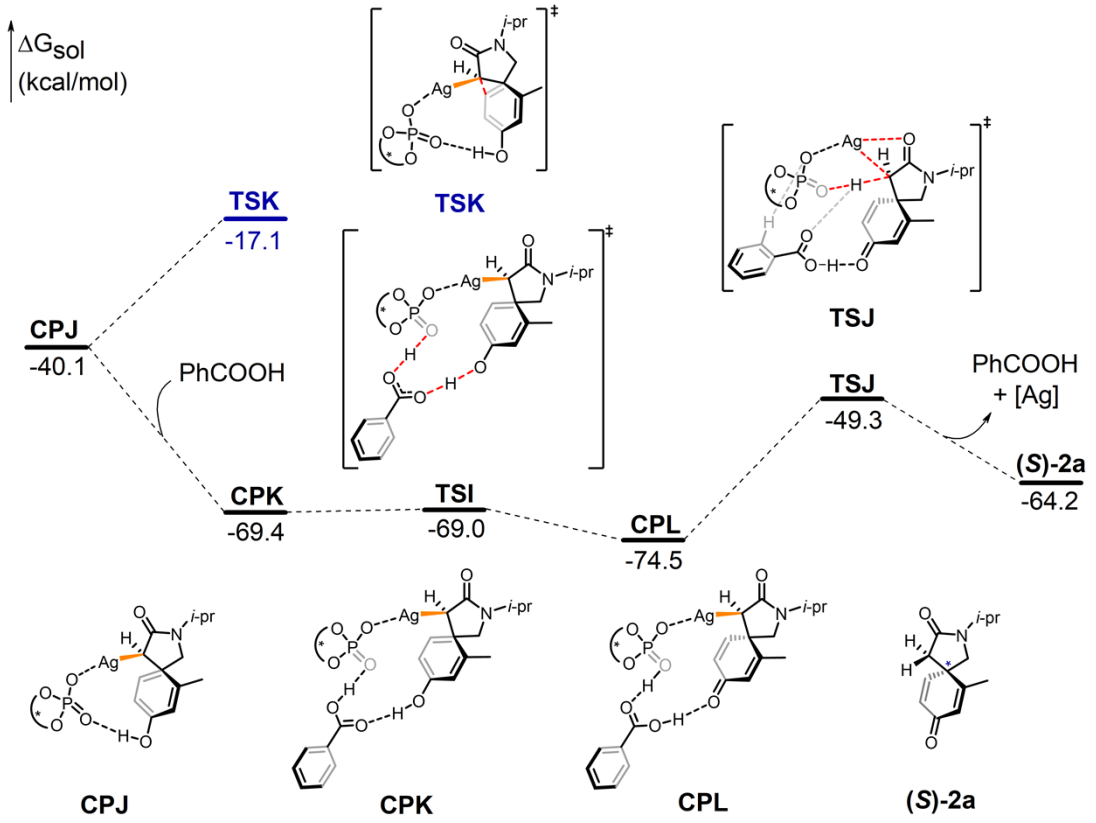
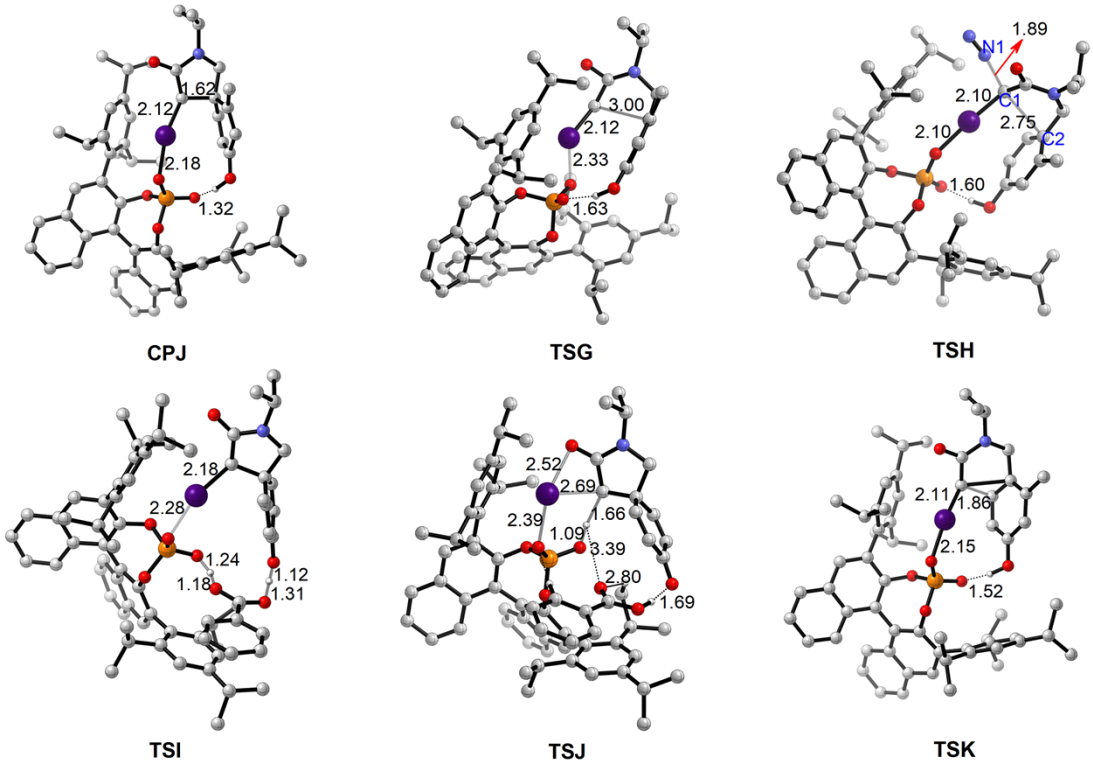


Fig. S7. Gibbs free energy profile (in kcal/mol) for the proto-demetalation process and Büchner reaction mechanism of S configuration catalyzed by chiral silver phosphate



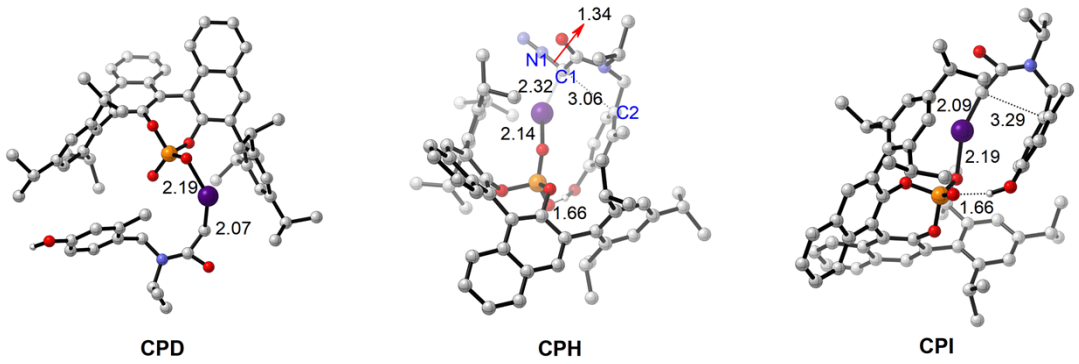


Figure S8. The 3D structures of key transition states and intermediates involved in the Ag-catalyzed asymmetric S-configuration de-aromatization reaction.

VII. Orbital interaction diagram of transition metal carbene

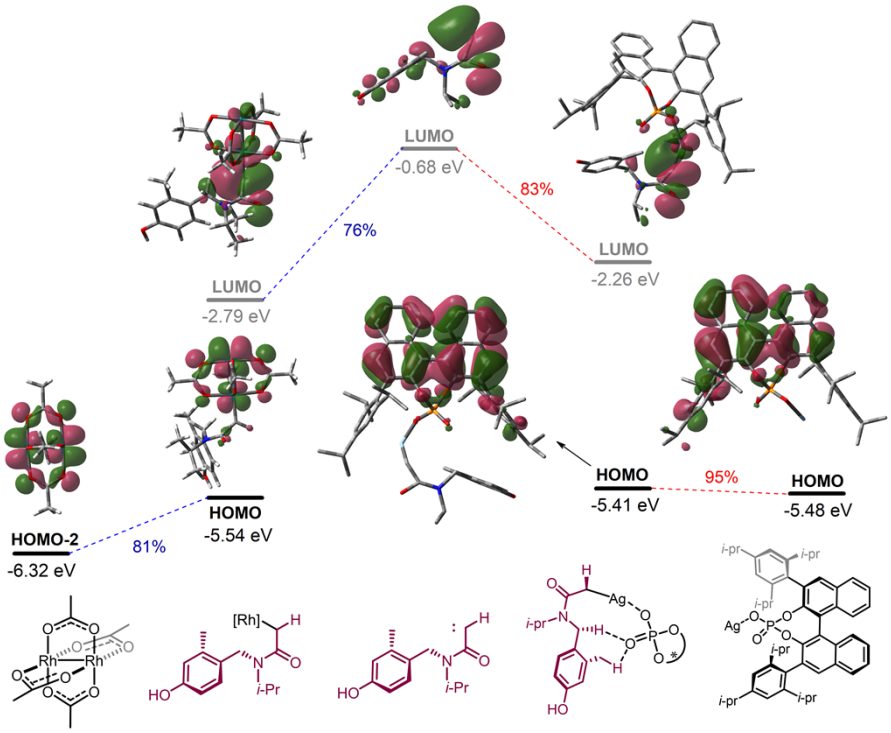


Fig. S9. Orbital interaction diagram of Ag-carbene and Rh-carbene

VIII. The orbital weight Fukui function diagram of donor metal carbenoid

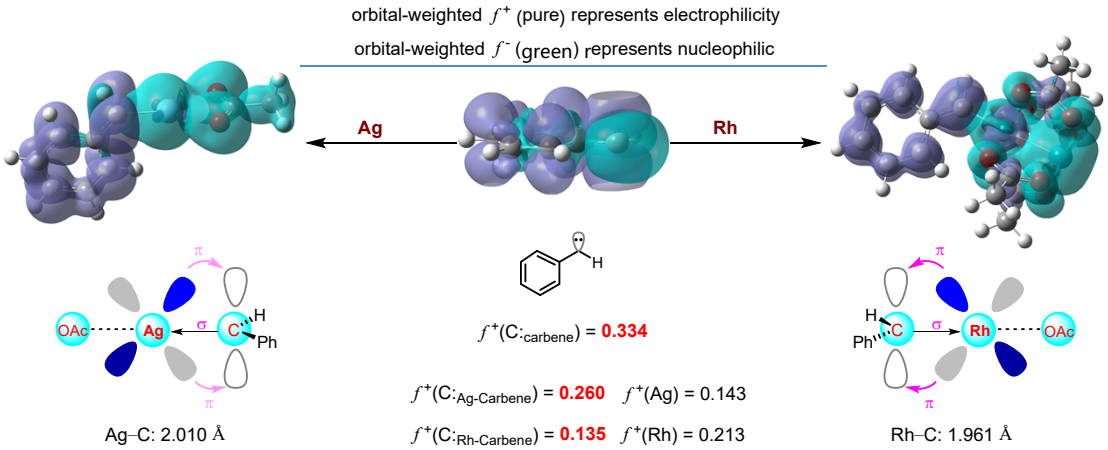


Fig. S10. The orbital weight Fukui function diagram of donor Ag-carbene and donor Rh-carbene.

Ⅸ. Cartesian Coordinates of the Computed Structures

$Rh_2(OAc)_4$

Zero-point correction=	0.210282 (Hartree/Particle)		
Thermal correction to Energy=	0.231500		
Thermal correction to Enthalpy=	0.232444		
Thermal correction to Gibbs Free Energy=	0.159203		
Sum of electronic and zero-point Energies=	-1135.037849		
Sum of electronic and thermal Energies=	-1135.016631		
Sum of electronic and thermal Enthalpies=	-1135.015687		
Sum of electronic and thermal Free Energies=	-1135.088928		

Rh	-0.00447900	-0.00466700	1.19365300
Rh	-0.00439100	-0.00452600	-1.19349000
O	1.44405800	1.44879900	1.13435100
O	-1.45765200	1.44346700	1.13397700
O	1.44850200	-1.45296600	1.13403100
O	-1.45242800	-1.45728900	1.13375900
O	-1.45163700	-1.45785400	-1.13401300
O	-1.45827200	1.44290700	-1.13376600
O	1.44928500	-1.45218500	-1.13370600
O	1.44341100	1.44974300	-1.13335300
C	1.86406600	-1.85874700	0.00017900
C	-1.86344200	1.85904400	0.00011800
C	-1.86747500	-1.86348400	-0.00016700
C	1.85892100	1.85542900	0.00059200
C	2.96083900	2.88412300	-0.00039800
H	3.92423100	2.36490800	-0.04252900
H	2.87912000	3.52309000	-0.88076200

H	2.92741500	3.47583400	0.91504900
C	2.96563800	-2.88774000	-0.00022600
H	2.89811300	-3.51247500	-0.89179700
H	3.92970000	-2.36831200	-0.01669700
H	2.91699700	-3.49406400	0.90501800
C	-2.97020400	-2.89108900	-0.00042900
H	-2.91608400	-3.50368200	0.90032900
H	-3.93353700	-2.37007400	-0.00590800
H	-2.90970900	-3.50971900	-0.89669200
C	-2.89103000	2.96187000	-0.00004600
H	-3.50259300	2.90892100	0.90148800
H	-2.36985100	3.92509500	-0.00718500
H	-3.51064000	2.90072800	-0.89561400

CP1

Zero-point correction=	0.501163 (Hartree/Particle)
Thermal correction to Energy=	0.540973
Thermal correction to Enthalpy=	0.541917
Thermal correction to Gibbs Free Energy=	0.429872
Sum of electronic and zero-point Energies=	-1955.035867
Sum of electronic and thermal Energies=	-1954.996057
Sum of electronic and thermal Enthalpies=	-1954.995113
Sum of electronic and thermal Free Energies=	-1955.107158

Rh	0.90343500	-0.00409100	0.34096700
Rh	2.96053600	-0.72118800	-0.71758800
O	0.47123900	1.01346000	-1.40788300
O	0.00454000	-1.71219800	-0.41789100
O	1.92082300	1.62610700	1.05071700
O	1.47751300	-1.06871900	2.00742700
O	3.43596100	-1.68125100	1.04157900
O	1.95703800	-2.41043900	-1.34209700
O	3.82851400	1.00531300	-0.01053000
O	2.37107600	0.28235900	-2.41188000
C	3.14378200	1.78400200	0.72347600
C	0.72777800	-2.54593500	-1.06304000
C	2.60845700	-1.66364300	2.00167600
C	1.28428200	0.93597100	-2.38837900
C	-3.99114800	-1.50669400	-0.95966600
C	-5.01434500	-2.29845900	-0.44292000
C	-5.76710200	-1.87414600	0.65747800
C	-5.49246400	-0.64158900	1.24921700
C	-4.46797400	0.15333600	0.73291100

C	-3.71097300	-0.25725700	-0.36344800
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H	-6.07042700	-0.30136800	2.10542800
H	-4.25446100	1.11061900	1.19538900
C	-3.19044800	-1.98091100	-2.14652500
H	-3.48263700	-2.99159800	-2.44099200
H	-3.33404500	-1.32555900	-3.01495100
H	-2.12052600	-1.98302500	-1.91825200
C	-2.57883800	0.58505000	-0.92305200
H	-2.76777200	0.81702500	-1.97636600
H	-1.65087900	0.01077700	-0.92954600
N	-2.35752500	1.85584600	-0.23921400
C	-1.55001300	1.95213000	0.85140400
O	-1.24046300	3.00720200	1.40129600
C	-1.03541300	0.63416800	1.39573100
H	-1.64101700	-0.26717800	1.32738300
N	-0.57290500	0.79971500	2.65578400
N	-0.10068600	0.96249400	3.66001500
C	-2.88660900	3.09209500	-0.86694100
C	-1.75469500	3.92247400	-1.48153900
C	-3.76850000	3.90684000	0.08431100
H	-3.52790900	2.72854700	-1.67592100
H	-1.15725600	3.30793200	-2.15918300
H	-2.16939800	4.76656200	-2.04199700
H	-1.10050500	4.30458400	-0.69630200
H	-4.59284700	3.29773800	0.46675600
H	-3.18530700	4.28504400	0.92398000
H	-4.19926900	4.75482800	-0.45757500
O	-6.75141100	-2.71048300	1.10280700
H	-7.19225800	-2.30150700	1.85858300
C	0.91649800	1.71637000	-3.62773700
H	-0.14010400	1.56850300	-3.86263500
H	1.06737800	2.78275300	-3.43221400
H	1.54039600	1.41377100	-4.46853000
C	3.83899300	2.99646700	1.29099000
H	3.13180900	3.82076000	1.39468000
H	4.22094600	2.74736700	2.28677600
H	4.68056900	3.28042900	0.65824600
C	2.96840000	-2.42816500	3.25190100
H	2.74300100	-1.82489700	4.13412300
H	2.35601700	-3.33417600	3.30293600
H	4.02173400	-2.70743000	3.23710700
C	0.04745500	-3.79873400	-1.56240300
H	-0.82773200	-4.02916400	-0.95408500

H	-0.27796200	-3.63848100	-2.59572500
H	0.75294600	-4.63099500	-1.55741600

TS1

Zero-point correction=	0.498329 (Hartree/Particle)
Thermal correction to Energy=	0.538355
Thermal correction to Enthalpy=	0.539299
Thermal correction to Gibbs Free Energy=	0.425765
Sum of electronic and zero-point Energies=	-1955.008857
Sum of electronic and thermal Energies=	-1954.968832
Sum of electronic and thermal Enthalpies=	-1954.967888
Sum of electronic and thermal Free Energies=	-1955.081421

Rh	0.90709000	0.02507100	0.34268300
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O	0.47825600	0.94800200	-1.45972800
O	-0.04259000	-1.70610600	-0.29705200
O	2.00846900	1.65432600	0.92260000
O	1.49813000	-0.95554900	2.05116800
O	3.40443200	-1.71049600	1.07577500
O	1.85817200	-2.51827100	-1.23871000
O	3.87216700	0.90451100	-0.13634100
O	2.33373300	0.10673700	-2.46377500
C	3.22758500	1.75309900	0.54789000
C	0.63874200	-2.59818600	-0.91439700
C	2.61026100	-1.59078600	2.05280500
C	1.27037600	0.79139700	-2.45208900
C	-4.10607300	-1.50721700	-0.87915600
C	-5.15041600	-2.24614800	-0.32781900
C	-5.85036400	-1.77937800	0.79014600
C	-5.49894300	-0.55902800	1.36623700
C	-4.45296500	0.18299700	0.81528200
C	-3.75256900	-0.26803600	-0.30202800
H	-5.43794500	-3.20089100	-0.75663000
H	-6.03362300	-0.18768600	2.23747400
H	-4.17871000	1.13039500	1.26579400
C	-3.35663000	-2.03151500	-2.07883100
H	-3.69706300	-3.03369800	-2.34932800
H	-3.49528200	-1.38468300	-2.95440300
H	-2.28134500	-2.07594100	-1.88003700
C	-2.59089300	0.50996800	-0.88969300
H	-2.73921000	0.66684100	-1.96381400
H	-1.67605600	-0.08586600	-0.83037800

N	-2.36018300	1.82010900	-0.28691700
C	-1.47125800	1.97280000	0.73235000
O	-1.17799700	3.05216100	1.24698300
C	-0.81542700	0.68236400	1.17130600
H	-1.49510900	-0.08109500	1.56322500
N	-0.26072400	1.26500000	2.90429300
N	0.50866300	1.49124600	3.66718800
C	-2.96237800	3.00599300	-0.94184700
C	-1.89008400	3.82171800	-1.67257100
C	-3.79806800	3.85544800	0.02041400
H	-3.64532100	2.58232700	-1.68551500
H	-1.32919700	3.18448200	-2.36124000
H	-2.35573400	4.63228300	-2.24209500
H	-1.19050700	4.25134400	-0.95335000
H	-4.58284100	3.25394700	0.48778800
H	-3.16944900	4.28737800	0.79902300
H	-4.28053600	4.66497400	-0.53658300
O	-6.86139500	-2.56427600	1.26810700
H	-7.25728700	-2.13266900	2.03607300
C	0.88428800	1.51383500	-3.72124500
H	-0.15824100	1.29764300	-3.96846400
H	0.96777500	2.59251800	-3.55738500
H	1.53697500	1.21754900	-4.54197900
C	3.93945800	3.01794300	0.96085500
H	3.50667200	3.86298200	0.41666100
H	3.78069900	3.19940300	2.02649200
H	5.00399500	2.94562000	0.73931400
C	2.99916500	-2.23332500	3.36217900
H	3.85071000	-2.89837800	3.22034500
H	3.26588300	-1.44903100	4.07769600
H	2.14893500	-2.78181500	3.77419900
C	-0.10050300	-3.85419100	-1.31304000
H	-0.98170000	-3.99854000	-0.68734600
H	-0.42088700	-3.76174500	-2.35613900
H	0.56865600	-4.71336800	-1.24352500

CP2

Zero-point correction=	0.490023 (Hartree/Particle)
Thermal correction to Energy=	0.528143
Thermal correction to Enthalpy=	0.529088
Thermal correction to Gibbs Free Energy=	0.420872
Sum of electronic and zero-point Energies=	-1845.517646
Sum of electronic and thermal Energies=	-1845.479526

Sum of electronic and thermal Enthalpies= -1845.478582
Sum of electronic and thermal Free Energies= -1845.586797

Rh	-1.08071500	0.56940100	-0.38336600
Rh	-2.41242900	-1.28072600	0.54486400
O	-0.10196700	0.65311600	1.43160100
O	0.20660800	-0.90324600	-1.05993900
O	-2.52764600	1.82639400	0.36229400
O	-2.15998000	0.38281500	-2.12441100
O	-3.34548500	-1.37277400	-1.29670400
O	-0.96304300	-2.59329100	-0.10465900
O	-3.78981800	0.11669800	1.16205800
O	-1.36429200	-1.02052300	2.30936500
C	-3.55763100	1.34186000	0.94497600
C	0.01541800	-2.13358400	-0.75832900
C	-3.04553500	-0.54021800	-2.20061600
C	-0.46399900	-0.13622000	2.37317700
C	4.30635200	-1.07003800	-1.09629200
C	4.78102800	-2.13858500	-0.33123900
C	4.29043600	-2.38112100	0.95468300
C	3.30318600	-1.54669200	1.48702100
C	2.82930400	-0.48083000	0.72759800
C	3.31863100	-0.22353500	-0.55524100
H	5.54263700	-2.80302100	-0.72624400
H	2.90458200	-1.73189300	2.48202400
H	2.04478600	0.15285600	1.12128900
C	4.85035200	-0.86529800	-2.49090300
H	5.60522500	-1.61849700	-2.72741300
H	4.06127700	-0.93600300	-3.24818900
H	5.31801300	0.11961200	-2.60515300
C	2.72224000	0.90931000	-1.36268000
H	1.79357600	0.56237100	-1.83174500
H	3.40006000	1.21226100	-2.16809500
N	2.40585700	2.08952100	-0.55649700
C	1.17192700	2.61257100	-0.58656300
O	0.78444200	3.67724400	-0.07187200
C	-0.00462000	1.97855600	-1.18214600
H	-0.35525800	2.46148200	-2.10111300
C	3.52846800	2.81204200	0.08797000
C	3.27422300	3.03856000	1.58062000
C	3.84160000	4.10884800	-0.66603000
H	4.37883600	2.13042800	-0.00998500
H	3.09376900	2.08699300	2.08607000
H	4.15312500	3.50858500	2.03260800

H	2.40996300	3.68631200	1.73330300
H	4.03528800	3.90782300	-1.72462700
H	3.00402800	4.80575600	-0.59069800
H	4.73078600	4.58449900	-0.24144500
O	4.81120700	-3.44275000	1.63556600
H	4.37457800	-3.51116800	2.49452700
C	-4.58980000	2.34814200	1.39233600
H	-4.09843000	3.18684900	1.89027900
H	-5.10619600	2.74258800	0.51151100
H	-5.31487000	1.87714500	2.05591900
C	0.26219800	0.03984300	3.68610600
H	1.33687400	0.13584800	3.51266200
H	-0.07655800	0.96865200	4.15578500
H	0.05395300	-0.79782700	4.35152900
C	1.08048300	-3.09360000	-1.22421000
H	1.33331500	-2.89044600	-2.26736800
H	1.98402300	-2.93534700	-0.62903500
H	0.73881000	-4.12200200	-1.10836700
C	-3.81200500	-0.60809200	-3.49997300
H	-4.52268000	0.22391200	-3.53532600
H	-3.12853400	-0.49704100	-4.34448700
H	-4.35825600	-1.54872900	-3.56812300

CP3

Zero-point correction=	0.490666 (Hartree/Particle)
Thermal correction to Energy=	0.528389
Thermal correction to Enthalpy=	0.529333
Thermal correction to Gibbs Free Energy=	0.422379
Sum of electronic and zero-point Energies=	-1845.517203
Sum of electronic and thermal Energies=	-1845.479480
Sum of electronic and thermal Enthalpies=	-1845.478536
Sum of electronic and thermal Free Energies=	-1845.585490

Rh	1.18139100	0.38525900	-0.44666400
Rh	2.63879700	-0.99920300	0.97564900
O	-0.41082400	-0.69877500	0.28262300
O	1.06582600	1.67010400	1.17512600
O	1.45840400	-1.04530000	-1.89618700
O	2.86518300	1.37691100	-1.08881500
O	4.22059900	0.07533500	0.19228600
O	2.42663700	0.40146600	2.47294300
O	2.77825800	-2.33803900	-0.57650700
O	0.92080500	-1.94718200	1.63468900

C	2.16869900	-2.08032200	-1.65563000
C	1.69974400	1.41045400	2.25771800
C	4.00604300	0.99901800	-0.64560300
C	-0.20016500	-1.61521200	1.15384400
C	-4.20865900	-0.97424900	-0.73366000
C	-4.93722100	-1.72893700	0.18644100
C	-5.97210300	-1.16205200	0.93794800
C	-6.30362600	0.18202600	0.76056900
C	-5.57860900	0.93890400	-0.15799100
C	-4.52901600	0.39244700	-0.89902200
H	-4.71648400	-2.78189400	0.32912400
H	-7.11614300	0.63036500	1.32714200
H	-5.83434100	1.98649400	-0.29600500
C	-3.09261400	-1.62718700	-1.50853100
H	-3.14865000	-2.71494300	-1.41625200
H	-3.12499100	-1.37327000	-2.57128900
H	-2.11631800	-1.30318600	-1.13748400
C	-3.73696100	1.28503300	-1.82428800
H	-4.30691300	2.19823100	-2.02991000
H	-3.52816400	0.79921100	-2.77828400
N	-2.42960300	1.68660200	-1.27023700
C	-1.32637500	1.32756400	-1.93724000
O	-1.27565600	0.67965200	-3.00448100
C	0.07099900	1.52743700	-1.58154200
H	0.56758300	2.29843300	-2.17971300
C	-2.42158300	2.53706900	-0.05663300
C	-1.33229400	3.61253900	-0.11684600
C	-2.34269300	1.72258800	1.23932900
H	-3.39242500	3.04510400	-0.08596400
H	-1.50001800	4.33429400	0.68826700
H	-0.33614800	3.18954300	0.04911800
H	-1.35346600	4.15162500	-1.06847800
H	-2.44823200	2.39896100	2.09462700
H	-3.14058600	0.98063800	1.28642900
H	-1.38205300	1.21461400	1.31007500
O	-6.62353900	-1.97686000	1.81769900
H	-7.31608500	-1.47164700	2.26270500
C	5.20324500	1.72660000	-1.20951800
H	6.08812200	1.52507500	-0.60596500
H	5.37866600	1.37805900	-2.23242500
H	5.00295800	2.79924100	-1.25416100
C	2.25910900	-3.08511600	-2.77827000
H	3.00729700	-3.84363700	-2.54888900
H	1.28234800	-3.56088400	-2.90941000

H	2.50305000	-2.57422400	-3.71251500
C	-1.41862500	-2.37683200	1.61723500
H	-2.30622100	-1.74380700	1.58146900
H	-1.58006400	-3.22204100	0.93978700
H	-1.25621300	-2.76821100	2.62206800
C	1.54061700	2.42534900	3.36415800
H	2.08451900	2.10700500	4.25298900
H	1.91599100	3.39485900	3.02436200
H	0.47875000	2.54605500	3.59609400

TS3

Zero-point correction=	0.489452 (Hartree/Particle)
Thermal correction to Energy=	0.526086
Thermal correction to Enthalpy=	0.527030
Thermal correction to Gibbs Free Energy=	0.422351
Sum of electronic and zero-point Energies=	-1845.503210
Sum of electronic and thermal Energies=	-1845.466576
Sum of electronic and thermal Enthalpies=	-1845.465632
Sum of electronic and thermal Free Energies=	-1845.570311

Rh	1.16782200	0.54440000	-0.20204100
Rh	2.51040000	-1.35932300	0.52546700
O	-0.39441800	-0.26277300	0.88555400
O	1.79826200	1.53705700	1.50958900
O	0.63305800	-0.58816100	-1.82823600
O	2.82453000	1.23514500	-1.21327300
O	4.07568900	-0.53472800	-0.53322500
O	3.04127500	-0.23885000	2.18083800
O	1.89354000	-2.35617900	-1.16298700
O	0.83827900	-2.06045900	1.51638800
C	1.09011400	-1.77125000	-1.95360500
C	2.59465700	0.93576600	2.31313900
C	3.90020500	0.54678700	-1.17099400
C	-0.22940800	-1.38295700	1.48378100
C	-3.95345600	-0.70626200	-0.74725600
C	-4.68602300	-1.70614700	-0.10430100
C	-5.86255000	-1.41574600	0.59340900
C	-6.33217600	-0.10264500	0.64377600
C	-5.60156200	0.89854600	0.00557600
C	-4.41504200	0.62750900	-0.67845700
H	-4.35633900	-2.73955300	-0.14857100
H	-7.25322700	0.13555200	1.17048800
H	-5.96483500	1.92281400	0.04731900

C	-2.68656400	-1.07266700	-1.47571300
H	-2.65562700	-2.14814300	-1.67214300
H	-2.57986700	-0.54203800	-2.42449800
H	-1.80835200	-0.80897700	-0.88239500
C	-3.66350200	1.76719500	-1.33357100
H	-4.25558400	2.68824500	-1.24126700
H	-3.50895700	1.57907400	-2.39972800
N	-2.32712200	2.01041800	-0.79624300
C	-1.23924300	1.94850200	-1.63839500
O	-1.28295200	1.60121900	-2.81268800
C	0.03557200	2.25387800	-0.93829400
H	0.81120400	2.77099300	-1.51219900
C	-2.16118900	2.71236700	0.47464600
C	-0.66703200	3.04007600	0.65048900
C	-2.65705000	1.93744100	1.69832500
H	-2.71959100	3.65991500	0.40709300
H	-0.50446500	4.09036900	0.93400800
H	-0.10401900	2.41545700	1.33478800
H	-0.18387400	3.37970100	-0.45387100
H	-2.42730600	2.50493700	2.60745900
H	-3.73444100	1.77961000	1.65649800
H	-2.15344600	0.97119900	1.73684700
O	-6.50836100	-2.45828600	1.19477300
H	-7.30846400	-2.12741300	1.62267200
C	5.05983700	1.06745500	-1.98650600
H	5.99652200	0.63630300	-1.63250200
H	4.91081600	0.77810100	-3.03208100
H	5.09440000	2.15770400	-1.94216900
C	0.59058500	-2.55049400	-3.14581800
H	1.27722900	-3.36312200	-3.38487900
H	-0.38753200	-2.97641600	-2.89861100
H	0.45889000	-1.88375500	-3.99947400
C	-1.43072500	-1.91868900	2.22615600
H	-2.33251000	-1.79459100	1.62183200
H	-1.28155100	-2.96714700	2.48378300
H	-1.56674200	-1.34275500	3.14783600
C	3.05423900	1.72853700	3.51434700
H	3.50598900	1.06880400	4.25497300
H	3.79776900	2.46392400	3.18992700
H	2.21441900	2.27469700	3.95010200

5a+[Rh]

Zero-point correction= 0.493698 (Hartree/Particle)

Thermal correction to Energy=	0.530025
Thermal correction to Enthalpy=	0.530970
Thermal correction to Gibbs Free Energy=	0.425962
Sum of electronic and zero-point Energies=	-1845.607615
Sum of electronic and thermal Energies=	-1845.571288
Sum of electronic and thermal Enthalpies=	-1845.570344
Sum of electronic and thermal Free Energies=	-1845.675351

Rh	1.30054500	0.58350200	-0.19967600
Rh	2.45484800	-1.39626000	0.48118600
O	-0.33362700	-0.10195600	0.84612400
O	1.97617700	1.49995300	1.51579300
O	0.69356300	-0.43278900	-1.86635500
O	3.00549800	1.16221400	-1.18517000
O	4.09896600	-0.71677100	-0.54019700
O	3.07320800	-0.37853200	2.15697700
O	1.77670000	-2.31635900	-1.22072400
O	0.75336800	-1.99072300	1.46338900
C	1.04237800	-1.64636500	-2.01961400
C	2.71658900	0.83306600	2.31104200
C	4.02230700	0.39486700	-1.15623000
C	-0.26465300	-1.22954100	1.44194500
C	-3.86619600	-0.77896400	-0.78758200
C	-4.45344000	-1.90437200	-0.20468900
C	-5.62684700	-1.80656000	0.54938900
C	-6.23965900	-0.56456300	0.71762200
C	-5.65533500	0.55958000	0.13607700
C	-4.47370300	0.48274700	-0.60348100
H	-4.00946000	-2.88585400	-0.34044200
H	-7.15950900	-0.47507200	1.29076600
H	-6.13360800	1.52742500	0.26608800
C	-2.59205400	-0.93568600	-1.57530000
H	-2.42525600	-1.98564900	-1.83222800
H	-2.59092800	-0.34517000	-2.49425300
H	-1.73566500	-0.58460200	-0.99669600
C	-3.89545900	1.74442900	-1.21020000
H	-4.60522200	2.56908800	-1.05912300
H	-3.74933900	1.62690400	-2.28815100
N	-2.59564800	2.15297400	-0.68884700
C	-1.52664400	2.30057100	-1.53562400
O	-1.48729000	1.94148400	-2.70439300
C	-0.42368900	3.03063800	-0.77850600
H	0.54169600	2.50320500	-0.88201400
C	-2.45157800	2.86466100	0.58595400

C	-0.93442400	3.17126300	0.65918000
C	-2.93451400	2.07105600	1.79660400
H	-3.02729600	3.80321400	0.52186000
H	-0.75206400	4.16314900	1.07827400
H	-0.45169500	2.44209600	1.31100500
H	-0.25123000	3.99065000	-1.27741100
H	-2.69144800	2.62558900	2.70979000
H	-4.01155700	1.89706100	1.77962600
H	-2.42570900	1.10549200	1.82380000
O	-6.12573000	-2.95988800	1.08662400
H	-6.94081700	-2.75616700	1.56292400
C	5.22906200	0.82984100	-1.94774300
H	6.13486100	0.38692600	-1.53238000
H	5.11285400	0.48204500	-2.97967200
H	5.29823100	1.91850500	-1.96200900
C	0.52589800	-2.35999700	-3.24181100
H	1.34638600	-2.88274000	-3.73896500
H	-0.20494100	-3.11210500	-2.92910100
H	0.05098700	-1.65191400	-3.92012000
C	-1.49554700	-1.68055500	2.18363500
H	-2.37066800	-1.59809800	1.53424900
H	-1.37577000	-2.70547100	2.53370400
H	-1.65736900	-1.01953900	3.04092000
C	3.24095800	1.55597100	3.52596600
H	3.43609800	0.84843300	4.33260800
H	4.18358200	2.04643300	3.26065700
H	2.53433100	2.32386100	3.84393300

CP4

Zero-point correction=	0.490682 (Hartree/Particle)
Thermal correction to Energy=	0.527551
Thermal correction to Enthalpy=	0.528495
Thermal correction to Gibbs Free Energy=	0.424266
Sum of electronic and zero-point Energies=	-1845.518461
Sum of electronic and thermal Energies=	-1845.481593
Sum of electronic and thermal Enthalpies=	-1845.480649
Sum of electronic and thermal Free Energies=	-1845.584878

Rh	-1.22149700	0.34035300	0.51390000
Rh	-2.67489600	-0.85235300	-1.07666200
O	0.33863700	-0.80273700	-0.19962200
O	-0.92351400	1.70663300	-1.02098200
O	-1.67377000	-1.14718600	1.85483800

O	-2.87506400	1.39993900	1.12292900
O	-4.22352200	0.29991000	-0.34076200
O	-2.25661400	0.59421900	-2.48159700
O	-3.01772200	-2.24782700	0.39327700
O	-0.99514600	-1.90216500	-1.67334700
C	-2.46136900	-2.09763400	1.51999000
C	-1.47787100	1.53516000	-2.16260600
C	-4.00431800	1.14702000	0.57295200
C	0.11582000	-1.67070700	-1.11758400
C	4.17414500	-1.03811400	0.74262600
C	4.92048800	-1.82706500	-0.13429700
C	5.97031800	-1.28957000	-0.88562800
C	6.30078700	0.05983000	-0.74998900
C	5.55526200	0.85102200	0.12187900
C	4.48656900	0.33490600	0.85737100
H	4.70425800	-2.88562900	-0.23770300
H	7.12738400	0.48599700	-1.31337200
H	5.80923300	1.90307800	0.22506600
C	3.05550300	-1.66710500	1.53289500
H	3.13381300	-2.75711700	1.50572800
H	3.05999000	-1.34916900	2.57850900
H	2.08091400	-1.38488500	1.12547200
C	3.69262500	1.26187700	1.74916700
H	4.22810900	2.21009500	1.85572400
H	3.56930600	0.84272100	2.75055200
N	2.32894600	1.54634000	1.27498600
C	1.29565400	1.19343700	2.05502800
O	1.33689600	0.59637500	3.14622700
C	-0.11563600	1.38524100	1.72893000
H	-0.61076700	2.14629900	2.34244600
C	2.06862000	2.34613700	0.05970700
C	2.38497100	1.59450600	-1.23590800
C	2.76855100	3.70606200	0.13257600
H	0.98665700	2.52219900	0.06205800
H	1.89710000	0.62066200	-1.22581700
H	1.99675900	2.17146500	-2.08115400
H	3.45798400	1.45548800	-1.37667700
H	2.43354900	4.33311400	-0.69852100
H	2.53720000	4.22301700	1.06890700
H	3.85508600	3.60615500	0.04967000
O	6.63919700	-2.13655500	-1.72138900
H	7.34239700	-1.64823400	-2.16847900
C	-5.17886400	1.93937000	1.09525700
H	-5.39850900	1.61822700	2.11820000

H	-4.92374100	3.00117100	1.13085100
H	-6.05473400	1.77813000	0.46730400
C	-2.75811800	-3.11227100	2.59681600
H	-1.84757600	-3.34509700	3.15229100
H	-3.47671600	-2.67976700	3.30052100
H	-3.18663400	-4.01357400	2.15829200
C	1.30411000	-2.49994800	-1.54218500
H	1.41708400	-3.33185600	-0.83900200
H	1.14061600	-2.90723700	-2.54013700
H	2.22180700	-1.91004000	-1.50653300
C	-1.12802800	2.55365500	-3.22097600
H	-0.13151200	2.32465100	-3.61302900
H	-1.84790800	2.51140600	-4.03832700
H	-1.09640900	3.55467300	-2.78619200

TS2

Zero-point correction=	0.485721 (Hartree/Particle)
Thermal correction to Energy=	0.523220
Thermal correction to Enthalpy=	0.524164
Thermal correction to Gibbs Free Energy=	0.417354
Sum of electronic and zero-point Energies=	-1845.506070
Sum of electronic and thermal Energies=	-1845.468571
Sum of electronic and thermal Enthalpies=	-1845.467627
Sum of electronic and thermal Free Energies=	-1845.574437

Rh	1.17868000	0.51949100	-0.15536500
Rh	2.80341000	-1.20788300	0.49248100
O	-0.30766500	-0.88697400	0.19832600
O	1.11577600	1.08845300	1.83721000
O	1.36905800	-0.18550700	-2.07591900
O	2.77065300	1.78865000	-0.45757100
O	4.27754000	0.18090800	0.10264700
O	2.64324900	-0.48703000	2.42481600
O	2.84722700	-1.80500600	-1.47723300
O	1.19408800	-2.46763600	0.83221100
C	2.14208200	-1.16969700	-2.31995200
C	1.86766600	0.48052400	2.67435500
C	3.95566100	1.34446800	-0.28288600
C	0.02146300	-2.05504400	0.61131200
C	-4.28962800	-0.84205800	-0.83730900
C	-5.05211500	-1.75865400	-0.11448900
C	-6.12973300	-1.34618100	0.67806300
C	-6.46483300	0.00714000	0.74896700

C	-5.70448200	0.92819300	0.02877800
C	-4.62244700	0.53118000	-0.75944800
H	-4.82575600	-2.81900600	-0.16208800
H	-7.30807700	0.33681900	1.35092700
H	-5.96921300	1.98230100	0.07440300
C	-3.12559200	-1.32452100	-1.66471700
H	-3.17792900	-2.40696600	-1.80528600
H	-3.09767800	-0.85307000	-2.65074900
H	-2.17429100	-1.08813200	-1.17821300
C	-3.78168200	1.56988300	-1.45534400
H	-4.29542200	2.53926400	-1.46198100
H	-3.55105300	1.31090600	-2.49342200
N	-2.45979700	1.68749600	-0.82621400
C	-1.27333200	1.66457000	-1.60670900
O	-1.29522600	1.38185900	-2.78925800
C	-0.11402500	2.04753700	-0.78347300
H	0.49562100	2.83562800	-1.23148600
C	-2.31447500	2.23839100	0.44423100
C	-2.10355800	1.31116800	1.58268700
C	-2.88865000	3.59218800	0.70560000
H	-0.57314100	2.42264400	0.19783600
H	-1.42857600	0.49645400	1.31835300
H	-1.78105900	1.81980600	2.49208700
H	-3.09789900	0.85878100	1.75252900
H	-2.38567100	4.07409000	1.54713400
H	-2.84406000	4.22990800	-0.17898000
H	-3.94518100	3.47160800	0.99177000
O	-6.81448500	-2.31506200	1.35071400
H	-7.54013100	-1.90866200	1.84187600
C	5.07818700	2.30556500	-0.59888400
H	5.23415600	2.31957000	-1.68270800
H	4.80898100	3.31628700	-0.28624300
H	6.00052700	1.98377500	-0.11471600
C	2.24032300	-1.59204300	-3.76694800
H	1.29175500	-1.41516700	-4.27604200
H	3.00831400	-0.98484600	-4.25781000
H	2.53239000	-2.64072500	-3.83528100
C	-1.11283500	-3.03227600	0.82281600
H	-1.27103400	-3.59039900	-0.10595700
H	-0.85274300	-3.74375300	1.60762200
H	-2.03838700	-2.50728300	1.06495900
C	1.82903900	0.99502400	4.09553500
H	0.79642500	1.18079400	4.40053000
H	2.30361200	0.28329600	4.77094400

H	2.36615400	1.94787900	4.14263200

4a+[Rh]

Zero-point correction=	0.491416 (Hartree/Particle)
Thermal correction to Energy=	0.528373
Thermal correction to Enthalpy=	0.529317
Thermal correction to Gibbs Free Energy=	0.423257
Sum of electronic and zero-point Energies=	-1845.604588
Sum of electronic and thermal Energies=	-1845.567631
Sum of electronic and thermal Enthalpies=	-1845.566686
Sum of electronic and thermal Free Energies=	-1845.672747

Rh	1.21775400	0.23458000	-0.47787300
Rh	2.99553500	-0.75951000	0.81271100
O	-0.01547400	-0.01960600	1.17044000
O	1.79732300	2.07124500	0.26296100
O	0.73568600	-1.65956300	-1.12801100
O	2.54704500	0.43064100	-2.02931700
O	4.22203900	-0.50066900	-0.81120900
O	3.47472800	1.13246600	1.47033300
O	2.41260900	-2.59255400	0.08407300
O	1.65485600	-0.97236100	2.37139300
C	1.41921500	-2.64821300	-0.70794000
C	2.78653600	2.12029000	1.06592400
C	3.74156900	0.02078600	-1.86812700
C	0.46118300	-0.57774600	2.21607300
C	-3.99089600	-1.18917000	-0.43218500
C	-4.86469800	-1.96805400	0.32689200
C	-6.21875500	-1.63999900	0.44487800
C	-6.72281200	-0.51765500	-0.21509700
C	-5.85472000	0.26144600	-0.97771200
C	-4.49867700	-0.04882200	-1.09439600
H	-4.50399700	-2.85348900	0.84076900
H	-7.77615600	-0.25868100	-0.13931300
H	-6.24384700	1.13608900	-1.49322900
C	-2.53373700	-1.56915000	-0.50407500
H	-2.39289200	-2.61210400	-0.20792900
H	-2.10959100	-1.44539500	-1.50325200
H	-1.91867800	-0.95360200	0.15944300
C	-3.59994800	0.86980700	-1.88926600
H	-4.21076300	1.56086400	-2.48169400
H	-2.95879500	0.31893000	-2.58413100
N	-2.69226300	1.63816500	-1.05154800

C	-1.34765900	1.66272200	-0.99451400
O	-0.51214500	1.03730500	-1.65822400
C	-1.33127400	2.67764700	0.14231100
H	-0.85602000	2.31052800	1.05070500
C	-2.89381500	2.58012000	0.09356100
C	-3.50255500	1.91628500	1.32623100
C	-3.62986200	3.84852500	-0.31653300
H	-0.91052700	3.64405000	-0.14240800
H	-2.96724600	0.99475500	1.56773400
H	-3.42715300	2.59743900	2.18051700
H	-4.55593500	1.67136800	1.17170900
H	-3.61337900	4.57891400	0.49829900
H	-3.16749800	4.30176700	-1.19842400
H	-4.67810100	3.63096900	-0.54807900
O	-6.99580600	-2.45782000	1.21362200
H	-7.90490000	-2.13188800	1.20135300
C	4.66552300	0.13635600	-3.05620400
H	4.58062100	-0.77627800	-3.65565800
H	4.37611900	0.98349200	-3.67948200
H	5.69950600	0.23348600	-2.72257400
C	0.98201100	-4.01679300	-1.17296800
H	0.14747800	-4.35086200	-0.54721100
H	0.63008000	-3.96750600	-2.20488800
H	1.79964500	-4.73152200	-1.07587000
C	-0.50706100	-0.79534100	3.35464200
H	0.01830900	-1.13248300	4.24777900
H	-1.05207200	0.12948300	3.56050500
H	-1.24166700	-1.55035000	3.05676700
C	3.14871300	3.48196000	1.61017400
H	2.98718400	4.24679500	0.84853100
H	2.49771300	3.70689800	2.46189100
H	4.18379700	3.49034900	1.95276300

CP5

Zero-point correction=	0.489870 (Hartree/Particle)
Thermal correction to Energy=	0.527132
Thermal correction to Enthalpy=	0.528077
Thermal correction to Gibbs Free Energy=	0.422395
Sum of electronic and zero-point Energies=	-1845.517602
Sum of electronic and thermal Energies=	-1845.480339
Sum of electronic and thermal Enthalpies=	-1845.479395
Sum of electronic and thermal Free Energies=	-1845.585077

Rh	-0.50941500	-0.02077000	-0.35560600
Rh	-2.79941700	0.14360200	0.54624500
O	-1.09239800	-1.84748800	-1.10695100
O	-3.21933400	-1.66764800	-0.33025100
O	-0.16867400	1.82861400	0.49448400
O	-2.25972600	1.95832900	1.36883000
O	-2.10448200	-0.85376300	2.22399600
O	0.00532000	-1.00301500	1.39520400
O	-1.20547500	0.95378200	-2.02808200
O	-3.31677500	1.10948500	-1.19864700
C	-2.28670500	-2.26760200	-0.94266500
C	-2.43621200	1.29902000	-2.08764800
C	-0.89642300	-1.21294200	2.28267200
C	-1.09703700	2.40766300	1.15466100
C	-0.43064000	-1.94475400	3.51985300
H	0.25735300	-1.30230100	4.07908000
H	-1.27923500	-2.20372500	4.15236400
H	0.11884200	-2.84464200	3.23206900
C	-2.58598400	-3.62897100	-1.52310500
H	-2.09830200	-3.73472800	-2.49384300
H	-2.17461400	-4.39466900	-0.85716600
H	-3.66292500	-3.77518000	-1.60900700
C	-0.74052700	3.74448800	1.76210600
H	0.02831300	4.23892900	1.16710700
H	-1.63118400	4.36891000	1.84301600
H	-0.34655000	3.57917900	2.77061500
C	-2.85904800	1.99106200	-3.36164800
H	-3.88792200	2.34081100	-3.28055800
H	-2.18742700	2.82877500	-3.56588000
H	-2.77247200	1.28836700	-4.19579400
C	1.24692800	-0.17710600	-1.23470400
C	1.95938000	-1.46297400	-1.34043000
C	3.25802400	-3.24671800	-0.30777200
O	1.61761400	-2.14432200	-2.31365000
N	2.84291500	-1.83897800	-0.38155600
C	3.10496600	-0.92924700	0.73398800
H	4.05394100	-1.23220000	1.19046400
H	2.32342900	-1.03048900	1.48829800
C	3.19803000	0.51137400	0.26690500
C	2.78059800	1.57590100	1.10717600
C	3.86948200	0.82279900	-0.93013600
C	2.97510000	2.88682200	0.68645600
C	4.05418400	2.13495400	-1.34635400
H	4.23778600	0.01224900	-1.55046900

C	3.58900300	3.17542200	-0.53655900
H	2.64595400	3.71476900	1.30481400
H	4.55611500	2.34843600	-2.28667400
H	2.85099500	-3.69420300	-1.21780100
C	4.78177100	-3.38553000	-0.33240800
H	5.06043100	-4.44299800	-0.36771000
H	5.20132900	-2.89011500	-1.21243900
H	5.24731000	-2.95497500	0.56083300
C	2.61847200	-3.93160100	0.90597500
H	3.00518400	-3.52338500	1.84622200
H	1.53383700	-3.79265500	0.89009400
H	2.83572700	-5.00399600	0.89462700
O	3.71539000	4.48713800	-0.87541500
H	4.14601800	4.55368800	-1.73775800
C	2.16950300	1.31243800	2.45830900
H	1.28884700	0.67476500	2.36571000
H	2.88201800	0.80910000	3.12314100
H	1.87297400	2.24864800	2.93546500
H	1.48240800	0.54317800	-2.02088500

TS4

Zero-point correction=	0.490433 (Hartree/Particle)
Thermal correction to Energy=	0.527553
Thermal correction to Enthalpy=	0.528498
Thermal correction to Gibbs Free Energy=	0.423213
Sum of electronic and zero-point Energies=	-1845.521398
Sum of electronic and thermal Energies=	-1845.484278
Sum of electronic and thermal Enthalpies=	-1845.483334
Sum of electronic and thermal Free Energies=	-1845.588619

Rh	0.40418400	-0.06576900	-0.25211700
Rh	2.78205300	-0.18000700	0.38478600
O	0.85602100	1.78461200	-1.04267200
O	3.06997100	1.62348200	-0.56112200
O	0.17923400	-1.91971100	0.62779000
O	2.35000900	-1.98857000	1.29126900
O	2.27332000	0.84268500	2.11299400
O	0.07529800	0.91959400	1.54710300
O	0.93717100	-1.02752800	-1.99362900
O	3.12496800	-1.16146700	-1.39154900
C	2.05545200	2.21608300	-1.03889600
C	2.15682100	-1.35569900	-2.18532500
C	1.07317600	1.18250800	2.30675300

C	1.18062100	-2.46315800	1.20601200
C	0.75513200	1.98570400	3.54673800
H	-0.06365100	1.51227800	4.09575100
H	1.63476700	2.07163800	4.18403400
H	0.41780200	2.98319100	3.24836500
C	2.26092500	3.58537400	-1.64241800
H	1.61523300	3.70709000	-2.51377700
H	1.97600600	4.34212400	-0.90353700
H	3.30860700	3.73080000	-1.90714700
C	0.91315700	-3.78890500	1.88190700
H	0.50899200	-3.60030400	2.88256500
H	0.17282400	-4.35815100	1.31687600
H	1.83900000	-4.35549700	1.98512300
C	2.46020300	-2.02138000	-3.50701500
H	3.45252500	-2.47192000	-3.48698000
H	1.70016300	-2.77343000	-3.72996800
H	2.42272100	-1.26609700	-4.29854500
C	-1.49704800	0.02493600	-1.05253500
C	-2.00298800	1.38933400	-1.36679900
C	-2.89282000	3.38834000	-0.26953000
O	-1.66550800	1.97645100	-2.39065000
N	-2.79590300	1.92942700	-0.38049500
C	-3.03180400	1.05490800	0.76205200
H	-3.99886200	1.30067000	1.21459900
H	-2.25222800	1.16945800	1.51844300
C	-3.04485400	-0.38338500	0.24681400
C	-2.68537800	-1.47871000	1.11629100
C	-3.89345500	-0.69081200	-0.86493200
C	-2.96784300	-2.77314000	0.72468500
C	-4.17717100	-1.98926300	-1.23923400
H	-4.28048900	0.13361700	-1.45340400
C	-3.67990400	-3.04050900	-0.45583800
H	-2.65902300	-3.61214200	1.33767700
H	-4.77305600	-2.19322700	-2.12459800
H	-2.76290600	3.74163500	-1.29605100
C	-4.26766600	3.82471400	0.23625900
H	-4.35749400	4.91324200	0.17699900
H	-5.06568100	3.38103400	-0.36676100
H	-4.42670000	3.54210200	1.28279300
C	-1.74185300	3.94295700	0.58228700
H	-1.81537100	3.59788700	1.61952500
H	-0.78458200	3.60718600	0.17577100
H	-1.76337800	5.03767100	0.58875800
O	-3.88331700	-4.33873500	-0.76592200

H	-4.38417000	-4.40380700	-1.59065800
C	-2.07276500	-1.22576400	2.46118200
H	-2.79873000	-0.72360600	3.11428300
H	-1.78140700	-2.16427800	2.93560400
H	-1.19904700	-0.57979000	2.37776100
H	-1.62819700	-0.70675400	-1.84978400

CP6

Zero-point correction=	0.491156 (Hartree/Particle)
Thermal correction to Energy=	0.528681
Thermal correction to Enthalpy=	0.529625
Thermal correction to Gibbs Free Energy=	0.423369
Sum of electronic and zero-point Energies=	-1845.536439
Sum of electronic and thermal Energies=	-1845.498914
Sum of electronic and thermal Enthalpies=	-1845.497969
Sum of electronic and thermal Free Energies=	-1845.604226

Rh	0.37830500	-0.07421600	-0.21133100
Rh	2.76839200	-0.25769600	0.31298200
O	0.83047200	1.78210200	-0.98493800
O	3.06034900	1.54913700	-0.62178200
O	0.13774800	-1.94258100	0.63411300
O	2.32937200	-2.06909400	1.21449300
O	2.37645200	0.74923600	2.07798800
O	0.15484400	0.87417200	1.62673100
O	0.80203700	-0.99857800	-2.00125500
O	3.00575900	-1.21544700	-1.49208600
C	2.03854000	2.17841200	-1.04002900
C	2.00006200	-1.35576900	-2.25333800
C	1.19262100	1.10741300	2.33819100
C	1.14601800	-2.51613600	1.16815100
C	0.95877200	1.90247700	3.60191000
H	0.12426100	1.47394900	4.16341900
H	1.85835000	1.92090200	4.21663500
H	0.68144200	2.92582300	3.32959200
C	2.25694000	3.54724900	-1.63975400
H	1.59079400	3.68538500	-2.49330000
H	2.00394700	4.30503900	-0.89040800
H	3.29967400	3.67482300	-1.93160500
C	0.87635000	-3.84355900	1.84029300
H	0.51777600	-3.65750400	2.85873400
H	0.10065800	-4.38950900	1.30013900
H	1.79191500	-4.43270700	1.89976600

C	2.23897300	-1.98118800	-3.60741500
H	3.17473900	-2.54071600	-3.60840900
H	1.40107400	-2.62674200	-3.87766600
H	2.30198900	-1.18311900	-4.35446300
C	-1.71725700	-0.01036900	-0.94386600
C	-1.99940100	1.39174500	-1.36223200
C	-2.69884200	3.46826100	-0.22336300
O	-1.64225500	1.94050800	-2.39545900
N	-2.73408200	2.01240100	-0.35662900
C	-2.95809700	1.13304900	0.78043500
H	-3.94411400	1.30483200	1.22531800
H	-2.18750700	1.25654200	1.54649300
C	-2.85754100	-0.28610300	0.18118400
C	-2.64557800	-1.41575700	1.12599900
C	-3.84287100	-0.56813300	-0.87695800
C	-3.04680800	-2.67230500	0.77480300
C	-4.22163400	-1.85279800	-1.21743100
H	-4.21435100	0.27716000	-1.44341900
C	-3.78220600	-2.90992900	-0.41603600
H	-2.84645300	-3.52010200	1.42010200
H	-4.84708500	-2.03842400	-2.08617500
H	-2.55521100	3.82249400	-1.24830400
C	-4.02620200	4.00552400	0.31299900
H	-4.02480200	5.09945300	0.29787300
H	-4.86441300	3.65317800	-0.29574400
H	-4.19824700	3.69377300	1.34967200
C	-1.49547100	3.92092100	0.61676600
H	-1.58481100	3.58126400	1.65471500
H	-0.57557600	3.50693600	0.19777800
H	-1.42717700	5.01389300	0.62633900
O	-4.07328700	-4.19231800	-0.68233200
H	-4.59134400	-4.25324500	-1.49795000
C	-2.06225000	-1.16332300	2.47726800
H	-2.77731300	-0.58790900	3.08143000
H	-1.85618400	-2.10226400	2.99398500
H	-1.14920200	-0.57224900	2.40572600
H	-1.64226900	-0.73690600	-1.74744200

TS5

Zero-point correction=	0.490671 (Hartree/Particle)
Thermal correction to Energy=	0.527666
Thermal correction to Enthalpy=	0.528610
Thermal correction to Gibbs Free Energy=	0.423244

Sum of electronic and zero-point Energies= -1845.535108
Sum of electronic and thermal Energies= -1845.498113
Sum of electronic and thermal Enthalpies= -1845.497169
Sum of electronic and thermal Free Energies= -1845.602535

Rh	0.37549700	-0.07295700	-0.21279200
Rh	2.74953200	-0.22446900	0.31745600
O	0.80064100	1.78167800	-1.00048500
O	3.03004400	1.57559800	-0.62922100
O	0.15403700	-1.93627600	0.64475100
O	2.34320100	-2.02952800	1.23599900
O	2.35325500	0.78627300	2.07455400
O	0.13169600	0.87162200	1.62032400
O	0.80600200	-0.99826100	-1.99870000
O	3.00692100	-1.19363300	-1.47674400
C	2.00310400	2.19252500	-1.05654200
C	2.00684600	-1.34896900	-2.24409700
C	1.16155200	1.12378600	2.33434500
C	1.16392500	-2.49260100	1.19016400
C	0.91389700	1.91437600	3.59728000
H	0.07669700	1.48052100	4.15029300
H	1.80838200	1.93623200	4.21926200
H	0.63437700	2.93700900	3.32441100
C	2.21049200	3.55827300	-1.66497300
H	1.97203800	4.31833500	-0.91311800
H	3.24798500	3.68499600	-1.97540300
H	1.52909200	3.69336400	-2.50671100
C	0.90815200	-3.81431200	1.87659300
H	0.54520400	-3.61928400	2.89169300
H	0.13854600	-4.37344800	1.34157500
H	1.82976200	-4.39302200	1.94462500
C	2.25931500	-1.98240400	-3.59094700
H	3.19594000	-2.54032400	-3.57973200
H	1.42481300	-2.63081800	-3.86448800
H	2.32832200	-1.18889300	-4.34232600
C	-1.83740400	-0.05981500	-0.97517300
C	-2.04237900	1.35498900	-1.37836300
C	-2.69838200	3.44365600	-0.23321500
O	-1.68323400	1.89543700	-2.41488300
N	-2.73664900	1.98737700	-0.35275400
C	-2.95556400	1.11728200	0.79549600
H	-3.94404800	1.28563400	1.23643000
H	-2.18716900	1.26037800	1.56028900
C	-2.84538100	-0.30597300	0.22084600

C	-2.64903200	-1.43861200	1.16893200
C	-3.75238200	-0.59058000	-0.90317600
C	-3.01107000	-2.69062000	0.78990200
C	-4.08488100	-1.90647800	-1.26831400
H	-4.20869500	0.24633500	-1.41559500
C	-3.67472800	-2.94239600	-0.45405400
H	-2.83864700	-3.53984500	1.44195500
H	-4.66002500	-2.09454900	-2.17038100
H	-2.54949600	3.78811800	-1.26068600
C	-4.02719600	3.98828800	0.29283700
H	-4.02273300	5.08213400	0.27123700
H	-4.86297800	3.63427500	-0.31808600
H	-4.20532500	3.68274900	1.33031000
C	-1.49897000	3.90340100	0.60856500
H	-1.59415300	3.57475700	1.64952000
H	-0.57743600	3.48493600	0.19825000
H	-1.43047700	4.99637000	0.60750400
O	-3.91734300	-4.24217700	-0.72183900
H	-4.38361900	-4.31944300	-1.56618100
C	-2.11235600	-1.17394200	2.53988600
H	-2.82649300	-0.57148100	3.11692400
H	-1.94573200	-2.10983900	3.07694600
H	-1.17959300	-0.61093700	2.48735500
H	-1.61140500	-0.80679600	-1.72247500

CP7

Zero-point correction=	0.492484 (Hartree/Particle)
Thermal correction to Energy=	0.529789
Thermal correction to Enthalpy=	0.530733
Thermal correction to Gibbs Free Energy=	0.423532
Sum of electronic and zero-point Energies=	-1845.571759
Sum of electronic and thermal Energies=	-1845.534454
Sum of electronic and thermal Enthalpies=	-1845.533510
Sum of electronic and thermal Free Energies=	-1845.640712

Rh	-0.93510600	0.31915300	-0.46087500
Rh	-2.76285100	-0.82039600	0.62815300
O	-1.94845600	2.08652800	-0.16383200
O	-3.68411100	1.00665000	0.82485800
O	-0.04778700	-1.53224400	-0.69782100
O	-1.73744600	-2.59162600	0.38112000
O	-3.62220200	-1.05096600	-1.22256200
O	-1.91604900	0.04574700	-2.24471900

O	-0.06641700	0.54337400	1.40646700
O	-1.78796100	-0.52616000	2.42498200
C	-3.09290600	2.04691500	0.39236600
C	-0.67193700	0.07507200	2.42718400
C	-3.03245500	-0.56620800	-2.24089400
C	-0.62527300	-2.56679500	-0.23218500
C	-3.73723400	-0.70002900	-3.56937400
H	-3.00897300	-0.75717200	-4.37962300
H	-4.38645900	-1.57650700	-3.56673800
H	-4.35683300	0.18898100	-3.72823000
C	-3.83195200	3.35754000	0.52127000
H	-4.43595600	3.50880500	-0.37971100
H	-4.50093300	3.33167800	1.38251000
H	-3.12560700	4.18498200	0.60179400
C	0.07602700	-3.88619200	-0.45675900
H	-0.13399800	-4.22796400	-1.47567300
H	1.15614500	-3.75644500	-0.36354500
H	-0.29126700	-4.63658100	0.24439200
C	0.03096800	0.24104500	3.75471000
H	0.37648300	1.27187800	3.86486600
H	-0.63220200	-0.02703300	4.57682400
H	0.91307200	-0.40765400	3.77623400
C	2.50565000	-0.13339100	-0.76835000
C	1.91262500	1.21221300	-0.91812800
C	2.39307900	3.52338700	-0.21026600
O	0.76645700	1.49020000	-1.32541900
N	2.80264700	2.14395700	-0.49921800
C	4.10591500	1.58884100	-0.12683300
H	4.38336700	1.89954300	0.88699400
H	4.88050100	1.94932100	-0.81239200
C	3.91409200	0.07508400	-0.22275100
C	5.02055200	-0.83265600	-0.59543800
C	2.80788800	-0.48778500	0.68038600
C	4.93264100	-2.14723500	-0.29015800
C	2.89982400	-1.90236500	1.05759100
H	2.36160000	0.18138400	1.40963000
C	3.86131200	-2.69007300	0.52528200
H	5.71032400	-2.83997100	-0.59578200
H	2.17068200	-2.29506100	1.76125600
H	1.51473500	3.68823200	-0.83921800
C	1.96764700	3.64795100	1.25825900
H	1.58916700	4.65493700	1.45976800
H	1.17818600	2.92492500	1.48073600
H	2.81331000	3.46671400	1.93178500

C	3.48957500	4.51278300	-0.60309100
H	4.38554700	4.39064800	0.01537700
H	3.77348800	4.39016000	-1.65244000
H	3.13094400	5.53627200	-0.46349000
O	3.97442900	-4.03559400	0.75221300
H	3.25525900	-4.31423200	1.33480500
C	6.21093900	-0.26770700	-1.31853100
H	6.76012300	0.44854400	-0.69469400
H	6.90586400	-1.06086300	-1.60296000
H	5.91043800	0.26802500	-2.22797000
H	2.22700900	-0.92694300	-1.44553600

TS6

Zero-point correction=	0.491080 (Hartree/Particle)
Thermal correction to Energy=	0.528203
Thermal correction to Enthalpy=	0.529148
Thermal correction to Gibbs Free Energy=	0.422596
Sum of electronic and zero-point Energies=	-1845.559811
Sum of electronic and thermal Energies=	-1845.522688
Sum of electronic and thermal Enthalpies=	-1845.521743
Sum of electronic and thermal Free Energies=	-1845.628295

Rh	-0.90651900	0.42828800	-0.29350100
Rh	-2.88657600	-0.80001500	0.33429600
O	-1.86027200	2.14853600	0.31162900
O	-3.73687700	0.99576600	0.86357600
O	-0.09371100	-1.38256900	-0.87569500
O	-1.92867700	-2.53785300	-0.21673800
O	-3.56187300	-0.54758300	-1.58934400
O	-1.71320000	0.63548000	-2.17294300
O	-0.22100400	0.15755700	1.63895700
O	-2.08859400	-0.98869800	2.22748700
C	-3.05180200	2.06167800	0.75173600
C	-0.95096200	-0.48004600	2.46642300
C	-2.85065500	0.11488200	-2.41046100
C	-0.75860600	-2.45543500	-0.70313100
C	-3.42245000	0.33369200	-3.79066500
H	-2.61920900	0.42914700	-4.52259900
H	-4.09485900	-0.48347800	-4.05511500
H	-3.99692100	1.26614300	-3.78777700
C	-3.70025600	3.34455400	1.21524800
H	-4.78370600	3.28052600	1.10598900
H	-3.46968400	3.49211700	2.27577100

H	-3.30290000	4.19292700	0.65632700
C	-0.08662300	-3.73750400	-1.13441800
H	0.00742200	-3.74066400	-2.22484900
H	0.92399400	-3.78856000	-0.72209800
H	-0.67365100	-4.60087100	-0.82102500
C	-0.41345400	-0.61651800	3.87231600
H	-0.93480800	-1.41207600	4.40492500
H	0.66109700	-0.81138000	3.84696400
H	-0.56881400	0.32740000	4.40506400
C	2.52449000	-0.15183000	-0.43412200
C	2.05612900	1.26838900	-0.53745200
C	2.93869000	3.54410700	-0.17144200
O	0.89784100	1.66413200	-0.75544200
N	3.10674600	2.09511700	-0.33110500
C	4.37284000	1.39495500	-0.10043000
H	4.79176200	1.66036800	0.87848700
H	5.11331100	1.67857000	-0.85944000
C	3.99726200	-0.07026900	-0.21775600
C	4.88167700	-1.12172400	-0.55025700
C	2.62590800	-0.64571300	0.95986600
C	4.48631900	-2.44540600	-0.43160200
C	2.72505000	-2.02375500	1.22883300
H	2.35396500	0.04195600	1.75281300
C	3.43318700	-2.88351800	0.40433800
H	5.12829300	-3.22774900	-0.82574800
H	2.31521000	-2.40167800	2.16319300
H	1.98670400	3.76770600	-0.65952200
C	2.82197800	3.90570600	1.31384600
H	2.64324500	4.97890000	1.42990000
H	1.98735800	3.36690100	1.77075000
H	3.74050100	3.65807200	1.85732700
C	4.05922800	4.30556300	-0.88010400
H	5.03048200	4.13339400	-0.40379800
H	4.13102400	4.01205400	-1.93139000
H	3.85816000	5.37951200	-0.83825200
O	3.32134300	-4.24940100	0.52146900
H	2.59700000	-4.44702200	1.12890900
C	6.29245800	-0.79080300	-0.97738800
H	6.85544600	-0.32914600	-0.15633600
H	6.82983100	-1.69448100	-1.27286700
H	6.31937700	-0.08846100	-1.81954200
H	2.11017900	-0.84720600	-1.15801400

3a+[Rh]

Zero-point correction=	0.492399 (Hartree/Particle)
Thermal correction to Energy=	0.530054
Thermal correction to Enthalpy=	0.530998
Thermal correction to Gibbs Free Energy=	0.423940
Sum of electronic and zero-point Energies=	-1845.576028
Sum of electronic and thermal Energies=	-1845.538373
Sum of electronic and thermal Enthalpies=	-1845.537429
Sum of electronic and thermal Free Energies=	-1845.644487

Rh	0.87881600	0.42953100	0.00365600
Rh	2.98047400	-0.75154000	0.12942000
O	1.90225400	2.03156100	-0.78205100
O	3.88344600	0.93375400	-0.62481400
O	0.00250100	-1.25313200	0.82777600
O	1.96570700	-2.38451000	0.87072000
O	3.19422600	-0.00957700	2.03536200
O	1.23267300	1.12699700	1.90610300
O	0.65909300	-0.33882700	-1.90501300
O	2.64566000	-1.42905700	-1.78688600
C	3.16393900	1.93913000	-0.92453700
C	1.57894800	-1.08147100	-2.38092600
C	2.29985700	0.76568800	2.50024900
C	0.71640300	-2.28018600	1.06966400
C	2.53849000	1.34037600	3.87614000
H	1.58843300	1.53706100	4.37500300
H	3.15494600	0.66194400	4.46734600
H	3.07402500	2.28990300	3.77085700
C	3.86663800	3.12648600	-1.53861800
H	4.90505900	3.16412100	-1.20695900
H	3.85583500	3.01621700	-2.62823900
H	3.34327400	4.04906300	-1.28341200
C	0.00185300	-3.46811600	1.66970500
H	-0.20814400	-3.25863500	2.72366400
H	-0.95769800	-3.62749200	1.17311600
H	0.62482500	-4.36043700	1.60447600
C	1.38793100	-1.56706300	-3.79879600
H	2.01231200	-2.44010800	-3.99019700
H	0.33601700	-1.79718900	-3.98020700
H	1.67934600	-0.76748400	-4.48786100
C	-2.64930900	-0.17318800	0.06465600
C	-2.16158700	1.25760800	-0.02391900
C	-3.06265600	3.55247600	-0.13177800
O	-0.98354600	1.64197100	-0.13054600

N	-3.21621600	2.10008000	0.00672900
C	-4.51563800	1.42641000	0.04927000
H	-5.09487300	1.65279900	-0.85708500
H	-5.10296900	1.78152300	0.90536600
C	-4.14573400	-0.03383400	0.17778900
C	-4.96699100	-1.07570900	0.42877300
C	-2.29616700	-0.98513000	-1.15286300
C	-4.48475800	-2.44397100	0.47709300
C	-2.64970500	-2.27945300	-1.23074500
H	-1.71909400	-0.52231700	-1.94602300
C	-3.45815700	-2.97466700	-0.24532300
H	-5.06410300	-3.15390300	1.06331400
H	-2.32637300	-2.86693700	-2.09002000
H	-1.99946300	3.73337200	0.04485100
C	-3.40611200	3.99875800	-1.55730000
H	-3.22682900	5.07218200	-1.66941800
H	-2.78488600	3.46941700	-2.28485100
H	-4.45895700	3.80983000	-1.79331800
C	-3.88042000	4.29253900	0.92857900
H	-4.95720900	4.17228600	0.76820000
H	-3.63603600	3.93371600	1.93251300
H	-3.65880400	5.36247400	0.88403600
O	-3.24397900	-4.32785000	-0.11485600
H	-2.45057600	-4.56522000	-0.61122200
C	-6.44710300	-0.88408800	0.67041800
H	-7.03489900	-1.23035400	-0.18793500
H	-6.77245000	-1.47221500	1.53571300
H	-6.70984700	0.16022600	0.85684900
H	-2.20802800	-0.66024600	0.94435700

TS7

Zero-point correction=	0.487099 (Hartree/Particle)
Thermal correction to Energy=	0.523720
Thermal correction to Enthalpy=	0.524664
Thermal correction to Gibbs Free Energy=	0.420640
Sum of electronic and zero-point Energies=	-1845.518626
Sum of electronic and thermal Energies=	-1845.482005
Sum of electronic and thermal Enthalpies=	-1845.481061
Sum of electronic and thermal Free Energies=	-1845.585085

Rh	0.37069100	0.00658900	-0.09558400
Rh	2.70017400	-0.83838800	0.11017000
O	-0.21556000	-1.92528800	-0.05106800

O	1.90939800	-2.72458100	-0.01464300
O	1.35124400	2.01080800	-0.06288500
O	3.39970100	1.11568100	0.20917300
O	2.79305400	-0.77292700	-1.95000200
O	0.66270500	0.00224000	-2.12827000
O	0.29785400	-0.05443400	1.98619500
O	2.42047000	-0.85315600	2.15926100
C	0.65138600	-2.86262600	-0.05622500
C	1.30651300	-0.48905800	2.63877600
C	1.77485200	-0.39718700	-2.60873400
C	2.65166900	2.09915600	0.09137200
C	1.86325200	-0.44081600	-4.11557100
H	2.90088400	-0.53562400	-4.43604900
H	1.29412400	-1.30553300	-4.47149500
H	1.40511500	0.45337500	-4.54348600
C	0.08655800	-4.26112400	-0.10544600
H	-0.66675400	-4.31664600	-0.89464800
H	0.88167700	-4.98647900	-0.27707900
H	-0.40878600	-4.48263700	0.84522000
C	3.23369000	3.48850300	0.10118400
H	2.64634000	4.14860300	0.74427500
H	4.26958300	3.44995200	0.43437400
H	3.19377700	3.90050700	-0.91267400
C	1.13159700	-0.59638300	4.13742900
H	0.56076700	-1.50379500	4.36112900
H	2.10132400	-0.66089300	4.63128900
H	0.56411700	0.25677700	4.51587300
C	-1.68999900	0.54811800	-0.56832300
C	-2.53511900	-0.60926500	-0.98045900
C	-4.42137300	-1.94074100	-0.10529300
O	-2.33615500	-1.36178000	-1.92792400
N	-3.63357400	-0.71266300	-0.14210700
C	-3.64913300	0.26554800	0.92321600
H	-3.35199000	-0.17510400	1.88502700
H	-4.64968800	0.69244500	1.05804800
C	-2.61357000	1.33574200	0.51318900
C	-3.09059000	2.47362900	-0.35084200
C	-1.77781800	1.79533600	1.64918300
C	-2.27594000	3.56230400	-0.49484600
C	-0.99526800	2.87712400	1.50515800
H	-1.67703400	1.14443200	2.50792500
C	-1.04027000	3.56059100	0.22809400
H	-2.41657900	4.28169500	-1.29475500
H	-0.22138600	3.14515300	2.21511600

H	-4.25892800	-2.38629000	-1.09102900
C	-3.87858100	-2.90722200	0.95712800
H	-4.40202700	-3.86766300	0.90943200
H	-2.81178600	-3.07803200	0.79023600
H	-4.01169300	-2.50650100	1.96861300
C	-5.91103700	-1.64432400	0.07505900
H	-6.12253400	-1.21489600	1.06101600
H	-6.26418300	-0.94432000	-0.68821500
H	-6.49242900	-2.56711900	-0.01030200
O	0.04640600	4.02600300	-0.27862200
H	0.79299600	3.08538400	-0.14475800
C	-4.30271700	2.28362600	-1.20934800
H	-5.19992000	2.20020600	-0.58379200
H	-4.43659500	3.12190200	-1.89567300
H	-4.23716100	1.35603500	-1.78537100
H	-1.47665100	1.16857200	-1.43779200

CP8

Zero-point correction=	0.491899 (Hartree/Particle)
Thermal correction to Energy=	0.529042
Thermal correction to Enthalpy=	0.529986
Thermal correction to Gibbs Free Energy=	0.424432
Sum of electronic and zero-point Energies=	-1845.528921
Sum of electronic and thermal Energies=	-1845.491778
Sum of electronic and thermal Enthalpies=	-1845.490834
Sum of electronic and thermal Free Energies=	-1845.596389

Rh	-0.42419500	-0.03178100	0.21319500
Rh	-2.87288600	0.00041200	-0.26372200
O	-0.56884100	-2.03366600	0.39867500
O	-2.81975300	-2.01051000	0.06468900
O	-0.53984200	2.11161700	-0.04902600
O	-2.70824000	2.09932300	-0.58435200
O	-3.15025500	0.30437400	1.75697700
O	-0.91591100	0.26319200	2.18585000
O	-0.14309700	-0.32863200	-1.83098600
O	-2.37835800	-0.33129700	-2.25140300
C	-1.71621800	-2.58687500	0.31322200
C	-1.16573000	-0.45622000	-2.59146500
C	-2.14268000	0.34306800	2.52973900
C	-1.66051300	2.72419200	-0.50155600
C	-2.40676600	0.47456200	4.01022200
H	-2.31382500	-0.51596700	4.46740900

H	-1.65879500	1.12268300	4.47070400
H	-3.41346200	0.85393700	4.18684000
C	-1.75105300	-4.07796200	0.53832500
H	-2.35512000	-4.28697800	1.42586500
H	-2.23393900	-4.56537500	-0.31261500
H	-0.74338000	-4.46601100	0.68242700
C	-1.51956300	4.17295000	-0.85019300
H	-0.78147600	4.29650800	-1.64976000
H	-2.48280300	4.56126500	-1.17649500
H	-1.16103200	4.73423100	0.01824700
C	-0.87935100	-0.81259800	-4.03165700
H	-0.69591000	-1.89054300	-4.09274400
H	-1.73284400	-0.56642800	-4.66359600
H	0.02081200	-0.30214700	-4.38038900
C	1.64057300	0.08589700	0.83005600
C	2.11259800	-1.29772400	1.11782100
C	3.24210100	-3.09917900	-0.14791300
O	1.82689800	-2.00256000	2.07956600
N	2.95143200	-1.69027500	0.08771400
C	3.14455800	-0.65685700	-0.90800400
H	2.51841300	-0.82106800	-1.79407700
H	4.18932000	-0.59818200	-1.23311700
C	2.69499900	0.65249400	-0.19012200
C	3.78878200	1.31934000	0.62825200
C	2.06459700	1.59142600	-1.16979700
C	3.89982300	2.66653100	0.67595900
C	2.18857700	2.93255700	-1.11385500
H	1.43384500	1.12367400	-1.91870900
C	3.07509800	3.58134500	-0.11836800
H	4.62941300	3.14067600	1.32635600
H	1.71981500	3.58834200	-1.84576700
H	3.01628100	-3.57556200	0.81085700
C	2.30467500	-3.68137700	-1.21594500
H	2.45207000	-4.76229900	-1.30995900
H	1.26458100	-3.48642400	-0.94185400
H	2.49322800	-3.23364900	-2.19851100
C	4.71892700	-3.32005800	-0.48222500
H	4.99053100	-2.85672000	-1.43758300
H	5.36108300	-2.90170200	0.29846600
H	4.93288800	-4.38993500	-0.56525500
O	3.11704400	4.80554700	-0.00330700
H	0.31997000	2.55574200	-0.27118500
C	4.68184100	0.45793000	1.47844700
H	5.20059600	-0.29424800	0.87600200

H	5.42710000	1.07044200	1.99045600
H	4.10786400	-0.09196500	2.23116200
H	1.55460500	0.70148800	1.72745500

TS8

Zero-point correction=	0.486606 (Hartree/Particle)
Thermal correction to Energy=	0.523467
Thermal correction to Enthalpy=	0.524411
Thermal correction to Gibbs Free Energy=	0.419916
Sum of electronic and zero-point Energies=	-1845.491083
Sum of electronic and thermal Energies=	-1845.454221
Sum of electronic and thermal Enthalpies=	-1845.453277
Sum of electronic and thermal Free Energies=	-1845.557772

Rh	-0.60558800	0.05237900	-0.28394100
Rh	-2.80860500	-0.73010900	0.35498100
O	-1.25069500	1.93725300	0.13177300
O	-3.39672800	1.21664300	0.37029900
O	-0.09566700	-1.91006500	-0.77078300
O	-1.84307900	-2.67349500	0.38383000
O	-3.23994700	-0.82877600	-1.64895200
O	-1.28379300	0.18243900	-2.21146100
O	-0.10818400	-0.14393800	1.72700900
O	-2.25103400	-0.56334200	2.33408400
C	-2.50372100	2.12202900	0.28747000
C	-1.03406300	-0.32131300	2.59161400
C	-2.42477400	-0.31450100	-2.48300800
C	-0.69071800	-2.85195700	-0.02289900
C	-2.86068900	-0.25812600	-3.92514000
H	-3.44620700	0.65512800	-4.07484000
H	-1.99197500	-0.22316400	-4.58297200
H	-3.49756200	-1.11245300	-4.15968200
C	-2.96089700	3.55568600	0.35735800
H	-2.94729700	3.97424300	-0.65404000
H	-3.97111200	3.61723000	0.76150400
H	-2.26425100	4.13726900	0.96465900
C	0.07282200	-4.11591300	0.19206600
H	1.06531200	-3.88038100	0.58494700
H	-0.47086500	-4.77451900	0.86752100
H	0.21856700	-4.61047300	-0.77404400
C	-0.62949000	-0.21117900	4.04022500
H	-0.52151100	0.84870100	4.29327800
H	-1.38771200	-0.65535500	4.68488400

H	0.33950000	-0.68965800	4.19857700
C	1.70344600	0.04827600	-0.95883600
C	1.63269300	1.54476000	-1.12527600
C	2.16731500	3.54448200	0.24175400
O	1.13883000	2.17502600	-2.05409400
N	2.28030600	2.11999500	-0.05027200
C	2.82326700	1.15254600	0.87917600
H	2.17274700	1.01784400	1.75094200
H	3.81866300	1.44354500	1.23199200
C	2.88046000	-0.17483500	0.05683600
C	4.17505200	-0.31166600	-0.73144400
C	2.62653900	-1.34446700	0.96473000
C	4.87910000	-1.46317500	-0.72350500
C	3.35840700	-2.46794600	0.97663200
H	1.77290000	-1.22937800	1.62522200
C	4.52563000	-2.63579200	0.08788400
H	5.77647000	-1.56858800	-1.32710800
H	3.13829700	-3.29604800	1.64561700
H	1.63236400	3.94727400	-0.62304300
C	1.32629400	3.78421000	1.50224700
H	1.16389400	4.85667900	1.65127600
H	0.35793800	3.28825900	1.40210300
H	1.82921800	3.39955600	2.39718600
C	3.54512100	4.20901700	0.32699900
H	4.13587800	3.80634500	1.15770000
H	4.10543400	4.05906600	-0.60001000
H	3.43869900	5.28563700	0.49241600
O	5.16411300	-3.68636800	0.04829000
H	0.86327700	-1.37557600	-0.73117500
C	4.63991100	0.84889900	-1.57010400
H	4.82833700	1.73252400	-0.95234500
H	5.56276700	0.59197300	-2.09473700
H	3.89091700	1.14470600	-2.31127200
H	1.88311800	-0.40972400	-1.93809800

（S）-TRIPAg

Zero-point correction=	0.943436 (Hartree/Particle)
Thermal correction to Energy=	0.999109
Thermal correction to Enthalpy=	1.000053
Thermal correction to Gibbs Free Energy=	0.851110
Sum of electronic and zero-point Energies=	-2727.908289
Sum of electronic and thermal Energies=	-2727.852616
Sum of electronic and thermal Enthalpies=	-2727.851672

Sum of electronic and thermal Free Energies= -2728.000614

C	-0.41318000	2.53201200	-0.11458700
C	-0.91955800	3.75946200	-0.65987400
C	-3.18579300	2.76783400	-0.68555200
C	-2.68862600	1.55351000	-0.27087400
C	0.99410000	2.33521700	0.33320500
C	1.58748200	3.22569700	1.29653500
C	2.95350200	3.03255200	1.68113800
C	3.66719900	1.91774800	1.17610900
C	3.07171800	0.99427000	0.34813000
H	-4.24547400	2.87952300	-0.89252500
H	4.69926700	1.77083200	1.47942300
C	-3.46359700	0.27875600	-0.17140800
C	-3.91819200	-0.37032500	-1.34452500
C	-3.55402300	-0.37931300	1.07639000
C	-4.42805100	-1.67262200	-1.24902900
C	-4.01020700	-1.71873100	1.12112300
C	-4.46290300	-2.38009200	-0.04828100
H	-4.77150900	-2.16945400	-2.14986700
H	-4.16840500	-2.18618300	2.08919400
C	3.78250500	-0.24591000	-0.08575500
C	3.80146600	-1.36662200	0.77333700
C	4.40967200	-0.29953000	-1.34272900
C	4.48750600	-2.51095300	0.36411100
C	5.07724300	-1.47188200	-1.71251600
C	5.13160000	-2.58408700	-0.87457500
H	4.50889700	-3.37398200	1.02159100
H	5.56176600	-1.52341500	-2.68423500
C	-2.32700400	3.87795200	-0.91043700
C	-0.60644300	6.01980800	-1.50596800
C	-1.99945000	6.15215000	-1.71106900
C	-2.83725500	5.09977500	-1.42294800
C	-0.08059200	4.85496300	-0.99376600
H	0.05493900	6.84252900	-1.75984900
H	-2.40184600	7.07837800	-2.10948900
H	-3.90648100	5.18058700	-1.59917200
H	0.98790800	4.75921000	-0.84432000
C	2.83670600	4.95910000	3.16189800
C	1.47179700	5.11920100	2.82947400
C	0.86443500	4.27661400	1.92558100
C	3.55587600	3.92944000	2.60232100
H	3.30585100	5.63541800	3.86983500
H	0.89336400	5.91066300	3.29655700

H	-0.18427200	4.40899700	1.69433500
H	4.59738700	3.77178600	2.86890800
C	-1.29546200	1.47745500	0.01575600
C	1.73588400	1.23183300	-0.07753400
O	1.23849100	0.32815600	-1.00051100
O	-0.80465600	0.26854600	0.45471300
P	-0.04438500	-0.65352100	-0.71691900
O	0.31874200	-1.91115900	0.08368500
O	-0.85065500	-0.76655100	-1.96155700
Ag	-1.75635200	-2.46545900	0.63381800
C	4.35526400	0.87121600	-2.31339500
C	3.53136900	0.51228700	-3.56197800
C	5.76143900	1.36604000	-2.68879100
H	3.84499800	1.69880600	-1.81217500
H	2.52198600	0.20258500	-3.28088300
H	3.45592600	1.37449900	-4.23392700
H	3.99858000	-0.30692300	-4.11943500
H	6.33216200	1.64470600	-1.79720400
H	6.32899100	0.59482700	-3.22026000
H	5.69864400	2.24189000	-3.34361500
C	5.85528300	-3.84811600	-1.30553700
C	4.88308300	-5.03276200	-1.43668300
C	7.01648700	-4.18842000	-0.35676900
H	6.28184100	-3.65537600	-2.29850000
H	4.07083600	-4.79778500	-2.13082300
H	5.40304000	-5.92580000	-1.80073000
H	4.43236600	-5.27812800	-0.46912900
H	7.72197800	-3.35517900	-0.28378900
H	6.64896200	-4.40309600	0.65242000
H	7.56112400	-5.07156800	-0.70823800
C	3.11091500	-1.33440900	2.13214200
C	4.11054900	-0.95844400	3.24046400
C	2.39309500	-2.64877000	2.47445200
H	2.34439800	-0.55434200	2.09364900
H	4.56709500	0.01727600	3.05429100
H	3.61319000	-0.92016700	4.21610100
H	4.91556900	-1.69962300	3.29809800
H	1.71759900	-2.93152600	1.66547500
H	3.09989900	-3.46615700	2.65466500
H	1.80840800	-2.52098900	3.39280700
C	-3.22358300	0.33107200	2.38114100
C	-2.28016000	-0.46413900	3.29649700
C	-4.53265900	0.69341100	3.10949100
H	-2.72109400	1.26755900	2.13061500

H	-1.34144600	-0.68706900	2.78109900
H	-2.04223500	0.12105700	4.19035800
H	-2.73355200	-1.40241700	3.63553000
H	-5.18300200	1.29920600	2.47148100
H	-5.08658300	-0.20713600	3.39715600
H	-4.31847900	1.26254900	4.01954600
C	-3.86576500	0.29957500	-2.70859500
C	-5.23899000	0.91599800	-3.03769100
C	-3.40182200	-0.64028700	-3.83118800
H	-3.13310700	1.10598900	-2.64770000
H	-5.56539900	1.62194900	-2.26785700
H	-5.19866600	1.44750700	-3.99389200
H	-6.00503200	0.13626200	-3.11728800
H	-2.44425900	-1.09072500	-3.56736300
H	-4.13399600	-1.42801800	-4.04163900
H	-3.27599600	-0.06562100	-4.75448900
C	-5.03981400	-3.78302300	0.01678700
C	-6.41983500	-3.76869600	0.70059800
C	-4.09686800	-4.78178600	0.70736900
H	-5.18002600	-4.11859400	-1.01778000
H	-7.10219700	-3.08075900	0.19341500
H	-6.86734200	-4.76745600	0.68955300
H	-6.33456500	-3.44931900	1.74497900
H	-3.12033800	-4.81247500	0.20639200
H	-3.93711700	-4.52061900	1.75923600
H	-4.51366600	-5.79343600	0.68120700

CPA

Zero-point correction=	1.231684 (Hartree/Particle)
Thermal correction to Energy=	1.294409
Thermal correction to Enthalpy=	1.295274
Thermal correction to Gibbs Free Energy=	1.139764
Sum of electronic and zero-point Energies=	-3547.504285
Sum of electronic and thermal Energies=	-3547.441560
Sum of electronic and thermal Enthalpies=	-3547.440695
Sum of electronic and thermal Free Energies=	-3547.596205

C	-2.41904500	2.80579500	0.10181300
C	-3.47131000	3.58468900	-0.48723400
C	-4.86645500	1.55772200	-0.56270400
C	-3.82122200	0.78109900	-0.11107600
C	-1.12727700	3.41067400	0.52385100
C	-1.07108000	4.51630100	1.43776900

C	0.19883200	5.11204400	1.72592300
C	1.37314000	4.55820200	1.15959800
C	1.34142900	3.42692000	0.37094100
H	-5.81407200	1.08691200	-0.80470700
H	2.33123200	5.01496200	1.38806000
C	-3.92917800	-0.70792700	-0.04663000
C	-3.98048600	-1.45302700	-1.25226600
C	-3.97076600	-1.37853100	1.19354900
C	-4.10022800	-2.84814400	-1.17892800
C	-4.11562400	-2.77159500	1.21245500
C	-4.18525400	-3.52755800	0.04357900
H	-4.15334000	-3.41527000	-2.10228300
H	-4.16540000	-3.28480800	2.16925400
C	2.60880400	2.79672500	-0.10385100
C	3.49788100	2.23809500	0.83733300
C	2.95429100	2.80303900	-1.47318000
C	4.75048700	1.78689400	0.40505900
C	4.20226600	2.31110900	-1.85709800
C	5.13855500	1.83492000	-0.93269300
H	5.43146400	1.38660900	1.14631100
H	4.46159100	2.32403200	-2.91162500
C	-4.72225700	2.95100500	-0.77917400
C	-4.36093100	5.67108400	-1.37361100
C	-5.61122600	5.05474700	-1.61510600
C	-5.78185300	3.72078200	-1.32836400
C	-3.31958600	4.95656500	-0.82588500
H	-4.21907400	6.71692700	-1.62862000
H	-6.42596900	5.63217100	-2.04114800
H	-6.72768900	3.22661800	-1.53339600
H	-2.36520400	5.43778100	-0.65357100
C	-0.87187100	6.71503900	3.20962200
C	-2.12101400	6.09806400	2.96364800
C	-2.21825300	5.02826700	2.10274900
C	0.26230100	6.22494300	2.60616700
H	-0.81051100	7.56248400	3.88557200
H	-3.01117300	6.46792100	3.46357000
H	-3.17906700	4.55967500	1.93075500
H	1.23280900	6.67157400	2.80459700
C	-2.61151000	1.44012800	0.24107000
C	0.06818800	2.87848500	0.06174600
O	0.03815500	1.78430200	-0.78693900
O	-1.60003500	0.67145200	0.78325400
P	-0.29271600	0.30284700	-0.16321000
O	0.75601400	-0.24290600	0.74822700

O	-0.76042000	-0.50226900	-1.37660200
Ag	-1.17181800	-2.48608300	-0.54610600
C	2.03035100	3.36875900	-2.54376400
C	1.62275100	2.29053300	-3.56159900
C	2.66452400	4.58662300	-3.23762700
H	1.11711600	3.71901600	-2.05812300
H	1.13204100	1.45345000	-3.06040300
H	0.92598800	2.70543200	-4.29824900
H	2.49386700	1.90919200	-4.10591600
H	2.92492400	5.36136700	-2.50947900
H	3.57977100	4.31094100	-3.77228500
H	1.97006200	5.01966800	-3.96582000
C	6.52493100	1.41013500	-1.40723300
C	7.46138700	0.98459800	-0.27078900
C	7.19660700	2.53092000	-2.22367800
H	6.39957900	0.54294700	-2.06897100
H	7.03890400	0.17200400	0.32485100
H	8.42190100	0.65438100	-0.68149500
H	7.66539800	1.82177600	0.40598400
H	6.59742000	2.82567100	-3.08844300
H	7.34257800	3.42103100	-1.60187200
H	8.17650900	2.20639300	-2.59048500
C	3.14541300	2.08449200	2.31267100
C	4.01702100	2.98877600	3.19954500
C	3.23555000	0.61330200	2.75336100
H	2.10530300	2.38950500	2.44610200
H	3.91400200	4.04203700	2.92013700
H	3.73318900	2.88715200	4.25278100
H	5.07695400	2.72578500	3.11116200
H	2.57020900	0.00824000	2.13627900
H	4.25515000	0.22388700	2.66119700
H	2.93283800	0.51543700	3.80254200
C	-3.86112300	-0.63774300	2.51795600
C	-2.61269100	-1.08430600	3.29909900
C	-5.13992100	-0.79964200	3.35673900
H	-3.74677900	0.42693600	2.30316100
H	-1.71136800	-0.92731000	2.70205800
H	-2.51427700	-0.50673700	4.22430800
H	-2.67816900	-2.14312100	3.57682000
H	-6.01809900	-0.44982300	2.80516700
H	-5.31107000	-1.84665700	3.62905000
H	-5.06562600	-0.22189700	4.28399500
C	-3.93941500	-0.79124400	-2.62574400
C	-5.34814800	-0.76674400	-3.24770200

C	-2.94115600	-1.45530500	-3.58812000
H	-3.60987300	0.24053100	-2.48961800
H	-6.06817300	-0.26155400	-2.59806900
H	-5.33420200	-0.24517200	-4.21035100
H	-5.71444500	-1.78506700	-3.41993700
H	-1.92960700	-1.41307000	-3.17974500
H	-3.20305300	-2.49746600	-3.80080200
H	-2.93919500	-0.92033900	-4.54359400
C	-4.37827700	-5.03277700	0.09642600
C	-3.34790300	-5.79576600	-0.75121000
C	-5.81458300	-5.40268000	-0.31611700
H	-4.24166800	-5.33896500	1.14190200
H	-2.32671000	-5.56332500	-0.44011400
H	-3.49907000	-6.87570300	-0.65128300
H	-3.44685000	-5.54827400	-1.81365900
H	-6.55008400	-4.88714900	0.30882300
H	-6.00240200	-5.11840300	-1.35732000
H	-5.98031300	-6.48149900	-0.22613300
C	3.53870500	-2.40812200	-0.73843600
C	4.71737400	-2.19143800	-1.44960100
C	5.95645300	-2.14989000	-0.80523600
C	6.02740300	-2.30933800	0.57960200
C	4.85021800	-2.52499100	1.29367900
C	3.60655100	-2.58983100	0.66155000
H	4.68936100	-2.04050400	-2.52357900
H	6.98509400	-2.27151300	1.09191800
H	4.90174600	-2.64506500	2.37271000
C	2.22242800	-2.41525600	-1.46811100
H	2.36334400	-2.24067900	-2.53684000
H	1.69785800	-3.37028900	-1.35096400
H	1.57114900	-1.63068700	-1.07850200
C	2.37694700	-2.87844600	1.48569000
H	1.56634200	-2.18456400	1.24267800
H	2.61199000	-2.76068600	2.54853000
N	1.88156500	-4.26917800	1.27711800
C	0.59932900	-4.47925600	1.10620900
O	-0.05966200	-5.54490600	0.86939600
C	-0.61221800	-3.74002600	1.00307400
H	-1.17763600	-3.74943400	1.93742100
C	2.84055800	-5.40874800	1.28933300
C	2.96450900	-6.02501600	-0.10588500
C	2.47123600	-6.42560200	2.37201000
H	3.79744200	-4.95176500	1.54788200
H	3.29447000	-5.27388800	-0.82725900

H	3.70301500	-6.83194100	-0.08808100
H	2.00852500	-6.44060300	-0.43440900
H	3.25234800	-7.18868000	2.43490400
H	2.38820600	-5.94064600	3.34934700
H	1.52414500	-6.92078000	2.14716200
O	7.05795100	-1.94606300	-1.58571700
H	7.82615900	-1.80170100	-1.01843400

TSB

Zero-point correction=	1.228488 (Hartree/Particle)
Thermal correction to Energy=	1.291587
Thermal correction to Enthalpy=	1.292452
Thermal correction to Gibbs Free Energy=	1.134674
Sum of electronic and zero-point Energies=	-3547.464377
Sum of electronic and thermal Energies=	-3547.401278
Sum of electronic and thermal Enthalpies=	-3547.400413
Sum of electronic and thermal Free Energies=	-3547.558191

C	-0.86867000	3.58075600	-0.23474800
C	-1.29879500	4.59064600	-1.15916800
C	-3.47078700	3.43841000	-1.32951700
C	-3.02324000	2.40893700	-0.53005700
C	0.48479500	3.57961200	0.37979600
C	0.96568700	4.70317900	1.13123100
C	2.31734100	4.69913700	1.59979700
C	3.13885100	3.57873500	1.32666500
C	2.65947900	2.45654100	0.68394100
H	-4.46398400	3.38348700	-1.76507900
H	4.17971400	3.60197500	1.63485600
C	-3.77691800	1.13378500	-0.36392000
C	-3.96171300	0.28879300	-1.48681100
C	-4.19569800	0.70553800	0.91493200
C	-4.59783400	-0.94595900	-1.31280900
C	-4.79390500	-0.56146300	1.04862500
C	-5.02080200	-1.40039300	-0.05797500
H	-4.74706200	-1.58276500	-2.17806300
H	-5.14628600	-0.88188600	2.02505700
C	3.59433900	1.32956800	0.37737100
C	3.87705600	0.34838100	1.34545400
C	4.27618900	1.32464700	-0.86056700
C	4.88017600	-0.59144700	1.08050300
C	5.24444500	0.34511200	-1.08936400
C	5.59039400	-0.60162000	-0.11825600

H	5.11208900	-1.32473100	1.84228300
H	5.77116900	0.33553400	-2.03976500
C	-2.63855100	4.53649800	-1.66575200
C	-0.91077000	6.59040800	-2.49248500
C	-2.24777400	6.56241600	-2.95367200
C	-3.08844600	5.55098800	-2.55181600
C	-0.44785100	5.63044400	-1.62093000
H	-0.24092900	7.37379700	-2.83382900
H	-2.60100200	7.32959800	-3.63581100
H	-4.10980900	5.50112200	-2.91945600
H	0.57944700	5.65885800	-1.28040300
C	1.98812900	6.88104500	2.62100600
C	0.63916800	6.86976200	2.19400200
C	0.14113000	5.81099000	1.46908300
C	2.80537800	5.81366300	2.33197000
H	2.36930800	7.72560200	3.18685500
H	-0.01136200	7.70180600	2.44611400
H	-0.89601500	5.80941500	1.15750800
H	3.83787300	5.79815800	2.67012500
C	-1.72859300	2.53592900	0.04658900
C	1.30597800	2.46469100	0.24978500
O	0.82244900	1.32166000	-0.37858500
O	-1.31857500	1.57839600	0.95055900
P	-0.28474900	0.39226500	0.43325700
O	0.24910900	-0.27976200	1.65502500
O	-0.99775400	-0.43010700	-0.63452900
Ag	-2.37191700	-1.68661600	0.78158800
C	3.98405700	2.37326400	-1.92909400
C	3.07771600	1.81225800	-3.03815600
C	5.26447200	2.98414400	-2.51929200
H	3.43612400	3.18811300	-1.44816600
H	2.13852700	1.43734700	-2.62490200
H	2.84516500	2.58990900	-3.77417600
H	3.57372100	0.98930800	-3.56484500
H	5.91755100	3.37187800	-1.73140600
H	5.83671300	2.25182700	-3.09831900
H	5.01377400	3.80907400	-3.19457800
C	6.75173100	-1.55304600	-0.37573200
C	6.90344000	-2.65226900	0.68039400
C	8.06847500	-0.76166500	-0.50031200
H	6.57026200	-2.04725200	-1.33787700
H	5.97350300	-3.20825600	0.82182400
H	7.68226800	-3.35740400	0.37407800
H	7.19921200	-2.23302500	1.64861900

H	8.01100400	-0.00336100	-1.28602400
H	8.29522700	-0.24838700	0.44072700
H	8.90346600	-1.43136000	-0.73379600
C	3.16528100	0.32646200	2.69110600
C	3.99737600	1.05647300	3.76040300
C	2.82507200	-1.09859400	3.15313800
H	2.21495100	0.85088200	2.57395400
H	4.16693100	2.10215600	3.48968200
H	3.48436500	1.03704100	4.72835700
H	4.97570300	0.57816400	3.88465600
H	2.31448100	-1.64577900	2.35925700
H	3.71880700	-1.65905200	3.44980900
H	2.15797700	-1.05625700	4.01982900
C	-4.07343800	1.58518600	2.15056600
C	-3.34502200	0.87946300	3.30574900
C	-5.46562600	2.08081600	2.58376500
H	-3.48525000	2.46413200	1.88161600
H	-2.34962800	0.55315100	2.99536000
H	-3.22801200	1.56557600	4.15078900
H	-3.90732000	0.01062300	3.66638000
H	-5.96386800	2.61568900	1.76926000
H	-6.10965900	1.24588100	2.88117300
H	-5.38081100	2.76021900	3.43808300
C	-3.45289000	0.63887200	-2.87962100
C	-4.62208600	0.99504400	-3.81417400
C	-2.58495700	-0.48324500	-3.47561700
H	-2.81409100	1.51891800	-2.79310500
H	-5.21247100	1.82827500	-3.42034100
H	-4.24968100	1.27892200	-4.80387900
H	-5.29755800	0.14159900	-3.94137600
H	-1.76683700	-0.72309700	-2.79375700
H	-3.16549600	-1.39224700	-3.66894100
H	-2.16433900	-0.15629300	-4.43248200
C	-5.76275400	-2.71683000	0.10719100
C	-4.98637800	-3.91751500	-0.45428200
C	-7.16230700	-2.61755600	-0.52695200
H	-5.89492800	-2.87864400	1.18516400
H	-4.03089800	-4.06283600	0.05693200
H	-5.56752600	-4.83724500	-0.33249200
H	-4.78220600	-3.79481500	-1.52292300
H	-7.72714600	-1.77747400	-0.11170300
H	-7.08753900	-2.46909700	-1.60946300
H	-7.73115000	-3.53620400	-0.35132400
C	2.78056800	-2.75999900	-1.42487900

C	4.04278500	-3.18558900	-1.84077900
C	4.65744600	-4.29864800	-1.26702200
C	4.01517000	-5.00100200	-0.24330800
C	2.75065800	-4.58836500	0.16605300
C	2.11424700	-3.48931400	-0.41832400
H	4.56913900	-2.64698500	-2.62089900
H	4.49281700	-5.86198900	0.21817800
H	2.23203400	-5.14602600	0.94085300
C	2.17924700	-1.52740700	-2.04980400
H	2.79311800	-1.18449400	-2.88358800
H	1.16430700	-1.69709700	-2.42229100
H	2.12276200	-0.70865200	-1.32751300
C	0.70520400	-3.14412400	-0.00645100
H	0.29768000	-2.33704900	-0.61655800
H	0.68718700	-2.75429700	1.01898900
N	-0.17820000	-4.32505400	-0.08703700
C	-1.20191200	-4.48401300	0.79677800
O	-2.01877800	-5.41060800	0.77328400
C	-1.39963100	-3.30973400	1.70215800
H	-0.68310300	-3.13385100	2.50601300
N	-2.68996400	-4.18953700	2.99799700
N	-3.66618600	-4.38091600	3.48219100
C	-0.24776700	-5.00447200	-1.40891000
C	-1.51708500	-4.59469500	-2.16414200
C	-0.07445700	-6.51879000	-1.28760800
H	0.61529700	-4.61254100	-1.95193300
H	-1.59884400	-3.50407200	-2.22204200
H	-1.48380200	-4.98719600	-3.18513200
H	-2.40652700	-4.98997500	-1.67027000
H	-0.03208600	-6.96305700	-2.28740200
H	0.86047200	-6.75144000	-0.77052200
H	-0.90476700	-6.96051300	-0.73609200
O	5.89286000	-4.64508900	-1.73908300
H	6.23619900	-5.37875300	-1.21327900

CPD

Zero-point correction=	1.220720 (Hartree/Particle)
Thermal correction to Energy=	1.282174
Thermal correction to Enthalpy=	1.283039
Thermal correction to Gibbs Free Energy=	1.129071
Sum of electronic and zero-point Energies=	-3437.980207
Sum of electronic and thermal Energies=	-3437.918753
Sum of electronic and thermal Enthalpies=	-3437.917888

Sum of electronic and thermal Free Energies= -3438.071857

C	-2.41904500	2.80579500	0.10181300
C	-3.47131000	3.58468900	-0.48723400
C	-4.86645500	1.55772200	-0.56270400
C	-3.82122200	0.78109900	-0.11107600
C	-1.12727700	3.41067400	0.52385100
C	-1.07108000	4.51630100	1.43776900
C	0.19883200	5.11204400	1.72592300
C	1.37314000	4.55820200	1.15959800
C	1.34142900	3.42692000	0.37094100
H	-5.81407200	1.08691200	-0.80470700
H	2.33123200	5.01496200	1.38806000
C	-3.92917800	-0.70792700	-0.04663000
C	-3.98048600	-1.45302700	-1.25226600
C	-3.97076600	-1.37853100	1.19354900
C	-4.10022800	-2.84814400	-1.17892800
C	-4.11562400	-2.77159500	1.21245500
C	-4.18525400	-3.52755800	0.04357900
H	-4.15334000	-3.41527000	-2.10228300
H	-4.16540000	-3.28480800	2.16925400
C	2.60880400	2.79672500	-0.10385100
C	3.49788100	2.23809500	0.83733300
C	2.95429100	2.80303900	-1.47318000
C	4.75048700	1.78689400	0.40505900
C	4.20226600	2.31110900	-1.85709800
C	5.13855500	1.83492000	-0.93269300
H	5.43146400	1.38660900	1.14631100
H	4.46159100	2.32403200	-2.91162500
C	-4.72225700	2.95100500	-0.77917400
C	-4.36093100	5.67108400	-1.37361100
C	-5.61122600	5.05474700	-1.61510600
C	-5.78185300	3.72078200	-1.32836400
C	-3.31958600	4.95656500	-0.82588500
H	-4.21907400	6.71692700	-1.62862000
H	-6.42596900	5.63217100	-2.04114800
H	-6.72768900	3.22661800	-1.53339600
H	-2.36520400	5.43778100	-0.65357100
C	-0.87187100	6.71503900	3.20962200
C	-2.12101400	6.09806400	2.96364800
C	-2.21825300	5.02826700	2.10274900
C	0.26230100	6.22494300	2.60616700
H	-0.81051100	7.56248400	3.88557200
H	-3.01117300	6.46792100	3.46357000

H	-3.17906700	4.55967500	1.93075500
H	1.23280900	6.67157400	2.80459700
C	-2.61151000	1.44012800	0.24107000
C	0.06818800	2.87848500	0.06174600
O	0.03815500	1.78430200	-0.78693900
O	-1.60003500	0.67145200	0.78325400
P	-0.29271600	0.30284700	-0.16321000
O	0.75601400	-0.24290600	0.74822700
O	-0.76042000	-0.50226900	-1.37660200
Ag	-1.17181800	-2.48608300	-0.54610600
C	2.03035100	3.36875900	-2.54376400
C	1.62275100	2.29053300	-3.56159900
C	2.66452400	4.58662300	-3.23762700
H	1.11711600	3.71901600	-2.05812300
H	1.13204100	1.45345000	-3.06040300
H	0.92598800	2.70543200	-4.29824900
H	2.49386700	1.90919200	-4.10591600
H	2.92492400	5.36136700	-2.50947900
H	3.57977100	4.31094100	-3.77228500
H	1.97006200	5.01966800	-3.96582000
C	6.52493100	1.41013500	-1.40723300
C	7.46138700	0.98459800	-0.27078900
C	7.19660700	2.53092000	-2.22367800
H	6.39957900	0.54294700	-2.06897100
H	7.03890400	0.17200400	0.32485100
H	8.42190100	0.65438100	-0.68149500
H	7.66539800	1.82177600	0.40598400
H	6.59742000	2.82567100	-3.08844300
H	7.34257800	3.42103100	-1.60187200
H	8.17650900	2.20639300	-2.59048500
C	3.14541300	2.08449200	2.31267100
C	4.01702100	2.98877600	3.19954500
C	3.23555000	0.61330200	2.75336100
H	2.10530300	2.38950500	2.44610200
H	3.91400200	4.04203700	2.92013700
H	3.73318900	2.88715200	4.25278100
H	5.07695400	2.72578500	3.11116200
H	2.57020900	0.00824000	2.13627900
H	4.25515000	0.22388700	2.66119700
H	2.93283800	0.51543700	3.80254200
C	-3.86112300	-0.63774300	2.51795600
C	-2.61269100	-1.08430600	3.29909900
C	-5.13992100	-0.79964200	3.35673900
H	-3.74677900	0.42693600	2.30316100

H	-1.71136800	-0.92731000	2.70205800
H	-2.51427700	-0.50673700	4.22430800
H	-2.67816900	-2.14312100	3.57682000
H	-6.01809900	-0.44982300	2.80516700
H	-5.31107000	-1.84665700	3.62905000
H	-5.06562600	-0.22189700	4.28399500
C	-3.93941500	-0.79124400	-2.62574400
C	-5.34814800	-0.76674400	-3.24770200
C	-2.94115600	-1.45530500	-3.58812000
H	-3.60987300	0.24053100	-2.48961800
H	-6.06817300	-0.26155400	-2.59806900
H	-5.33420200	-0.24517200	-4.21035100
H	-5.71444500	-1.78506700	-3.41993700
H	-1.92960700	-1.41307000	-3.17974500
H	-3.20305300	-2.49746600	-3.80080200
H	-2.93919500	-0.92033900	-4.54359400
C	-4.37827700	-5.03277700	0.09642600
C	-3.34790300	-5.79576600	-0.75121000
C	-5.81458300	-5.40268000	-0.31611700
H	-4.24166800	-5.33896500	1.14190200
H	-2.32671000	-5.56332500	-0.44011400
H	-3.49907000	-6.87570300	-0.65128300
H	-3.44685000	-5.54827400	-1.81365900
H	-6.55008400	-4.88714900	0.30882300
H	-6.00240200	-5.11840300	-1.35732000
H	-5.98031300	-6.48149900	-0.22613300
C	3.53870500	-2.40812200	-0.73843600
C	4.71737400	-2.19143800	-1.44960100
C	5.95645300	-2.14989000	-0.80523600
C	6.02740300	-2.30933800	0.57960200
C	4.85021800	-2.52499100	1.29367900
C	3.60655100	-2.58983100	0.66155000
H	4.68936100	-2.04050400	-2.52357900
H	6.98509400	-2.27151300	1.09191800
H	4.90174600	-2.64506500	2.37271000
C	2.22242800	-2.41525600	-1.46811100
H	2.36334400	-2.24067900	-2.53684000
H	1.69785800	-3.37028900	-1.35096400
H	1.57114900	-1.63068700	-1.07850200
C	2.37694700	-2.87844600	1.48569000
H	1.56634200	-2.18456400	1.24267800
H	2.61199000	-2.76068600	2.54853000
N	1.88156500	-4.26917800	1.27711800
C	0.59932900	-4.47925600	1.10620900

O	-0.05966200	-5.54490600	0.86939600
C	-0.61221800	-3.74002600	1.00307400
H	-1.17763600	-3.74943400	1.93742100
C	2.84055800	-5.40874800	1.28933300
C	2.96450900	-6.02501600	-0.10588500
C	2.47123600	-6.42560200	2.37201000
H	3.79744200	-4.95176500	1.54788200
H	3.29447000	-5.27388800	-0.82725900
H	3.70301500	-6.83194100	-0.08808100
H	2.00852500	-6.44060300	-0.43440900
H	3.25234800	-7.18868000	2.43490400
H	2.38820600	-5.94064600	3.34934700
H	1.52414500	-6.92078000	2.14716200
O	7.05795100	-1.94606300	-1.58571700
H	7.82615900	-1.80170100	-1.01843400

CPE

Zero-point correction=	1.220669 (Hartree/Particle)
Thermal correction to Energy=	1.281758
Thermal correction to Enthalpy=	1.282623
Thermal correction to Gibbs Free Energy=	1.129455
Sum of electronic and zero-point Energies=	-3437.996670
Sum of electronic and thermal Energies=	-3437.935581
Sum of electronic and thermal Enthalpies=	-3437.934716
Sum of electronic and thermal Free Energies=	-3438.087885

C	1.98947500	2.64577100	0.75329400
C	2.55885400	3.96228500	0.78054400
C	0.41140700	4.85244600	-0.02213600
C	-0.11121400	3.58264800	-0.14280700
C	2.74735600	1.45788600	1.22773600
C	3.27802000	1.37475400	2.55819200
C	4.07605200	0.23959400	2.91255400
C	4.28968900	-0.78943900	1.96042600
C	3.70196600	-0.76461300	0.71394900
H	-0.21235500	5.70638600	-0.26752800
H	4.92228000	-1.62877400	2.23053600
C	-1.52530900	3.37115800	-0.58104200
C	-1.85876500	3.35126300	-1.95414300
C	-2.52930500	3.22060000	0.39574000
C	-3.19918000	3.19160200	-2.31433900
C	-3.85574300	3.05077500	-0.01705400
C	-4.21181000	3.03230300	-1.36470000

H	-3.45750000	3.17012900	-3.36725100
H	-4.63526900	2.93104500	0.73165900
C	3.89489600	-1.87107800	-0.27047400
C	3.26024600	-3.11863800	-0.07489600
C	4.72269200	-1.66638500	-1.39229500
C	3.49719100	-4.14333900	-0.99316500
C	4.91816900	-2.72098800	-2.28946500
C	4.32000800	-3.96603500	-2.10805900
H	3.01319000	-5.10312900	-0.84331400
H	5.55436500	-2.56711900	-3.15719100
C	1.74423200	5.07759000	0.40390800
C	4.41775700	5.48773600	1.15861600
C	3.59921000	6.59229800	0.82442900
C	2.29180700	6.38683500	0.45086500
C	3.91239000	4.20757600	1.13779300
H	5.45676500	5.65097000	1.42824700
H	4.00983400	7.59699200	0.85039200
H	1.65739200	7.22342600	0.17102200
H	4.55081500	3.36913900	1.38685400
C	4.37365100	1.13520300	5.15455600
C	3.55270300	2.23708400	4.81817900
C	3.01942800	2.35470300	3.55421100
C	4.62394600	0.15757500	4.22000300
H	4.79340400	1.05844900	6.15289000
H	3.33833600	2.99562700	5.56498100
H	2.38904100	3.20039000	3.30849100
H	5.23635700	-0.70427500	4.47064600
C	0.71092600	2.48852800	0.24124000
C	2.92773500	0.37904100	0.38008400
O	2.35765600	0.42693100	-0.88574000
O	0.17181900	1.21330200	0.15746900
P	0.74741300	0.16126400	-0.99054300
O	0.41916800	-1.21715400	-0.43488100
O	0.30790100	0.54857600	-2.36783000
C	5.42224000	-0.33926700	-1.65414900
C	4.95703200	0.28963600	-2.97800500
C	6.95139400	-0.49984500	-1.61229200
H	5.15294600	0.35340500	-0.85295000
H	3.87291700	0.42256000	-2.98078600
H	5.42691300	1.26892300	-3.12121500
H	5.22931400	-0.33837300	-3.83320100
H	7.27677600	-0.91488000	-0.65302400
H	7.30374000	-1.17092000	-2.40277900
H	7.44407500	0.46848500	-1.75227200

C	4.54283800	-5.09057700	-3.10407400
C	3.23026500	-5.49071600	-3.79891600
C	5.21328300	-6.30729000	-2.44491600
H	5.22573700	-4.71056200	-3.87492400
H	2.76544700	-4.62830700	-4.28553400
H	3.40945400	-6.26149900	-4.55659200
H	2.51132900	-5.89178500	-3.07648800
H	6.16015200	-6.02745400	-1.97323700
H	4.56993300	-6.73865800	-1.67047300
H	5.41466100	-7.08955900	-3.18486400
C	2.32658200	-3.37638300	1.10180700
C	3.04803100	-4.12910700	2.23362800
C	1.05797300	-4.14216200	0.68699400
H	2.00809000	-2.40441000	1.48796400
H	3.91075500	-3.57059000	2.60540500
H	2.36945100	-4.30472000	3.07611800
H	3.40836600	-5.10157300	1.87996800
H	0.59897100	-3.68350100	-0.19132000
H	1.27272100	-5.19109400	0.45509400
H	0.33326400	-4.13887200	1.51028300
C	-2.20047200	3.21895200	1.88329900
C	-2.32549400	1.80194900	2.46763300
C	-3.05099800	4.22717200	2.67070400
H	-1.15624400	3.52090300	1.99572400
H	-1.68609900	1.10775600	1.91638300
H	-2.02869400	1.78564400	3.52261100
H	-3.36230100	1.44864300	2.40351200
H	-2.94740100	5.23461900	2.25673400
H	-4.11425500	3.96567800	2.64968800
H	-2.73808700	4.25398700	3.71988000
C	-0.79390300	3.51428200	-3.03113400
C	-0.61857600	4.99822700	-3.40355800
C	-1.08025500	2.68648900	-4.29269700
H	0.14867300	3.14844700	-2.61607300
H	-0.31431000	5.59925600	-2.54339500
H	0.14514200	5.10992100	-4.18064500
H	-1.55775500	5.41112900	-3.78902900
H	-1.31376800	1.64977400	-4.04841300
H	-1.91110200	3.10376900	-4.87308300
H	-0.19882200	2.68837300	-4.94069800
C	-5.65910200	2.84528200	-1.78691900
C	-5.84473800	1.59943700	-2.66983700
C	-6.19855600	4.10360900	-2.48817100
H	-6.24687200	2.69668700	-0.87093100

H	-5.49848300	0.69676200	-2.16042800
H	-6.90008600	1.46959400	-2.93382600
H	-5.27741500	1.68963500	-3.60178900
H	-6.09383200	4.98620100	-1.84987400
H	-5.65089500	4.29674500	-3.41663300
H	-7.25735500	3.98480000	-2.74258600
Ag	-1.15161400	-1.57819000	0.92402200
C	-2.74030000	-1.70309800	2.20938700
C	-3.78257800	-2.67374100	2.31509500
C	-5.81253700	-4.02730200	2.19901600
O	-3.18585200	-3.25559400	3.26903100
N	-4.93150700	-2.92734200	1.72120600
C	-5.44805600	-1.92696400	0.73672300
H	-5.69215200	-1.00135100	1.26896300
H	-6.38618200	-2.34508700	0.36514900
C	-4.47614200	-1.64981100	-0.37468300
C	-4.22658700	-2.60907000	-1.38040100
C	-3.75494400	-0.44952500	-0.39027000
C	-3.25797000	-2.34278900	-2.34284400
C	-2.77684900	-0.18751900	-1.34953400
H	-3.96639700	0.31500400	0.35101100
C	-2.50968900	-1.15112300	-2.33792700
H	-3.04525700	-3.06757500	-3.12230300
H	-2.24339300	0.75327800	-1.34267000
H	-6.56192300	-4.13375500	1.40912900
C	-5.06296600	-5.35573900	2.32530700
H	-5.78581200	-6.15358300	2.51814800
H	-4.52752100	-5.59512600	1.40278900
H	-4.34297000	-5.33314200	3.14439400
C	-6.51053700	-3.61884800	3.49981900
H	-5.77539900	-3.48219400	4.29786300
H	-7.06780000	-2.68584100	3.37336900
H	-7.21372300	-4.39672800	3.81110000
O	-1.58757000	-0.99498200	-3.29593500
H	-0.87948800	-0.35229700	-3.00562000
C	-4.97477700	-3.91886000	-1.41665300
H	-4.71938900	-4.55004600	-0.55872500
H	-6.06119100	-3.77022300	-1.39658200
H	-4.73472900	-4.47950200	-2.32243100
H	-2.90066800	-0.88950800	2.92239100

TSC

Zero-point correction= 1.220798 (Hartree/Particle)

Thermal correction to Energy=	1.281077
Thermal correction to Enthalpy=	1.281942
Thermal correction to Gibbs Free Energy=	1.131241
Sum of electronic and zero-point Energies=	-3437.995024
Sum of electronic and thermal Energies=	-3437.934745
Sum of electronic and thermal Enthalpies=	-3437.933880
Sum of electronic and thermal Free Energies=	-3438.084582

C	2.06373100	2.61682700	0.74916700
C	2.65426400	3.92426300	0.75675700
C	0.51506100	4.83914700	-0.03953900
C	-0.02848300	3.57651600	-0.14277900
C	2.80843200	1.42194600	1.22692800
C	3.35386800	1.34353700	2.55163200
C	4.14026200	0.20063700	2.90698500
C	4.32681200	-0.84056900	1.96248100
C	3.72391100	-0.81922300	0.72317900
H	-0.09647200	5.69994500	-0.29154200
H	4.95039900	-1.68651000	2.23289000
C	-1.44702300	3.38617200	-0.57657900
C	-1.78451900	3.37341200	-1.94889500
C	-2.45152800	3.25633600	0.40242000
C	-3.12934300	3.24545300	-2.30568200
C	-3.78266600	3.11663300	-0.00685300
C	-4.14306600	3.10955500	-1.35354500
H	-3.39086000	3.23217100	-3.35796600
H	-4.56264400	3.01520400	0.74418600
C	3.88740100	-1.93900500	-0.25158400
C	3.23062100	-3.17204200	-0.03772000
C	4.70940000	-1.76168400	-1.38212100
C	3.44044800	-4.21050100	-0.94701800
C	4.87737500	-2.82903000	-2.26984200
C	4.25726600	-4.06048800	-2.07037300
H	2.93952600	-5.15926100	-0.78325900
H	5.50894100	-2.69622600	-3.14442000
C	1.85406300	5.04811000	0.37485000
C	4.54017500	5.42423100	1.10153900
C	3.73595600	6.53797300	0.76300400
C	2.42227300	6.34910400	0.40308000
C	4.01476200	4.15201600	1.09895800
H	5.58403800	5.57393800	1.36002500
H	4.16242600	7.53631000	0.77467200
H	1.79853100	7.19248200	0.11964900
H	4.64238100	3.30642900	1.35114900

C	4.47904700	1.11345300	5.13610600
C	3.66930400	2.22349900	4.79939600
C	3.12159000	2.33646500	3.54123500
C	4.70361900	0.12340700	4.20814300
H	4.91033000	1.04035300	6.12978400
H	3.47494000	2.99198400	5.54148100
H	2.49973100	3.18839400	3.29534400
H	5.30692000	-0.74462500	4.45951800
C	0.77809300	2.47422800	0.25054400
C	2.96328800	0.33283100	0.38733100
O	2.38082100	0.37829100	-0.87329800
O	0.21867000	1.20594400	0.18733800
P	0.76585800	0.14072500	-0.96054500
O	0.42469100	-1.23285700	-0.39985500
O	0.31751600	0.53248600	-2.33418300
C	5.43047500	-0.45028500	-1.66378800
C	4.96226600	0.17473300	-2.98844700
C	6.95678500	-0.63843700	-1.63694600
H	5.18246800	0.25447000	-0.86621300
H	3.88084700	0.32800100	-2.98048300
H	5.44873700	1.14358700	-3.14646300
H	5.21297100	-0.46652900	-3.84040000
H	7.28505400	-1.05064100	-0.67744800
H	7.28822700	-1.32296500	-2.42493100
H	7.46545600	0.31939400	-1.79119900
C	4.45015200	-5.19942600	-3.05623100
C	3.12463800	-5.58001100	-3.73741100
C	5.10078300	-6.42267100	-2.38938200
H	5.13482400	-4.84117100	-3.83587600
H	2.67390400	-4.71344500	-4.22988500
H	3.28251200	-6.36222000	-4.48808700
H	2.40307000	-5.95870200	-3.00558100
H	6.05650900	-6.15721600	-1.92736300
H	4.45461500	-6.83316100	-1.60598200
H	5.28097800	-7.21628400	-3.12267600
C	2.30149700	-3.39860800	1.14899600
C	3.01948000	-4.14473100	2.28742700
C	1.01946700	-4.15274900	0.75456900
H	1.99920100	-2.41644000	1.52194500
H	3.89127100	-3.59228400	2.64671500
H	2.34342600	-4.29962700	3.13595900
H	3.36509900	-5.12667400	1.94545400
H	0.56508800	-3.70615000	-0.13242600
H	1.21640800	-5.20967800	0.54417200

H	0.29743200	-4.12064100	1.57955800
C	-2.11992300	3.24736700	1.88901400
C	-2.29411300	1.83701700	2.47604100
C	-2.93363000	4.28731900	2.67414000
H	-1.06559500	3.51270700	1.99917300
H	-1.67780200	1.12119800	1.92628500
H	-1.99966100	1.81171900	3.53129500
H	-3.34271000	1.52041700	2.41093400
H	-2.79286700	5.28956700	2.25847800
H	-4.00569100	4.06470000	2.65227000
H	-2.62086700	4.30453300	3.72354000
C	-0.71986800	3.51083500	-3.02970500
C	-0.52253600	4.98837400	-3.41618300
C	-1.02297600	2.67625000	-4.28300300
H	0.21784100	3.13390200	-2.61375100
H	-0.20641300	5.59247600	-2.56247700
H	0.24054300	5.08099000	-4.19638800
H	-1.45620700	5.41248200	-3.80287100
H	-1.27071900	1.64531600	-4.02858200
H	-1.84966800	3.10047700	-4.86423100
H	-0.14398200	2.65941500	-4.93413500
C	-5.59665600	2.96587800	-1.77120400
C	-5.81889500	1.74996300	-2.68638900
C	-6.10917700	4.25581800	-2.43456300
H	-6.18226400	2.80686300	-0.85556000
H	-5.48654800	0.82592800	-2.20681800
H	-6.87971400	1.65010300	-2.94107300
H	-5.26121200	1.85427500	-3.62264600
H	-5.98055900	5.11740900	-1.77241700
H	-5.56013800	4.46135800	-3.35958000
H	-7.17155700	4.16956500	-2.68721900
Ag	-1.21126400	-1.60102700	0.87411300
C	-2.87444600	-1.65593700	2.05822300
C	-3.92197300	-2.61296000	2.25603300
C	-6.02738000	-3.85472300	2.22988900
O	-3.37038600	-3.16648300	3.24627100
N	-5.08977700	-2.84167700	1.67788200
C	-5.57016700	-1.85157200	0.67087200
H	-5.83586300	-0.91923200	1.18215000
H	-6.49166400	-2.27190100	0.26181000
C	-4.55363900	-1.58937600	-0.40412200
C	-4.27571200	-2.56701200	-1.38533400
C	-3.82389800	-0.39290800	-0.41311800
C	-3.27859300	-2.31889400	-2.32166300

C	-2.81243500	-0.15157500	-1.34536900
H	-4.05603700	0.38616400	0.30701400
C	-2.52579200	-1.12883800	-2.31471900
H	-3.04503900	-3.05610800	-3.08327000
H	-2.27116500	0.78498900	-1.33441200
H	-6.80858700	-3.94278100	1.46860400
C	-5.36271400	-5.22411300	2.39004500
H	-6.12468600	-5.96110400	2.65948100
H	-4.89293500	-5.54414700	1.45616900
H	-4.60165000	-5.20822700	3.17138700
C	-6.65454500	-3.34801400	3.53262500
H	-5.88679000	-3.23101700	4.30222100
H	-7.15104700	-2.38447200	3.38322900
H	-7.39919400	-4.06217600	3.89588600
O	-1.58209800	-0.99326500	-3.25305800
H	-0.87164100	-0.35217700	-2.96018600
C	-5.02681000	-3.87496100	-1.42120100
H	-4.82068500	-4.47782000	-0.53043700
H	-6.11197100	-3.72205700	-1.46346100
H	-4.74149800	-4.46389600	-2.29527100
H	-3.03814100	-0.78922000	2.70670500

CPB

Zero-point correction=	1.233417 (Hartree/Particle)
Thermal correction to Energy=	1.295212
Thermal correction to Enthalpy=	1.296077
Thermal correction to Gibbs Free Energy=	1.142545
Sum of electronic and zero-point Energies=	-3547.514702
Sum of electronic and thermal Energies=	-3547.452906
Sum of electronic and thermal Enthalpies=	-3547.452041
Sum of electronic and thermal Free Energies=	-3547.605573

C	1.20173500	-2.82425600	0.86135400
C	1.90017000	-4.01894100	1.22955800
C	3.96053100	-3.02897300	0.32087400
C	3.28076700	-1.90139800	-0.08744100
C	-0.21471100	-2.58479100	1.24031100
C	-0.62590400	-2.53218300	2.61308800
C	-2.00824900	-2.30109600	2.90655300
C	-2.92163000	-2.09514200	1.84221700
C	-2.51955700	-2.04964900	0.52298000
H	5.03659400	-3.07689600	0.18272100
H	-3.96864800	-1.93776800	2.07870900

C	3.98912400	-0.68730500	-0.59624000
C	4.19757900	-0.47947300	-1.97627400
C	4.41537900	0.27472700	0.34352600
C	4.81191700	0.70591500	-2.38760600
C	5.00396600	1.45651300	-0.12043400
C	5.20243900	1.69478900	-1.47986400
H	4.96144500	0.87707500	-3.44745600
H	5.31771400	2.21398500	0.59258800
C	-3.48450300	-1.73047200	-0.56925000
C	-4.10481700	-0.45811500	-0.62264800
C	-3.79508600	-2.70524700	-1.53992000
C	-5.03124200	-0.20404000	-1.63497000
C	-4.72119200	-2.39425800	-2.54031500
C	-5.35143300	-1.15406800	-2.60709700
H	-5.50628500	0.77121600	-1.67543600
H	-4.96174100	-3.14413100	-3.28912600
C	3.29986800	-4.11849300	0.94421300
C	1.95985200	-6.25641400	2.18265900
C	3.34775300	-6.34449700	1.92166500
C	3.99971800	-5.29723600	1.31297500
C	1.25394300	-5.12343100	1.84650800
H	1.44634800	-7.09288900	2.64680900
H	3.89237900	-7.24313700	2.19446400
H	5.06273800	-5.35784500	1.09637900
H	0.18944800	-5.06697300	2.04118500
C	-1.53064000	-2.40700200	5.28998100
C	-0.15844300	-2.59439000	5.00202000
C	0.28395200	-2.65454700	3.69863000
C	-2.43204800	-2.25706800	4.26177300
H	-1.86601700	-2.36703100	6.32161000
H	0.55333100	-2.69106600	5.81629800
H	1.33652500	-2.80007900	3.48882700
H	-3.48571100	-2.09171300	4.46895100
C	1.87836000	-1.85158000	0.14399200
C	-1.14489800	-2.30552000	0.25457200
O	-0.69680000	-2.25363500	-1.06123700
O	1.19220800	-0.72763200	-0.28068600
P	0.02241100	-0.83596700	-1.48068600
O	-0.92352000	0.30781500	-1.15764500
O	0.63320800	-0.95252800	-2.83733100
C	-3.19308500	-4.10428300	-1.51638900
C	-2.42410300	-4.41644500	-2.81022600
C	-4.27710800	-5.16017200	-1.23695800
H	-2.47815100	-4.15915500	-0.69243100

H	-1.64604500	-3.67075900	-2.98598700
H	-1.94992200	-5.40156400	-2.74202100
H	-3.09228900	-4.42997900	-3.67795300
H	-4.79500500	-4.95250300	-0.29513000
H	-5.02838800	-5.17891800	-2.03348700
H	-3.83326600	-6.15952400	-1.17171800
C	-6.34630000	-0.84151200	-3.71073300
C	-5.84420000	0.30271100	-4.60763300
C	-7.74140200	-0.52974400	-3.14418800
H	-6.43250200	-1.74088100	-4.33401600
H	-4.86104600	0.07005100	-5.02689600
H	-6.53974900	0.48352200	-5.43440900
H	-5.75093600	1.23401900	-4.03870300
H	-8.10940900	-1.35500000	-2.52705900
H	-7.71992700	0.36978500	-2.51953500
H	-8.45996200	-0.35682900	-3.95262200
C	-3.79681800	0.65963900	0.36763500
C	-4.92364900	0.84920400	1.39704600
C	-3.49896700	1.99844100	-0.33381500
H	-2.89570600	0.37174400	0.92079400
H	-5.12370300	-0.06921300	1.95563300
H	-4.65752100	1.63457200	2.11327900
H	-5.85468700	1.14168900	0.89919300
H	-2.75525700	1.87356600	-1.12276000
H	-4.40347400	2.42997600	-0.77554100
H	-3.12490500	2.72362700	0.39809400
C	4.21907500	0.05905000	1.84132200
C	2.95143500	0.77295100	2.34102300
C	5.44256600	0.46930200	2.67322100
H	4.06502200	-1.01060200	2.00301300
H	2.08295900	0.47856700	1.74689300
H	2.75813700	0.53337200	3.39355600
H	3.07430100	1.86024100	2.25669900
H	6.34876900	-0.02391300	2.30994600
H	5.61531600	1.55018700	2.64383800
H	5.29784400	0.19021600	3.72225300
C	3.78418700	-1.53238100	-2.99466900
C	4.87836600	-2.60765400	-3.13166600
C	3.44196500	-0.94761200	-4.37138300
H	2.87639500	-2.01105400	-2.61812400
H	5.06924700	-3.11356200	-2.18209600
H	4.57954200	-3.36533200	-3.86384600
H	5.81839300	-2.15843200	-3.47157600
H	2.76585700	-0.09521900	-4.28916600

H	4.34078000	-0.62450900	-4.90944500
H	2.94985100	-1.70903100	-4.98260500
C	5.79648500	3.00651800	-1.96210600
C	4.76281800	3.81617200	-2.76489600
C	7.08298600	2.78852000	-2.77477100
H	6.06027500	3.59053600	-1.07036300
H	3.85897800	3.99592800	-2.17624700
H	5.17936300	4.78185300	-3.07138900
H	4.46064700	3.27733900	-3.66892900
H	7.82506300	2.22868100	-2.19740200
H	6.87913400	2.22583900	-3.69174100
H	7.52438000	3.74774300	-3.06538700
Ag	-0.52955400	1.29650400	0.69969200
C	-0.15291400	2.35715100	2.58843000
C	-1.15155800	3.49974000	2.65118400
C	-1.74589100	5.79005100	2.03941600
O	-2.11358500	3.40227900	3.41142900
N	-0.91727200	4.56542700	1.83238600
C	0.33073500	4.71756800	1.03748600
H	1.19704200	4.47854800	1.66504300
H	0.40890500	5.78786200	0.82955100
C	0.43386400	3.92640500	-0.25507900
C	-0.42321600	4.15090000	-1.35878000
C	1.46989400	2.98514600	-0.40333600
C	-0.26292300	3.38324500	-2.51138000
C	1.62420600	2.22197600	-1.55989300
H	2.18691400	2.84669200	0.40082200
C	0.71764700	2.38810700	-2.61435600
H	-0.93713300	3.51705600	-3.35119700
H	2.41180800	1.48442200	-1.62897900
H	-1.45790700	6.44599800	1.21531800
C	-3.25576300	5.55527300	1.92472300
H	-3.75141200	6.52467700	1.80920300
H	-3.49986500	4.94512900	1.05231100
H	-3.64865500	5.05482500	2.80759600
C	-1.36991300	6.47563700	3.35781600
H	-1.62347600	5.83198700	4.20321400
H	-0.29931400	6.70214700	3.39328000
H	-1.91947300	7.41596000	3.46419700
O	0.75504200	1.63665000	-3.73921400
H	0.82926600	0.68007400	-3.49895800
C	-1.51903100	5.18438700	-1.32120100
H	-2.32430100	4.88783000	-0.64486900
H	-1.14923600	6.15938100	-0.98367100

H	-1.95301900	5.32111000	-2.31397100
H	0.91263000	2.55121400	2.50013800
N	-0.60175200	0.74392500	4.41736000
N	-0.37260200	1.47944900	3.60063800

TSA

Zero-point correction=	1.229104 (Hartree/Particle)
Thermal correction to Energy=	1.290974
Thermal correction to Enthalpy=	1.291839
Thermal correction to Gibbs Free Energy=	1.137248
Sum of electronic and zero-point Energies=	-3547.483893
Sum of electronic and thermal Energies=	-3547.422024
Sum of electronic and thermal Enthalpies=	-3547.421159
Sum of electronic and thermal Free Energies=	-3547.575749

C	-0.05543700	-2.98567800	1.09226400
C	0.13366500	-4.33464900	1.53471700
C	2.34413700	-4.32067100	0.45670900
C	2.14410700	-3.04210200	-0.01862200
C	-1.24727800	-2.18862600	1.48251200
C	-1.53897400	-1.88459600	2.85251100
C	-2.71628200	-1.12606200	3.15112100
C	-3.54787600	-0.68086100	2.09188900
C	-3.22774600	-0.89130100	0.76675700
H	3.29586200	-4.81002600	0.27198600
H	-4.45146400	-0.13200500	2.33561700
C	3.23935500	-2.26661500	-0.67727600
C	3.39451500	-2.25896900	-2.07993900
C	4.10908200	-1.51701900	0.14155100
C	4.41179700	-1.47875100	-2.63521100
C	5.09871800	-0.73435000	-0.46407400
C	5.26128500	-0.69515200	-1.84829100
H	4.52884600	-1.46112900	-3.71282500
H	5.76431100	-0.13972900	0.15581800
C	-4.06968800	-0.35143900	-0.34066700
C	-4.19689900	1.04586400	-0.53030300
C	-4.75210000	-1.24198200	-1.19623100
C	-5.01447600	1.51273000	-1.56102700
C	-5.54978900	-0.72139200	-2.21953800
C	-5.69572200	0.64903700	-2.42094100
H	-5.11193700	2.58410200	-1.70565300
H	-6.07625100	-1.40581700	-2.87931400
C	1.35337700	-5.00757600	1.20337800

C	-0.63511300	-6.34257500	2.67339000
C	0.58084300	-6.99806200	2.36682700
C	1.55062700	-6.34246300	1.64452900
C	-0.85372200	-5.04511100	2.26886300
H	-1.40504400	-6.87050900	3.22775500
H	0.74061100	-8.02059700	2.69468900
H	2.48332600	-6.83917300	1.39162300
H	-1.79136900	-4.55383200	2.49982200
C	-2.17754300	-1.20944200	5.52229800
C	-0.99643800	-1.92926900	5.22492500
C	-0.68465000	-2.25967100	3.92451000
C	-3.01501800	-0.81531100	4.50447500
H	-2.41366400	-0.96023100	6.55214000
H	-0.32902500	-2.22284700	6.02952900
H	0.22204400	-2.81055200	3.70570200
H	-3.91641800	-0.24750900	4.71808300
C	0.90283400	-2.41242200	0.27278400
C	-2.05425200	-1.64986400	0.49748100
O	-1.67640000	-1.84469600	-0.82835300
O	0.69649000	-1.13210400	-0.21299100
P	-0.49668600	-0.82612800	-1.34110100
O	-0.92924300	0.60393500	-1.04421000
O	-0.06472500	-1.20037200	-2.72027900
C	-4.68887900	-2.75431100	-1.02371100
C	-4.14133700	-3.44967800	-2.28053800
C	-6.06449500	-3.31595200	-0.62340500
H	-4.00437400	-2.98084500	-0.20322000
H	-3.15824300	-3.05322700	-2.54275600
H	-4.04552400	-4.52713700	-2.10754200
H	-4.80967300	-3.30993300	-3.13691000
H	-6.43037800	-2.84314200	0.29360600
H	-6.80849000	-3.14211100	-1.40794800
H	-6.00427700	-4.39628800	-0.45243300
C	-6.55979300	1.18517700	-3.54850800
C	-5.72083000	1.97281400	-4.56907500
C	-7.72438300	2.03574100	-3.01490700
H	-6.98981600	0.31886400	-4.06756600
H	-4.90542100	1.35961700	-4.96354400
H	-6.34090400	2.30646600	-5.40826700
H	-5.27548800	2.86087800	-4.10792200
H	-8.33610500	1.46698800	-2.30804300
H	-7.35483600	2.92611000	-2.49486200
H	-8.36803600	2.37211900	-3.83488200
C	-3.47888900	2.07077400	0.34055100

C	-4.44211000	2.73156200	1.34177000
C	-2.76119300	3.14946700	-0.49260300
H	-2.71527800	1.54012000	0.91798400
H	-4.92914600	1.99333900	1.98488700
H	-3.90652700	3.44140600	1.98235200
H	-5.23045900	3.27946200	0.81421600
H	-2.13364300	2.69569100	-1.26175000
H	-3.47428400	3.82245600	-0.98019000
H	-2.13234400	3.76845000	0.15959900
C	3.96644800	-1.52197200	1.66014400
C	3.17455900	-0.29381800	2.13941900
C	5.31294300	-1.62737400	2.39016600
H	3.38270200	-2.40397800	1.93429400
H	2.21755800	-0.22128300	1.61717700
H	2.98602800	-0.34678200	3.21807300
H	3.74697200	0.62109400	1.94119400
H	5.88556000	-2.49063700	2.03868900
H	5.92996900	-0.73459100	2.24419000
H	5.15130400	-1.73932900	3.46746400
C	2.49603300	-3.10624800	-2.96970400
C	3.04691500	-4.54065900	-3.07605800
C	2.28765700	-2.51202600	-4.36889700
H	1.51298200	-3.15131500	-2.49404100
H	3.10987700	-5.02177400	-2.09679700
H	2.39925100	-5.15295000	-3.71252400
H	4.05043500	-4.53578100	-3.51638600
H	2.00390700	-1.45962200	-4.31833600
H	3.18859200	-2.60137300	-4.98678900
H	1.48471700	-3.04952200	-4.88084500
C	6.31986300	0.18958900	-2.48329300
C	5.68031700	1.28679900	-3.35185600
C	7.33841300	-0.63249700	-3.28983300
H	6.86232500	0.68325300	-1.66601300
H	4.97349300	1.88739100	-2.77287500
H	6.44765700	1.95041200	-3.76502800
H	5.12776500	0.85010700	-4.19027300
H	7.81024600	-1.39801500	-2.66633600
H	6.85565100	-1.13879400	-4.13226700
H	8.12379000	0.01381200	-3.69597600
Ag	-0.05304900	1.60576700	0.57996700
C	1.16707200	2.57551200	1.91032500
C	1.12037800	4.03914200	2.27106300
C	1.94798200	6.30665300	1.80317200
O	0.43482800	4.42419300	3.22031600

N	1.84843200	4.86069300	1.46112600
C	2.82484300	4.30539300	0.49497800
H	3.59443900	3.72957800	1.02745900
H	3.33545600	5.17232700	0.06675800
C	2.24451600	3.44903300	-0.60987100
C	1.31461400	3.97351500	-1.54351500
C	2.70827800	2.13493600	-0.79761000
C	0.87474800	3.16706200	-2.58780200
C	2.24762600	1.32574300	-1.83306900
H	3.44979800	1.72576500	-0.11773100
C	1.30817600	1.83940800	-2.73956000
H	0.14866700	3.54448100	-3.30053900
H	2.60512600	0.30991800	-1.93508300
H	2.47264800	6.74630800	0.94952700
C	0.59217400	7.01042900	1.91439300
H	0.76205600	8.09052100	1.96860500
H	-0.02848300	6.81085900	1.03814600
H	0.05176700	6.68974100	2.80329400
C	2.80759300	6.50575900	3.05688900
H	2.31608100	6.05722100	3.92303600
H	3.79488700	6.04891800	2.93423300
H	2.94929100	7.57305300	3.25289400
O	0.80702300	1.12802000	-3.76751700
H	0.59635300	0.20239900	-3.48172800
C	0.76647500	5.37143600	-1.41684100
H	0.03854500	5.43208500	-0.60204700
H	1.55011200	6.10629900	-1.20327500
H	0.26412100	5.67406200	-2.33825900
H	2.15224200	2.11919800	2.01856100
N	0.04189100	1.32290700	4.41455500
N	0.61582200	1.87414100	3.64583800

CPC

Zero-point correction=	1.219603 (Hartree/Particle)
Thermal correction to Energy=	1.280069
Thermal correction to Enthalpy=	1.280934
Thermal correction to Gibbs Free Energy=	1.128554
Sum of electronic and zero-point Energies=	-3438.026042
Sum of electronic and thermal Energies=	-3437.965576
Sum of electronic and thermal Enthalpies=	-3437.964711
Sum of electronic and thermal Free Energies=	-3438.117092

C	2.39578700	2.51299100	0.68919400

C	3.06217600	3.77969300	0.57829200
C	0.92813200	4.78722600	-0.11488900
C	0.30685300	3.55667800	-0.11520300
C	3.10588600	1.29773600	1.16834000
C	3.77404600	1.25288600	2.43768900
C	4.52502000	0.08259200	2.78002800
C	4.54914600	-1.01979500	1.88831500
C	3.82242200	-1.02762800	0.71728700
H	0.35573300	5.66916600	-0.38432300
H	5.14100100	-1.89082200	2.14960400
C	-1.12792600	3.42590500	-0.51183200
C	-1.49365400	3.52364200	-1.87309500
C	-2.11691600	3.26265300	0.47786200
C	-2.85149800	3.50742500	-2.20780700
C	-3.46122800	3.23349200	0.09096300
C	-3.85234600	3.36706700	-1.24217800
H	-3.13242300	3.60271600	-3.25118000
H	-4.22869900	3.12101800	0.85340700
C	3.79225400	-2.21457500	-0.18928500
C	3.05763000	-3.36692700	0.17345200
C	4.49790100	-2.17846700	-1.40794800
C	3.07540200	-4.46911600	-0.68332600
C	4.47475100	-3.30497900	-2.23642700
C	3.77424900	-4.45922900	-1.89317400
H	2.51435700	-5.35580100	-0.40634900
H	5.01676400	-3.28167200	-3.17830900
C	2.30215700	4.93214500	0.19897300
C	5.05502600	5.17309700	0.69377000
C	4.29301800	6.31821100	0.36267400
C	2.94601200	6.19512300	0.11570400
C	4.45727900	3.93763400	0.79868300
H	6.12351600	5.26860400	0.86105100
H	4.77688000	7.28732900	0.29002000
H	2.35208400	7.06129900	-0.16280800
H	5.05332400	3.06791000	1.04440100
C	5.13907300	1.08663000	4.90845600
C	4.36208300	2.22504100	4.59009100
C	3.69736300	2.30687200	3.38727800
C	5.21239800	0.03793100	4.02178000
H	5.66311800	1.03814400	5.85799900
H	4.28477000	3.03979400	5.30356500
H	3.09980900	3.18021500	3.15711600
H	5.78656600	-0.85231700	4.26313000
C	1.06923400	2.43162800	0.29590600

C	3.11205600	0.15640500	0.38636700
O	2.41125500	0.17216800	-0.81835700
O	0.41536600	1.20727500	0.35809400
P	0.79241200	0.02998700	-0.72142100
O	0.40864000	-1.28107400	-0.07672200
O	0.26133600	0.38913600	-2.09925200
C	5.29305900	-0.95668500	-1.84844100
C	4.74176000	-0.36947500	-3.15840100
C	6.79213300	-1.28099300	-1.96339200
H	5.19130100	-0.18736500	-1.07876700
H	3.68398000	-0.11808400	-3.05249800
H	5.28865100	0.54030600	-3.42949300
H	4.84563900	-1.07918400	-3.98625900
H	7.18460600	-1.66445800	-1.01627600
H	6.97826200	-2.03811600	-2.73244300
H	7.36081700	-0.38435900	-2.23282400
C	3.75591100	-5.66402000	-2.81755700
C	2.33529100	-5.95067700	-3.33330100
C	4.36047200	-6.90654800	-2.14318700
H	4.38183800	-5.41736100	-3.68495100
H	1.91597900	-5.07298100	-3.83421400
H	2.33862400	-6.78573000	-4.04247000
H	1.66564500	-6.21475600	-2.50772400
H	5.38036900	-6.71020900	-1.79901000
H	3.76780400	-7.20926900	-1.27330400
H	4.38817600	-7.75252000	-2.83852600
C	2.24924000	-3.43836200	1.46373100
C	3.03751000	-4.15153800	2.57710000
C	0.88635300	-4.12614400	1.27085700
H	2.05116900	-2.41281700	1.78527200
H	3.97640400	-3.63972200	2.80169600
H	2.44789600	-4.19727200	3.49938100
H	3.28034400	-5.17742000	2.27834300
H	0.37318900	-3.73062300	0.39151000
H	0.98901900	-5.21000000	1.14783800
H	0.25506400	-3.96157200	2.15137000
C	-1.76535200	3.14635700	1.95442000
C	-2.18887100	1.78539200	2.52815400
C	-2.36228800	4.31059900	2.76264000
H	-0.67894100	3.21309300	2.04899800
H	-1.72124400	0.97046700	1.97006500
H	-1.88786900	1.69695500	3.57725200
H	-3.27642400	1.65555200	2.48486700
H	-2.02874000	5.27469100	2.36630400

H	-3.45712100	4.29792100	2.73438000
H	-2.05537000	4.24610200	3.81173600
C	-0.45198200	3.66299500	-2.97721500
C	-0.33558500	5.12715100	-3.43779500
C	-0.73390800	2.74805700	-4.17924500
H	0.51213100	3.35850000	-2.56206200
H	-0.06038000	5.78877100	-2.61247200
H	0.42492600	5.22586900	-4.21957500
H	-1.28889600	5.48095600	-3.84622800
H	-0.83073600	1.70805900	-3.86579600
H	-1.64335400	3.04174600	-4.71440700
H	0.09513800	2.80723500	-4.89150900
C	-5.32663600	3.40590400	-1.61163900
C	-5.67065100	2.53437700	-2.82930000
C	-5.78097300	4.85965300	-1.83582800
H	-5.88541400	3.01338500	-0.75072800
H	-5.33664100	1.50189900	-2.69313100
H	-6.75205700	2.52742900	-3.00001400
H	-5.19952400	2.91744700	-3.74016200
H	-5.57935600	5.47440900	-0.95373600
H	-5.24305200	5.30199600	-2.68126500
H	-6.85351600	4.90710100	-2.05323800
Ag	-1.51362500	-1.69635000	0.83774500
C	-3.60814200	-1.50653600	1.10270200
C	-4.55055700	-2.29063900	1.97368600
C	-7.00523400	-2.82898300	2.03569700
O	-4.29374000	-2.75054800	3.08087500
N	-5.78769000	-2.36444200	1.35726900
C	-5.85938400	-1.52936600	0.17244500
H	-6.23087700	-0.51748400	0.39977500
H	-6.52916700	-1.96785100	-0.57564100
C	-4.39437400	-1.44764400	-0.31520800
C	-3.97900800	-2.62797700	-1.14730900
C	-3.96211300	-0.14724200	-0.85976900
C	-3.04234900	-2.47580100	-2.11937000
C	-2.92053300	-0.02907400	-1.71816200
H	-4.38317800	0.74626700	-0.41125400
C	-2.37763500	-1.22087500	-2.31433900
H	-2.65546700	-3.32623800	-2.67057500
H	-2.49508600	0.93453800	-1.96892000
H	-7.80046300	-2.75606600	1.28332900
C	-6.87518600	-4.29699400	2.45440600
H	-7.81251300	-4.64351800	2.90069900
H	-6.65259000	-4.92776900	1.58847000

H	-6.07101400	-4.40936500	3.18275200
C	-7.36274200	-1.91664700	3.21613700
H	-6.57409600	-1.96309100	3.97034800
H	-7.47260700	-0.87764300	2.88811800
H	-8.30660200	-2.23065900	3.67264600
O	-1.30265900	-1.21217600	-3.02238500
H	-0.60522100	-0.43415900	-2.69813400
C	-4.48126200	-3.99890200	-0.81145700
H	-4.10311100	-4.30074600	0.17162200
H	-5.57223700	-4.03633300	-0.75011000
H	-4.13950100	-4.72563300	-1.55133200
H	-3.63946200	-0.49056200	1.52136000

TSF

Zero-point correction=	1.220526 (Hartree/Particle)
Thermal correction to Energy=	1.279681
Thermal correction to Enthalpy=	1.280546
Thermal correction to Gibbs Free Energy=	1.133056
Sum of electronic and zero-point Energies=	-3438.007411
Sum of electronic and thermal Energies=	-3437.948256
Sum of electronic and thermal Enthalpies=	-3437.947391
Sum of electronic and thermal Free Energies=	-3438.094881

C	-2.68272600	-2.49822700	0.18505000
C	-3.27280100	-3.75263300	-0.18646500
C	-1.01262800	-4.63554800	-0.63080400
C	-0.44625600	-3.40485300	-0.38005600
C	-3.47771300	-1.35534000	0.71394100
C	-4.32877400	-1.48105600	1.86510800
C	-5.08918500	-0.34329200	2.29111400
C	-4.91527200	0.90397600	1.63749900
C	-4.01224500	1.06362000	0.61038200
H	-0.37681500	-5.46856400	-0.91356800
H	-5.48172000	1.76041200	1.98821100
C	1.01600300	-3.13675800	-0.52485400
C	1.61205800	-3.12787700	-1.80307200
C	1.79911600	-2.85826700	0.61869200
C	2.99000300	-2.89293100	-1.90756600
C	3.16171800	-2.59771700	0.46171800
C	3.78296000	-2.62793200	-0.79221500
H	3.44251300	-2.91488800	-2.89232700
H	3.76195200	-2.36448700	1.33485700
C	-3.65477700	2.38957300	0.02096800

C	-2.82753900	3.27581600	0.75141100
C	-4.03925000	2.70571800	-1.29570400
C	-2.40681700	4.45691900	0.13992500
C	-3.58365600	3.89775800	-1.86749400
C	-2.75301300	4.77567400	-1.17526000
H	-1.75699400	5.12945700	0.68998000
H	-3.86414400	4.13688000	-2.88985200
C	-2.41606600	-4.83555600	-0.57019000
C	-5.20521000	-5.18047200	-0.57878400
C	-4.35699600	-6.26161800	-0.91420600
C	-2.99277100	-6.08690200	-0.91384400
C	-4.67775400	-3.95906100	-0.22492600
H	-6.28246800	-5.31326200	-0.60672600
H	-4.78577500	-7.22148300	-1.18535400
H	-2.33043600	-6.90202800	-1.19233200
H	-5.33586900	-3.13510300	0.02194600
C	-6.06133700	-1.65135300	4.09756900
C	-5.27080000	-2.75890700	3.71261400
C	-4.42660300	-2.67598600	2.62797500
C	-5.96353700	-0.46841900	3.40291200
H	-6.72891200	-1.73263100	4.94990500
H	-5.32535500	-3.68239700	4.28107500
H	-3.82144000	-3.52932700	2.34986300
H	-6.54243500	0.40023000	3.70469400
C	-1.31325000	-2.35625700	0.02637800
C	-3.34277500	-0.10089200	0.14256200
O	-2.52874000	0.04594800	-0.97248900
O	-0.72285800	-1.13745600	0.31634200
P	-0.91257000	0.09522400	-0.75730100
O	-0.52212600	1.33151800	0.04093800
O	-0.27460000	-0.20126700	-2.08473800
C	-4.93775000	1.78853900	-2.11317500
C	-4.27629900	1.36091900	-3.43342000
C	-6.30622800	2.44751800	-2.35893100
H	-5.11686000	0.88211400	-1.52856600
H	-3.30970200	0.88848400	-3.24616100
H	-4.91463300	0.64571900	-3.96356400
H	-4.11879400	2.21749500	-4.09756800
H	-6.79234500	2.70923900	-1.41370300
H	-6.20178400	3.36651600	-2.94581700
H	-6.96833400	1.77074400	-2.90992900
C	-2.17680100	6.00261900	-1.85907200
C	-0.66641200	5.81552800	-2.09878300
C	-2.45993700	7.29916400	-1.08536700

H	-2.65992600	6.08623900	-2.84101500
H	-0.47411700	4.89762700	-2.66285700
H	-0.24650400	6.66252400	-2.65278700
H	-0.13518500	5.73875800	-1.14264300
H	-3.53396000	7.43768900	-0.92925200
H	-1.97901600	7.28746100	-0.10136800
H	-2.07665600	8.16849700	-1.63046600
C	-2.36850000	2.96652000	2.17215200
C	-3.31372700	3.60321400	3.20795400
C	-0.92439100	3.41423500	2.45972100
H	-2.40118200	1.88137800	2.30063800
H	-4.34055100	3.25096300	3.08858200
H	-2.99051600	3.36664900	4.22786800
H	-3.32126300	4.69329700	3.09712000
H	-0.25509400	3.09406000	1.65657900
H	-0.84263500	4.50258600	2.55455500
H	-0.58087300	2.98065200	3.40529300
C	1.22437500	-2.90214800	2.02970700
C	1.41628700	-1.57619100	2.78470600
C	1.83589800	-4.07492200	2.81768100
H	0.15018400	-3.08769100	1.95956300
H	0.87211500	-0.77403900	2.27060100
H	1.00733400	-1.64965100	3.79850900
H	2.47154000	-1.29830000	2.86006000
H	1.67810700	-5.02209500	2.29248600
H	2.91414900	-3.94012000	2.95139600
H	1.37967200	-4.15253800	3.81042800
C	0.81365000	-3.38016400	-3.07652600
C	1.07340100	-4.80081400	-3.60890800
C	1.09533700	-2.33421100	-4.16694800
H	-0.24679300	-3.30031100	-2.82709800
H	0.82742300	-5.56252500	-2.86321100
H	0.47327400	-4.99446000	-4.50449600
H	2.12856800	-4.92878900	-3.87557500
H	0.90036300	-1.33023800	-3.78914000
H	2.12789700	-2.38692000	-4.52953600
H	0.44104700	-2.50815400	-5.02773900
C	5.29021700	-2.42550400	-0.87063600
C	5.81589100	-2.13831400	-2.28155900
C	6.02190400	-3.64060600	-0.26942500
H	5.53367200	-1.56691200	-0.23198000
H	5.29371600	-1.30318300	-2.75942700
H	6.88299100	-1.89657200	-2.24623200
H	5.70171400	-3.01131400	-2.93284200

H	5.70246100	-3.82242400	0.75991200
H	5.80803000	-4.54250900	-0.85326000
H	7.10595600	-3.48169600	-0.26860100
Ag	1.44506200	1.25856900	0.91429200
C	3.68075200	0.87754000	0.52050400
C	4.80543000	0.48184500	1.39895600
C	7.13834100	1.24774700	1.88913700
O	4.78832500	-0.42756500	2.22846800
N	5.88646500	1.28206100	1.11774000
C	5.51273000	2.47323500	0.37518600
H	6.26906900	2.72544300	-0.37656000
H	5.40817200	3.33194300	1.04988800
C	4.16963100	2.15934200	-0.29851400
C	3.28150700	3.30961400	-0.62335000
C	4.15981000	1.00589900	-1.19346500
C	2.33000900	3.12813000	-1.56207400
C	3.06007800	0.84227000	-2.10375700
H	5.05983800	0.41361300	-1.30336600
C	2.13658000	1.85272400	-2.23788100
H	1.61672800	3.90964200	-1.80058700
H	2.94122900	-0.08902400	-2.64416500
H	7.78675800	1.99149900	1.41044900
C	6.90497900	1.66223100	3.34709100
H	7.85519200	1.70770900	3.88780500
H	6.43553800	2.65003400	3.40397000
H	6.25376000	0.93728500	3.83994000
C	7.81167500	-0.12263200	1.76678500
H	7.18825900	-0.89321400	2.22225200
H	7.97066500	-0.37916400	0.71499400
H	8.78317700	-0.10774800	2.26995400
O	1.04046000	1.78187500	-2.99359200
H	0.53832600	0.92787000	-2.79053000
C	3.41753200	4.59887000	0.13436600
H	3.32885200	4.43055800	1.21617900
H	4.38551800	5.08420600	-0.03593700
H	2.63410100	5.29816300	-0.16486100
H	3.01244800	0.04979700	0.27042200

CPF

Zero-point correction=	1.339234 (Hartree/Particle)
Thermal correction to Energy=	1.405466
Thermal correction to Enthalpy=	1.406331
Thermal correction to Gibbs Free Energy=	1.243410

Sum of electronic and zero-point Energies= -3858.743029
Sum of electronic and thermal Energies= -3858.676797
Sum of electronic and thermal Enthalpies= -3858.675932
Sum of electronic and thermal Free Energies= -3858.838853

C	-1.71517100	3.09199000	-0.26203400
C	-2.27619300	4.13846800	0.54683200
C	-0.07383900	4.42128100	1.62751300
C	0.44362500	3.35132500	0.93137300
C	-2.51399100	2.37714500	-1.29745100
C	-3.19520900	3.06757900	-2.35754000
C	-4.07238200	2.33128200	-3.22011400
C	-4.25759500	0.93786000	-3.01346400
C	-3.54599500	0.25595800	-2.05390900
H	0.55826800	4.96025500	2.32603200
H	-4.98720800	0.40800300	-3.61831100
C	1.83974700	2.85127300	1.12419000
C	2.17831600	2.13697800	2.29248200
C	2.81183200	3.06168700	0.12127600
C	3.50217700	1.71633100	2.46914600
C	4.11022800	2.59246200	0.32784300
C	4.48520600	1.93915000	1.50470800
H	3.76083800	1.18967500	3.38058900
H	4.85640300	2.72783200	-0.44946800
C	-3.76758500	-1.17467500	-1.67664300
C	-3.00960900	-2.21210400	-2.26009500
C	-4.64907500	-1.44542300	-0.61144400
C	-3.13682000	-3.50308100	-1.74453300
C	-4.73159800	-2.75325400	-0.12032000
C	-3.97523500	-3.79035500	-0.66227300
H	-2.55025600	-4.30315700	-2.18188600
H	-5.38907200	-2.96514800	0.71877700
C	-1.42711800	4.82314200	1.47746400
C	-4.14205000	5.52045800	1.27989900
C	-3.29321200	6.22542100	2.16440000
C	-1.96625100	5.87684200	2.26176000
C	-3.64774100	4.50465100	0.49274100
H	-5.19521000	5.77884800	1.22459100
H	-3.69430900	7.02926800	2.77406300
H	-1.30769000	6.39413200	2.95416800
H	-4.30988700	3.96703600	-0.17411000
C	-4.56267800	4.36240500	-4.46701600
C	-3.67160200	5.08249100	-3.63819300
C	-3.00687100	4.45247900	-2.61001300

C	-4.75317500	3.01557400	-4.26077500
H	-5.08507500	4.87197300	-5.27085200
H	-3.50578100	6.14043200	-3.81745300
H	-2.31996000	5.01047100	-1.98541800
H	-5.42296900	2.44755900	-4.90059500
C	-0.40896800	2.71420800	-0.00812600
C	-2.63558400	0.99901900	-1.25416800
O	-1.91339300	0.27045600	-0.32012400
O	0.14447400	1.68880900	-0.74996600
P	-0.29033200	0.13909500	-0.45700300
O	0.17931200	-0.58485400	-1.70235800
O	0.14480400	-0.36149100	0.90358800
C	-5.49366700	-0.35189200	0.03168800
C	-5.05372800	-0.07747700	1.47778300
C	-6.99282900	-0.68558400	-0.03837600
H	-5.34348900	0.56864900	-0.53712000
H	-3.98609600	0.15087800	1.52988500
H	-5.60867500	0.77027800	1.89502500
H	-5.24292400	-0.94503000	2.11594300
H	-7.31131600	-0.85553400	-1.07165500
H	-7.22981800	-1.58681100	0.53684400
H	-7.58787500	0.13675800	0.37353300
C	-4.08192600	-5.20078000	-0.10755800
C	-2.71775100	-5.75351000	0.33712000
C	-4.75547400	-6.14292100	-1.12006100
H	-4.72798800	-5.14961800	0.77922400
H	-2.24827700	-5.09855000	1.07467400
H	-2.83042100	-6.75240200	0.77335800
H	-2.03077300	-5.83645600	-0.51130400
H	-5.74078200	-5.76715100	-1.41202100
H	-4.15039000	-6.23188900	-2.02877000
H	-4.87908400	-7.14693000	-0.69919100
C	-2.10212100	-1.93288000	-3.45049100
C	-2.91113900	-1.98763900	-4.75950100
C	-0.88767000	-2.86726800	-3.52913500
H	-1.71154600	-0.91832100	-3.33335000
H	-3.72965200	-1.26302000	-4.75470600
H	-2.26966200	-1.76872700	-5.62032700
H	-3.34551600	-2.98365200	-4.90197600
H	-0.35816300	-2.88227600	-2.57597100
H	-1.17569400	-3.89030500	-3.79829500
H	-0.19669900	-2.50847300	-4.29898500
C	2.49899000	3.80734800	-1.16926900
C	2.75076200	2.93582800	-2.41083700

C	3.29290700	5.12358400	-1.24298700
H	1.43857200	4.07186900	-1.16485400
H	2.11727100	2.04389200	-2.38421200
H	2.51149800	3.49176100	-3.32411100
H	3.79454900	2.61314600	-2.47344800
H	3.08805400	5.75397400	-0.37189400
H	4.37099300	4.93397500	-1.27298800
H	3.02549200	5.68575700	-2.14418700
C	1.14447800	1.79897300	3.36022000
C	1.20839800	2.78749700	4.53734800
C	1.28532700	0.35487400	3.87004900
H	0.15559800	1.88149400	2.90094100
H	1.02601100	3.81462900	4.21146100
H	0.46051500	2.53472600	5.29704300
H	2.19612700	2.75813900	5.01098000
H	1.34898100	-0.33446000	3.02722100
H	2.17488800	0.22946500	4.49715200
H	0.41460000	0.08359800	4.47473900
C	5.94098700	1.54223900	1.69639900
C	6.14660900	0.36374500	2.65436000
C	6.75974900	2.76032700	2.16402200
H	6.31692600	1.24433400	0.71088100
H	5.56463900	-0.50962500	2.34375300
H	7.20170300	0.07550200	2.67847000
H	5.85453800	0.61583100	3.67945500
H	6.65846200	3.59283800	1.46202000
H	6.41118300	3.10488000	3.14421900
H	7.82304200	2.50931500	2.24763100
Ag	2.40242400	-0.49523500	-1.50444000
C	4.13809300	-1.05706400	-0.40637700
C	5.54712700	-0.96588300	-0.88795800
C	7.67151600	-2.30656300	-0.76738400
O	6.05576900	0.00367700	-1.45008600
N	6.22643500	-2.12978700	-0.57349200
C	5.49502300	-2.94923500	0.37279100
H	5.77458400	-2.72317100	1.41301100
H	5.68896100	-4.01427500	0.20437800
C	4.00916800	-2.57707600	0.13183500
C	3.36915400	-3.38481600	-0.96095900
C	3.18653200	-2.46654100	1.35447900
C	2.05010000	-3.71092300	-0.88887000
C	1.86268500	-2.74357400	1.38753800
H	3.66034200	-2.01256600	2.22018900
C	1.24678900	-3.30959600	0.22218000

H	1.54097000	-4.19870600	-1.71246700
H	1.24692300	-2.52495500	2.24958700
H	7.88106600	-3.33441500	-0.44547300
C	8.04229000	-2.18663700	-2.24898400
H	9.10776700	-2.39569900	-2.38612400
H	7.47057800	-2.90193400	-2.84803400
H	7.82743600	-1.18013400	-2.61008200
C	8.47925000	-1.34571900	0.11423400
H	8.27185800	-0.31406200	-0.17768400
H	8.21805900	-1.47011800	1.16946100
H	9.55173800	-1.53473400	0.00428200
O	-0.02705300	-3.49571900	0.12326800
H	-0.57984200	-3.13773900	0.91538100
C	4.15269300	-3.70742400	-2.19491700
H	4.44469900	-2.77856400	-2.69660400
H	5.07777100	-4.24287700	-1.96225900
H	3.55791400	-4.30643300	-2.88706800
H	4.02983500	-0.35849800	0.42936300
C	-4.77052600	-1.45570300	5.21744500
C	-3.64439600	-1.22555700	4.43169400
C	-3.18131600	-2.22624800	3.56823100
C	-3.84768800	-3.45554300	3.49627600
C	-4.98153400	-3.67654500	4.27344600
C	-5.44298100	-2.67752100	5.13451400
H	-5.13081000	-0.68063500	5.88650700
H	-3.12630600	-0.27453400	4.46418300
H	-3.47562700	-4.21440500	2.81900900
H	-5.50631400	-4.62462300	4.20829100
H	-6.32776200	-2.85061700	5.73993500
C	-2.01441000	-1.98742800	2.68309000
O	-1.49931000	-2.93076900	2.05572100
O	-1.60369700	-0.75074900	2.63651800
H	-0.86231300	-0.60132400	1.92314000

TSD

Zero-point correction=	1.330637 (Hartree/Particle)
Thermal correction to Energy=	1.396599
Thermal correction to Enthalpy=	1.397464
Thermal correction to Gibbs Free Energy=	1.234422
Sum of electronic and zero-point Energies=	-3858.743446
Sum of electronic and thermal Energies=	-3858.677483
Sum of electronic and thermal Enthalpies=	-3858.676618
Sum of electronic and thermal Free Energies=	-3858.839661

C	-1.78685900	3.02472200	-0.32896200
C	-2.37771200	4.04561800	0.49138400
C	-0.17053500	4.41569700	1.53562500
C	0.37996100	3.36690100	0.83176400
C	-2.57794000	2.27658000	-1.34653300
C	-3.30873400	2.93895100	-2.39142800
C	-4.18565100	2.17054400	-3.22552800
C	-4.33324600	0.77642700	-2.99548500
C	-3.58100500	0.12305900	-2.04665700
H	0.44987400	4.97809900	2.22574900
H	-5.07132100	0.22225100	-3.56742300
C	1.79334600	2.91459800	1.01508500
C	2.16881500	2.23866400	2.19542000
C	2.74643900	3.13144000	-0.00501400
C	3.50654400	1.86036200	2.36247500
C	4.06004200	2.70403400	0.19453100
C	4.46971800	2.08740700	1.37965500
H	3.79239600	1.35992300	3.28034300
H	4.79220700	2.84519100	-0.59499600
C	-3.79329600	-1.29497400	-1.62047300
C	-3.02512400	-2.34763000	-2.15959900
C	-4.68802600	-1.53202300	-0.55728600
C	-3.16047900	-3.62315700	-1.60945000
C	-4.77691600	-2.82522000	-0.02985500
C	-4.01591700	-3.87880900	-0.53307100
H	-2.56650400	-4.43467000	-2.01390500
H	-5.44453300	-3.01263000	0.80678600
C	-1.54081900	4.76339400	1.40779100
C	-4.28573800	5.34687900	1.26071800
C	-3.45081800	6.08597200	2.13053000
C	-2.10892000	5.79331100	2.20333400
C	-3.76413300	4.35359800	0.46252500
H	-5.34956700	5.56107800	1.22535500
H	-3.87395800	6.87182500	2.74861800
H	-1.46012800	6.33686600	2.88463500
H	-4.41553700	3.78980600	-0.19309600
C	-4.76440500	4.17641300	-4.47463800
C	-3.87624500	4.92917900	-3.67206800
C	-3.16857800	4.32710900	-2.65592400
C	-4.91083000	2.82630700	-4.25448900
H	-5.32039900	4.66426400	-5.26928800
H	-3.74689800	5.99020800	-3.86235900
H	-2.48398200	4.90975700	-2.05154700

H	-5.57958500	2.23439400	-4.87323800
C	-0.46294100	2.70288900	-0.09685400
C	-2.65748600	0.89622400	-1.29404800
O	-1.87095900	0.19001600	-0.38746400
O	0.11881100	1.69971200	-0.85586400
P	-0.25555500	0.14554700	-0.57180300
O	0.25747100	-0.58693300	-1.78419300
O	0.22357400	-0.32003200	0.80824800
C	-5.52539800	-0.41382800	0.05334400
C	-5.01264300	-0.03383600	1.45168200
C	-7.01976300	-0.77074000	0.09193200
H	-5.42447300	0.46793100	-0.58355800
H	-3.94452700	0.19912700	1.43409300
H	-5.54879700	0.84131200	1.83548700
H	-5.16444000	-0.85490400	2.15733900
H	-7.39060800	-1.02808500	-0.90508900
H	-7.21413200	-1.62281700	0.75155600
H	-7.60406500	0.07624200	0.46745000
C	-4.13996400	-5.27489900	0.05328200
C	-2.78182200	-5.84861500	0.48905100
C	-4.84786600	-6.22128000	-0.93195800
H	-4.77305400	-5.19363500	0.94746300
H	-2.28447400	-5.18859700	1.20287300
H	-2.91150200	-6.83411100	0.94993400
H	-2.11050300	-5.96839900	-0.36733700
H	-5.82976000	-5.83103100	-1.21647400
H	-4.25765800	-6.33790800	-1.84730000
H	-4.98495200	-7.21488300	-0.49117000
C	-2.09439400	-2.10058800	-3.33843100
C	-2.87669800	-2.18956300	-4.66158400
C	-0.87798700	-3.03548400	-3.36263600
H	-1.70737100	-1.08220900	-3.24408700
H	-3.69298500	-1.46258000	-4.69269200
H	-2.21701300	-1.99561600	-5.51447000
H	-3.31082000	-3.18805700	-4.78570500
H	-0.37894700	-3.04116300	-2.39260100
H	-1.15918800	-4.06223100	-3.62472300
H	-0.16181800	-2.68892100	-4.11435900
C	2.39815300	3.84414500	-1.30506000
C	2.68278900	2.96743000	-2.53563800
C	3.13585400	5.19154600	-1.39875800
H	1.32771600	4.06481500	-1.30099500
H	2.10369500	2.04057100	-2.48753700
H	2.40199600	3.49456100	-3.45408600

H	3.74239800	2.70398500	-2.60758600
H	2.90455100	5.82565400	-0.53701700
H	4.22083400	5.04626600	-1.42565000
H	2.84574200	5.72861800	-2.30823700
C	1.16184400	1.89054700	3.28596600
C	1.21319100	2.90152200	4.44472200
C	1.35774300	0.46259200	3.82327500
H	0.16294600	1.93295400	2.84263800
H	0.99324700	3.91695600	4.10600500
H	0.48680000	2.63826700	5.22158800
H	2.20913100	2.91110300	4.90137100
H	1.44941900	-0.24461500	2.99817300
H	2.25348100	0.38417100	4.44900700
H	0.50004000	0.17031600	4.43653500
C	5.93731300	1.72915700	1.55568700
C	6.18953400	0.59802000	2.55861300
C	6.73922800	2.98343200	1.95171500
H	6.29718200	1.39484700	0.57593600
H	5.61967400	-0.29990900	2.30024200
H	7.25073100	0.33275100	2.56759900
H	5.91737500	0.88932100	3.57904600
H	6.60580600	3.78292100	1.21732700
H	6.40551400	3.36320200	2.92415400
H	7.80903700	2.75755500	2.02152300
Ag	2.49482400	-0.52388000	-1.51466300
C	4.20548900	-1.03728500	-0.35724300
C	5.61250300	-0.95722300	-0.84390200
C	7.73035800	-2.30262200	-0.67823400
O	6.13137300	-0.00766200	-1.43248300
N	6.28577200	-2.11637800	-0.49646800
C	5.54870100	-2.90578000	0.47227100
H	5.83586000	-2.65539100	1.50529200
H	5.73267400	-3.97657400	0.33114100
C	4.06564600	-2.52125300	0.22385700
C	3.41519000	-3.37672500	-0.83626200
C	3.25437200	-2.40081400	1.46170200
C	2.10573500	-3.71458600	-0.73836200
C	1.94420900	-2.70916700	1.52721600
H	3.73781600	-1.92160600	2.30911400
C	1.28911200	-3.29668700	0.37533900
H	1.59586000	-4.23631900	-1.54106200
H	1.34863000	-2.49597600	2.40666600
H	7.93603800	-3.32121800	-0.32574000
C	8.10921800	-2.22668500	-2.16075600

H	9.17475600	-2.44290900	-2.28698300
H	7.53747400	-2.95716300	-2.74115000
H	7.89845300	-1.23033700	-2.55119900
C	8.53649200	-1.31852200	0.17936700
H	8.33016900	-0.29555800	-0.14243700
H	8.27072300	-1.41328000	1.23672000
H	9.60939900	-1.51123100	0.07930300
O	0.03503400	-3.46209700	0.30718700
H	-0.71780400	-3.08548200	1.22557200
C	4.19480200	-3.73443400	-2.06572500
H	4.49957900	-2.82360800	-2.59156700
H	5.11230600	-4.27841400	-1.82162500
H	3.59188600	-4.34357800	-2.74220900
H	4.08785000	-0.30386000	0.44625200
C	-4.53519600	-1.07359600	5.20815200
C	-3.41517000	-0.98066300	4.38724200
C	-3.06980900	-2.05328600	3.55581000
C	-3.84785100	-3.21781800	3.54877200
C	-4.97535400	-3.30084700	4.36167900
C	-5.31889200	-2.23036300	5.19138200
H	-4.80472500	-0.24282400	5.85250800
H	-2.80964400	-0.08224300	4.36408100
H	-3.57016900	-4.03348900	2.89283000
H	-5.58722000	-4.19739300	4.34801100
H	-6.19912700	-2.29682100	5.82386600
C	-1.91297500	-1.93128300	2.63689200
O	-1.53832400	-2.99555800	2.04212300
O	-1.38031100	-0.78547200	2.51406500
H	-0.57547500	-0.58315000	1.65157400

CPG

Zero-point correction=	1.337625 (Hartree/Particle)
Thermal correction to Energy=	1.404831
Thermal correction to Enthalpy=	1.405696
Thermal correction to Gibbs Free Energy=	1.240147
Sum of electronic and zero-point Energies=	-3858.740449
Sum of electronic and thermal Energies=	-3858.673242
Sum of electronic and thermal Enthalpies=	-3858.672377
Sum of electronic and thermal Free Energies=	-3858.837926

C	-1.74714900	3.01884600	-0.37802600
C	-2.33715300	4.03862000	0.44350700
C	-0.12121300	4.42649000	1.46226900

C	0.43016400	3.37675500	0.75938200
C	-2.54621000	2.25739600	-1.37890500
C	-3.28575700	2.90923000	-2.42360600
C	-4.17010800	2.13232200	-3.24121300
C	-4.32460300	0.74410800	-2.98517800
C	-3.57203800	0.09994200	-2.02910100
H	0.50190200	4.99344800	2.14590400
H	-5.07344600	0.18498100	-3.53800600
C	1.84231000	2.92360700	0.94769100
C	2.21518200	2.26857000	2.14122000
C	2.79642500	3.11920200	-0.07574200
C	3.55174300	1.89043800	2.31562000
C	4.10865900	2.69206900	0.13280900
C	4.51614500	2.09678400	1.32953800
H	3.83530500	1.40422100	3.24167300
H	4.84182300	2.81678500	-0.65850100
C	-3.82654700	-1.29986600	-1.56820300
C	-3.07891000	-2.38733600	-2.06256600
C	-4.77060200	-1.48568200	-0.53590200
C	-3.28361600	-3.64937700	-1.50206100
C	-4.92938800	-2.76741600	0.00132300
C	-4.19215300	-3.85721600	-0.46045000
H	-2.70686200	-4.48800400	-1.87463200
H	-5.63750100	-2.91988400	0.81045500
C	-1.49435000	4.76636200	1.34630400
C	-4.24557000	5.32830400	1.22848500
C	-3.40572500	6.07776400	2.08478400
C	-2.06083900	5.79609300	2.14343300
C	-3.72615300	4.33533600	0.42856100
H	-5.31125100	5.53452000	1.20502500
H	-3.82764400	6.86321900	2.70413900
H	-1.40855900	6.34772300	2.81472000
H	-4.38069300	3.76342300	-0.21686400
C	-4.75239800	4.12318600	-4.51148800
C	-3.85890900	4.88469900	-3.72290800
C	-3.14568800	4.29422200	-2.70399100
C	-4.90027500	2.77625100	-4.27422000
H	-5.31220600	4.60241700	-5.30864200
H	-3.73002800	5.94325200	-3.92652700
H	-2.45675800	4.88307700	-2.11063300
H	-5.57446200	2.17825400	-4.88096200
C	-0.41898700	2.71010900	-0.16013700
C	-2.63096400	0.87840200	-1.30678400
O	-1.81891600	0.18027000	-0.40566100

O	0.15787200	1.70343400	-0.92715000
P	-0.21517900	0.16151000	-0.63318600
O	0.30731900	-0.61010500	-1.80851500
O	0.31162100	-0.25168100	0.76850500
C	-5.57662700	-0.32012200	0.02878800
C	-4.97664500	0.17887900	1.35448700
C	-7.06514000	-0.65857900	0.20076500
H	-5.51871500	0.50247400	-0.68792800
H	-3.90527600	0.37721300	1.26359300
H	-5.46926500	1.10224200	1.67922800
H	-5.11138300	-0.56834900	2.13998700
H	-7.49984100	-1.02802500	-0.73312800
H	-7.22159800	-1.42163800	0.97014100
H	-7.62144000	0.23294300	0.50927900
C	-4.40891500	-5.24168600	0.12680100
C	-3.09714400	-5.90687100	0.57303900
C	-5.17133800	-6.13759100	-0.86549000
H	-5.04316400	-5.11898900	1.01557100
H	-2.55714500	-5.27864900	1.28434900
H	-3.29974300	-6.87664800	1.04055200
H	-2.43315200	-6.08358900	-0.27922000
H	-6.12332800	-5.68286200	-1.15593300
H	-4.58296500	-6.29020100	-1.77673000
H	-5.37666000	-7.12085000	-0.42809100
C	-2.10136200	-2.19512900	-3.21278400
C	-2.84036600	-2.29418800	-4.55991000
C	-0.91199400	-3.16392300	-3.16973600
H	-1.69003900	-1.18536100	-3.13235000
H	-3.63289100	-1.54426200	-4.63653200
H	-2.14613300	-2.14082400	-5.39335000
H	-3.29972600	-3.28230800	-4.67529900
H	-0.45743000	-3.17769600	-2.17775700
H	-1.21212800	-4.18511500	-3.43260500
H	-0.15291600	-2.84788900	-3.89196400
C	2.45183700	3.81089700	-1.38806300
C	2.74306800	2.91599900	-2.60389900
C	3.18780000	5.15794800	-1.49956100
H	1.38103200	4.03048600	-1.39179500
H	2.17141200	1.98547900	-2.54179100
H	2.46018000	3.42643500	-3.53106100
H	3.80434400	2.65826800	-2.67048800
H	2.95152000	5.80517300	-0.64899900
H	4.27301100	5.01360400	-1.51870500
H	2.90144700	5.68018200	-2.41882400

C	1.20770900	1.93785500	3.23717300
C	1.25911400	2.96549700	4.38140300
C	1.40338900	0.51880600	3.79878900
H	0.20850400	1.97359800	2.79364200
H	1.03839700	3.97644000	4.03013600
H	0.53396200	2.71197400	5.16261500
H	2.25550000	2.98155300	4.83672100
H	1.51338300	-0.20422300	2.99001600
H	2.29009100	0.45634900	4.43901400
H	0.53812500	0.22988700	4.40259900
C	5.98206200	1.73577000	1.51232300
C	6.23058300	0.63348700	2.54765600
C	6.79168500	2.99695900	1.86899100
H	6.33700900	1.37046700	0.54193300
H	5.65449800	-0.26826100	2.31829200
H	7.29013400	0.36227000	2.56042600
H	5.96429300	0.95707900	3.55998000
H	6.66093300	3.77552900	1.11193600
H	6.46338600	3.40695100	2.83098800
H	7.86031300	2.76688600	1.94217100
Ag	2.56173300	-0.59543700	-1.51347400
C	4.24835900	-1.08530500	-0.31444100
C	5.65903500	-1.02078400	-0.79301100
C	7.76530100	-2.37716600	-0.57723500
O	6.19049900	-0.09025000	-1.40184400
N	6.32209800	-2.17348700	-0.40804500
C	5.56833900	-2.93797400	0.56915100
H	5.84748900	-2.66756800	1.59939600
H	5.74664600	-4.01264500	0.45251900
C	4.09078600	-2.54677000	0.29504600
C	3.44883200	-3.43368400	-0.75011900
C	3.26772500	-2.40689600	1.52813400
C	2.14410600	-3.77882400	-0.65230000
C	1.96303300	-2.72755700	1.59477800
H	3.74493900	-1.90570400	2.36692000
C	1.30358700	-3.34471500	0.44960500
H	1.64655000	-4.32804100	-1.44495900
H	1.35966700	-2.50251200	2.46737400
H	7.96060500	-3.38710500	-0.19524200
C	8.15227800	-2.34611100	-2.05941100
H	9.21663300	-2.57447500	-2.17434100
H	7.57706700	-3.08779200	-2.62185700
H	7.95142100	-1.35933400	-2.47843000
C	8.57630400	-1.37645800	0.25630000

H	8.37846000	-0.36116000	-0.09388500
H	8.30603400	-1.44087600	1.31478900
H	9.64813600	-1.57975900	0.16532600
O	0.06226500	-3.50708800	0.38800300
H	-0.96183000	-3.11894200	1.36965700
C	4.24240200	-3.81718500	-1.96465900
H	4.55695400	-2.91975800	-2.50737500
H	5.15476800	-4.36059700	-1.70021700
H	3.64491900	-4.43897300	-2.63474900
H	4.12584200	-0.33019100	0.46797700
C	-4.54843800	-0.76899800	5.12168700
C	-3.40820200	-0.82322300	4.32577900
C	-3.17811100	-1.93879700	3.51157000
C	-4.09053200	-3.00134600	3.49819000
C	-5.23641800	-2.93731900	4.28720000
C	-5.46593100	-1.82281400	5.09804800
H	-4.72931500	0.09630500	5.75142700
H	-2.69554900	-0.00681900	4.30560200
H	-3.90199000	-3.85346900	2.85752400
H	-5.95119300	-3.75415900	4.26963900
H	-6.36113000	-1.77486600	5.71090400
C	-1.99108500	-1.94855900	2.62379800
O	-1.78298800	-3.07234200	2.00189700
O	-1.27817600	-0.93074600	2.52287200
H	-0.37211500	-0.58181500	1.48679900

TSE

Zero-point correction=	1.337391 (Hartree/Particle)
Thermal correction to Energy=	1.403405
Thermal correction to Enthalpy=	1.404270
Thermal correction to Gibbs Free Energy=	1.242766
Sum of electronic and zero-point Energies=	-3858.717853
Sum of electronic and thermal Energies=	-3858.651839
Sum of electronic and thermal Enthalpies=	-3858.650974
Sum of electronic and thermal Free Energies=	-3858.812478

C	2.67455700	-1.35572400	-1.14902000
C	3.59028300	-2.37685800	-0.72564600
C	1.74826200	-4.01306200	-0.82001400
C	0.83919000	-3.01364300	-1.08715100
C	3.10201900	0.04046700	-1.42317700
C	4.17920100	0.31795000	-2.33415400
C	4.62672300	1.66774800	-2.49347100

C	3.97867900	2.70281900	-1.77745800
C	2.88666400	2.46160500	-0.97287400
H	1.40252800	-5.03386000	-0.69392900
H	4.34417100	3.71937200	-1.88013200
C	-0.63634500	-3.23055400	-1.07936600
C	-1.28124000	-3.54113000	0.14150300
C	-1.39761400	-3.04712100	-2.25548700
C	-2.66808400	-3.73606000	0.14527200
C	-2.80132400	-3.19242200	-2.18983200
C	-3.45150700	-3.57096400	-0.99695400
H	-3.15204100	-4.00357900	1.07811600
H	-3.38410400	-3.14271100	-3.10646600
C	2.18838700	3.56732300	-0.24821200
C	1.24398400	4.35827300	-0.93676000
C	2.48508100	3.81270700	1.11214300
C	0.59571800	5.38454100	-0.24224700
C	1.80990100	4.85365900	1.75673800
C	0.85957100	5.64147000	1.10460400
H	-0.13249000	5.99527400	-0.76616900
H	2.01056000	5.04713100	2.80440500
C	3.12588600	-3.72909100	-0.63772900
C	5.79508300	-3.11882100	-0.01352100
C	5.35578500	-4.46395900	-0.00404900
C	4.04518400	-4.75773700	-0.30047100
C	4.93604100	-2.10241900	-0.36664700
H	6.81739800	-2.88546400	0.26683400
H	6.04839200	-5.25682700	0.26120100
H	3.68245900	-5.78078500	-0.25565800
H	5.27709900	-1.07530700	-0.35973200
C	6.29140000	0.94874900	-4.11342700
C	5.81927100	-0.37944700	-3.99570500
C	4.79280200	-0.68677900	-3.13169900
C	5.69947800	1.94965200	-3.38026800
H	7.10733300	1.17543300	-4.79272600
H	6.26620700	-1.16437800	-4.59827200
H	4.43549400	-1.70615800	-3.06429500
H	6.03326000	2.97915800	-3.47583500
C	1.34894100	-1.70564400	-1.29677200
C	2.44616200	1.11871100	-0.84331600
O	1.31525900	0.91576100	-0.05150200
O	0.44783500	-0.74779500	-1.73547700
P	-0.06736600	0.42280200	-0.72613000
O	-0.88647100	1.36187000	-1.53638300
O	-0.78765500	-0.25947100	0.49008400

C	3.53597900	2.98835900	1.85444900
C	3.44596500	3.08861300	3.38335500
C	4.96111200	3.39176600	1.42321600
H	3.37420500	1.93599400	1.59407100
H	2.43642200	2.88560500	3.73732800
H	4.12219000	2.35445000	3.83255700
H	3.75869000	4.07749200	3.73949900
H	5.13481100	3.24292000	0.35712100
H	5.13946500	4.44842700	1.65303100
H	5.70152800	2.79840200	1.97045700
C	0.11579100	6.73361700	1.85466200
C	-1.38930900	6.42617800	1.94318500
C	0.36027000	8.11942500	1.23572700
H	0.51211200	6.74999700	2.87792300
H	-1.56490400	5.44605600	2.39618700
H	-1.90689700	7.18367800	2.54201600
H	-1.84555100	6.41887600	0.94732400
H	1.42927400	8.34921900	1.19643800
H	-0.02890100	8.16791300	0.21305500
H	-0.13889600	8.90053800	1.81942100
C	0.97507500	4.16336600	-2.42556900
C	1.82662800	5.15184700	-3.24448600
C	-0.50513400	4.28972400	-2.81122500
H	1.28623800	3.14931300	-2.69178400
H	2.89354400	5.03506100	-3.03703900
H	1.66971600	5.00082800	-4.31809300
H	1.55237300	6.18479800	-3.00273300
H	-1.10622500	3.56577500	-2.26243200
H	-0.89289800	5.29831600	-2.63059000
H	-0.62336400	4.08658600	-3.88109900
C	-0.74977900	-2.78759200	-3.60830400
C	-1.33799100	-1.56116300	-4.32402400
C	-0.84494100	-4.04853500	-4.48770400
H	0.31013900	-2.58955900	-3.44074400
H	-1.23271800	-0.66353700	-3.70541900
H	-0.80717800	-1.37751400	-5.26373000
H	-2.39582000	-1.70409600	-4.57133300
H	-0.39052100	-4.90962200	-3.98830700
H	-1.88775400	-4.29955300	-4.71011600
H	-0.32619500	-3.89155200	-5.43878800
C	-0.52448600	-3.63641300	1.46127000
C	-0.32382400	-5.10108000	1.88734000
C	-1.21025800	-2.83683700	2.58065400
H	0.46278000	-3.19386400	1.31677200

H	0.20748000	-5.67531300	1.12298200
H	0.25855800	-5.14787700	2.81146300
H	-1.28855600	-5.59173000	2.06121500
H	-1.35404600	-1.79882300	2.28213400
H	-2.18103600	-3.26417700	2.85586500
H	-0.58084000	-2.84757700	3.47356900
C	-4.94422000	-3.85209800	-0.98708400
C	-5.69287100	-3.06166200	0.09723600
C	-5.19300700	-5.36511800	-0.84615400
H	-5.34008100	-3.53424600	-1.96011300
H	-5.59115400	-1.98703700	-0.06798400
H	-6.75878900	-3.31141200	0.07639700
H	-5.31721400	-3.30365800	1.09724300
H	-4.68341700	-5.92719200	-1.63484200
H	-4.82287700	-5.73063100	0.11769000
H	-6.26375500	-5.58638400	-0.90253700
Ag	-2.95255100	-0.75906200	-1.54139200
C	-3.49240700	0.23873200	0.71883100
C	-4.73770100	0.66922600	0.02920800
C	-6.64841400	2.26571500	0.34325900
O	-5.17384000	0.17878000	-1.04198200
N	-5.35643100	1.66806500	0.71050000
C	-4.71878300	1.92260100	1.99580000
H	-5.24414600	1.39752800	2.80672900
H	-4.72657000	2.99204100	2.22878900
C	-3.27523800	1.36258300	1.82108900
C	-2.33839600	2.43444800	1.29258400
C	-2.77567300	0.69773300	3.06039900
C	-1.08945500	2.56773200	1.78542500
C	-1.51478700	0.80263500	3.50319100
H	-3.47420700	0.02215900	3.55050500
C	-0.56835800	1.69958700	2.83157800
H	-0.39139700	3.28110700	1.36439700
H	-1.14506800	0.22598200	4.34410100
H	-6.82401700	3.04702700	1.09169300
C	-6.58006900	2.92768500	-1.03691800
H	-7.52831000	3.42765600	-1.25714200
H	-5.78051000	3.67284400	-1.07047500
H	-6.38904500	2.17799300	-1.80639000
C	-7.77668300	1.23181800	0.44049600
H	-7.61064600	0.43357100	-0.28640700
H	-7.81648800	0.79085300	1.44160200
H	-8.74369600	1.70109500	0.23451000
O	0.63433700	1.73023400	3.14652200

H	1.25000800	0.35726700	3.71553500
C	-2.78524000	3.28500000	0.14129500
H	-2.97036000	2.66088200	-0.73749600
H	-3.70808100	3.82932800	0.36728900
H	-2.00720300	4.00255600	-0.11798200
H	-3.71042200	-0.71779700	1.21336600
C	3.41290200	-4.81901000	3.16970800
C	3.21713800	-3.48305000	2.82825900
C	2.40341800	-2.66814500	3.62178200
C	1.79681600	-3.19676900	4.76880500
C	1.99388500	-4.53423000	5.10878000
C	2.80020100	-5.34753200	4.30820100
H	4.04387900	-5.44295700	2.54579300
H	3.68797000	-3.04992800	1.95613200
H	1.17763600	-2.55279800	5.38195300
H	1.52089300	-4.94226700	5.99710200
H	2.95229800	-6.38985300	4.57363400
C	2.19795200	-1.24591800	3.20468200
O	1.44263200	-0.56396500	4.06782600
O	2.67566600	-0.77846300	2.18282400
H	-1.83089400	-0.07952900	0.44292200

(*R*)-2a

Zero-point correction=	0.280591 (Hartree/Particle)
Thermal correction to Energy=	0.293097
Thermal correction to Enthalpy=	0.293962
Thermal correction to Gibbs Free Energy=	0.244557
Sum of electronic and zero-point Energies=	-710.531968
Sum of electronic and thermal Energies=	-710.519462
Sum of electronic and thermal Enthalpies=	-710.518597
Sum of electronic and thermal Free Energies=	-710.568002

C	-0.10129700	-0.83049000	1.17352500
C	1.32249700	-0.35663000	1.04987800
C	2.97777300	0.03451900	-0.78557000
O	2.10122900	-0.12465100	1.99677500
N	1.63525200	-0.27008200	-0.25872900
C	0.50370100	-0.59205500	-1.13366200
H	0.60231700	-1.60926300	-1.53584000
H	0.46457100	0.10283100	-1.97681300
C	-0.74041500	-0.47748500	-0.20808600
C	-1.28151200	0.94495900	-0.14222100
C	-1.79397700	-1.50908700	-0.47321100

C	-2.60710700	1.16707800	-0.04361100
C	-3.10265600	-1.27033900	-0.32480800
H	-1.43669800	-2.51610800	-0.68166900
C	-3.58788600	0.08890600	-0.04085500
H	-2.99883200	2.17065800	0.08347800
H	-3.85019800	-2.05156500	-0.41431700
H	2.86397000	0.01778800	-1.87489700
C	3.43566600	1.43489400	-0.36437400
H	4.40532700	1.65795900	-0.81927500
H	2.72040700	2.19537700	-0.68700500
H	3.53557800	1.49191900	0.72096600
C	3.97564600	-1.05622200	-0.38153500
H	4.09992000	-1.07085700	0.70346900
H	3.63012400	-2.04191500	-0.70787200
H	4.94915700	-0.86391000	-0.84192800
O	-4.79189900	0.31113300	0.15268000
C	-0.32148600	2.09571600	-0.07852600
H	0.27491900	2.05213800	0.83577000
H	0.35825100	2.10942000	-0.93736900
H	-0.87121400	3.03566900	-0.05508400
H	-0.07261200	-1.91755200	1.32014400
H	-0.67007500	-0.40645000	2.00204600

CPN

Zero-point correction=	1.221430 (Hartree/Particle)
Thermal correction to Energy=	1.282552
Thermal correction to Enthalpy=	1.283417
Thermal correction to Gibbs Free Energy=	1.130407
Sum of electronic and zero-point Energies=	-3437.976549
Sum of electronic and thermal Energies=	-3437.915428
Sum of electronic and thermal Enthalpies=	-3437.914563
Sum of electronic and thermal Free Energies=	-3438.067573

C	-3.45637400	1.70621000	0.19854300
C	-4.81207500	1.93898800	-0.21499400
C	-5.25870900	-0.47053400	0.03966600
C	-3.93026400	-0.72046700	0.30531000
C	-2.47420900	2.80713100	0.38667400
C	-2.75451900	3.93159800	1.23746500
C	-1.79710400	4.99357900	1.32284800
C	-0.54947800	4.86007400	0.66529300
C	-0.21827100	3.72389400	-0.04112600
H	-5.95909300	-1.29826500	-0.01352500

H	0.19137800	5.64564100	0.78147200
C	-3.36833500	-2.10027200	0.39148800
C	-3.35244300	-2.91837100	-0.76282100
C	-2.77225700	-2.56261800	1.58647500
C	-2.73608900	-4.17932700	-0.69316300
C	-2.17137600	-3.82325500	1.60519300
C	-2.13581400	-4.65072600	0.47991700
H	-2.74214700	-4.80719900	-1.57644600
H	-1.71378900	-4.17541100	2.52591100
C	1.18053800	3.48320800	-0.50158700
C	2.18572700	3.29714300	0.47252200
C	1.50895000	3.43125900	-1.87280400
C	3.50690600	3.12074700	0.04824600
C	2.83753400	3.21345300	-2.24435500
C	3.85684700	3.06562300	-1.29994200
H	4.29003900	3.02696800	0.79564200
H	3.08454900	3.17489200	-3.30132200
C	-5.72756600	0.83754200	-0.24377500
C	-6.59585400	3.39774000	-1.00316300
C	-7.51081700	2.31928600	-0.97934500
C	-7.07968500	1.06577200	-0.61315400
C	-5.28304100	3.21294100	-0.63201700
H	-6.93044100	4.37980800	-1.32332400
H	-8.54519700	2.48049900	-1.26709500
H	-7.76383800	0.22150600	-0.61812100
H	-4.59021200	4.04444900	-0.66180400
C	-3.24750200	6.20699100	2.85300200
C	-4.16816200	5.13383500	2.81744800
C	-3.92800900	4.02731400	2.03424500
C	-2.08330200	6.12977100	2.12556000
H	-3.45322100	7.07746800	3.46842000
H	-5.07089200	5.17938700	3.41919200
H	-4.63810200	3.21057600	2.02688000
H	-1.34976100	6.93040500	2.16678500
C	-3.05468000	0.39665400	0.41006100
C	-1.22102500	2.72980200	-0.20697000
O	-0.91852300	1.67095300	-1.04156100
O	-1.74471000	0.14177500	0.76737900
P	-0.60529000	0.17558500	-0.43255600
O	0.72759200	0.03811500	0.22871800
O	-1.02911400	-0.76144600	-1.55863800
Ag	-0.26489700	-2.78073500	-1.26127800
C	0.46478900	3.64871200	-2.95888000
C	0.36429900	2.44354200	-3.90815800

C	0.74658600	4.94949200	-3.73128400
H	-0.50784000	3.76486400	-2.47504200
H	0.11958400	1.53421500	-3.35539600
H	-0.42072700	2.61290700	-4.65317700
H	1.30340500	2.28118100	-4.44843900
H	0.78197000	5.80902200	-3.05433000
H	1.70627900	4.89946000	-4.25695400
H	-0.03466400	5.13198000	-4.47705900
C	5.30299000	2.86851100	-1.72202100
C	5.83798700	4.10221100	-2.46875600
C	5.48735400	1.59354400	-2.56054900
H	5.89628600	2.74756500	-0.80653100
H	5.73231000	5.00609100	-1.86114200
H	6.89668600	3.97690100	-2.72072300
H	5.28835800	4.26299500	-3.40227700
H	5.16806000	0.70911700	-2.00394000
H	4.90374000	1.64053400	-3.48571400
H	6.53947200	1.45848900	-2.83301500
C	1.88905700	3.24241600	1.96764100
C	2.52024500	4.42861200	2.71389900
C	2.32433800	1.89825600	2.57613300
H	0.80830600	3.30837800	2.10177100
H	2.16170700	5.38357600	2.31700500
H	2.27465200	4.38904600	3.78067100
H	3.61198500	4.42107500	2.62126700
H	1.86219300	1.07683900	2.02433200
H	3.41300400	1.77582000	2.55024700
H	2.01483700	1.83866900	3.62562000
C	-2.79822000	-1.74765300	2.87205900
C	-1.39002200	-1.51872400	3.44436800
C	-3.72255300	-2.41273900	3.90752200
H	-3.22097900	-0.76730100	2.64454700
H	-0.74190200	-1.05508100	2.69808100
H	-1.43963800	-0.85701600	4.31547700
H	-0.93576900	-2.45973700	3.77416100
H	-4.73518200	-2.53341000	3.51021800
H	-3.35331900	-3.40507400	4.18890400
H	-3.78142800	-1.80573800	4.81719400
C	-3.99157600	-2.49931400	-2.08270200
C	-5.31733700	-3.25489300	-2.29092600
C	-3.06666400	-2.68719600	-3.29646200
H	-4.21689400	-1.43363200	-2.02323200
H	-6.00228600	-3.10548600	-1.45093300
H	-5.81645700	-2.91342900	-3.20376200

H	-5.14152600	-4.33245600	-2.38520200
H	-2.16184200	-2.08578400	-3.18352000
H	-2.78635000	-3.73547000	-3.44685400
H	-3.57821400	-2.35552800	-4.20619000
C	-1.49141500	-6.02503600	0.58361700
C	-1.12146600	-6.64929900	-0.76659600
C	-2.40039000	-6.97655700	1.38487800
H	-0.56251900	-5.89602800	1.15811200
H	-0.51254300	-5.97212500	-1.37243700
H	-0.55948000	-7.57561600	-0.61218100
H	-2.01530600	-6.90574000	-1.34531900
H	-2.63313400	-6.56773700	2.37212600
H	-3.34700800	-7.13094800	0.85569300
H	-1.92214600	-7.95248800	1.52039100
C	6.17922600	-2.03027200	0.28420700
C	7.47808700	-1.82506700	0.75226200
C	7.86840800	-0.60427100	1.31005400
C	6.94547000	0.43820200	1.40566900
C	5.64626300	0.23191100	0.95037400
C	5.23928800	-0.98319600	0.39439800
H	8.21750400	-2.61619100	0.67991600
H	7.23339900	1.39644800	1.83156000
H	4.92515900	1.03735300	1.01860900
C	5.82466200	-3.36790200	-0.31774500
H	5.19333300	-3.95390900	0.35997300
H	5.27237600	-3.26351900	-1.25561800
H	6.72632500	-3.95143800	-0.51762900
C	3.82612300	-1.07405800	-0.13054600
H	3.82746200	-1.16321000	-1.22024800
H	3.25878200	-0.16983100	0.10597600
N	3.00323300	-2.21154300	0.36109000
C	2.54506900	-3.02586100	-0.55265300
O	2.87364300	-3.18423100	-1.78274900
C	1.47780200	-3.90399000	-0.87694700
H	1.71949300	-4.96450900	-0.80856600
C	2.35693500	-2.13248600	1.70957000
C	3.39184400	-1.80570400	2.78547000
C	1.62125200	-3.42913400	2.05089800
H	1.63327400	-1.31628200	1.62542600
H	3.85875000	-0.83427300	2.63156800
H	2.88453300	-1.78123000	3.75402200
H	4.18122000	-2.56296500	2.82522700
H	1.23790400	-3.34643600	3.07027100
H	0.75783300	-3.60699200	1.40522000

H	2.29381500	-4.29312200	2.01179800
O	9.16009300	-0.49491000	1.73715700
H	9.30104900	0.39369400	2.08848600

TSL

Zero-point correction=	1.220603 (Hartree/Particle)
Thermal correction to Energy=	1.280773
Thermal correction to Enthalpy=	1.281638
Thermal correction to Gibbs Free Energy=	1.127942
Sum of electronic and zero-point Energies=	-3437.974286
Sum of electronic and thermal Energies=	-3437.914116
Sum of electronic and thermal Enthalpies=	-3437.913251
Sum of electronic and thermal Free Energies=	-3438.066947

C	3.46747300	-1.64431600	0.20347900
C	4.83842600	-1.81739500	-0.18642500
C	5.17695400	0.60714900	0.07934900
C	3.83344700	0.79963300	0.31953900
C	2.53453700	-2.78896400	0.38276700
C	2.84856500	-3.89443600	1.24671600
C	1.92884200	-4.98945200	1.33207700
C	0.68195600	-4.90666300	0.66410800
C	0.31616200	-3.79130800	-0.05814800
H	5.84166900	1.46460300	0.04182300
H	-0.03211900	-5.71562200	0.78555900
C	3.23254000	2.16414400	0.39987600
C	3.23255300	2.98829900	-0.75063100
C	2.62753200	2.62644200	1.59068800
C	2.64839200	4.26265500	-0.67552100
C	2.06682100	3.90658700	1.61594800
C	2.06533500	4.74587500	0.49792900
H	2.66019400	4.88710500	-1.56073500
H	1.63003100	4.26989400	2.54375800
C	-1.08810000	-3.59274700	-0.52278800
C	-2.09668500	-3.40580600	0.44811300
C	-1.41467300	-3.56394800	-1.89473000
C	-3.41795000	-3.24549900	0.01934700
C	-2.74443300	-3.36334800	-2.27138600
C	-3.76504200	-3.20626500	-1.33003000
H	-4.20279800	-3.13805500	0.76318500
H	-2.99015900	-3.33788100	-3.32902400
C	5.70667500	-0.67813100	-0.19773700
C	6.69602700	-3.19785200	-0.94349200

C	7.56380700	-2.08122600	-0.90294900
C	7.07381900	-0.84780500	-0.54328000
C	5.37038800	-3.06993500	-0.59539800
H	7.07789300	-4.16418000	-1.25847900
H	8.60886500	-2.19804900	-1.17289000
H	7.72144400	0.02474600	-0.53555600
H	4.71389400	-3.92993700	-0.63751100
C	3.40714900	-6.13641100	2.88680600
C	4.28868200	-5.03103100	2.85091300
C	4.01635700	-3.94038000	2.05592500
C	2.24808800	-6.10749000	2.14765800
H	3.63807000	-6.99373300	3.51164900
H	5.18655500	-5.03894700	3.46152800
H	4.69673200	-3.09874600	2.04846800
H	1.54347600	-6.93362200	2.18922400
C	3.00416400	-0.35241000	0.40521100
C	1.28902100	-2.76905500	-0.22891300
O	0.96488600	-1.72517300	-1.07924100
O	1.68015000	-0.15040300	0.74092800
P	0.54252300	-0.26826700	-0.45671800
O	-0.79001900	-0.23302100	0.21587900
O	0.88560700	0.71718900	-1.57355200
Ag	0.08658300	2.67374300	-1.14307600
C	-0.36497200	-3.78212600	-2.97525000
C	-0.28406900	-2.59310200	-3.94646000
C	-0.62253300	-5.10130000	-3.72450600
H	0.60890100	-3.87266000	-2.48772000
H	-0.06596400	-1.66772200	-3.40930100
H	0.51046200	-2.75807800	-4.68239900
H	-1.22217700	-2.46220300	-4.49663800
H	-0.64089800	-5.94932600	-3.03253000
H	-1.58407900	-5.07804200	-4.24857000
H	0.16067500	-5.28226200	-4.46869800
C	-5.20852200	-2.99873100	-1.75523200
C	-5.75399400	-4.22537100	-2.50542700
C	-5.37531300	-1.71953400	-2.59161400
H	-5.80215900	-2.87252100	-0.84060300
H	-5.66142300	-5.13140500	-1.89870600
H	-6.81010700	-4.08764500	-2.76157600
H	-5.20277100	-4.39120800	-3.43720700
H	-5.03444900	-0.84223200	-2.03668300
H	-4.79784400	-1.77641600	-3.52019500
H	-6.42639700	-1.56540600	-2.85785000
C	-1.80472900	-3.33657700	1.94352600

C	-2.36949700	-4.56143700	2.68145700
C	-2.31853800	-2.02566200	2.56368200
H	-0.72172100	-3.34114600	2.07808800
H	-1.95742500	-5.49320000	2.28162300
H	-2.13149300	-4.51415800	3.74975700
H	-3.45949800	-4.61295300	2.58216800
H	-1.91998100	-1.17353700	2.00915600
H	-3.41289800	-1.97317300	2.55589300
H	-1.99688800	-1.95269500	3.60883300
C	2.58836500	1.79209500	2.86353000
C	1.14596200	1.55502100	3.34355900
C	3.44899000	2.43471600	3.96511700
H	3.02131400	0.81499600	2.64309900
H	0.54986300	1.08490400	2.55833600
H	1.13957900	0.89299800	4.21551700
H	0.66772900	2.49469800	3.64680200
H	4.48201600	2.56673100	3.62895500
H	3.06249000	3.41891300	4.25191800
H	3.45832600	1.80521100	4.86101100
C	3.85014900	2.55861500	-2.07748400
C	5.16857500	3.31521600	-2.32305800
C	2.89560300	2.73370600	-3.27044300
H	4.07963900	1.49415200	-2.01291200
H	5.87479100	3.17255800	-1.49977700
H	5.64507900	2.96726500	-3.24529400
H	4.98945100	4.39177700	-2.42189000
H	1.99557200	2.13073800	-3.13209000
H	2.60837300	3.78003600	-3.42132500
H	3.38644900	2.39629400	-4.18928300
C	1.46532500	6.13976200	0.60748000
C	1.15749800	6.79859800	-0.74195500
C	2.37959800	7.04894700	1.45076800
H	0.51521100	6.03813900	1.15514800
H	0.55513700	6.15142700	-1.38645400
H	0.61555100	7.73701800	-0.59073100
H	2.07808000	7.03913100	-1.28379600
H	2.56977900	6.61843700	2.43777300
H	3.34568000	7.17866900	0.95157800
H	1.92994700	8.03813800	1.58711700
C	-6.25330100	1.95780200	0.48333600
C	-7.40503200	1.59381200	1.18290900
C	-7.54707500	0.31691400	1.73487100
C	-6.52386300	-0.62068700	1.58658400
C	-5.37010600	-0.25685300	0.89543800

C	-5.21205900	1.01611700	0.34501500
H	-8.22175700	2.29901300	1.30165400
H	-6.62314600	-1.61978300	2.00526400
H	-4.57104700	-0.97913300	0.77291900
C	-6.14655100	3.34665200	-0.09836500
H	-5.51973200	3.98781000	0.53215300
H	-5.68581900	3.34361400	-1.08978600
H	-7.13264800	3.81213000	-0.17357300
C	-3.95025200	1.31007000	-0.42812800
H	-4.17925000	1.51183500	-1.47844700
H	-3.27815500	0.44390000	-0.39530600
N	-3.18493700	2.48496800	0.02524300
C	-2.75492400	3.35376700	-0.94850000
O	-3.26506900	3.50548100	-2.05544600
C	-1.47949900	4.03718100	-0.59722700
H	-1.36931200	5.07771700	-0.91562400
C	-2.26082400	2.31627300	1.15797300
C	-2.95529400	1.89701600	2.45180700
C	-1.55165700	3.65289300	1.37349800
H	-1.51856900	1.55291500	0.89445000
H	-3.35540300	0.88767300	2.36276500
H	-2.22759600	1.89472400	3.27003700
H	-3.77857400	2.57414100	2.69982100
H	-0.50592600	3.59727100	1.65596300
H	-1.71309700	4.53097000	0.53694400
H	-2.12219100	4.30978700	2.04981900
O	-8.70906900	0.04789600	2.40264600
H	-8.68379800	-0.86503100	2.71677800

5a

Zero-point correction=	0.281528 (Hartree/Particle)
Thermal correction to Energy=	0.296611
Thermal correction to Enthalpy=	0.297555
Thermal correction to Gibbs Free Energy=	0.239531
Sum of electronic and zero-point Energies=	-710.658592
Sum of electronic and thermal Energies=	-710.643510
Sum of electronic and thermal Enthalpies=	-710.642565
Sum of electronic and thermal Free Energies=	-710.700589

C	-1.25949900	0.98722100	0.21409000
C	-2.55009100	0.84819100	0.72434200
C	-3.43550900	-0.10410400	0.21205400
C	-3.03182200	-0.93482600	-0.83349900

C	-1.74335700	-0.79620000	-1.34644400
C	-0.84636200	0.14781300	-0.84388600
H	-2.89097100	1.48460600	1.53472300
H	-3.71287500	-1.67662500	-1.24370700
H	-1.42731600	-1.44320800	-2.16066200
C	-0.33014000	2.00104400	0.83368600
H	0.31412800	1.52490300	1.58242800
H	0.33907100	2.46387200	0.10551600
H	-0.89696300	2.78634300	1.34008900
C	0.54041100	0.23875800	-1.44277200
H	0.76379400	1.25366600	-1.78430800
H	0.59056300	-0.42277100	-2.31766500
N	1.62493500	-0.10387000	-0.53533200
C	2.62399500	0.78444900	-0.23329200
O	2.67892900	1.94884900	-0.60534600
C	3.62554500	0.05559100	0.65881500
H	4.64440400	0.34707200	0.39829500
C	1.80489000	-1.43631100	0.04934800
C	0.89643000	-1.69382200	1.25673900
C	3.30722800	-1.42748700	0.42647000
H	1.59616300	-2.18945900	-0.72125000
H	-0.15823800	-1.62313000	0.98781200
H	1.08637000	-2.69482100	1.65799700
H	1.09547200	-0.96505500	2.04932400
H	3.89923400	-1.80540300	-0.41265300
H	3.45124200	0.36274400	1.69663600
H	3.51080300	-2.06055300	1.29320700
O	-4.67895100	-0.17134900	0.77557900
H	-5.18955400	-0.85701200	0.32577600

CPM

Zero-point correction=	1.220841 (Hartree/Particle)
Thermal correction to Energy=	1.282635
Thermal correction to Enthalpy=	1.283500
Thermal correction to Gibbs Free Energy=	1.126782
Sum of electronic and zero-point Energies=	-3437.980751
Sum of electronic and thermal Energies=	-3437.918957
Sum of electronic and thermal Enthalpies=	-3437.918092
Sum of electronic and thermal Free Energies=	-3438.074810

C	-3.10215000	-1.68195900	1.12534600
C	-4.08115000	-2.73326900	1.11220900
C	-2.28633600	-4.33070600	0.59066400

C	-1.36402100	-3.31184500	0.48092000
C	-3.48226300	-0.27512900	1.41916300
C	-4.18599700	0.08888800	2.61597200
C	-4.67645800	1.42705100	2.75305500
C	-4.42549800	2.36940800	1.72438900
C	-3.65592900	2.05795400	0.62396700
H	-1.97313100	-5.35224900	0.39873300
H	-4.82690100	3.37365800	1.82228000
C	0.02214100	-3.60151400	0.00463700
C	0.22177800	-3.99360800	-1.34155100
C	1.12062000	-3.53560000	0.88617700
C	1.50861300	-4.35934600	-1.75559100
C	2.38751200	-3.91198700	0.42303800
C	2.60286300	-4.34092600	-0.88744500
H	1.65272400	-4.67478600	-2.78332400
H	3.23038000	-3.88427600	1.11000400
C	-3.34415200	3.07061600	-0.42625600
C	-2.50687700	4.16569300	-0.12036400
C	-3.89227600	2.94023300	-1.71960400
C	-2.25555000	5.11983900	-1.10911800
C	-3.60368600	3.91758200	-2.67623000
C	-2.79148200	5.01494300	-2.39365800
H	-1.61165500	5.96142000	-0.87067600
H	-4.02560500	3.82253800	-3.67340000
C	-3.64820700	-4.07933800	0.88674100
C	-6.37340600	-3.54043500	1.27952600
C	-5.93530500	-4.87465300	1.10871500
C	-4.59980000	-5.13335000	0.90943100
C	-5.47323900	-2.49896200	1.28029900
H	-7.43209600	-3.33429300	1.40464100
H	-6.65591800	-5.68667600	1.11744600
H	-4.24989800	-6.14931600	0.74743400
H	-5.82575400	-1.48304400	1.40229600
C	-5.59493600	0.87993000	4.93818300
C	-5.07654800	-0.43124900	4.82179500
C	-4.39178600	-0.81671300	3.69139900
C	-5.39290000	1.78774400	3.92491700
H	-6.13910600	1.16911300	5.83212000
H	-5.21562600	-1.13861000	5.63383200
H	-3.99272100	-1.82081600	3.61532900
H	-5.76775100	2.80420300	4.00903400
C	-1.79373400	-1.99097100	0.78597900
C	-3.17148300	0.72621400	0.51124100
O	-2.42002900	0.41974300	-0.60983100

O	-0.84419300	-0.98944400	0.78910600
P	-0.81179300	0.12221500	-0.44264800
O	0.01582800	1.26465400	0.03527300
O	-0.46998500	-0.60909700	-1.74770200
Ag	1.60488100	-1.06680300	-1.67918300
C	-4.81024100	1.78746900	-2.10465800
C	-4.22225900	0.95533700	-3.25661700
C	-6.22241900	2.29653500	-2.44163600
H	-4.90885800	1.12451100	-1.24208500
H	-3.23092100	0.58037600	-2.99342100
H	-4.86960700	0.09892200	-3.47556900
H	-4.13707000	1.54960900	-4.17298000
H	-6.64859900	2.85659400	-1.60316700
H	-6.20973300	2.95937700	-3.31341700
H	-6.88978000	1.45803500	-2.66888100
C	-2.48944500	6.05541700	-3.45794300
C	-0.99030100	6.08585100	-3.80059600
C	-2.99083700	7.44969900	-3.04707100
H	-3.03248900	5.75951100	-4.36486600
H	-0.64101000	5.09848800	-4.11706100
H	-0.78813000	6.79978300	-4.60671500
H	-0.39647500	6.38562300	-2.93039000
H	-4.06282000	7.43326700	-2.82846900
H	-2.47341300	7.80424200	-2.14915800
H	-2.81267700	8.17907400	-3.84482900
C	-1.84630500	4.33328200	1.24208900
C	-2.42446300	5.54100100	1.99766200
C	-0.31839100	4.42578200	1.11143000
H	-2.05726100	3.43906700	1.83237200
H	-3.50655300	5.44580400	2.13419000
H	-1.96325900	5.63633500	2.98691700
H	-2.24201800	6.47257300	1.45057900
H	0.05589600	3.54332600	0.59064500
H	-0.01074600	5.32263600	0.56212500
H	0.14380900	4.47322000	2.10459900
C	0.96604300	-3.08879700	2.33241700
C	1.74317900	-1.78827200	2.59350300
C	1.37999100	-4.19986500	3.31174600
H	-0.09068200	-2.87729100	2.50970700
H	1.37809900	-0.99321200	1.93990600
H	1.61379000	-1.46400000	3.63176500
H	2.81626300	-1.92901500	2.42138900
H	0.80705600	-5.11470700	3.13186300
H	2.44281600	-4.44649400	3.21518900

H	1.20452400	-3.88385000	4.34539800
C	-0.91869400	-4.05745200	-2.35223300
C	-1.29247800	-5.52039300	-2.65276200
C	-0.60313100	-3.30180400	-3.65371000
H	-1.78891700	-3.57138200	-1.90689200
H	-1.56488500	-6.06181700	-1.74238500
H	-2.14185400	-5.56584700	-3.34223800
H	-0.45314400	-6.05092500	-3.11621600
H	-0.42681200	-2.24433100	-3.44860300
H	0.26794400	-3.71839500	-4.17083300
H	-1.45474800	-3.37329200	-4.33853900
C	3.97914400	-4.81116900	-1.32982000
C	4.39761300	-4.27291500	-2.70705400
C	4.04557000	-6.34941300	-1.30264200
H	4.70209000	-4.43828000	-0.59001100
H	4.35550200	-3.18121000	-2.74937400
H	5.42115700	-4.58387400	-2.93967300
H	3.75099200	-4.66255000	-3.49969100
H	3.79037600	-6.73672000	-0.31181500
H	3.33585600	-6.77422500	-2.02075800
H	5.04809200	-6.70353900	-1.56573000
C	7.32692500	1.63976900	0.85040800
C	8.23403200	1.99626400	1.84725000
C	8.18345700	3.25236000	2.46051300
C	7.21480400	4.17792200	2.06751600
C	6.30647900	3.82432500	1.07271300
C	6.33821800	2.56967400	0.46004600
H	9.00338600	1.29996200	2.16495600
H	7.17049400	5.16109500	2.52914700
H	5.55373400	4.54519000	0.76595000
C	7.41065400	0.26127500	0.24198300
H	6.66458900	-0.40895700	0.68556400
H	7.23049600	0.26574600	-0.83626900
H	8.39351700	-0.18074100	0.42046400
C	5.31717700	2.24849400	-0.60400900
H	5.79199600	1.93957400	-1.53935100
H	4.71555400	3.13378600	-0.82332100
N	4.39779100	1.15261800	-0.23957300
C	4.35029100	0.08576500	-1.00152000
O	4.96877100	-0.22088500	-2.06716600
C	3.56553500	-1.09895500	-1.09322200
H	4.07937300	-1.97934200	-0.70847000
C	3.45957600	1.23585500	0.91667200
C	2.78033500	2.59831500	0.97572300

C	4.14680900	0.85294200	2.22870400
H	2.67948300	0.50039100	0.69567400
H	2.31859300	2.84794000	0.01891300
H	1.97445700	2.54959500	1.70879300
H	3.47580900	3.38696300	1.27609300
H	3.39468400	0.79066500	3.01974800
H	4.63133700	-0.12462100	2.14933300
H	4.89780100	1.59004200	2.51924900
O	9.10782900	3.51130000	3.42772300
H	8.97180600	4.40545400	3.76701000

TSM

Zero-point correction=	1.217168 (Hartree/Particle)
Thermal correction to Energy=	1.278209
Thermal correction to Enthalpy=	1.279074
Thermal correction to Gibbs Free Energy=	1.124852
Sum of electronic and zero-point Energies=	-3437.980482
Sum of electronic and thermal Energies=	-3437.919441
Sum of electronic and thermal Enthalpies=	-3437.918576
Sum of electronic and thermal Free Energies=	-3438.072798

C	-3.33339900	-1.61501500	0.88599200
C	-4.31861100	-2.65357900	0.78229800
C	-2.50772200	-4.26283900	0.36116300
C	-1.56898500	-3.25310200	0.33940900
C	-3.70547800	-0.21260500	1.21113800
C	-4.45154300	0.12513300	2.39019800
C	-4.86876500	1.48190600	2.58024200
C	-4.48970800	2.46819900	1.63503200
C	-3.68218300	2.17233400	0.55823300
H	-2.19111300	-5.28601000	0.18481800
H	-4.81914800	3.49163000	1.78495600
C	-0.14592500	-3.55726300	-0.00446500
C	0.18860400	-3.90849800	-1.33600600
C	0.85366400	-3.55240900	0.99029800
C	1.50468700	-4.29585500	-1.62258200
C	2.14847800	-3.96829000	0.65690500
C	2.49588600	-4.35384900	-0.63784000
H	1.75298600	-4.57778000	-2.64001900
H	2.91098000	-3.99380400	1.43223900
C	-3.20123700	3.22854800	-0.38038500
C	-2.24264500	4.17054700	0.05625400
C	-3.69739300	3.28260200	-1.69818000

C	-1.82842400	5.16701600	-0.82985300
C	-3.24238200	4.29320600	-2.55044000
C	-2.31258000	5.24568300	-2.13738300
H	-1.09544200	5.89388600	-0.49322800
H	-3.62301600	4.33965900	-3.56751000
C	-3.88561100	-3.99968700	0.55747000
C	-6.62569100	-3.43315100	0.77659300
C	-6.19186600	-4.76870100	0.60338200
C	-4.84894300	-5.04104700	0.49021000
C	-5.71568500	-2.40403700	0.86294900
H	-7.68805000	-3.21668000	0.83549200
H	-6.92079500	-5.57107200	0.54359500
H	-4.50116900	-6.05801000	0.32989700
H	-6.06161500	-1.38570800	0.98643800
C	-5.94246100	0.87252300	4.67650400
C	-5.49309500	-0.45876800	4.51285600
C	-4.76745300	-0.82262400	3.40086800
C	-5.62967600	1.82049300	3.73046100
H	-6.51999100	1.14470700	5.55470300
H	-5.71809300	-1.19977600	5.27405200
H	-4.42247700	-1.84321100	3.29067500
H	-5.94783500	2.85214500	3.85387200
C	-2.00723800	-1.93166200	0.62855100
C	-3.30534800	0.81482600	0.37119400
O	-2.53771300	0.51361900	-0.74237800
O	-1.05048800	-0.94050900	0.70436000
P	-0.94416000	0.18793900	-0.51434900
O	-0.13492300	1.31542100	0.02501000
O	-0.53599300	-0.53287600	-1.80340700
Ag	1.51575700	-1.07417700	-1.46406000
C	-4.72560200	2.28788900	-2.21941700
C	-4.18002600	1.48576100	-3.41264000
C	-6.04761300	2.99158100	-2.57066400
H	-4.94563800	1.57491700	-1.42105700
H	-3.25474700	0.97354000	-3.13993600
H	-4.91070900	0.73482600	-3.73300500
H	-3.97601100	2.13719700	-4.26941900
H	-6.44835800	3.52943100	-1.70553600
H	-5.90985600	3.71683800	-3.37971400
H	-6.79678700	2.26287500	-2.89902900
C	-1.82848100	6.32586300	-3.08894300
C	-0.32290600	6.18734900	-3.37184000
C	-2.16603300	7.73328400	-2.56984800
H	-2.36027300	6.18430700	-4.03874300

H	-0.08844900	5.19363200	-3.76504500
H	0.00841200	6.93554400	-4.10044800
H	0.26115900	6.32903300	-2.45609600
H	-3.24062500	7.83994800	-2.39351400
H	-1.65177300	7.93709700	-1.62448800
H	-1.85704200	8.49914100	-3.28968300
C	-1.64679900	4.13468600	1.45887100
C	-2.24391100	5.24749600	2.33750700
C	-0.11184300	4.21439200	1.43969100
H	-1.90601100	3.17286100	1.90742400
H	-3.33258000	5.16461000	2.40728900
H	-1.83381300	5.20376500	3.35269000
H	-2.01405500	6.23526200	1.92241700
H	0.28583500	3.42058000	0.80708600
H	0.24298700	5.18366200	1.07198900
H	0.28016400	4.08803100	2.45581800
C	0.56824000	-3.10237000	2.41541100
C	1.35186600	-1.81887800	2.74312100
C	0.85675500	-4.21533200	3.43563600
H	-0.49432500	-2.86127200	2.48867400
H	1.08345900	-1.02338200	2.04340100
H	1.12181300	-1.47440900	3.75711000
H	2.43202100	-1.99931900	2.68903800
H	0.27908600	-5.11589900	3.20625400
H	1.91675600	-4.49102500	3.44388900
H	0.59110700	-3.88683700	4.44584100
C	-0.84395100	-3.91523200	-2.45847300
C	-1.26521800	-5.35823000	-2.79286600
C	-0.35786600	-3.19556400	-3.72696700
H	-1.72460700	-3.37561100	-2.10368000
H	-1.66314900	-5.87659700	-1.91659100
H	-2.03738700	-5.36209300	-3.56905500
H	-0.41102200	-5.93641700	-3.16280700
H	-0.12140100	-2.15111400	-3.51412500
H	0.52045300	-3.68023300	-4.16628600
H	-1.14937700	-3.20765900	-4.48334700
C	3.89646300	-4.85535800	-0.94947800
C	4.50309300	-4.22798600	-2.21437800
C	3.89645400	-6.39216300	-1.04926100
H	4.53531100	-4.58048400	-0.09826900
H	4.54155900	-3.13618500	-2.16413700
H	5.52498100	-4.59177700	-2.36296800
H	3.92943300	-4.49807700	-3.10679700
H	3.50156500	-6.84638800	-0.13560700

H	3.26911400	-6.72124200	-1.88474100
H	4.90957200	-6.77324100	-1.21591300
C	7.55226400	1.48978200	0.69100900
C	8.42973000	1.83395900	1.71860000
C	8.26591800	3.01583900	2.44901200
C	7.21037700	3.87858500	2.14732600
C	6.33339700	3.53927600	1.11869600
C	6.48199500	2.35977000	0.38603700
H	9.26371600	1.18635400	1.96968200
H	7.07695700	4.80356700	2.70273800
H	5.51468200	4.21287000	0.87852600
C	7.75055300	0.18508800	-0.04172300
H	7.11247800	-0.60157800	0.37833500
H	7.49592500	0.25139600	-1.10199300
H	8.78584600	-0.15332200	0.04465400
C	5.47495100	2.02638800	-0.68812700
H	5.95215100	1.78324800	-1.64259900
H	4.81747400	2.88559700	-0.86211900
N	4.66570000	0.85449900	-0.37254900
C	4.52080500	-0.22610000	-1.18687100
O	5.13267600	-0.50215000	-2.21120800
C	3.42180800	-1.07253100	-0.65600100
H	3.75350100	-1.95530400	-0.10112700
C	3.79989200	0.72185000	0.78252300
C	2.78278200	1.83074800	0.94311700
C	4.49536700	0.27621100	2.05609400
H	3.10106000	-0.21800400	0.43755200
H	2.21278000	1.99342700	0.02799000
H	2.06838600	1.59599200	1.73291900
H	3.31530900	2.74907000	1.21873500
H	3.76322600	0.00403300	2.81938100
H	5.16000500	-0.57033300	1.87042200
H	5.10168500	1.10642700	2.43176100
O	9.16940800	3.26710300	3.43866000
H	8.95859400	4.11308000	3.85454500

4a

Zero-point correction=	0.278786 (Hartree/Particle)
Thermal correction to Energy=	0.294608
Thermal correction to Enthalpy=	0.295552
Thermal correction to Gibbs Free Energy=	0.235834
Sum of electronic and zero-point Energies=	-710.637673
Sum of electronic and thermal Energies=	-710.621851

Sum of electronic and thermal Enthalpies= -710.620907
Sum of electronic and thermal Free Energies= -710.680625

C	-1.25638700	1.08590100	-0.00533700
C	-2.54473500	0.96351100	0.51466500
C	-3.35479300	-0.13033300	0.19730400
C	-2.87797200	-1.12204100	-0.66064900
C	-1.59267100	-0.99958600	-1.18542400
C	-0.77107800	0.08473700	-0.87450600
H	-2.94297400	1.72309400	1.17976400
H	-3.50107100	-1.97501300	-0.91847500
H	-1.21977700	-1.76991600	-1.85564400
C	-0.40876100	2.26634900	0.40141800
H	0.24976500	2.00489000	1.23760600
H	0.24598800	2.61685300	-0.39946200
H	-1.03712100	3.09959600	0.72567100
C	0.62540000	0.14699400	-1.45308400
H	0.80657600	1.09315200	-1.97434400
H	0.74711500	-0.65551300	-2.19159700
N	1.67030200	0.05432000	-0.45546800
C	2.66525600	0.92905100	-0.11225800
O	2.93678100	2.04193700	-0.51435500
C	3.22543000	-0.05620600	0.93292300
H	4.23296800	-0.41682600	0.71343100
C	2.06372100	-1.01144200	0.50146800
C	2.50389600	-2.29358900	-0.19903500
C	1.02264000	-1.28058200	1.58592000
H	3.17750800	0.30197400	1.96384200
H	3.25364500	-2.08002700	-0.96651000
H	2.93309500	-2.99830300	0.52005400
H	1.65096800	-2.78580100	-0.67872900
H	1.44399100	-1.93315300	2.35766900
H	0.70250500	-0.34770600	2.05735400
H	0.13645500	-1.76734300	1.17033500
O	-4.60106700	-0.16974700	0.75645800
H	-5.05713400	-0.96430000	0.45006200

CPI

Zero-point correction= 1.221254 (Hartree/Particle)
Thermal correction to Energy= 1.282384
Thermal correction to Enthalpy= 1.283249
Thermal correction to Gibbs Free Energy= 1.129923
Sum of electronic and zero-point Energies= -3437.982903

Sum of electronic and thermal Energies= -3437.921773
Sum of electronic and thermal Enthalpies= -3437.920908
Sum of electronic and thermal Free Energies= -3438.074234

C	4.00505500	-0.12451000	-0.35792600
C	5.04511500	0.16328800	-1.31038300
C	4.51255200	2.56449700	-1.11771000
C	3.44023600	2.29021400	-0.30007500
C	3.66322600	-1.52205500	0.03421600
C	4.61602500	-2.47592900	0.52842400
C	4.19942500	-3.83518400	0.72211800
C	2.84730300	-4.20856100	0.48838700
C	1.90146800	-3.27682100	0.12686700
H	4.71338300	3.59017000	-1.41096500
H	2.55980500	-5.24378400	0.63980200
C	2.43624100	3.31917400	0.10890000
C	1.49184500	3.77453200	-0.84046700
C	2.37033600	3.76653800	1.44209200
C	0.52333700	4.69479900	-0.43539300
C	1.37602400	4.68228900	1.80088300
C	0.44345100	5.15749500	0.88047000
H	-0.20019900	5.04808300	-1.16342600
H	1.32202200	5.03059100	2.82898200
C	0.42850400	-3.50509200	0.00282500
C	-0.34933500	-3.72344400	1.16329500
C	-0.20754400	-3.29386200	-1.24107600
C	-1.74177500	-3.73073100	1.04912300
C	-1.60598000	-3.27418000	-1.29731900
C	-2.39133100	-3.48511100	-0.16081300
H	-2.33462500	-3.89720400	1.94137600
H	-2.10099400	-3.11275200	-2.25097000
C	5.32746600	1.52917000	-1.64323700
C	6.78693500	-0.53253700	-2.86780600
C	7.10286100	0.81688100	-3.14725600
C	6.37881000	1.82268600	-2.55141000
C	5.78539300	-0.85025000	-1.97781900
H	7.33435800	-1.32769000	-3.36492800
H	7.90051900	1.05410500	-3.84456800
H	6.58636400	2.86452900	-2.78002400
H	5.54983300	-1.88860500	-1.78540000
C	6.43880900	-4.41805900	1.47811700
C	6.83678100	-3.06927600	1.33047600
C	5.94878600	-2.12381500	0.86817200
C	5.14634500	-4.78688600	1.18415100

H	7.14975300	-5.15568500	1.83758200
H	7.84939700	-2.77533100	1.58958000
H	6.25934500	-1.09121400	0.76409000
H	4.82174600	-5.81535000	1.31710500
C	3.24077900	0.94053900	0.09900700
C	2.35327300	-1.94700400	-0.09308800
O	1.39366100	-1.04557500	-0.50158700
O	2.23694100	0.72925300	1.02859200
P	0.82375800	0.03031700	0.59630400
O	0.25108000	-0.57717400	1.84017800
C	0.57856800	-3.12369500	-2.53454900
C	0.16416900	-1.87411300	-3.32855800
C	0.45285500	-4.39383300	-3.39590400
H	1.63516400	-3.01169300	-2.27975700
H	0.27539100	-0.97496900	-2.71740200
H	0.79650200	-1.76242500	-4.21611100
H	-0.87395700	-1.93891300	-3.67212500
H	0.79059200	-5.27629800	-2.84379800
H	-0.58748500	-4.56383000	-3.69421600
H	1.05579100	-4.30633300	-4.30626800
C	-3.90648700	-3.47629700	-0.25043800
C	-4.52293800	-2.50448100	0.76341700
C	-4.47575200	-4.89450400	-0.07437300
H	-4.17589800	-3.12298300	-1.25330300
H	-4.17510000	-1.48270900	0.59610700
H	-5.61487300	-2.51734300	0.69396000
H	-4.25730800	-2.76956500	1.79107400
H	-4.05326400	-5.58232000	-0.81296000
H	-4.24006400	-5.28742000	0.92057800
H	-5.56567700	-4.89526100	-0.18799700
C	0.28204800	-3.94130400	2.53186900
C	0.43354800	-5.44767400	2.81571700
C	-0.48965400	-3.26250100	3.67385300
H	1.27967700	-3.49608000	2.50904000
H	1.01823500	-5.95312700	2.04197900
H	0.92712500	-5.61253400	3.77963100
H	-0.54989400	-5.93006800	2.85226100
H	-0.69183800	-2.21589700	3.44684800
H	-1.44186800	-3.76526000	3.87812300
H	0.10003400	-3.31059200	4.59524200
C	3.35450400	3.28921000	2.50021900
C	2.63893800	2.61838400	3.68429500
C	4.25596300	4.44398600	2.97006700
H	4.00402500	2.53832000	2.04265400

H	2.01814700	1.78782600	3.34147100
H	3.37118400	2.22793500	4.39929600
H	2.00053200	3.32896500	4.22026900
H	4.79435000	4.89017200	2.12783800
H	3.66851700	5.23567500	3.44757500
H	4.99250500	4.08759200	3.69836100
C	1.50318700	3.29352700	-2.28736800
C	2.18402400	4.33023100	-3.19873600
C	0.10124100	2.95041300	-2.81820300
H	2.09086000	2.37295600	-2.32849500
H	3.20840100	4.53615500	-2.87656700
H	2.21775400	3.97569500	-4.23485200
H	1.63408800	5.27794600	-3.18129700
H	-0.39060500	2.24642000	-2.14513500
H	-0.52661800	3.84260900	-2.92224000
H	0.18193900	2.49296300	-3.81066100
C	-0.63560600	6.14040600	1.30104400
C	-2.03971500	5.53123100	1.14817600
C	-0.52254000	7.46848300	0.53451800
H	-0.48188800	6.35551900	2.36630300
H	-2.13305300	4.60548300	1.72221600
H	-2.80907500	6.23100200	1.49311700
H	-2.24865000	5.29575400	0.09831200
H	0.46845200	7.91372700	0.66391900
H	-0.68176200	7.31750500	-0.53866200
H	-1.27165500	8.18664200	0.88552500
O	-0.04548800	0.93333700	-0.26598200
Ag	-1.89120300	-0.04055700	-0.93584800
C	-3.68116500	0.31680600	-1.95281600
C	-5.06661000	0.10915500	-1.68793000
C	-7.46130400	0.24489600	-1.20585000
O	-5.05035400	-0.86190800	-2.50939500
N	-6.04085300	0.63681600	-0.97672200
C	-5.73750000	1.84355500	-0.14075700
H	-6.69746100	2.14829000	0.28162500
H	-5.39857000	2.65170800	-0.79693600
C	-4.70697200	1.56024300	0.91642600
C	-3.40233800	2.04022900	0.75535000
C	-4.99867700	0.73700400	2.02541200
C	-2.36947900	1.65784400	1.60927800
C	-3.96285200	0.34898000	2.87188300
C	-2.63493100	0.74539800	2.64335000
H	-1.36456900	2.02418800	1.44338400
H	-4.15688500	-0.31906200	3.70502100

H	-7.99442400	0.65192300	-0.34219800
C	-7.98005700	0.92037800	-2.47920900
H	-9.04486800	0.70846000	-2.61198800
H	-7.85137100	2.00586600	-2.43342700
H	-7.44449900	0.54132300	-3.35461500
C	-7.67344400	-1.26927200	-1.22093400
H	-7.20358100	-1.73497300	-2.08796800
H	-7.26872100	-1.73393600	-0.32009900
H	-8.74801500	-1.47033600	-1.25678900
O	-1.67070100	0.24833000	3.43767600
H	-0.85042300	0.08607800	2.89733100
H	-3.58342400	0.94661400	-2.84426700
H	-3.17976400	2.72323100	-0.06134400
C	-6.39667600	0.22947600	2.27804700
H	-7.13343800	1.04153800	2.27414800
H	-6.70345200	-0.49432400	1.51607900
H	-6.45951900	-0.26984200	3.24719300

TSG

Zero-point correction=	1.220569 (Hartree/Particle)
Thermal correction to Energy=	1.281072
Thermal correction to Enthalpy=	1.281937
Thermal correction to Gibbs Free Energy=	1.130478
Sum of electronic and zero-point Energies=	-3437.977645
Sum of electronic and thermal Energies=	-3437.917141
Sum of electronic and thermal Enthalpies=	-3437.916276
Sum of electronic and thermal Free Energies=	-3438.067736

C	4.04964800	-0.19235800	-0.31871800
C	5.13631300	0.05975800	-1.22855400
C	4.67654500	2.47730300	-1.05990000
C	3.56493200	2.23903900	-0.28533300
C	3.64000800	-1.57836600	0.04892400
C	4.52944900	-2.57370900	0.57689300
C	4.04499400	-3.91329100	0.74909100
C	2.68613400	-4.22435100	0.46824000
C	1.79668100	-3.25072200	0.07402800
H	4.92020900	3.49522200	-1.34795500
H	2.34682300	-5.24454200	0.61341100
C	2.57340500	3.29700200	0.07771100
C	1.63572200	3.71739400	-0.89376500
C	2.50731100	3.79756900	1.39068000
C	0.67114400	4.65820600	-0.52975500

C	1.51755900	4.73317400	1.70902300
C	0.58989300	5.17357900	0.76659300
H	-0.05022900	4.98286800	-1.27284800
H	1.46031300	5.12140100	2.72267000
C	0.31729300	-3.41071600	-0.08080400
C	-0.49311000	-3.65144700	1.05398600
C	-0.28924600	-3.12126100	-1.32528400
C	-1.88516100	-3.60685500	0.91827300
C	-1.68810300	-3.04610800	-1.40364700
C	-2.50747000	-3.29183200	-0.29028000
H	-2.49743200	-3.79809700	1.79162800
H	-2.15998900	-2.85921700	-2.36450900
C	5.47855100	1.41472900	-1.54965000
C	6.91497300	-0.69635400	-2.71525900
C	7.28818800	0.64112900	-2.98084500
C	6.57514600	1.67142400	-2.41430700
C	5.86780400	-0.97880500	-1.86686300
H	7.45433900	-1.51027700	-3.19035400
H	8.12103900	0.85040400	-3.64516600
H	6.82688800	2.70541500	-2.63398700
H	5.58934400	-2.00848200	-1.68559200
C	6.22474400	-4.59764400	1.58925200
C	6.68771800	-3.26743200	1.46366000
C	5.86176600	-2.28199300	0.97084900
C	4.92974900	-4.90776300	1.24334200
H	6.88755700	-5.36716100	1.97296000
H	7.70134400	-3.01975000	1.76385300
H	6.22149400	-1.26393500	0.88312600
H	4.55477400	-5.92104700	1.35939600
C	3.30490500	0.89883100	0.11078300
C	2.31979200	-1.94517500	-0.13587800
O	1.42298000	-0.99785600	-0.57826000
O	2.26076700	0.72956300	1.00374500
P	0.84149000	0.05769600	0.53824600
O	0.27393500	-0.61262300	1.75799500
C	0.51751600	-2.94532600	-2.60502500
C	0.14443000	-1.67234400	-3.38202100
C	0.36844900	-4.19859400	-3.48808500
H	1.57272100	-2.86661900	-2.33561300
H	0.26176400	-0.78657300	-2.75326000
H	0.79708700	-1.55923500	-4.25418900
H	-0.88689000	-1.70900100	-3.74958000
H	0.67577700	-5.09879500	-2.94692600
H	-0.67155500	-4.33552500	-3.80413200

H	0.98619100	-4.11143300	-4.38820200
C	-4.01900900	-3.29734900	-0.44348500
C	-4.73043200	-2.53316700	0.67857400
C	-4.53629500	-4.74386400	-0.54059500
H	-4.25266400	-2.78941900	-1.38705600
H	-4.38761400	-1.49780600	0.73184400
H	-5.81156400	-2.53403200	0.50983300
H	-4.55211500	-2.98843500	1.65796600
H	-4.05435800	-5.28063900	-1.36326200
H	-4.32722000	-5.29194500	0.38457700
H	-5.61893100	-4.75977200	-0.70760300
C	0.09855000	-3.95363700	2.42377800
C	0.16000500	-5.47602100	2.65194500
C	-0.65803800	-3.27628700	3.57672400
H	1.11865100	-3.56343500	2.43522600
H	0.72463400	-5.98669400	1.86673100
H	0.63045200	-5.70337700	3.61452800
H	-0.84960700	-5.90242100	2.66018700
H	-0.79846200	-2.21204100	3.38916700
H	-1.64041900	-3.73253300	3.74436300
H	-0.09030500	-3.39285500	4.50564900
C	3.47798100	3.34334800	2.47086800
C	2.74442100	2.68458200	3.65092600
C	4.36614700	4.50793200	2.94081100
H	4.13798700	2.58899700	2.03338700
H	2.13994300	1.84216300	3.30756300
H	3.46427200	2.31430800	4.38899900
H	2.08600300	3.39746400	4.15899700
H	4.91514900	4.94731000	2.10187700
H	3.76811700	5.30221600	3.40049700
H	5.09316300	4.16381300	3.68441400
C	1.65734800	3.17501200	-2.31885800
C	2.39908300	4.14570900	-3.25507000
C	0.25659300	2.85964700	-2.86881200
H	2.21106600	2.23225400	-2.30662200
H	3.42418300	4.32310700	-2.91870700
H	2.43943900	3.74814700	-4.27520000
H	1.88731200	5.11420900	-3.28739600
H	-0.27489100	2.20231100	-2.17896900
H	-0.33410200	3.76891400	-3.02883700
H	0.34540800	2.35796000	-3.83893600
C	-0.49361100	6.16835400	1.14600800
C	-1.89236100	5.53750700	1.03431400
C	-0.40060500	7.45795500	0.31422500

H	-0.33452200	6.43735300	2.19818100
H	-1.97123100	4.64163400	1.65627800
H	-2.66777100	6.24532400	1.34803400
H	-2.10369800	5.24590600	-0.00090800
H	0.58681600	7.91865700	0.41309800
H	-0.56719400	7.25346500	-0.74887400
H	-1.15401600	8.18517200	0.63623100
O	-0.04746800	0.96603300	-0.28479600
Ag	-1.93062600	-0.33041800	-0.71884700
C	-3.68700500	0.53782300	-1.54109000
C	-5.10344300	0.33136100	-1.53440300
C	-7.52195200	0.53565900	-1.25025800
O	-5.10007300	-0.47123300	-2.51033700
N	-6.12113500	0.82713800	-0.84330600
C	-5.84341000	1.95253300	0.09523700
H	-6.78604100	2.15073800	0.60903800
H	-5.58948900	2.84949000	-0.48159400
C	-4.74123600	1.61299300	1.05810100
C	-3.44525300	2.09700200	0.84195300
C	-4.97167000	0.72193600	2.12844900
C	-2.36493000	1.67025100	1.61582000
C	-3.89289000	0.30056800	2.89940000
C	-2.57889300	0.72338900	2.63043400
H	-1.36853600	2.03709100	1.40511400
H	-4.03912300	-0.40887100	3.70771000
H	-8.13175600	0.97752900	-0.45634000
C	-7.85213900	1.23199300	-2.57467600
H	-8.90630300	1.08321900	-2.82597400
H	-7.66600200	2.30834500	-2.51047200
H	-7.24369100	0.81856900	-3.38308400
C	-7.80780500	-0.96694200	-1.28716100
H	-7.22389200	-1.46287100	-2.06386000
H	-7.57408500	-1.43220300	-0.32666900
H	-8.87015000	-1.12470800	-1.49457700
O	-1.58526000	0.21243100	3.37617100
H	-0.78191300	0.04677700	2.80529200
H	-3.45758500	1.35369600	-2.23965300
H	-3.26930700	2.82918600	0.05692500
C	-6.35416400	0.19120700	2.41638000
H	-7.06743000	1.00035200	2.61415200
H	-6.74284600	-0.38688200	1.57172900
H	-6.34532100	-0.46375100	3.29001300

CPH

Zero-point correction=	1.230825 (Hartree/Particle)
Thermal correction to Energy=	1.292836
Thermal correction to Enthalpy=	1.293701
Thermal correction to Gibbs Free Energy=	1.139387
Sum of electronic and zero-point Energies=	-3547.509002
Sum of electronic and thermal Energies=	-3547.446990
Sum of electronic and thermal Enthalpies=	-3547.446125
Sum of electronic and thermal Free Energies=	-3547.600439

C	-3.77441600	-0.59207400	0.46842100
C	-4.93618200	-0.49164600	1.30598500
C	-4.70587400	1.96462200	1.26424200
C	-3.53382300	1.87338500	0.54736800
C	-3.25652400	-1.89768200	-0.03178800
C	-4.05558800	-2.81798600	-0.79128900
C	-3.47859400	-4.06712900	-1.19484700
C	-2.11547900	-4.34369800	-0.90692300
C	-1.31551600	-3.42676100	-0.26401400
H	-5.08624900	2.94175300	1.54529900
H	-1.69607400	-5.28849600	-1.23745600
C	-2.72335100	3.06808300	0.15649800
C	-1.89864200	3.70883800	1.10665600
C	-2.76452900	3.53059100	-1.17442300
C	-1.17472600	4.83848300	0.71361800
C	-2.02424300	4.66613800	-1.51832200
C	-1.23194100	5.34042000	-0.58897100
H	-0.55087000	5.34094200	1.44603600
H	-2.06423900	5.03758400	-2.53809000
C	0.15742300	-3.57121500	-0.04626100
C	1.05653700	-3.46188200	-1.12876100
C	0.65189600	-3.65314200	1.27679100
C	2.43643900	-3.36019200	-0.85739300
C	2.02302300	-3.52474700	1.50525700
C	2.93926800	-3.35348900	0.45893600
H	3.13152100	-3.33751900	-1.68988700
H	2.39859000	-3.56562600	2.52363500
C	-5.41568500	0.80710100	1.67771000
C	-6.73343600	-1.49329700	2.60933400
C	-7.23151000	-0.21092800	2.93746000
C	-6.57962600	0.91210400	2.48394100
C	-5.61599100	-1.63004000	1.81676600
H	-7.23322400	-2.37840500	2.99119000
H	-8.11723300	-0.11683400	3.55821600

H	-6.93702200	1.90370600	2.74794600
H	-5.23843200	-2.61707700	1.58008500
C	-5.56757600	-4.69657600	-2.27184500
C	-6.12207200	-3.44536700	-1.91614400
C	-5.38597900	-2.53027800	-1.19721500
C	-4.27087100	-4.99391400	-1.92216900
H	-6.16098500	-5.41179100	-2.83306700
H	-7.13606400	-3.20113200	-2.21787700
H	-5.81814500	-1.57204000	-0.93787900
H	-3.82368300	-5.94119700	-2.21115600
C	-3.09712100	0.57869200	0.15960500
C	-1.92899000	-2.22135400	0.18613800
O	-1.13651300	-1.32989300	0.88645900
O	-1.95419200	0.52538600	-0.61677500
P	-0.55557200	-0.03814800	0.04091800
O	0.19398000	-0.53213000	-1.19215300
C	-0.27967100	-3.94774100	2.44504300
C	-0.17423400	-2.93087400	3.58886500
C	-0.03102000	-5.38209500	2.94834000
H	-1.30524400	-3.91229100	2.07013400
H	-0.35717200	-1.91851100	3.22400100
H	-0.91739200	-3.16079000	4.35968200
H	0.81098300	-2.95517800	4.06389700
H	-0.15346900	-6.11108500	2.14110900
H	0.98430500	-5.48891100	3.34549200
H	-0.73404300	-5.63474800	3.74900400
C	4.42771300	-3.28487900	0.77039400
C	5.25862100	-2.54870900	-0.28551900
C	4.97926000	-4.70622700	0.99477200
H	4.53559600	-2.72473100	1.70655400
H	4.87355900	-1.53630100	-0.45943200
H	6.29296000	-2.44823200	0.05222700
H	5.26837300	-3.07729500	-1.24487000
H	4.42554000	-5.22449800	1.78266400
H	4.89383200	-5.30084400	0.07826100
H	6.03486700	-4.67145500	1.28302200
C	0.58378600	-3.48890800	-2.57584300
C	0.67254900	-4.92933100	-3.11840700
C	1.33708200	-2.52906400	-3.50807500
H	-0.46566800	-3.18599300	-2.58320600
H	0.12107600	-5.63396500	-2.49006800
H	0.26647300	-4.98469900	-4.13375200
H	1.71564100	-5.26427900	-3.15192400
H	1.25337700	-1.49820500	-3.16326600

H	2.39735400	-2.78963700	-3.60219900
H	0.90584400	-2.57938600	-4.51296200
C	-3.63003800	2.85012100	-2.22573300
C	-2.90231000	2.66332400	-3.56529000
C	-4.95138600	3.61850000	-2.40369400
H	-3.88380500	1.85299800	-1.85875700
H	-1.93939400	2.16321500	-3.43177200
H	-3.51421500	2.05737000	-4.24182900
H	-2.71874900	3.62003500	-4.06613700
H	-5.49713900	3.68254500	-1.45698000
H	-4.76324600	4.63978400	-2.75296500
H	-5.59530400	3.12158700	-3.13760700
C	-1.80135800	3.21484500	2.54492100
C	-2.73295900	4.02870300	3.46097100
C	-0.36379100	3.23043900	3.08715000
H	-2.13461700	2.17363000	2.55904900
H	-3.77397500	3.96853000	3.13228500
H	-2.68038900	3.66168600	4.49181100
H	-2.44462600	5.08596500	3.46197700
H	0.29087400	2.66704300	2.42149100
H	0.01989900	4.25021300	3.20296100
H	-0.33746800	2.76157900	4.07678000
C	-0.46509300	6.59065800	-0.98662000
C	1.05406500	6.40610900	-0.84044300
C	-0.95014200	7.81697000	-0.19510700
H	-0.67515000	6.77446200	-2.04808300
H	1.40810000	5.56415200	-1.44119600
H	1.58736000	7.30771500	-1.16107900
H	1.32648000	6.21269600	0.20328000
H	-2.02699200	7.96448100	-0.32022600
H	-0.75309100	7.69545200	0.87543800
H	-0.43633600	8.72493900	-0.52913900
O	0.10462400	0.86184300	1.02914600
Ag	2.41173100	-0.73639100	-0.57179200
C	3.08167100	0.58099800	1.34620800
C	4.57216200	0.64623000	1.44613600
C	6.69672600	1.74853800	0.90733600
O	5.15830200	-0.17577400	2.15833900
N	5.22698900	1.60125300	0.71162200
C	4.52873500	2.76303300	0.11497300
H	5.31487400	3.38433500	-0.32308700
H	4.05767700	3.36807000	0.90001500
C	3.49208000	2.42302600	-0.93107000
C	2.18915500	2.91010600	-0.78100100

C	3.79034200	1.57562300	-2.01989800
C	1.15426300	2.52006500	-1.62671300
C	2.73757000	1.15826500	-2.84702100
C	1.42150400	1.59137400	-2.63243200
H	0.14109400	2.86867600	-1.46309000
H	2.92708500	0.47925000	-3.67298100
H	6.99026300	2.49174800	0.15943400
C	7.01349200	2.31446600	2.29681300
H	8.08607500	2.51132400	2.39014100
H	6.47984400	3.25473300	2.46875700
H	6.72259500	1.59829500	3.06780500
C	7.49660900	0.47728100	0.60611100
H	7.31945900	-0.28790000	1.35946500
H	7.23704900	0.07122100	-0.37436600
H	8.56202500	0.72941900	0.59333700
O	0.41272200	1.04010000	-3.37612200
H	-0.04317700	0.43972400	-2.74429500
H	2.41132300	1.36134500	1.00720100
H	1.95708600	3.56598800	0.05337100
C	5.19439600	1.10440300	-2.31318900
H	5.25974500	0.70690500	-3.32908600
H	5.91875100	1.92066000	-2.22332000
H	5.51412400	0.32174300	-1.62149900
N	2.15525400	-0.69426300	3.23809500
N	2.55569500	-0.09327500	2.37639700

TSH

Zero-point correction=	1.228471 (Hartree/Particle)
Thermal correction to Energy=	1.291248
Thermal correction to Enthalpy=	1.292113
Thermal correction to Gibbs Free Energy=	1.135692
Sum of electronic and zero-point Energies=	-3547.472663
Sum of electronic and thermal Energies=	-3547.409887
Sum of electronic and thermal Enthalpies=	-3547.409022
Sum of electronic and thermal Free Energies=	-3547.565442

C	-3.79143900	-0.32148500	0.50280900
C	-4.93958900	-0.12550600	1.34156700
C	-4.51056400	2.30359400	1.29443200
C	-3.35243300	2.11585600	0.57367800
C	-3.38891600	-1.66287900	-0.00825200
C	-4.26535900	-2.50103900	-0.77675900
C	-3.79779800	-3.78952400	-1.19734400

C	-2.46224300	-4.18358200	-0.91828600
C	-1.58438200	-3.34540700	-0.26911400
H	-4.81218000	3.30944600	1.56982800
H	-2.12818800	-5.15884200	-1.25652700
C	-2.46157800	3.24346800	0.15872000
C	-1.57675200	3.83254800	1.08793800
C	-2.49357600	3.69664600	-1.17574900
C	-0.78190200	4.90479400	0.67138800
C	-1.68137300	4.77424400	-1.54337000
C	-0.82683800	5.39862300	-0.63501200
H	-0.11238700	5.36921500	1.38852600
H	-1.71312800	5.13820600	-2.56625000
C	-0.13265800	-3.63844800	-0.04934900
C	0.78700100	-3.56452800	-1.12341400
C	0.33578600	-3.86989400	1.26104700
C	2.16364100	-3.66919600	-0.84635900
C	1.71225000	-3.98365500	1.49094300
C	2.64807500	-3.87758500	0.46115300
H	2.86489900	-3.68356200	-1.67495400
H	2.06694400	-4.17202800	2.50023900
C	-5.30957200	1.20820600	1.71456000
C	-6.81190200	-0.97637100	2.64629700
C	-7.20073800	0.34252700	2.97744900
C	-6.45901100	1.40827300	2.52356900
C	-5.71115800	-1.20428500	1.85135500
H	-7.38322300	-1.81737400	3.02755500
H	-8.07435500	0.50899800	3.60018800
H	-6.73298500	2.42578600	2.78883300
H	-5.41736600	-2.21879700	1.61163900
C	-5.93623500	-4.22734600	-2.27207200
C	-6.38119500	-2.93761400	-1.90011700
C	-5.56783900	-2.09662000	-1.17409100
C	-4.66830100	-4.63755600	-1.93134400
H	-6.59012600	-4.88310600	-2.83869300
H	-7.37179900	-2.60476800	-2.19479200
H	-5.91650800	-1.10834400	-0.90212100
H	-4.30395700	-5.61589000	-2.23298600
C	-3.01843400	0.78855500	0.19350000
C	-2.09326700	-2.10138100	0.20240400
O	-1.22992000	-1.29282200	0.91728600
O	-1.88309800	0.63932800	-0.57864300
P	-0.53724500	-0.04972400	0.08079500
O	0.15733100	-0.60774400	-1.15634200
C	-0.62689800	-4.05277600	2.42632100

C	-0.37659300	-3.05457800	3.56606900
C	-0.57608600	-5.50598400	2.93175000
H	-1.63884000	-3.87683800	2.05456700
H	-0.42369900	-2.02845800	3.19557900
H	-1.13787500	-3.17584600	4.34391700
H	0.60014900	-3.21387600	4.03332600
H	-0.79799600	-6.21224100	2.12555800
H	0.41359200	-5.75289500	3.33094100
H	-1.30767500	-5.65822700	3.73215500
C	4.12311500	-4.12813300	0.73220500
C	5.06479400	-3.11145000	0.07003700
C	4.48367100	-5.56623200	0.31126300
H	4.26728300	-4.05202900	1.81735900
H	4.89953600	-2.10519500	0.46265500
H	6.10746700	-3.37719200	0.27283200
H	4.93774100	-3.09473100	-1.01821300
H	3.83418100	-6.29617500	0.80346300
H	4.36897400	-5.69146600	-0.77118700
H	5.52200800	-5.79733100	0.57046100
C	0.32506400	-3.44270700	-2.56926600
C	0.18529000	-4.85015500	-3.18449300
C	1.23700300	-2.58440800	-3.45724800
H	-0.65949400	-2.96967700	-2.55938800
H	-0.47599300	-5.48986600	-2.59552500
H	-0.21690800	-4.78655700	-4.20083100
H	1.16246400	-5.34369800	-3.23650400
H	1.34818600	-1.57593700	-3.05744100
H	2.22915800	-3.03174600	-3.58441500
H	0.79735500	-2.49235000	-4.45521400
C	-3.41893000	3.06847000	-2.20861100
C	-2.70919100	2.77567800	-3.53905900
C	-4.66320000	3.94991700	-2.41461800
H	-3.76455700	2.11059200	-1.81340200
H	-1.80355200	2.18233600	-3.38828700
H	-3.37733800	2.21946800	-4.20509700
H	-2.42557400	3.69623100	-4.06042300
H	-5.20050400	4.09400900	-1.47185500
H	-4.38222700	4.93804700	-2.79547500
H	-5.35033400	3.49160300	-3.13428700
C	-1.49274000	3.34603800	2.52940400
C	-2.34997200	4.23326100	3.44988500
C	-0.04983000	3.26231900	3.04990700
H	-1.89866100	2.33130800	2.55833200
H	-3.39713700	4.24522500	3.13567500

H	-2.30954300	3.87253100	4.48348500
H	-1.98640800	5.26701600	3.43664500
H	0.54758500	2.63536000	2.38712100
H	0.41317200	4.25141800	3.13936600
H	-0.04316000	2.81150100	4.04819600
C	0.01689000	6.58979300	-1.05790300
C	1.52253300	6.30867200	-0.92688300
C	-0.37734500	7.85530900	-0.27766700
H	-0.19344500	6.77342000	-2.11932500
H	1.81204000	5.43364100	-1.51468200
H	2.10861100	7.16762700	-1.27156900
H	1.79641500	6.11749100	0.11692800
H	-1.44337900	8.07224700	-0.39393100
H	-0.17725300	7.73389300	0.79235300
H	0.19172800	8.72313300	-0.62847900
O	0.18361700	0.78944700	1.07905300
Ag	2.36482600	-1.03771300	-0.48809000
C	3.23499900	0.42824900	0.86923600
C	4.67508200	0.62894400	1.25197500
C	6.76683300	1.90755800	1.06356400
O	5.22915600	-0.20312900	1.98243400
N	5.34274600	1.68391600	0.69920000
C	4.63817200	2.78277800	0.01406300
H	5.40602400	3.34159000	-0.53006200
H	4.20444000	3.47569700	0.74775000
C	3.56289500	2.32322800	-0.93621600
C	2.24453900	2.77031200	-0.75288800
C	3.86463200	1.49613700	-2.04551400
C	1.21154400	2.35596500	-1.58026700
C	2.81741300	1.07560500	-2.86707400
C	1.49423700	1.46065800	-2.61574000
H	0.19190200	2.67140300	-1.39527300
H	3.00766700	0.40369200	-3.69832900
H	7.06132000	2.77703600	0.46724900
C	6.91661800	2.27703900	2.54387400
H	7.95473100	2.54962100	2.75841600
H	6.28177100	3.13175900	2.79841700
H	6.63819800	1.43160100	3.17480900
C	7.67399200	0.74336300	0.65176900
H	7.44678500	-0.15106300	1.23040700
H	7.55661000	0.51617200	-0.41109000
H	8.71793500	1.02354700	0.82494900
O	0.49253000	0.89830900	-3.35328500
H	-0.00514100	0.35299800	-2.70082200

H	2.49033400	1.17951600	1.11785100
H	2.01123200	3.41692500	0.08747100
C	5.26625800	1.01578600	-2.32314000
H	5.33972300	0.60846200	-3.33436700
H	6.00133300	1.82201900	-2.22830000
H	5.56316400	0.23165800	-1.61908300
N	2.39546400	-1.24561800	3.24313300
N	2.74267900	-0.53238500	2.47294800

CPJ

Zero-point correction=	1.219781 (Hartree/Particle)
Thermal correction to Energy=	1.279223
Thermal correction to Enthalpy=	1.280088
Thermal correction to Gibbs Free Energy=	1.130851
Sum of electronic and zero-point Energies=	-3438.024932
Sum of electronic and thermal Energies=	-3437.965489
Sum of electronic and thermal Enthalpies=	-3437.964624
Sum of electronic and thermal Free Energies=	-3438.113861

C	-2.63744000	-2.58693800	-0.23278100
C	-2.97756100	-3.80197000	-0.91767000
C	-0.62989700	-4.51695400	-0.72041600
C	-0.26721400	-3.30465900	-0.17147100
C	-3.66519300	-1.57835900	0.14454400
C	-4.82175800	-1.91898400	0.92672600
C	-5.79942300	-0.90531500	1.19170200
C	-5.56645800	0.42632700	0.76242700
C	-4.40460900	0.78770300	0.11628900
H	0.13088000	-5.27407400	-0.88240900
H	-6.30293700	1.18779800	0.99851100
C	1.15718000	-2.99195900	0.15229000
C	2.11443900	-2.90608400	-0.88939400
C	1.56435000	-2.81505100	1.49208000
C	3.45585700	-2.68912400	-0.55620500
C	2.92084200	-2.61624800	1.77218400
C	3.88721800	-2.57222800	0.76847700
H	4.19445800	-2.60723600	-1.34759800
H	3.22399600	-2.51456600	2.80874500
C	-4.03687700	2.20647700	-0.16778000
C	-3.71700300	3.06901600	0.90855000
C	-3.93053800	2.66574900	-1.49584200
C	-3.30306500	4.37158100	0.62373600
C	-3.50659700	3.97791200	-1.72670800

C	-3.17916700	4.84317600	-0.68485700
H	-3.05221500	5.03236800	1.44745900
H	-3.42145800	4.33456200	-2.74970100
C	-1.95932700	-4.78646400	-1.12971000
C	-4.56649500	-5.24328400	-2.06870400
C	-3.57060100	-6.23425700	-2.23553400
C	-2.29402700	-6.00445900	-1.77933600
C	-4.27858700	-4.05971100	-1.42761500
H	-5.56614700	-5.41516900	-2.45596400
H	-3.81342500	-7.16594900	-2.73716000
H	-1.51247800	-6.74553100	-1.92264200
H	-5.04678000	-3.30515700	-1.31390200
C	-7.14708000	-2.50907900	2.42876100
C	-6.15826800	-3.49693500	2.21315500
C	-5.02630000	-3.20994100	1.48380100
C	-6.96376300	-1.23958100	1.93292000
H	-8.03859700	-2.75091700	2.99919900
H	-6.28973100	-4.49006400	2.63184800
H	-4.27380600	-3.97357900	1.33410500
H	-7.70076100	-0.46220300	2.11486200
C	-1.30101200	-2.35895300	0.06135700
C	-3.49167800	-0.25159400	-0.20850800
O	-2.37143500	0.10238800	-0.95198500
O	-0.93139200	-1.16984100	0.67575600
P	-0.94170700	0.21564700	-0.18552700
O	-0.94998700	1.28783600	0.89629900
C	-4.29421400	1.78963700	-2.68656600
C	-3.13425900	1.66277300	-3.68758200
C	-5.57025000	2.31134900	-3.37057800
H	-4.51679700	0.78607500	-2.31562400
H	-2.23516300	1.28807000	-3.19360600
H	-3.40178400	0.96817200	-4.49122800
H	-2.89845800	2.62686200	-4.15088000
H	-6.40453900	2.35720800	-2.66342000
H	-5.41858400	3.31859900	-3.77331400
H	-5.85894600	1.65737400	-4.20061400
C	-2.68120800	6.24948700	-0.96733400
C	-1.23219000	6.43177200	-0.48352700
C	-3.60709500	7.31619700	-0.36042300
H	-2.68802600	6.38259000	-2.05694600
H	-0.57930700	5.66868700	-0.91502000
H	-0.85265300	7.42268200	-0.75679400
H	-1.16888200	6.33454800	0.60546800
H	-4.63205200	7.20222800	-0.72614000

H	-3.63244500	7.23938000	0.73186700
H	-3.26034700	8.32353000	-0.61544900
C	-3.82061600	2.63427200	2.36707000
C	-5.09069500	3.21981900	3.01085100
C	-2.58088600	3.00245400	3.19789400
H	-3.90384300	1.54557100	2.39061400
H	-5.99078700	2.92994000	2.46084300
H	-5.19702300	2.87585500	4.04552800
H	-5.04971200	4.31466800	3.01993600
H	-1.68369300	2.56834800	2.75534800
H	-2.44500300	4.08606800	3.27780500
H	-2.68698100	2.61184600	4.21574700
C	0.59367800	-2.89029200	2.66381100
C	0.57510800	-1.57693300	3.46467900
C	0.91125600	-4.09434200	3.56775200
H	-0.41281900	-3.04547200	2.27116800
H	0.30698100	-0.73722400	2.81986900
H	-0.15952900	-1.63438400	4.27509000
H	1.55278700	-1.37496000	3.91701600
H	0.89258200	-5.02802400	2.99699200
H	1.90244100	-4.00247700	4.02438000
H	0.17659100	-4.17225200	4.37639800
C	1.74966400	-3.08459300	-2.36090600
C	2.32763100	-4.40631400	-2.89920200
C	2.19896900	-1.90423500	-3.23818500
H	0.66209000	-3.14175000	-2.43857600
H	1.99985500	-5.26079900	-2.29909800
H	2.01038700	-4.57370500	-3.93394300
H	3.42260900	-4.39036000	-2.88008100
H	1.66858100	-0.98957900	-2.95561300
H	3.27500000	-1.71991000	-3.16413400
H	1.96417600	-2.10644900	-4.28902500
C	5.37622800	-2.47803200	1.06134100
C	5.99708400	-3.88830000	1.04081800
C	5.71624600	-1.77020400	2.37865400
H	5.82294700	-1.90466300	0.24267700
H	5.80556900	-4.38655100	0.08618200
H	7.08136600	-3.84031600	1.19095800
H	5.56874100	-4.51007400	1.83514900
H	5.26915200	-0.77191300	2.43048400
H	5.36840000	-2.33871900	3.24796300
H	6.80024800	-1.65877500	2.47611200
O	0.08635500	0.25102800	-1.29205000
Ag	2.21902700	0.40089400	-0.87168200

C	4.04605300	0.87268800	0.09114700
C	5.44249000	0.74909300	-0.44355400
C	7.71527600	1.71494600	0.03729800
O	5.83602500	-0.08531700	-1.25788600
N	6.25172900	1.69051100	0.16112900
C	5.57025600	2.38709900	1.23832100
H	5.93199000	3.41736400	1.32674300
H	5.72646200	1.89362900	2.21019500
C	4.07779300	2.30852200	0.84530300
C	3.11981500	2.10041900	1.94874000
C	3.66295600	3.37063700	-0.13342900
C	1.80917100	2.41443400	1.82299800
C	2.37710300	3.80487200	-0.15442700
C	1.38873200	3.19788600	0.68687500
H	1.06037800	2.08728700	2.53405800
H	2.02096000	4.49023800	-0.91602600
H	8.03912700	2.58210100	0.62602500
C	8.34562600	0.45362600	0.64116900
H	9.43773200	0.51585300	0.60459700
H	8.04519300	0.32860300	1.68593600
H	8.02532000	-0.42605200	0.07865900
C	8.14269500	1.93746400	-1.41718100
H	7.81267800	1.10314900	-2.03744800
H	7.70658000	2.85981900	-1.81220000
H	9.23238200	2.01869300	-1.47827100
O	0.15046500	3.37035000	0.39112400
H	-0.44594400	2.48491500	0.67677700
H	3.97519800	0.10004300	0.86893200
H	3.46092300	1.50853000	2.79387800
C	4.61561300	3.83034600	-1.19437000
H	5.57702900	4.14702500	-0.78122000
H	4.82646900	3.00434500	-1.88277800
H	4.18452300	4.65423100	-1.76685100

TSK

Zero-point correction=	1.221439 (Hartree/Particle)
Thermal correction to Energy=	1.281498
Thermal correction to Enthalpy=	1.282363
Thermal correction to Gibbs Free Energy=	1.131027
Sum of electronic and zero-point Energies=	-3437.986868
Sum of electronic and thermal Energies=	-3437.926810
Sum of electronic and thermal Enthalpies=	-3437.925945
Sum of electronic and thermal Free Energies=	-3438.077281

C	-2.70793600	-2.52521700	-0.27986700
C	-3.09754200	-3.72616700	-0.96257600
C	-0.78144000	-4.53885000	-0.76271200
C	-0.37134900	-3.34266900	-0.21256200
C	-3.69396100	-1.48454600	0.12184000
C	-4.84545500	-1.79415900	0.92490100
C	-5.77837200	-0.74920100	1.22775500
C	-5.50606200	0.57953400	0.81237800
C	-4.34722200	0.90637100	0.14382500
H	-0.05482900	-5.33098800	-0.91468500
H	-6.20963100	1.36351100	1.07377000
C	1.05809900	-3.09867300	0.14843100
C	2.04574500	-3.05788700	-0.86542900
C	1.43819400	-2.94778700	1.50045800
C	3.38745000	-2.92010000	-0.49579400
C	2.79556400	-2.82028100	1.81759100
C	3.78981200	-2.82686500	0.83868700
H	4.14861500	-2.87662700	-1.26744800
H	3.07702400	-2.74090200	2.86288600
C	-3.93799300	2.31360300	-0.14297300
C	-3.51919400	3.14599400	0.92234000
C	-3.89215300	2.78595700	-1.46917900
C	-3.07134900	4.43532700	0.62912100
C	-3.43642400	4.08575100	-1.70938200
C	-3.01366000	4.92252700	-0.67852400
H	-2.73864100	5.07084100	1.44322900
H	-3.40011700	4.45411900	-2.73130700
C	-2.11993600	-4.75059600	-1.17811900
C	-4.74719900	-5.10248900	-2.10792300
C	-3.79150000	-6.13123800	-2.28094000
C	-2.50517500	-5.95293100	-1.82863200
C	-4.41011700	-3.93232000	-1.46610800
H	-5.75463700	-5.23458600	-2.49070800
H	-4.07264900	-7.05176300	-2.78326100
H	-1.75450000	-6.72478200	-1.97509100
H	-5.14712300	-3.14791700	-1.34656300
C	-7.15799200	-2.32075700	2.47147300
C	-6.21207600	-3.34107700	2.21864500
C	-5.08656500	-3.08495300	1.46797000
C	-6.93753400	-1.05144500	1.99035100
H	-8.04513600	-2.53789100	3.05851600
H	-6.37119000	-4.33516900	2.62545000
H	-4.36705600	-3.87394800	1.29069000

H	-7.64024000	-0.24977000	2.20061700
C	-1.36169200	-2.34764200	0.00549900
C	-3.47886200	-0.15959900	-0.21625300
O	-2.36867400	0.16537200	-0.98232100
O	-0.93930700	-1.17456000	0.60345400
P	-0.90947700	0.22194500	-0.25777600
O	-0.78959900	1.28738600	0.80078600
C	-4.34530700	1.93375600	-2.64637500
C	-3.23159500	1.75975900	-3.69198300
C	-5.62282600	2.51387200	-3.27795100
H	-4.59700100	0.93934200	-2.26885200
H	-2.33445400	1.33770100	-3.23390500
H	-3.56201000	1.08633900	-4.49042600
H	-2.96661400	2.71617800	-4.15559100
H	-6.42537900	2.59422800	-2.53785900
H	-5.44317700	3.51484400	-3.68489300
H	-5.97340000	1.87643700	-4.09705400
C	-2.47532700	6.31104100	-0.97647800
C	-0.96709300	6.39043200	-0.68085100
C	-3.24610200	7.40483500	-0.22020100
H	-2.61458800	6.48870300	-2.05089400
H	-0.42120200	5.62875900	-1.24411300
H	-0.57179400	7.37895000	-0.94213100
H	-0.76712400	6.20752100	0.37939200
H	-4.31658900	7.35772000	-0.44196400
H	-3.12478400	7.29708600	0.86284400
H	-2.88046900	8.39964100	-0.49725200
C	-3.55844100	2.68921700	2.37700200
C	-4.79069200	3.27816400	3.08807500
C	-2.27892300	3.02973800	3.15713000
H	-3.65380800	1.60093600	2.38518300
H	-5.71928000	3.00556000	2.57839700
H	-4.85137500	2.92096100	4.12206100
H	-4.73616000	4.37234400	3.10978200
H	-1.40518500	2.60823600	2.66046700
H	-2.13605000	4.11039800	3.26206700
H	-2.34040400	2.61072900	4.16754000
C	0.43254800	-2.97541000	2.64463900
C	0.44379500	-1.65638000	3.43632600
C	0.67360900	-4.18490600	3.56475600
H	-0.56752300	-3.09189900	2.22341000
H	0.21041500	-0.81429700	2.78096500
H	-0.30578100	-1.68359100	4.23450800
H	1.41984800	-1.48328600	3.90432600

H	0.63700200	-5.12096000	2.99875300
H	1.65185600	-4.12903500	4.05409600
H	-0.08971300	-4.22859700	4.34898300
C	1.71013300	-3.19717800	-2.34747700
C	2.22790800	-4.54083600	-2.89218100
C	2.24756400	-2.02891500	-3.19096700
H	0.62336400	-3.19196700	-2.45281600
H	1.83528900	-5.38433800	-2.31594800
H	1.93075800	-4.67394600	-3.93781100
H	3.32119100	-4.58808700	-2.84341100
H	1.75238400	-1.09450200	-2.91105200
H	3.32774400	-1.89847900	-3.07485100
H	2.03998600	-2.20450300	-4.25224900
C	5.27345600	-2.82464900	1.17293000
C	5.76883900	-4.27511500	1.32904800
C	5.64473400	-2.00158900	2.41374100
H	5.78516000	-2.37844000	0.31466900
H	5.55461600	-4.85973000	0.42969200
H	6.84936500	-4.30431500	1.50911100
H	5.26888900	-4.76480200	2.17231400
H	5.30106100	-0.96546000	2.33182000
H	5.21706800	-2.42534400	3.32864100
H	6.73195700	-1.98301000	2.54126300
O	0.06850100	0.16586000	-1.42114900
Ag	2.12149800	0.35669300	-0.81326500
C	3.85405700	0.61302200	0.35877900
C	5.21771400	0.56704800	-0.24474100
C	7.54838900	1.38243700	-0.49301300
O	5.44884600	-0.40117400	-0.97952800
N	6.16012700	1.53561900	-0.00176000
C	5.91005600	2.49432700	1.07041500
H	6.54125300	3.37047800	0.91034600
H	6.16454100	2.07894700	2.05663600
C	4.45718900	2.86174100	1.00773300
C	3.53758600	1.94888000	1.61507200
C	3.98397000	3.89514900	0.19368100
C	2.12686600	2.20792200	1.54887600
C	2.60355400	4.07529100	0.10152800
C	1.65394600	3.24588300	0.74761600
H	1.42788300	1.55085500	2.05355000
H	2.20431300	4.86539800	-0.52817500
H	8.06314400	2.28388700	-0.14087600
C	8.23914100	0.16459300	0.13292700
H	9.29469000	0.14177400	-0.15530200

H	8.18549800	0.20309000	1.22577800
H	7.76180200	-0.75515100	-0.20799900
C	7.60954200	1.37689300	-2.02280300
H	7.11371200	0.49226600	-2.42217800
H	7.11991400	2.26651000	-2.43111100
H	8.65414300	1.37949700	-2.34966000
O	0.37024300	3.51451500	0.53098800
H	-0.18771200	2.67374300	0.65043900
H	3.75566800	-0.23033800	1.04488100
H	3.88698500	1.43194500	2.50663100
C	4.92404700	4.77108600	-0.59702500
H	5.59477100	5.34105900	0.05524900
H	5.54659700	4.16465900	-1.26310900
H	4.36896200	5.48466900	-1.20892300

CPK

Zero-point correction=	1.339761 (Hartree/Particle)
Thermal correction to Energy=	1.406425
Thermal correction to Enthalpy=	1.407290
Thermal correction to Gibbs Free Energy=	1.245069
Sum of electronic and zero-point Energies=	-3858.734578
Sum of electronic and thermal Energies=	-3858.667914
Sum of electronic and thermal Enthalpies=	-3858.667049
Sum of electronic and thermal Free Energies=	-3858.829270

C	-2.45297700	2.91037100	-0.92212700
C	-3.31620100	3.49400600	-1.90588000
C	-4.82581200	1.58322500	-1.63301800
C	-3.92719300	0.93863000	-0.80509700
C	-1.32780100	3.66344500	-0.31989000
C	-1.54728200	4.94449300	0.29913000
C	-0.43517800	5.61992500	0.89442000
C	0.79894800	4.93755000	1.01250600
C	0.97223500	3.65084400	0.55073000
H	-5.76350400	1.09089600	-1.87202800
H	1.60860600	5.40930400	1.56092500
C	-4.22445100	-0.43957400	-0.32284500
C	-4.38438500	-1.48047000	-1.26302500
C	-4.40875100	-0.70149300	1.05486800
C	-4.73192900	-2.75855300	-0.80705100
C	-4.75704900	-1.99053200	1.45474200
C	-4.93154100	-3.03638000	0.54301500
H	-4.84683700	-3.55152900	-1.53678300

H	-4.90321300	-2.19332000	2.51237600
C	2.14341900	2.85785000	1.02592600
C	2.05576800	2.27061200	2.31182500
C	3.31306200	2.73116400	0.26114900
C	3.16961500	1.59296200	2.80410600
C	4.39952300	2.01438300	0.78657800
C	4.34909300	1.45192200	2.06422800
H	3.12592400	1.15345200	3.79646800
H	5.28420300	1.88071300	0.17925100
C	-4.53721700	2.82934800	-2.23704700
C	-3.86194900	5.23928200	-3.51046800
C	-5.09125900	4.60196400	-3.80521400
C	-5.41756000	3.42020800	-3.18264800
C	-2.99837500	4.70184200	-2.58346800
H	-3.59642500	6.15815200	-4.02429900
H	-5.76630400	5.04155800	-4.53315900
H	-6.34701200	2.90803400	-3.41597800
H	-2.05773000	5.19314800	-2.36517600
C	-1.85447600	7.50479300	1.47873400
C	-2.97045100	6.81127400	0.95577500
C	-2.82335500	5.56633400	0.38635200
C	-0.61462800	6.91149500	1.45661900
H	-1.98431000	8.48986400	1.91640400
H	-3.95708700	7.26140300	1.01016600
H	-3.69326700	5.04978400	0.00451900
H	0.24780000	7.41029200	1.89028600
C	-2.72919500	1.62633700	-0.46797100
C	-0.07909800	3.07318600	-0.21325100
O	0.15370800	1.86983800	-0.88125500
O	-1.83673200	1.00332900	0.40475600
P	-0.41005800	0.46809400	-0.23006100
O	0.48179000	0.04245400	0.92027100
O	-0.67336200	-0.53728600	-1.33547800
C	3.43148800	3.39562200	-1.10296300
C	3.59894300	2.36841400	-2.23279200
C	4.57376000	4.42521700	-1.11529600
H	2.49909300	3.93835100	-1.28727200
H	2.73229200	1.70158500	-2.26736200
H	3.67974900	2.87532100	-3.20115400
H	4.49943400	1.76507300	-2.08243700
H	4.43976300	5.17047300	-0.32478400
H	5.54306000	3.94075900	-0.95857300
H	4.61138600	4.94826200	-2.07705100
C	5.50379900	0.67447400	2.67863400

C	6.88082500	1.09057800	2.14890300
C	5.28411000	-0.84100900	2.50825100
H	5.48049600	0.88515600	3.75694500
H	7.04284900	2.16617600	2.27173900
H	7.67077800	0.56342600	2.69467000
H	6.98019300	0.84575800	1.08905300
H	4.31393500	-1.14567800	2.91382500
H	5.31226300	-1.10254600	1.44860200
H	6.06713300	-1.41054400	3.02178000
C	0.80407800	2.39060300	3.17600200
C	0.93910600	3.55873700	4.16999700
C	0.46216200	1.09381900	3.92629700
H	-0.04009600	2.60604200	2.51553500
H	1.09834000	4.51004900	3.65698100
H	0.03449300	3.65097600	4.78097900
H	1.78780100	3.39254200	4.84308100
H	0.40391400	0.25587700	3.23027800
H	1.20058600	0.86459500	4.70275000
H	-0.50629400	1.20274500	4.42557600
C	-4.30324400	0.38935600	2.11304800
C	-3.20810800	0.08113100	3.14612700
C	-5.66340700	0.62658300	2.79188600
H	-4.02762000	1.32260200	1.61855100
H	-2.24334800	-0.05805200	2.65450700
H	-3.11021600	0.90849100	3.85723000
H	-3.44708200	-0.82061600	3.72161100
H	-6.43105500	0.87938400	2.05386900
H	-6.00071200	-0.26462000	3.33188500
H	-5.59567000	1.44915300	3.51208500
C	-4.20148500	-1.28510200	-2.76538600
C	-5.50868300	-1.56883200	-3.52462800
C	-3.04059500	-2.12913500	-3.30859300
H	-3.93761200	-0.24313500	-2.94823200
H	-6.33045600	-0.94940600	-3.15043600
H	-5.38365200	-1.36165600	-4.59281900
H	-5.81314200	-2.61584200	-3.42168000
H	-2.09981700	-1.79731400	-2.86871400
H	-3.17444500	-3.19423700	-3.09327800
H	-2.96175500	-2.01560000	-4.39551400
C	-5.36579200	-4.40350300	1.04939600
C	-5.16262500	-5.53348100	0.03438300
C	-6.83438000	-4.35734400	1.51249400
H	-4.74951000	-4.62890200	1.92871500
H	-4.14679500	-5.53624600	-0.36878100

H	-5.34618400	-6.50307900	0.50761500
H	-5.85899300	-5.44167200	-0.80664400
H	-6.98788200	-3.58964000	2.27633900
H	-7.49362200	-4.12452000	0.66908000
H	-7.14228900	-5.32234300	1.93006400
Ag	2.48683400	-0.40744500	-0.00107700
C	3.93095200	-1.13101500	-1.46568400
C	5.38431300	-1.08243200	-1.16752400
C	7.38221500	-2.60427100	-1.19770800
O	6.04150900	-0.07562900	-0.89753400
N	5.93179000	-2.35636800	-1.24408000
C	5.10751300	-3.23597400	-2.04576400
H	5.12682900	-4.26103800	-1.66241800
H	5.46038200	-3.27609700	-3.08790200
C	3.67430400	-2.62061000	-1.98745600
C	3.06821300	-2.47225800	-3.33055500
C	2.79360000	-3.31453900	-0.99458000
C	1.77284000	-2.73383900	-3.60199800
C	1.49488800	-3.59890700	-1.28855200
C	0.94449100	-3.29155000	-2.57062900
H	1.31804200	-2.53908000	-4.56592000
H	0.85401900	-4.06418900	-0.55164900
H	7.48542300	-3.68971800	-1.32179900
C	8.11292900	-1.90952600	-2.35481900
H	9.17365200	-2.17889800	-2.35292000
H	7.69302100	-2.20539400	-3.32230900
H	8.02235600	-0.82649900	-2.25214700
C	7.96715300	-2.23294900	0.16672800
H	7.90393900	-1.15769800	0.33168000
H	7.42277000	-2.73830800	0.96920500
H	9.01764600	-2.53670400	0.21425400
O	-0.28845200	-3.52793700	-2.86887300
H	-0.85712800	-3.82904800	-2.04600800
H	3.70378000	-0.40419600	-2.24629700
C	-2.37609200	-4.16286800	3.85486600
C	-2.07799400	-3.52347300	2.65510000
C	-1.93566800	-4.27853800	1.48321800
C	-2.06636600	-5.67174100	1.52276200
C	-2.36259200	-6.30717700	2.72576500
C	-2.52343700	-5.55263000	3.89059800
H	-2.49506400	-3.57827100	4.76169700
H	-1.96908800	-2.44835000	2.60736700
H	-1.94224600	-6.23567300	0.60573000
H	-2.47149100	-7.38667400	2.75617700

H	-2.76007000	-6.04796100	4.82761400
C	-1.63973800	-3.61392600	0.19196500
O	-1.54126700	-4.28498100	-0.85811900
O	-1.45635400	-2.33216800	0.28198300
H	-1.18781100	-1.77879500	-0.54172000
C	3.36979400	-3.68629200	0.33753000
H	3.95532200	-4.61015900	0.24512400
H	4.04428700	-2.91080700	0.70411000
H	2.58208500	-3.85837900	1.07335500
H	3.71068700	-2.04716000	-4.09710300

TSI

Zero-point correction=	1.333735 (Hartree/Particle)
Thermal correction to Energy=	1.400010
Thermal correction to Enthalpy=	1.400875
Thermal correction to Gibbs Free Energy=	1.239823
Sum of electronic and zero-point Energies=	-3858.734648
Sum of electronic and thermal Energies=	-3858.668372
Sum of electronic and thermal Enthalpies=	-3858.667507
Sum of electronic and thermal Free Energies=	-3858.828559

C	-2.59463800	2.80545000	-0.93583600
C	-3.48235700	3.33263800	-1.93000900
C	-4.90263800	1.35720700	-1.62820600
C	-3.97776200	0.76709700	-0.78859900
C	-1.49933600	3.61595200	-0.35207100
C	-1.76592200	4.89975400	0.24246400
C	-0.67835400	5.62834800	0.82067100
C	0.58166000	4.99666500	0.94971300
C	0.80385900	3.70874500	0.51281200
H	-5.81486500	0.81773100	-1.86273000
H	1.37262100	5.50901200	1.48870600
C	-4.19995300	-0.61927000	-0.29041400
C	-4.30318100	-1.67889700	-1.21786800
C	-4.36089700	-0.87456900	1.09152200
C	-4.56877200	-2.96973500	-0.74407300
C	-4.62213000	-2.17814000	1.50886100
C	-4.73565100	-3.24370700	0.61079600
H	-4.64033000	-3.77738400	-1.46292300
H	-4.74503500	-2.37808100	2.56981900
C	1.99803500	2.96090300	1.00459400
C	1.92251600	2.39072900	2.29893300
C	3.17198300	2.85264300	0.24361300

C	3.05180700	1.74779800	2.80247500
C	4.27416600	2.16925900	0.78039300
C	4.23515100	1.62360600	2.06609600
H	3.01713000	1.32117500	3.80067300
H	5.16314200	2.04760300	0.17672900
C	-4.67101400	2.60653300	-2.25013500
C	-4.10507800	5.02273500	-3.56476000
C	-5.30377400	4.32504400	-3.84833700
C	-5.57650400	3.14042400	-3.20587900
C	-3.21867300	4.54147200	-2.62848900
H	-3.88116600	5.94352200	-4.09461200
H	-5.99743500	4.72078700	-4.58382400
H	-6.48105400	2.58224300	-3.43096800
H	-2.30161700	5.07903100	-2.41922800
C	-2.16799000	7.46788400	1.37310300
C	-3.25798500	6.72228500	0.86732300
C	-3.06475500	5.47315400	0.32146500
C	-0.90616600	6.92275000	1.35843600
H	-2.33455300	8.45545500	1.79216900
H	-4.26089800	7.13536600	0.91632700
H	-3.91485600	4.91624100	-0.04802600
H	-0.06274400	7.46281700	1.77966300
C	-2.81818300	1.51989100	-0.45998200
C	-0.22758000	3.08148800	-0.23710700
O	0.05052700	1.86758500	-0.88052200
O	-1.89856200	0.95007600	0.43000200
P	-0.45344300	0.48090700	-0.18207400
O	0.45756000	0.06783500	0.94691600
O	-0.67875500	-0.54398200	-1.30928900
C	3.27899600	3.50540300	-1.12697500
C	3.50156700	2.47454300	-2.24356200
C	4.37974900	4.57951200	-1.13620500
H	2.32813900	4.00899900	-1.32819300
H	2.66310300	1.77287500	-2.28271100
H	3.57554000	2.97451400	-3.21598700
H	4.42238700	1.90778000	-2.07557000
H	4.20564900	5.32755700	-0.35621000
H	5.36469600	4.13488600	-0.96033800
H	4.41029400	5.09287200	-2.10338500
C	5.40680500	0.88165800	2.69219300
C	6.77582700	1.33752900	2.17395500
C	5.23430100	-0.63999700	2.52197800
H	5.36706000	1.09356100	3.76973500
H	6.90294700	2.41849700	2.29101700

H	7.57547600	0.83917000	2.73249200
H	6.89467300	1.08760000	1.11737200
H	4.27022700	-0.97369700	2.91950900
H	5.28117800	-0.90099000	1.46290900
H	6.02942900	-1.18478100	3.04354900
C	0.66696200	2.49163000	3.16023700
C	0.76693000	3.68309500	4.13050700
C	0.36254500	1.20166500	3.93812100
H	-0.18341800	2.66990000	2.49616800
H	0.89883300	4.62828900	3.59884600
H	-0.14022300	3.76092600	4.73963600
H	1.61984700	3.55491100	4.80640000
H	0.33599000	0.34470700	3.26360800
H	1.10401300	1.01432600	4.72261000
H	-0.61124800	1.29050300	4.43059700
C	-4.33588000	0.23537700	2.13524800
C	-3.24262500	0.01176500	3.19148200
C	-5.71990100	0.39577300	2.78862400
H	-4.11179600	1.17785700	1.63169300
H	-2.25962300	-0.05511200	2.72173600
H	-3.22273100	0.84532800	3.90191700
H	-3.42207800	-0.90527200	3.76363300
H	-6.48929200	0.58801200	2.03434500
H	-6.00833300	-0.50786300	3.33601400
H	-5.71714000	1.23117400	3.49719500
C	-4.15392300	-1.49081600	-2.72501900
C	-5.47158300	-1.81371500	-3.45098800
C	-2.98969100	-2.31274900	-3.29445700
H	-3.92001600	-0.44387500	-2.92179900
H	-6.30057100	-1.21279900	-3.06298200
H	-5.37771600	-1.61449600	-4.52391200
H	-5.74526900	-2.86713200	-3.32927200
H	-2.04231600	-1.96653300	-2.88221700
H	-3.09250700	-3.37959000	-3.07348600
H	-2.94154300	-2.20054400	-4.38322600
C	-5.06883900	-4.63057500	1.13870300
C	-4.80373500	-5.75649000	0.13354600
C	-6.52990000	-4.67834500	1.62492100
H	-4.42447000	-4.80152600	2.00998300
H	-3.79618900	-5.69517100	-0.28506200
H	-4.91448800	-6.73008200	0.62110500
H	-5.51774900	-5.72313200	-0.69718400
H	-6.72423600	-3.91346000	2.38238600
H	-7.21669900	-4.50223400	0.78969800

H	-6.76438600	-5.65670600	2.05866800
Ag	2.48576300	-0.34263900	-0.00099200
C	3.94381700	-1.01077000	-1.47447900
C	5.39238900	-0.91118300	-1.15960500
C	7.44710000	-2.35389600	-1.20586100
O	6.00737300	0.11130500	-0.84946700
N	5.99057500	-2.15786700	-1.27679300
C	5.20927600	-3.03291600	-2.12580600
H	5.28754500	-4.07665800	-1.80573300
H	5.55348600	-2.98985600	-3.17079800
C	3.74744200	-2.49605400	-2.01878700
C	3.10590300	-2.36078100	-3.34963100
C	2.93435000	-3.28023600	-1.02990400
C	1.82843800	-2.70327400	-3.60654100
C	1.65833600	-3.65017800	-1.31171200
C	1.04850100	-3.33683500	-2.57449500
H	1.34584800	-2.51837200	-4.55911200
H	1.06750400	-4.18611900	-0.58068300
H	7.59397500	-3.42997000	-1.36323200
C	8.17757400	-1.59381000	-2.32128400
H	9.24769600	-1.82239500	-2.30155800
H	7.79233000	-1.87337300	-3.30777000
H	8.04230300	-0.51906200	-2.18593900
C	7.98540500	-2.00713500	0.18439500
H	7.87843100	-0.94077900	0.38210600
H	7.44033800	-2.55823100	0.95590900
H	9.04487400	-2.27430400	0.24924200
O	-0.17167800	-3.62137300	-2.83573900
H	-0.74950200	-3.98178000	-1.95007200
H	3.70401300	-0.28253500	-2.25055400
C	-2.00486200	-3.97081700	3.84489700
C	-1.76888300	-3.41381600	2.59145200
C	-1.63111900	-4.24668800	1.47382500
C	-1.70229900	-5.63661400	1.62146700
C	-1.93479500	-6.19124800	2.87820900
C	-2.09275600	-5.35878400	3.98892900
H	-2.12062500	-3.32404400	4.70915100
H	-1.70305300	-2.34256500	2.45602200
H	-1.58232600	-6.26346400	0.74576200
H	-1.99634800	-7.26909000	2.99200500
H	-2.27986000	-5.79129800	4.96744300
C	-1.39581400	-3.64975800	0.13143400
O	-1.33211100	-4.42807700	-0.86910300
O	-1.23023900	-2.38903200	0.10574800

H	-0.96803500	-1.60882400	-0.74378600
C	3.55041800	-3.62294600	0.29208100
H	4.33044400	-4.38363900	0.16939200
H	4.02891100	-2.74472700	0.73188100
H	2.80115300	-4.00742400	0.98649100
H	3.70548200	-1.87742500	-4.11670600

CPL

Zero-point correction=	1.340776 (Hartree/Particle)
Thermal correction to Energy=	1.407437
Thermal correction to Enthalpy=	1.408302
Thermal correction to Gibbs Free Energy=	1.246122
Sum of electronic and zero-point Energies=	-3858.742627
Sum of electronic and thermal Energies=	-3858.675965
Sum of electronic and thermal Enthalpies=	-3858.675100
Sum of electronic and thermal Free Energies=	-3858.837280

C	-3.06281900	2.29178400	-1.13482800
C	-3.97965000	2.58864600	-2.19643300
C	-4.91678100	0.32923900	-1.94992700
C	-3.95874400	-0.01376400	-1.01795200
C	-2.18740100	3.32500200	-0.52455300
C	-2.72278200	4.53603200	0.03814700
C	-1.82186900	5.46350600	0.65585800
C	-0.46411100	5.10064400	0.83968300
C	0.02815700	3.88558400	0.41575800
H	-5.66555400	-0.40407200	-2.22830700
H	0.18419000	5.76240300	1.40524500
C	-3.91405100	-1.37652300	-0.41122800
C	-3.62491300	-2.50272600	-1.21184100
C	-4.20720400	-1.54040500	0.96313600
C	-3.66582200	-3.77466400	-0.62645300
C	-4.21040300	-2.82638000	1.50028600
C	-3.96260900	-3.96148600	0.72229000
H	-3.45313200	-4.63628300	-1.24764700
H	-4.42939200	-2.95699200	2.55681200
C	1.32095600	3.34549100	0.92968700
C	1.34104700	2.85808800	2.25821600
C	2.47288000	3.27837800	0.12854300
C	2.54875500	2.38558900	2.77160000
C	3.65248100	2.75084800	0.67249800
C	3.71559500	2.32872300	2.00462300
H	2.58694700	2.03712700	3.80007800

H	4.52918900	2.65987700	0.04448000
C	-4.93135900	1.59445400	-2.58634600
C	-4.86266600	4.07215200	-3.90917500
C	-5.83200800	3.10440800	-4.26518900
C	-5.86089200	1.89124600	-3.61854100
C	-3.96069700	3.82245100	-2.90004300
H	-4.82696400	5.01791300	-4.44093700
H	-6.54157200	3.31804400	-5.05850900
H	-6.58538500	1.13129000	-3.89729900
H	-3.21794500	4.56591300	-2.63713800
C	-3.66922100	6.97376900	1.12421300
C	-4.56851400	6.03210500	0.57273600
C	-4.10994400	4.84466400	0.04791900
C	-2.32553200	6.68681200	1.17212600
H	-4.04451900	7.90942200	1.52691100
H	-5.63334100	6.24376900	0.56880800
H	-4.81464700	4.13274900	-0.36041000
H	-1.62559400	7.38282900	1.62581200
C	-3.03528400	0.99573600	-0.64189600
C	-0.84035400	3.07066300	-0.35312500
O	-0.29454000	1.92131300	-0.94920700
O	-2.06166400	0.64340400	0.31470900
P	-0.54462900	0.50201600	-0.23367000
O	0.38956200	0.17765700	0.89099200
O	-0.53348100	-0.48237600	-1.46365900
C	2.47497600	3.81228300	-1.29629600
C	2.85686600	2.73296900	-2.32080600
C	3.39985800	5.03654400	-1.41148500
H	1.45899000	4.14734100	-1.52929400
H	2.14610900	1.90256100	-2.28414400
H	2.84312600	3.14979600	-3.33422000
H	3.85736700	2.33686700	-2.12404800
H	3.11099100	5.81656700	-0.69977200
H	4.43903000	4.76099900	-1.20446900
H	3.35747000	5.45963300	-2.42096800
C	4.99092400	1.79233600	2.63712900
C	6.26436200	2.45498800	2.09537400
C	5.07226900	0.26225100	2.48786500
H	4.92281800	2.01524400	3.71077000
H	6.21246400	3.54486900	2.18308300
H	7.13811600	2.10923500	2.65812800
H	6.41798300	2.19823500	1.04453300
H	4.17480700	-0.22266000	2.88625700
H	5.16985900	0.00317700	1.43193900

H	5.94380900	-0.13715100	3.01881500
C	0.09474700	2.83103300	3.13873900
C	0.09549300	4.00309500	4.13539700
C	-0.07596600	1.49358500	3.87973600
H	-0.77926200	2.94655100	2.49190800
H	0.13583700	4.96691000	3.62098200
H	-0.80749000	3.98598800	4.75533400
H	0.96454400	3.94258000	4.79971500
H	-0.01825600	0.65886100	3.17943600
H	0.69103600	1.35304100	4.64875700
H	-1.04951600	1.46923300	4.38142000
C	-4.60853100	-0.37000800	1.85441300
C	-3.67134400	-0.19870400	3.05885100
C	-6.07361100	-0.51526100	2.30324800
H	-4.54966100	0.54829700	1.26582800
H	-2.64460800	-0.03291600	2.72868200
H	-3.98172300	0.66207400	3.66142900
H	-3.68215100	-1.08195700	3.70485500
H	-6.74082000	-0.60402400	1.44024100
H	-6.21162300	-1.40642800	2.92440100
H	-6.38495500	0.35536600	2.89059000
C	-3.30846300	-2.39315900	-2.70054700
C	-4.51844800	-2.83157100	-3.54685500
C	-2.06927300	-3.20300200	-3.11219700
H	-3.09973700	-1.34382100	-2.92461600
H	-5.41474900	-2.24993200	-3.31459300
H	-4.30459300	-2.71594800	-4.61486600
H	-4.75380900	-3.88533400	-3.36216900
H	-1.19845700	-2.95884000	-2.50678500
H	-2.23378500	-4.28095500	-3.01871800
H	-1.82401500	-3.00346400	-4.16050000
C	-4.09133000	-5.33683000	1.35960200
C	-3.43791700	-6.46622200	0.55606900
C	-5.57639900	-5.65485300	1.62124900
H	-3.58706600	-5.28162900	2.33268000
H	-2.39736300	-6.24088600	0.31112900
H	-3.46570000	-7.39861900	1.12916100
H	-3.97496800	-6.64781400	-0.38177200
H	-6.04790700	-4.88506900	2.23908100
H	-6.12715400	-5.70675900	0.67557500
H	-5.68443000	-6.61819900	2.13159900
Ag	2.47702300	-0.12917000	-0.03838100
C	3.98910800	-0.66550000	-1.48488600
C	5.37677700	-0.21020100	-1.19441500

C	7.70695700	-1.14501000	-1.22031100
O	5.74207500	0.93814400	-0.92144500
N	6.24569400	-1.28293500	-1.29050800
C	5.66326400	-2.36514400	-2.06004800
H	6.01168800	-3.34077700	-1.70611500
H	5.93338700	-2.28931600	-3.12471300
C	4.12044500	-2.18914200	-1.87446300
C	3.40333600	-2.40381500	-3.16612400
C	3.62415400	-3.08560500	-0.76286700
C	2.32542600	-3.18980400	-3.31764800
C	2.54881800	-3.88434300	-0.93538300
C	1.80595700	-3.95226100	-2.18673300
H	1.79269900	-3.27873900	-4.25842700
H	2.18928600	-4.50333300	-0.12039300
H	8.09371700	-2.16423300	-1.34508400
C	8.24995900	-0.27455300	-2.36160900
H	9.34406200	-0.25067400	-2.33786300
H	7.94185900	-0.66772800	-3.33621500
H	7.87066900	0.74420800	-2.26075900
C	8.14747300	-0.64144600	0.15709800
H	7.79869600	0.37820900	0.32007100
H	7.73784000	-1.27756000	0.94716600
H	9.23966500	-0.65825000	0.22858000
O	0.76384400	-4.63416500	-2.30845500
H	0.03057100	-4.86311000	-0.97322700
H	3.60906500	-0.08482000	-2.32975900
C	-1.03478100	-2.38915900	3.97127700
C	-0.79294700	-2.44535900	2.60142800
C	-0.73082700	-3.68642100	1.95570800
C	-0.90034000	-4.86914000	2.68796000
C	-1.15586700	-4.80644100	4.05569700
C	-1.22495900	-3.56701400	4.69762200
H	-1.07829800	-1.42600800	4.46869300
H	-0.63665700	-1.54284000	2.02499300
H	-0.83480900	-5.82311700	2.17926700
H	-1.29582800	-5.72201600	4.62209100
H	-1.41971300	-3.52063000	5.76514000
C	-0.45378700	-3.71769700	0.49892900
O	-0.32585600	-4.92697500	-0.01499000
O	-0.30942200	-2.68827700	-0.16467500
H	-0.42976300	-1.41730300	-1.12242500
C	4.34527800	-3.05632100	0.55296500
H	5.38577900	-3.38111600	0.44718000
H	4.37429300	-2.03836200	0.94985100

H	3.85124400	-3.70234100	1.28187000
H	3.77771100	-1.82465100	-4.00769500

TSJ

Zero-point correction=	1.336869 (Hartree/Particle)
Thermal correction to Energy=	1.403145
Thermal correction to Enthalpy=	1.404010
Thermal correction to Gibbs Free Energy=	1.242286
Sum of electronic and zero-point Energies=	-3858.702534
Sum of electronic and thermal Energies=	-3858.636258
Sum of electronic and thermal Enthalpies=	-3858.635393
Sum of electronic and thermal Free Energies=	-3858.797118

C	-1.94761500	2.67281700	-1.35724600
C	-2.68127000	3.23052400	-2.45846400
C	-4.22703700	1.33514400	-2.31770500
C	-3.46799100	0.73265800	-1.33555100
C	-0.93295200	3.48279000	-0.63657100
C	-1.26425200	4.76715300	-0.08031800
C	-0.22994600	5.52812500	0.55430000
C	1.05601200	4.95573000	0.72211800
C	1.34116700	3.67314100	0.30666300
H	-5.16252700	0.86995300	-2.61217400
H	1.81489100	5.52128900	1.25411000
C	-3.98023700	-0.48947600	-0.64838000
C	-4.12681000	-1.70450900	-1.35285900
C	-4.41110100	-0.38104600	0.69524600
C	-4.69841600	-2.79595900	-0.68854400
C	-4.97109200	-1.50229400	1.30715300
C	-5.13134500	-2.71447000	0.63358100
H	-4.79510600	-3.73577900	-1.21263800
H	-5.29542100	-1.43926800	2.33999600
C	2.59290600	2.97271300	0.71000400
C	2.77326500	2.63058000	2.07344600
C	3.54416200	2.57400500	-0.25057500
C	3.90725600	1.90193300	2.43916100
C	4.65672300	1.81715900	0.15993600
C	4.85495500	1.46241500	1.50416100
H	4.04924400	1.63998500	3.48348200
H	5.37505600	1.50257600	-0.58563200
C	-3.83309600	2.54019300	-2.94707400
C	-3.01654200	4.93790500	-4.15901900
C	-4.17476100	4.26928900	-4.62090400

C	-4.57102400	3.09419100	-4.02616400
C	-2.29090100	4.43481700	-3.10280600
H	-2.69440300	5.85358900	-4.64535400
H	-4.74156200	4.68109200	-5.45024900
H	-5.45074500	2.56297900	-4.37862800
H	-1.40123500	4.94993400	-2.76104300
C	-1.80531300	7.32420100	1.00554600
C	-2.84012500	6.55110700	0.42968200
C	-2.57854600	5.30688200	-0.09867800
C	-0.52932500	6.81619500	1.07189900
H	-2.02531600	8.30715600	1.41043900
H	-3.85370000	6.93955800	0.40941600
H	-3.38378800	4.72422100	-0.52646100
H	0.27002600	7.38428700	1.53967700
C	-2.26835000	1.38860500	-0.93773800
C	0.33178500	2.97882000	-0.41474700
O	0.64096300	1.73809800	-0.95855800
O	-1.47382200	0.73349300	0.01322300
P	0.08924500	0.38294600	-0.22104500
O	0.78037900	0.15639700	1.09513200
O	0.30947600	-0.68865800	-1.31929900
C	3.42805700	2.96511700	-1.71747100
C	3.41931000	1.74420500	-2.65262900
C	4.55156200	3.94812800	-2.09417700
H	2.47894600	3.49072700	-1.85054600
H	2.56294800	1.10229900	-2.43658000
H	3.34480500	2.07102800	-3.69539400
H	4.32733400	1.14339400	-2.54760600
H	4.53933400	4.82930400	-1.44503900
H	5.53594800	3.47662000	-2.00262500
H	4.43568900	4.28340200	-3.13002000
C	6.02649100	0.60760200	1.97258900
C	7.13362800	0.44314800	0.92594300
C	5.52690100	-0.77339300	2.44415400
H	6.45490300	1.11534900	2.84808000
H	7.51756400	1.41185800	0.59087900
H	7.96967100	-0.11996000	1.35223800
H	6.76659400	-0.10572300	0.05380900
H	4.75744800	-0.68365000	3.21618000
H	5.10420300	-1.32760100	1.59705800
H	6.35083000	-1.36966200	2.85050500
C	1.76104600	2.98689500	3.15551500
C	2.30045000	4.10688100	4.06166000
C	1.33888400	1.75960100	3.98000800

H	0.86075100	3.36159500	2.66550100
H	2.54925900	5.00369900	3.48590500
H	1.55773000	4.38217200	4.81775500
H	3.20886500	3.78539100	4.58315700
H	0.97448700	0.96914000	3.32148700
H	2.16552100	1.36238100	4.57902100
H	0.53988400	2.04036100	4.67481800
C	-4.36096400	0.94829800	1.44726500
C	-4.38120500	0.80240900	2.97433000
C	-5.51436400	1.86694500	0.99806200
H	-3.42140800	1.44694600	1.19747200
H	-3.61831300	0.10582500	3.32433600
H	-4.19280100	1.77631600	3.43795600
H	-5.35561300	0.45675000	3.33640900
H	-5.48862300	2.05625100	-0.07737600
H	-6.47938700	1.40651500	1.23702800
H	-5.46030000	2.83134800	1.51566100
C	-3.67221000	-1.84346900	-2.80858400
C	-4.03207100	-3.19483500	-3.44101200
C	-2.16118400	-1.59713500	-2.94552600
H	-4.18859700	-1.07013300	-3.39187400
H	-5.10517000	-3.40455400	-3.38696700
H	-3.74820700	-3.18666600	-4.49850400
H	-3.49136300	-4.01202500	-2.95326200
H	-1.89731700	-0.55274500	-2.78690800
H	-1.61211900	-2.17825300	-2.20796500
H	-1.81635200	-1.87401500	-3.94798000
C	-5.81912300	-3.86650600	1.35015900
C	-5.52270900	-5.24954600	0.76169400
C	-7.33904700	-3.61625900	1.39760100
H	-5.45135400	-3.85804200	2.38505800
H	-4.44880300	-5.43955100	0.71487600
H	-5.98329600	-6.02669700	1.38046800
H	-5.93605300	-5.35252000	-0.24756900
H	-7.56949400	-2.65304200	1.86235000
H	-7.75330400	-3.60416500	0.38327300
H	-7.84901200	-4.40323900	1.96445100
Ag	2.98812800	-0.32719100	0.31300300
C	2.62583700	-2.06534600	-1.70289800
C	4.09739500	-2.14946800	-1.45781100
C	5.95293200	-3.84341100	-1.53155500
O	4.84949900	-1.19890900	-1.13649000
N	4.54421200	-3.42733500	-1.60567800
C	3.51166700	-4.32066600	-2.10248500

H	3.56410900	-5.29605800	-1.60723300
H	3.62126500	-4.48832800	-3.18329100
C	2.17280900	-3.57103100	-1.78455100
C	1.20445000	-3.78593000	-2.90279100
C	1.63928400	-4.02901600	-0.44079800
C	-0.04668300	-4.24267000	-2.74893200
C	0.38260700	-4.49202300	-0.30690700
C	-0.56491300	-4.55433500	-1.41522400
H	-0.73331600	-4.34636000	-3.58150300
H	0.00688700	-4.79372200	0.66430700
H	5.93807900	-4.92414000	-1.71327000
C	6.78418900	-3.17618800	-2.63345600
H	7.81317000	-3.54835700	-2.61293800
H	6.36278900	-3.38858400	-3.62093100
H	6.79659400	-2.09434200	-2.48557000
C	6.53689600	-3.60324100	-0.13548900
H	6.57753700	-2.53572300	0.08062600
H	5.92816100	-4.09096700	0.63168600
H	7.55056500	-4.01214400	-0.08025500
O	-1.76334600	-4.84467200	-1.24079100
H	-2.23606600	-4.40142300	0.31599900
H	2.50013000	-1.57076800	-2.67605300
C	-1.41173000	-0.83664200	4.57125900
C	-1.31655500	-1.29676700	3.25906200
C	-2.02576800	-2.44007900	2.87145200
C	-2.82934300	-3.11591500	3.79776900
C	-2.93761100	-2.63878800	5.10242000
C	-2.22626200	-1.50096000	5.49143600
H	-0.85885200	0.04724400	4.87184600
H	-0.70047000	-0.78805800	2.52653400
H	-3.36271600	-4.00544800	3.48447500
H	-3.57149600	-3.15537700	5.81702900
H	-2.30741500	-1.13297000	6.51026700
C	-1.89279400	-2.90984500	1.46487900
O	-2.36352800	-4.15036400	1.27500400
O	-1.36786600	-2.24982500	0.58298400
H	1.26841600	-1.20734200	-1.26855600
C	2.52614300	-3.91332400	0.76514200
H	2.02358100	-4.29738500	1.65485300
H	3.47484700	-4.44349700	0.63731200
H	2.77361100	-2.85963700	0.94946100
H	1.56802400	-3.51661200	-3.89257700

(*S*)-2a

Zero-point correction=	0.280073 (Hartree/Particle)
Thermal correction to Energy=	0.292790
Thermal correction to Enthalpy=	0.293655
Thermal correction to Gibbs Free Energy=	0.243529
Sum of electronic and zero-point Energies=	-710.536580
Sum of electronic and thermal Energies=	-710.523863
Sum of electronic and thermal Enthalpies=	-710.522998
Sum of electronic and thermal Free Energies=	-710.573124

C	-0.06561700	-0.61353600	1.44513900
C	-1.50237900	-0.23330700	1.09890200
C	-2.87906300	-0.02474300	-0.98249600
O	-2.40097500	-0.02050000	1.90069600
N	-1.60686800	-0.20108900	-0.26388400
C	-0.38515000	-0.57396800	-0.95330700
H	-0.19756500	0.07960800	-1.81134400
H	-0.43584300	-1.60578600	-1.32848800
C	0.74381100	-0.43428800	0.12557300
C	1.74933300	-1.53727100	-0.03610000
C	1.35935200	0.95482400	0.06748900
C	3.06298100	-1.34771500	-0.20102100
C	2.68416500	1.12237300	-0.09901200
C	3.63933800	0.01127600	-0.24786200
H	3.75810200	-2.17463100	-0.30555800
H	3.11882400	2.11734300	-0.13300900
H	-2.61525200	-0.05902400	-2.04570500
C	-3.84268800	-1.17767600	-0.68009200
H	-4.75826800	-1.07083700	-1.26945900
H	-3.38691300	-2.14140400	-0.92782500
H	-4.10492000	-1.17668100	0.37979000
C	-3.49432000	1.34528100	-0.67983100
H	-3.73388100	1.42282200	0.38170400
H	-2.80067700	2.14978700	-0.94176100
H	-4.41085800	1.48033800	-1.26196300
O	4.84254700	0.20178100	-0.40324300
H	0.31634200	-0.01628300	2.27416700
H	-0.06260800	-1.66032500	1.76825700
H	1.34087700	-2.54610800	-0.00346200
C	0.44501800	2.14207800	0.20471000
H	-0.30180300	2.16746500	-0.59580600
H	-0.11540400	2.11962700	1.14564400
H	1.01666200	3.07149400	0.16983700