Supplementary Information (SI) for Organic Chemistry Frontiers.

Supporting Information

NCI-driven Regioselectivity and Enantioreversal in Chiral Phosphoric Acid-Catalyzed Arylamine Functionalization

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Content

1. Computational Method Screening

In the preliminary calculations, we selected the Gibbs free energy barrier difference between TS-A_2' and TS-A_2 in reaction (2) (***ΔΔG‡***), the energy barrier of TS-A_2 in reaction (2) (***ΔG‡ (TS-A₂)***), as well as the energy barrier of TS-C_1 in reaction (1) (***Highest ΔG‡***) as evaluation metrics to screen for suitable computational methods. Considering that the different reaction conditions in these experiments need to be compared with each other, along with enantioselectivity, the cost of computational time and resources, and the errors encountered with some other methods, we ultimately chose M06-2X-D3/6-311+G(d,p), SMD // M06-2X/6-31G(d,p), vacuum.

Table S1. Comparison of DFT methods for calculations. All energies are in kcal/mol.

Geometry Optimizations	***Single-point Calculations***	***ΔΔG‡***	***ΔG‡ (TS-A₂)***	***Highest ΔG‡***
M06-2X/6-31G(d,p), vac.	M06-2X/6-311+G(d,p), SMD	1.1	10.0	23.3
M06-2X/6-31G(d,p), vac.	**M06-2X-D3/6-311+G(d,p), SMD**	**1.1**	**1.6**	**18.2**
M06-2X/6-31G(d,p), vac.	M06-2X/6-311+G(d,p), PCM	2.5		
M06-2X/6-31G(d,p), vac.	M06-2X/Def2-TZVP, SMD	1.6	18.4	
M06-2X/6-31G(d,p), vac.	M06-2X-D3/Def2-TZVP, SMD	1.6	10.0	24.6
M06-2X-D3/6-31G(d,p), vac.	M06-2X-D3/6-311+G(d,p), SMD	-0.1		
M06-2X/6-31G(d,p), vac.	wB97-XD/6-311+G(d,p), SMD	4.1		
M06-2X/6-31G(d,p), vac.	wB97-XD/Def2-TZVP, SMD	4.7		

2. Additional Computational Results

We referenced Goodman's transition state models for this type of reaction, combined with CREST conformational search and manual placement, to select the lowest energy pair of key transition states. The structure names and the numbering from 1 to 4 refer to Table 2 in the main text.

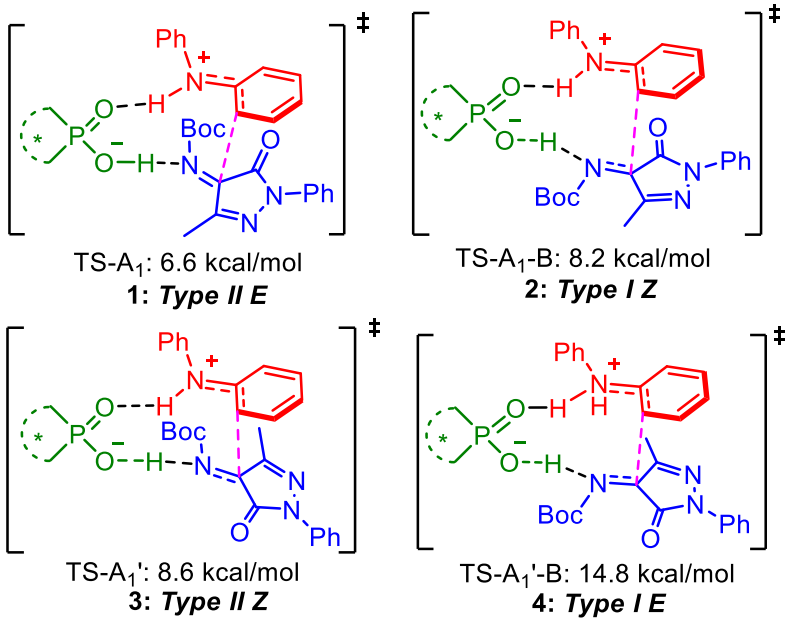

Figure S1. Conformers of the key transition states in reaction (1). All energies are in kcal/mol.

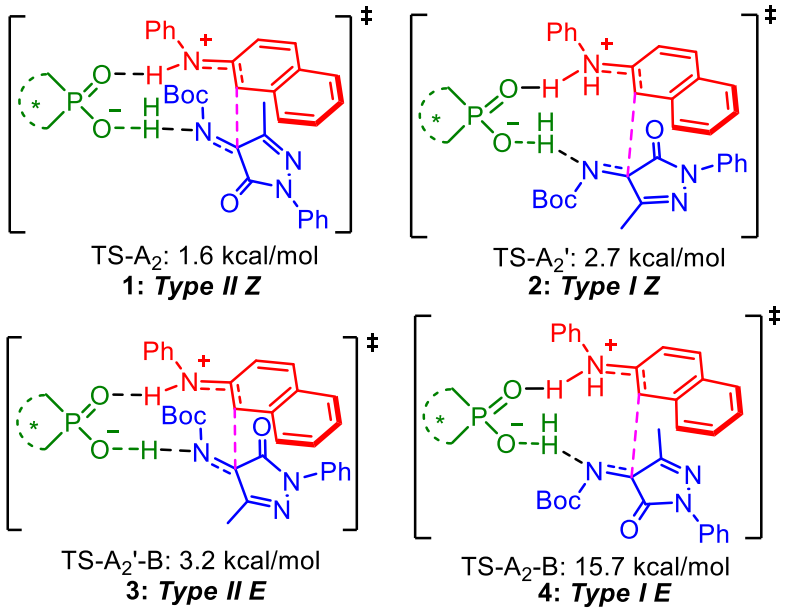

Figure S2. Conformers of the key transition states in reaction (2). All energies are in kcal/mol.

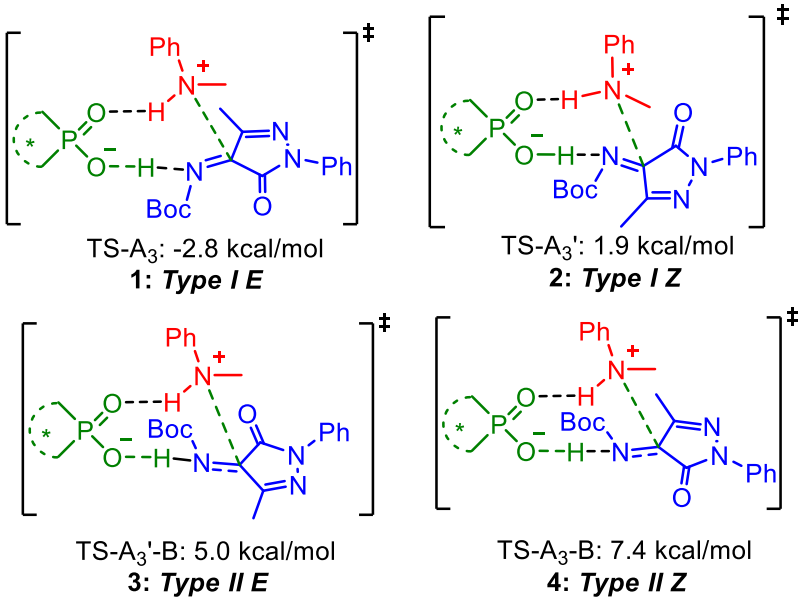

Figure S3. Conformers of the key transition states in reaction (3). All energies are in kcal/mol.

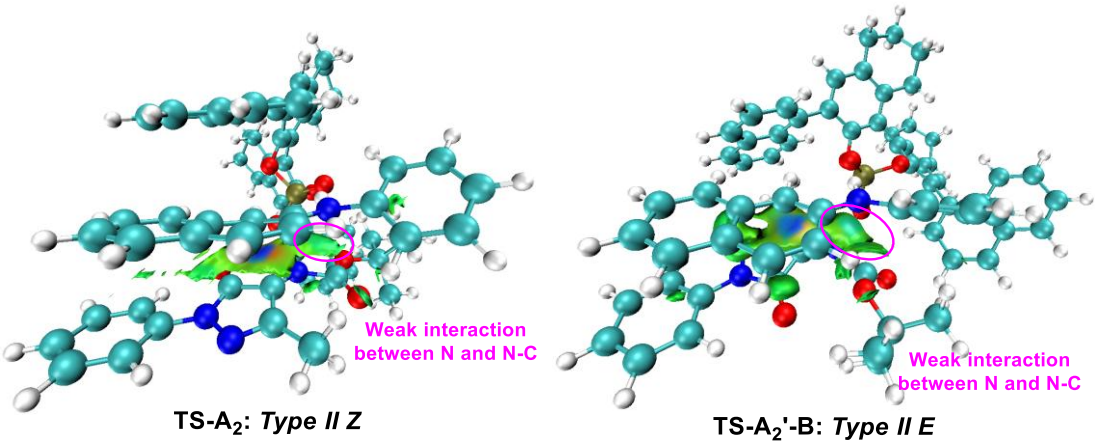

Figure S4. The independent gradient model based on Hirshfeld partition (IGMH) analysis between two substrates (Sub0 and Sub2) of reaction (2) in **TS-A₂** and **TS-A₂'-B**. The *sign*(λ_2)ρ colored isosurfaces were plotted with 0.01 isovalue by VMD.

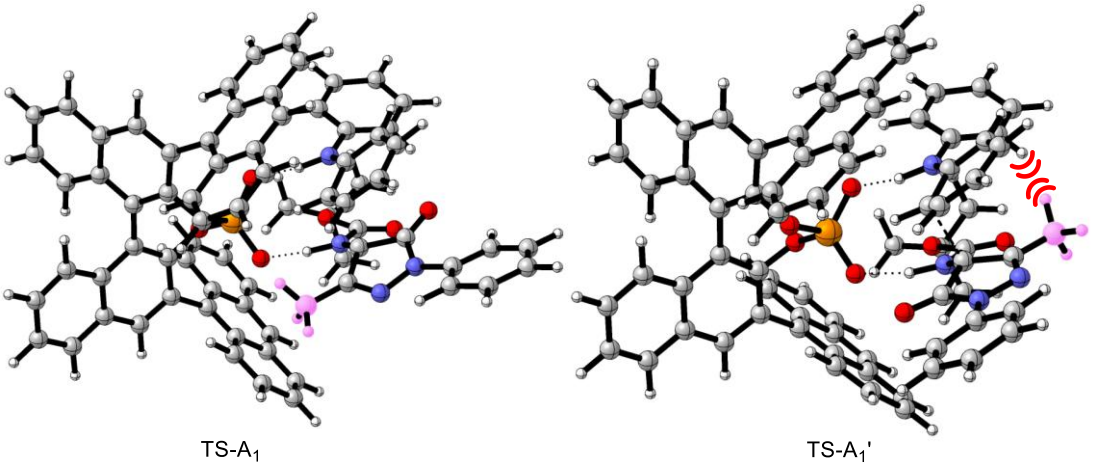

Figure S5. 3D structures of TS-A_1 and TS-A_1' in reaction (1).

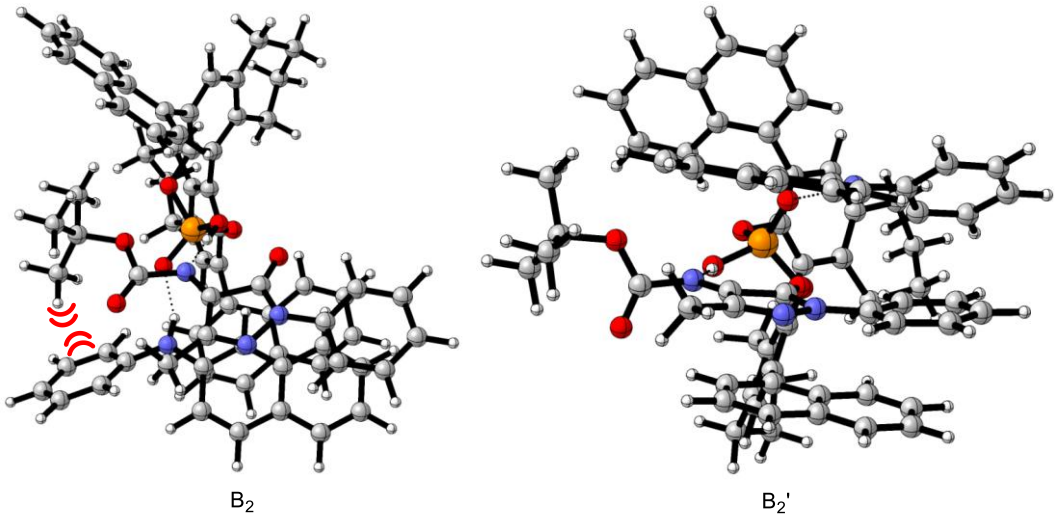

Figure S6. 3D structures of B_2 and B_2' in reaction (2).

3. Cartesian coordinates of the calculated species.

Reaction (1):

Sub0

Zero-point correction=	0.307402 (Hartree/Particle)
Thermal correction to Energy=	0.327397
Thermal correction to Enthalpy=	0.328342
Thermal correction to Gibbs Free Energy=	0.257498
Sum of electronic and zero-point Energies=	-971.061611
Sum of electronic and thermal Energies=	-971.041615
Sum of electronic and thermal Enthalpies=	-971.040671
Sum of electronic and thermal Free Energies=	-971.111515

SCF Done: E(RM062X) = -971.639262761

C	-0.75712800	2.49273100	0.17103900
C	-0.42562700	0.19470600	-0.25747100
C	0.30712200	1.51995900	-0.13383700
O	0.06874600	-0.88458400	-0.50100000
N	-1.89723300	1.90346100	0.22742000
N	-1.73685400	0.53500300	-0.02351100
C	-2.88237800	-0.29904700	0.00003800
C	-2.77156200	-1.65911400	-0.30400900
C	-4.12131500	0.25583600	0.32987300
C	-3.91342100	-2.45293000	-0.27127900
H	-1.81076200	-2.08311300	-0.56010300
C	-5.24781000	-0.55731400	0.35448600
H	-4.18972000	1.31064800	0.56027200
C	-5.15329300	-1.91352500	0.05590900
H	-3.82453600	-3.50815400	-0.50801900
H	-6.20772300	-0.12099200	0.61080700
H	-6.03657500	-2.54255800	0.07728500
C	-0.56477900	3.95083400	0.38480300
H	0.11998800	4.12044600	1.21999000
H	-0.11364900	4.40298800	-0.50246900
H	-1.52284400	4.42687800	0.59278200
N	1.54272700	1.74904100	-0.25178300
C	2.41144800	0.66947200	-0.60101900
O	2.75166200	0.47901900	-1.73693200
O	2.81980600	0.06486200	0.50409400

C	3.74257900	-1.07189600	0.41550100
C	3.91145800	-1.47590300	1.87417700
H	4.32611400	-0.64791900	2.45468300
H	2.94693900	-1.75730000	2.30364900
H	4.59031300	-2.32942300	1.94481000
C	5.06952300	-0.61198300	-0.17868600
H	5.79268300	-1.42969700	-0.11205400
H	4.95565400	-0.32650300	-1.22439200
H	5.46031300	0.23846700	0.38707900
C	3.09671300	-2.19426100	-0.38887700
H	2.97652800	-1.91104500	-1.43480800
H	3.73224700	-3.08264000	-0.33112400
H	2.11365700	-2.43238500	0.02354700

Sub0 (Z-imine)

Zero-point correction=	0.307580 (Hartree/Particle)
Thermal correction to Energy=	0.327437
Thermal correction to Enthalpy=	0.328381
Thermal correction to Gibbs Free Energy=	0.257485
Sum of electronic and zero-point Energies=	-971.056764
Sum of electronic and thermal Energies=	-971.036907
Sum of electronic and thermal Enthalpies=	-971.035963
Sum of electronic and thermal Free Energies=	-971.106859

SCF Done: E(RM062X) = -971.635788615

C	0.10421600	1.02864800	-0.28303600
C	1.20193900	-1.06558900	-0.17218500
C	-0.17098100	-0.42483900	-0.31717800
O	1.46634600	-2.24202200	-0.14648300
N	1.36601100	1.23240100	-0.14561600
N	2.05018400	0.02435700	-0.08062900
C	3.45931800	0.04593900	0.07007400
C	4.18058200	-1.14931200	0.14698100
C	4.11793200	1.27632600	0.14042900
C	5.56282200	-1.09535300	0.29495800
H	3.66763700	-2.09895100	0.09132000
C	5.49917100	1.30425200	0.28844700
H	3.54623400	2.19274500	0.07854300
C	6.23076100	0.12268300	0.36682200
H	6.11906600	-2.02519500	0.35419300
H	6.00442600	2.26313200	0.34234300
H	7.30882300	0.15149800	0.48215400
C	-0.88946000	2.13474000	-0.37055500

H	-1.39909900	2.11786000	-1.33764300
H	-1.65240200	2.01616300	0.40565300
H	-0.38174600	3.08979500	-0.23442100
N	-1.22839600	-1.10675700	-0.42605900
C	-2.46824300	-0.45797800	-0.63519800
O	-2.81970000	-0.06283300	-1.71853300
O	-3.15811400	-0.44946900	0.49882900
C	-4.56065000	-0.01901700	0.50575500
C	-4.96945600	-0.24146900	1.95578800
H	-4.87060300	-1.29646400	2.22183200
H	-4.33742900	0.34786400	2.62468900
H	-6.00967200	0.06210000	2.09731400
C	-5.37574200	-0.90485000	-0.43049900
H	-6.43786800	-0.68372500	-0.29431500
H	-5.11105200	-0.73227800	-1.47358300
H	-5.21061100	-1.95769700	-0.18616400
C	-4.65402200	1.45701000	0.13427100
H	-4.31255900	1.62914600	-0.88710000
H	-5.69554500	1.78030700	0.21547800
H	-4.05955700	2.06113100	0.82609000

CPA1

Zero-point correction=	0.638471 (Hartree/Particle)
Thermal correction to Energy=	0.677366
Thermal correction to Enthalpy=	0.678310
Thermal correction to Gibbs Free Energy=	0.565896
Sum of electronic and zero-point Energies=	-2487.502087
Sum of electronic and thermal Energies=	-2487.463192
Sum of electronic and thermal Enthalpies=	-2487.462248
Sum of electronic and thermal Free Energies=	-2487.574662

SCF Done: E(RM062X) = -2488.73280773

H	1.31249500	-2.63961200	-1.12307500
C	0.96319200	4.97370800	-2.23230000
C	0.41891300	3.97675600	-1.46381000
C	1.21351100	2.88597400	-1.01757500
C	2.57762000	2.83305100	-1.42163300
C	3.11382100	3.88777800	-2.20671100
C	2.32878800	4.93873700	-2.60020600
H	0.33853500	5.79526500	-2.56728300
H	-0.63140100	4.00925300	-1.19665500
C	0.68503100	1.82142300	-0.21556900
C	3.37571000	1.71726900	-1.06019700

H	4.15943700	3.83624500	-2.49664000
H	2.74580300	5.73806000	-3.20366600
C	2.85835100	0.66361900	-0.34920400
C	1.50012700	0.74415100	0.05600600
H	4.41551100	1.68660400	-1.37556200
C	-0.71852800	1.80377800	0.27743700
C	-1.26345200	2.84559300	1.09764200
C	-1.51722000	0.71743200	-0.01116800
C	-0.48581800	3.94054700	1.56372800
C	-2.62694200	2.76495600	1.49862500
C	-2.87543200	0.61199400	0.38410000
C	-1.04565700	4.91545100	2.34896600
H	0.56426300	3.99381900	1.29884500
C	-3.17942800	3.79724600	2.30219500
C	-3.40786500	1.64527700	1.11385600
C	-2.41090400	4.85289100	2.71502000
H	-0.43386100	5.74042900	2.69902100
H	-4.22424200	3.72433700	2.59026600
H	-4.44789900	1.59313900	1.42507300
H	-2.84045100	5.63477600	3.33238100
O	0.99267000	-0.32418300	0.77854100
O	-0.99384400	-0.32798900	-0.75996900
P	0.00240800	-1.34068200	-0.00001200
O	0.80275500	-1.83392800	-1.28543900
O	-0.55020600	-2.35288700	0.89796100
C	4.83769300	-3.32695700	-2.97758400
C	5.26009500	-3.49315400	-1.69397900
C	4.88043400	-2.57009600	-0.66746500
C	4.05538100	-1.44309400	-1.00812400
C	3.62292900	-1.31478600	-2.37087500
C	3.99833300	-2.22350700	-3.31564600
C	5.28891900	-2.74941900	0.65314300
C	3.68094800	-0.53078600	-0.00173800
C	4.09261800	-0.72795500	1.33113900
C	4.91099600	-1.86050000	1.65911700
C	5.32633100	-2.05208800	3.01468100
H	5.94387100	-2.91557600	3.24529000
C	4.95619200	-1.17664100	3.98965300
C	4.14711900	-0.04759600	3.66669100
C	3.73249200	0.17075100	2.38668100
H	5.91259800	-3.60407800	0.90523300
H	5.12855100	-4.03432500	-3.74718600
H	5.89111000	-4.33371200	-1.41907800
H	2.96718500	-0.49277600	-2.63473500

H	3.65149800	-2.11184300	-4.33772500
H	5.27410200	-1.33140200	5.01540900
H	3.85969900	0.64319500	4.45249900
H	3.12020700	1.03554100	2.15433700
C	-4.69625700	-3.51060600	2.90156100
C	-5.16563100	-3.62943900	1.62933400
C	-4.83098400	-2.66236800	0.62907700
C	-4.00165000	-1.54511400	0.98660500
C	-3.51367500	-1.47096700	2.33229700
C	-3.84978000	-2.41747100	3.25273500
C	-5.29066800	-2.78625400	-0.68074900
C	-3.68523000	-0.58268200	0.01035200
C	-4.14368800	-0.72278000	-1.31321600
C	-4.96066600	-1.85012000	-1.66073800
C	-5.42528700	-1.98428500	-3.00704000
H	-6.04217000	-2.84407800	-3.25345800
C	-5.10293700	-1.06113700	-3.95513900
C	-4.29424400	0.06225000	-3.61219700
C	-3.83409500	0.22723700	-2.33945800
H	-5.91689700	-3.63516100	-0.94608800
H	-4.95280500	-4.25124000	3.65201700
H	-5.80028300	-4.46386000	1.34412900
H	-2.85203800	-0.65651700	2.60527800
H	-3.46027200	-2.34950400	4.26309400
H	-5.45914000	-1.17344800	-4.97394500
H	-4.04464300	0.79161900	-4.37597900
H	-3.22292100	1.08860300	-2.09030800

Sub1

Zero-point correction=	0.199837 (Hartree/Particle)
Thermal correction to Energy=	0.210131
Thermal correction to Enthalpy=	0.211075
Thermal correction to Gibbs Free Energy=	0.162792
Sum of electronic and zero-point Energies=	-518.239195
Sum of electronic and thermal Energies=	-518.228900
Sum of electronic and thermal Enthalpies=	-518.227956
Sum of electronic and thermal Free Energies=	-518.276239

SCF Done: E(RM062X) = -518.580168159

C	-3.83552600	0.64849700	0.09830800
C	-3.63387100	-0.63257700	-0.40947300
C	-2.35899800	-1.18049800	-0.45702400
C	-1.25544900	-0.46073800	0.02096100

C	-1.46239300	0.81960000	0.55227500
C	-2.74133400	1.36415700	0.57657400
H	-4.83000400	1.07980200	0.12485400
H	-4.47397300	-1.20933000	-0.78347300
H	-2.20407400	-2.17222600	-0.87336700
H	-0.62569200	1.37255700	0.96386600
H	-2.88235900	2.35726300	0.99174500
N	0.00003800	-1.06909500	0.00048300
H	-0.00001400	-2.07716400	0.00024300
C	1.25546400	-0.46074700	-0.02051300
C	2.35925800	-1.18047900	0.45685400
C	1.46216600	0.81971300	-0.55178900
C	3.63412600	-0.63249700	0.40880900
H	2.20458200	-2.17227400	0.87313900
C	2.74103400	1.36429900	-0.57657100
H	0.62525700	1.37267500	-0.96294900
C	3.83550100	0.64863300	-0.09881500
H	4.47434900	-1.20934100	0.78239600
H	2.88188100	2.35746000	-0.99167100
H	4.82991400	1.08006400	-0.12573400

A_1

Zero-point correction= 0.839770 (Hartree/Particle)
Thermal correction to Energy= 0.890470
Thermal correction to Enthalpy= 0.891414
Thermal correction to Gibbs Free Energy= 0.751719
Sum of electronic and zero-point Energies= -3005.767894
Sum of electronic and thermal Energies= -3005.717194
Sum of electronic and thermal Enthalpies= -3005.716250
Sum of electronic and thermal Free Energies= -3005.855944
SCF Done: E(RM062X) = -3007.33577776

H	0.49200800	2.20869000	1.40514900
C	-5.01372900	-0.06432200	3.35493800
C	-3.65336400	-0.12408700	3.05475400
C	-3.14097100	0.55369300	1.95937500
C	-3.98185900	1.30297500	1.11851000
C	-5.35526700	1.33506000	1.40496100
C	-5.85346400	0.66594800	2.51928900
H	-5.41083000	-0.59060300	4.21647500
H	-2.98403300	-0.71638900	3.67188400
H	-2.07732500	0.50449100	1.74213300
H	-6.03313900	1.84812600	0.73315500

H	-6.91982800	0.70701300	2.72293200
N	-3.41514200	1.90875000	0.00496900
H	-2.54434200	1.50230400	-0.32405000
C	-3.86991300	2.98659700	-0.74191100
C	-3.27310500	3.20153600	-1.99765400
C	-4.83169100	3.90352600	-0.29220300
C	-3.65938900	4.27226400	-2.78898400
H	-2.49565600	2.51637200	-2.32347500
C	-5.21401900	4.96827100	-1.10314600
H	-5.25441100	3.80553300	0.70002500
C	-4.64555700	5.15966100	-2.35783100
H	-3.18316600	4.41550200	-3.75448800
H	-5.96157300	5.66471000	-0.73486100
H	-4.95253900	5.99141300	-2.98244200
C	3.27363600	-4.63568700	-3.05940300
C	3.10020700	-3.65793800	-2.11388600
C	1.80116700	-3.32655000	-1.64079700
C	0.68313800	-4.00951800	-2.19625300
C	0.89784200	-5.02554600	-3.16492000
C	2.16316300	-5.33720800	-3.58571000
H	4.27237500	-4.87000200	-3.41287800
H	3.95795500	-3.11991700	-1.72584000
C	1.57346300	-2.30712500	-0.65927300
C	-0.62803700	-3.65959900	-1.78517400
H	0.03358100	-5.54289300	-3.57126400
H	2.31755700	-6.11158600	-4.32962000
C	-0.85984800	-2.64148600	-0.89379300
C	0.26928700	-1.96373700	-0.36897000
H	-1.47461600	-4.20337900	-2.19569300
C	2.68898700	-1.58816200	0.01417500
C	3.70039400	-2.26465900	0.77337500
C	2.73099100	-0.21361100	-0.03837700
C	3.68035000	-3.66789700	0.99764200
C	4.74724300	-1.49944000	1.36165900
C	3.75386900	0.57247500	0.55189200
C	4.66689200	-4.27499100	1.73177100
H	2.86784400	-4.25730500	0.58787300
C	5.76020400	-2.16047500	2.10547100
C	4.75312900	-0.08741200	1.22212500
C	5.72686100	-3.51794400	2.28371800
H	4.63123900	-5.34686500	1.89624300
H	6.55716400	-1.56269900	2.53836700
H	5.55651000	0.48589000	1.67743300
H	6.50276800	-4.01411800	2.85701200

O	0.02541400	-0.92378300	0.52556000
O	1.72750900	0.46479400	-0.72047700
P	0.29411900	0.56907200	0.00030200
O	-0.69401900	1.19482900	-0.88836300
O	0.52727100	1.24142000	1.42081500
C	-4.74251300	0.23698200	-2.74967000
C	-5.24160900	-0.37957300	-1.64363800
C	-4.42557500	-1.25203800	-0.85577200
C	-3.05830600	-1.46758300	-1.23907700
C	-2.57490500	-0.80537100	-2.41557800
C	-3.38847600	0.01255700	-3.14138000
C	-4.92724400	-1.87694900	0.28400400
C	-2.24813200	-2.30890000	-0.45575600
C	-2.75354000	-2.90877300	0.71344700
C	-4.12359800	-2.69276700	1.07910300
C	-4.63247000	-3.30484700	2.26723100
H	-5.66968100	-3.11897400	2.53196400
C	-3.83542400	-4.08030100	3.05385100
C	-2.47181900	-4.29553600	2.69431800
C	-1.95105600	-3.73634500	1.56474200
H	-5.95868100	-1.69819500	0.57806500
H	-5.35942700	0.91631500	-3.32844200
H	-6.26554000	-0.20983200	-1.32216200
H	-1.54107000	-0.94930100	-2.71135000
H	-3.00065300	0.51680300	-4.02092400
H	-4.22959800	-4.53585000	3.95641500
H	-1.84496400	-4.91326900	3.32955900
H	-0.91285400	-3.91098200	1.30089700
C	4.62627500	3.92970500	-3.26418800
C	4.32368300	4.69407800	-2.17865900
C	4.01532900	4.09094000	-0.91858400
C	4.02675900	2.66025600	-0.80612300
C	4.35612200	1.89538000	-1.97144600
C	4.64278800	2.50796300	-3.15497400
C	3.70569400	4.86522900	0.19937600
C	3.72519100	2.05865300	0.43137100
C	3.40309800	2.84878100	1.55245200
C	3.39812200	4.28103600	1.42713000
C	3.06622800	5.08045800	2.56759300
H	3.07370800	6.16095600	2.45533400
C	2.74266600	4.50389800	3.75782500
C	2.72703700	3.08235000	3.88162500
C	3.04741700	2.28418400	2.82341900
H	3.69881100	5.94912400	0.11009600

H	4.85671400	4.39598000	-4.21632400
H	4.30842600	5.77814000	-2.24649900
H	4.37694800	0.81296900	-1.90107400
H	4.88669900	1.91029600	-4.02710100
H	2.48830700	5.11885300	4.61464000
H	2.45181600	2.63361300	4.83041800
H	3.01420600	1.20517800	2.92476400

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Zero-point correction= 1.148901 (Hartree/Particle)
Thermal correction to Energy= 1.219997
Thermal correction to Enthalpy= 1.220942
Thermal correction to Gibbs Free Energy= 1.039892
Sum of electronic and zero-point Energies= -3976.869058
Sum of electronic and thermal Energies= -3976.797962
Sum of electronic and thermal Enthalpies= -3976.797017
Sum of electronic and thermal Free Energies= -3976.978067
SCF Done: E(RM062X) = -3979.00871131

H	0.19584100	1.43824800	-0.79139600
C	4.18956500	-2.39249300	-1.72004500
C	2.85527900	-2.00447800	-1.73237900
C	2.31726800	-1.28644100	-0.67257500
C	3.10013500	-0.94965300	0.45006800
C	4.43976900	-1.38724800	0.47838900
C	4.96525100	-2.08851200	-0.59781800
H	4.62037900	-2.92793100	-2.55919200
H	2.21654400	-2.26199500	-2.57359500
H	1.26765500	-1.00182300	-0.69155900
H	5.05898000	-1.18305500	1.34221500
H	6.00905400	-2.38865000	-0.56758600
N	2.49433800	-0.20475200	1.44307700
H	1.47500400	-0.21024300	1.41193400
C	2.99640100	0.14847400	2.70286400
C	2.11405800	0.06669700	3.79031600
C	4.29121300	0.63770700	2.91176500
C	2.53734100	0.40612900	5.06883300
H	1.10119300	-0.27888500	3.60616900
C	4.70600000	0.96568100	4.20021200
H	4.94540400	0.80795700	2.06526600
C	3.84377900	0.84249000	5.28652400
H	1.84048400	0.33027000	5.89863400
H	5.71277100	1.34377900	4.34847400

H	4.17762100	1.10449900	6.28485200
C	-6.79768600	-3.33271200	1.75797900
C	-5.99551200	-2.49126900	1.03087800
C	-4.61469100	-2.77790200	0.85207500
C	-4.07748100	-3.93999400	1.47294600
C	-4.93764500	-4.79757100	2.20887500
C	-6.26860500	-4.50589800	2.34646300
H	-7.84802000	-3.09395000	1.88902700
H	-6.40881300	-1.58960000	0.59237900
C	-3.73910700	-1.92356400	0.10649500
C	-2.69157400	-4.21759300	1.36049400
H	-4.51276100	-5.68547200	2.66823700
H	-6.91746700	-5.16411100	2.91454000
C	-1.83358200	-3.36902800	0.70497700
C	-2.38927400	-2.20952700	0.10522400
H	-2.29341100	-5.11736300	1.82229200
C	-4.22392200	-0.73051600	-0.63814000
C	-5.21433400	-0.82212800	-1.67079200
C	-3.64862000	0.49735200	-0.39135600
C	-5.77592700	-2.05897800	-2.09088700
C	-5.62788500	0.36710200	-2.33494200
C	-4.02062100	1.68900100	-1.06474500
C	-6.72289100	-2.09947700	-3.08185500
H	-5.44148400	-2.97825900	-1.62383300
C	-6.61997900	0.29254000	-3.34861000
C	-5.01915100	1.60347800	-2.00397400
C	-7.16204900	-0.91116200	-3.71206000
H	-7.13589500	-3.05413100	-3.39075800
H	-6.93062900	1.21215500	-3.83625300
H	-5.32980200	2.50256300	-2.53000100
H	-7.91651700	-0.95983100	-4.49011200
O	-1.52016000	-1.33970100	-0.54186100
O	-2.66785700	0.59800700	0.58396200
P	-1.19450300	0.04031500	0.24208100
O	-0.39041200	-0.09399200	1.46889200
O	-0.64445400	0.89482700	-0.94691600
C	2.20796700	-3.21793800	3.92754600
C	2.69523400	-3.71826000	2.76017300
C	1.83928900	-3.91135100	1.62841600
C	0.45795100	-3.52537200	1.72015600
C	-0.01200400	-2.99413800	2.96731500
C	0.82792200	-2.86574600	4.03200600
C	2.32184700	-4.46754900	0.44707000
C	-0.37831600	-3.68307000	0.60083400

C	0.12811400	-4.21503000	-0.60236600
C	1.49735800	-4.63613300	-0.66544700
C	2.00087700	-5.19134000	-1.88300500
H	3.04333300	-5.49665100	-1.91192000
C	1.20289800	-5.31546000	-2.98065400
C	-0.15786500	-4.89230600	-2.92357700
C	-0.67791000	-4.36747300	-1.77673500
H	3.36983100	-4.75104000	0.38045000
H	2.86388700	-3.06223300	4.77776600
H	3.74481700	-3.97910100	2.65717100
H	-1.04714600	-2.68094500	3.04605800
H	0.45584800	-2.45822400	4.96724200
H	1.59571200	-5.73402400	-3.90159500
H	-0.78474200	-4.99423300	-3.80365000
H	-1.71746700	-4.05744500	-1.74483600
C	-3.82521600	4.96552200	2.93228900
C	-3.10590300	5.55971100	1.94004100
C	-2.93433500	4.91871300	0.67234600
C	-3.52700100	3.63065600	0.45202300
C	-4.29854200	3.05559800	1.51357300
C	-4.43470200	3.69535300	2.70981000
C	-2.18847500	5.51562900	-0.34459900
C	-3.33812800	2.98346400	-0.78504800
C	-2.53429700	3.56904600	-1.78369800
C	-1.96111700	4.86689900	-1.55686400
C	-1.15465000	5.46476400	-2.57739200
H	-0.73509600	6.44876700	-2.38844300
C	-0.91062200	4.81411400	-3.74787000
C	-1.45436900	3.51292300	-3.96667500
C	-2.23255800	2.91072300	-3.02204800
H	-1.75026200	6.49715600	-0.17605100
H	-3.94329600	5.45522700	3.89333800
H	-2.63958500	6.52951400	2.09147500
H	-4.77082900	2.09162800	1.35826800
H	-5.01288600	3.23592000	3.50469800
H	-0.29532000	5.27412200	-4.51401500
H	-1.23737800	2.99479200	-4.89583400
H	-2.61847000	1.91179900	-3.19112300
C	2.58572500	0.98232500	-2.68460600
C	4.17826000	1.52127400	-1.02231700
C	2.68918600	1.59338400	-1.35130100
O	4.72559100	1.85091200	0.00305800
N	3.75261100	0.67039600	-3.12563900
N	4.71305400	0.94191200	-2.15339900

C	6.03857900	0.49423700	-2.36345300
C	6.32261700	-0.27615900	-3.49455700
C	7.04530500	0.79485300	-1.44196800
C	7.61362200	-0.74707400	-3.69512600
H	5.52899000	-0.50442900	-4.19373400
C	8.33082800	0.30822200	-1.66174700
H	6.82267200	1.39162900	-0.56903500
C	8.62542900	-0.46275000	-2.78115900
H	7.82661400	-1.34580800	-4.57497400
H	9.10921400	0.54266200	-0.94273800
H	9.63113800	-0.83597500	-2.94182100
C	1.32949900	0.79159100	-3.45624000
H	1.56858900	0.49153400	-4.47686300
H	0.71262800	0.02000000	-2.98344100
H	0.73777100	1.71225700	-3.46492800
N	1.73078600	2.07145400	-0.66744400
C	1.97079400	2.95329100	0.44177500
O	2.72153800	3.88838500	0.36660900
O	1.12376300	2.64875300	1.40684400
C	0.92050200	3.58404600	2.52530500
C	2.18210600	3.65929200	3.37441700
H	1.99282000	4.32414200	4.22285300
H	2.45088800	2.67483500	3.75916200
H	3.01506200	4.06017100	2.79479000
C	-0.23937500	2.94292400	3.27475900
H	-0.46879500	3.53083200	4.16769200
H	-1.13141700	2.90409400	2.64059600
H	0.02152400	1.92422900	3.56967900
C	0.51994900	4.95182900	1.98099300
H	0.12231000	5.55204500	2.80499000
H	1.36758100	5.47437200	1.53758900
H	-0.26871900	4.83642000	1.23379700

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Zero-point correction= 1.149722 (Hartree/Particle)
Thermal correction to Energy= 1.220526
Thermal correction to Enthalpy= 1.221471
Thermal correction to Gibbs Free Energy= 1.041483
Sum of electronic and zero-point Energies= -3976.870438
Sum of electronic and thermal Energies= -3976.799633
Sum of electronic and thermal Enthalpies= -3976.798689
Sum of electronic and thermal Free Energies= -3976.978676
SCF Done: E(RM062X) = -3979.01091429

H	0.29083000	1.30947300	-1.02042900
C	5.35805100	-1.36344200	-0.48267100
C	4.01191100	-1.30527800	-0.83068500
C	3.09331500	-0.68142300	0.00300200
C	3.49289400	-0.10761100	1.23035900
C	4.84259500	-0.23004100	1.60717200
C	5.75149100	-0.83987300	0.75003600
H	6.07995000	-1.82341200	-1.14888700
H	3.66394100	-1.74068500	-1.76445600
H	2.03953400	-0.66654000	-0.27019400
H	5.17303400	0.11263900	2.57834800
H	6.79006700	-0.91298800	1.05978700
N	2.51191000	0.52431900	1.97093300
H	1.55717900	0.29861900	1.68577500
C	2.57056600	1.09030800	3.24822600
C	1.39952800	1.01769000	4.02334200
C	3.67602800	1.77646300	3.76913000
C	1.35370000	1.57679500	5.29177000
H	0.53901900	0.50487400	3.60495600
C	3.61570000	2.33402400	5.04533700
H	4.57431700	1.90666000	3.17954100
C	2.46587300	2.23323100	5.82008500
H	0.43770700	1.50201300	5.87073500
H	4.48347800	2.86232900	5.42787000
H	2.43083100	2.66930100	6.81244400
C	-5.97238300	-4.23103900	1.87971400
C	-5.29298200	-3.34958700	1.07862700
C	-3.87382600	-3.38365700	0.99979300
C	-3.17424600	-4.32959100	1.79992500
C	-3.90795800	-5.23710600	2.60939200
C	-5.27618800	-5.19502000	2.64689400
H	-7.05532700	-4.18556500	1.93070800
H	-5.83702900	-2.60903700	0.50305400
C	-3.12102100	-2.48067100	0.18056800
C	-1.75679100	-4.33754500	1.79684200
H	-3.35734800	-5.95902800	3.20574300
H	-5.82865700	-5.88923900	3.27129300
C	-1.02671000	-3.43089100	1.06750500
C	-1.74513600	-2.50050500	0.27198900
H	-1.23188400	-5.06581800	2.40969700
C	-3.77128000	-1.49342700	-0.72202400
C	-4.67529500	-1.89089200	-1.76075800
C	-3.46070100	-0.15503100	-0.59853200

C	-4.95079400	-3.25350000	-2.05895100
C	-5.29688600	-0.88684700	-2.55423100
C	-4.06652900	0.86225100	-1.38070000
C	-5.82272400	-3.58971000	-3.06238800
H	-4.45394600	-4.03046900	-1.48899300
C	-6.20511000	-1.26736600	-3.57777700
C	-4.98451100	0.47613000	-2.32736600
C	-6.46861800	-2.58801300	-3.82530500
H	-6.01511800	-4.63551500	-3.27845600
H	-6.67775200	-0.48609400	-4.16615100
H	-5.46791200	1.23657600	-2.93524700
H	-7.16027700	-2.87064500	-4.61190300
O	-1.01880500	-1.57876800	-0.46872300
O	-2.54739500	0.24317300	0.36566200
P	-0.98140300	-0.07599300	0.13254600
O	-0.23682300	0.05919700	1.39836900
O	-0.53987800	0.74601600	-1.11374800
C	2.52932900	-2.15976800	4.59391100
C	3.22757500	-2.67856100	3.54776900
C	2.55549200	-3.13867100	2.36924400
C	1.12552700	-3.02409000	2.28647500
C	0.42983300	-2.47040700	3.41267700
C	1.10606100	-2.06867000	4.52481600
C	3.26550900	-3.67565100	1.29920000
C	0.46432000	-3.44473900	1.11755200
C	1.19594200	-3.95574100	0.02640700
C	2.62073400	-4.08253900	0.13061500
C	3.35794800	-4.59760400	-0.98088300
H	4.43836200	-4.67002100	-0.88796300
C	2.72596500	-4.96929800	-2.12958400
C	1.30842700	-4.85502400	-2.23243300
C	0.57009700	-4.37138000	-1.19280500
H	4.34972100	-3.74317700	1.35984300
H	3.04472000	-1.79561500	5.47690400
H	4.31189200	-2.74343100	3.57380300
H	-0.64685800	-2.35469400	3.35698700
H	0.56366300	-1.63993800	5.36167900
H	3.29518000	-5.35204800	-2.97041300
H	0.81525200	-5.15504000	-3.15130600
H	-0.50812300	-4.29103800	-1.28433100
C	-1.85564800	4.49797500	-4.29490800
C	-2.31412500	5.15033800	-3.19157100
C	-2.94091800	4.43448400	-2.12214800
C	-3.10841300	3.01164100	-2.23358500

C	-2.59099100	2.36411500	-3.40408400
C	-1.98659200	3.08084100	-4.39331900
C	-3.37503400	5.08880500	-0.97070800
C	-3.74355900	2.30505500	-1.19288200
C	-4.14125300	2.97119700	-0.01587200
C	-3.93951800	4.38822800	0.09544400
C	-4.31435600	5.05500700	1.30434200
H	-4.14648800	6.12665500	1.37195700
C	-4.86360700	4.36545300	2.34311400
C	-5.08819700	2.96214800	2.22773800
C	-4.75016800	2.29191900	1.08915400
H	-3.23981000	6.16522500	-0.88698700
H	-1.37547500	5.04840000	-5.09732800
H	-2.20538100	6.22686800	-3.09366500
H	-2.65968000	1.28500400	-3.47851000
H	-1.58620700	2.56825600	-5.26166500
H	-5.13902900	4.87883400	3.25868300
H	-5.53575600	2.42447600	3.05713300
H	-4.93251600	1.22530900	1.01652700
C	4.23765900	2.24571000	-0.81962300
C	2.93364300	1.03774900	-2.37885900
C	2.83403900	1.92045200	-1.14298100
O	2.02009400	0.51473100	-2.96964500
N	5.01579800	1.70701100	-1.69671400
N	4.28457600	1.04043700	-2.66634900
C	4.97328800	0.24379200	-3.61101600
C	4.27441900	-0.37821400	-4.64959000
C	6.35680800	0.08610400	-3.49216400
C	4.97510800	-1.16304500	-5.56037300
H	3.20361500	-0.25375000	-4.73415000
C	7.03587000	-0.69645300	-4.41814000
H	6.87771100	0.57256100	-2.67769200
C	6.35255600	-1.32662600	-5.45500300
H	4.42957100	-1.64676600	-6.36408900
H	8.11055500	-0.81436000	-4.32303100
H	6.88871700	-1.93765000	-6.17311500
C	4.77717100	2.99493000	0.34942700
H	4.70705300	4.07196500	0.18532300
H	4.18710500	2.76667800	1.24000400
H	5.81551300	2.69915900	0.50706000
N	1.69137900	2.21272100	-0.66547500
C	1.54750800	3.25427100	0.30156500
O	2.20478400	4.26687300	0.27819600
O	0.53233200	2.96028200	1.08653900

C	-0.06146900	3.99306100	1.95019800
C	-1.24446300	3.25690600	2.56375200
H	-1.92885400	2.91223800	1.78142800
H	-0.89521300	2.38793100	3.12613000
H	-1.79103600	3.92758400	3.23227500
C	-0.53174900	5.14858200	1.07325000
H	-1.18633500	5.79776300	1.66298900
H	0.30793500	5.73653000	0.70014300
H	-1.10960500	4.76167400	0.23014700
C	0.94043200	4.44481500	3.00588000
H	1.77363400	4.98096100	2.55017000
H	0.43072400	5.11612200	3.70363900
H	1.32273500	3.59080700	3.56812100

TS-A_1

Zero-point correction= 1.148935 (Hartree/Particle)
Thermal correction to Energy= 1.218404
Thermal correction to Enthalpy= 1.219348
Thermal correction to Gibbs Free Energy= 1.043791
Sum of electronic and zero-point Energies= -3976.858886
Sum of electronic and thermal Energies= -3976.789418
Sum of electronic and thermal Enthalpies= -3976.788473
Sum of electronic and thermal Free Energies= -3976.964030
SCF Done: E(RM062X) = -3978.99932384
Number of Imaginary Frequencies = -159.52

H	0.93190600	1.38226300	-0.43551500
C	4.80695100	-2.17659800	-1.04080800
C	3.56576200	-1.76599700	-1.42869400
C	2.69200800	-1.11161400	-0.50321800
C	3.04750900	-1.06401200	0.88583700
C	4.32605200	-1.56032600	1.27369000
C	5.17186000	-2.07969500	0.33390700
H	5.49968800	-2.60730300	-1.75526200
H	3.23302600	-1.88631200	-2.45495800
H	1.63474600	-1.02268600	-0.75412000
H	4.60313100	-1.54612700	2.31992400
H	6.14045700	-2.45563900	0.64893900
N	2.17152000	-0.51704200	1.74468400
H	1.15616700	-0.49347200	1.48823100
C	2.44194000	-0.12954400	3.07432800
C	1.44206200	-0.33810200	4.02977200
C	3.63859700	0.50517500	3.42304700

C	1.68847400	-0.00974900	5.35727900
H	0.49751300	-0.76460500	3.70867700
C	3.86762300	0.83046600	4.75712300
H	4.35524900	0.76421700	2.64818900
C	2.90863700	0.55570700	5.72915100
H	0.92071600	-0.18881500	6.10348800
H	4.79670100	1.31889300	5.03210900
H	3.09779400	0.80904500	6.76705300
C	-6.86278300	-3.38448000	1.28331200
C	-6.03692000	-2.50096400	0.63690400
C	-4.65819500	-2.79411600	0.45255500
C	-4.14755500	-4.01025200	0.98787200
C	-5.03165000	-4.90964000	1.64074500
C	-6.36043700	-4.60944500	1.78283200
H	-7.91138900	-3.13999000	1.41835800
H	-6.42917500	-1.56082000	0.26465200
C	-3.76079100	-1.90011600	-0.21536600
C	-2.76184700	-4.29467500	0.88480600
H	-4.62698400	-5.83796400	2.03419200
H	-7.02743300	-5.30096200	2.28690900
C	-1.88581600	-3.40878600	0.30746700
C	-2.41565700	-2.20716800	-0.23335300
H	-2.38248100	-5.22570100	1.29869400
C	-4.20194900	-0.63481900	-0.86103300
C	-5.17941100	-0.61525500	-1.90900100
C	-3.58392700	0.54982000	-0.50728100
C	-5.77368200	-1.79783300	-2.43064800
C	-5.54636400	0.63199700	-2.48762000
C	-3.91666400	1.79705100	-1.09915500
C	-6.70741400	-1.73325500	-3.43277200
H	-5.47355900	-2.76038200	-2.03255100
C	-6.52545000	0.66670700	-3.51592200
C	-4.90153900	1.81718000	-2.05608200
C	-7.10079300	-0.48732500	-3.97631300
H	-7.14505000	-2.64845700	-3.81816700
H	-6.79917300	1.63048000	-3.93601600
H	-5.17409500	2.76356800	-2.51630200
H	-7.84537000	-0.45244300	-4.76468200
O	-1.53738300	-1.32156700	-0.81528700
O	-2.62440300	0.54601800	0.48169700
P	-1.13569200	-0.02107200	0.10849300
O	-0.49114700	-0.46361700	1.38192500
O	-0.42658800	0.90572700	-0.84104300
C	1.91091400	-3.79367100	3.78966900

C	2.48570700	-4.10081800	2.59518200
C	1.72108600	-4.08296800	1.38375500
C	0.33053000	-3.72534900	1.43625700
C	-0.23072500	-3.39663500	2.71547200
C	0.52785600	-3.44340700	3.84621300
C	2.30761100	-4.38947600	0.15833200
C	-0.42370000	-3.69339400	0.24758200
C	0.18824300	-3.97598200	-0.99146000
C	1.57561100	-4.33949600	-1.02900400
C	2.18706400	-4.63088400	-2.28939900
H	3.23997300	-4.90098200	-2.29612300
C	1.47308100	-4.56117000	-3.44782900
C	0.09286700	-4.20288900	-3.41441500
C	-0.52771000	-3.92745100	-2.23172600
H	3.36304100	-4.65135400	0.12288600
H	2.49828800	-3.80096700	4.70216200
H	3.53913000	-4.35977600	2.53002600
H	-1.26640600	-3.08117100	2.76406100
H	0.08710300	-3.18185200	4.80338600
H	1.94648600	-4.78230000	-4.39907400
H	-0.46743000	-4.15388200	-4.34236700
H	-1.57950200	-3.66298700	-2.22030800
C	-3.99419600	4.97864200	2.97424500
C	-3.20193300	5.59210800	2.05082200
C	-2.92576400	4.97161200	0.79164500
C	-3.50063900	3.68766500	0.50414100
C	-4.34131600	3.08702300	1.49615200
C	-4.57068300	3.70536800	2.68969400
C	-2.10418400	5.58427100	-0.15449800
C	-3.21801200	3.05993900	-0.72363500
C	-2.33283300	3.65676800	-1.64187300
C	-1.78018700	4.95075200	-1.35356800
C	-0.89568600	5.55895900	-2.30088600
H	-0.49222200	6.54088700	-2.06951300
C	-0.56285900	4.92113600	-3.45676100
C	-1.08851600	3.62356800	-3.73409400
C	-1.93878400	3.01216300	-2.86056200
H	-1.68250100	6.56384200	0.06147300
H	-4.19233700	5.45434900	3.92938900
H	-2.75840400	6.56356800	2.25279600
H	-4.78368200	2.11814700	1.29022900
H	-5.19892300	3.22717100	3.43398500
H	0.11047900	5.38953100	-4.16727200
H	-0.79747500	3.11587500	-4.64860600

H	-2.30991400	2.01414300	-3.06514100
C	2.74864800	0.89229000	-2.37702400
C	4.41298600	1.10975900	-0.70851400
C	2.90538100	1.00926600	-0.90454700
O	5.05918700	1.16178900	0.31180700
N	3.89501100	0.91339900	-2.95772400
N	4.89506400	1.03492100	-2.00200200
C	6.23974600	0.83501600	-2.39452400
C	6.50281000	0.24275400	-3.63252500
C	7.28933600	1.21906100	-1.55557600
C	7.81919500	0.03582600	-4.02635800
H	5.67569400	-0.04006000	-4.27133400
C	8.59953400	0.99387100	-1.96594900
H	7.07885800	1.68001800	-0.60075900
C	8.87438800	0.40513300	-3.19634800
H	8.01788600	-0.42116900	-4.99046000
H	9.41289100	1.29302600	-1.31280300
H	9.90014300	0.23900800	-3.50750000
C	1.46827400	0.79011200	-3.12793700
H	1.69170500	0.76677800	-4.19517700
H	0.91353200	-0.10960200	-2.84139800
H	0.80971300	1.63311900	-2.89842000
N	1.96286100	1.56877300	-0.15271600
C	2.13200900	2.33874800	1.02206900
O	3.13046900	2.94590500	1.30711700
O	0.97300100	2.30099200	1.66537900
C	0.58923000	3.35088900	2.61113300
C	1.50161300	3.34715200	3.82913200
H	1.13540400	4.09366800	4.54089000
H	1.48207300	2.36977200	4.31413000
H	2.52860800	3.59028200	3.55475800
C	-0.82976000	2.93549600	2.97448500
H	-1.26668200	3.65260900	3.67472700
H	-1.45564400	2.89293100	2.07812100
H	-0.81804100	1.94092600	3.42915200
C	0.61833300	4.68622400	1.87697500
H	0.14110700	5.45150700	2.49672800
H	1.64463200	4.99510300	1.66536800
H	0.05993300	4.60688500	0.94045200

TS-A_1'

Zero-point correction=	1.149525 (Hartree/Particle)
Thermal correction to Energy=	1.218806

Thermal correction to Enthalpy= 1.219750
Thermal correction to Gibbs Free Energy= 1.044898
Sum of electronic and zero-point Energies= -3976.853341
Sum of electronic and thermal Energies= -3976.784059
Sum of electronic and thermal Enthalpies= -3976.783115
Sum of electronic and thermal Free Energies= -3976.957968
SCF Done: E(RM062X) = -3978.99718902
Number of Imaginary Frequencies = -264.36

H	-1.09955500	-1.57753100	-0.60869000
C	-5.33588200	1.32795200	-0.01243700
C	-4.11518700	1.19512800	-0.59593300
C	-3.07078400	0.45608200	0.06456400
C	-3.20592200	0.17424000	1.48629500
C	-4.49408800	0.36395400	2.08243100
C	-5.50952000	0.90059300	1.34153700
H	-6.15485400	1.81018000	-0.53448100
H	-3.91691100	1.58415500	-1.59063300
H	-2.05505000	0.59337100	-0.31087200
H	-4.62995600	0.15049400	3.13515900
H	-6.47228800	1.05924900	1.81912800
N	-2.13179100	-0.27230900	2.12827800
H	-1.15875200	-0.08173000	1.71676900
C	-2.06683100	-0.81381900	3.43452000
C	-0.91894800	-0.52969900	4.18322900
C	-3.04682700	-1.66565000	3.94981200
C	-0.80397500	-1.02609100	5.47551000
H	-0.14012200	0.07557500	3.73377100
C	-2.91433100	-2.16278500	5.24257500
H	-3.87951700	-1.97611700	3.33096700
C	-1.80524300	-1.83202800	6.01583200
H	0.08107400	-0.79159800	6.05833000
H	-3.67631400	-2.82671100	5.63704900
H	-1.70882800	-2.22139500	7.02384000
C	6.20276600	4.12138200	1.30527800
C	5.43542700	3.22592800	0.60516400
C	4.01691600	3.31854400	0.61323200
C	3.41130000	4.34091200	1.39754500
C	4.23421600	5.25998900	2.10085600
C	5.59940100	5.15929500	2.05405300
H	7.28401300	4.03020200	1.28957400
H	5.90737700	2.42898800	0.04115400
C	3.17701000	2.40748800	-0.10589700
C	1.99733300	4.41067000	1.48907700

H	3.75477100	6.04020300	2.68557800
H	6.21977200	5.86395500	2.59794100
C	1.18999700	3.49544900	0.86034000
C	1.81152100	2.49592700	0.06344800
H	1.54660800	5.19241400	2.09568700
C	3.71155300	1.33954200	-0.99278700
C	4.56068200	1.63760400	-2.10840000
C	3.33172800	0.02682100	-0.77771700
C	4.88489900	2.96822200	-2.49322800
C	5.07248400	0.56800900	-2.89412000
C	3.84507200	-1.05127000	-1.54905500
C	5.69890000	3.21117000	-3.56963700
H	4.47024900	3.79687700	-1.93038700
C	5.92266400	0.85140700	-3.99552800
C	4.71140200	-0.76421900	-2.57400500
C	6.23605900	2.14279100	-4.32613000
H	5.92834400	4.23446600	-3.84885900
H	6.31041800	0.01902900	-4.57614800
H	5.12089500	-1.57940900	-3.16505900
H	6.88278600	2.35104300	-5.17206600
O	1.00414800	1.59764100	-0.58837600
O	2.47131500	-0.27638600	0.25378900
P	0.88452700	0.10395500	0.08777600
O	0.33278400	0.22596500	1.48071800
O	0.19952800	-0.73711700	-0.93688000
C	-2.12160600	2.67646800	4.74228000
C	-2.89488200	3.01419100	3.67439600
C	-2.30531000	3.32034400	2.40491000
C	-0.87786100	3.24627600	2.25692600
C	-0.10422800	2.86970100	3.40506800
C	-0.70247900	2.61307300	4.60217600
C	-3.09247100	3.68317400	1.31451200
C	-0.29301100	3.53088800	1.00746900
C	-1.10221600	3.87915800	-0.09388100
C	-2.52436800	3.96898100	0.07190500
C	-3.33532900	4.34155800	-1.04674700
H	-4.41082000	4.40437100	-0.90085000
C	-2.77604000	4.60147200	-2.26157600
C	-1.36264100	4.51253300	-2.43032400
C	-0.55616800	4.16955500	-1.38621000
H	-4.17270400	3.74000100	1.43194600
H	-2.57548600	2.44341400	5.70018700
H	-3.97741600	3.06306700	3.75954800
H	0.96988800	2.77066600	3.29907500

H	-0.09859100	2.32312700	5.45656700
H	-3.40002700	4.87920800	-3.10493400
H	-0.92830500	4.72047600	-3.40248200
H	0.51730300	4.10879700	-1.52730500
C	0.42157100	-4.50470600	-3.30066500
C	1.22022400	-5.19558900	-2.43997200
C	2.26712000	-4.53469100	-1.72072700
C	2.48190900	-3.13045100	-1.93771100
C	1.62220900	-2.44596300	-2.85721200
C	0.62226700	-3.10704300	-3.50506600
C	3.06905900	-5.22209900	-0.80962000
C	3.51231700	-2.47416800	-1.23983400
C	4.29953700	-3.17128800	-0.30311800
C	4.07071000	-4.57249500	-0.08843100
C	4.86796300	-5.26731800	0.87500700
H	4.68354400	-6.32773100	1.02505600
C	5.82832800	-4.61709700	1.58988000
C	6.05749400	-3.22508300	1.37966100
C	5.32482700	-2.52910800	0.46427000
H	2.89993900	-6.28492500	-0.64820000
H	-0.37547500	-5.01398000	-3.83332400
H	1.07402000	-6.25957700	-2.27243800
H	1.74780100	-1.37856600	-2.99486100
H	-0.04117700	-2.56117700	-4.16719500
H	6.42410900	-5.15309200	2.32167900
H	6.82302600	-2.71818500	1.95812500
H	5.50368400	-1.46980900	0.31239700
C	-4.56752000	-1.87593700	-0.45301200
C	-3.14712600	-0.94587300	-2.08928400
C	-3.15660800	-1.42675500	-0.63981500
O	-2.19403000	-0.58695800	-2.73421400
N	-5.27307100	-1.54234400	-1.48137900
N	-4.47987300	-0.97672900	-2.45487700
C	-5.08930100	-0.37375000	-3.58090300
C	-4.31261000	0.08708600	-4.64842000
C	-6.47950900	-0.22830400	-3.59939900
C	-4.94474400	0.69636600	-5.72814100
H	-3.23802700	-0.02977000	-4.62854500
C	-7.08813900	0.37589100	-4.69256700
H	-7.06240400	-0.59327600	-2.76366500
C	-6.32768700	0.84358800	-5.76112800
H	-4.33987000	1.05354300	-6.55522500
H	-8.16809300	0.48255100	-4.70414300
H	-6.80863800	1.31589500	-6.61086500

C	-5.26203100	-2.58677700	0.66318300
H	-4.99710100	-3.64397400	0.66418500
H	-4.98015000	-2.18495000	1.63379400
H	-6.33607900	-2.46575500	0.51174300
N	-2.00050700	-1.99210900	-0.21598600
C	-1.83863700	-2.84782600	0.87207700
O	-2.72709800	-3.49055000	1.38813700
O	-0.55639700	-2.83171000	1.20445700
C	0.07487900	-3.92806500	1.93828700
C	1.52346300	-3.46116100	1.97517200
H	1.87532800	-3.27277500	0.95756000
H	1.59695400	-2.52514800	2.53662800
H	2.16371500	-4.21657000	2.43969100
C	-0.09398000	-5.20525900	1.12377500
H	0.49983400	-6.00557800	1.57483600
H	-1.14146700	-5.51671400	1.10580400
H	0.25650300	-5.04590000	0.10075100
C	-0.50562600	-4.06875600	3.33897700
H	-1.55202300	-4.37356000	3.30660300
H	0.07145900	-4.82626700	3.87857800
H	-0.42390300	-3.12518200	3.88203800

TS-N_1

Zero-point correction= 1.151857 (Hartree/Particle)
Thermal correction to Energy= 1.221032
Thermal correction to Enthalpy= 1.221977
Thermal correction to Gibbs Free Energy= 1.048232
Sum of electronic and zero-point Energies= -3976.848571
Sum of electronic and thermal Energies= -3976.779396
Sum of electronic and thermal Enthalpies= -3976.778451
Sum of electronic and thermal Free Energies= -3976.952196
SCF Done: E(RM062X) = -3978.99208467
Number of Imaginary Frequencies = -136.76

H	0.88457700	1.75865200	-0.47459000
C	2.94141100	-3.17371300	-3.16719600
C	1.72545600	-2.96294000	-2.52445200
C	1.65551700	-2.12439900	-1.41748500
C	2.80594400	-1.48109800	-0.96625100
C	4.02914600	-1.67864000	-1.61023500
C	4.08966400	-2.53604000	-2.70411200
H	2.99332900	-3.83531400	-4.02567000
H	0.82361700	-3.46189300	-2.86597600

H	0.71668600	-1.99416700	-0.88869200
H	4.91988100	-1.14904600	-1.29041600
H	5.04010100	-2.68690800	-3.20484000
N	2.65099400	-0.53214600	0.11213500
H	1.63549000	-0.43371900	0.33066300
C	3.30225700	-0.75892800	1.38052000
C	2.69750400	-0.16683900	2.49013600
C	4.51236000	-1.43937600	1.50818500
C	3.33444100	-0.21822200	3.72334000
H	1.72005500	0.29451100	2.37396000
C	5.12990500	-1.49440400	2.75363200
H	4.96514500	-1.93798400	0.66130700
C	4.55687600	-0.87022300	3.85802600
H	2.86616900	0.24947400	4.58371600
H	6.07071300	-2.02579700	2.85446000
H	5.05447700	-0.90420600	4.82167200
C	-6.94984700	-2.38038600	1.93315200
C	-6.06333900	-1.72053000	1.12157400
C	-4.74811900	-2.22281100	0.91978700
C	-4.36521000	-3.40771000	1.60696800
C	-5.30962000	-4.07363600	2.43236200
C	-6.57594600	-3.57675600	2.59054100
H	-7.94745400	-1.97860600	2.07819900
H	-6.35746300	-0.79947900	0.63041700
C	-3.78879800	-1.56535800	0.08550400
C	-3.04201000	-3.89482300	1.46644200
H	-5.00118300	-4.98207500	2.94219100
H	-7.29048900	-4.08942900	3.22597600
C	-2.10227300	-3.23545800	0.71252700
C	-2.49551900	-2.04740400	0.03817400
H	-2.75909600	-4.80978500	1.98083000
C	-4.11609000	-0.34272500	-0.69134100
C	-5.14646000	-0.31992000	-1.68600000
C	-3.35725800	0.79158300	-0.48547900
C	-5.89090000	-1.47656400	-2.04677800
C	-5.41437700	0.89614900	-2.37334700
C	-3.62486500	2.01728900	-1.15515400
C	-6.86532500	-1.41260300	-3.00953100
H	-5.67286900	-2.41863700	-1.55607300
C	-6.43706500	0.93275200	-3.35760100
C	-4.64808300	2.04920000	-2.06962100
C	-7.15213000	-0.19334300	-3.66803600
H	-7.41912000	-2.30765600	-3.27383300
H	-6.63355300	1.87336600	-3.86449400

H	-4.87300500	2.98245600	-2.57985700
H	-7.92966600	-0.15777700	-4.42392700
O	-1.56402300	-1.37737300	-0.72406600
O	-2.32096300	0.74564800	0.42610600
P	-0.93990300	0.02055000	-0.09485200
O	-0.07633100	-0.30897300	1.08221200
O	-0.33827400	0.78469400	-1.23743900
C	2.12701700	-3.33598000	3.67732800
C	2.43686000	-4.09139400	2.58885400
C	1.49416200	-4.26598000	1.52477200
C	0.21655300	-3.61243800	1.60970800
C	-0.05201000	-2.79439900	2.75654300
C	0.86595900	-2.67134000	3.75479400
C	1.77761300	-5.08490600	0.43297800
C	-0.72828700	-3.80561100	0.58567000
C	-0.42629400	-4.62616600	-0.51946900
C	0.84637700	-5.28668700	-0.58542200
C	1.13748700	-6.12668200	-1.70596500
H	2.10599500	-6.61824800	-1.74004200
C	0.23157600	-6.29679400	-2.70998100
C	-1.03031000	-5.63363200	-2.65341100
C	-1.34958000	-4.83148000	-1.59615100
H	2.74277600	-5.58363700	0.37751600
H	2.84582900	-3.21427600	4.48087700
H	3.40047500	-4.58735800	2.50978100
H	-0.99139000	-2.25639300	2.80275200
H	0.64835000	-2.04460300	4.61430600
H	0.46371000	-6.93459400	-3.55678800
H	-1.74222200	-5.77272800	-3.46058100
H	-2.31295500	-4.33335200	-1.56020100
C	-3.90709400	5.44287300	2.66037100
C	-2.92330400	5.90890200	1.84068400
C	-2.56284000	5.20432000	0.64803700
C	-3.24335700	3.98167600	0.32905500
C	-4.28381000	3.53702600	1.20955900
C	-4.60236100	4.24139400	2.33291400
C	-1.56293700	5.67566200	-0.20364600
C	-2.87486800	3.26194000	-0.82285900
C	-1.87413500	3.75019000	-1.68140600
C	-1.21187600	4.98504400	-1.36312900
C	-0.21357400	5.48971100	-2.25664100
H	0.28230900	6.42164300	-2.00003300
C	0.09494300	4.82643200	-3.40509900
C	-0.56157900	3.59898700	-3.72298600

C	-1.49695000	3.06878400	-2.88455200
H	-1.05497000	6.60761700	0.03618600
H	-4.17023300	5.98497500	3.56288800
H	-2.38931100	6.82573500	2.07654700
H	-4.81299700	2.62012800	0.97301900
H	-5.38886900	3.88494200	2.98999900
H	0.84426400	5.22359200	-4.08239200
H	-0.29644200	3.07477500	-4.63604100
H	-1.95990100	2.11459100	-3.10777200
C	3.04212000	1.23119600	-1.95324000
C	4.30948700	1.53293700	0.03131200
C	2.86741200	1.36791300	-0.47838000
O	4.71573000	1.67021100	1.15446600
N	4.28722600	1.26195400	-2.26480600
N	5.05944600	1.35060500	-1.11754000
C	6.46892600	1.26690300	-1.23048900
C	7.05520300	1.42489900	-2.48893600
C	7.25697900	0.99536800	-0.10742100
C	8.43449200	1.31910200	-2.61737400
H	6.42595600	1.62221100	-3.34727900
C	8.63673100	0.89947700	-0.26039800
H	6.79715800	0.87130300	0.86378800
C	9.23346200	1.05957100	-1.50691600
H	8.88554800	1.44444100	-3.59633800
H	9.24788600	0.69349900	0.61232200
H	10.31009400	0.98189300	-1.61306900
C	1.97161000	1.15096200	-2.97948600
H	2.43794200	1.18531100	-3.96477400
H	1.39026900	0.23344900	-2.86196000
H	1.26393000	1.97684100	-2.86572700
N	1.78724100	2.00806600	-0.00550200
C	1.70652900	2.69715600	1.23342000
O	2.62185700	3.29590800	1.72902800
O	0.46511400	2.57678600	1.67862700
C	0.10125200	3.09518100	3.00177600
C	0.92821700	2.38814500	4.07092300
H	0.65218800	2.79043500	5.04991900
H	0.70249300	1.31670000	4.06775400
H	1.99821100	2.54388200	3.91821700
C	-1.36240900	2.70162800	3.11362700
H	-1.74421600	2.96944700	4.10289400
H	-1.95259200	3.21903400	2.35787500
H	-1.46911600	1.62520400	2.95481400
C	0.28463700	4.60849800	3.03460800

H	-0.20833500	5.00630800	3.92657800
H	1.33984000	4.88263300	3.05421600
H	-0.19035200	5.05274000	2.15603300

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Zero-point correction=	1.151348 (Hartree/Particle)
Thermal correction to Energy=	1.220786
Thermal correction to Enthalpy=	1.221730
Thermal correction to Gibbs Free Energy=	1.047083
Sum of electronic and zero-point Energies=	-3976.867650
Sum of electronic and thermal Energies=	-3976.798211
Sum of electronic and thermal Enthalpies=	-3976.797267
Sum of electronic and thermal Free Energies=	-3976.971915

SCF Done: E(RM062X) = -3979.01341894

H	1.25341000	1.15432100	-0.18162200
C	4.18326400	-2.75968600	-1.85864200
C	3.22161800	-1.84788000	-2.07353900
C	2.50923100	-1.18157900	-0.94609600
C	2.70872500	-1.82824600	0.39279700
C	3.76529300	-2.79611500	0.56243000
C	4.45412700	-3.23310500	-0.51553900
H	4.73248200	-3.19215000	-2.68793400
H	2.96722400	-1.52753400	-3.07941500
H	1.43956900	-1.04924200	-1.16426600
H	3.93473600	-3.21448700	1.54601700
H	5.21162700	-3.99950300	-0.38105600
N	1.92860000	-1.43354400	1.36493100
H	0.95271000	-1.00624300	1.13483900
C	2.18031400	-1.58839000	2.75210600
C	1.08923800	-1.82221400	3.59017000
C	3.46502000	-1.39632600	3.26592900
C	1.31003800	-1.96722000	4.95490600
H	0.09752400	-1.88839100	3.15561500
C	3.66614200	-1.54192300	4.63481500
H	4.26787200	-1.08800200	2.60052800
C	2.59789200	-1.84551500	5.47651600
H	0.47106600	-2.16324500	5.61475900
H	4.65858600	-1.39207100	5.04634900
H	2.76308200	-1.95466600	6.54334700
C	-7.35715100	-2.24592300	1.34411100
C	-6.41751400	-1.43156200	0.76567400
C	-5.17786500	-1.95748700	0.31096600

C	-4.91882400	-3.34389000	0.50650600
C	-5.91860400	-4.16299200	1.09527400
C	-7.11357200	-3.63091300	1.50146100
H	-8.29513200	-1.82368500	1.68975100
H	-6.60950000	-0.36980300	0.65553300
C	-4.17261300	-1.14350500	-0.30467000
C	-3.65661400	-3.88128700	0.14477700
H	-5.70888700	-5.22093800	1.22651500
H	-7.86918400	-4.26395200	1.95474200
C	-2.65631100	-3.08791700	-0.36106500
C	-2.94670100	-1.71339600	-0.58090900
H	-3.46882400	-4.93964000	0.30864600
C	-4.37193100	0.29071100	-0.64708300
C	-5.43724200	0.72472000	-1.50439100
C	-3.44421200	1.22346800	-0.21978600
C	-6.35798900	-0.17609400	-2.10872700
C	-5.56100300	2.10990800	-1.80723900
C	-3.52656700	2.60028700	-0.56134400
C	-7.36649400	0.28250300	-2.91687300
H	-6.25095200	-1.24006200	-1.93280600
C	-6.62408900	2.55516000	-2.63702900
C	-4.59163100	3.02013900	-1.31800500
C	-7.51483400	1.66552200	-3.17533800
H	-8.05433200	-0.42447200	-3.36941400
H	-6.70598400	3.61843200	-2.84444700
H	-4.67336900	4.07143500	-1.58220000
H	-8.32194400	2.01362200	-3.81138300
O	-1.95583400	-0.93487000	-1.12479900
O	-2.40396000	0.83088600	0.59388800
P	-1.14074500	0.04459100	-0.08983100
O	-0.51159500	-0.77361800	1.00646300
O	-0.29566600	0.92285200	-0.95047500
C	1.10857400	-5.18690200	2.49058700
C	1.58235700	-5.17819300	1.21447900
C	0.80085400	-4.64295000	0.13993900
C	-0.50841200	-4.11918400	0.41475900
C	-0.95481100	-4.12453800	1.77855800
C	-0.18210600	-4.64819700	2.77187900
C	1.29809600	-4.60762900	-1.16132000
C	-1.29082500	-3.61255000	-0.64397100
C	-0.77941300	-3.59426600	-1.95896200
C	0.54354000	-4.08798500	-2.21355700
C	1.06248300	-4.04661700	-3.54721000
H	2.06942300	-4.41955200	-3.71562000

C	0.31377500	-3.55730200	-4.57423600
C	-1.01150300	-3.08922900	-4.33069500
C	-1.53865900	-3.11061500	-3.07409300
H	2.29327900	-4.99784800	-1.36241100
H	1.70933900	-5.58976000	3.29963000
H	2.56602400	-5.57676300	0.98018200
H	-1.91535900	-3.68216700	2.01497700
H	-0.53753300	-4.63176900	3.79753000
H	0.71445200	-3.53169800	-5.58255600
H	-1.60449500	-2.71415500	-5.15819900
H	-2.54930500	-2.75590900	-2.90605300
C	-2.33128000	5.14298100	3.77308700
C	-1.43621700	5.57827000	2.84247400
C	-1.45423400	5.06263800	1.50773500
C	-2.43418300	4.07499300	1.15492700
C	-3.35681100	3.64665600	2.16344500
C	-3.30445100	4.15954800	3.42606500
C	-0.53878300	5.49515400	0.54732700
C	-2.46182500	3.56233200	-0.15449700
C	-1.52055700	3.98878900	-1.11012900
C	-0.54347700	4.97657900	-0.74684400
C	0.40437100	5.41328300	-1.72698200
H	1.13702000	6.16068600	-1.43562000
C	0.38836900	4.90541900	-2.99013300
C	-0.57248000	3.91306500	-3.35043600
C	-1.48647600	3.46475500	-2.44437800
H	0.19826100	6.24900900	0.81677600
H	-2.30705200	5.53847500	4.78350800
H	-0.68602500	6.32307200	3.09493600
H	-4.09833000	2.89714200	1.90684200
H	-4.00753000	3.81755500	4.17856500
H	1.11125600	5.24351600	-3.72575300
H	-0.55987500	3.49951500	-4.35408700
H	-2.19039800	2.68691500	-2.71745000
C	3.09153000	1.01146200	-2.17299500
C	4.56980200	0.28776600	-0.48869700
C	3.05804700	0.33993900	-0.81101400
O	5.10991900	-0.29051200	0.42841900
N	4.27655800	1.33309100	-2.53061800
N	5.17592900	0.92810700	-1.54307500
C	6.56048800	1.10819700	-1.76708400
C	7.00095200	1.45648700	-3.04687200
C	7.47642500	0.95326100	-0.72187700
C	8.35882500	1.64059500	-3.27727700

H	6.27627100	1.58680700	-3.83996600
C	8.83116000	1.13767700	-0.97704300
H	7.12851400	0.69389100	0.26806800
C	9.28237300	1.47929300	-2.24829200
H	8.69389300	1.91290900	-4.27299400
H	9.53912800	1.01779700	-0.16326500
H	10.34135900	1.62291100	-2.43428400
C	1.88752300	1.34535300	-2.97925300
H	2.19874400	1.80811400	-3.91680000
H	1.28393000	0.45368600	-3.18148600
H	1.23237400	2.02487100	-2.42590200
N	2.24815100	1.08858600	0.08752900
C	2.55996800	1.47218200	1.37362500
O	3.67311000	1.66079800	1.81151200
O	1.40380000	1.60865500	2.04050900
C	1.33015600	2.35920300	3.28701800
C	2.15827600	1.69350800	4.38017600
H	1.99735900	2.23223900	5.31943500
H	1.83385600	0.65960800	4.51976600
H	3.22051400	1.70635500	4.13636000
C	-0.15575700	2.28122500	3.61259000
H	-0.37296800	2.82894100	4.53376200
H	-0.74736800	2.70986800	2.79968900
H	-0.45055200	1.23471900	3.73355600
C	1.77590700	3.79421700	3.02854400
H	1.58022800	4.40286500	3.91649300
H	2.84361800	3.83320500	2.80211600
H	1.21010400	4.21160700	2.19093900

C_1'

Zero-point correction= 1.150544 (Hartree/Particle)
Thermal correction to Energy= 1.219799
Thermal correction to Enthalpy= 1.220743
Thermal correction to Gibbs Free Energy= 1.045744
Sum of electronic and zero-point Energies= -3976.864425
Sum of electronic and thermal Energies= -3976.795170
Sum of electronic and thermal Enthalpies= -3976.794226
Sum of electronic and thermal Free Energies= -3976.969226
SCF Done: E(RM062X) = -3979.00741820

H	1.03599700	1.29856800	-1.11979600
C	5.87021100	0.83803600	1.38146700
C	4.93575700	0.22792900	0.63669700

C	3.50724500	0.65605100	0.64865000
C	3.15031900	1.62316500	1.74272000
C	4.20815000	2.29880600	2.46402000
C	5.48900600	1.89810000	2.29528800
H	6.91226600	0.54454900	1.32122600
H	5.19681900	-0.56560300	-0.06044400
H	2.83829600	-0.21374400	0.74631200
H	3.95463100	3.04113500	3.20786200
H	6.26609200	2.36763500	2.89150700
N	1.88286900	1.74934400	2.01569700
H	1.13011600	1.06287200	1.55472200
C	1.27567500	2.69557400	2.88547700
C	0.16889500	2.25759300	3.61616500
C	1.67971900	4.03092600	2.93031200
C	-0.49149400	3.15035400	4.45146800
H	-0.16464000	1.23221700	3.49786800
C	1.00969500	4.91183300	3.77418600
H	2.45517200	4.38185700	2.25701400
C	-0.06562900	4.47431500	4.54333500
H	-1.35031100	2.81290500	5.02173900
H	1.31642100	5.95232400	3.80817200
H	-0.58609500	5.16918300	5.19396200
C	-4.69567500	-4.57750600	3.21417900
C	-4.25472600	-3.82071000	2.15901100
C	-2.86538100	-3.60037100	1.95079000
C	-1.94662700	-4.15150800	2.88769900
C	-2.43466000	-4.94009600	3.96339100
C	-3.77766500	-5.15527500	4.12320900
H	-5.76041000	-4.73114200	3.35724700
H	-4.96740700	-3.37544000	1.47365700
C	-2.35810700	-2.81705900	0.86541700
C	-0.56243400	-3.87919200	2.75195900
H	-1.71750600	-5.36161300	4.66232900
H	-4.14201400	-5.75643300	4.94973100
C	-0.07611800	-3.08103400	1.74436100
C	-1.00397300	-2.56032900	0.80298000
H	0.12907200	-4.29468600	3.48088000
C	-3.23613900	-2.19527300	-0.16022500
C	-4.10041100	-2.96934600	-0.99853500
C	-3.16978800	-0.82614700	-0.34674200
C	-4.13323400	-4.39095300	-0.96398600
C	-4.93345000	-2.29857500	-1.93592400
C	-4.01340000	-0.14190100	-1.26212800
C	-4.97179000	-5.09461200	-1.78972200

H	-3.47635700	-4.91722300	-0.28021600
C	-5.79864800	-3.05508000	-2.77012800
C	-4.87867000	-0.88619200	-2.02696000
C	-5.82390900	-4.42234800	-2.69810800
H	-4.97794400	-6.17917000	-1.75143200
H	-6.43407600	-2.52353300	-3.47298800
H	-5.53551200	-0.37730400	-2.72788400
H	-6.48511100	-4.99324600	-3.34164900
O	-0.52933000	-1.77578800	-0.21928600
O	-2.29007900	-0.08308000	0.40701300
P	-0.69957800	-0.15680600	-0.01393200
O	0.05409400	0.22593100	1.23860900
O	-0.45388300	0.51241800	-1.31909600
C	3.25003600	-0.47067600	4.70526100
C	4.01587500	-1.11424300	3.77916200
C	3.41398500	-1.90079500	2.74595500
C	1.98470300	-2.02814700	2.70275100
C	1.21943700	-1.33800900	3.69923200
C	1.82959100	-0.58417300	4.65996000
C	4.18599000	-2.49571500	1.74745800
C	1.38260200	-2.78233300	1.67102700
C	2.16797200	-3.30667800	0.62738200
C	3.59526700	-3.14411000	0.66451800
C	4.38511900	-3.64709500	-0.41833700
H	5.46260500	-3.50752800	-0.37892500
C	3.80136600	-4.28093200	-1.47196500
C	2.38760700	-4.47368000	-1.49570200
C	1.60131000	-4.01263600	-0.48318500
H	5.26955700	-2.40787700	1.79124700
H	3.71520400	0.13704500	5.47512300
H	5.09941300	-1.02732200	3.79132400
H	0.13757700	-1.39527800	3.65030700
H	1.23041300	-0.05004800	5.39066000
H	4.40436600	-4.63836800	-2.30050000
H	1.93662900	-4.98970800	-2.33769400
H	0.52777200	-4.15900000	-0.51943700
C	-2.55111200	3.27140500	-4.84100800
C	-3.29142600	3.98194000	-3.94596000
C	-3.78047600	3.36981200	-2.74748100
C	-3.51751200	1.97518200	-2.52004000
C	-2.71315000	1.27127200	-3.47580900
C	-2.24363700	1.90008200	-4.59044200
C	-4.50744400	4.09417600	-1.80445100
C	-4.04824700	1.34638700	-1.37876100

C	-4.75129500	2.09606100	-0.41455300
C	-4.97463700	3.49745700	-0.63267700
C	-5.68301800	4.25061000	0.35563500
H	-5.83970000	5.31124800	0.17799900
C	-6.14863700	3.65591700	1.48943600
C	-5.93994500	2.26164900	1.70279300
C	-5.27194200	1.50825100	0.78333700
H	-4.70646600	5.14950100	-1.98053800
H	-2.17840000	3.74671500	-5.74278000
H	-3.51651600	5.03170300	-4.11545800
H	-2.45036900	0.23938600	-3.27285100
H	-1.62029500	1.35744400	-5.29332300
H	-6.68289000	4.23759600	2.23378300
H	-6.31805100	1.79899000	2.60868100
H	-5.11707100	0.44850400	0.95633500
C	4.32156100	1.81144900	-1.56866500
C	2.99018000	-0.12949900	-1.64508800
C	3.14732300	1.17532700	-0.83225200
O	2.19611500	-1.00750200	-1.39836200
N	4.72740200	1.07802900	-2.53935900
N	3.94167400	-0.07020200	-2.62802800
C	4.22388300	-1.03135200	-3.62718700
C	3.32647100	-2.07404200	-3.87683100
C	5.40736100	-0.92011800	-4.36135300
C	3.63699100	-3.00756400	-4.86078200
H	2.41396200	-2.15679600	-3.30076500
C	5.69401200	-1.86281400	-5.34114400
H	6.08118700	-0.09720100	-4.16077300
C	4.81529500	-2.91273400	-5.59543600
H	2.93901500	-3.81680700	-5.05300800
H	6.61400200	-1.77208400	-5.90962700
H	5.04450300	-3.64556900	-6.36169600
C	5.02549300	3.08958300	-1.25955100
H	4.43168800	3.94135700	-1.59362400
H	5.15188000	3.20727800	-0.18133500
H	5.99455200	3.08402000	-1.76083200
N	1.89250100	1.85101700	-0.89980900
C	1.68630000	3.08604000	-0.36239400
O	2.57212500	3.88434400	-0.09850800
O	0.38630700	3.23507500	-0.07629700
C	-0.37421400	4.41730200	-0.45132900
C	-1.70977700	4.16776000	0.23311800
H	-2.13239000	3.21793000	-0.10965800
H	-1.56717600	4.11764800	1.31744500

H	-2.41333200	4.97171300	0.00164000
C	-0.50321100	4.38566900	-1.96899700
H	-1.18385900	5.16999800	-2.31231900
H	0.47280400	4.54697100	-2.44058600
H	-0.89521200	3.41393200	-2.28653600
C	0.26565900	5.70896500	0.04573200
H	1.22718100	5.89499300	-0.43344900
H	-0.41147300	6.53873500	-0.17934600
H	0.41441600	5.66561500	1.12736700

TS-B_1

Zero-point correction= 1.148285 (Hartree/Particle)
Thermal correction to Energy= 1.217780
Thermal correction to Enthalpy= 1.218725
Thermal correction to Gibbs Free Energy= 1.041623
Sum of electronic and zero-point Energies= -3976.865041
Sum of electronic and thermal Energies= -3976.795545
Sum of electronic and thermal Enthalpies= -3976.794601
Sum of electronic and thermal Free Energies= -3976.971702
SCF Done: E(RM062X) = -3979.00583573
Number of Imaginary Frequencies = -131.99

H	1.39012000	1.02622500	0.20912800
C	3.79968400	-3.18724500	-1.35593300
C	2.90682700	-2.24608700	-1.69107700
C	2.28709600	-1.35721600	-0.65426600
C	2.42251100	-1.86123900	0.76713500
C	3.45770300	-2.84148300	1.05321700
C	4.09052700	-3.47003600	0.04142400
H	4.28416100	-3.78519700	-2.12099300
H	2.64643800	-2.06368300	-2.72924200
H	1.23298200	-1.15458800	-0.88734200
H	3.63125400	-3.12300900	2.08421200
H	4.81078900	-4.25028300	0.26972800
N	1.62413700	-1.35468300	1.65479400
H	0.34253800	-0.93580100	1.38737700
C	1.92672900	-1.33305200	3.03734500
C	3.21709900	-1.00699200	3.47376000
C	0.88758300	-1.48137100	3.95877100
C	3.47227600	-0.91033700	4.83720400
H	3.98879600	-0.79642500	2.73666600
C	1.15934300	-1.39027300	5.31872000
H	-0.11651400	-1.66896000	3.59602100

C	2.45120000	-1.11542800	5.76300300
H	4.47160100	-0.65595500	5.17546800
H	0.35363400	-1.51917900	6.03451900
H	2.65606500	-1.03627000	6.82561300
C	-7.63314700	-1.93824000	1.25071900
C	-6.62390900	-1.21486900	0.66868600
C	-5.37623400	-1.82265200	0.36239400
C	-5.18588400	-3.19003100	0.70919400
C	-6.25573200	-3.91505400	1.29805100
C	-7.45499700	-3.30756500	1.55963300
H	-8.57651500	-1.45467800	1.48224200
H	-6.76741100	-0.16381500	0.44348700
C	-4.29641500	-1.10490400	-0.24789900
C	-3.92498300	-3.80127200	0.49009400
H	-6.09686900	-4.96068900	1.54613400
H	-8.26510800	-3.86808100	2.01410800
C	-2.86182900	-3.09625500	-0.01786000
C	-3.07957500	-1.73979400	-0.37640400
H	-3.79036400	-4.84530800	0.76159200
C	-4.41863000	0.29871300	-0.72328000
C	-5.40004700	0.69120300	-1.69258600
C	-3.50342200	1.23969100	-0.29484900
C	-6.29616200	-0.23174700	-2.29952000
C	-5.45754700	2.05250500	-2.10334900
C	-3.52099200	2.59161500	-0.72517100
C	-7.22146300	0.18814600	-3.22021200
H	-6.23620400	-1.28101500	-2.03461500
C	-6.43614400	2.45830200	-3.04937700
C	-4.50991200	2.97585600	-1.59659900
C	-7.30554300	1.55068000	-3.59237200
H	-7.89250000	-0.53388200	-3.67397200
H	-6.47037800	3.50430800	-3.34043400
H	-4.54539700	4.00841400	-1.93415100
H	-8.04759400	1.86789600	-4.31746400
O	-2.00949200	-1.04525600	-0.90826200
O	-2.52869300	0.87323600	0.61950500
P	-1.26546800	0.02261400	0.06707300
O	-0.76178700	-0.71928500	1.31790100
O	-0.27462800	0.77694400	-0.73455000
C	0.71713900	-4.95840700	3.21044300
C	1.22261400	-5.14631000	1.96093100
C	0.49212600	-4.73425400	0.80012600
C	-0.79251700	-4.11199800	0.96155500
C	-1.27816700	-3.91780900	2.29789400

C	-0.55644200	-4.33630700	3.37561600
C	1.01302800	-4.91481400	-0.47896500
C	-1.51389300	-3.70780700	-0.17945400
C	-0.97236900	-3.88886600	-1.46911600
C	0.31628800	-4.50125300	-1.61463800
C	0.86315700	-4.67802400	-2.92533400
H	1.84341200	-5.13906500	-3.01229800
C	0.17582000	-4.27737000	-4.03067800
C	-1.11269000	-3.68145500	-3.89148100
C	-1.66748000	-3.49830400	-2.65988300
H	1.98716600	-5.38424100	-0.59496000
H	1.27951000	-5.26715100	4.08547900
H	2.19498900	-5.60880100	1.81402900
H	-2.22506100	-3.41030300	2.44193800
H	-0.93844900	-4.17035700	4.37824500
H	0.59848600	-4.41523000	-5.02059800
H	-1.65584700	-3.37426300	-4.77912800
H	-2.65142300	-3.05073200	-2.57178200
C	0.54131200	4.82709600	-2.96953400
C	0.45351400	5.39930600	-1.73692700
C	-0.54828900	4.98433200	-0.80187100
C	-1.48011100	3.96046500	-1.18490200
C	-1.33984400	3.37279100	-2.48518000
C	-0.36899200	3.79397500	-3.34437000
C	-0.64370900	5.55998600	0.46465000
C	-2.48448600	3.56691300	-0.28071800
C	-2.55418500	4.13261300	1.00528900
C	-1.61462700	5.15037700	1.37981000
C	-1.69920000	5.72723600	2.68665400
H	-0.97891500	6.49513600	2.95654200
C	-2.65246500	5.32097400	3.57068600
C	-3.58993000	4.31227900	3.19923800
C	-3.54566100	3.74198300	1.96183300
H	0.05642300	6.34393500	0.74800900
H	1.30653300	5.14721700	-3.66907300
H	1.14217800	6.18496300	-1.43785200
H	-2.01007300	2.56995300	-2.77127600
H	-0.27487200	3.33049500	-4.32147100
H	-2.70517500	5.76206200	4.56067000
H	-4.34412400	3.99784000	3.91323500
H	-4.26384500	2.97610200	1.68777100
C	3.04257900	0.55734700	-2.16553800
C	4.51518500	-0.11610100	-0.46668900
C	3.00378400	0.06888500	-0.73061700

O	5.02456400	-0.47009000	0.57532900
N	4.22620800	0.56246000	-2.65089700
N	5.12257100	0.12346600	-1.67538600
C	6.49536700	0.05712200	-1.99773100
C	7.45076700	-0.23532200	-1.01808700
C	6.89163000	0.27796800	-3.32081500
C	8.79228300	-0.30692500	-1.37919500
H	7.14213000	-0.39663800	0.00454300
C	8.23745000	0.20321100	-3.65692600
H	6.14235000	0.51077200	-4.06561100
C	9.19720100	-0.09111200	-2.69251000
H	9.52862500	-0.53147500	-0.61391700
H	8.53471300	0.37836900	-4.68608400
H	10.24672800	-0.14815400	-2.96084600
C	1.84822700	1.00754100	-2.92806500
H	1.10758100	0.20430900	-3.01067500
H	1.34487700	1.82048500	-2.39604500
H	2.15101000	1.34011800	-3.92187600
N	2.40861500	0.97331700	0.20644900
C	3.09831000	2.08991800	0.60619000
O	4.21858300	2.36923200	0.22605000
O	2.35818200	2.77985000	1.48179700
C	2.91207100	3.95710500	2.13333600
C	1.78822700	4.37560000	3.07359600
H	0.87295400	4.56034400	2.50677000
H	1.58853700	3.58517900	3.80156100
H	2.06908400	5.28679700	3.60940000
C	3.18451200	5.04208800	1.09612100
H	3.44988300	5.97435600	1.60372100
H	3.99885200	4.75297800	0.43149800
H	2.28059900	5.21019000	0.50329700
C	4.16130400	3.58019000	2.92560800
H	4.98102600	3.30336700	2.26322000
H	4.46781700	4.43261000	3.53904800
H	3.93717700	2.74005800	3.58978400

TS-B_1'

Zero-point correction=	1.147597 (Hartree/Particle)
Thermal correction to Energy=	1.217039
Thermal correction to Enthalpy=	1.217983
Thermal correction to Gibbs Free Energy=	1.040293
Sum of electronic and zero-point Energies=	-3976.851522

Sum of electronic and thermal Energies= -3976.782079
Sum of electronic and thermal Enthalpies= -3976.781135
Sum of electronic and thermal Free Energies= -3976.958825
SCF Done: E(RM062X) = -3978.99641181
Number of Imaginary Frequencies = -485.75

H	-1.29237400	-1.30309600	-0.01664100
C	-5.34849700	1.84319500	-0.43642700
C	-4.31316600	1.19755700	-0.99035700
C	-3.19370600	0.65788100	-0.15794700
C	-3.08898100	1.25911200	1.21974500
C	-4.29903600	1.83547200	1.78801700
C	-5.35758800	2.10245400	0.99322800
H	-6.18329000	2.18265700	-1.03983100
H	-4.27074000	0.99395800	-2.05591000
H	-2.24395000	0.74120800	-0.70455000
H	-4.33288700	2.04592100	2.84930000
H	-6.24940100	2.53892400	1.43415000
N	-1.97708400	1.10244200	1.86542400
H	-0.88591200	0.73588900	1.39310100
C	-1.78048700	1.34812600	3.25463600
C	-1.12284000	0.33578100	3.95956900
C	-2.13144300	2.54013100	3.88337700
C	-0.86730200	0.50508000	5.31469400
H	-0.81601100	-0.56022300	3.42552600
C	-1.85760900	2.70252900	5.23821500
H	-2.57430900	3.34370300	3.30687000
C	-1.23708500	1.68547200	5.95808600
H	-0.36409800	-0.28256900	5.86633800
H	-2.12152900	3.63606400	5.72551000
H	-1.02671700	1.81764300	7.01422800
C	6.36814400	4.05800800	-0.32127700
C	5.56213400	2.98645700	-0.60860700
C	4.14936400	3.13395300	-0.66546500
C	3.59134800	4.41191700	-0.38603600
C	4.45361700	5.50545700	-0.10635800
C	5.81226900	5.33665500	-0.07762000
H	7.44402100	3.92403500	-0.27576400
H	5.99814100	2.00979800	-0.78769000
C	3.26806200	2.04777100	-0.97104200
C	2.18406200	4.57020100	-0.37453000
H	4.00961600	6.47659000	0.09395900
H	6.46423600	6.17572200	0.14154900
C	1.32838600	3.51214100	-0.57738300

C	1.90685800	2.24362900	-0.86384800
H	1.77021000	5.55639900	-0.17986200
C	3.77398600	0.71219700	-1.38415300
C	4.61796100	0.55537700	-2.53245600
C	3.38576900	-0.41356500	-0.68405500
C	4.94872500	1.63405300	-3.39855900
C	5.11318400	-0.73876100	-2.85099900
C	3.90124200	-1.70634400	-0.96737900
C	5.75156200	1.43595300	-4.49250800
H	4.54790700	2.62024800	-3.19363700
C	5.95270500	-0.90956100	-3.98337900
C	4.75621700	-1.83914800	-2.03403400
C	6.27132500	0.15302500	-4.78613400
H	5.98570100	2.27129100	-5.14444800
H	6.32829600	-1.90502200	-4.20264400
H	5.16638400	-2.81979100	-2.26105500
H	6.90948500	0.01395700	-5.65246800
O	1.06664300	1.18927800	-1.12698500
O	2.49582400	-0.28175100	0.36582500
P	0.93644300	-0.02736900	-0.03846400
O	0.31584400	0.54417200	1.22881500
O	0.29542900	-1.16552700	-0.73932400
C	-1.89863400	5.72861300	2.78194200
C	-2.66840700	5.40364100	1.70527100
C	-2.11847600	4.67943400	0.59819400
C	-0.73007600	4.30708600	0.61779200
C	0.00894600	4.57796800	1.81869200
C	-0.54754600	5.27623500	2.85009800
C	-2.89574500	4.37810200	-0.51888100
C	-0.14640400	3.72511300	-0.53158700
C	-0.93642700	3.47575300	-1.67645600
C	-2.33818300	3.78732200	-1.65266100
C	-3.13435200	3.53618400	-2.81624200
H	-4.19353100	3.77549000	-2.77091200
C	-2.57932400	3.01933800	-3.94650900
C	-1.18179500	2.73871000	-3.98725800
C	-0.39088200	2.96574100	-2.90132000
H	-3.95034500	4.64598400	-0.52385300
H	-2.31675600	6.30034500	3.60476600
H	-3.71081600	5.70643600	1.65022300
H	1.02721000	4.21607900	1.89813000
H	0.03639800	5.47304600	3.74324800
H	-3.19015700	2.83229100	-4.82365900
H	-0.74434000	2.34344800	-4.89766800

H	0.67026200	2.75926100	-2.96273900
C	1.17987300	-6.05217300	-1.53681400
C	1.92448700	-6.23694800	-0.41174700
C	2.73408800	-5.17944400	0.11370500
C	2.78773500	-3.92730200	-0.59013100
C	1.96712100	-3.76665400	-1.75484000
C	1.18805200	-4.79052700	-2.20491500
C	3.46692900	-5.33875400	1.28860600
C	3.62840400	-2.90312100	-0.11712700
C	4.34357800	-3.06406100	1.08663200
C	4.25003400	-4.30454600	1.80334800
C	4.97027000	-4.45506000	3.02989400
H	4.88618800	-5.39889200	3.56196400
C	5.73957300	-3.44302300	3.51978500
C	5.84389400	-2.21416100	2.80444700
C	5.17702100	-2.03315700	1.62891700
H	3.42184300	-6.28748200	1.81968400
H	0.56127600	-6.85653000	-1.92170400
H	1.90749500	-7.18421700	0.12055100
H	1.94278200	-2.80036400	-2.24583900
H	0.55537900	-4.64386700	-3.07378900
H	6.27881400	-3.56668300	4.45336600
H	6.46100000	-1.41600000	3.20402500
H	5.26361200	-1.09313800	1.09406400
C	-4.64138200	-1.29437100	0.77869200
C	-3.73211000	-1.44558700	-1.38484400
C	-3.37304200	-0.94599100	0.02526800
O	-3.00175800	-1.42642100	-2.34993400
N	-5.55852700	-1.71582300	-0.00750600
N	-5.05752000	-1.80509400	-1.30695100
C	-5.91727600	-2.23910500	-2.34181800
C	-5.44021200	-2.39134700	-3.64845000
C	-7.25702900	-2.50654400	-2.04385700
C	-6.31790700	-2.80774100	-4.64440000
H	-4.40173700	-2.19152500	-3.87199000
C	-8.11338900	-2.92293000	-3.05538800
H	-7.60723500	-2.38917500	-1.02702200
C	-7.65328200	-3.07519100	-4.36053900
H	-5.94300800	-2.92644100	-5.65598600
H	-9.15134400	-3.13091300	-2.81577200
H	-8.32697100	-3.40142300	-5.14559900
C	-4.88959900	-1.18022200	2.25291800
H	-5.05982700	-2.17892500	2.65551500
H	-4.02253000	-0.76078700	2.76870700

H	-5.76119200	-0.55167700	2.44505500
N	-2.15176300	-1.45681100	0.53818000
C	-2.04636400	-2.45297000	1.47576500
O	-2.94525600	-3.17202800	1.86291600
O	-0.78147800	-2.45681100	1.91832600
C	-0.24487400	-3.58255900	2.66668100
C	1.21029800	-3.17310800	2.84812300
H	1.67681300	-3.01756800	1.87143300
H	1.27497300	-2.23588000	3.40997400
H	1.76290800	-3.94786900	3.38623800
C	-0.36344000	-4.83993900	1.81393600
H	0.22041400	-5.64909400	2.26366300
H	-1.40430600	-5.15795600	1.72672400
H	0.03943200	-4.64146700	0.81644400
C	-0.95031500	-3.71756400	4.01287500
H	-1.99442900	-4.00131000	3.88404100
H	-0.43980000	-4.47977000	4.60902500
H	-0.90367400	-2.77057900	4.56059700

TS-E_1

Zero-point correction= 1.147783 (Hartree/Particle)
Thermal correction to Energy= 1.217661
Thermal correction to Enthalpy= 1.218605
Thermal correction to Gibbs Free Energy= 1.038886
Sum of electronic and zero-point Energies= -3976.843100
Sum of electronic and thermal Energies= -3976.773223
Sum of electronic and thermal Enthalpies= -3976.772279
Sum of electronic and thermal Free Energies= -3976.951998
SCF Done: E(RM062X) = -3978.98521107
Number of Imaginary Frequencies = -636.92

H	-1.46434600	-1.26860300	0.17286700
C	-1.63442500	3.66245900	-0.96820700
C	-1.87223600	2.35490300	-1.21367600
C	-1.98483500	1.36371200	-0.14190600
C	-2.02154000	1.89275600	1.23772900
C	-1.74513200	3.27608200	1.44667000
C	-1.60139700	4.11756700	0.38470900
H	-1.48416600	4.36457800	-1.77922900
H	-1.92506900	1.99656600	-2.23603100
H	-0.81325000	1.04044600	0.06631000
H	-1.72048800	3.65550100	2.46137100
H	-1.46318900	5.17476400	0.58019600

N	-2.16176500	1.06601500	2.26314400
H	-2.48053900	0.12256600	2.05139300
C	-1.76264100	1.35364400	3.60205900
C	-0.42441900	1.65249300	3.85610900
C	-2.69968600	1.28077600	4.62813000
C	-0.03092300	1.89771600	5.16760500
H	0.27647700	1.66265000	3.02424700
C	-2.28955800	1.51960400	5.93659500
H	-3.73199300	1.04497700	4.38936600
C	-0.95901500	1.83166300	6.20571400
H	1.00996200	2.11821400	5.38273800
H	-3.01093500	1.46471200	6.74494000
H	-0.64294700	2.01575000	7.22721800
C	7.71020000	0.04348400	1.45510500
C	6.58617700	-0.40686100	0.81217600
C	5.58270200	0.50278400	0.37707200
C	5.75730400	1.88483700	0.66193500
C	6.93842200	2.32186700	1.31922400
C	7.89828200	1.42454000	1.70359700
H	8.46210200	-0.66702500	1.78288000
H	6.44898300	-1.46799200	0.63722000
C	4.39298200	0.07985200	-0.29634400
C	4.73768800	2.79897600	0.30652800
H	7.05745900	3.38337500	1.51758800
H	8.79645900	1.76467200	2.20835400
C	3.56494900	2.39190100	-0.28728000
C	3.40753500	1.00958400	-0.57260600
H	4.87923600	3.85438700	0.52508000
C	4.14383700	-1.34334200	-0.63885100
C	5.01437200	-2.10165600	-1.48579200
C	2.99311700	-1.93636600	-0.16377600
C	6.15692300	-1.53782300	-2.11681700
C	4.70463600	-3.46638300	-1.74225000
C	2.66198400	-3.29304500	-0.42030700
C	6.96170600	-2.30067400	-2.92368800
H	6.38302500	-0.48895100	-1.95913500
C	5.56419000	-4.23225200	-2.57363700
C	3.53067900	-4.03265000	-1.18465100
C	6.67145700	-3.66729300	-3.14869600
H	7.82702600	-1.85076500	-3.39961700
H	5.31734000	-5.27535100	-2.75048900
H	3.29960300	-5.07523100	-1.38803000
H	7.32046400	-4.25936700	-3.78548100
O	2.24271000	0.59505000	-1.17963000

O	2.12493100	-1.18161400	0.60213200
P	1.13611000	-0.19691900	-0.25318100
O	0.51252600	0.77650400	0.72605700
O	0.21272000	-0.95378000	-1.13921600
C	0.90342800	5.77135300	2.51697000
C	0.78100000	6.19122500	1.22686400
C	1.27017500	5.39324600	0.14187100
C	1.97787600	4.17912200	0.43480800
C	2.06718500	3.76484300	1.80494200
C	1.53503300	4.52415400	2.80549900
C	1.05896100	5.75998000	-1.18632300
C	2.54814900	3.43251700	-0.61625300
C	2.29174600	3.78859100	-1.95553300
C	1.51472800	4.96372000	-2.23843200
C	1.25247200	5.31425500	-3.60075200
H	0.65991500	6.20368300	-3.79792600
C	1.73704600	4.55655100	-4.62363000
C	2.52947300	3.40386600	-4.34677000
C	2.80479500	3.03823900	-3.06249200
H	0.52150900	6.68012600	-1.40866200
H	0.51786900	6.37774100	3.33043600
H	0.28943900	7.13222300	0.99102000
H	2.54160300	2.81475000	2.02694300
H	1.58956800	4.18243300	3.83415000
H	1.53035500	4.82944800	-5.65340100
H	2.91645600	2.81335100	-5.17058900
H	3.40676600	2.15822200	-2.86688200
C	1.10414900	-4.85070500	4.24355700
C	0.08779000	-5.17524800	3.39749100
C	0.16589800	-4.87069100	2.00158000
C	1.33395300	-4.20801200	1.49516200
C	2.38295100	-3.89243700	2.41876300
C	2.27044700	-4.20021300	3.74189900
C	-0.86453000	-5.20856600	1.12711000
C	1.41710900	-3.90228800	0.12407200
C	0.35719100	-4.22080200	-0.74644500
C	-0.79758900	-4.89640300	-0.22915200
C	-1.87284800	-5.21900000	-1.11648500
H	-2.73525100	-5.73671400	-0.70699300
C	-1.81642100	-4.88761900	-2.43631800
C	-0.67592600	-4.19948200	-2.95103900
C	0.36875300	-3.87357500	-2.13799200
H	-1.75596800	-5.69503800	1.51503600
H	1.03428100	-5.08452200	5.30098900

H	-0.80693000	-5.67087400	3.76376500
H	3.27589900	-3.39894600	2.04963000
H	3.07500700	-3.94826100	4.42532900
H	-2.63709700	-5.13895200	-3.10130000
H	-0.65135900	-3.91859200	-3.99946700
H	1.21185900	-3.31552800	-2.52813000
C	-3.07203600	-0.09574600	-1.96399700
C	-4.31590300	0.57528700	-0.09232900
C	-2.87968100	0.12864900	-0.46903200
O	-4.75340100	0.73686100	1.02798600
N	-4.21109900	0.31721900	-2.37651000
N	-4.93544200	0.82211000	-1.29260600
C	-6.25900200	1.26779800	-1.51252200
C	-6.82379900	1.12184700	-2.78304600
C	-6.99577700	1.85166500	-0.47613400
C	-8.12455200	1.55574200	-3.00826800
H	-6.23809700	0.67307600	-3.57436700
C	-8.29769500	2.27481100	-0.72455400
H	-6.55642400	1.95950000	0.50552500
C	-8.87100400	2.13178900	-1.98410500
H	-8.55600900	1.43841400	-3.99718500
H	-8.86592400	2.72441500	0.08343900
H	-9.88674300	2.46592500	-2.16605300
C	-2.10496200	-0.76662700	-2.87106800
H	-2.54352700	-0.84086200	-3.86701000
H	-1.14875100	-0.23877600	-2.89890700
H	-1.86606200	-1.76510400	-2.48889300
N	-2.45445600	-1.03355800	0.28623800
C	-3.28568700	-2.14341800	0.42348400
O	-2.98936700	-3.11746200	1.07163700
O	-4.43934400	-1.94484100	-0.22778900
C	-5.61203700	-2.76774900	0.05298200
C	-5.36302800	-4.19351800	-0.42446900
H	-6.29630200	-4.76142500	-0.37116100
H	-5.01644100	-4.18583100	-1.46215200
H	-4.61074000	-4.67900000	0.19704700
C	-6.69876400	-2.08712500	-0.76979000
H	-7.62032900	-2.67336500	-0.72797900
H	-6.90402700	-1.08623500	-0.37930100
H	-6.38400600	-1.99359100	-1.81358000
C	-5.93814700	-2.69624900	1.54117000
H	-6.90700200	-3.17106800	1.72003600
H	-5.17966000	-3.20619000	2.13640200
H	-5.99910200	-1.64855300	1.85027400

D_1

Zero-point correction= 1.149411 (Hartree/Particle)
Thermal correction to Energy= 1.219541
Thermal correction to Enthalpy= 1.220486
Thermal correction to Gibbs Free Energy= 1.041569
Sum of electronic and zero-point Energies= -3976.863924
Sum of electronic and thermal Energies= -3976.793793
Sum of electronic and thermal Enthalpies= -3976.792849
Sum of electronic and thermal Free Energies= -3976.971766
SCF Done: E(RM062X) = -3979.00571714

H	1.40989300	1.01239100	0.24056800
C	3.80040200	-3.19493200	-1.35016600
C	2.91293600	-2.24955700	-1.68745100
C	2.29416500	-1.35823100	-0.65169500
C	2.42272800	-1.86365000	0.77058300
C	3.45542200	-2.84783300	1.05812400
C	4.08772300	-3.47910600	0.04803800
H	4.28399300	-3.79485900	-2.11432800
H	2.65646500	-2.06572800	-2.72638700
H	1.24105600	-1.15271800	-0.88645700
H	3.62657000	-3.12926000	2.08962000
H	4.80500500	-4.26178800	0.27745200
N	1.62197500	-1.35615700	1.65429600
H	0.28666300	-0.93457400	1.39102500
C	1.92556000	-1.34073300	3.03633400
C	3.21442400	-1.00783500	3.47315500
C	0.88997300	-1.50125200	3.95994300
C	3.47145200	-0.91526300	4.83653700
H	3.98387900	-0.79037400	2.73559400
C	1.16348100	-1.41519700	5.31989800
H	-0.11363600	-1.69537000	3.59919800
C	2.45383800	-1.13226900	5.76342500
H	4.46969300	-0.65551700	5.17405400
H	0.36005100	-1.55423500	6.03643200
H	2.66001800	-1.05655600	6.82603500
C	-7.65073000	-1.92303000	1.23729100
C	-6.63837900	-1.20063000	0.65946500
C	-5.39192700	-1.81101900	0.35354900
C	-5.20596300	-3.17999800	0.69638500
C	-6.27899400	-3.90390900	1.28079600
C	-7.47702600	-3.29384900	1.54202400

H	-8.59312900	-1.43754800	1.46870200
H	-6.77851300	-0.14844500	0.43747500
C	-4.30884700	-1.09440000	-0.25247900
C	-3.94621800	-3.79408400	0.47839800
H	-6.12355200	-4.95075200	1.52587300
H	-8.28957500	-3.85353500	1.99314000
C	-2.87976800	-3.09053400	-0.02460100
C	-3.09386700	-1.73273700	-0.37999300
H	-3.81501900	-4.83920400	0.74732500
C	-4.42640100	0.31082400	-0.72438600
C	-5.40558000	0.70872300	-1.69388000
C	-3.50939700	1.24846800	-0.29298300
C	-6.30340800	-0.21009400	-2.30447900
C	-5.45880700	2.07136000	-2.10086900
C	-3.52140300	2.60125200	-0.72030300
C	-7.22651300	0.21497700	-3.22499000
H	-6.24655800	-1.26028900	-2.04264100
C	-6.43531000	2.48253600	-3.04675200
C	-4.50864900	2.99061300	-1.59134300
C	-7.30655600	1.57880500	-3.59323700
H	-7.89891700	-0.50393400	-3.68164700
H	-6.46634200	3.52942900	-3.33491600
H	-4.54022800	4.02389500	-1.92701200
H	-8.04695700	1.90008400	-4.31821400
O	-2.01962200	-1.03923000	-0.90730100
O	-2.53626300	0.87737500	0.62245300
P	-1.27707900	0.02323800	0.07174700
O	-0.79041600	-0.72653300	1.33039100
O	-0.26941700	0.76956500	-0.71401400
C	0.68842400	-4.96255800	3.21059000
C	1.19947000	-5.14350600	1.96234600
C	0.47217600	-4.72907400	0.80041900
C	-0.81459800	-4.11052900	0.95926800
C	-1.30615900	-3.92352900	2.29450100
C	-0.58773100	-4.34511400	3.37323100
C	0.99803300	-4.90456200	-0.47736400
C	-1.53208200	-3.70337700	-0.18320400
C	-0.98622900	-3.88047400	-1.47155700
C	0.30404100	-4.49002100	-1.61435700
C	0.85515100	-4.66328700	-2.92374600
H	1.83662700	-5.12205500	-3.00851600
C	0.17032800	-4.26200500	-4.03041000
C	-1.11970900	-3.66879500	-3.89392300
C	-1.67844900	-3.48884700	-2.66364000

H	1.97377500	-5.37103300	-0.59118700
H	1.24838700	-5.27292400	4.08657100
H	2.17390800	-5.60212400	1.81726600
H	-2.25504600	-3.41943600	2.43731600
H	-0.97444100	-4.18483000	4.37499800
H	0.59619000	-4.39723400	-5.01930900
H	-1.66090900	-3.36118900	-4.78263300
H	-2.66370200	-3.04365400	-2.57775800
C	0.55177700	4.81540000	-2.96539200
C	0.46936700	5.38545900	-1.73140700
C	-0.53411000	4.97538300	-0.79601300
C	-1.47363400	3.95902900	-1.18022100
C	-1.33920700	3.37359100	-2.48215800
C	-0.36630000	3.78969000	-3.34148600
C	-0.62376100	5.54861200	0.47205300
C	-2.47932600	3.57030500	-0.27532000
C	-2.54327100	4.13325600	1.01213400
C	-1.59608000	5.14351300	1.38773900
C	-1.67488700	5.71791600	2.69602300
H	-0.94904500	6.48029600	2.96665200
C	-2.62966700	5.31611600	3.58046400
C	-3.57452200	4.31472500	3.20800000
C	-3.53599800	3.74711000	1.96917900
H	0.08206100	6.32714100	0.75618800
H	1.31850100	5.13160000	-3.66505100
H	1.16382500	6.16565700	-1.43152200
H	-2.01615100	2.57706100	-2.77013700
H	-0.27671800	3.32785000	-4.31977900
H	-2.67795000	5.75519000	4.57155700
H	-4.32982100	4.00377600	3.92235600
H	-4.25997500	2.98696100	1.69432400
C	3.05113600	0.55737000	-2.15962600
C	4.52673200	-0.12584000	-0.46782700
C	3.01521100	0.06451300	-0.72631100
O	5.03845700	-0.48052500	0.57266700
N	4.23268800	0.55776400	-2.64991100
N	5.13073800	0.11193700	-1.67893200
C	6.50192200	0.04056400	-2.00649800
C	7.45837200	-0.27140300	-1.03381600
C	6.89580600	0.27544100	-3.32792900
C	8.79822800	-0.34767300	-1.40005100
H	7.15182800	-0.44377100	-0.01236600
C	8.24001700	0.19544900	-3.66922500
H	6.14591200	0.52268500	-4.06741400

C	9.20070900	-0.11785600	-2.71173500
H	9.53526500	-0.58743400	-0.64005700
H	8.53527300	0.38159700	-4.69704100
H	10.24898200	-0.17880700	-2.98409300
C	1.85553800	1.01627200	-2.91498900
H	1.11175700	0.21614500	-2.99958200
H	1.35770400	1.82813900	-2.37609700
H	2.15525200	1.35377700	-3.90807600
N	2.42754000	0.96933900	0.21502700
C	3.11762800	2.08737200	0.60674600
O	4.23470600	2.36730800	0.21743600
O	2.38264600	2.77882300	1.48608100
C	2.94153300	3.95510600	2.13451700
C	1.82277000	4.37595300	3.07985600
H	0.90528400	4.56238700	2.51703000
H	1.62471100	3.58594300	3.80870400
H	2.10775600	5.28662300	3.61436400
C	3.21116000	5.03963400	1.09604800
H	3.47966900	5.97172100	1.60233600
H	4.02222000	4.74927900	0.42801600
H	2.30498100	5.20860900	0.50695100
C	4.19379500	3.57598100	2.92086800
H	5.00924400	3.29629700	2.25437900
H	4.50589900	4.42821400	3.53174200
H	3.97095000	2.73707200	3.58700800

D_1'

Zero-point correction= 1.150817 (Hartree/Particle)
Thermal correction to Energy= 1.220640
Thermal correction to Enthalpy= 1.221584
Thermal correction to Gibbs Free Energy= 1.043243
Sum of electronic and zero-point Energies= -3976.849784
Sum of electronic and thermal Energies= -3976.779961
Sum of electronic and thermal Enthalpies= -3976.779016
Sum of electronic and thermal Free Energies= -3976.957358
SCF Done: E(RM062X) = -3978.99532309

H	-1.41286700	-1.26825400	-0.03356000
C	-5.41042400	1.96160700	-0.37268900
C	-4.42931700	1.25640700	-0.94946700
C	-3.29259900	0.69107300	-0.15298000
C	-3.11210700	1.30850500	1.21657300
C	-4.28696400	1.94799100	1.81253000

C	-5.35835900	2.25195800	1.05347000
H	-6.25200000	2.32391400	-0.95365500
H	-4.44196700	1.02803100	-2.01096000
H	-2.36330800	0.76746300	-0.73508700
H	-4.27404800	2.17441600	2.87160300
H	-6.21543100	2.73475700	1.51464200
N	-1.98427600	1.12557500	1.81549400
H	-0.57936300	0.65909000	1.36037900
C	-1.76190700	1.45378400	3.17997600
C	-1.18708100	0.45311600	3.97031600
C	-1.99747600	2.71904900	3.71518000
C	-0.90288000	0.70877700	5.30597900
H	-0.96677600	-0.50812100	3.51325000
C	-1.69124000	2.97115300	5.04903500
H	-2.39115100	3.50238800	3.07843300
C	-1.15497600	1.96738700	5.85063400
H	-0.46758900	-0.07360800	5.91980400
H	-1.86744200	3.96260600	5.45573100
H	-0.91983100	2.16779700	6.89071200
C	6.46192500	3.94920200	-0.45687800
C	5.63907600	2.87908900	-0.69828200
C	4.22805200	3.04385200	-0.74462100
C	3.68950100	4.33776100	-0.50490000
C	4.56875700	5.42893900	-0.27297400
C	5.92525000	5.24275400	-0.25227400
H	7.53635400	3.80262500	-0.41770100
H	6.06071300	1.89120700	-0.84764400
C	3.32877900	1.95972600	-1.00362300
C	2.28476600	4.51601200	-0.48801700
H	4.13965000	6.41225800	-0.10230900
H	6.59041700	6.08002300	-0.06906900
C	1.41078200	3.46406500	-0.63914000
C	1.97283400	2.17869500	-0.88000500
H	1.88648600	5.51513700	-0.33150800
C	3.81788700	0.61117700	-1.39613200
C	4.64445300	0.42479100	-2.55360700
C	3.43657300	-0.49964200	-0.67179200
C	4.96701400	1.48260500	-3.44771700
C	5.12839000	-0.87890000	-2.85082900
C	3.93394400	-1.80270000	-0.93486600
C	5.75273000	1.25637000	-4.54864700
H	4.57370300	2.47500900	-3.25938200
C	5.95112800	-1.07836900	-3.99084100
C	4.77529700	-1.96163100	-2.00852300

C	6.26278000	-0.03500500	-4.82100600
H	5.98063800	2.07583800	-5.22244800
H	6.31881900	-2.08012500	-4.19384100
H	5.17373200	-2.94976200	-2.22328500
H	6.88778600	-0.19600500	-5.69305700
O	1.11050200	1.12457500	-1.09287000
O	2.55601600	-0.34284400	0.38982800
P	1.00997000	-0.08822200	-0.01508900
O	0.45288500	0.51142800	1.30156000
O	0.31063200	-1.21582200	-0.65936800
C	-1.76123900	5.92708300	2.60562800
C	-2.54291600	5.54485500	1.55657400
C	-2.01084200	4.74590100	0.49347800
C	-0.62669100	4.35867900	0.52438600
C	0.12487900	4.69657900	1.69993700
C	-0.41494500	5.46503800	2.68978300
C	-2.80291100	4.38349600	-0.59491400
C	-0.06069500	3.70189500	-0.59395400
C	-0.86256300	3.40057900	-1.71786800
C	-2.26191700	3.72378900	-1.69762900
C	-3.07233000	3.41513700	-2.83731800
H	-4.12900900	3.66435000	-2.79311400
C	-2.53403100	2.83178200	-3.94274100
C	-1.13812200	2.54384000	-3.98408200
C	-0.33361500	2.82595000	-2.92140200
H	-3.85577300	4.65741800	-0.60395300
H	-2.16634800	6.55268900	3.39482200
H	-3.58323100	5.85245000	1.49210400
H	1.14001700	4.33013100	1.79609600
H	0.17970900	5.71064600	3.56363100
H	-3.15587500	2.59916000	-4.80092000
H	-0.71229300	2.10000500	-4.87751300
H	0.72674600	2.61653000	-2.98785500
C	1.13494300	-6.11278400	-1.40654500
C	1.85691900	-6.27391800	-0.26339700
C	2.68745500	-5.21951600	0.23450200
C	2.78664400	-3.99666400	-0.51397400
C	1.99009900	-3.86023600	-1.69827500
C	1.19023100	-4.87907700	-2.12252200
C	3.39557400	-5.35350100	1.42753900
C	3.64219300	-2.97604200	-0.06002700
C	4.33411000	-3.11072800	1.16019500
C	4.19817300	-4.32240800	1.91778300
C	4.89449200	-4.44770200	3.16084900

H	4.77885600	-5.37023500	3.72332600
C	5.67962500	-3.43766300	3.62919700
C	5.82502300	-2.23711800	2.87420400
C	5.18252800	-2.08137200	1.68158900
H	3.31533000	-6.27993700	1.99268500
H	0.49959200	-6.91368400	-1.77045300
H	1.80515300	-7.19885400	0.30464700
H	2.00446600	-2.91632800	-2.23134600
H	0.57743500	-4.74963800	-3.00820600
H	6.20020400	-3.54144700	4.57562700
H	6.45441500	-1.44031800	3.25690500
H	5.30260900	-1.16301100	1.11640200
C	-4.74635300	-1.23478200	0.80503700
C	-3.87790500	-1.40540300	-1.37298900
C	-3.49007600	-0.89785500	0.02538100
O	-3.16672700	-1.38648600	-2.35376400
N	-5.67491600	-1.67258300	0.04158400
N	-5.19555700	-1.78127100	-1.26543000
C	-6.06875800	-2.24331100	-2.27597800
C	-5.61271900	-2.41938000	-3.58715600
C	-7.40078300	-2.51661200	-1.94960200
C	-6.50307200	-2.86533200	-4.55873000
H	-4.58025600	-2.21359600	-3.83220300
C	-8.27019200	-2.96242500	-2.93714600
H	-7.73457900	-2.38009000	-0.92965600
C	-7.83093500	-3.13878500	-4.24641500
H	-6.14436200	-3.00220700	-5.57393400
H	-9.30203500	-3.17423400	-2.67542100
H	-8.51476600	-3.48776000	-5.01273500
C	-4.98057100	-1.07465100	2.27731400
H	-5.17915800	-2.05601800	2.70860700
H	-4.09879700	-0.66660300	2.77573500
H	-5.83138400	-0.41412900	2.45546500
N	-2.26711500	-1.44590100	0.50462400
C	-2.13414200	-2.36474500	1.50962000
O	-3.01748600	-3.06025800	1.96871800
O	-0.85784500	-2.32883500	1.92557500
C	-0.27573800	-3.42460800	2.68287000
C	1.17636800	-2.98336800	2.80685700
H	1.61867100	-2.87650300	1.81188000
H	1.23654800	-2.01494300	3.31376100
H	1.75416800	-3.71804600	3.37391600
C	-0.39749900	-4.70334600	1.86311400
H	0.20787700	-5.49426300	2.31688700

H	-1.43621800	-5.03645600	1.80985000
H	-0.02202400	-4.52291400	0.85120500
C	-0.93290900	-3.54598300	4.05467900
H	-1.98132400	-3.82851400	3.96446000
H	-0.40283000	-4.30490900	4.63793800
H	-0.86463600	-2.59622100	4.59487600

E_1

Zero-point correction= 0.510770 (Hartree/Particle)
Thermal correction to Energy= 0.541603
Thermal correction to Enthalpy= 0.542547
Thermal correction to Gibbs Free Energy= 0.445487
Sum of electronic and zero-point Energies= -1489.315707
Sum of electronic and thermal Energies= -1489.284874
Sum of electronic and thermal Enthalpies= -1489.283929
Sum of electronic and thermal Free Energies= -1489.380990
SCF Done: E(RM062X) = -1490.23369394

H	1.62962400	0.56962900	1.24804600
C	-1.27020300	-3.33298800	1.57791900
C	-1.04058300	-2.21163800	2.26826300
C	0.11722900	-1.30628600	1.94813400
C	1.15599900	-1.91931000	1.01408500
C	0.77205100	-3.10126900	0.23627200
C	-0.36338400	-3.76323900	0.51631700
H	-2.12977500	-3.95309600	1.80902500
H	-1.71347500	-1.90314900	3.06269200
H	0.63088500	-1.00860900	2.87120300
H	1.45570800	-3.45451500	-0.52590100
H	-0.61267500	-4.66237500	-0.03866500
N	2.29926200	-1.33681600	0.97859200
C	3.24571700	-1.65660900	-0.01940000
C	2.93591800	-1.45603800	-1.37030000
C	4.52723800	-2.07089400	0.34945200
C	3.90303700	-1.69619700	-2.34066200
H	1.94085900	-1.10128000	-1.62922000
C	5.48066500	-2.32252100	-0.63102700
H	4.75682100	-2.19677100	1.40237600
C	5.17415700	-2.13579400	-1.97739000
H	3.66080200	-1.53722600	-3.38674400
H	6.47134400	-2.65795400	-0.34094000
H	5.92452700	-2.32380600	-2.73801800
C	-1.59851300	0.55475000	2.08836300

C	-1.06471700	-0.25425200	-0.03750400
C	-0.39974700	0.04347600	1.32206700
O	-0.49232600	-0.58971700	-1.05359900
N	-2.69381500	0.41727300	1.44517000
N	-2.41324800	-0.10477300	0.18105500
C	-3.47791600	-0.28261200	-0.73133500
C	-3.25244400	-0.86405600	-1.98356400
C	-4.76605600	0.11424300	-0.36085200
C	-4.32428000	-1.03780200	-2.85289100
H	-2.25377500	-1.16416700	-2.26736200
C	-5.82143800	-0.07137600	-1.24517600
H	-4.92371300	0.56272000	0.61089700
C	-5.61062100	-0.64670200	-2.49509500
H	-4.14337700	-1.48689000	-3.82432900
H	-6.81813100	0.24106400	-0.95017500
H	-6.43851400	-0.78716500	-3.18176300
C	-1.52747100	1.13644500	3.45475300
H	-0.90612500	2.03674600	3.43645000
H	-2.52813100	1.39235700	3.80324600
H	-1.06566800	0.43443200	4.15820200
N	0.69402100	0.97238500	1.24789900
C	0.49262900	2.12719800	0.53677700
O	-0.61026400	2.50261000	0.18852500
O	1.65685700	2.75324800	0.33079800
C	1.69342300	3.98571900	-0.44749200
C	3.17848900	4.32763700	-0.46253300
H	3.54633300	4.47114800	0.55659900
H	3.74916100	3.52068400	-0.92875700
H	3.34229800	5.24815400	-1.02850300
C	0.89549200	5.07673300	0.26032900
H	1.04421200	6.02700700	-0.26041900
H	-0.16814800	4.83964700	0.27032200
H	1.25019100	5.19070000	1.28879600
C	1.18643800	3.72202100	-1.86227600
H	0.12289300	3.48404800	-1.86121600
H	1.35213200	4.61201200	-2.47603900
H	1.73939600	2.88922400	-2.30602600

E_1'

Zero-point correction=	0.510760 (Hartree/Particle)
Thermal correction to Energy=	0.541668
Thermal correction to Enthalpy=	0.542612
Thermal correction to Gibbs Free Energy=	0.445250

Sum of electronic and zero-point Energies= -1489.313714
Sum of electronic and thermal Energies= -1489.282805
Sum of electronic and thermal Enthalpies= -1489.281861
Sum of electronic and thermal Free Energies= -1489.379223
SCF Done: E(RM062X) = -1490.23287302

H	-1.39679800	0.74124500	-0.98861200
C	0.49040200	-3.74622500	-0.32976200
C	0.73056400	-2.64950400	-1.05511100
C	-0.23307600	-1.49521500	-1.09257800
C	-1.62060100	-1.81963900	-0.55686500
C	-1.75313100	-2.98785800	0.32219900
C	-0.74935900	-3.87696000	0.43190000
H	1.20998400	-4.55693700	-0.29756400
H	1.64748900	-2.54302000	-1.62745800
H	-0.33290700	-1.14695500	-2.12824000
H	-2.67826200	-3.11045200	0.87473700
H	-0.86109900	-4.73306000	1.09085200
N	-2.55614400	-0.99335200	-0.85776700
C	-3.87196200	-1.15610300	-0.37856500
C	-4.43812700	-0.11152600	0.35932100
C	-4.64395800	-2.28043600	-0.68931300
C	-5.74746300	-0.21092200	0.81376200
H	-3.83364900	0.76645500	0.56857700
C	-5.95995500	-2.36329700	-0.24481700
H	-4.20825800	-3.07209400	-1.29148400
C	-6.51420900	-1.33539600	0.51309300
H	-6.17503200	0.59852600	1.39664600
H	-6.55425800	-3.23639300	-0.49471500
H	-7.53989300	-1.40480400	0.85903400
C	0.65861200	-0.48469100	1.11137000
C	1.80358200	-0.09945600	-0.89524800
C	0.36734800	-0.24001000	-0.35451600
O	2.10642900	0.15379600	-2.03948400
N	1.90578500	-0.64446300	1.34314300
N	2.61355700	-0.47520900	0.15245500
C	4.01915700	-0.62087100	0.17029700
C	4.78099900	-0.34855100	-0.97125300
C	4.64077600	-1.05764400	1.34429100
C	6.16059600	-0.52150800	-0.92151400
H	4.29772600	-0.00309000	-1.87401200
C	6.02010700	-1.22021800	1.37019300
H	4.03759500	-1.25902800	2.21949200
C	6.78975700	-0.95609800	0.24051300

H	6.74701900	-0.30697200	-1.80925500
H	6.49464700	-1.55736100	2.28628300
H	7.86646600	-1.08520700	0.26697700
C	-0.34656000	-0.41581100	2.20851700
H	-0.69534700	0.61879600	2.30379200
H	-1.21730800	-1.04576400	2.01144200
H	0.11813500	-0.71542300	3.14834400
N	-0.45923200	0.89641800	-0.63239500
C	-0.07790800	2.11796700	-0.16663900
O	0.98286400	2.30709700	0.39896600
O	-1.02976100	3.02903400	-0.41905700
C	-0.83178300	4.41607400	-0.01884200
C	-2.11465100	5.08804300	-0.49390500
H	-2.22173800	4.97992300	-1.57603500
H	-2.98392900	4.63425100	-0.01068500
H	-2.09121100	6.15240900	-0.24698500
C	0.38099200	5.00201000	-0.73543100
H	0.43594500	6.07521900	-0.53160400
H	1.30245900	4.52796300	-0.39828400
H	0.27948600	4.86159500	-1.81515800
C	-0.70650500	4.50745000	1.49946800
H	0.21359500	4.03684200	1.84546500
H	-0.70334400	5.55914500	1.79960500
H	-1.56338800	4.01938700	1.97401300

F_1

Zero-point correction= 1.151120 (Hartree/Particle)
Thermal correction to Energy= 1.221325
Thermal correction to Enthalpy= 1.222270
Thermal correction to Gibbs Free Energy= 1.044208
Sum of electronic and zero-point Energies= -3976.849279
Sum of electronic and thermal Energies= -3976.779073
Sum of electronic and thermal Enthalpies= -3976.778129
Sum of electronic and thermal Free Energies= -3976.956190
SCF Done: E(RM062X) = -3978.99125063

H	4.85980800	1.05230900	-2.81182600
C	5.84115400	-2.20593600	-0.72846400
C	4.81796200	-1.64948400	-1.38766300
C	3.70637600	-0.92297000	-0.68196100
C	3.86044000	-0.82239600	0.83456600
C	5.02200700	-1.47515000	1.46013400
C	5.93211800	-2.13819300	0.72830100

H	6.61526300	-2.73776200	-1.27343700
H	4.74830800	-1.71453600	-2.46965000
H	2.78105700	-1.49760900	-0.82717400
H	5.09005300	-1.43878400	2.54108100
H	6.75923700	-2.64323500	1.21877900
N	2.90082800	-0.26361200	1.46562900
H	-0.08309500	1.23004200	-0.25392000
C	2.99421700	0.02319600	2.84164700
C	4.06835900	0.76731100	3.35021500
C	1.94333300	-0.34931500	3.68239600
C	4.10119000	1.09998900	4.70095800
H	4.85546400	1.08521500	2.67017200
C	1.99800000	-0.02709100	5.03319000
H	1.08998600	-0.87116300	3.26457400
C	3.07314100	0.69515600	5.54919700
H	4.93202000	1.68089400	5.08982000
H	1.18040400	-0.32904800	5.68068200
H	3.10124700	0.95643100	6.60222400
C	-6.15591000	-1.22029700	-3.40526800
C	-5.44983100	-1.34765100	-2.23615900
C	-5.02910200	-0.19920700	-1.50944000
C	-5.33252800	1.08560000	-2.04420000
C	-6.08104900	1.18251500	-3.24735600
C	-6.48701600	0.05749500	-3.91498300
H	-6.45865200	-2.10959300	-3.94840200
H	-5.19124100	-2.33307100	-1.86610300
C	-4.24762700	-0.28519700	-0.31019700
C	-4.82275000	2.24782700	-1.41116300
H	-6.30801700	2.17128500	-3.63569400
H	-7.05034500	0.14167300	-4.83836100
C	-4.02088200	2.17006600	-0.30023500
C	-3.75854800	0.88209300	0.24049300
H	-5.03618700	3.22173500	-1.84402800
C	-3.83260400	-1.59424900	0.26433500
C	-4.75508700	-2.60811000	0.67976200
C	-2.48554200	-1.85130200	0.39544100
C	-6.15934600	-2.39613500	0.70182900
C	-4.24763700	-3.86339400	1.12054100
C	-1.95616200	-3.10900300	0.78425600
C	-7.01147100	-3.38744800	1.11710600
H	-6.55045300	-1.43176700	0.39503100
C	-5.15752500	-4.87134000	1.53427200
C	-2.84581700	-4.09319700	1.13281700
C	-6.50855200	-4.64307400	1.53129300

H	-8.08109300	-3.20580800	1.13442100
H	-4.75722900	-5.82695700	1.86080300
H	-2.47232400	-5.07129300	1.42488500
H	-7.19488700	-5.41886600	1.85399200
O	-2.98601600	0.81243700	1.38411100
O	-1.58006600	-0.84512000	0.10172900
P	-1.45484300	0.29935100	1.25642700
O	-0.73861000	1.45122100	0.47364800
O	-0.94215000	-0.16295300	2.54710300
C	0.01415700	5.13254100	-1.52639700
C	-0.49471400	5.67360300	-0.38448200
C	-1.64959000	5.11124700	0.24805000
C	-2.28462100	3.96989700	-0.34751700
C	-1.72555000	3.44464300	-1.55850300
C	-0.61264100	3.99543500	-2.11960400
C	-2.15409600	5.63683800	1.43687400
C	-3.38791000	3.38031800	0.29742500
C	-3.87779100	3.90589200	1.50624500
C	-3.25238100	5.06372400	2.07814700
C	-3.76549200	5.59661400	3.30262900
H	-3.28218700	6.47396000	3.72340800
C	-4.82819700	5.01738500	3.92731700
C	-5.44798300	3.86314900	3.36356200
C	-4.99092800	3.32729200	2.19657900
H	-1.67190900	6.50436600	1.88192000
H	0.89465900	5.56376300	-1.99230400
H	-0.02828400	6.53945100	0.07744900
H	-2.19028200	2.58085500	-2.02138600
H	-0.19792400	3.56185000	-3.02469900
H	-5.20769900	5.42787400	4.85729300
H	-6.29106100	3.40901400	3.87392600
H	-5.46987700	2.44995000	1.77411700
C	1.93645800	-3.69928500	4.16072700
C	2.50561200	-3.79468700	2.92711500
C	1.71099400	-3.68394900	1.74227600
C	0.29643300	-3.45927500	1.86652300
C	-0.25704700	-3.34350200	3.18384000
C	0.53432500	-3.46791400	4.28734500
C	2.28597300	-3.77720600	0.47514400
C	-0.48517300	-3.33462100	0.70375800
C	0.10863600	-3.40275900	-0.57294300
C	1.51926400	-3.63906400	-0.68314000
C	2.12194700	-3.66878000	-1.98274100
H	3.19383900	-3.84095700	-2.04439300

C	1.38006000	-3.45470500	-3.10600800
C	-0.02668100	-3.24316300	-3.00113100
C	-0.63908000	-3.22890300	-1.78376500
H	3.36153600	-3.92915600	0.38696700
H	2.54797500	-3.77391000	5.05396500
H	3.57517500	-3.95028100	2.81250900
H	-1.31372100	-3.12412100	3.28786600
H	0.09967000	-3.36644600	5.27656200
H	1.85322300	-3.44384400	-4.08274800
H	-0.61049100	-3.06889700	-3.89979100
H	-1.70939900	-3.06074700	-1.72799200
C	2.32855900	1.24372900	-0.76388000
C	2.69191500	0.01083100	-2.71531200
C	3.42745800	0.44538300	-1.43742500
O	3.22220800	-0.44521300	-3.70962800
N	1.19255700	1.02732600	-1.32637800
N	1.36334500	0.22605800	-2.46767300
C	0.26634700	0.00612200	-3.34073800
C	-1.03442700	0.15885200	-2.85641200
C	0.48224900	-0.38096900	-4.66741000
C	-2.11532900	-0.08724800	-3.69565200
H	-1.21072500	0.44682400	-1.82954900
C	-0.61368600	-0.62494700	-5.49066700
H	1.48855400	-0.49874300	-5.04245100
C	-1.91369800	-0.48497800	-5.01490200
H	-3.12234100	0.02978200	-3.30713300
H	-0.43888500	-0.92590800	-6.51878100
H	-2.76301600	-0.67847600	-5.66156100
C	2.48321600	2.28007500	0.29756200
H	2.45110100	3.26456600	-0.18239400
H	1.66094600	2.21795500	1.01322600
H	3.43333600	2.16104900	0.81468300
N	4.60542000	1.17607500	-1.83745900
C	5.66174200	1.33672400	-0.97582000
O	5.57218000	1.23895700	0.23229700
O	6.76598400	1.64256500	-1.66657900
C	8.03907900	1.80089100	-0.97066400
C	7.97099700	2.98198900	-0.00750100
H	8.96985300	3.17589700	0.39356600
H	7.63542800	3.87734400	-0.53830500
H	7.29065600	2.77874100	0.81889500
C	9.00857100	2.09225700	-2.10979800
H	10.01731900	2.23033500	-1.71286600
H	9.02121700	1.26251600	-2.82094100

H	8.71206700	3.00133100	-2.63899700
C	8.40758200	0.49651700	-0.26892200
H	8.38018200	-0.33025600	-0.98533200
H	9.42358600	0.57559700	0.12821700
H	7.72028500	0.27967300	0.54983200

F_1'

Zero-point correction=	1.150893 (Hartree/Particle)
Thermal correction to Energy=	1.221079
Thermal correction to Enthalpy=	1.222023
Thermal correction to Gibbs Free Energy=	1.043867
Sum of electronic and zero-point Energies=	-3976.857619
Sum of electronic and thermal Energies=	-3976.787433
Sum of electronic and thermal Enthalpies=	-3976.786489
Sum of electronic and thermal Free Energies=	-3976.964645

SCF Done: E(RM062X) = -3978.99943838

H	-0.77841200	-0.10401600	-1.43097800
C	-6.44321500	-0.71860700	3.28357900
C	-5.13813500	-0.77518700	2.99463200
C	-4.66059300	-1.09551800	1.60727300
C	-5.70676300	-0.89567800	0.52378200
C	-7.11279000	-0.94885400	0.92913700
C	-7.44268700	-0.85137700	2.23149100
H	-6.77768700	-0.55129300	4.30149700
H	-4.38265100	-0.66278800	3.76401600
H	-4.43363000	-2.17452900	1.62912400
H	-7.87312600	-0.95550800	0.15736100
H	-8.49180700	-0.82107900	2.51256600
N	-5.25823600	-0.67464900	-0.65548800
C	-6.07761200	-0.56725000	-1.79056300
C	-5.95342600	0.58140600	-2.58019500
C	-6.92816600	-1.59875300	-2.20510800
C	-6.70494100	0.71235400	-3.74120200
H	-5.26410200	1.35870700	-2.26233500
C	-7.66543500	-1.46520200	-3.37771700
H	-6.99055000	-2.50518000	-1.60965000
C	-7.56404500	-0.30842700	-4.14575200
H	-6.61087700	1.61278600	-4.33992700
H	-8.32038700	-2.27169900	-3.69252400
H	-8.14150100	-0.20704100	-5.05854000
C	6.93728200	0.41335000	-3.27143500
C	6.02700800	0.57203900	-2.25793500

C	5.04498000	-0.42200100	-1.99944900
C	5.00799500	-1.57212800	-2.83856800
C	5.97280700	-1.71180000	-3.87055200
C	6.91998200	-0.74517300	-4.08258400
H	7.67470700	1.18730000	-3.45726900
H	6.04243600	1.46919200	-1.64920900
C	4.07035300	-0.28858500	-0.95494900
C	4.01096200	-2.56289900	-2.63522400
H	5.93672000	-2.60003500	-4.49484800
H	7.64990800	-0.85896700	-4.87708000
C	3.03925300	-2.41159600	-1.67971700
C	3.07503500	-1.23816100	-0.88201200
H	4.01949900	-3.45794800	-3.25170300
C	4.07851500	0.84325300	0.01368800
C	5.20887300	1.13665300	0.84740800
C	2.95084600	1.62130200	0.15908400
C	6.36875700	0.31602700	0.88124500
C	5.15829600	2.27265200	1.70472600
C	2.88196000	2.76796700	0.99575800
C	7.42759500	0.62862400	1.69504600
H	6.40604400	-0.57227900	0.26051500
C	6.27608500	2.57475300	2.52608900
C	3.99084200	3.08107300	1.73848000
C	7.38921600	1.77626500	2.52061200
H	8.30159100	-0.01430600	1.71032600
H	6.22420700	3.45029700	3.16696300
H	3.97384100	3.96094700	2.37614700
H	8.23646000	2.01347600	3.15534200
O	2.06811600	-1.10082000	0.05704700
O	1.82770300	1.31954300	-0.59433200
P	0.94541200	0.03761700	-0.16148100
O	0.21506900	-0.27507800	-1.51543300
O	0.11708200	0.15108400	1.04707200
C	-1.49706800	-3.91838600	-3.69470500
C	-1.25970100	-4.76785500	-2.65684900
C	-0.08168200	-4.63638600	-1.85363100
C	0.86229400	-3.59670100	-2.16217700
C	0.56880300	-2.72109900	-3.25836900
C	-0.56907200	-2.87553900	-3.99386700
C	0.16476000	-5.49502000	-0.78331000
C	2.02652400	-3.46875300	-1.38449400
C	2.26771100	-4.34310300	-0.30565700
C	1.31779100	-5.37699300	-0.00665400
C	1.57920500	-6.27204800	1.07852400

H	0.84983100	-7.04905400	1.28967800
C	2.71197000	-6.15515000	1.82661400
C	3.65416400	-5.12380400	1.53840000
C	3.44030200	-4.24978000	0.51309900
H	-0.55326400	-6.27910100	-0.55387200
H	-2.39515200	-4.02265900	-4.29455300
H	-1.96095900	-5.56123100	-2.41355400
H	1.26095400	-1.91646900	-3.48051400
H	-0.77813300	-2.19703500	-4.81428700
H	2.90197700	-6.84142700	2.64536000
H	4.55070200	-5.03707400	2.14373800
H	4.16714100	-3.47214400	0.30300900
C	-1.67151900	2.66646000	3.43355700
C	-1.79066200	3.63245600	2.47938800
C	-0.66779600	4.01342400	1.67938200
C	0.57493600	3.31112000	1.84079400
C	0.66346000	2.32412200	2.87480000
C	-0.41510700	2.02414500	3.65299300
C	-0.76520300	5.03446400	0.73474700
C	1.64309600	3.59968500	0.97229900
C	1.53150500	4.62064000	0.01001200
C	0.31440100	5.37556100	-0.07840500
C	0.22061400	6.43482600	-1.03556500
H	-0.70591200	7.00064200	-1.07952600
C	1.25487400	6.71588100	-1.87626500
C	2.45542500	5.94731600	-1.81150100
C	2.58998100	4.93933700	-0.90314200
H	-1.71002800	5.56015200	0.61524400
H	-2.53875800	2.36499000	4.01225900
H	-2.74718100	4.11172300	2.29169700
H	1.60133400	1.79638800	3.01519200
H	-0.33672100	1.25006000	4.40970300
H	1.17248300	7.52064500	-2.59969000
H	3.26967400	6.17342700	-2.49255300
H	3.51055200	4.36668100	-0.85808800
C	-2.62774200	-0.84057400	-0.03060200
C	-3.59292100	1.09028800	0.88051400
C	-3.34338500	-0.38729100	1.23409000
O	-4.27370000	1.87089100	1.50604900
N	-2.29244900	0.15300200	-0.76886400
N	-2.84111200	1.32804400	-0.24847200
C	-2.70642600	2.54110200	-0.95998200
C	-1.58247600	2.74868200	-1.76386200
C	-3.69782600	3.52237100	-0.86292900

C	-1.46722300	3.92723100	-2.48941400
H	-0.79700300	2.00416900	-1.81480100
C	-3.56038200	4.70017300	-1.59315100
H	-4.55680300	3.35688000	-0.22581900
C	-2.45552200	4.90589500	-2.41371900
H	-0.58164500	4.09172500	-3.09509600
H	-4.33596500	5.45649600	-1.52291100
H	-2.35577000	5.82528000	-2.98149700
C	-2.17448200	-2.22060700	-0.35248800
H	-1.77286900	-2.25449600	-1.36792900
H	-1.40440000	-2.55109200	0.35209400
H	-3.01215500	-2.91906200	-0.27341900
C	-1.88173200	-1.55478900	2.82901900
O	-2.41998200	-2.63936800	2.70254900
O	-0.75493500	-1.30807400	3.50384200
C	0.20421300	-2.37944000	3.74316000
C	-0.30270400	-3.26621900	4.87383500
H	-1.22718400	-3.76451400	4.57803000
H	0.44996800	-4.02335300	5.11283100
H	-0.48857100	-2.66677400	5.76950400
C	1.45674600	-1.60859200	4.14243700
H	1.76046300	-0.95843800	3.31665300
H	1.26266000	-0.99432700	5.02654200
H	2.26964300	-2.30371200	4.36840100
C	0.46598700	-3.16655600	2.46183500
H	0.68529400	-2.47463900	1.64168500
H	1.34281600	-3.80483400	2.60500400
H	-0.38185300	-3.79937900	2.19403900
N	-2.37607000	-0.37019500	2.33067400
H	-1.63857500	0.32633000	2.22357000

TS-C_1

Zero-point correction=	1.148282 (Hartree/Particle)
Thermal correction to Energy=	1.217407
Thermal correction to Enthalpy=	1.218351
Thermal correction to Gibbs Free Energy=	1.043128
Sum of electronic and zero-point Energies=	-3976.837655
Sum of electronic and thermal Energies=	-3976.768530
Sum of electronic and thermal Enthalpies=	-3976.767586
Sum of electronic and thermal Free Energies=	-3976.942810

SCF Done: E(RM062X) = -3978.98281262

Number of Imaginary Frequencies = -216.89

H	-5.03491600	-2.61826700	-1.15609700
C	-6.16082900	1.30558800	-2.60612700
C	-5.33773100	0.25110200	-2.56131200
C	-4.07351900	0.31430100	-1.76264200
C	-3.98116700	1.45220200	-0.77664100
C	-4.84337900	2.61072700	-0.97727700
C	-5.87148800	2.52107100	-1.84304200
H	-7.05169500	1.28582600	-3.22490100
H	-5.51120600	-0.64814500	-3.14647000
H	-3.25701500	0.51675900	-2.47969600
H	-4.65811200	3.50253400	-0.38911300
H	-6.53110200	3.37351000	-1.97639600
N	-3.09180300	1.26589500	0.11595200
H	-0.48296800	-1.00032800	0.14160800
C	-2.80396700	2.07940300	1.22617400
C	-3.82164300	2.62083700	2.02078400
C	-1.46616300	2.20644100	1.60347600
C	-3.47921600	3.33898300	3.16224800
H	-4.85969500	2.43269800	1.76177800
C	-1.13525900	2.90603100	2.75716500
H	-0.69178400	1.76575700	0.98362000
C	-2.14180700	3.48662700	3.52733600
H	-4.26324000	3.76320200	3.78180900
H	-0.08898900	2.97089000	3.03986400
H	-1.88198400	4.04063900	4.42366200
C	5.67976900	-1.48977800	-3.85078400
C	5.21818900	-0.74465700	-2.79474900
C	4.62093100	-1.36592600	-1.66185200
C	4.47838700	-2.78258400	-1.67726700
C	4.98224000	-3.52713800	-2.77643500
C	5.57669500	-2.90099200	-3.83992800
H	6.12738900	-0.99009000	-4.70398600
H	5.29463900	0.33630700	-2.82716100
C	4.09069600	-0.62424300	-0.55279600
C	3.78715300	-3.43194500	-0.62314700
H	4.87177100	-4.60785200	-2.75974100
H	5.95514400	-3.47865900	-4.67688000
C	3.24124700	-2.72712900	0.41901100
C	3.42534700	-1.31594700	0.44167600
H	3.66161500	-4.51114200	-0.66080700
C	4.11217400	0.86538900	-0.50190000
C	5.31363200	1.63875700	-0.60456600
C	2.91495000	1.53930400	-0.33146800
C	6.60534800	1.04549300	-0.62005500

C	5.22160300	3.05861600	-0.65504700
C	2.80207500	2.95576700	-0.38084000
C	7.73371500	1.81857100	-0.71850400
H	6.68822500	-0.03322100	-0.54178100
C	6.40831700	3.83007700	-0.77118900
C	3.95212300	3.68413800	-0.56372800
C	7.63778700	3.22759000	-0.80743300
H	8.71070700	1.34621700	-0.72107000
H	6.31845100	4.91175500	-0.81881400
H	3.89477000	4.76882900	-0.60992700
H	8.53901700	3.82600900	-0.89025700
O	2.93602400	-0.62671900	1.52219800
O	1.75876900	0.82707600	-0.14508100
P	1.50798700	0.15731000	1.35244100
O	0.42584400	-0.86911300	1.07447600
O	1.39212000	1.18585200	2.40053800
C	-1.45004000	-4.88294900	0.69319000
C	-0.92700200	-4.98745100	1.94659200
C	0.38720100	-4.50197400	2.24010700
C	1.16106700	-3.89356800	1.19409500
C	0.56866200	-3.79716900	-0.10891500
C	-0.68479700	-4.27961300	-0.34888600
C	0.92038300	-4.60384700	3.52390800
C	2.44360900	-3.39116100	1.48920300
C	2.96864800	-3.49247000	2.79116400
C	2.19187200	-4.11704700	3.82321200
C	2.73960100	-4.22314900	5.14072500
H	2.13744400	-4.69830900	5.91023700
C	3.98055800	-3.73938800	5.42350700
C	4.75520300	-3.11667100	4.40047600
C	4.26864700	-2.99768600	3.13300100
H	0.32932600	-5.06766600	4.31056100
H	-2.44552000	-5.26023900	0.47954700
H	-1.49587400	-5.44388600	2.75222900
H	1.12874500	-3.32437200	-0.91008900
H	-1.10677300	-4.20513700	-1.34715700
H	4.38624200	-3.82236600	6.42657200
H	5.74123800	-2.73169900	4.63922100
H	4.86633400	-2.52137800	2.36315700
C	0.75612400	6.18934600	3.07958800
C	-0.16284500	6.10744100	2.07851100
C	0.04446900	5.23975800	0.95963200
C	1.26076200	4.47892800	0.87640900
C	2.18905700	4.57755700	1.96582200

C	1.94197200	5.39746200	3.02657200
C	-0.93836000	5.07500000	-0.01253800
C	1.47910300	3.62929400	-0.22755300
C	0.46087900	3.44674200	-1.18805400
C	-0.77450200	4.16840400	-1.05932900
C	-1.82391100	3.93260300	-2.00239400
H	-2.74979900	4.49075000	-1.88941900
C	-1.67316100	3.03132200	-3.01444400
C	-0.43987500	2.33054300	-3.16256100
C	0.59166000	2.54745200	-2.29497400
H	-1.87159400	5.62771100	0.07440000
H	0.58384900	6.83996100	3.93104900
H	-1.08697300	6.67737000	2.11985200
H	3.07405900	3.95266000	1.95501300
H	2.64670100	5.43813000	3.85056500
H	-2.48175000	2.85840500	-3.71960800
H	-0.31644700	1.62057400	-3.97486200
H	1.52841500	2.01672900	-2.43253100
C	-2.63717700	-0.72551500	0.04429100
C	-2.90437300	-1.79802200	-2.06711000
C	-3.70708900	-1.01764600	-1.02188200
O	-3.38451900	-2.42340500	-2.99396900
N	-1.46512700	-1.00989300	-0.49042100
N	-1.60295400	-1.51874400	-1.79468600
C	-0.46658500	-1.72215100	-2.60937700
C	0.63262300	-0.89169000	-2.40652000
C	-0.45057600	-2.71641700	-3.58959000
C	1.76228300	-1.05472500	-3.19598800
H	0.59942400	-0.12020300	-1.64869900
C	0.70051200	-2.87377800	-4.35872800
H	-1.32021000	-3.34232000	-3.74548000
C	1.80960600	-2.05342800	-4.16674700
H	2.60996200	-0.39539100	-3.04506300
H	0.72456300	-3.65224400	-5.11431000
H	2.70809200	-2.18874800	-4.76029300
C	-2.81434200	-0.96043100	1.51174100
H	-2.85373400	-2.04457500	1.66134800
H	-1.94656500	-0.57397900	2.05195300
H	-3.73201800	-0.49805100	1.87393800
N	-4.83307100	-1.79851200	-0.59519100
C	-5.89326100	-1.20146700	0.03851100
O	-5.83792700	-0.09100300	0.53241100
O	-6.94804000	-2.02126300	0.03598400
C	-8.21871400	-1.57422400	0.60198000

C	-8.06318900	-1.30320600	2.09490300
H	-9.04860200	-1.11178300	2.52889100
H	-7.63531900	-2.17901800	2.59056300
H	-7.42252600	-0.44047200	2.27526500
C	-9.13035800	-2.77167100	0.36395700
H	-10.13096600	-2.55828700	0.74777900
H	-9.20311000	-2.98991800	-0.70441500
H	-8.73956700	-3.65486000	0.87522600
C	-8.71963800	-0.35304700	-0.16435000
H	-8.75159400	-0.57392800	-1.23553500
H	-9.73307600	-0.11067200	0.16740600
H	-8.07417100	0.50990500	0.00299600

TS-C_1'

Zero-point correction= 1.147709 (Hartree/Particle)
Thermal correction to Energy= 1.216772
Thermal correction to Enthalpy= 1.217716
Thermal correction to Gibbs Free Energy= 1.044591
Sum of electronic and zero-point Energies= -3976.851193
Sum of electronic and thermal Energies= -3976.782131
Sum of electronic and thermal Enthalpies= -3976.781187
Sum of electronic and thermal Free Energies= -3976.954312
SCF Done: E(RM062X) = -3978.99044531
Number of Imaginary Frequencies = -577.80

H	-1.19649000	0.27510300	-1.18484700
C	-6.85306300	1.00439500	2.60032800
C	-5.52100600	0.87334800	2.69311900
C	-4.78399700	0.00521600	1.72898100
C	-5.52683900	-0.30783500	0.45849700
C	-6.97442700	-0.23407200	0.46217200
C	-7.57918500	0.40578400	1.48983700
H	-7.40993800	1.57440700	3.33488500
H	-4.94729800	1.31984500	3.49860200
H	-4.63848200	-0.96172100	2.24453800
H	-7.52919900	-0.59460300	-0.39613300
H	-8.65943000	0.52200100	1.46915900
N	-4.74838200	-0.59067700	-0.52255800
C	-5.09267300	-1.07131800	-1.79274700
C	-4.58436500	-0.40820000	-2.91527200
C	-5.84775600	-2.24027400	-1.94546400
C	-4.87065100	-0.89839700	-4.18540900
H	-3.98599700	0.48586300	-2.77577700

C	-6.13075500	-2.71554500	-3.22074900
H	-6.19611900	-2.76703200	-1.06174200
C	-5.64908700	-2.04349300	-4.34363600
H	-4.48731400	-0.37723500	-5.05658200
H	-6.72469700	-3.61625200	-3.33795100
H	-5.87372600	-2.41603700	-5.33755200
C	6.77958000	-1.04745200	-3.13197400
C	5.91527300	-0.60664700	-2.16255300
C	4.74747800	-1.34776800	-1.83495000
C	4.48015400	-2.54317600	-2.56165600
C	5.40102000	-2.97808900	-3.55056400
C	6.52868700	-2.25204800	-3.82946100
H	7.66195900	-0.46283800	-3.37112500
H	6.11128200	0.32424400	-1.64214400
C	3.81609900	-0.91562600	-0.83306900
C	3.30156800	-3.28601600	-2.28669600
H	5.18586500	-3.89754700	-4.08777200
H	7.22406800	-2.59066200	-4.59033300
C	2.37891000	-2.84610400	-1.37329500
C	2.64260400	-1.62754600	-0.69141400
H	3.13254900	-4.22394900	-2.80931400
C	4.05074000	0.28359100	0.01990200
C	5.20950300	0.43207800	0.85331600
C	3.09833500	1.27864600	0.05530200
C	6.18582800	-0.59057600	0.99735300
C	5.37627300	1.63522400	1.59792700
C	3.25023700	2.49180900	0.78276800
C	7.27892000	-0.41217100	1.80674300
H	6.05261300	-1.52513700	0.46354600
C	6.52458400	1.79248200	2.41719600
C	4.38987600	2.65587900	1.52509700
C	7.45968200	0.79620800	2.51862300
H	8.00964400	-1.20828200	1.90624500
H	6.64029800	2.72016300	2.97067400
H	4.54019500	3.57827500	2.07997100
H	8.33170600	0.92571200	3.15104500
O	1.68836400	-1.20108100	0.20283700
O	1.95305000	1.13640600	-0.69672500
P	0.80142600	0.12402300	-0.15263000
O	-0.04447800	-0.11835900	-1.40634500
O	0.11292300	0.52587900	1.09267200
C	-2.44570200	-3.53681900	-3.16872700
C	-2.32635000	-4.38368700	-2.10820300
C	-1.11512500	-4.44208100	-1.34623600

C	-0.00553800	-3.61184900	-1.73228500
C	-0.17347500	-2.73861900	-2.85641700
C	-1.35241300	-2.69745700	-3.54103600
C	-1.00254000	-5.26329200	-0.22561100
C	1.18717500	-3.66185600	-0.98937700
C	1.28977900	-4.49574500	0.14271400
C	0.17028200	-5.30728600	0.52900500
C	0.28549400	-6.15297700	1.67735300
H	-0.57228500	-6.75864900	1.95641900
C	1.43937400	-6.20119900	2.40019400
C	2.55389100	-5.39626100	2.02033100
C	2.48196700	-4.57305400	0.93508400
H	-1.84677300	-5.88388800	0.06676800
H	-3.37654300	-3.48034800	-3.72431600
H	-3.15648400	-5.01610100	-1.80453500
H	0.64309300	-2.07901600	-3.12733300
H	-1.47088400	-2.01071300	-4.37299900
H	1.51658800	-6.84894400	3.26742400
H	3.46707000	-5.44059800	2.60504600
H	3.33620500	-3.96463800	0.65739500
C	-1.23186600	3.48084800	3.14204200
C	-1.20316600	4.30239400	2.05486300
C	-0.03662400	4.38576500	1.23101400
C	1.08543900	3.53765800	1.52279300
C	1.02182300	2.71064300	2.69052500
C	-0.08906500	2.69431200	3.48000700
C	0.01686600	5.25046700	0.13835300
C	2.18089400	3.52303200	0.64075800
C	2.22370100	4.39317400	-0.46474900
C	1.13397500	5.29751300	-0.69451100
C	1.20038700	6.19928500	-1.80328400
H	0.36991000	6.88371600	-1.95333000
C	2.26627000	6.19223200	-2.65170800
C	3.33840400	5.27437300	-2.44264100
C	3.31831500	4.40777500	-1.39003900
H	-0.83835500	5.88623700	-0.08014000
H	-2.13336400	3.40601900	3.74195800
H	-2.07465500	4.88939900	1.77903600
H	1.86618600	2.06996000	2.92201600
H	-0.12995500	2.03605400	4.34195700
H	2.30628300	6.88069600	-3.48982800
H	4.17862700	5.27140500	-3.12965700
H	4.14210400	3.71854000	-1.23595700
C	-2.87023000	-0.28107100	0.07460500

C	-3.40706800	1.90704400	0.76959200
C	-3.38131000	0.46316200	1.31548800
O	-3.95165700	2.85056000	1.30707500
N	-2.31354000	0.57816200	-0.75983900
N	-2.69737000	1.88735700	-0.39725400
C	-2.40382600	2.97667000	-1.24967700
C	-1.32175700	2.88990200	-2.13084500
C	-3.19528000	4.12983500	-1.20887700
C	-1.04629500	3.95671700	-2.97837700
H	-0.68493500	2.01254600	-2.14705900
C	-2.89971600	5.18534900	-2.06574100
H	-4.02304300	4.19084900	-0.51575400
C	-1.83282800	5.10504400	-2.95626300
H	-0.19009100	3.89475200	-3.64224900
H	-3.52050000	6.07548600	-2.03727900
H	-1.60842600	5.93287800	-3.62109800
C	-2.35236800	-1.68308200	0.06218700
H	-2.20203300	-1.98975100	-0.97468000
H	-1.38754700	-1.71814200	0.58003400
H	-3.04068000	-2.36407100	0.56273700
C	-2.11024100	-0.72360500	3.05302000
O	-2.82135200	-1.71333800	3.08135900
O	-0.94420200	-0.57777900	3.67984200
C	-0.15697200	-1.74707900	4.06125800
C	-0.78998000	-2.40793600	5.27965800
H	-1.76912400	-2.81699800	5.02681900
H	-0.14486800	-3.21783800	5.63259000
H	-0.90330200	-1.67877700	6.08696400
C	1.19621600	-1.12769400	4.38831900
H	1.58050700	-0.61373800	3.50242300
H	1.10029500	-0.40677300	5.20553200
H	1.90273200	-1.90639800	4.68728100
C	-0.01981800	-2.70430500	2.88086400
H	0.38010200	-2.16711800	2.01468400
H	0.68791400	-3.49802700	3.13907600
H	-0.97366000	-3.16777100	2.62184300
N	-2.41275900	0.45117300	2.39413200
H	-1.56328700	0.98342200	2.19111400

G_1

Zero-point correction=	1.154812 (Hartree/Particle)
Thermal correction to Energy=	1.223603
Thermal correction to Enthalpy=	1.224547

Thermal correction to Gibbs Free Energy= 1.051598
Sum of electronic and zero-point Energies= -3976.857464
Sum of electronic and thermal Energies= -3976.788673
Sum of electronic and thermal Enthalpies= -3976.787729
Sum of electronic and thermal Free Energies= -3976.960678
SCF Done: E(RM062X) = -3979.01479454

H	-4.93898100	-2.49928800	-1.32539000
C	-5.98274900	1.76797200	-2.56165700
C	-5.25322700	0.64672600	-2.67018700
C	-4.00204000	0.50026400	-1.87766300
C	-3.85697100	1.47249500	-0.75948800
C	-4.56531600	2.72200700	-0.76872100
C	-5.59570300	2.83059800	-1.63950700
H	-6.86869700	1.91435000	-3.16931500
H	-5.50150800	-0.14328800	-3.37296600
H	-3.14828100	0.73229200	-2.54471900
H	-4.31672500	3.48890800	-0.04454500
H	-6.18903000	3.74017500	-1.63895000
N	-3.07422000	1.00935100	0.16417900
H	-0.61941000	-0.65209900	-0.23816900
C	-2.76618200	1.68604000	1.39187900
C	-3.81331500	1.96543000	2.27028200
C	-1.44578200	1.99870000	1.68168500
C	-3.51380900	2.60480000	3.46806400
H	-4.82281600	1.65942100	2.01053100
C	-1.15845600	2.61324300	2.89804700
H	-0.65842600	1.77924600	0.96741600
C	-2.19149900	2.92451200	3.77818300
H	-4.31106700	2.83598300	4.16688200
H	-0.11936600	2.81828000	3.13460800
H	-1.96190200	3.41350900	4.71943700
C	5.72538400	-1.39951400	-3.80245400
C	5.25873100	-0.66683300	-2.74009700
C	4.62437600	-1.29834000	-1.63285700
C	4.45650400	-2.71199700	-1.67878000
C	4.96554500	-3.44357700	-2.78413000
C	5.59184700	-2.80818200	-3.82375200
H	6.20066200	-0.89216900	-4.63602400
H	5.35708400	0.41280900	-2.74837800
C	4.08494500	-0.56939000	-0.52213800
C	3.73512400	-3.36799200	-0.64976700
H	4.83294200	-4.52200400	-2.79209300
H	5.97382000	-3.37632900	-4.66573000

C	3.19145700	-2.67371900	0.40118900
C	3.39894200	-1.26674500	0.45705200
H	3.58840300	-4.44342500	-0.71204200
C	4.09868600	0.91901900	-0.45383800
C	5.28859300	1.71330100	-0.51631300
C	2.88722500	1.56854900	-0.29548600
C	6.58937400	1.14018700	-0.52590200
C	5.17590200	3.13321800	-0.52669100
C	2.75690100	2.98397200	-0.30332100
C	7.70785000	1.93182000	-0.58264500
H	6.68581900	0.06066100	-0.47730900
C	6.35294100	3.92414200	-0.59936700
C	3.89537400	3.73852000	-0.43842500
C	7.59213700	3.34117700	-0.63194800
H	8.69176700	1.47390700	-0.58229700
H	6.24807200	5.00551200	-0.61687100
H	3.82266000	4.82332200	-0.45080800
H	8.48537800	3.95514400	-0.68156800
O	2.91920100	-0.59392300	1.54524000
O	1.74308000	0.83886500	-0.13894900
P	1.49133700	0.22212500	1.40032400
O	0.35640700	-0.73483900	1.19522300
O	1.49751500	1.32597400	2.38593600
C	-1.47654200	-4.89391100	0.56812600
C	-0.96163200	-5.03440500	1.82121200
C	0.33348800	-4.51959100	2.14798900
C	1.09842500	-3.84823800	1.13436300
C	0.50526800	-3.69597600	-0.16308700
C	-0.73084200	-4.20612600	-0.43631700
C	0.86142800	-4.66414700	3.42967800
C	2.37842300	-3.35239900	1.45086500
C	2.89784800	-3.49723600	2.75128000
C	2.12225600	-4.16693300	3.75560300
C	2.66444500	-4.31611800	5.07128800
H	2.06298900	-4.82514100	5.81952300
C	3.89948000	-3.83194800	5.37824800
C	4.67385800	-3.16634000	4.38248400
C	4.19265700	-3.00606300	3.11749400
H	0.27688100	-5.17439200	4.19218200
H	-2.45544000	-5.29749200	0.32699200
H	-1.52021900	-5.54686500	2.59998100
H	1.05585600	-3.16516800	-0.93370200
H	-1.15580800	-4.09166400	-1.42958300
H	4.30077400	-3.94800200	6.37990300

H	5.65517800	-2.78147400	4.64014600
H	4.78950800	-2.49608500	2.36912700
C	0.46452100	5.93982900	3.25159800
C	-0.41851700	5.87726200	2.21696000
C	-0.13636900	5.08524700	1.05874900
C	1.11434700	4.38157800	0.97872800
C	2.00065300	4.45160400	2.10445800
C	1.68446900	5.20123700	3.19830500
C	-1.06953400	4.94832900	0.03345200
C	1.41080300	3.61154400	-0.16368300
C	0.44060900	3.44863400	-1.17582400
C	-0.82325000	4.12184300	-1.06336000
C	-1.80632100	3.93222400	-2.08558300
H	-2.74377400	4.47568000	-2.00239500
C	-1.57458000	3.10029600	-3.14165900
C	-0.32121600	2.43029200	-3.25825600
C	0.65467500	2.61932500	-2.32345600
H	-2.01880500	5.47649200	0.10329700
H	0.23730900	6.53541400	4.13018900
H	-1.36468000	6.41009700	2.25678400
H	2.90271900	3.85202000	2.09203100
H	2.35747800	5.22256800	4.04898500
H	-2.33137400	2.96745400	-3.91066600
H	-0.13804700	1.77029200	-4.10039800
H	1.61128400	2.11952000	-2.43677300
C	-2.65323500	-0.40615600	-0.11472200
C	-2.81341500	-1.72763200	-2.11296700
C	-3.66964600	-0.86382800	-1.19452700
O	-3.27810900	-2.55044200	-2.88945100
N	-1.39598400	-0.37044200	-0.87627600
N	-1.53592500	-1.36115000	-1.90176900
C	-0.41682700	-1.64952400	-2.71896300
C	0.72872600	-0.86528700	-2.57326800
C	-0.45302500	-2.69852400	-3.64517300
C	1.83468200	-1.12350400	-3.37414000
H	0.75443800	-0.06213700	-1.84860000
C	0.67667100	-2.95062500	-4.41828600
H	-1.34709400	-3.29619100	-3.75774500
C	1.82237500	-2.16999500	-4.29247500
H	2.71689800	-0.50212900	-3.26852000
H	0.65162000	-3.77092200	-5.12842900
H	2.70258800	-2.37465700	-4.89295500
C	-2.62169100	-1.23789800	1.14713000
H	-2.41435600	-2.27591000	0.86830600

H	-1.81307100	-0.90212800	1.79868400
H	-3.58815000	-1.17796600	1.65466800
N	-4.80089100	-1.64058100	-0.80306600
C	-5.85258000	-1.10255700	-0.12207200
O	-5.82126200	0.00925200	0.38081100
O	-6.87426700	-1.95985100	-0.09135800
C	-8.12091800	-1.59614300	0.57904300
C	-7.86835200	-1.37058900	2.06613400
H	-8.82642800	-1.24157300	2.57722900
H	-7.36556900	-2.24115200	2.49620200
H	-7.25653000	-0.48438400	2.23374600
C	-8.98879100	-2.82925900	0.36048500
H	-9.96715600	-2.68104200	0.82395500
H	-9.13008400	-3.01227400	-0.70759700
H	-8.51874400	-3.70907500	0.80644000
C	-8.73551300	-0.37594700	-0.10068600
H	-8.82848600	-0.55587800	-1.17584700
H	-9.73603900	-0.20392600	0.30558000
H	-8.12809200	0.51431500	0.06313300

G_1'

Zero-point correction= 1.154439 (Hartree/Particle)
Thermal correction to Energy= 1.223065
Thermal correction to Enthalpy= 1.224010
Thermal correction to Gibbs Free Energy= 1.051935
Sum of electronic and zero-point Energies= -3976.861194
Sum of electronic and thermal Energies= -3976.792567
Sum of electronic and thermal Enthalpies= -3976.791623
Sum of electronic and thermal Free Energies= -3976.963698
SCF Done: E(RM062X) = -3979.01603486

H	-1.68138800	0.41274500	-1.13030400
C	-6.69820600	0.20617700	2.94133700
C	-5.35566400	0.32241600	2.97031300
C	-4.53960300	-0.42461800	1.98496600
C	-5.26701300	-0.89979300	0.78441300
C	-6.67929400	-1.10092900	0.82997200
C	-7.34058900	-0.54154600	1.88321100
H	-7.31851000	0.67820400	3.69348400
H	-4.82913600	0.87187400	3.74289100
H	-4.19728600	-1.34164300	2.51511400
H	-7.19981300	-1.57608600	0.00800900
H	-8.42394500	-0.62280600	1.90821500

N	-4.46167800	-1.04354000	-0.23826400
C	-4.82554300	-1.67078200	-1.47268600
C	-4.75416800	-0.96159900	-2.67077300
C	-5.25948600	-2.99633100	-1.43910700
C	-5.15289300	-1.59554300	-3.84473700
H	-4.38996600	0.05835100	-2.66756200
C	-5.66655500	-3.61117500	-2.61785100
H	-5.27105800	-3.53223300	-0.49429400
C	-5.61941200	-2.90802700	-3.82017400
H	-5.10655700	-1.05250100	-4.78247500
H	-6.01151500	-4.63940800	-2.59726500
H	-5.93682400	-3.38761200	-4.74024700
C	7.08968800	-0.46099500	-2.77573900
C	6.08601100	-0.06378400	-1.92963400
C	4.95142900	-0.89046700	-1.70458400
C	4.87234400	-2.12996200	-2.39914000
C	5.93266700	-2.51809000	-3.25920700
C	7.02049100	-1.70616300	-3.44390900
H	7.94304000	0.18910000	-2.93979000
H	6.14254400	0.89755100	-1.43073700
C	3.87924800	-0.50277300	-0.83566700
C	3.74344100	-2.96602000	-2.20176700
H	5.85786300	-3.47208700	-3.77385100
H	7.82406900	-2.00880600	-4.10722300
C	2.68831500	-2.57048200	-1.42057200
C	2.74303700	-1.29128300	-0.79612700
H	3.72417200	-3.94838100	-2.66695000
C	3.94489500	0.71745100	0.01376600
C	4.97874100	0.93323300	0.98499400
C	2.92950800	1.64359600	-0.07614000
C	6.00196500	-0.01867200	1.24532000
C	4.96388400	2.13340400	1.75274300
C	2.88667100	2.83664700	0.69818600
C	6.97258900	0.22732400	2.18306900
H	6.00446300	-0.95335900	0.69564400
C	5.98939700	2.36207600	2.70719500
C	3.91030500	3.07072200	1.57852900
C	6.97703600	1.43590900	2.91705200
H	7.74217000	-0.51542200	2.36738200
H	5.96697800	3.28746500	3.27619900
H	3.90537500	3.97779100	2.17765200
H	7.75410900	1.61993200	3.65165900
O	1.65789900	-0.90540900	-0.05544400
O	1.92045000	1.43131900	-0.97979500

P	0.73142400	0.38915600	-0.54805600
O	-0.03284600	0.08841200	-1.79844200
O	0.00253100	0.81629300	0.67826700
C	-2.07051300	-3.62063700	-3.20843900
C	-1.86589700	-4.50108100	-2.18746800
C	-0.64352400	-4.48820500	-1.44319200
C	0.37496900	-3.53561600	-1.79461400
C	0.11513400	-2.62546700	-2.86847800
C	-1.06798300	-2.66425100	-3.54631200
C	-0.42303600	-5.37192900	-0.38667300
C	1.58649500	-3.52043600	-1.08128700
C	1.80195200	-4.42412800	-0.02138000
C	0.77285700	-5.36268100	0.33050500
C	0.99814100	-6.26956300	1.41460700
H	0.20968000	-6.97358300	1.66651800
C	2.16771400	-6.25275600	2.11286900
C	3.18926100	-5.31670200	1.77257700
C	3.01353000	-4.43504100	0.74690600
H	-1.19691000	-6.08909300	-0.12105600
H	-3.00398800	-3.63490600	-3.76189100
H	-2.62857800	-5.22714600	-1.91631700
H	0.85753200	-1.87360400	-3.10808000
H	-1.25674400	-1.94865600	-4.33957900
H	2.32734000	-6.94638500	2.93210700
H	4.11344300	-5.30637500	2.34143100
H	3.79340600	-3.72149100	0.50377100
C	-1.59967200	3.52241400	3.13645200
C	-1.66572800	4.31461800	2.03061100
C	-0.54454500	4.44252700	1.15056000
C	0.65014500	3.69620800	1.43051400
C	0.67627500	2.87746500	2.60720500
C	-0.40267200	2.80438500	3.43558400
C	-0.60753100	5.24597100	0.01277200
C	1.71824600	3.74410600	0.51785900
C	1.64644900	4.55683100	-0.62885100
C	0.46743100	5.33602700	-0.87139800
C	0.41116400	6.16765000	-2.03424900
H	-0.48800800	6.75583100	-2.19701500
C	1.45059900	6.21535100	-2.91398100
C	2.61791800	5.42864300	-2.68371000
C	2.71214600	4.62942900	-1.58306200
H	-1.52184100	5.79528300	-0.20213700
H	-2.46964200	3.40923000	3.77517400
H	-2.58286100	4.83897700	1.77743600

H	1.55942900	2.28202500	2.80979700
H	-0.37178000	2.15319700	4.30371000
H	1.39781600	6.85037600	-3.79275800
H	3.43721300	5.47014400	-3.39429200
H	3.60544400	4.03705400	-1.41327400
C	-3.04162200	-0.56541800	0.04637100
C	-3.55406800	1.61066600	0.89718100
C	-3.26179400	0.18215800	1.39983900
O	-4.12609600	2.46289300	1.55249200
N	-2.69553200	0.43462300	-0.92491900
N	-3.10045800	1.68401200	-0.37909200
C	-3.03639700	2.83282100	-1.20284600
C	-2.08780600	2.86827100	-2.22936500
C	-3.89783100	3.91229200	-0.98423000
C	-2.01430700	3.99375500	-3.04260700
H	-1.39667100	2.04253400	-2.37671000
C	-3.80710700	5.02623900	-1.81280600
H	-4.61629300	3.87265500	-0.17673200
C	-2.87283600	5.07216500	-2.84433700
H	-1.26071500	4.03272300	-3.82217400
H	-4.47975400	5.86238900	-1.64884200
H	-2.80827200	5.94565200	-3.48537200
C	-2.08486900	-1.73634100	0.00444600
H	-1.92564000	-2.03301400	-1.03530000
H	-1.12639700	-1.42163400	0.42473100
H	-2.47088000	-2.57854200	0.58295200
C	-1.69700100	-0.88062700	2.94310700
O	-2.36543300	-1.88804600	3.13503000
O	-0.44794400	-0.68163800	3.34576000
C	0.42160900	-1.80587700	3.68773900
C	0.01072000	-2.36325100	5.04484400
H	-0.98565300	-2.80495700	4.99197500
H	0.72477400	-3.13171100	5.35461900
H	0.01211800	-1.56734900	5.79506500
C	1.79506500	-1.14672000	3.73130700
H	2.01510100	-0.69879000	2.75743200
H	1.82147200	-0.36502300	4.49599700
H	2.55934000	-1.89360000	3.96268000
C	0.38479200	-2.85806800	2.58529200
H	0.64040500	-2.39653500	1.62553200
H	1.13616400	-3.62460900	2.79834200
H	-0.59055600	-3.34260000	2.51592500
N	-2.14746700	0.24932700	2.29885600
H	-1.36681600	0.81928400	1.94991800

TS-D_1

Zero-point correction= 1.152269 (Hartree/Particle)
Thermal correction to Energy= 1.220464
Thermal correction to Enthalpy= 1.221409
Thermal correction to Gibbs Free Energy= 1.049710
Sum of electronic and zero-point Energies= -3976.863257
Sum of electronic and thermal Energies= -3976.795061
Sum of electronic and thermal Enthalpies= -3976.794116
Sum of electronic and thermal Free Energies= -3976.965815
SCF Done: E(RM062X) = -3979.01052151
Number of Imaginary Frequencies = -75.85

H	-5.40497800	-1.31977900	-0.42108400
C	-2.15970500	0.30856200	-3.28000300
C	-2.72526400	-0.48578700	-2.34536600
C	-2.53852600	-0.16063500	-0.92611100
C	-2.11333700	1.21157100	-0.63504500
C	-1.44028100	1.99133400	-1.61227900
C	-1.48080800	1.52082500	-2.89161400
H	-2.18750000	0.03781100	-4.32916800
H	-3.19332700	-1.43385800	-2.59501800
H	-1.51694600	-0.69574000	-0.74095700
H	-0.97322600	2.93668400	-1.35611600
H	-0.99404800	2.10906000	-3.66434600
N	-2.40438500	1.54536100	0.60598700
H	-1.27622700	-0.22851100	1.74755600
C	-2.12088500	2.80303800	1.22788600
C	-2.86352600	3.91327700	0.83523600
C	-1.17708000	2.86418500	2.25003700
C	-2.66050800	5.12147900	1.49678500
H	-3.59647800	3.80193400	0.04100800
C	-1.00275200	4.07362700	2.91328100
H	-0.58424700	1.98522200	2.48383300
C	-1.74264900	5.19512700	2.54173400
H	-3.23193500	5.99741100	1.20730800
H	-0.26322700	4.14733400	3.70363800
H	-1.59133700	6.13461400	3.06468300
C	6.25383500	-1.80674600	-3.84727700
C	5.61836000	-1.22028600	-2.78206000
C	4.55939200	-1.88521700	-2.10556100
C	4.14209100	-3.15502200	-2.59663100
C	4.82932700	-3.74120200	-3.69185300

C	5.86779900	-3.08878100	-4.30226400
H	7.05765000	-1.27830800	-4.34971100
H	5.91875400	-0.23251400	-2.45179000
C	3.86865800	-1.31681700	-0.98279900
C	3.01289500	-3.79543900	-2.02306000
H	4.50316300	-4.71636400	-4.04290000
H	6.38432400	-3.54360400	-5.14112000
C	2.29845900	-3.21854100	-1.00432200
C	2.77383200	-1.98386800	-0.47862600
H	2.68046000	-4.74473800	-2.43589300
C	4.23247300	0.00449200	-0.40213300
C	5.55682300	0.28141100	0.06851800
C	3.26641500	0.99318500	-0.29525600
C	6.56209200	-0.72048600	0.16179400
C	5.88295100	1.60066900	0.48646000
C	3.57961200	2.32133800	0.11984400
C	7.82143400	-0.41409500	0.60927600
H	6.31684200	-1.73946100	-0.11623100
C	7.20078900	1.89110600	0.93003300
C	4.88031000	2.59915400	0.47127200
C	8.15321000	0.90905500	0.98730100
H	8.57092200	-1.19571000	0.68031600
H	7.43172500	2.90847700	1.23360800
H	5.14370500	3.61076400	0.76983300
H	9.15615700	1.13684800	1.33289800
O	2.09041900	-1.41869000	0.57346900
O	1.97982800	0.74960500	-0.69189200
P	0.98868400	-0.29412000	0.11785900
O	0.08486500	-0.86615200	-0.93115400
O	0.42633700	0.32494800	1.35529600
C	-2.42560400	-3.97184200	-2.95756900
C	-2.49387200	-4.40625900	-1.66851500
C	-1.34334200	-4.35975200	-0.81533800
C	-0.10706400	-3.83896000	-1.32771500
C	-0.10245500	-3.33023100	-2.66931100
C	-1.21121400	-3.41055000	-3.45736100
C	-1.40766800	-4.81902300	0.49964800
C	1.02863500	-3.80584200	-0.49338300
C	0.95904900	-4.29523000	0.82443900
C	-0.28207200	-4.81308600	1.32398800
C	-0.33823300	-5.31945100	2.65982800
H	-1.28830100	-5.69703000	3.02571100
C	0.76467300	-5.31090100	3.45830500
C	1.99979900	-4.79560700	2.96675800

C	2.09395100	-4.30587500	1.69808000
H	-2.35461000	-5.18621300	0.88907700
H	-3.29649300	-4.03282700	-3.60412300
H	-3.41800100	-4.79804000	-1.25493700
H	0.79785700	-2.85873400	-3.04416900
H	-1.17945600	-3.02550300	-4.47233400
H	0.70492000	-5.68806500	4.47462100
H	2.87230300	-4.79378300	3.61233900
H	3.03921400	-3.91907100	1.33233000
C	2.10640600	5.73719300	3.68963000
C	1.48295900	6.11976800	2.54139500
C	1.56280400	5.32049500	1.35609200
C	2.37369700	4.13527700	1.35846900
C	2.95667000	3.73682000	2.60859500
C	2.82588700	4.50530100	3.72805100
C	0.85941300	5.67041500	0.20682200
C	2.56307100	3.41238400	0.15865700
C	1.87778000	3.80656800	-1.01190400
C	0.97866100	4.92693500	-0.96640000
C	0.25395000	5.29604700	-2.14519900
H	-0.43731900	6.13188700	-2.08032400
C	0.44015500	4.62997800	-3.31927900
C	1.37788700	3.55667200	-3.38546600
C	2.06777900	3.16056200	-2.27753200
H	0.21262800	6.54487700	0.22210600
H	2.04215900	6.35061800	4.58271300
H	0.90242500	7.03771700	2.49909800
H	3.49822600	2.79942700	2.65613500
H	3.27275900	4.17755300	4.66102300
H	-0.10522000	4.92481300	-4.21064700
H	1.54678000	3.05234300	-4.33189600
H	2.77644800	2.34499700	-2.35233900
C	-3.16893000	0.49351100	1.29413500
C	-3.45801200	-1.84199000	0.86255700
C	-3.58894800	-0.48083200	0.15481900
O	-4.06344500	-2.84201800	0.51797800
N	-2.23877800	-0.31203000	2.11566000
N	-2.68729300	-1.65335200	1.96387800
C	-2.51991700	-2.53268800	3.06379400
C	-3.39741800	-3.59899300	3.28342600
C	-1.48340900	-2.26943100	3.96069100
C	-3.24151400	-4.37673700	4.42697800
H	-4.18970000	-3.80302500	2.57558100
C	-1.34333700	-3.06055800	5.09445100

H	-0.80059000	-1.45084700	3.76408700
C	-2.22321800	-4.11124900	5.33904200
H	-3.93169700	-5.19559100	4.60500600
H	-0.53329700	-2.85423000	5.78631900
H	-2.11266800	-4.72267600	6.22857300
C	-4.30327400	1.03919500	2.13173100
H	-4.97658900	1.63811600	1.51464200
H	-4.85517100	0.20060300	2.56384700
H	-3.89753900	1.64560300	2.94298800
N	-4.94856100	-0.42008200	-0.31247600
C	-5.38757900	0.62930200	-1.06589600
O	-4.80250800	1.69750800	-1.13264800
O	-6.53450600	0.31458100	-1.67898200
C	-7.16792400	1.27047900	-2.58136500
C	-8.39515000	0.50881000	-3.06740400
H	-8.09599500	-0.41171700	-3.57471500
H	-9.04017300	0.24887300	-2.22442100
H	-8.96331300	1.12686700	-3.76696200
C	-6.22966800	1.58053300	-3.74447200
H	-6.76140500	2.18314100	-4.48614900
H	-5.34932700	2.12723100	-3.40610500
H	-5.91012400	0.64994900	-4.22280600
C	-7.58182600	2.52404200	-1.81672200
H	-6.71091500	3.08608600	-1.48092600
H	-8.18574400	3.16026300	-2.46987400
H	-8.18945100	2.24882300	-0.95005000

TS-D_1'

Zero-point correction= 1.151442 (Hartree/Particle)
Thermal correction to Energy= 1.219735
Thermal correction to Enthalpy= 1.220679
Thermal correction to Gibbs Free Energy= 1.049173
Sum of electronic and zero-point Energies= -3976.863871
Sum of electronic and thermal Energies= -3976.795578
Sum of electronic and thermal Enthalpies= -3976.794634
Sum of electronic and thermal Free Energies= -3976.966139
SCF Done: E(RM062X) = -3979.00841356
Number of Imaginary Frequencies = -142.07

H	-4.82956800	-0.86572100	-2.19573700
C	-3.54434400	-2.16521500	2.05763100
C	-3.43059400	-1.99494600	0.71924100
C	-2.84229500	-0.76125900	0.21226400

C	-2.71774700	0.34995900	1.13739600
C	-2.79313800	0.14240200	2.53799800
C	-3.19504000	-1.09414000	2.95423000
H	-3.87533900	-3.11185700	2.46935900
H	-3.64788400	-2.79401500	0.01681300
H	-2.54956300	0.94204200	3.22531900
H	-1.67090800	-1.02362700	0.17347200
H	-3.26762100	-1.27969500	4.02187200
N	-2.48541900	1.48483700	0.49049600
H	-0.57006200	0.82313100	-0.81735300
C	-2.39143700	2.74453700	1.17541100
C	-3.56590700	3.46352500	1.39989800
C	-1.16792900	3.16036300	1.68705900
C	-3.50209100	4.64264300	2.13426600
H	-4.50530300	3.06953700	1.02462900
C	-1.12878000	4.32148200	2.45531800
H	-0.28129800	2.55395900	1.53035400
C	-2.28472500	5.06713300	2.66549100
H	-4.40630000	5.21544900	2.31260000
H	-0.18747000	4.63521500	2.89270400
H	-2.23766600	5.97609100	3.25729600
C	7.56642700	-0.18649900	1.17960800
C	6.28983800	-0.57660800	0.86460900
C	5.26268300	0.38624400	0.67075300
C	5.58508900	1.76207000	0.82506600
C	6.91840600	2.13498800	1.13975100
C	7.89003600	1.18477700	1.31276000
H	8.33584400	-0.93623300	1.33303100
H	6.04705000	-1.63005400	0.77121500
C	3.91957700	0.01863600	0.34155300
C	4.57195700	2.73442100	0.63586900
H	7.14921100	3.19133000	1.24595100
H	8.90543200	1.47800900	1.55801900
C	3.26333200	2.38711500	0.39629300
C	2.94258800	0.99818300	0.32591300
H	4.84078700	3.78718300	0.67349400
C	3.55370700	-1.37235200	-0.03880200
C	4.14640800	-2.02132800	-1.17328600
C	2.52671500	-2.00747800	0.62211000
C	5.13000800	-1.40161900	-1.99312100
C	3.68062300	-3.31566100	-1.54103500
C	2.04585800	-3.29903400	0.26983300
C	5.63427000	-2.04487900	-3.09610900
H	5.47007800	-0.40164800	-1.75054400

C	4.22934600	-3.95719100	-2.68258200
C	2.64504300	-3.93096300	-0.79142800
C	5.18636400	-3.34029900	-3.44522600
H	6.37871300	-1.55002200	-3.71144000
H	3.86188100	-4.94503800	-2.94568700
H	2.29670900	-4.91700200	-1.08817100
H	5.59447300	-3.83662500	-4.31945200
O	1.63506700	0.65844600	0.10281200
O	1.90498900	-1.33740500	1.65257200
P	0.75228500	-0.29476400	1.14473800
O	0.22190300	0.47453200	2.28894000
O	-0.15121000	-1.02056600	0.16681800
C	1.61700300	6.67782100	2.78567200
C	1.00569100	6.67686800	1.56834200
C	1.16491500	5.57966600	0.66283200
C	2.01763000	4.48189500	1.02816200
C	2.59280800	4.49867900	2.34288600
C	2.40346100	5.55620600	3.18506300
C	0.49117600	5.54995200	-0.55568600
C	2.25024100	3.44098000	0.10273200
C	1.61500100	3.46203500	-1.16020300
C	0.68206200	4.51118300	-1.46576700
C	0.01362700	4.51134800	-2.73174000
H	-0.70837100	5.29972900	-2.92839400
C	0.29820300	3.56956300	-3.67260900
C	1.28017300	2.57296100	-3.40525200
C	1.90342400	2.51255400	-2.19446300
H	-0.18356200	6.36431700	-0.81036600
H	1.49195600	7.51528500	3.46439100
H	0.37375200	7.50546200	1.26023800
H	3.17833700	3.64591100	2.66705800
H	2.84862900	5.54231600	4.17466900
H	-0.20471300	3.58030700	-4.63461500
H	1.52502400	1.84387600	-4.17222300
H	2.64122200	1.73707000	-2.01779800
C	-2.66533900	-4.99542500	-0.99018300
C	-2.47678000	-5.37912700	0.30376700
C	-1.29251700	-5.00452400	1.01745200
C	-0.27640100	-4.24630900	0.34119500
C	-0.54796500	-3.81185300	-0.99970100
C	-1.69585500	-4.17397400	-1.64243600
C	-1.10458300	-5.37501900	2.34792200
C	0.92757600	-3.94741600	1.01272500
C	1.10483900	-4.32669400	2.35904900

C	0.05972500	-5.03979500	3.03802900
C	0.24656000	-5.42078700	4.40458300
H	-0.55695900	-5.95740600	4.90177300
C	1.40062000	-5.12391100	5.06302100
C	2.44798400	-4.43070700	4.38808800
C	2.30806700	-4.05100400	3.08660000
H	-1.87796100	-5.94750600	2.85623200
H	-3.56185000	-5.29181200	-1.52641400
H	-3.21681600	-5.98443000	0.82150000
H	0.16931700	-3.16656300	-1.49485300
H	-1.88802400	-3.81010100	-2.64564000
H	1.53237700	-5.41653000	6.09966500
H	3.36601200	-4.20404400	4.92022500
H	3.11649700	-3.52791300	2.58829800
C	-2.45547700	-0.68825100	-2.31865700
C	-3.22024000	-0.10621000	-1.13163700
O	-2.86784100	-1.59600800	-3.02102100
N	-1.20586300	1.13855400	-1.55271900
N	-1.32893500	0.03607400	-2.45500800
C	-0.29163400	-0.26019800	-3.38427500
C	0.94566700	-0.70469000	-2.91796700
C	-0.54410900	-0.12059600	-4.74541700
C	1.94852700	-0.99182000	-3.84069900
H	1.10556400	-0.81214200	-1.84735500
C	0.46271300	-0.41754000	-5.65958200
H	-1.52227300	0.21645800	-5.07178600
C	1.70862300	-0.84635200	-5.20683100
H	2.91770200	-1.33571100	-3.49367500
H	0.27393000	-0.31257400	-6.72296400
H	2.49492300	-1.07585500	-5.91893100
N	-4.61240700	-0.18538100	-1.47406100
C	-5.58596100	0.14836500	-0.57922700
O	-5.37933500	0.82180100	0.41636900
O	-6.76734100	-0.34326500	-0.97104900
C	-7.95516800	-0.13574800	-0.14954600
C	-7.75493800	-0.77533000	1.22160800
H	-8.69851300	-0.74648500	1.77372000
H	-7.45681600	-1.82131600	1.10441800
H	-6.99125800	-0.24918500	1.79440900
C	-9.03601900	-0.87002700	-0.93384900
H	-9.99306400	-0.78970400	-0.41247700
H	-9.14210700	-0.43788600	-1.93199300
H	-8.77952700	-1.92730500	-1.03685300
C	-8.27684300	1.35261300	-0.05529900

H	-7.51954200	1.88278100	0.52163100
H	-8.33658200	1.78584500	-1.05774800
H	-9.24774000	1.48071400	0.43151900
C	-2.57462600	1.30337300	-0.97277000
C	-3.28280000	2.43491100	-1.68026500
H	-3.29782100	2.21279500	-2.75048600
H	-4.30627500	2.54391600	-1.31659100
H	-2.72229800	3.35979700	-1.52828500

Pro1

Zero-point correction=	0.514239 (Hartree/Particle)
Thermal correction to Energy=	0.543769
Thermal correction to Enthalpy=	0.544714
Thermal correction to Gibbs Free Energy=	0.453161
Sum of electronic and zero-point Energies=	-1489.365184
Sum of electronic and thermal Energies=	-1489.335654
Sum of electronic and thermal Enthalpies=	-1489.334710
Sum of electronic and thermal Free Energies=	-1489.426263

SCF Done: E(RM062X) = -1490.28283747

H	0.21841100	-2.66577200	-0.34542300
C	0.82325700	-0.47464600	3.96724800
C	0.28494000	-1.08629000	2.83500900
C	0.12502800	-0.33012900	1.68620400
C	0.49265200	1.01812300	1.64471600
C	1.03754000	1.63728300	2.76826400
C	1.19760900	0.86993100	3.92028300
H	0.95447600	-1.04169400	4.88199600
H	-0.00307700	-2.13395700	2.84063000
H	1.32934200	2.68153500	2.74000000
H	1.61998800	1.33574600	4.80517600
N	0.18868100	1.58480100	0.40598200
H	-2.07089000	1.31408500	0.79833400
C	0.86412300	2.70005200	-0.14187200
C	2.25156500	2.81460900	-0.02525800
C	0.13348300	3.69066300	-0.80195200
C	2.89532300	3.92768800	-0.55526600
H	2.80336600	2.01427600	0.45674300
C	0.79000100	4.78507800	-1.35511100
H	-0.94635100	3.58925600	-0.86873200
C	2.17076800	4.91185700	-1.22488000
H	3.97305100	4.01634700	-0.46242400
H	0.21879700	5.54855600	-1.87330800

H	2.68028700	5.77274000	-1.64486200
C	-0.56057400	0.62340400	-0.38518700
C	-1.72410800	-1.39124700	0.27073800
C	-0.33098500	-0.75691800	0.30735800
O	-1.92772600	-2.58458200	0.39544800
N	-2.01866000	0.87575000	-0.12368000
N	-2.62271600	-0.40270800	-0.00279800
C	-4.00302500	-0.53637700	-0.28480100
C	-4.68060700	-1.73047000	-0.01161700
C	-4.68857400	0.55291800	-0.83043600
C	-6.03775900	-1.81946900	-0.30148800
H	-4.14782500	-2.56966100	0.41219900
C	-6.04511100	0.44034000	-1.11103200
H	-4.14880100	1.46873200	-1.03347700
C	-6.72884500	-0.74312500	-0.84995300
H	-6.55828500	-2.74781400	-0.08926200
H	-6.56847700	1.29005100	-1.53759300
H	-7.78812400	-0.82487600	-1.06843900
C	-0.28585700	0.63595400	-1.87138000
H	0.78001000	0.48453000	-2.05085400
H	-0.85332200	-0.17072100	-2.34255600
H	-0.60095100	1.58443700	-2.30672600
N	0.54184000	-1.70515800	-0.34124800
C	1.87982400	-1.46693200	-0.46634700
O	2.38891300	-0.37106900	-0.32351900
O	2.51539200	-2.60081200	-0.80126600
C	3.94697700	-2.58379600	-1.07103400
C	4.23712400	-4.03583000	-1.43275500
H	3.97346300	-4.69448100	-0.60147100
H	3.65736800	-4.33267000	-2.31035500
H	5.30002800	-4.15898700	-1.65525000
C	4.71107300	-2.17996900	0.18651900
H	5.78397900	-2.30079800	0.01149900
H	4.50773100	-1.14280900	0.45177400
H	4.42403100	-2.82616300	1.02083900
C	4.24969900	-1.66591500	-2.25212900
H	4.06297500	-0.62275100	-1.99801500
H	5.29932200	-1.78047100	-2.53748600
H	3.62959300	-1.94447700	-3.10908300

Reaction (2):

Sub2

Zero-point correction= 0.247221 (Hartree/Particle)
Thermal correction to Energy= 0.256549
Thermal correction to Enthalpy= 0.257351
Thermal correction to Gibbs Free Energy= 0.214761
Sum of electronic and zero-point Energies= -671.777011
Sum of electronic and thermal Energies= -671.767683
Sum of electronic and thermal Enthalpies= -671.766881
Sum of electronic and thermal Free Energies= -671.809471
SCF Done: E(RM062X) = -672.205083371

C	-2.54019600	0.74288400	-0.26144600
C	-2.37170600	-0.61926900	0.11193200
C	-1.07373200	-1.18642900	0.10158800
C	0.02538400	-0.44955500	-0.28378800
C	-0.15113900	0.90806200	-0.68423400
C	-1.39253300	1.47961000	-0.65960500
H	-0.94891200	-2.22138900	0.41125100
H	0.70939300	1.47122400	-1.02836800
H	-1.51788500	2.51327600	-0.97041800
N	1.28264300	-1.04967800	-0.36125200
H	1.28467400	-2.05622000	-0.42417400
C	2.52002600	-0.45749300	-0.09069300
C	3.67903400	-1.08404900	-0.56815900
C	2.64638900	0.71357400	0.66767400
C	4.93144800	-0.54974300	-0.29783600
H	3.58425100	-1.98942000	-1.16132200
C	3.90570400	1.25040700	0.91292800
H	1.76177800	1.18703500	1.07899600
C	5.05557100	0.62773300	0.43629300
H	5.81632800	-1.05274000	-0.67492200
H	3.98510900	2.15920900	1.50134400
H	6.03379600	1.05011800	0.63735700
C	-3.51615300	-1.36426400	0.50338200
H	-3.38902500	-2.40419400	0.79140100
C	-3.83686500	1.31505600	-0.23588300
H	-3.95250900	2.35595200	-0.52608500
C	-4.92424300	0.57135600	0.14579200
H	-5.91344000	1.01663900	0.16203100
C	-4.75836200	-0.78396400	0.52031200
H	-5.62382300	-1.36524300	0.82212400

CPA2

Zero-point correction= 0.637903 (Hartree/Particle)

Thermal correction to Energy= 0.663802
Thermal correction to Enthalpy= 0.664603
Thermal correction to Gibbs Free Energy= 0.584415
Sum of electronic and zero-point Energies= -2185.164320
Sum of electronic and thermal Energies= -2185.138421
Sum of electronic and thermal Enthalpies= -2185.137619
Sum of electronic and thermal Free Energies= -2185.217807
SCF Done: E(RM062X) = -2186.32229733

H	-1.20505100	-3.10223000	1.11726900
C	0.34417700	4.18180900	-2.95104000
C	0.01958700	3.46969900	-1.63888600
C	1.01222100	2.36746600	-1.31211600
C	2.24456800	2.28657700	-1.97423700
C	2.68405200	3.32923200	-2.98417400
C	1.81602600	4.58438800	-2.96862700
H	0.14219800	3.51319100	-3.79727200
H	-0.00030100	4.21755300	-0.83507600
C	0.66768200	1.35933300	-0.38780500
C	3.08744300	1.19732900	-1.73744700
H	3.73486000	3.58046400	-2.80400800
H	2.04697700	5.20897200	-3.83639800
C	2.73531000	0.14899600	-0.89305800
C	1.50457500	0.25470200	-0.24382600
H	4.04527400	1.14624300	-2.25019700
C	-0.61323100	1.38147100	0.37534600
C	-0.92660700	2.38388000	1.31216400
C	-1.50208100	0.32183600	0.19311300
C	0.12373900	3.38971000	1.74556600
C	-2.17803800	2.35650300	1.94693800
C	-2.72967300	0.24501400	0.84966400
C	-0.47813200	4.64888900	2.36355300
H	0.75112200	2.89214000	2.49918000
C	-2.61813000	3.46174700	2.88831900
C	-3.05448600	1.29854200	1.70078100
C	-1.45674200	4.26429000	3.47070500
H	0.31988400	5.28786300	2.75317800
H	-3.27522200	4.14287700	2.33041800
H	-4.01460000	1.27373400	2.21108000
H	-1.83909800	5.15141200	3.98427300
O	1.08008000	-0.79872300	0.56562800
O	-1.13050600	-0.71889700	-0.64947400
P	-0.03243000	-1.76604000	-0.08521400
O	0.36694300	-2.73065800	-1.10910700

O	-0.63497500	-2.33755700	1.27639500
C	4.71717700	-2.94340600	-1.78406300
C	3.89035700	-1.79966200	-1.86172900
C	5.25206000	-3.32243600	-0.58268300
C	3.60371200	-1.04888300	-0.74492700
C	4.15694400	-1.41996900	0.52218100
C	4.98916700	-2.57306600	0.59402600
C	5.54754000	-2.94854400	1.84441000
H	6.17733700	-3.83308300	1.88527300
C	5.30156600	-2.21348700	2.97373400
C	4.48473100	-1.06034500	2.90158600
C	3.92904100	-0.67383500	1.70944500
H	5.88426200	-4.20297800	-0.50881600
H	5.73326500	-2.50965500	3.92430000
H	4.29815700	-0.47845400	3.79840300
H	3.30745200	0.21440400	1.66316900
C	-4.67702000	-2.84710500	1.81499500
C	-3.86494200	-1.69030300	1.86172200
C	-5.22506000	-3.25214000	0.62675200
C	-3.60506300	-0.95151500	0.72789000
C	-4.17687000	-1.34886300	-0.52269100
C	-4.99392900	-2.51487400	-0.56413500
C	-5.56823800	-2.91573100	-1.79972600
H	-6.18614300	-3.80920200	-1.81855600
C	-5.35120900	-2.19183000	-2.94168600
C	-4.54877300	-1.02661700	-2.89952800
C	-3.97779800	-0.61599500	-1.72339800
H	-5.84734400	-4.14134000	0.57657600
H	-5.79387600	-2.50676400	-3.88097400
H	-4.38433400	-0.45630000	-3.80779800
H	-3.36453400	0.27855100	-1.69818800
H	4.91361000	-3.52160500	-2.68072400
H	3.44706900	-1.51915200	-2.81217100
H	-3.41324800	-1.38449200	2.80087700
H	-4.85763400	-3.41075300	2.72450700
H	2.64432900	2.87951400	-3.98522400
H	2.03691700	5.18032700	-2.07370800
H	-0.30651900	5.05354000	-3.06605100
H	-0.98709400	3.03996500	-1.66968200
H	0.79865100	3.63579300	0.92508900
H	-1.00629800	5.22470000	1.59165000
H	-0.92843900	3.66100800	4.21945800
H	-3.23142300	3.03419200	3.68814300

A_2

Zero-point correction=	0.887214 (Hartree/Particle)
Thermal correction to Energy=	0.923216
Thermal correction to Enthalpy=	0.924018
Thermal correction to Gibbs Free Energy=	0.820858
Sum of electronic and zero-point Energies=	-2856.972568
Sum of electronic and thermal Energies=	-2856.936565
Sum of electronic and thermal Enthalpies=	-2856.935764
Sum of electronic and thermal Free Energies=	-2857.038924

SCF Done: E(RM062X) = -2858.55021562

H	-0.93101000	1.95687600	0.69327600
C	-3.57346600	2.53193000	2.79563600
C	-2.66560800	1.48472300	2.47589000
C	-2.79169000	0.80789300	1.23580000
C	-3.75922000	1.16627700	0.31404400
C	-4.65458000	2.23246500	0.63300000
C	-4.56648500	2.87466700	1.83732300
H	-2.16107200	-0.05581200	1.03860900
H	-5.39018500	2.53956600	-0.10229300
H	-5.25029900	3.68803400	2.06571600
N	-3.79249100	0.53389600	-0.91826800
H	-2.89959700	0.18118500	-1.25558500
C	-4.90574000	0.29215400	-1.71247200
C	-4.70420500	0.01011400	-3.07219900
C	-6.20833800	0.23902500	-1.19568100
C	-5.77828300	-0.31083300	-3.88988800
H	-3.69182400	0.04147000	-3.46597600
C	-7.27789400	-0.06695700	-2.03158500
H	-6.37400800	0.40665800	-0.13645200
C	-7.07615200	-0.34512700	-3.38039000
H	-5.60026900	-0.52840300	-4.93865000
H	-8.27965500	-0.10376200	-1.61413600
H	-7.91447700	-0.58781900	-4.02399700
C	4.98648900	-4.24542800	-1.18240300
C	4.35788100	-2.87236600	-0.95873900
C	2.87381400	-2.94107600	-0.64324100
C	2.11503200	-4.05170300	-1.04095400
C	2.76331400	-5.29859900	-1.61146200
C	4.15649100	-5.04610900	-2.18179500
H	6.01545600	-4.12562500	-1.53414300
H	4.90096900	-2.32343000	-0.18688900
C	2.21640300	-1.84284800	-0.05470900

C	0.72588200	-4.02203300	-0.90970700
H	2.83781700	-6.04571100	-0.80946400
H	4.07662200	-4.47929700	-3.11781800
C	0.04179700	-2.91599400	-0.40991800
C	0.82384100	-1.84309200	0.02067300
H	0.14385600	-4.87939100	-1.23948000
C	2.94799500	-0.62597200	0.40566000
C	3.89543400	-0.66026700	1.44851300
C	2.63660200	0.59849400	-0.18494500
C	4.08167900	-1.92161300	2.27360100
C	4.58211100	0.51515700	1.78369400
C	3.29831400	1.78422800	0.13502100
C	5.39956900	-1.94252300	3.04360300
H	3.24846600	-1.96915300	2.98920200
C	5.66230300	0.53388700	2.84866300
C	4.28681500	1.70310400	1.11187000
C	5.57250300	-0.64013200	3.82007700
H	5.41957700	-2.80539400	3.71585500
H	6.63980100	0.50748200	2.34803900
H	4.82695100	2.60996100	1.37370500
H	4.71238000	-0.50392000	4.48756900
O	0.20376600	-0.69018300	0.50375900
O	1.59971700	0.64770700	-1.11919100
P	0.10212000	0.53659400	-0.55365800
O	-0.91484500	0.36479700	-1.60111000
O	-0.01523500	1.79027800	0.40505700
C	-3.46192300	-2.93330300	-1.81546000
C	-2.05789600	-3.00729400	-1.68230700
C	-4.24161600	-2.68123800	-0.71792900
C	-1.44251000	-2.85091600	-0.45881800
C	-2.23807500	-2.62284800	0.70738000
C	-3.65131500	-2.51029800	0.56054800
C	-4.44402900	-2.21189600	1.70107200
H	-5.51677500	-2.10023000	1.56760800
C	-3.87207400	-2.06164500	2.93671900
C	-2.47432900	-2.22285800	3.09207800
C	-1.67899900	-2.49652700	2.00852700
H	-5.31865000	-2.57640300	-0.81830300
H	-4.48446200	-1.82062100	3.79923600
H	-2.03053300	-2.11820400	4.07712500
H	-0.60703200	-2.61367900	2.13408000
C	2.14631200	5.36925200	-0.18186700
C	2.49908400	4.10437800	0.34051300
C	2.23354600	5.60327500	-1.52785800

C	2.93230700	3.08757600	-0.47982200
C	3.04441700	3.31137000	-1.88929100
C	2.68527800	4.58724100	-2.41014800
C	2.79451400	4.82267200	-3.80628500
H	2.51159200	5.79893000	-4.19029000
C	3.24786900	3.84442900	-4.65072500
C	3.61957000	2.58107400	-4.13288300
C	3.52176300	2.32204400	-2.79046800
H	1.95945900	6.56918900	-1.94298700
H	3.32666200	4.03443200	-5.71618700
H	3.98431900	1.81210400	-4.80607300
H	3.81362000	1.35151400	-2.40298000
C	-1.65210600	1.14223600	3.41263500
H	-0.95514500	0.34988500	3.15105600
C	-3.45242200	3.19624000	4.04163400
H	-4.15086700	3.99488600	4.27732400
C	-2.47009900	2.84177900	4.93196100
H	-2.38319000	3.35686200	5.88295800
C	-1.56059000	1.80490400	4.61020900
H	-0.78247100	1.53824900	5.31856200
H	-3.91661900	-3.04052000	-2.79463000
H	-1.44124800	-3.15769000	-2.56334300
H	2.40278700	3.91463000	1.40529100
H	1.79831200	6.14665000	0.49023800
H	2.10559500	-5.73166100	-2.37190200
H	4.63923400	-5.99806900	-2.42169500
H	5.03327000	-4.78973600	-0.22951700
H	4.46788200	-2.27447300	-1.87486100
H	3.98364800	-2.81543600	1.65405100
H	6.23591600	-2.06163300	2.34159400
H	6.46666000	-0.67222200	4.44958400
H	5.62122300	1.48617400	3.38722200

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Zero-point correction= 1.196753 (Hartree/Particle)
Thermal correction to Energy= 1.247739
Thermal correction to Enthalpy= 1.248541
Thermal correction to Gibbs Free Energy= 1.116310
Sum of electronic and zero-point Energies= -3828.071199
Sum of electronic and thermal Energies= -3828.020212
Sum of electronic and thermal Enthalpies= -3828.019411
Sum of electronic and thermal Free Energies= -3828.151642
SCF Done: E(RM062X) = -3830.22133265

H	0.52863400	1.14536300	-0.78709100
C	5.60882300	-1.17714600	0.35220300
C	4.32241700	-1.24590700	-0.24917800
C	3.21719800	-0.64581700	0.40272700
C	3.34415600	-0.05178200	1.65667200
C	4.63859300	-0.00323300	2.26035400
C	5.72184900	-0.53583800	1.61683500
H	2.23164900	-0.72694700	-0.05587300
H	4.75399100	0.42228200	3.24934700
H	6.69736700	-0.50109600	2.09520700
N	2.20961600	0.43244800	2.27326400
H	1.32366800	0.07738800	1.90846000
C	2.09635200	0.93148200	3.58328500
C	1.03485600	0.46830400	4.37263300
C	2.94186100	1.91988400	4.09820700
C	0.84242600	0.96586000	5.65488600
H	0.34728500	-0.25194100	3.94119000
C	2.75201500	2.39919500	5.39081900
H	3.71585300	2.34632700	3.47364100
C	1.70661400	1.92564400	6.17800800
H	0.00991600	0.60093800	6.24826800
H	3.41666600	3.16728500	5.77337400
H	1.55899900	2.30930700	7.18181000
C	-6.70532800	-2.68989400	2.20826900
C	-5.90283200	-2.35094000	0.95340500
C	-4.43296800	-2.71093200	1.08453300
C	-3.98792400	-3.56322500	2.10421900
C	-4.94895800	-4.22938100	3.07080200
C	-6.40827100	-4.12359500	2.63761300
H	-6.43279100	-2.00496100	3.02100900
H	-6.35083400	-2.88082400	0.10229800
C	-3.48075200	-2.12396700	0.22238800
C	-2.61745400	-3.78324400	2.28143800
H	-4.65663000	-5.27716000	3.19969600
H	-7.06420800	-4.43873900	3.45432000
C	-1.65784800	-3.15287900	1.49849500
C	-2.12926000	-2.32238800	0.48003300
H	-2.28482800	-4.44402100	3.07890300
C	-3.86793800	-1.21874000	-0.89961900
C	-4.68281700	-1.65666600	-1.96112700
C	-3.40099400	0.10076100	-0.90005200
C	-4.95271400	-3.13652400	-2.16551600
C	-5.14134200	-0.72377800	-2.90323200

C	-3.83234000	1.04246200	-1.83611000
C	-6.19348100	-3.40390600	-3.01296100
H	-4.07666700	-3.55160500	-2.68433500
C	-6.10128800	-1.11179200	-4.01246800
C	-4.73183500	0.60556100	-2.80655300
C	-6.11110600	-2.60874900	-4.31375000
H	-6.27959400	-4.47562100	-3.21555800
H	-7.11241800	-0.80429300	-3.71210000
H	-5.09331800	1.32779500	-3.53553100
H	-6.94776500	-2.84870700	-4.97666900
O	-1.21027500	-1.60936700	-0.28199100
O	-2.53047700	0.51052000	0.10070000
P	-1.02653200	-0.07618400	0.19120200
O	-0.50551200	0.11963300	1.56108600
O	-0.19272500	0.46371600	-1.00820600
C	1.67887300	-2.79949700	3.24596300
C	0.29168300	-2.79311200	2.96446500
C	2.55990100	-3.30842100	2.32956900
C	-0.19974900	-3.26728700	1.77055100
C	0.69964300	-3.82417000	0.80594500
C	2.09254400	-3.84937400	1.10179100
C	2.99191000	-4.40404000	0.15466300
H	4.05574900	-4.39140000	0.37830100
C	2.53352500	-4.92309700	-1.02817800
C	1.14995900	-4.90390500	-1.32090300
C	0.25689800	-4.36546200	-0.42974000
H	3.63075900	-3.29304800	2.51729600
H	3.23333600	-5.33574900	-1.74802600
H	0.79428800	-5.31509000	-2.26020400
H	-0.80355500	-4.35291800	-0.66039400
C	-1.59104100	4.08522500	-2.15288800
C	-2.05304600	2.74892500	-2.12353600
C	-2.44999400	5.11988200	-1.88953200
C	-3.36245200	2.45653900	-1.81712300
C	-4.27595000	3.51760000	-1.51482100
C	-3.80775400	4.86317100	-1.56310400
C	-4.70687200	5.92157300	-1.26704400
H	-4.33696800	6.94232900	-1.31190400
C	-6.00901500	5.66526900	-0.92749800
C	-6.47158900	4.32964400	-0.86115600
C	-5.62951100	3.28538100	-1.14557600
H	-2.10675800	6.15070900	-1.91992700
H	-6.68667000	6.48234800	-0.70220500
H	-7.50040200	4.13220000	-0.57761500

H	-5.98795600	2.26339100	-1.08257800
C	4.30670300	2.45945300	-0.27786500
C	3.15516000	1.17138800	-1.89568200
C	2.93994800	1.98936700	-0.62427000
O	2.30722000	0.59570600	-2.53683700
N	5.14089600	2.02109300	-1.16190900
N	4.50184900	1.29334200	-2.14384100
C	5.27496400	0.66277900	-3.14782200
C	4.65127700	0.10883100	-4.26892300
C	6.65921800	0.59043100	-2.99320500
C	5.42948500	-0.54089400	-5.22049700
H	3.57683300	0.16911100	-4.37702800
C	7.41815200	-0.05820200	-3.95998100
H	7.11976200	1.02065100	-2.11322400
C	6.81096000	-0.63322200	-5.07282000
H	4.94451500	-0.97704100	-6.08794800
H	8.49428100	-0.12062000	-3.83307800
H	7.40882700	-1.14223600	-5.82140100
C	4.82559800	3.29056800	0.84603100
H	5.90583300	3.37878100	0.72279000
H	4.36054900	4.27600800	0.86064100
H	4.60432600	2.81377700	1.80042900
N	1.73361400	2.13836600	-0.22942500
C	1.36146000	2.98869900	0.85630000
O	2.12155800	3.60207900	1.56576000
O	0.04030700	3.00754000	0.87477500
C	-0.69510500	3.82356700	1.85002600
C	-2.14768800	3.50230200	1.53131700
H	-2.37951900	3.75933900	0.49585100
H	-2.33746800	2.43668400	1.67902500
H	-2.80103200	4.07871000	2.19210700
C	-0.38690600	5.29420900	1.59226700
H	-1.02278700	5.90828400	2.23587500
H	0.65710600	5.52589600	1.80724300
H	-0.61306200	5.54111600	0.55038800
C	-0.35258400	3.37400000	3.26288600
H	0.68843500	3.57455500	3.52201400
H	-1.00077100	3.90498200	3.96645700
H	-0.54437600	2.30250000	3.35168200
C	4.18326200	-1.91893900	-1.49333200
H	3.20043500	-1.96028400	-1.95565500
C	6.71240300	-1.79044200	-0.29210700
H	7.68967300	-1.73529600	0.18049800
C	6.54713700	-2.44730100	-1.48630100

H	7.39605800	-2.91109800	-1.97798100
C	5.26952500	-2.50610400	-2.09215700
H	5.15346400	-3.00621900	-3.04875400
H	2.03617200	-2.37326200	4.17865700
H	-0.40462700	-2.37110300	3.68354500
H	-1.36922700	1.93940400	-2.35316500
H	-0.55084600	4.28101500	-2.39337900
H	-4.83338600	-3.75631500	4.05514900
H	-6.59701600	-4.79849200	1.79276100
H	-7.77195000	-2.54823700	2.01099400
H	-5.98444300	-1.28507800	0.71649800
H	-5.00275500	-3.66625800	-1.21354500
H	-7.09376600	-3.10603800	-2.45839000
H	-5.19083200	-2.88602700	-4.84275100
H	-5.86369700	-0.53835700	-4.91419100

B_2'

Zero-point correction= 1.196429 (Hartree/Particle)
Thermal correction to Energy= 1.248018
Thermal correction to Enthalpy= 1.248819
Thermal correction to Gibbs Free Energy= 1.112361
Sum of electronic and zero-point Energies= -3828.073544
Sum of electronic and thermal Energies= -3828.021956
Sum of electronic and thermal Enthalpies= -3828.021154
Sum of electronic and thermal Free Energies= -3828.157612
SCF Done: E(RM062X) = -3830.22771665

H	0.63551400	1.34173400	1.16686800
C	5.53211000	0.37103900	-1.86163700
C	4.43277000	1.23076500	-1.58043700
C	3.11684300	0.79155000	-1.85505200
C	2.86844300	-0.44334500	-2.44425700
C	3.97575400	-1.31315900	-2.69478400
C	5.25122500	-0.91332900	-2.40139400
H	2.27556800	1.44546200	-1.63243700
H	3.79527400	-2.31927900	-3.05564700
H	6.07684700	-1.59932100	-2.57271000
N	1.55722100	-0.79808300	-2.66771700
H	0.86674300	-0.22052900	-2.18555500
C	1.01990100	-1.88746300	-3.34723400
C	-0.25152600	-2.32851100	-2.94027100
C	1.64675100	-2.52502700	-4.42492600
C	-0.85731500	-3.40207600	-3.57606100

H	-0.73670900	-1.81776000	-2.11140600
C	1.03498600	-3.61422300	-5.03933900
H	2.59412200	-2.15467500	-4.79868600
C	-0.21280100	-4.06610600	-4.62129800
H	-1.83857000	-3.72921700	-3.24535000
H	1.53800400	-4.10153600	-5.86904200
H	-0.68351300	-4.91218800	-5.11037200
C	-6.59105000	-2.75588200	-1.07145400
C	-5.89434500	-1.87357500	-0.03766100
C	-5.25331900	-0.64524500	-0.65523200
C	-5.62546000	-0.20987600	-1.93479000
C	-6.70202200	-0.91000900	-2.74277900
C	-7.52437400	-1.90283400	-1.92578100
H	-5.84409900	-3.23514300	-1.71695900
H	-6.63845000	-1.56634100	0.70760800
C	-4.22649900	0.03750300	0.02830100
C	-4.96065500	0.87066500	-2.51879200
H	-7.34982300	-0.15726400	-3.20480500
H	-8.13104700	-2.52245300	-2.59262000
C	-3.90615700	1.52584500	-1.89050600
C	-3.55663900	1.07659300	-0.61691800
H	-5.25624500	1.20272000	-3.51145300
C	-3.75271200	-0.36373200	1.38411000
C	-4.56952600	-0.35323500	2.52338500
C	-2.40296200	-0.71088400	1.53703100
C	-5.97417300	0.20056200	2.55477200
C	-4.04186900	-0.75445100	3.76045400
C	-1.85796700	-1.10895800	2.75498800
C	-6.96666500	-0.67729600	3.35181800
H	-5.90671900	1.17478900	3.05760300
C	-4.98027600	-0.76104700	4.93977400
C	-2.71157800	-1.14424100	3.85990600
C	-6.30108700	-1.42424300	4.52568100
H	-7.76742600	-0.03028600	3.72233600
H	-4.52564200	-1.28662700	5.78431800
H	-2.31019300	-1.46421500	4.81808000
H	-6.98507900	-1.48159400	5.37709300
O	-2.47466100	1.66677200	0.02977300
O	-1.57384400	-0.64603000	0.42376400
P	-1.09681700	0.82694200	-0.05080800
O	-0.45820800	0.77604600	-1.37737300
O	-0.33765900	1.51150000	1.14124800
C	-1.75456700	3.29538800	-4.44459600
C	-2.48056600	2.30677500	-3.74211600

C	-1.70888600	4.57919800	-3.97192000
C	-3.14923700	2.60606800	-2.57767800
C	-3.11850000	3.94098600	-2.06332200
C	-2.38755300	4.93329200	-2.77643300
C	-2.35713000	6.26284100	-2.27858000
H	-1.79455800	7.00998700	-2.83198400
C	-3.02305100	6.59931800	-1.12975800
C	-3.75624300	5.61578600	-0.42430500
C	-3.80347100	4.32332400	-0.87888900
H	-1.15118400	5.34686800	-4.50138300
H	-2.99376300	7.61885700	-0.75882100
H	-4.28488100	5.88911200	0.48322500
H	-4.37042100	3.57573200	-0.33391500
C	1.78705600	-0.94808500	3.78753800
C	0.43706700	-0.59899100	3.53396600
C	2.25490000	-2.18463700	3.42620200
C	-0.42038800	-1.47574400	2.91199400
C	0.05226800	-2.76584800	2.50477400
C	1.40052500	-3.12543600	2.78757400
C	1.86673500	-4.41441100	2.42111400
H	2.90154500	-4.67191700	2.63093900
C	1.03808100	-5.30837600	1.79424900
C	-0.29636600	-4.94642100	1.49798600
C	-0.77844400	-3.70891000	1.84550700
H	3.28860600	-2.46500200	3.61531800
H	1.41042700	-6.28460000	1.50146800
H	-0.94289200	-5.65475500	0.98969600
H	-1.80498600	-3.43682800	1.62090700
C	4.46130700	-0.22848900	1.41323000
C	2.35785900	-0.89263100	0.58265200
C	3.07777200	0.25659200	1.25845700
O	1.18445600	-0.92545400	0.29343800
N	4.55522700	-1.41648200	0.91877900
N	3.33489000	-1.85446700	0.44149400
C	3.26219400	-3.08815500	-0.24801300
C	2.05472400	-3.49989900	-0.81179800
C	4.41678100	-3.86158700	-0.38989400
C	2.02188600	-4.67190200	-1.56051100
H	1.15651500	-2.91319600	-0.67428200
C	4.35603100	-5.04256000	-1.11991500
H	5.34523600	-3.52296800	0.05159700
C	3.16514400	-5.44889600	-1.71951100
H	1.08597000	-4.96124600	-2.03001200
H	5.25459200	-5.64123100	-1.23172000

H	3.13142400	-6.36025900	-2.30706200
C	5.63729000	0.50949300	1.94953300
H	5.72646500	1.47463300	1.43864800
H	5.52651200	0.69810200	3.02022400
H	6.53937500	-0.07235100	1.75819500
N	2.45599400	1.32233300	1.55461900
C	3.09158400	2.30509400	2.35477500
O	3.45138500	2.08511600	3.48717300
O	3.12888300	3.45404700	1.70313700
C	3.69031200	4.64967100	2.34119000
C	3.60028900	5.68849400	1.23126600
H	4.20997600	5.38649800	0.37478900
H	2.56552200	5.80350500	0.90005400
H	3.96389900	6.65227900	1.59599800
C	5.14324700	4.39779000	2.73102300
H	5.60136800	5.34492400	3.02902700
H	5.21950600	3.69319600	3.55928900
H	5.69405800	4.00423200	1.87138500
C	2.82304900	5.04167000	3.53181300
H	2.87615600	4.29137200	4.32123100
H	3.17482600	5.99701300	3.93096400
H	1.78344500	5.16174000	3.21572600
C	4.69606100	2.51943900	-1.03642000
H	3.85538000	3.17132300	-0.81355900
C	6.84962800	0.81655300	-1.59109000
H	7.67913000	0.14691700	-1.80361100
C	7.07975100	2.07381900	-1.08873600
H	8.09315600	2.41281800	-0.90123200
C	5.98719800	2.93408800	-0.81684400
H	6.17820800	3.93458300	-0.43752600
H	-1.22766500	3.02462100	-5.35347500
H	-2.48857000	1.28379500	-4.10575600
H	0.06971600	0.38017300	3.82707300
H	2.44520100	-0.21966800	4.25295000
H	-6.21685900	-1.44436200	-3.57047000
H	-8.21749100	-1.36233000	-1.26843900
H	-7.13959700	-3.55454900	-0.56340200
H	-5.13424200	-2.43881700	0.51172400
H	-6.34943100	0.40848900	1.55094000
H	-7.44262400	-1.40393900	2.68673100
H	-6.07551300	-2.45342100	4.22799300
H	-5.17684500	0.26833000	5.27154300

TS-A_2

Zero-point correction= 1.194521 (Hartree/Particle)
Thermal correction to Energy= 1.244625
Thermal correction to Enthalpy= 1.245427
Thermal correction to Gibbs Free Energy= 1.115611
Sum of electronic and zero-point Energies= -3828.065667
Sum of electronic and thermal Energies= -3828.015563
Sum of electronic and thermal Enthalpies= -3828.014761
Sum of electronic and thermal Free Energies= -3828.144577
SCF Done: E(RM062X) = -3830.21520945
Number of Imaginary Frequencies = -124.24

H	0.85387700	1.55268600	-0.59553200
C	5.35653900	-1.11580400	0.26931400
C	4.07377300	-1.10629300	-0.33256400
C	3.00426900	-0.41401000	0.31484500
C	3.14239200	0.04263300	1.64993700
C	4.44601200	-0.00143600	2.25455000
C	5.49674800	-0.53326000	1.57186900
H	2.00524700	-0.49521400	-0.11324200
H	4.57471500	0.34869500	3.27094700
H	6.47419800	-0.57178300	2.04640500
N	2.04197300	0.47699800	2.29551100
H	1.10792600	0.23286600	1.89279700
C	1.94978500	0.94117000	3.62674100
C	0.88905200	0.45210500	4.39867200
C	2.80642900	1.90527600	4.16331000
C	0.71564800	0.89684700	5.70276200
H	0.19038300	-0.23744400	3.93702200
C	2.62986200	2.33632500	5.47469200
H	3.57004200	2.35658100	3.54430800
C	1.59135400	1.83187300	6.25158900
H	-0.11276000	0.51502800	6.29052100
H	3.29816600	3.08879600	5.88034000
H	1.45487400	2.17723300	7.27081900
C	-6.50300600	-2.89567600	2.25308500
C	-5.73282800	-2.50534500	0.99305300
C	-4.24866000	-2.81267300	1.09516900
C	-3.75694900	-3.66459200	2.09329700
C	-4.67696600	-4.38081100	3.06420000
C	-6.14561700	-4.32401400	2.65364600
H	-6.24402600	-2.21484500	3.07377700
H	-6.17464600	-3.03564100	0.13892800
C	-3.33439900	-2.17680000	0.22702700

C	-2.37663700	-3.83713900	2.24229000
H	-4.34419400	-5.41886700	3.17337600
H	-6.77731200	-4.67790700	3.47382300
C	-1.45660600	-3.15769100	1.45318000
C	-1.96963500	-2.32295100	0.45737000
H	-2.00603500	-4.50048000	3.02096600
C	-3.77611200	-1.27451500	-0.87732000
C	-4.58571000	-1.73317300	-1.93374600
C	-3.35880300	0.06253800	-0.86443600
C	-4.80096400	-3.22034500	-2.15099100
C	-5.08928300	-0.80971300	-2.86183200
C	-3.83465800	0.99410200	-1.79112400
C	-6.03874800	-3.52679700	-2.98962700
H	-3.91491600	-3.59733700	-2.68196300
C	-6.04583300	-1.22292500	-3.96503300
C	-4.72639500	0.53237900	-2.75758400
C	-6.00003500	-2.71580100	-4.28267700
H	-6.08649500	-4.59906900	-3.20264700
H	-7.06560700	-0.95958300	-3.65174000
H	-5.11848100	1.24590300	-3.47955700
H	-6.83275300	-2.98201400	-4.94079400
O	-1.09414300	-1.57135100	-0.30284000
O	-2.50448400	0.48825200	0.13344400
P	-0.95237200	-0.01431100	0.17485600
O	-0.51056300	0.10079600	1.60067300
O	-0.12155300	0.61865500	-0.91608400
C	1.90466500	-2.77377900	3.15130700
C	0.51511500	-2.76888200	2.88478000
C	2.77721400	-3.28652700	2.22783200
C	0.00953600	-3.24022100	1.69546700
C	0.90043100	-3.79381300	0.72139100
C	2.29581500	-3.83112000	1.00693400
C	3.18036500	-4.41459900	0.06308700
H	4.24618200	-4.41414700	0.28025500
C	2.70672900	-4.94431300	-1.10864100
C	1.32273900	-4.89944300	-1.39817300
C	0.44342900	-4.33470100	-0.50973800
H	3.84913300	-3.28515800	2.41093600
H	3.39447100	-5.38401800	-1.82432900
H	0.95590400	-5.31380300	-2.33174700
H	-0.61747700	-4.30263800	-0.73528100
C	-1.66504000	4.08616700	-2.10423500
C	-2.09092800	2.73868800	-2.04843100
C	-2.55772900	5.10583200	-1.90054400

C	-3.40313600	2.42037800	-1.77926800
C	-4.35155800	3.46565100	-1.53294700
C	-3.91728400	4.82182900	-1.60594200
C	-4.85216500	5.86390000	-1.36735900
H	-4.50736900	6.89248900	-1.43200700
C	-6.15673300	5.58344000	-1.05772200
C	-6.58587700	4.23827200	-0.96405200
C	-5.70901900	3.20932000	-1.19412700
H	-2.24133700	6.14443500	-1.95354100
H	-6.86151400	6.38850800	-0.87630700
H	-7.61667200	4.02129900	-0.70253400
H	-6.04192000	2.18035500	-1.10936600
C	4.27390100	2.35973900	-0.14124400
C	3.12220400	1.23281700	-1.86158000
C	2.92617500	1.87705700	-0.50023100
O	2.27630300	0.75518100	-2.57952700
N	5.11695800	1.99645400	-1.05610300
N	4.47928500	1.35008400	-2.08489500
C	5.24900300	0.77779600	-3.12632400
C	4.62811400	0.28983000	-4.27898700
C	6.63308300	0.68818600	-2.97108400
C	5.40809700	-0.31220800	-5.26108900
H	3.55527300	0.36509900	-4.39110200
C	7.39318200	0.08907300	-3.96789200
H	7.09232500	1.06947400	-2.06808400
C	6.78771400	-0.42140900	-5.11316500
H	4.92434200	-0.69633300	-6.15339600
H	8.46871600	0.01638900	-3.84137200
H	7.38608000	-0.89193200	-5.88606100
C	4.79026500	3.15216300	1.01273300
H	5.87393200	3.21721400	0.90533800
H	4.34964300	4.14839000	1.03560000
H	4.54897700	2.66751500	1.95648800
N	1.69390300	2.17417600	-0.14390800
C	1.30645900	3.02910100	0.91444900
O	2.07442800	3.62516400	1.63280500
O	-0.01294100	3.07177200	0.90326400
C	-0.76531900	3.87140400	1.87946900
C	-2.21236800	3.55122600	1.53452200
H	-2.44171800	3.85602200	0.51174200
H	-2.39162700	2.47738900	1.62794200
H	-2.87416400	4.08911700	2.21908700
C	-0.45156100	5.34466700	1.64960500
H	-1.09221200	5.95067600	2.29618200

H	0.59147600	5.56903000	1.87825200
H	-0.66633600	5.60816700	0.60947900
C	-0.44294400	3.39701400	3.28914900
H	0.59336100	3.59757900	3.56687300
H	-1.10322600	3.91256200	3.99267500
H	-0.63495700	2.32343400	3.35305900
C	3.88805600	-1.76232900	-1.57064800
H	2.89796100	-1.76885400	-2.01823400
C	6.42524200	-1.76721100	-0.38134100
H	7.40470600	-1.77081300	0.08941200
C	6.22559700	-2.39317200	-1.59351800
H	7.05191800	-2.88485600	-2.09597100
C	4.94855600	-2.39019700	-2.18712000
H	4.79902600	-2.88363000	-3.14211100
H	2.27025800	-2.35233100	4.08359000
H	-0.17605500	-2.36236300	3.61650100
H	-1.37443000	1.94251900	-2.21912100
H	-0.62279700	4.30234700	-2.31813300
H	-4.56593500	-3.91844700	4.05431500
H	-6.32060200	-4.99118700	1.79966600
H	-7.57726700	-2.79128600	2.07424600
H	-5.85670400	-1.43923500	0.77688700
H	-4.82212700	-3.76114600	-1.20409100
H	-6.94419600	-3.26865400	-2.42355300
H	-5.07425000	-2.95120200	-4.82241300
H	-5.84091200	-0.63132800	-4.86316400

TS-A_2'

Zero-point correction= 1.195657 (Hartree/Particle)
Thermal correction to Energy= 1.245758
Thermal correction to Enthalpy= 1.246560
Thermal correction to Gibbs Free Energy= 1.114788
Sum of electronic and zero-point Energies= -3828.054671
Sum of electronic and thermal Energies= -3828.004570
Sum of electronic and thermal Enthalpies= -3828.003769
Sum of electronic and thermal Free Energies= -3828.135541
SCF Done: E(RM062X) = -3830.21267096
Number of Imaginary Frequencies = -163.18

H	1.18878600	1.45493100	1.05339900
C	5.25201600	1.54129600	-1.75608800
C	3.96923400	1.94308900	-1.31952300
C	2.91466200	0.95932600	-1.27006400

C	3.05237700	-0.26421600	-2.01199200
C	4.39169800	-0.69422200	-2.33119400
C	5.42561000	0.17454800	-2.18743400
H	1.89447000	1.30520400	-1.11205900
H	4.57024900	-1.71180000	-2.65109600
H	6.43332000	-0.15829400	-2.42404500
N	1.93376900	-0.93513300	-2.26948300
H	1.03015900	-0.46867900	-1.95137500
C	1.70888500	-2.19209000	-2.86627300
C	0.50871500	-2.81992200	-2.49907100
C	2.54842100	-2.78897100	-3.80985600
C	0.18235300	-4.05235600	-3.04292600
H	-0.13760000	-2.32540700	-1.77844300
C	2.21382400	-4.03559000	-4.33271800
H	3.42660200	-2.27413200	-4.17709000
C	1.04008800	-4.67522900	-3.95020900
H	-0.74551100	-4.53324100	-2.75039600
H	2.87283600	-4.49677600	-5.06112600
H	0.78620800	-5.64386100	-4.36782500
C	-6.43887200	-3.23667100	-0.47566400
C	-5.74312600	-2.11353500	0.29061500
C	-5.10292300	-1.08716700	-0.62544000
C	-5.46921100	-1.00797700	-1.97611900
C	-6.53960700	-1.90051300	-2.57622100
C	-7.36787800	-2.63952300	-1.52865000
H	-5.69116300	-3.87014100	-0.96982200
H	-6.48724300	-1.62442400	0.93139000
C	-4.08630400	-0.23972700	-0.13900500
C	-4.80511400	-0.11463500	-2.81911100
H	-7.18475300	-1.29996000	-3.22678600
H	-7.97509600	-3.41273400	-2.00889200
C	-3.76112900	0.69190000	-2.37730100
C	-3.41124800	0.60047800	-1.02771500
H	-5.09728600	-0.05526900	-3.86543900
C	-3.62266500	-0.27633500	1.27858600
C	-4.44802200	0.00936000	2.37549000
C	-2.27149700	-0.56997600	1.51759800
C	-5.85147700	0.55568900	2.25819800
C	-3.93111900	-0.07896500	3.67695700
C	-1.74400300	-0.67479200	2.80447200
C	-6.85459700	-0.08933200	3.24292000
H	-5.78322400	1.62517000	2.49941600
C	-4.87768600	0.20327700	4.81550600
C	-2.60408600	-0.44128000	3.87896800

C	-6.19825700	-0.53720400	4.56456400
H	-7.64643800	0.63863500	3.44443900
H	-4.43126100	-0.10338600	5.76596900
H	-2.21402200	-0.52793000	4.89018700
H	-6.88795200	-0.39017500	5.40080700
O	-2.36559700	1.36306200	-0.55268000
O	-1.43958200	-0.75794500	0.43472600
P	-0.93058600	0.60621000	-0.32715400
O	-0.34766800	0.17358800	-1.63743900
O	-0.17134600	1.51186500	0.60070200
C	-1.66105600	1.75934800	-5.33375300
C	-2.36527100	0.98130300	-4.38714700
C	-1.61784100	3.12173900	-5.20751300
C	-3.01664500	1.56407000	-3.32444900
C	-2.98880300	2.98698300	-3.17264300
C	-2.27930700	3.76679000	-4.12999400
C	-2.25475300	5.18011300	-3.99247300
H	-1.70787100	5.76238100	-4.72942000
C	-2.90733600	5.79746900	-2.95851500
C	-3.62013000	5.02450800	-2.01129600
C	-3.66034100	3.65836400	-2.11578900
H	-1.07797000	3.73089200	-5.92751900
H	-2.88278700	6.87846600	-2.86351500
H	-4.13752900	5.51918800	-1.19558300
H	-4.20781800	3.07265900	-1.38523700
C	1.89990100	-0.34715500	3.81011700
C	0.54995700	-0.04515700	3.49865800
C	2.36820300	-1.62737100	3.67743300
C	-0.31275700	-1.01568500	3.04888800
C	0.15734400	-2.36139000	2.89268700
C	1.50697300	-2.66702400	3.22958200
C	1.96634900	-4.00385500	3.11262600
H	2.99970400	-4.22227800	3.36860000
C	1.13045000	-4.99850800	2.67300500
C	-0.20252000	-4.69253800	2.31474700
C	-0.67722100	-3.40777300	2.42180000
H	3.40205400	-1.86909400	3.91127900
H	1.49498600	-6.01661600	2.58109500
H	-0.85627200	-5.48157800	1.95635800
H	-1.70265200	-3.17700100	2.15119500
C	4.48365800	0.24998700	1.10786500
C	2.47520900	-0.84963000	0.61282400
C	3.05007000	0.51116000	0.89661900
O	1.32339300	-1.14477600	0.39450600

N	4.74065100	-0.99868200	0.86244600
N	3.59097300	-1.67704000	0.56504100
C	3.67041500	-2.97502100	0.00140000
C	2.52459700	-3.76322800	-0.11618600
C	4.90500300	-3.43784800	-0.46418800
C	2.62317700	-5.00658700	-0.73288300
H	1.57326800	-3.40590000	0.25818000
C	4.98189100	-4.68683100	-1.06885900
H	5.78190800	-2.81189200	-0.35154000
C	3.84128000	-5.47302700	-1.21602600
H	1.72615700	-5.60877800	-0.83612500
H	5.94104900	-5.04272200	-1.43142900
H	3.90309000	-6.44180100	-1.70049700
C	5.61281300	1.16942900	1.44565500
H	5.45869100	2.15995900	1.01604600
H	5.69176000	1.29613200	2.52571800
H	6.53360800	0.73364100	1.05298500
N	2.25009600	1.48508600	1.35646200
C	2.63176900	2.50514800	2.21365300
O	3.66006900	2.53794700	2.85525700
O	1.64742100	3.40297400	2.24511400
C	1.72673800	4.55929500	3.12831600
C	0.39366200	5.25465400	2.88184000
H	0.29565500	5.52413000	1.82765500
H	-0.43296100	4.58960900	3.14253800
H	0.32905200	6.16130900	3.48891500
C	2.89280100	5.44558100	2.70055200
H	2.88700400	6.36428300	3.29376000
H	3.84649300	4.93645700	2.84481200
H	2.78288000	5.71856900	1.64655600
C	1.84110200	4.10952700	4.58229600
H	2.80446100	3.64017700	4.78058700
H	1.72933300	4.97977100	5.23516000
H	1.03968200	3.40288400	4.81768800
C	3.76923700	3.25733400	-0.86344200
H	2.77812200	3.56011000	-0.53465600
C	6.31019300	2.46252600	-1.73290900
H	7.29493700	2.14703100	-2.06695100
C	6.10234100	3.75640300	-1.28512200
H	6.92303400	4.46528700	-1.27108100
C	4.82895600	4.15139500	-0.84996100
H	4.67088100	5.16737300	-0.50260800
H	-1.15034800	1.26708600	-6.15507600
H	-2.37319600	-0.10059400	-4.47701800

H	0.18984300	0.97691300	3.58403200
H	2.56439600	0.44756800	4.13992300
H	-6.05127900	-2.63773500	-3.22787700
H	-8.06063000	-1.94199900	-1.04039000
H	-6.99027000	-3.87291900	0.22327900
H	-4.98243000	-2.51501500	0.96837700
H	-6.21841200	0.50509000	1.23113600
H	-7.34188500	-0.94945000	2.77400500
H	-5.97334500	-1.60792300	4.52032200
H	-5.07368100	1.28274300	4.88738900

TS-N_2

Zero-point correction= 1.199468 (Hartree/Particle)
Thermal correction to Energy= 1.248997
Thermal correction to Enthalpy= 1.249799
Thermal correction to Gibbs Free Energy= 1.122187
Sum of electronic and zero-point Energies= -3828.054556
Sum of electronic and thermal Energies= -3828.005027
Sum of electronic and thermal Enthalpies= -3828.004226
Sum of electronic and thermal Free Energies= -3828.131838
SCF Done: E(RM062X) = -3830.20821495
Number of Imaginary Frequencies = -115.89

H	0.71646800	2.23491300	-0.54215500
C	4.43914300	-2.09872800	-1.84443100
C	3.08890600	-1.66946800	-1.92758600
C	2.55370900	-0.83992600	-0.91045000
C	3.32541200	-0.44868000	0.16075000
C	4.65918900	-0.92958300	0.28000500
C	5.18961700	-1.72735800	-0.69787000
H	1.54721900	-0.45651600	-1.04526900
H	5.25701600	-0.70413500	1.14980800
H	6.21224200	-2.08200700	-0.60256300
N	2.73682200	0.51414600	1.06783300
H	1.69892100	0.37266000	1.06975200
C	3.16469200	0.57309400	2.44708100
C	2.17244700	0.45574800	3.42345500
C	4.48815600	0.82152800	2.81614400
C	2.51861600	0.53308700	4.76671300
H	1.14085400	0.31871100	3.11172000
C	4.82226000	0.88994200	4.16655100
H	5.24585000	1.01618000	2.06764200
C	3.84492700	0.73672200	5.14462500

H	1.74415400	0.43791100	5.52066500
H	5.85237800	1.08112700	4.44802700
H	4.11146400	0.79375600	6.19471400
C	-5.83399700	-2.75892300	3.06540600
C	-5.26953300	-2.43764200	1.68248600
C	-3.77512300	-2.69172600	1.58629800
C	-3.10711600	-3.44654500	2.55846500
C	-3.84167800	-4.10544900	3.71026900
C	-5.35467300	-4.13654500	3.51360900
H	-5.49543400	-2.00679200	3.78927600
H	-5.80615300	-3.04160400	0.93842700
C	-3.02514500	-2.10756200	0.54458200
C	-1.71735800	-3.57684700	2.49379600
H	-3.44744400	-5.11720200	3.85514300
H	-5.84678600	-4.44680600	4.44021900
C	-0.95005500	-2.94484700	1.52001600
C	-1.63579400	-2.19608100	0.56119000
H	-1.20629000	-4.17693800	3.24357100
C	-3.66888100	-1.31494500	-0.54029300
C	-4.58153300	-1.89794200	-1.43717300
C	-3.33529700	0.03982500	-0.66131400
C	-4.73667100	-3.40637200	-1.50846500
C	-5.25699800	-1.07622800	-2.35031500
C	-4.00354300	0.87705600	-1.56288900
C	-6.04402000	-3.83931400	-2.16653500
H	-3.89711500	-3.78890600	-2.10691800
C	-6.31185400	-1.62262100	-3.29395300
C	-4.97449600	0.28730000	-2.37423300
C	-6.20859700	-3.13091300	-3.50904000
H	-6.05239500	-4.92603900	-2.29451600
H	-7.30144000	-1.39211900	-2.87561800
H	-5.50412600	0.92357600	-3.08037000
H	-7.09394900	-3.49301000	-4.04047100
O	-0.93009000	-1.47552200	-0.38721000
O	-2.36381400	0.55148600	0.18295800
P	-0.79137800	0.12452000	-0.04286000
O	-0.08496600	0.30513200	1.27481000
O	-0.20743900	0.78545700	-1.25333000
C	2.62114300	-2.80275000	2.76418100
C	1.22515300	-2.61020700	2.63788100
C	3.30669500	-3.48366800	1.79402500
C	0.53193200	-3.07029700	1.54159100
C	1.23501800	-3.75285600	0.49747900
C	2.63446600	-3.97500300	0.64398700

C	3.33112300	-4.69154700	-0.36438800
H	4.40036100	-4.84722500	-0.24347500
C	2.67875000	-5.16065700	-1.47370100
C	1.29046300	-4.93337700	-1.62312300
C	0.58648700	-4.25132900	-0.66431100
H	4.37717400	-3.65014000	1.88057900
H	3.22526500	-5.69265300	-2.24569300
H	0.78114300	-5.29919900	-2.50921000
H	-0.47891300	-4.08675800	-0.78503800
C	-2.19815700	4.13244000	-2.28506300
C	-2.46586300	2.76008100	-2.07194400
C	-3.19050800	5.06563400	-2.14432300
C	-3.72165500	2.33250900	-1.70570500
C	-4.76906300	3.29276700	-1.50556400
C	-4.49451300	4.67117900	-1.74492400
C	-5.52369900	5.63032000	-1.55204900
H	-5.29924600	6.67518000	-1.74967300
C	-6.76686500	5.25406400	-1.11659800
C	-7.03318400	3.89206700	-0.84341800
C	-6.06378500	2.94002600	-1.03257100
H	-2.99643300	6.11990000	-2.32331700
H	-7.54426400	5.99690300	-0.96955300
H	-8.01172800	3.59982100	-0.47580700
H	-6.27508100	1.90046500	-0.80688200
C	3.63090400	3.11770600	1.05931700
C	3.20694500	2.09714200	-1.02227800
C	2.54569200	2.42193000	0.30436200
O	2.65647000	1.72060600	-2.02549500
N	4.73868800	2.99942000	0.40736300
N	4.54222800	2.31665500	-0.77901700
C	5.63909700	2.03514800	-1.62946000
C	5.49950300	1.07518100	-2.63382000
C	6.85351500	2.69049400	-1.42712200
C	6.59320700	0.78009000	-3.43966400
H	4.55369400	0.56758300	-2.77873000
C	7.93532200	2.37840000	-2.24298200
H	6.93945900	3.42491800	-0.63597200
C	7.81218100	1.42599900	-3.25123300
H	6.48346800	0.02776200	-4.21411700
H	8.88068000	2.88774700	-2.08695300
H	8.66067700	1.18850500	-3.88395800
C	3.60909200	3.88334600	2.33964600
H	4.62170800	4.24622900	2.52297200
H	2.92010700	4.72821700	2.26843400

H	3.26842700	3.26240700	3.16840900
N	1.23310100	2.67778500	0.24747700
C	0.47467200	2.99380900	1.40106600
O	0.98211600	3.07450100	2.49325700
O	-0.77800300	3.20117500	1.06383200
C	-1.76169000	3.50273500	2.12503500
C	-3.07072800	3.60490000	1.36062000
H	-2.98442700	4.32934700	0.54627800
H	-3.33411200	2.63416500	0.93923300
H	-3.86463200	3.92945800	2.03890900
C	-1.40182100	4.84011900	2.76462400
H	-2.19705900	5.12103800	3.46052100
H	-0.46174300	4.78307400	3.31359400
H	-1.33130600	5.61625100	1.99704200
C	-1.81362700	2.35639500	3.12898300
H	-0.90626600	2.30567200	3.73187600
H	-2.66938900	2.52170500	3.79052800
H	-1.94621400	1.40954100	2.60090300
C	2.30951500	-2.03032000	-3.05656300
H	1.27716900	-1.69407400	-3.09878600
C	4.98413800	-2.87184800	-2.89919500
H	6.01958300	-3.19543600	-2.83301900
C	4.21238000	-3.20146200	-3.98597700
H	4.63569200	-3.79019700	-4.79394500
C	2.86268400	-2.77956200	-4.06418100
H	2.26693300	-3.05082700	-4.92966200
H	3.13723400	-2.40834700	3.63491500
H	0.67933500	-2.09005700	3.41954500
H	-1.67316000	2.03139100	-2.20595700
H	-1.19771400	4.43493000	-2.57832400
H	-3.61367100	-3.55330700	4.63206300
H	-5.61569900	-4.87597700	2.74538900
H	-6.92658500	-2.70950000	3.03696900
H	-5.46793500	-1.39443300	1.41556400
H	-4.62209000	-3.86343700	-0.52443500
H	-6.89001300	-3.58430100	-1.51372200
H	-5.33928700	-3.35617700	-4.13952300
H	-6.25377100	-1.09139200	-4.24952400

TS-P_2

Zero-point correction=	1.196802 (Hartree/Particle)
Thermal correction to Energy=	1.246846
Thermal correction to Enthalpy=	1.247648

Thermal correction to Gibbs Free Energy= 1.117050
Sum of electronic and zero-point Energies= -3828.050588
Sum of electronic and thermal Energies= -3828.000543
Sum of electronic and thermal Enthalpies= -3827.999742
Sum of electronic and thermal Free Energies= -3828.130339
SCF Done: E(RM062X) = -3830.20515287
Number of Imaginary Frequencies = -235.19

H	-1.23916400	-1.42976600	0.97849000
C	-2.53603400	5.24629300	2.36215500
C	-1.43499300	4.91894400	1.52290000
C	-1.44742700	3.70258100	0.80111600
C	-2.51949200	2.84432800	0.89261100
C	-3.59894700	3.14435500	1.76606600
C	-3.60444400	4.31800000	2.47082800
H	-0.59507400	3.41920700	0.19155100
H	-4.38814000	2.41985800	1.91446800
H	-4.42493900	4.53977700	3.14708000
N	-2.43716400	1.62804000	0.17400600
H	-1.43366400	1.29590500	0.07569300
C	-3.42134200	0.97729100	-0.43928500
C	-3.14935600	-0.35373400	-0.95442300
C	-4.74114100	1.50243500	-0.61575300
C	-4.10046500	-0.95440600	-1.84518100
H	-2.10243200	-0.64357800	-1.06534900
C	-5.66941100	0.78614400	-1.32055600
H	-4.97807100	2.48989800	-0.24047200
C	-5.36374700	-0.45690400	-1.95150300
H	-3.80363800	-1.85596200	-2.37365600
H	-6.66164300	1.20876300	-1.45043500
H	-6.11179800	-0.95582600	-2.55713200
C	6.73784400	2.52288900	-1.57401600
C	5.90749400	1.24112500	-1.60995100
C	4.48955100	1.47562000	-2.10178600
C	4.14137900	2.67043100	-2.74734100
C	5.16898300	3.73737400	-3.07640400
C	6.60740400	3.25787100	-2.90477200
H	6.38360100	3.17448100	-0.76519600
H	6.42065500	0.51488400	-2.25387800
C	3.48265600	0.52013100	-1.85045600
C	2.80393600	2.92466900	-3.05722000
H	4.99806300	4.09573100	-4.09749700
H	7.29443300	4.10747300	-2.96048800
C	1.77529700	2.04481200	-2.72691500

C	2.15392000	0.83600000	-2.13070500
H	2.54694800	3.86215100	-3.54611600
C	3.78284100	-0.78632300	-1.19177500
C	4.67399900	-1.71675200	-1.75948300
C	3.16339100	-1.08747300	0.02897400
C	5.11373900	-1.58086800	-3.20651100
C	5.05273700	-2.84419600	-1.01629900
C	3.51547700	-2.21430500	0.77727400
C	6.40249000	-2.33968000	-3.51099000
H	4.30678800	-1.99835600	-3.82567400
C	6.08388800	-3.83282400	-1.52858100
C	4.49130600	-3.05369000	0.24264200
C	6.27121200	-3.78710600	-3.04343900
H	6.61578800	-2.29373100	-4.58332900
H	7.04518000	-3.60695500	-1.04657600
H	4.78945300	-3.92797100	0.81784500
H	7.14916400	-4.37512100	-3.32788300
O	1.19218900	-0.08328500	-1.77798700
O	2.21426500	-0.21659000	0.52918200
P	0.75405200	-0.13575800	-0.20386400
O	0.14615600	1.16919000	0.22875600
O	-0.03713300	-1.40334800	-0.07866200
C	-1.34162300	4.14971100	-2.37796800
C	-0.00362500	3.69311600	-2.36364900
C	-2.33007200	3.35218500	-2.88596200
C	0.35165800	2.45773300	-2.86203200
C	-0.65945300	1.63583100	-3.46337400
C	-2.01117900	2.08959700	-3.45303000
C	-3.02221100	1.27843600	-4.03166100
H	-4.05123500	1.62734300	-3.99303800
C	-2.70989500	0.08399800	-4.62706100
C	-1.36535900	-0.35240300	-4.67110000
C	-0.36927600	0.40201800	-4.10519300
H	-3.36851700	3.67333800	-2.87756400
H	-3.49192500	-0.52726900	-5.06734700
H	-1.12027600	-1.29153700	-5.15595300
H	0.65817100	0.05995900	-4.14553500
C	0.93572400	-3.28049200	3.34392400
C	1.54692200	-2.89348000	2.12840000
C	1.66290900	-3.32594200	4.50418000
C	2.87715500	-2.54154400	2.08465500
C	3.65353100	-2.54835100	3.28887600
C	3.03422200	-2.95717300	4.50644300
C	3.79911100	-2.97272000	5.70281500

H	3.31444300	-3.29095900	6.62203100
C	5.11482800	-2.59107100	5.70384300
C	5.72694700	-2.16659800	4.50080400
C	5.01706400	-2.14550800	3.32763300
H	1.20407900	-3.63447300	5.44002900
H	5.68843900	-2.60599800	6.62501900
H	6.76531200	-1.85076200	4.50990000
H	5.48928600	-1.80939800	2.41060000
C	-4.69436400	-1.32046900	1.23919900
C	-3.24207000	-2.74622600	0.05521300
C	-3.27333800	-1.42847800	0.82269300
O	-2.27334700	-3.31856600	-0.37668300
N	-5.38892900	-2.25325100	0.67295200
N	-4.57527800	-3.10150100	-0.04075600
C	-5.15660500	-4.06619300	-0.89700900
C	-4.36768200	-5.05937500	-1.48470900
C	-6.52758400	-3.99765000	-1.16053900
C	-4.96784600	-5.97698100	-2.34172300
H	-3.30830400	-5.10733900	-1.27345800
C	-7.10572600	-4.93114100	-2.01223200
H	-7.11967100	-3.22183800	-0.69202600
C	-6.33199800	-5.92274500	-2.60961300
H	-4.35424500	-6.74713100	-2.79749700
H	-8.17129100	-4.87758900	-2.21080400
H	-6.78874600	-6.64687400	-3.27550900
C	-5.40487800	-0.37172000	2.14650000
H	-6.47422400	-0.56750500	2.05337300
H	-5.08360200	-0.50883700	3.17912300
H	-5.19492300	0.66170100	1.88045600
N	-2.13028900	-1.13341100	1.47666400
C	-1.95507700	-0.22536300	2.52703300
O	-2.84854200	0.40566100	3.04800800
O	-0.67014600	-0.23990300	2.84143900
C	-0.12314900	0.63990100	3.88061300
C	1.37095100	0.35794900	3.80799000
H	1.57732900	-0.69047300	4.03312800
H	1.74624200	0.58101800	2.80602000
H	1.89294200	0.98420400	4.53689600
C	-0.70374400	0.22416400	5.22678000
H	-0.21638800	0.79782200	6.02003300
H	-1.77830100	0.40940400	5.26713400
H	-0.50766300	-0.83831900	5.40040900
C	-0.40096400	2.09504000	3.52792500
H	-1.46608100	2.33240900	3.56892900

H	0.12960900	2.73703600	4.23733000
H	-0.02047900	2.29086700	2.52226200
C	-0.34482800	5.82561500	1.42927200
H	0.49626400	5.56264200	0.79365200
C	-2.51781100	6.47136500	3.07725600
H	-3.36020700	6.71506900	3.71866700
C	-1.45517100	7.33022600	2.96274700
H	-1.44947800	8.26528700	3.51326800
C	-0.35604100	7.00312500	2.13013600
H	0.47992100	7.69061000	2.05333000
H	-1.57870500	5.11787600	-1.94747600
H	0.76354700	4.31010900	-1.90390100
H	0.96314400	-2.87695200	1.21410600
H	-0.11647300	-3.54816700	3.34281600
H	5.00052500	4.59976200	-2.41734300
H	6.87269500	2.57332300	-3.72087200
H	7.78177600	2.27807300	-1.35690200
H	5.86268500	0.77872000	-0.61848300
H	5.19205000	-0.53381400	-3.50189900
H	7.24619400	-1.86359200	-2.99271800
H	5.40391400	-4.24286700	-3.53729400
H	5.81074400	-4.84231500	-1.20464500

C_2

Zero-point correction= 1.198922 (Hartree/Particle)
Thermal correction to Energy= 1.249037
Thermal correction to Enthalpy= 1.249839
Thermal correction to Gibbs Free Energy= 1.119372
Sum of electronic and zero-point Energies= -3828.078854
Sum of electronic and thermal Energies= -3828.028739
Sum of electronic and thermal Enthalpies= -3828.027938
Sum of electronic and thermal Free Energies= -3828.158405
SCF Done: E(RM062X) = -3830.23151948

H	1.28702500	1.81508800	-0.31964400
C	5.23890900	-1.51900900	0.38715700
C	4.14660900	-1.06189000	-0.36884200
C	3.06329900	-0.24112100	0.29421000
C	2.94360600	-0.45674000	1.78716400
C	4.13094300	-0.92096200	2.50622000
C	5.20093800	-1.38814000	1.83624800
H	2.09733700	-0.44047500	-0.18672400
H	4.10610300	-0.94762300	3.58813200

H	6.05511100	-1.76666300	2.39333900
N	1.80516000	-0.20649800	2.34181500
H	0.41995800	-0.18479300	1.65606900
C	1.62829900	-0.16118400	3.74815600
C	0.52612400	-0.82608500	4.29364800
C	2.43768200	0.62899700	4.57142800
C	0.27363700	-0.74889700	5.65878100
H	-0.13489200	-1.37156200	3.63063100
C	2.17111500	0.70713600	5.93380900
H	3.22172600	1.22995500	4.12412400
C	1.09753100	0.01184300	6.48490400
H	-0.58155200	-1.27179000	6.07453700
H	2.79614800	1.33190000	6.56369700
H	0.89155300	0.08016400	7.54786000
C	-6.72647900	-2.86496400	1.70715200
C	-5.95249500	-2.28848200	0.52310200
C	-4.50084300	-2.73521700	0.49960000
C	-4.06585700	-3.81242800	1.28415100
C	-5.02630600	-4.63535800	2.12223600
C	-6.49209300	-4.37034900	1.79106300
H	-6.38864400	-2.39373200	2.63871800
H	-6.46019600	-2.59101900	-0.40218800
C	-3.55191900	-2.01716900	-0.26059600
C	-2.70425600	-4.12608300	1.34341600
H	-4.78622900	-5.69729700	2.00117400
H	-7.13521200	-4.83239000	2.54573600
C	-1.74002100	-3.37938100	0.67525300
C	-2.20238400	-2.32242900	-0.11371000
H	-2.38021400	-4.96397800	1.95711600
C	-3.93675200	-0.88179600	-1.15136300
C	-4.81635100	-1.05239600	-2.23780100
C	-3.39716500	0.38654400	-0.90852400
C	-5.17690100	-2.44264300	-2.72984700
C	-5.25622400	0.07602600	-2.94629500
C	-3.79871300	1.51965600	-1.61811400
C	-6.46819900	-2.46927600	-3.54288100
H	-4.35056300	-2.77757000	-3.37327300
C	-6.28355000	-0.02731900	-4.05847900
C	-4.76112900	1.33525800	-2.60895000
C	-6.39755200	-1.42763300	-4.65687700
H	-6.62645300	-3.47059400	-3.95460700
H	-7.26052100	0.26288500	-3.64799000
H	-5.10206200	2.20670400	-3.16397800
H	-7.27656800	-1.48377500	-5.30594800

O	-1.27578000	-1.51523300	-0.75249900
O	-2.46771500	0.53491400	0.11184100
P	-0.98250700	-0.07233800	-0.07638100
O	-0.58656500	-0.30107600	1.40983800
O	-0.04646400	0.66004200	-0.95197400
C	1.60481900	-3.65226300	2.41530600
C	0.21902300	-3.54937900	2.15533100
C	2.48100400	-3.83992800	1.37897800
C	-0.28293100	-3.60490000	0.87399500
C	0.61008600	-3.84368200	-0.21993200
C	2.00458400	-3.96497100	0.04682700
C	2.89873200	-4.21550800	-1.02672400
H	3.96349800	-4.27631900	-0.81171500
C	2.43366900	-4.35593100	-2.30733600
C	1.04782500	-4.24931100	-2.57312100
C	0.16092200	-3.99587000	-1.55894900
H	3.55156200	-3.90579900	1.55599900
H	3.12755200	-4.54161200	-3.12130800
H	0.68618600	-4.36514600	-3.58963300
H	-0.89994300	-3.91428900	-1.77074800
C	-1.31543400	4.37635400	-1.42908600
C	-1.88760800	3.09828500	-1.62783400
C	-2.08335200	5.41451400	-0.97060800
C	-3.21684100	2.86591500	-1.35474500
C	-4.03611600	3.92620000	-0.84903200
C	-3.45584400	5.21543700	-0.66624600
C	-4.26016900	6.27327500	-0.16580500
H	-3.80494100	7.25137000	-0.03546600
C	-5.57690000	6.06837400	0.15194900
C	-6.15032800	4.78509100	-0.01065100
C	-5.40164800	3.74371200	-0.49599400
H	-1.65461400	6.40231700	-0.82280900
H	-6.18096600	6.88446700	0.53509700
H	-7.18982700	4.62446400	0.25700000
H	-5.84493800	2.75971300	-0.60637800
C	4.62019600	1.84575500	0.48572900
C	3.45635000	1.44596300	-1.50878200
C	3.25714100	1.35015900	0.01524900
O	2.59325700	1.31074700	-2.34474000
N	5.45156500	1.91852900	-0.49041900
N	4.79990000	1.66393400	-1.69039300
C	5.55857700	1.45274300	-2.86195800
C	4.93287700	1.38136800	-4.11038500
C	6.93901400	1.26620200	-2.74863800

C	5.70386400	1.11241700	-5.23747900
H	3.86470500	1.52982400	-4.18857900
C	7.68911000	1.00737700	-3.88872100
H	7.40135600	1.31819100	-1.77129200
C	7.07896200	0.92484600	-5.13805800
H	5.21615000	1.05729800	-6.20548900
H	8.76093200	0.86396000	-3.79543300
H	7.67004700	0.72026100	-6.02436200
C	5.10147400	2.22367800	1.84878300
H	6.19276400	2.23221900	1.83217500
H	4.72005100	3.21098400	2.11277600
H	4.74643200	1.53469200	2.61293500
N	2.05461300	2.06881700	0.31143700
C	1.65471800	2.54800900	1.52991600
O	2.39091100	2.83743100	2.45503600
O	0.31995300	2.67430900	1.51040000
C	-0.39496200	3.41792000	2.54231100
C	-1.85013400	3.24425100	2.12646400
H	-2.00686700	3.63058400	1.11748800
H	-2.11798900	2.18422600	2.13510700
H	-2.50166900	3.78586400	2.81803900
C	0.03310400	4.87943400	2.47166100
H	-0.55385900	5.46848800	3.18203500
H	1.09149800	4.98437800	2.71949100
H	-0.14812200	5.26889900	1.46541600
C	-0.16654200	2.81409200	3.92355000
H	0.85681000	2.96294100	4.26554000
H	-0.85491200	3.28853200	4.62976100
H	-0.38388100	1.74207600	3.90215900
C	4.11286400	-1.33372600	-1.73637700
H	3.25239000	-1.02566000	-2.32284600
C	6.29850500	-2.18475600	-0.24114700
H	7.13439700	-2.53322100	0.35943900
C	6.28121300	-2.39502600	-1.61351400
H	7.11437700	-2.89106800	-2.09996000
C	5.18008000	-1.97597200	-2.35833700
H	5.14889400	-2.14433100	-3.43007900
H	1.96473400	-3.55706600	3.43568200
H	-0.47186900	-3.39093800	2.97777500
H	-1.26470200	2.28990900	-1.99568800
H	-0.26218600	4.52223600	-1.64684000
H	-4.85197700	-4.40106800	3.18097500
H	-6.74554200	-4.82824600	0.82619200
H	-7.79021500	-2.63496400	1.59688400

H	-5.98292100	-1.19411500	0.53470100
H	-5.21205100	-3.15903600	-1.90840000
H	-7.32345300	-2.24901800	-2.88950400
H	-5.52094800	-1.63535200	-5.28304400
H	-6.05008300	0.70651400	-4.83651600

C_2'

Zero-point correction= 1.198467 (Hartree/Particle)
Thermal correction to Energy= 1.249131
Thermal correction to Enthalpy= 1.249932
Thermal correction to Gibbs Free Energy= 1.115709
Sum of electronic and zero-point Energies= -3828.074610
Sum of electronic and thermal Energies= -3828.023946
Sum of electronic and thermal Enthalpies= -3828.023144
Sum of electronic and thermal Free Energies= -3828.157367
SCF Done: E(RM062X) = -3830.23308455

H	-1.49917100	-0.99688500	-1.80703900
C	-4.83690900	2.27155700	-1.97471500
C	-3.64633700	1.55107400	-2.17281700
C	-2.83776600	1.11229500	-0.97710000
C	-3.05653000	1.99631100	0.23033800
C	-4.41011700	2.51670000	0.44085100
C	-5.23267500	2.64259200	-0.61529800
H	-1.77130200	1.12572700	-1.21812800
H	-4.70143000	2.83404600	1.43605000
H	-6.22742800	3.06126900	-0.48093200
N	-2.04720200	2.19149300	1.00003800
H	-0.57880800	1.70094200	0.66158700
C	-2.12286500	2.95552400	2.18983200
C	-1.63867200	2.36152400	3.35724800
C	-2.57710400	4.27654500	2.20625100
C	-1.66533500	3.07123300	4.55103000
H	-1.26649800	1.34304600	3.30716200
C	-2.57692600	4.98640900	3.40345600
H	-2.90529200	4.74046900	1.28110400
C	-2.13265800	4.38434100	4.57791000
H	-1.31414800	2.59679800	5.46147900
H	-2.92507800	6.01424100	3.41637800
H	-2.14206700	4.93989300	5.50976000
C	6.95228100	-0.26003900	2.53934000
C	6.11526300	-0.65134300	1.32347400
C	5.31019600	0.50793000	0.76637500

C	5.63340400	1.82882800	1.10817100
C	6.81461100	2.16729000	1.99881900
C	7.76300400	0.99265100	2.22110500
H	6.29561900	-0.05984200	3.39545400
H	6.79260500	-1.03446800	0.55030300
C	4.18640000	0.26579100	-0.05270700
C	4.82163700	2.87663500	0.66813500
H	7.35019500	3.02280400	1.57314500
H	8.46616200	1.22730000	3.02569500
C	3.67865100	2.66231300	-0.09430600
C	3.38655800	1.34124800	-0.43788400
H	5.07475600	3.89745600	0.94605200
C	3.73912800	-1.11621400	-0.39805700
C	4.52333000	-2.04893000	-1.09428700
C	2.46090600	-1.51472700	0.01413600
C	5.81216800	-1.69797600	-1.79968900
C	4.05328400	-3.35889400	-1.27249200
C	1.99634900	-2.82290100	-0.10149300
C	6.92881600	-2.75701900	-1.63730900
H	5.56349000	-1.63137600	-2.86739900
C	4.96042300	-4.32294400	-1.99336300
C	2.82359600	-3.74282400	-0.74453100
C	6.38234300	-4.18306100	-1.43354300
H	7.55938600	-2.72242100	-2.53097200
H	4.59291600	-5.34690700	-1.87986000
H	2.48929500	-4.77300000	-0.83856400
H	7.05263500	-4.91541600	-1.89264300
O	2.25333800	1.08750300	-1.19060800
O	1.61914500	-0.57200700	0.58687800
P	0.94953900	0.47211700	-0.45481500
O	0.43027200	1.60184900	0.47215400
O	0.06462900	-0.09469500	-1.49540500
C	1.25183900	5.53544900	0.28539500
C	2.14257800	4.47307200	0.56121900
C	0.99944600	5.90030000	-1.00993900
C	2.76410900	3.78016000	-0.45223500
C	2.51929100	4.14501100	-1.81366300
C	1.62715600	5.22069900	-2.08672600
C	1.38511200	5.59439600	-3.43530400
H	0.70092400	6.41587000	-3.63041800
C	2.00026000	4.93764700	-4.46803300
C	2.89187900	3.87235600	-4.19749700
C	3.14462400	3.48717200	-2.90654000
H	0.31510100	6.71368900	-1.23586500

H	1.80802300	5.23167600	-5.49491000
H	3.37715200	3.35715000	-5.02013000
H	3.82877400	2.66946100	-2.70530800
C	-1.63163800	-3.88279600	0.28772800
C	-0.39319700	-3.49990200	-0.28633300
C	-1.75864100	-3.99136400	1.64700100
C	0.69365800	-3.21616300	0.50462600
C	0.58534700	-3.32080800	1.92916100
C	-0.65239000	-3.73251000	2.49735000
C	-0.76042800	-3.86556800	3.90723600
H	-1.71544600	-4.17118200	4.32618700
C	0.30605200	-3.59238000	4.72320500
C	1.53572500	-3.17384900	4.16110200
C	1.67223400	-3.04479000	2.80276400
H	-2.70646900	-4.27813800	2.09516400
H	0.21148700	-3.69625400	5.79978600
H	2.37696800	-2.95686700	4.81169100
H	2.62086300	-2.73007300	2.38012800
C	-4.58847200	-0.68496200	-0.35771000
C	-2.51848300	-0.68382300	0.76356100
C	-3.11779300	-0.42592800	-0.63509300
O	-1.34529800	-0.66918500	1.07165900
N	-4.81584300	-0.84120300	0.89198200
N	-3.60561800	-0.82223900	1.59062900
C	-3.62913900	-0.87727600	3.00160500
C	-2.45270500	-1.09022300	3.72781600
C	-4.84651900	-0.69874200	3.66685800
C	-2.50879300	-1.10718100	5.11866600
H	-1.51419400	-1.24426600	3.21230400
C	-4.87834000	-0.72242100	5.05546000
H	-5.74838700	-0.54786600	3.08783500
C	-3.71235400	-0.92145700	5.79119800
H	-1.59077700	-1.28428400	5.67095300
H	-5.82660000	-0.58252900	5.56468700
H	-3.74465700	-0.93843100	6.87547600
C	-5.71626900	-0.69811700	-1.34421000
H	-5.34781100	-0.57566200	-2.36289600
H	-6.22928100	-1.65766200	-1.27719500
H	-6.42176800	0.10622600	-1.11966000
N	-2.49473300	-1.19892000	-1.67281400
C	-2.97289100	-2.37512900	-2.16420200
O	-4.04172300	-2.88626600	-1.88411000
O	-2.07138200	-2.87973800	-3.02840000
C	-2.38763900	-4.05447900	-3.82707900

C	-1.13083000	-4.22756900	-4.67250900
H	-0.95305300	-3.33487500	-5.27707200
H	-0.26096700	-4.38982300	-4.03022600
H	-1.24320600	-5.08856200	-5.33641800
C	-3.59797200	-3.76701400	-4.71116500
H	-3.74075600	-4.59447400	-5.41192200
H	-4.50077900	-3.65092600	-4.11125500
H	-3.42874500	-2.85277800	-5.28779800
C	-2.60308700	-5.27467300	-2.93648100
H	-3.50926500	-5.17071700	-2.33931800
H	-2.69324900	-6.16537400	-3.56531900
H	-1.74544000	-5.41235400	-2.27071800
C	-3.25936700	1.20319900	-3.46432300
H	-2.32746500	0.66657100	-3.61214100
C	-5.63593200	2.60339400	-3.07169400
H	-6.55931100	3.15288300	-2.90965300
C	-5.25406200	2.23605100	-4.35674300
H	-5.87937500	2.49637400	-5.20416400
C	-4.06156300	1.54295300	-4.55254300
H	-3.75095800	1.26838400	-5.55524000
H	0.76347100	6.04832900	1.10776500
H	2.31688700	4.16946700	1.58884400
H	-0.30787300	-3.39662100	-1.36496100
H	-2.48693400	-4.08237100	-0.35018800
H	6.42837400	2.50205900	2.97090400
H	8.35678400	0.81488100	1.31530000
H	7.60429300	-1.09272900	2.81965500
H	5.43844500	-1.47772100	1.56502300
H	6.16489600	-0.70450500	-1.51455900
H	7.57748400	-2.49667100	-0.79570000
H	6.34097200	-4.41351000	-0.36370000
H	4.96932500	-4.10273100	-3.07043000

D_2

Zero-point correction= 0.558480 (Hartree/Particle)
Thermal correction to Energy= 0.583139
Thermal correction to Enthalpy= 0.583940
Thermal correction to Gibbs Free Energy= 0.505599
Sum of electronic and zero-point Energies= -1642.869639
Sum of electronic and thermal Energies= -1642.844980
Sum of electronic and thermal Enthalpies= -1642.844178
Sum of electronic and thermal Free Energies= -1642.922519
SCF Done: E(RM062X) = -1643.87667806

H	-1.78811600	0.66788400	-0.87309100
C	1.02077400	-3.16007900	0.32608100
C	1.10721100	-2.12161300	-0.61701300
C	-0.08246400	-1.20489400	-0.83211900
C	-1.41686700	-1.81827900	-0.43785500
C	-1.41439500	-2.87210300	0.58250300
C	-0.26579700	-3.47141700	0.94070300
H	-0.14861300	-0.91153400	-1.88636200
H	-2.36516200	-3.18868800	0.99581400
H	-0.28307300	-4.27410300	1.67443200
N	-2.45806200	-1.34430300	-1.01760800
C	-3.75241200	-1.71836700	-0.59382800
C	-4.58002600	-2.44800700	-1.44981700
C	-4.24285600	-1.28389300	0.64229900
C	-5.87476300	-2.76676400	-1.05475500
H	-4.19378800	-2.76056500	-2.41416800
C	-5.54350400	-1.59698100	1.02318400
H	-3.59676800	-0.68884900	1.28275600
C	-6.36237800	-2.34383700	0.17999200
H	-6.50891800	-3.34442500	-1.71966500
H	-5.91755300	-1.25406900	1.98265700
H	-7.37589600	-2.58822300	0.47925500
C	0.56435800	0.02637000	1.35990800
C	1.40076000	0.77545300	-0.69041800
C	0.11821100	0.17709800	-0.08073200
O	1.52960100	1.15963500	-1.83266300
N	1.81871900	0.23161000	1.50808800
N	2.35657500	0.63444900	0.28470500
C	3.75654600	0.71844400	0.14199600
C	4.32274900	1.35481100	-0.96719500
C	4.57154900	0.11620800	1.10528000
C	5.70781700	1.37422000	-1.10113500
H	3.68476900	1.82144900	-1.70479400
C	5.95188200	0.15655800	0.95542600
H	4.11187600	-0.37506200	1.95336800
C	6.52933100	0.78083700	-0.14772700
H	6.14483900	1.86952000	-1.96234100
H	6.57979700	-0.31004000	1.70781200
H	7.60791600	0.80674500	-0.26080500
C	-0.33913000	-0.18898900	2.52337700
H	0.25617000	-0.35452600	3.42200400
H	-0.94327700	0.71460400	2.66276600
H	-1.01610100	-1.03094900	2.36711600

N	-1.03973900	0.99879100	-0.27401100
C	-0.96899200	2.31497100	0.07993600
O	-0.02149600	2.78127300	0.68493100
O	-2.07530200	2.96293700	-0.30623000
C	-2.22441600	4.38395300	-0.01671000
C	-3.58720800	4.70662000	-0.61782900
H	-3.58790100	4.49836400	-1.69059700
H	-4.36503600	4.10174600	-0.14491100
H	-3.82073000	5.76319800	-0.46432300
C	-1.12483800	5.17865100	-0.71461000
H	-1.32874700	6.24765500	-0.60499000
H	-0.14786200	4.95701500	-0.28574100
H	-1.11094100	4.93836500	-1.78131500
C	-2.23340800	4.61157900	1.49222400
H	-1.25846200	4.39177100	1.92699100
H	-2.48797600	5.65512500	1.69813400
H	-2.99054400	3.97579900	1.96070600
C	2.30730400	-1.92471900	-1.29695000
H	2.38026900	-1.14023600	-2.04509500
C	2.14626400	-3.93997200	0.60991000
H	2.06407600	-4.73880300	1.34182300
C	3.35112600	-3.70236000	-0.03824900
H	4.22369100	-4.30255200	0.19646500
C	3.42705100	-2.69923700	-1.00095400
H	4.36029300	-2.50677600	-1.51995800

D_2'

Zero-point correction= 0.558459 (Hartree/Particle)
Thermal correction to Energy= 0.583094
Thermal correction to Enthalpy= 0.583895
Thermal correction to Gibbs Free Energy= 0.505057
Sum of electronic and zero-point Energies= -1642.868414
Sum of electronic and thermal Energies= -1642.843779
Sum of electronic and thermal Enthalpies= -1642.842977
Sum of electronic and thermal Free Energies= -1642.921816
SCF Done: E(RM062X) = -1643.87751265

H	-1.94656900	-0.24121800	1.09160000
C	1.86369100	2.59801300	0.19549000
C	1.46492700	1.83791300	1.30900700
C	0.08804700	1.20417300	1.33781700
C	-0.92174900	1.90064600	0.42992400
C	-0.41190900	2.62672400	-0.73610400

C	0.89341600	2.91257300	-0.85080900
H	-0.31905100	1.23652600	2.35461100
H	-1.11958200	2.89985200	-1.51010500
H	1.26195500	3.42906400	-1.73321800
N	-2.15929200	1.73036100	0.72602800
C	-3.19213100	2.30670100	-0.04135900
C	-4.17245700	1.46292700	-0.57357200
C	-3.30868300	3.69100200	-0.20423700
C	-5.23368700	1.99875700	-1.29239700
H	-4.07801400	0.39099700	-0.42458200
C	-4.38493700	4.21938500	-0.91040000
H	-2.56005900	4.34101800	0.23871400
C	-5.34664300	3.37774600	-1.46205400
H	-5.98202700	1.33633000	-1.71550400
H	-4.47066900	5.29493500	-1.02813400
H	-6.18304700	3.79284600	-2.01411800
C	1.17025900	-1.05302000	1.83009900
C	0.82967600	-0.48060800	-0.40642400
C	0.15440600	-0.33740300	0.97180500
O	0.33938400	-0.20280800	-1.47731200
N	2.25246000	-1.31477000	1.20349800
N	2.10783900	-0.91426500	-0.12497400
C	3.20771600	-1.04101400	-1.00004500
C	3.06177100	-0.80518600	-2.37136500
C	4.45686000	-1.38397200	-0.47344000
C	4.17444000	-0.91484100	-3.19927200
H	2.09246800	-0.54766900	-2.77400900
C	5.55218700	-1.49194000	-1.32071200
H	4.55163400	-1.56265400	0.58948100
C	5.42159400	-1.25757700	-2.68694400
H	4.05544500	-0.73348400	-4.26284900
H	6.51759400	-1.76116400	-0.90392900
H	6.28078900	-1.34342200	-3.34356900
C	0.93269800	-1.45980700	3.24072900
H	0.52028900	-0.63494200	3.83103700
H	0.20014900	-2.27292000	3.26186100
H	1.86373400	-1.80622400	3.69077700
N	-1.16574500	-0.89117300	1.05409100
C	-1.37162200	-2.14660100	0.55686800
O	-0.46378400	-2.90383600	0.27273700
O	-2.68676000	-2.39680600	0.46529000
C	-3.14803000	-3.68556400	-0.03605100
C	-4.66459000	-3.54263600	0.01541700
H	-4.99427200	-3.34375400	1.03828400

H	-4.99137200	-2.71809500	-0.62370500
H	-5.13725500	-4.46409100	-0.33376000
C	-2.68183600	-4.80465500	0.89068800
H	-3.14598900	-5.74557500	0.58175900
H	-1.59823900	-4.91543200	0.85536200
H	-2.99056800	-4.59143700	1.91825000
C	-2.67384500	-3.88761800	-1.47208800
H	-1.59086400	-4.00006300	-1.51579100
H	-3.14375900	-4.78547500	-1.88369800
H	-2.96903700	-3.03182400	-2.08575900
C	2.36605000	1.64355100	2.35168500
H	2.05693500	1.08776800	3.23238000
C	3.16885400	3.09202400	0.12485500
H	3.46809700	3.66722800	-0.74661000
C	4.07027400	2.86177200	1.15684200
H	5.08242500	3.24618900	1.09080000
C	3.66202700	2.15017700	2.28044100
H	4.35064800	1.98334900	3.10184300

E_2

Zero-point correction=	1.198664 (Hartree/Particle)
Thermal correction to Energy=	1.249417
Thermal correction to Enthalpy=	1.250218
Thermal correction to Gibbs Free Energy=	1.116673
Sum of electronic and zero-point Energies=	-3828.072096
Sum of electronic and thermal Energies=	-3828.021344
Sum of electronic and thermal Enthalpies=	-3828.020542
Sum of electronic and thermal Free Energies=	-3828.154088

SCF Done: E(RM062X) = -3830.22644458

H	-1.43112000	-0.64609100	2.00958800
C	-6.00553400	-0.05593000	2.37934700
C	-5.12882500	-1.14050600	2.21479000
C	-4.53466900	-1.42479000	0.85797400
C	-5.32090200	-0.84769200	-0.31051500
C	-6.14893700	0.33613600	-0.05236700
C	-6.44094000	0.70072000	1.20925900
H	-4.43416300	-2.50240200	0.70828700
H	-6.56611200	0.86895600	-0.89904900
H	-7.08569000	1.55882100	1.38634400
N	-5.14513100	-1.42105100	-1.44283000
H	-0.65670600	-0.05305800	-1.85351600
C	-5.65185300	-0.86887500	-2.63569600

C	-6.51911000	-1.63377000	-3.42187100
C	-5.22796500	0.38373100	-3.09670900
C	-6.98564000	-1.13440500	-4.63212200
H	-6.82035900	-2.61287400	-3.06437700
C	-5.68741400	0.86772900	-4.31732200
H	-4.52961300	0.96078200	-2.49687900
C	-6.57198900	0.11650100	-5.08671500
H	-7.66988800	-1.72997300	-5.22832800
H	-5.34877300	1.83851800	-4.66553900
H	-6.93003700	0.49815300	-6.03703300
C	7.05929200	1.40925800	-2.61665600
C	6.15363600	1.31530500	-1.38993300
C	5.25664500	0.08893700	-1.41778800
C	5.51882700	-0.97296100	-2.29393300
C	6.73309900	-0.98760900	-3.20224700
C	7.76600700	0.07546900	-2.83990000
H	6.46191600	1.65491300	-3.50360900
H	6.78593800	1.30532700	-0.49261100
C	4.10916600	0.03507800	-0.59724000
C	4.62301100	-2.04195400	-2.36729900
H	7.17946900	-1.98778500	-3.18559300
H	8.51784900	0.15083200	-3.63073800
C	3.42966300	-2.06392000	-1.65300200
C	3.18800700	-0.99397900	-0.79148000
H	4.84060400	-2.87338300	-3.03415500
C	3.84431000	1.08625400	0.42829300
C	4.74120400	1.35130700	1.48143100
C	2.67069600	1.83623600	0.33707800
C	5.86364100	0.38233800	1.80740700
C	4.50852200	2.46044300	2.30888000
C	2.39643400	2.92102900	1.16656200
C	6.99081600	1.02665800	2.61022500
H	5.42281000	-0.42603100	2.40826400
C	5.48585400	2.86475900	3.39667500
C	3.36296600	3.23475400	2.11967100
C	6.41404800	1.73401100	3.83422100
H	7.71717900	0.26390100	2.90627300
H	6.09447700	3.69615700	3.01538400
H	3.18665100	4.09122600	2.76656000
H	7.20975900	2.13197400	4.47089700
O	1.99874500	-0.98017200	-0.06726400
O	1.74830200	1.48093000	-0.64593100
P	0.89101400	0.14715800	-0.37136800
O	0.33749500	-0.13565500	-1.82047100

O	-0.09922100	0.21088900	0.71774500
C	0.49744600	-4.16277500	-2.83589300
C	1.36783400	-3.06884900	-2.61254900
C	0.74824600	-5.37658400	-2.25387100
C	2.47618900	-3.20000000	-1.80901700
C	2.74490100	-4.44954600	-1.16521100
C	1.87272700	-5.54974000	-1.40541100
C	2.13173500	-6.79144200	-0.76751800
H	1.46336300	-7.62504100	-0.96512400
C	3.18967100	-6.93273400	0.09252800
C	4.04172800	-5.83251200	0.35281300
C	3.82980300	-4.62563000	-0.26424900
H	0.08894700	-6.22263900	-2.42656800
H	3.37450000	-7.88430400	0.58033300
H	4.86992600	-5.94821900	1.04458200
H	4.48541800	-3.78453200	-0.06241700
C	-1.22312200	3.97109200	1.60667500
C	-0.03144200	3.20601300	1.59926000
C	-1.22488100	5.23880700	1.09122600
C	1.13465800	3.71070800	1.07259600
C	1.14687700	5.01738300	0.48984100
C	-0.05133500	5.78625900	0.50926000
C	-0.05254700	7.07752400	-0.08049600
H	-0.97447100	7.65322400	-0.06023400
C	1.07636500	7.58658900	-0.66819700
C	2.26720600	6.82233500	-0.69029800
C	2.30204000	5.57314300	-0.12439400
H	-2.13258100	5.83589500	1.09132100
H	1.06160100	8.57389400	-1.11870000
H	3.15668900	7.22865600	-1.16121300
H	3.21578600	4.98744500	-0.14857800
C	-2.47019900	-1.09278700	-0.62975600
C	-3.10084600	0.68533100	0.76726900
C	-3.06284700	-0.85708700	0.75196400
O	-3.37234400	1.40798900	1.69629700
N	-2.30899100	0.00158400	-1.28330800
N	-2.77894100	1.06548800	-0.51817200
C	-2.67546300	2.39797700	-0.98942900
C	-3.74874500	3.26047900	-0.76937000
C	-1.53061500	2.83470500	-1.65499400
C	-3.67411500	4.57086700	-1.22994400
H	-4.62174700	2.89153200	-0.24007200
C	-1.47184500	4.14528600	-2.11476800
H	-0.68983400	2.16655100	-1.80344200

C	-2.54130300	5.01378900	-1.90794000
H	-4.50828100	5.24475100	-1.06233700
H	-0.57423900	4.49545900	-2.61405900
H	-2.48129600	6.03832300	-2.26100700
C	-2.01127800	-2.39062700	-1.19335900
H	-1.77313200	-2.25586200	-2.25029800
H	-1.11657700	-2.74912500	-0.67064000
H	-2.79130800	-3.14573100	-1.08292500
N	-2.19307700	-1.29043100	1.82336400
C	-1.82759900	-2.60396400	1.95905800
O	-2.47220900	-3.55248500	1.54600600
O	-0.67704900	-2.66959200	2.64051000
C	0.06997300	-3.91882600	2.70627100
C	1.36639200	-3.49502100	3.38689900
H	1.87459300	-2.73922200	2.78192900
H	1.16000600	-3.07520900	4.37482000
H	2.02566300	-4.35989000	3.49866200
C	0.36206500	-4.42506400	1.29737500
H	1.09722600	-5.23446300	1.34645100
H	-0.53860500	-4.79736800	0.80587400
H	0.79582200	-3.61734900	0.69609300
C	-0.68906900	-4.93685600	3.55027900
H	-1.61947000	-5.22735600	3.06200200
H	-0.06760300	-5.82584800	3.69196300
H	-0.91467800	-4.51370200	4.53336200
C	-4.80674500	-1.93175900	3.31392900
H	-4.15852200	-2.79167400	3.17370800
C	-6.51351100	0.23956400	3.64728800
H	-7.18939300	1.08232100	3.76370300
C	-6.16977700	-0.54138000	4.74314000
H	-6.56816300	-0.30641300	5.72463200
C	-5.32433900	-1.63505700	4.57237700
H	-5.06650500	-2.26044300	5.42089700
H	-0.36522000	-4.03421200	-3.48195500
H	1.16744000	-2.11231700	-3.08425700
H	-0.03822700	2.20459300	2.01585800
H	-2.12926500	3.53021900	2.00945800
H	6.39544100	-0.82056600	-4.23368000
H	8.29188700	-0.21204800	-1.92020600
H	7.77931100	2.22092800	-2.47812200
H	5.52652500	2.20843200	-1.30170500
H	6.24630800	-0.10079000	0.90731700
H	7.52392400	1.75529500	1.98437300
H	5.85405300	1.00660300	4.43494400

H	4.93070000	3.26125800	4.25265100

E_2'

Zero-point correction= 1.198106 (Hartree/Particle)
Thermal correction to Energy= 1.249412
Thermal correction to Enthalpy= 1.250214
Thermal correction to Gibbs Free Energy= 1.112496
Sum of electronic and zero-point Energies= -3828.057244
Sum of electronic and thermal Energies= -3828.005939
Sum of electronic and thermal Enthalpies= -3828.005137
Sum of electronic and thermal Free Energies= -3828.142854
SCF Done: E(RM062X) = -3830.21474054

H	-5.09470500	0.53901100	2.31805800
C	-7.12265500	-0.96270300	-0.99824100
C	-6.32852600	-1.28615300	0.11488100
C	-4.83044300	-1.46589700	-0.03550000
C	-4.34619200	-1.55945400	-1.47523200
C	-5.20971600	-1.04255000	-2.54185700
C	-6.50071800	-0.76817800	-2.30564900
H	-4.58459500	-2.43823900	0.40308200
H	-4.77434100	-0.90451600	-3.52550000
H	-7.13412100	-0.39474100	-3.10679500
N	-3.17768400	-2.06045900	-1.62539300
H	-0.16363600	0.55745900	0.91535200
C	-2.60072700	-2.20272000	-2.90415600
C	-1.35674400	-1.60422800	-3.12833000
C	-3.18406300	-2.98881900	-3.90442800
C	-0.72630100	-1.75797700	-4.35767200
H	-0.88417300	-1.03334600	-2.33466400
C	-2.53368500	-3.15255700	-5.12446000
H	-4.13424600	-3.47783200	-3.71002500
C	-1.30899900	-2.53274600	-5.35979900
H	0.23174500	-1.27269900	-4.51901000
H	-2.98821700	-3.76960200	-5.89332900
H	-0.80784800	-2.66173000	-6.31344700
C	7.33107500	0.63981600	2.92560900
C	6.71957900	0.41309000	1.54440000
C	5.66778900	1.45205800	1.19876500
C	5.59977100	2.65718000	1.91210600
C	6.60962200	3.02338000	2.98408500
C	7.81128700	2.08381500	3.03612100
H	6.58251800	0.44327400	3.70340400

H	7.53339800	0.43212300	0.81060000
C	4.67887100	1.17186500	0.23084100
C	4.54279800	3.53958100	1.68062900
H	6.93297700	4.05906900	2.83247300
H	8.37320600	2.24838700	3.96012800
C	3.51038600	3.25089800	0.79421100
C	3.59894000	2.04453200	0.09795100
H	4.50129400	4.47514000	2.23408400
C	4.68588700	-0.09321900	-0.56163300
C	5.70984400	-0.43222900	-1.46969300
C	3.61500600	-0.97074200	-0.39906000
C	6.75512300	0.59817700	-1.85676200
C	5.68953500	-1.69637500	-2.07677900
C	3.58354400	-2.24156800	-0.97238400
C	7.42813900	0.27160800	-3.18866900
H	6.28381200	1.58589900	-1.88755500
C	6.73873500	-2.12173600	-3.08672200
C	4.65409800	-2.59073100	-1.78658200
C	7.92950100	-1.16965000	-3.16396600
H	6.71104600	0.39389200	-4.01007400
H	7.06967600	-3.13968600	-2.85328700
H	4.66095400	-3.57870300	-2.24170700
H	8.53172700	-1.39740200	-4.04831200
O	2.56219600	1.70342900	-0.76118200
O	2.53461800	-0.55509500	0.37115100
P	1.55377100	0.51502500	-0.35639600
O	0.70836700	1.04878100	0.85053100
O	0.81391000	0.01995000	-1.52862500
C	0.46572500	5.28711500	1.72497800
C	1.58553400	4.42655200	1.78185000
C	0.11062000	5.87269100	0.53973500
C	2.33792900	4.15625100	0.66143000
C	1.99348900	4.76573700	-0.58739500
C	0.86343400	5.63082700	-0.63922600
C	0.51528800	6.24455300	-1.87157800
H	-0.35179000	6.89902000	-1.89737300
C	1.25553300	6.02098700	-3.00198200
C	2.38667800	5.17235800	-2.94918900
C	2.74613800	4.56300800	-1.77516700
H	-0.75033600	6.53305900	0.48144400
H	0.98042700	6.49454300	-3.93885300
H	2.97250500	5.00329500	-3.84680600
H	3.61645000	3.91598500	-1.74352700
C	0.16906200	-3.90142300	-1.02769900

C	1.27412400	-3.08338100	-1.36545800
C	0.26069100	-4.78536800	0.01475500
C	2.45465300	-3.16513400	-0.66494800
C	2.58065800	-4.08971200	0.41852800
C	1.46126700	-4.89991700	0.76302600
C	1.56077200	-5.77758600	1.87433400
H	0.69534700	-6.37975500	2.13681100
C	2.71361100	-5.85449800	2.61165500
C	3.83178800	-5.05994500	2.26208500
C	3.76865900	-4.20225700	1.19278900
H	-0.58850000	-5.40220800	0.29534600
H	2.77368700	-6.52378600	3.46381400
H	4.74367600	-5.13010000	2.84669600
H	4.62561600	-3.58929100	0.93117700
C	-2.67487300	0.08551100	0.19732700
C	-3.41483500	-1.16306500	2.04785900
C	-3.97946800	-0.41873500	0.82073400
O	-4.08167400	-1.68936200	2.91805200
N	-1.65735500	-0.29171500	0.88068000
N	-2.05951500	-1.07998500	1.95760500
C	-1.08111400	-1.66688400	2.80238200
C	-1.38337900	-1.91714900	4.14220500
C	0.17279200	-1.97879300	2.27606100
C	-0.41022800	-2.48620300	4.95637200
H	-2.36539000	-1.67818500	4.52845700
C	1.14009600	-2.52270100	3.11421000
H	0.38738100	-1.82394100	1.22244800
C	0.85237900	-2.78276700	4.45088400
H	-0.64352600	-2.68818800	5.99679100
H	2.11869400	-2.75629800	2.70842400
H	1.61006300	-3.22161200	5.09171900
C	-2.49531900	1.02548000	-0.94587500
H	-3.12599400	0.74362300	-1.78957800
H	-2.80261900	2.03087300	-0.64477200
H	-1.44413300	1.02882900	-1.24446600
N	-4.72611300	0.68641100	1.38583300
C	-5.45767100	1.52097000	0.57701600
O	-5.32709900	1.56591500	-0.62884600
O	-6.27876200	2.26473300	1.32639000
C	-7.12364900	3.27650000	0.70101100
C	-7.86153500	3.87707500	1.89148100
H	-8.43981500	3.10604100	2.40676900
H	-7.15217400	4.31369400	2.59904900
H	-8.54388700	4.65937500	1.54983600

C	-8.10359600	2.61278900	-0.26008300
H	-8.81823200	3.35968600	-0.61822700
H	-7.58273600	2.17816200	-1.11442500
H	-8.65299400	1.82157800	0.25768500
C	-6.25748600	4.32911300	0.01564800
H	-5.73668700	3.90981500	-0.84507200
H	-6.89262600	5.15342000	-0.32086100
H	-5.52401500	4.72797300	0.72224400
C	-6.93712700	-1.46204100	1.35683300
H	-6.31895000	-1.71900700	2.21351600
C	-8.50676000	-0.83383100	-0.84634300
H	-9.11040200	-0.58581300	-1.71548300
C	-9.10582700	-1.01449000	0.39427100
H	-10.18126800	-0.91402200	0.49931800
C	-8.31635000	-1.32373900	1.49912600
H	-8.77316600	-1.46904400	2.47262100
H	-0.11186400	5.47187300	2.62478800
H	1.84825800	3.94531100	2.71898800
H	1.17893300	-2.35578900	-2.16438500
H	-0.75347100	-3.80203700	-1.59069900
H	6.09851300	3.00272100	3.95568600
H	8.49182900	2.29901100	2.20246000
H	8.15405200	-0.06370900	3.08235700
H	6.27105900	-0.58319100	1.47424300
H	7.53602700	0.65957000	-1.09038000
H	8.24860700	0.97269500	-3.36768300
H	8.57703500	-1.30822700	-2.28865300
H	6.26083500	-2.17565000	-4.07383900

TS-B_2

Zero-point correction= 1.195939 (Hartree/Particle)
Thermal correction to Energy= 1.245985
Thermal correction to Enthalpy= 1.246787
Thermal correction to Gibbs Free Energy= 1.114689
Sum of electronic and zero-point Energies= -3828.056640
Sum of electronic and thermal Energies= -3828.006594
Sum of electronic and thermal Enthalpies= -3828.005792
Sum of electronic and thermal Free Energies= -3828.137891
SCF Done: E(RM062X) = -3830.21057955
Number of Imaginary Frequencies = -253.86

H	1.51919700	-0.31737300	-1.72111300
C	6.93583100	-0.09289300	-2.00985900

C	5.55716300	-0.33933300	-2.14898000
C	4.79900500	-0.91169500	-0.97041400
C	5.49400100	-0.75495900	0.35993300
C	6.92921100	-0.56508400	0.41904800
C	7.58465700	-0.25259100	-0.71601800
H	4.72979300	-1.99690100	-1.14918500
H	7.42595700	-0.60741600	1.38134300
H	8.65534400	-0.06414800	-0.67707600
N	4.69017700	-0.80009700	1.35746900
H	0.86800400	-0.03961900	1.47861900
C	5.00920700	-0.73446300	2.72273000
C	5.70724200	-1.77431300	3.34552400
C	4.53285600	0.34926000	3.46665200
C	5.94918400	-1.71420100	4.71278600
H	6.04243200	-2.61960900	2.75162400
C	4.78132800	0.39343100	4.83503800
H	3.98779900	1.14173000	2.96438700
C	5.48743900	-0.63161500	5.45956200
H	6.49492000	-2.51746100	5.19692500
H	4.41923100	1.23620100	5.41437000
H	5.67596200	-0.58951700	6.52702800
C	-7.11416600	0.75622600	2.59671400
C	-6.22648900	0.80738300	1.35460000
C	-5.24980200	-0.35525000	1.28475700
C	-5.42533700	-1.48821400	2.09056900
C	-6.61958200	-1.64637300	3.01217100
C	-7.72717700	-0.63397500	2.73640100
H	-6.51839200	0.97976200	3.49065600
H	-6.87279500	0.81753000	0.46731400
C	-4.11722500	-0.27693900	0.44558900
C	-4.45736700	-2.49425100	2.08098800
H	-6.99867600	-2.67115900	2.93333100
H	-8.46943600	-0.66333400	3.53943700
C	-3.27782300	-2.38577500	1.35120700
C	-3.12153600	-1.24905500	0.55624100
H	-4.60517800	-3.37995400	2.69536200
C	-3.94550800	0.86085600	-0.50474500
C	-4.88309800	1.14323400	-1.51747200
C	-2.82518300	1.68307800	-0.37020000
C	-5.94057800	0.12343800	-1.90121300
C	-4.75069600	2.32956100	-2.25426300
C	-2.65634200	2.85438000	-1.10781900
C	-7.12677600	0.74369400	-2.63516300
H	-5.45626900	-0.60348500	-2.56881200

C	-5.77695600	2.74534800	-3.29159700
C	-3.66340200	3.17177900	-2.01607600
C	-6.62660900	1.58586500	-3.80634100
H	-7.80182400	-0.04489600	-2.98120700
H	-6.43886500	3.49522700	-2.83686500
H	-3.56749900	4.09132300	-2.58942100
H	-7.46115200	1.97096200	-4.40005100
O	-1.95987200	-1.11189100	-0.18797600
O	-1.86035000	1.31730700	0.55858000
P	-0.90697600	0.07079200	0.15976800
O	-0.22376700	-0.25920100	1.50813500
O	-0.03904200	0.30530400	-1.01445900
C	-0.14339300	-4.29061800	2.31992500
C	-1.09285700	-3.25308600	2.15923100
C	-0.35301200	-5.51831500	1.75028200
C	-2.24285100	-3.45578500	1.43103900
C	-2.46775000	-4.71734400	0.79339000
C	-1.51250500	-5.75940500	0.96886800
C	-1.72333300	-7.00850600	0.32729200
H	-0.98923300	-7.79639400	0.47305800
C	-2.81738900	-7.21228000	-0.47253800
C	-3.75819800	-6.17188700	-0.66292900
C	-3.59168500	-4.95999300	-0.04257000
H	0.36811700	-6.32129500	1.87629600
H	-2.96442800	-8.16816000	-0.96485700
H	-4.61664400	-6.33691900	-1.30608900
H	-4.31268900	-4.16332800	-0.19412200
C	0.88513500	4.18064500	-1.41478900
C	-0.25280000	3.34156900	-1.48907200
C	0.79169000	5.41101300	-0.82246300
C	-1.45949800	3.73080700	-0.95586200
C	-1.57187400	4.99489100	-0.29526500
C	-0.42945400	5.84328700	-0.24181400
C	-0.52810600	7.09312700	0.42421500
H	0.35259800	7.72955400	0.45918000
C	-1.69885000	7.48672900	1.01840200
C	-2.83337800	6.64181800	0.97152100
C	-2.77191200	5.43069600	0.33039800
H	1.65852000	6.06273900	-0.75754500
H	-1.75999500	8.44316200	1.52793800
H	-3.75601900	6.95522500	1.44974100
H	-3.64209800	4.78234400	0.30246600
C	2.86514700	-0.82434100	0.69667400
C	3.26456700	1.10515500	-0.60080800

C	3.35091500	-0.44083900	-0.71834700
O	3.70872300	1.91382600	-1.39158200
N	2.21385800	0.18508200	1.25446200
N	2.60100100	1.35760200	0.56232900
C	2.35097900	2.62814700	1.13398500
C	3.32497900	3.62480600	1.04610600
C	1.14317000	2.86879000	1.79187900
C	3.08297800	4.86584400	1.62627500
H	4.24857100	3.42409200	0.51625400
C	0.91628500	4.11567900	2.36262300
H	0.38432900	2.09608800	1.84648100
C	1.88352400	5.11536500	2.28722700
H	3.84062300	5.64048300	1.55934600
H	-0.03352800	4.31203800	2.84960800
H	1.69183400	6.08911000	2.72648900
C	2.42161300	-2.20368200	1.08448300
H	2.30891700	-2.23533900	2.17132900
H	1.44646500	-2.42236800	0.63397800
H	3.13361300	-2.96016600	0.75586000
N	2.38948900	-0.85742500	-1.72028900
C	2.18399300	-2.18420300	-2.01513400
O	2.96823600	-3.08819800	-1.77979900
O	1.00248000	-2.30803400	-2.62638300
C	0.38011400	-3.61535600	-2.79120000
C	-0.99795300	-3.25874200	-3.33615000
H	-1.51937700	-2.61039300	-2.62689700
H	-0.90691700	-2.73465400	-4.29115500
H	-1.58436300	-4.16959400	-3.48429900
C	0.24333700	-4.29823600	-1.43494700
H	-0.36146000	-5.20353300	-1.54548400
H	1.21560200	-4.57363200	-1.02209800
H	-0.27644700	-3.63363400	-0.73398700
C	1.17409700	-4.44956600	-3.79046600
H	2.15971300	-4.69579900	-3.39494200
H	0.63074700	-5.37530600	-4.00120300
H	1.29082200	-3.89806700	-4.72773000
C	4.96219500	-0.15516100	-3.39530700
H	3.89866400	-0.32627700	-3.50823200
C	7.68842500	0.33306000	-3.11199000
H	8.75110600	0.52063100	-2.98421200
C	7.08512800	0.51976300	-4.34516100
H	7.66995500	0.85352200	-5.19545100
C	5.71861500	0.27819800	-4.47940300
H	5.23382900	0.43052900	-5.43815100

H	0.74791500	-4.10821900	2.91201300
H	-0.91929400	-2.28439700	2.61666700
H	-0.17373500	2.37071800	-1.96481100
H	1.83187600	3.82799500	-1.81394400
H	-6.27663800	-1.52612300	4.04846300
H	-8.24751100	-0.89325000	1.80517400
H	-7.88864800	1.52549200	2.52493100
H	-5.66095600	1.74426000	1.32056300
H	-6.26998900	-0.45264300	-1.03518000
H	-7.69921800	1.37998700	-1.94635800
H	-6.02475500	0.95177600	-4.46925600
H	-5.27006000	3.24938200	-4.12066000

TS-B_2'

Zero-point correction= 1.195174 (Hartree/Particle)
Thermal correction to Energy= 1.245440
Thermal correction to Enthalpy= 1.246241
Thermal correction to Gibbs Free Energy= 1.111537
Sum of electronic and zero-point Energies= -3828.036501
Sum of electronic and thermal Energies= -3827.986235
Sum of electronic and thermal Enthalpies= -3827.985433
Sum of electronic and thermal Free Energies= -3828.120137
SCF Done: E(RM062X) = -3830.19653393
Number of Imaginary Frequencies = -570.67

H	4.49432500	1.02743900	-2.09346700
C	7.23204200	-1.74364100	0.42586200
C	6.31193300	-1.39528000	-0.57966100
C	4.84292200	-1.59170500	-0.31663600
C	4.45329500	-1.90857400	1.09970700
C	5.45399800	-2.35742800	2.04179800
C	6.75653100	-2.22763500	1.71402000
H	4.58430600	-2.52293400	-0.84763400
H	5.14618300	-2.67029100	3.03202600
H	7.51357500	-2.47505500	2.45459600
N	3.18993500	-1.74969100	1.30054900
H	0.53272200	0.08006200	-0.54182900
C	2.42881000	-2.36421000	2.31856300
C	1.32270900	-1.71497300	2.86917200
C	2.71325600	-3.68833300	2.69105600
C	0.54815400	-2.36450100	3.82572500
H	1.02321800	-0.72903600	2.54824500
C	1.94005900	-4.32094200	3.65556700

H	3.52065400	-4.22361900	2.20079000
C	0.85865900	-3.65762000	4.23510500
H	-0.31540900	-1.84428400	4.22690900
H	2.16934300	-5.34351200	3.93698500
H	0.24628000	-4.15960000	4.97648900
C	-6.52001600	1.62417300	-3.44817200
C	-6.17763500	1.35179800	-1.98473900
C	-4.99818800	2.17666700	-1.50128500
C	-4.57488000	3.30179400	-2.22331000
C	-5.31607700	3.80460100	-3.44855000
C	-6.66697900	3.12755200	-3.66370200
H	-5.72277100	1.23907200	-4.09628000
H	-7.06954100	1.56834000	-1.38518700
C	-4.24427000	1.75758000	-0.38363800
C	-3.39874900	3.96004400	-1.85565200
H	-5.43480400	4.89136700	-3.37508700
H	-7.04192800	3.35308900	-4.66649400
C	-2.59648800	3.51912900	-0.80906300
C	-3.04444500	2.40535200	-0.09630300
H	-3.07585500	4.82784600	-2.42697400
C	-4.61565100	0.55207700	0.41609000
C	-5.81389800	0.46575800	1.15113700
C	-3.73264700	-0.53224400	0.41842500
C	-6.65618000	1.70834000	1.37768000
C	-6.16510500	-0.75807700	1.73864800
C	-4.09100200	-1.77922200	0.94189400
C	-7.59298400	1.56663300	2.57608200
H	-5.98994700	2.56810400	1.50234400
C	-7.42028300	-0.91920600	2.57530200
C	-5.32552600	-1.86260900	1.58158900
C	-8.37851000	0.26330400	2.45896500
H	-7.01073100	1.55675400	3.50612000
H	-7.92080600	-1.85370900	2.29830500
H	-5.62525400	-2.81945500	2.00485200
H	-9.15259800	0.19409700	3.22910800
O	-2.25618700	1.90479800	0.92160800
O	-2.49399200	-0.37430400	-0.16715400
P	-1.39107200	0.56591900	0.60354800
O	-0.38046000	0.87566800	-0.50138500
O	-0.90749900	0.00157000	1.88558800
C	0.96146600	4.69659000	-1.29724600
C	-0.31705700	4.13266600	-1.51040900
C	1.26778200	5.26963600	-0.09181800
C	-1.27648800	4.14276500	-0.52396600

C	-0.98358900	4.74494500	0.74093600
C	0.30591300	5.31153700	0.95141400
C	0.60239800	5.91518600	2.20220800
H	1.59097500	6.34178100	2.35035300
C	-0.33505900	5.96269300	3.19961400
C	-1.61984500	5.40783900	2.98896300
C	-1.93506400	4.81616900	1.79346500
H	2.24835500	5.70397600	0.08574800
H	-0.09785000	6.42621800	4.15188100
H	-2.35894800	5.45041300	3.78235400
H	-2.92155700	4.39202000	1.63864400
C	-1.07435200	-4.07552100	1.16037800
C	-1.93755700	-2.96616000	1.31920000
C	-1.49250500	-5.18365600	0.47351800
C	-3.20644400	-2.96712200	0.78207700
C	-3.66126100	-4.10808900	0.04005900
C	-2.78866400	-5.22757300	-0.10170200
C	-3.22033000	-6.35600900	-0.84794500
H	-2.54389000	-7.20133900	-0.94179100
C	-4.45167100	-6.37786400	-1.44761000
C	-5.30905800	-5.25841100	-1.33314400
C	-4.92568500	-4.15640100	-0.61181400
H	-0.83636500	-6.03992900	0.34272400
H	-4.76796400	-7.24460400	-2.01903500
H	-6.27568900	-5.27002500	-1.82672400
H	-5.58480200	-3.29788700	-0.54493900
C	2.60689900	-0.40390600	0.14672500
C	3.15239400	-1.05621400	-2.08876700
C	3.82677900	-0.51152000	-0.81680500
O	3.75080300	-1.26608500	-3.13381400
N	1.49982700	-0.71879500	-0.53291800
N	1.86117700	-1.30118100	-1.76725300
C	0.86879600	-1.98636000	-2.51077400
C	1.11323200	-2.40001700	-3.82450300
C	-0.35673600	-2.25333200	-1.89596900
C	0.11701500	-3.09180200	-4.50542000
H	2.06202700	-2.18167200	-4.29465700
C	-1.33965400	-2.93964500	-2.59833900
H	-0.54701400	-1.93704000	-0.87859000
C	-1.10824800	-3.36554800	-3.90299400
H	0.30624900	-3.41488700	-5.52425300
H	-2.28902100	-3.13576500	-2.10937700
H	-1.87796200	-3.90325500	-4.44648800
C	2.45132200	0.77842400	1.07513100

H	3.17975900	0.76353200	1.88311400
H	2.59840400	1.68324600	0.47815500
H	1.43230300	0.81290400	1.46254400
N	4.41523900	0.76495100	-1.11991000
C	5.29312600	1.33073100	-0.23385800
O	5.43976800	0.91950900	0.90248700
O	5.92231600	2.36226700	-0.80105300
C	6.94227200	3.09215800	-0.05186000
C	7.40402600	4.14321400	-1.05369400
H	7.80392600	3.66390500	-1.95077100
H	6.56940200	4.78652600	-1.34335100
H	8.18629400	4.76250900	-0.60797700
C	8.08627700	2.14895000	0.30777200
H	8.90455700	2.72621100	0.74785200
H	7.76323700	1.38955900	1.02089900
H	8.45721000	1.65175500	-0.59328000
C	6.31753400	3.75202300	1.17341000
H	6.00295100	3.00797900	1.90469400
H	7.05116300	4.41830900	1.63594000
H	5.45151500	4.34982900	0.87451600
C	6.77901400	-0.99067400	-1.82785500
H	6.06480700	-0.79309300	-2.62204100
C	8.60505500	-1.63277800	0.17712600
H	9.30780100	-1.89783500	0.96221800
C	9.06486200	-1.19966800	-1.05914300
H	10.13029100	-1.11840900	-1.24592000
C	8.14902200	-0.88818900	-2.06279400
H	8.50115100	-0.57403800	-3.04003300
H	1.69837900	4.66412600	-2.09346800
H	-0.54315900	3.64876800	-2.45535900
H	-1.58904700	-2.09046500	1.85980400
H	-0.07511300	-4.03075700	1.58433900
H	-4.68418100	3.62573400	-4.32868800
H	-7.40117000	3.52089300	-2.94888600
H	-7.43936000	1.09446700	-3.71538500
H	-5.95663500	0.29140100	-1.82648700
H	-7.26631400	1.92589400	0.49355100
H	-8.26366500	2.42982000	2.62323000
H	-8.88729000	0.23806200	1.48660800
H	-7.12250600	-1.03265900	3.62631700

F_2

Zero-point correction= 1.200443 (Hartree/Particle)

Thermal correction to Energy= 1.250452
Thermal correction to Enthalpy= 1.251254
Thermal correction to Gibbs Free Energy= 1.118426
Sum of electronic and zero-point Energies= -3828.073186
Sum of electronic and thermal Energies= -3828.023177
Sum of electronic and thermal Enthalpies= -3828.022375
Sum of electronic and thermal Free Energies= -3828.155203
SCF Done: E(RM062X) = -3830.24147539

H	-1.22783400	-0.38729800	1.48328600
C	-6.64389400	0.10997100	2.33642900
C	-5.25331100	-0.11157300	2.38151500
C	-4.61126400	-0.79338400	1.20903700
C	-5.39969900	-0.75505600	-0.04857500
C	-6.82027100	-0.59638700	-0.03868800
C	-7.38372300	-0.18027000	1.12496800
H	-4.54661900	-1.86796500	1.47277200
H	-7.39303000	-0.72399500	-0.94884100
H	-8.45686000	-0.00356400	1.15030200
N	-4.63436000	-0.87308100	-1.09951100
H	-1.50437000	-0.02046900	-1.59781200
C	-5.10882200	-0.97600100	-2.44705300
C	-5.71437600	-2.16267500	-2.85534900
C	-4.94841400	0.10030500	-3.31695600
C	-6.17657700	-2.27176300	-4.16279600
H	-5.80858800	-2.98576300	-2.15308000
C	-5.41207800	-0.02604000	-4.62298700
H	-4.46180600	1.00456100	-2.96945000
C	-6.02341800	-1.20456200	-5.04483600
H	-6.64849800	-3.19111800	-4.49182300
H	-5.29210900	0.80218200	-5.31265600
H	-6.37973800	-1.29278100	-6.06569000
C	7.17915300	0.65492500	-2.42015300
C	6.22590700	0.77349500	-1.23236500
C	5.24007100	-0.38086500	-1.15482200
C	5.45137300	-1.55395800	-1.89122300
C	6.69014300	-1.76303500	-2.74116900
C	7.78881200	-0.74343300	-2.45584100
H	6.63396000	0.83420100	-3.35551600
H	6.82370600	0.82872000	-0.31310800
C	4.06781800	-0.25869400	-0.37977000
C	4.47621800	-2.55143000	-1.88029300
H	7.05819300	-2.78441900	-2.59361100
H	8.57474300	-0.81677900	-3.21358900

C	3.26086700	-2.40351900	-1.21655400
C	3.06709400	-1.22931500	-0.48244900
H	4.64665600	-3.46489400	-2.44692400
C	3.85638900	0.92576200	0.50184400
C	4.74420800	1.24579100	1.54692500
C	2.74958900	1.74662900	0.26539200
C	5.76803300	0.23392000	2.03079400
C	4.59049300	2.46536800	2.22123500
C	2.56574300	2.95470300	0.94050800
C	6.92197000	0.87469200	2.79720400
H	5.24155600	-0.45844000	2.70328000
C	5.56679400	2.91820900	3.29133400
C	3.52802400	3.30489600	1.88525000
C	6.37288800	1.77399600	3.90200700
H	7.56940900	0.09626800	3.21281500
H	6.26272800	3.63914700	2.84016300
H	3.41384900	4.25229600	2.40816700
H	7.18028400	2.17583700	4.52207200
O	1.89049700	-1.04443900	0.20885200
O	1.83680000	1.34708200	-0.68947600
P	0.83470900	0.11558600	-0.28922000
O	0.16690200	-0.29362100	-1.56990900
O	0.01541600	0.47415800	0.91151500
C	0.16400200	-4.28538900	-2.32826200
C	1.08304200	-3.23940000	-2.07326500
C	0.39379100	-5.54953000	-1.85242500
C	2.22789300	-3.47079900	-1.34257400
C	2.46364700	-4.76954400	-0.78677800
C	1.53928900	-5.81894300	-1.06015200
C	1.76435000	-7.10488100	-0.50069900
H	1.05437300	-7.89745900	-0.72218400
C	2.84041400	-7.33936800	0.31484700
C	3.74895700	-6.29317100	0.60474100
C	3.56985600	-5.04570000	0.06352400
H	-0.30145300	-6.35917200	-2.05791700
H	2.99746700	-8.32386500	0.74386900
H	4.59205500	-6.48184900	1.26167400
H	4.26450500	-4.24410300	0.29207600
C	-0.93711500	4.40761700	1.08518900
C	0.16066400	3.52122600	1.20477100
C	-0.78059900	5.61707500	0.46412800
C	1.39717000	3.85011700	0.69917800
C	1.57405500	5.08953600	0.00497200
C	0.46794500	5.98018900	-0.10536200

C	0.63310600	7.20405300	-0.80566100
H	-0.21987500	7.87414600	-0.88187000
C	1.83401200	7.53466600	-1.37819100
C	2.93281700	6.64914200	-1.27353300
C	2.80649700	5.46139700	-0.59851300
H	-1.61597600	6.30576700	0.36809200
H	1.94602800	8.47224400	-1.91371200
H	3.87979900	6.91199800	-1.73443300
H	3.64885300	4.78067300	-0.52609700
C	-3.15218200	-0.88182900	-0.77127300
C	-3.02801800	1.10805800	0.56990100
C	-3.18753700	-0.43053300	0.73317500
O	-3.21204500	1.93238800	1.44149100
N	-2.52795400	0.16975200	-1.51970400
N	-2.72128000	1.33913800	-0.73381900
C	-2.46351600	2.60682900	-1.32089000
C	-3.42501800	3.61085200	-1.22891400
C	-1.25588000	2.82057600	-1.98612500
C	-3.17688800	4.84505900	-1.82193600
H	-4.34493500	3.41962800	-0.68623200
C	-1.02171300	4.05920500	-2.57273100
H	-0.51210700	2.02916500	-2.03021000
C	-1.97989800	5.06832600	-2.49711500
H	-3.92011500	5.63316900	-1.75242900
H	-0.07463100	4.24365800	-3.06905100
H	-1.78033900	6.03623000	-2.94628800
C	-2.53968100	-2.22238700	-1.11619800
H	-2.58595700	-2.36219200	-2.20014300
H	-1.48522000	-2.21786400	-0.82176300
H	-3.05580600	-3.03595500	-0.60515900
N	-2.12998100	-0.90835600	1.56864500
C	-2.02679100	-2.21519000	1.95137500
O	-2.91483600	-3.05438800	1.84976000
O	-0.81742000	-2.41927300	2.47473100
C	-0.28958400	-3.76868800	2.64026100
C	1.17028200	-3.51124200	2.99487600
H	1.64979200	-2.94392000	2.19218900
H	1.24232600	-2.93593100	3.92166700
H	1.69388000	-4.46273500	3.12221700
C	-0.37688900	-4.52053500	1.31824900
H	0.19278500	-5.45172700	1.39272600
H	-1.40898000	-4.75655100	1.05359300
H	0.07461000	-3.91437100	0.52504700
C	-1.02640600	-4.47583400	3.77169800

H	-2.07297600	-4.63649200	3.51031800
H	-0.55303800	-5.44312600	3.96391300
H	-0.97155800	-3.87777700	4.68573300
C	-4.54351600	0.19906500	3.53792000
H	-3.46960700	0.05064500	3.55877200
C	-7.30449800	0.64165900	3.45538900
H	-8.37672400	0.81032700	3.40889600
C	-6.59087600	0.95337300	4.59919700
H	-7.09833500	1.36943800	5.46247000
C	-5.21053700	0.73625500	4.63291600
H	-4.64699200	0.99496000	5.52315100
H	-0.71929200	-4.07904900	-2.92529600
H	0.89244300	-2.24214000	-2.45814900
H	0.02674000	2.56390800	1.69605700
H	-1.90065800	4.10094100	1.47998100
H	6.40451200	-1.69087300	-3.79925500
H	8.25428900	-0.95740400	-1.48477600
H	7.95441700	1.42352500	-2.34649600
H	5.66477000	1.71254700	-1.27767300
H	6.13581700	-0.38334800	1.20976100
H	7.53667600	1.47415000	2.11160200
H	5.72812800	1.17661200	4.55882500
H	5.02423900	3.46509600	4.06939500

F_2'

Zero-point correction= 1.201738 (Hartree/Particle)
Thermal correction to Energy= 1.251809
Thermal correction to Enthalpy= 1.252611
Thermal correction to Gibbs Free Energy= 1.119231
Sum of electronic and zero-point Energies= -3828.042713
Sum of electronic and thermal Energies= -3827.992643
Sum of electronic and thermal Enthalpies= -3827.991841
Sum of electronic and thermal Free Energies= -3828.125220
SCF Done: E(RM062X) = -3830.22090102

H	-4.25251100	1.08389100	2.08552000
C	-7.23377500	-1.50414200	-0.49152400
C	-6.29602000	-1.22763200	0.52133900
C	-4.84558900	-1.44353700	0.21521000
C	-4.49114000	-1.61400300	-1.22102900
C	-5.47786600	-2.01230900	-2.17895900
C	-6.77850400	-1.90961300	-1.80914300
H	-4.60237300	-2.43646100	0.63492500

H	-5.19071300	-2.24628300	-3.19596200
H	-7.54644700	-2.10579900	-2.55382100
N	-3.21696800	-1.38976400	-1.41934200
H	-0.75824600	-0.32733100	0.44416600
C	-2.44885000	-2.00259900	-2.46196800
C	-1.34098200	-1.37779600	-3.02931100
C	-2.78690400	-3.31204800	-2.83200900
C	-0.60183400	-2.05686000	-3.99448900
H	-0.98786500	-0.40847100	-2.71221000
C	-2.05747500	-3.96477100	-3.81588100
H	-3.59251300	-3.83094300	-2.32256000
C	-0.96186400	-3.33563000	-4.40492500
H	0.27641300	-1.56751300	-4.40153700
H	-2.32412500	-4.97869900	-4.09392800
H	-0.37493200	-3.85503600	-5.15465500
C	6.73258700	1.19337100	3.34455500
C	6.30139100	0.98612100	1.89405400
C	5.17848300	1.92251500	1.48140200
C	4.88192800	3.05581200	2.25170500
C	5.71719200	3.46322000	3.45197500
C	7.01611500	2.67320200	3.58372600
H	5.93598700	0.86169300	4.02247000
H	7.18189800	1.13284300	1.25759600
C	4.34641100	1.60065300	0.38681200
C	3.74755500	3.81503600	1.95591700
H	5.92164100	4.53849400	3.39881300
H	7.45820600	2.84201500	4.57038900
C	2.86666000	3.46915700	0.93730600
C	3.18532300	2.34425000	0.17141100
H	3.52188500	4.68963100	2.56280900
C	4.59139000	0.39057100	-0.45237400
C	5.75682100	0.21577600	-1.22398400
C	3.62320600	-0.61757900	-0.43902000
C	6.68214300	1.39380300	-1.47286400
C	5.99744700	-1.02897900	-1.82282000
C	3.86925400	-1.88405900	-0.98263700
C	7.58588000	1.18041400	-2.68593900
H	6.07484300	2.29684300	-1.59316900
C	7.21810300	-1.28338500	-2.68685500
C	5.07717600	-2.06629900	-1.64923300
C	8.26854200	-0.18083900	-2.58224600
H	6.98972200	1.21655800	-3.60656800
H	7.64910900	-2.25631800	-2.42510000
H	5.29092400	-3.04226100	-2.08149300

H	9.02447600	-0.30819300	-3.36318700
O	2.32410100	1.94700600	-0.82253700
O	2.42833600	-0.37714100	0.18777300
P	1.34478500	0.66171600	-0.52066300
O	0.36199500	0.93668200	0.57936800
O	0.88112600	0.17660700	-1.85334500
C	-0.53875500	4.95382800	1.63470300
C	0.68594100	4.26024800	1.76475100
C	-0.84340600	5.59871000	0.46599200
C	1.59468200	4.21254200	0.73247800
C	1.30084500	4.88357100	-0.49726200
C	0.06634400	5.58239000	-0.62347100
C	-0.22748700	6.25767000	-1.83784500
H	-1.17359400	6.78639600	-1.92077200
C	0.66059000	6.24781800	-2.88052300
C	1.89084500	5.55971600	-2.75418100
C	2.20202400	4.89699000	-1.59543200
H	-1.78238800	6.13471500	0.35293600
H	0.42585100	6.76733900	-3.80423200
H	2.59082800	5.55575400	-3.58345600
H	3.14535300	4.36912400	-1.50550700
C	0.64379000	-3.87047400	-1.15605100
C	1.61656300	-2.86196700	-1.34301200
C	0.94007700	-4.99343800	-0.43065400
C	2.87833600	-2.98177200	-0.80436400
C	3.20605800	-4.13418900	-0.01822200
C	2.21916800	-5.14757400	0.16228900
C	2.51756400	-6.26942600	0.98018100
H	1.75248000	-7.03033500	1.11072700
C	3.72930700	-6.38357400	1.60928100
C	4.70565800	-5.37222700	1.44503400
C	4.45306200	-4.28153100	0.65206300
H	0.19548700	-5.76851800	-0.26879500
H	3.94148400	-7.24174600	2.23912300
H	5.65938600	-5.45895100	1.95610900
H	5.20107800	-3.50336700	0.54361400
C	-2.62067400	-0.47348900	-0.34177000
C	-3.08427900	-1.09715100	1.95563600
C	-3.75779800	-0.45374500	0.73983900
O	-3.64339300	-1.21867100	3.03579100
N	-1.47067100	-1.07680800	0.27416100
N	-1.89012500	-1.57092500	1.54423500
C	-0.99415900	-2.40000600	2.27229700
C	-1.48957600	-3.27229000	3.24414700

C	0.36907000	-2.34476100	1.98193300
C	-0.60245400	-4.10589100	3.91578000
H	-2.54773600	-3.28603600	3.47308000
C	1.23871100	-3.18872600	2.66505300
H	0.75921200	-1.65208600	1.24544300
C	0.75941100	-4.07501100	3.62506400
H	-0.98439400	-4.78752900	4.66912800
H	2.29831900	-3.15011400	2.43264300
H	1.44584900	-4.73662900	4.14312700
C	-2.28257400	0.88622800	-0.94069400
H	-3.06722300	1.20634200	-1.62573300
H	-2.18954200	1.59880900	-0.11875900
H	-1.30945300	0.86564300	-1.42837200
N	-4.27452400	0.82878700	1.10673000
C	-5.14742200	1.47488800	0.27771000
O	-5.36834300	1.09992200	-0.86236600
O	-5.69043600	2.52391700	0.89395600
C	-6.71050900	3.32164700	0.21541000
C	-7.05380500	4.37964400	1.25660000
H	-7.42058100	3.90889100	2.17212400
H	-6.17068000	4.97558400	1.49949500
H	-7.82956800	5.04386800	0.86792900
C	-7.92211200	2.44438200	-0.08532900
H	-8.72827800	3.06647200	-0.48446500
H	-7.67734300	1.67040000	-0.81424300
H	-8.27531600	1.96712500	0.83358900
C	-6.12580400	3.96756200	-1.03654000
H	-5.90586200	3.22305800	-1.80095100
H	-6.84526700	4.68731800	-1.43698000
H	-5.20711200	4.50485300	-0.78465200
C	-6.73082200	-0.87163800	1.79415400
H	-5.99823300	-0.71831600	2.58193400
C	-8.60230800	-1.37682200	-0.22002800
H	-9.32182400	-1.58495500	-1.00686300
C	-9.03229800	-0.99352200	1.04228300
H	-10.09238600	-0.89575500	1.24914000
C	-8.09590600	-0.74958500	2.04764300
H	-8.43075300	-0.46962600	3.04115700
H	-1.23612500	4.96487800	2.46648300
H	0.90845600	3.72462600	2.68211500
H	1.36065100	-1.96119000	-1.89382200
H	-0.34542400	-3.73060700	-1.58121700
H	5.11577200	3.31184100	4.35838200
H	7.74406500	3.02218500	2.83993900

H	7.61464600	0.58156400	3.55710700
H	5.97833400	-0.04660600	1.72759700
H	7.31996000	1.57609000	-0.60042200
H	8.32121400	1.98863300	-2.74490800
H	8.78659900	-0.24892000	-1.61672700
H	6.89359900	-1.36527600	-3.73307400

TS-C_2

Zero-point correction= 1.198005 (Hartree/Particle)
Thermal correction to Energy= 1.247524
Thermal correction to Enthalpy= 1.248325
Thermal correction to Gibbs Free Energy= 1.118435
Sum of electronic and zero-point Energies= -3828.080443
Sum of electronic and thermal Energies= -3828.030924
Sum of electronic and thermal Enthalpies= -3828.030123
Sum of electronic and thermal Free Energies= -3828.160013
SCF Done: E(RM062X) = -3830.23769630
Number of Imaginary Frequencies = -452.88

H	-1.33607500	-2.01756700	-0.39499800
C	-0.22446900	2.14181600	-2.07621400
C	-0.85241200	0.88069400	-1.96311800
C	-1.50508400	0.57046300	-0.68159000
C	-1.74726300	1.65547600	0.23984800
C	-1.07805300	2.90409200	0.11956300
C	-0.37378700	3.11819100	-1.02560300
H	-0.65373900	-0.00316800	-0.00254500
H	-1.18384100	3.66781400	0.88163500
H	0.08473600	4.09069800	-1.18602400
N	-2.62080300	1.31489000	1.17992500
H	-5.12019800	-0.73045600	0.84202500
C	-2.81436600	2.02965200	2.40421300
C	-1.78710800	2.03375600	3.34812800
C	-4.02602900	2.67823300	2.63472500
C	-1.99197200	2.70741600	4.54991400
H	-0.85346700	1.50453800	3.15090600
C	-4.21182700	3.34643800	3.84101300
H	-4.79664700	2.64916000	1.87175500
C	-3.19748600	3.36050400	4.79654300
H	-1.20637100	2.70731500	5.29884100
H	-5.14892800	3.85819500	4.03301700
H	-3.34910400	3.87963300	5.73741300
C	7.62912100	-0.13146800	-0.31575300

C	6.19671000	-0.47901900	-0.71776600
C	5.20032200	0.60089100	-0.33146400
C	5.63220000	1.88478600	0.02922500
C	7.09599200	2.27973400	-0.00165100
C	7.96534700	1.28678600	-0.76791100
H	7.73573900	-0.19623700	0.77442800
H	6.17106800	-0.65024700	-1.80228900
C	3.82535700	0.30004500	-0.27524400
C	4.69580000	2.82323800	0.46504800
H	7.18795600	3.28603100	-0.42496500
H	9.02347300	1.51440500	-0.60838700
C	3.34596200	2.51715700	0.61862000
C	2.93275300	1.22912600	0.26585200
H	5.03217000	3.82412200	0.72903200
C	3.29839200	-1.02192400	-0.71873700
C	3.38279700	-1.46627800	-2.05177300
C	2.64860500	-1.81438200	0.22621300
C	3.81713400	-0.51287500	-3.14969800
C	2.92060800	-2.75184600	-2.36962400
C	2.16762200	-3.09190900	-0.07020500
C	4.25586400	-1.22842500	-4.42419700
H	2.94947900	0.12325500	-3.37904100
C	3.04642200	-3.31700300	-3.77181300
C	2.34377900	-3.54488700	-1.37498700
C	3.19082900	-2.23864200	-4.84300600
H	4.43278600	-0.49594600	-5.21797700
H	3.92913600	-3.97043500	-3.80611900
H	1.98614500	-4.54019600	-1.63024500
H	3.43606100	-2.69747900	-5.80571800
O	1.60782100	0.87334500	0.40584900
O	2.42811600	-1.28094600	1.48319700
P	1.18187900	-0.22808900	1.56628300
O	1.11206800	0.36588800	2.91901500
O	-0.04641600	-0.88206000	0.93774400
C	0.85845900	4.34884300	2.82072700
C	1.75700100	3.37206200	2.33123700
C	0.57414000	5.46872100	2.08314200
C	2.38363500	3.53683500	1.11631800
C	2.09712700	4.69055600	0.31878100
C	1.16919500	5.65635500	0.80819500
C	0.82753800	6.76751800	-0.00936100
H	0.11947000	7.49564500	0.37715400
C	1.36306100	6.91374400	-1.26237500
C	2.27919800	5.95240300	-1.75444700

C	2.64009200	4.87491600	-0.98463300
H	-0.11953400	6.21930600	2.45264900
H	1.08663600	7.76176700	-1.88032600
H	2.69711000	6.07008600	-2.74951900
H	3.32891200	4.13314600	-1.37471000
C	-0.69453700	-4.91018200	1.59245500
C	0.10900700	-4.23500600	0.64692900
C	-0.17957200	-5.25363000	2.81380800
C	1.40636000	-3.87639800	0.93624500
C	1.97385900	-4.24188700	2.19856400
C	1.16615000	-4.94278300	3.13939000
C	1.72425700	-5.31805900	4.39036200
H	1.09472700	-5.84750700	5.10039800
C	3.02601100	-5.02270200	4.69541900
C	3.83349700	-4.33618800	3.75744300
C	3.32177900	-3.95555100	2.54465400
H	-0.78978300	-5.76657000	3.55222800
H	3.44293500	-5.31382700	5.65414900
H	4.86523500	-4.10769300	4.00402100
H	3.94723100	-3.42949800	1.83126800
C	-3.25208700	-0.00612900	0.93248200
C	-3.83416400	0.00517300	-1.41908900
C	-2.67820600	-0.39437600	-0.47325700
O	-3.78488800	-0.04179500	-2.62726600
N	-4.68799100	0.19222900	0.73819300
N	-4.83280000	0.52847700	-0.63257900
C	-6.00568300	1.19946400	-1.03699000
C	-6.24056600	1.49598800	-2.38608600
C	-6.93799100	1.58157700	-0.06536900
C	-7.39877300	2.17907700	-2.73823200
H	-5.52773700	1.18847000	-3.13747300
C	-8.08927400	2.26417100	-0.44265200
H	-6.75304600	1.34264800	0.97438500
C	-8.32888400	2.56868900	-1.77822100
H	-7.57306800	2.40563100	-3.78528500
H	-8.80397100	2.55535100	0.32055700
H	-9.22955200	3.09869600	-2.06851200
C	-2.99837200	-0.97015400	2.07348900
H	-3.44934000	-0.57587100	2.98772000
H	-3.45289200	-1.93741100	1.84455300
H	-1.92345500	-1.10207500	2.21401300
N	-2.28509900	-1.76430600	-0.66035000
C	-3.25242300	-2.72623900	-0.70406500
O	-4.44295300	-2.47723900	-0.59041200

O	-2.71894700	-3.93550500	-0.90590400
C	-3.57926000	-5.08348600	-1.19299100
C	-2.57319000	-6.20235300	-1.43645800
H	-1.92130500	-5.94839400	-2.27630000
H	-1.95107600	-6.36679700	-0.55277600
H	-3.10173900	-7.12976900	-1.67087800
C	-4.39281900	-4.80962200	-2.45442000
H	-4.92584800	-5.72028000	-2.74149100
H	-5.11725700	-4.01157800	-2.29226900
H	-3.72679900	-4.52811500	-3.27474700
C	-4.46967500	-5.39933500	0.00474600
H	-5.19425000	-4.60367400	0.17517300
H	-5.00599600	-6.33291900	-0.18738500
H	-3.86700400	-5.53661700	0.90713200
C	-0.73947400	-0.03728600	-3.01384900
H	-1.24808000	-0.99173300	-2.94240200
C	0.51789400	2.45493000	-3.22957500
H	1.00190000	3.42639400	-3.28937700
C	0.62263100	1.54014300	-4.25913400
H	1.19046000	1.78122700	-5.15172100
C	-0.01810200	0.29701600	-4.14834800
H	0.04267300	-0.41250300	-4.96774200
H	0.38826700	4.19922900	3.78712300
H	1.94246800	2.47274200	2.91054600
H	-0.31449700	-3.97798900	-0.32012900
H	-1.72734700	-5.13035100	1.34283800
H	7.46100200	2.34836300	1.03188700
H	7.77382100	1.37637200	-1.84521100
H	8.31961600	-0.86007600	-0.75075500
H	5.88551400	-1.42470000	-0.26190200
H	4.59239700	0.16904200	-2.79660000
H	5.20597000	-1.75159100	-4.25038800
H	2.23520200	-1.71276500	-4.96620200
H	2.18430300	-3.95836000	-3.98308400

TS-C_2'

Zero-point correction=	1.197829 (Hartree/Particle)
Thermal correction to Energy=	1.247324
Thermal correction to Enthalpy=	1.248126
Thermal correction to Gibbs Free Energy=	1.118983
Sum of electronic and zero-point Energies=	-3828.080776
Sum of electronic and thermal Energies=	-3828.031280
Sum of electronic and thermal Enthalpies=	-3828.030479

Sum of electronic and thermal Free Energies= -3828.159622

SCF Done: E(RM062X) = -3830.23703585

Number of Imaginary Frequencies = -475.30

H	4.29921000	-3.02904000	-0.22454200
C	3.11434700	0.57818200	2.55842500
C	3.05271900	-0.59906200	1.78109100
C	2.63599300	-0.46289600	0.37301200
C	2.76158900	0.85186900	-0.20905900
C	2.69902100	2.02709100	0.59658200
C	2.86155300	1.86138700	1.93437900
H	1.42416800	-0.50044600	0.58184800
H	2.55913600	2.99969000	0.13977800
H	2.81895200	2.73707900	2.57947300
N	2.88191000	0.80501600	-1.52364200
H	0.87632000	-0.27262400	-2.12822600
C	2.96498900	1.94052600	-2.38881200
C	4.16927800	2.63791900	-2.45169000
C	1.86998400	2.29870600	-3.17196100
C	4.28367700	3.71246200	-3.32876000
H	4.99448600	2.31433900	-1.82359100
C	2.00647700	3.36216600	-4.06088500
H	0.93091500	1.76770000	-3.05065200
C	3.20778800	4.06460800	-4.14213400
H	5.21663600	4.26282900	-3.38892500
H	1.16586500	3.64874500	-4.68475400
H	3.30444300	4.89209900	-4.83776700
C	-6.28889600	2.15857700	-2.72863600
C	-5.74488200	1.58889600	-1.41984300
C	-4.50325300	2.32059800	-0.94121100
C	-4.15037000	3.56582100	-1.47909200
C	-5.03698800	4.29556600	-2.47091700
C	-6.42402500	3.67395800	-2.60926700
H	-5.60521200	1.91925400	-3.55283500
H	-6.54064300	1.64042800	-0.66809800
C	-3.62638700	1.70106300	-0.02774800
C	-2.92760400	4.14721800	-1.13452000
H	-5.11078400	5.34906400	-2.17890400
H	-6.93901900	4.09873000	-3.47603500
C	-1.99928500	3.50856500	-0.31627100
C	-2.37487400	2.26899500	0.20723500
H	-2.67071500	5.12030000	-1.54805600
C	-3.96550300	0.42959100	0.67619800
C	-5.04852900	0.37001300	1.57626900

C	-3.14479300	-0.69108900	0.49994500
C	-5.76968500	1.64113100	1.99293200
C	-5.37967400	-0.86070100	2.15889000
C	-3.44021000	-1.91890400	1.10333100
C	-6.55265900	1.46948900	3.29347800
H	-5.03447300	2.44729300	2.08656300
C	-6.53452000	-1.01353200	3.13100100
C	-4.58890300	-1.97715200	1.89085300
C	-7.42699000	0.22220700	3.20284500
H	-5.85860300	1.36388300	4.13695000
H	-7.11819300	-1.89954500	2.85753300
H	-4.83956300	-2.92599800	2.36150600
H	-8.10416300	0.14602700	4.05875800
O	-1.46064500	1.54031300	0.94434700
O	-2.04774600	-0.58283100	-0.32980800
P	-0.75999000	0.32895000	0.09650500
O	-0.12298400	0.83931400	-1.15518400
O	0.09586200	-0.41744500	1.09384300
C	1.34775400	5.10023700	-1.07094900
C	0.09763100	4.45110100	-1.19488700
C	1.84051100	5.40639100	0.16990300
C	-0.65466900	4.10764400	-0.09270400
C	-0.14379300	4.39195700	1.21725300
C	1.11619200	5.04906200	1.33844300
C	1.63164700	5.33577600	2.63146900
H	2.59150700	5.84085600	2.70558300
C	0.93338900	4.99007700	3.75913900
C	-0.32456500	4.35291700	3.64106300
C	-0.85069700	4.06926100	2.40703800
H	2.79748500	5.90972500	0.28123500
H	1.33512400	5.21360100	4.74245600
H	-0.87831000	4.08953500	4.53615700
H	-1.81762000	3.58536500	2.33053600
C	-0.50057200	-4.22779600	1.71048900
C	-1.30709300	-3.07026400	1.61203000
C	-0.95976900	-5.43398600	1.25118800
C	-2.55555500	-3.11816300	1.03241900
C	-3.03561200	-4.35495400	0.49409700
C	-2.23261200	-5.52564500	0.62994700
C	-2.71460100	-6.76026800	0.11748000
H	-2.09606700	-7.64585400	0.23654000
C	-3.92212400	-6.83323800	-0.52724300
C	-4.70514800	-5.66552300	-0.69304900
C	-4.27630300	-4.46262600	-0.19218100

H	-0.35305600	-6.33133100	1.33524200
H	-4.27659100	-7.78096400	-0.91981400
H	-5.65060500	-5.72456500	-1.22276600
H	-4.87643900	-3.56889700	-0.32759500
C	2.90845300	-0.57850900	-2.02723100
C	2.05822900	-2.57987000	-0.98583000
C	3.06130400	-1.43977100	-0.73958000
O	2.08244000	-3.64030800	-0.38327900
N	1.56543400	-0.91810600	-2.54868900
N	1.25945700	-2.20026400	-2.01174600
C	0.24647700	-2.95451500	-2.65931600
C	-0.46732400	-3.92943200	-1.96143500
C	-0.03660500	-2.68174900	-3.99952300
C	-1.46090600	-4.64167200	-2.62731600
H	-0.24982900	-4.11953700	-0.91779700
C	-1.03232200	-3.40342300	-4.64576800
H	0.51857800	-1.90426000	-4.50880900
C	-1.74639400	-4.38587000	-3.96538700
H	-2.02426800	-5.39474000	-2.08524500
H	-1.25183000	-3.19014600	-5.68716800
H	-2.52904500	-4.94228500	-4.47059400
C	3.96525300	-0.79442600	-3.08706600
H	4.95191600	-0.52859600	-2.70262600
H	3.95849200	-1.84812900	-3.37619900
H	3.72567400	-0.19047900	-3.96453400
N	4.34456300	-2.06123900	-0.52622400
C	5.38408400	-1.30535500	-0.05496000
O	5.44907400	-0.09715700	-0.20322300
O	6.28850100	-2.07827000	0.55491100
C	7.40683100	-1.46393100	1.26366100
C	8.10837000	-2.66666100	1.88305200
H	7.42998400	-3.19353800	2.55884500
H	8.43460900	-3.36049100	1.10417700
H	8.98310300	-2.33671500	2.44897300
C	6.88002900	-0.53053600	2.35134700
H	7.71462200	-0.20563000	2.97944200
H	6.39674800	0.34736500	1.92183500
H	6.15687300	-1.05838800	2.98072400
C	8.32597700	-0.75158200	0.27651700
H	7.82913500	0.11080900	-0.16718800
H	9.22509300	-0.41450700	0.80028800
H	8.62912000	-1.44089700	-0.51663300
C	3.23127500	-1.84307700	2.39478000
H	3.11230500	-2.74919000	1.80693800

C	3.40233200	0.48691900	3.92935700
H	3.44297200	1.39762400	4.52043300
C	3.62059200	-0.74530200	4.52064300
H	3.84472700	-0.81043700	5.57982000
C	3.52645100	-1.91008100	3.74980300
H	3.67538700	-2.87858100	4.21694200
H	1.91278000	5.34384200	-1.96531700
H	-0.28067900	4.20346500	-2.18210600
H	-0.93788500	-2.13059900	2.00592500
H	0.48450900	-4.14842100	2.15791500
H	-4.54265100	4.28407100	-3.45158300
H	-7.02978200	3.91137400	-1.72518300
H	-7.25079700	1.69211800	-2.96104600
H	-5.50260900	0.52680700	-1.52744500
H	-6.47046600	1.96601000	1.21563200
H	-7.15494300	2.36361700	3.48027200
H	-8.05084700	0.28685500	2.30195800
H	-6.12391200	-1.21499200	4.12932900

Pro2

Zero-point correction=	0.561755 (Hartree/Particle)
Thermal correction to Energy=	0.585363
Thermal correction to Enthalpy=	0.586165
Thermal correction to Gibbs Free Energy=	0.511596
Sum of electronic and zero-point Energies=	-1642.904540
Sum of electronic and thermal Energies=	-1642.880931
Sum of electronic and thermal Enthalpies=	-1642.880129
Sum of electronic and thermal Free Energies=	-1642.954698

SCF Done: E(RM062X) = -1643.91163202

H	-2.08050700	1.57506900	-0.74111400
C	0.51814900	3.86106400	1.41724300
C	-0.33042500	2.74951100	1.12842200
C	0.22277100	1.69424800	0.36591000
C	1.55395400	1.68016000	0.00180900
C	2.41266200	2.75663600	0.33445400
C	1.87973600	3.82365900	1.00939000
H	3.46056300	2.72965900	0.05900900
H	2.51425900	4.66860200	1.26293600
N	1.90159200	0.50010300	-0.64024500
H	0.06557900	-2.16878400	-1.00839400
C	3.09000600	0.33034600	-1.39524100
C	3.54167500	1.32366100	-2.26961400

C	3.79787500	-0.86866000	-1.28041800
C	4.70407400	1.12480400	-3.00731400
H	2.97474600	2.24528300	-2.36642100
C	4.94594000	-1.06878700	-2.04044100
H	3.43143100	-1.62157400	-0.59148500
C	5.40628400	-0.07322100	-2.89903000
H	5.05315700	1.90233800	-3.67919200
H	5.49221900	-2.00206600	-1.94915000
H	6.30899100	-0.22917700	-3.48034200
C	0.68663800	-0.26076600	-0.98941000
C	-0.53814500	-0.57447300	1.07679600
C	-0.41808700	0.41533200	-0.10664900
O	-1.23980900	-0.39736900	2.04955200
N	0.78886900	-1.64209200	-0.50959400
N	0.34416000	-1.59656400	0.83913000
C	0.72844400	-2.63814400	1.70818300
C	0.27247200	-2.67891300	3.03247000
C	1.58644900	-3.63695100	1.23455000
C	0.68949500	-3.71319600	3.86201600
H	-0.39920100	-1.91391700	3.39445200
C	1.98940900	-4.66177900	2.08324900
H	1.93216400	-3.59925000	0.20943400
C	1.54606200	-4.70902900	3.40063500
H	0.33285200	-3.73654800	4.88689600
H	2.65643600	-5.42951300	1.70398900
H	1.86133100	-5.51157100	4.05869900
C	0.42800300	-0.24462900	-2.48570700
H	1.25859600	-0.72567700	-3.00772700
H	-0.49897900	-0.76961300	-2.72293700
H	0.34858600	0.79060600	-2.82679400
N	-1.69254400	0.64316800	-0.74346800
C	-2.51138000	-0.40312200	-1.03896500
O	-2.14106300	-1.56625100	-0.99112600
O	-3.72253000	0.03108100	-1.40047700
C	-4.75406800	-0.91986300	-1.80602800
C	-5.93089900	-0.01158000	-2.14113200
H	-6.22001400	0.57432800	-1.26519100
H	-5.66553100	0.67496000	-2.94908500
H	-6.78579600	-0.61377900	-2.45839000
C	-5.09773400	-1.84263000	-0.64123500
H	-5.96062200	-2.45740000	-0.91260400
H	-4.26000300	-2.49475200	-0.39544200
H	-5.36054300	-1.25047700	0.23959300
C	-4.29885200	-1.68926200	-3.04250900

H	-3.47223500	-2.35928900	-2.80700100
H	-5.13522600	-2.28027100	-3.42606900
H	-3.98714300	-0.99028300	-3.82423500
C	-1.66355600	2.75999500	1.62753600
H	-2.28047800	1.87642500	1.50140500
C	-0.00750900	4.96398400	2.13646600
H	0.64655500	5.80682400	2.34383700
C	-1.30750300	4.96599400	2.57209800
H	-1.69948900	5.81356900	3.12409400
C	-2.13362900	3.84400500	2.32484000
H	-3.14888700	3.83391700	2.70861100

Reaction (3):

Sub3

Zero-point correction=	0.147001 (Hartree/Particle)
Thermal correction to Energy=	0.154135
Thermal correction to Enthalpy=	0.155079
Thermal correction to Gibbs Free Energy=	0.115833
Sum of electronic and zero-point Energies=	-326.621208
Sum of electronic and thermal Energies=	-326.614074
Sum of electronic and thermal Enthalpies=	-326.613130
Sum of electronic and thermal Free Energies=	-326.652376
SCF Done: E(RM062X) =	-326.860334358

C	2.80868200	0.37094600	0.10090300
N	1.78713400	-0.62228000	-0.14393100
H	1.99744400	-1.54171200	0.21460100
C	0.44304100	-0.28204100	-0.05894400
C	-0.52641600	-1.29816500	-0.00867900
C	0.01393200	1.05228500	-0.05469300
C	-1.87574600	-0.98662600	0.04130200
H	-0.20435500	-2.33639800	-0.01580400
C	-1.34581200	1.35035700	-0.01068300
H	0.73758800	1.85874600	-0.08674500
C	-2.30090800	0.34222500	0.03915900
H	-2.60427500	-1.79066000	0.08162300
H	-1.65568000	2.39103400	-0.01002400
H	-3.35734400	0.58318500	0.07717400
H	2.68246200	0.89628300	1.05938700
H	3.78383900	-0.11755000	0.09496100
H	2.80974000	1.11914900	-0.69783800

CPA3

Zero-point correction=	1.054827 (Hartree/Particle)
Thermal correction to Energy=	1.110845
Thermal correction to Enthalpy=	1.111790
Thermal correction to Gibbs Free Energy=	0.963351
Sum of electronic and zero-point Energies=	-2584.919977
Sum of electronic and thermal Energies=	-2584.863958
Sum of electronic and thermal Enthalpies=	-2584.863014
Sum of electronic and thermal Free Energies=	-2585.011453

SCF Done: E(RM062X) = -2586.57249083

H	-1.77545100	-2.16148300	0.54423300
C	0.71160000	2.01734400	-0.28587700
C	3.43083900	1.87834300	-0.84476600
C	2.83675800	0.79074600	-0.21256800
C	1.47318900	0.89709600	0.05358700
H	4.50161200	1.84606600	-1.03039600
C	-3.42075300	1.99045700	0.80825400
C	-2.89356900	0.90709500	0.11303800
C	-1.54857200	0.99675400	-0.24543200
C	-0.72369400	2.05706000	0.12436700
H	-4.47669900	1.98113200	1.06582600
C	1.31934800	3.04707800	-1.03335100
C	2.69768500	2.98409700	-1.28217000
C	3.43375900	4.10104100	-1.99807700
C	2.51761800	4.99924700	-2.82551500
C	1.29361000	5.39306000	-2.00308000
C	0.47938700	4.15015400	-1.65333200
H	3.94517900	4.71347800	-1.24284300
H	3.06773000	5.88303200	-3.16196800
H	1.61871000	5.89420400	-1.08105500
H	-0.36666800	4.40978700	-1.01412700
C	-2.63004000	3.06028300	1.23518600
C	-1.25833300	3.07607000	0.93964400
C	-0.34972300	4.10722200	1.58597400
C	-1.09238900	5.36518000	2.02875500
C	-2.31167200	4.98634300	2.86481900
C	-3.29173300	4.17995900	2.01650900
H	0.10356200	3.63070400	2.46706700
H	-0.41557200	6.01212700	2.59463600
H	-1.98470800	4.38680700	3.72354900
H	-3.78150500	4.85535000	1.30165200
P	-0.06265100	-1.10031000	-0.24163200

O	0.84360500	-0.16681000	0.70519600
O	-1.00368100	-0.03275400	-1.00507000
O	-0.97286600	-1.74380900	0.89809400
O	0.59660700	-1.99367700	-1.19545900
C	-3.66582700	-0.34185800	-0.16578200
C	3.61320600	-0.43042700	0.15780700
C	-3.94114700	-0.73330900	-1.48931000
C	-4.62358600	-1.93203400	-1.71310900
H	-4.84271400	-2.23145300	-2.73577300
C	-4.73651500	-2.35957400	0.63279700
H	-5.04595500	-2.99425600	1.45976300
C	-4.06375800	-1.16952900	0.91366300
C	4.05385700	-1.31138500	-0.85185600
C	4.83130200	-2.40886500	-0.48659400
H	5.18009600	-3.08523800	-1.26346900
C	-5.02832300	-2.75962000	-0.67233600
C	5.16140000	-2.67471600	0.84190200
C	3.91161300	-0.69037900	1.50637100
C	4.68419100	-1.81020300	1.82090100
H	4.92254600	-2.01486000	2.86298500
H	4.22075300	3.66939500	-2.62512400
H	2.18692500	4.46372900	-3.72416400
H	0.66634400	6.10304200	-2.55032700
H	0.03725900	3.74355300	-2.57393100
H	0.48594700	4.36358400	0.93272400
H	-1.41718400	5.93252300	1.14598200
H	-2.80847100	5.87583700	3.26341100
H	-4.09010900	3.76265300	2.63906600
C	3.43350600	0.20638500	2.63830000
H	2.85046000	1.02600700	2.20807600
C	4.61746700	0.83212200	3.38514200
H	5.23118200	0.06308500	3.86508800
H	5.25907700	1.39537500	2.70172800
H	4.26265400	1.51193400	4.16599000
C	2.51586100	-0.55754800	3.60006900
H	2.14081300	0.11173800	4.38088100
H	1.66208600	-0.98150900	3.06605000
H	3.05529600	-1.37374600	4.09169500
C	6.00246200	-3.88267300	1.20810800
H	6.13016000	-3.87257500	2.29801300
C	7.39349100	-3.81023400	0.56898400
H	7.90947400	-2.88879000	0.85113100
H	8.00697500	-4.66127100	0.88020500
H	7.31940700	-3.83287800	-0.52314700

C	5.29586200	-5.18823400	0.82674900
H	4.30960900	-5.25217300	1.29320500
H	5.15754100	-5.25073900	-0.25746200
H	5.88699600	-6.05412200	1.14052200
C	3.71387600	-1.10063800	-2.32127800
H	2.88757900	-0.38498400	-2.37671400
C	3.23637100	-2.38888100	-3.00072800
H	2.89465200	-2.16251900	-4.01548500
H	4.04469400	-3.12254000	-3.08743500
H	2.40653100	-2.82953500	-2.44688400
C	4.91426700	-0.51643200	-3.07776200
H	5.23685800	0.43945100	-2.65580200
H	5.76479200	-1.20523100	-3.02947200
H	4.66546300	-0.35931500	-4.13198500
C	-3.80322400	-0.80425400	2.37168400
H	-3.03574400	-0.02551300	2.39518700
C	-3.28270400	-1.97798200	3.21067300
H	-4.03253900	-2.76788700	3.31696800
H	-2.37593500	-2.41236100	2.78472600
H	-3.04070400	-1.62609500	4.21764500
C	-5.08287300	-0.24771800	3.01254200
H	-5.86332300	-1.01622700	3.02603800
H	-4.89352800	0.06189400	4.04486600
H	-5.47584100	0.61047200	2.46195800
C	-3.55683500	0.11536900	-2.69155500
H	-2.97000600	0.96754700	-2.33920200
C	-2.69144400	-0.66423200	-3.68800700
H	-2.37410100	-0.00641400	-4.50268500
H	-1.79874400	-1.06700200	-3.20392600
H	-3.24974400	-1.49356700	-4.13436600
C	-4.81374400	0.67270900	-3.37222500
H	-4.53947300	1.31599900	-4.21370300
H	-5.44092100	-0.13731200	-3.75883500
H	-5.41472400	1.25832800	-2.67084900
C	-5.75831500	-4.06108500	-0.94249000
H	-5.87014000	-4.15114300	-2.03008000
C	-7.15944200	-4.05431800	-0.32137400
H	-7.74661100	-3.20556100	-0.68118300
H	-7.69446400	-4.97607400	-0.56826800
H	-7.10028400	-3.98438800	0.76971100
C	-4.94898900	-5.26554400	-0.44873300
H	-3.95522200	-5.28685800	-0.90348900
H	-4.82212900	-5.22873000	0.63830000
H	-5.46123600	-6.20068000	-0.69344300

A_3

Zero-point correction=	1.203938 (Hartree/Particle)
Thermal correction to Energy=	1.267788
Thermal correction to Enthalpy=	1.268732
Thermal correction to Gibbs Free Energy=	1.102626
Sum of electronic and zero-point Energies=	-2911.571922
Sum of electronic and thermal Energies=	-2911.508071
Sum of electronic and thermal Enthalpies=	-2911.507127
Sum of electronic and thermal Free Energies=	-2911.673233

SCF Done: E(RM062X) = -2913.45952697

H	-0.56269600	-2.22577700	0.44864400
C	1.53767000	-3.54381900	0.35036500
N	0.13694900	-3.53766200	-0.08018200
H	0.09441600	-3.24359900	-1.05685900
C	-0.65735600	-4.69765100	0.14951200
C	-1.96908700	-4.69731900	-0.34214700
C	-0.19458700	-5.79300000	0.87674200
C	-2.79233800	-5.79364600	-0.13000500
H	-2.33682200	-3.82427200	-0.87731600
C	-1.03625800	-6.88298200	1.09706500
H	0.81653800	-5.80547400	1.26749300
C	-2.33034400	-6.89419900	0.59256000
H	-3.80280900	-5.78567400	-0.52651400
H	-0.66636300	-7.73120800	1.66423000
H	-2.97713800	-7.74813700	0.76200000
H	2.10186300	-4.37302000	-0.09184300
H	1.99529700	-2.60222300	0.03554900
H	1.59114800	-3.61623900	1.44003600
C	1.04317900	2.64417700	-0.12212800
C	3.72124300	2.27683500	-0.78439700
C	3.03059900	1.20184300	-0.23426000
C	1.69317600	1.42848600	0.08414000
H	4.77763900	2.15581200	-1.01143800
C	-3.03472100	2.93703800	1.13608800
C	-2.65515700	1.88106500	0.31512600
C	-1.31630200	1.84361100	-0.07348800
C	-0.36806800	2.77516700	0.35270300
H	-4.08235400	3.03108300	1.41106000
C	1.73852300	3.67317900	-0.78941200
C	3.09615300	3.48953600	-1.09071100
C	3.92805200	4.58842900	-1.72585800

C	3.09049400	5.64987400	-2.43490100
C	1.93900600	6.09106600	-1.53525000
C	1.00552000	4.91310800	-1.26931700
H	4.51997500	5.07175500	-0.93645500
H	3.72250500	6.49901200	-2.71159500
H	2.34169200	6.46635500	-0.58449200
H	0.21314500	5.19563700	-0.57314400
C	-2.11360400	3.85708900	1.64353100
C	-0.76081900	3.75694900	1.28734000
C	0.27751600	4.61725300	1.98757700
C	-0.30755900	5.89370400	2.58615000
C	-1.52780600	5.55986800	3.43946900
C	-2.62044400	4.95130900	2.56451100
H	0.70950500	4.00958600	2.79579500
H	0.45631000	6.40641600	3.17840100
H	-1.23519600	4.84407300	4.21783300
H	-3.06333200	5.74437400	1.94640800
P	-0.01498800	-0.36848700	-0.41094800
O	0.96430500	0.38338800	0.63675700
O	-0.92787200	0.83945800	-0.95383500
O	-0.88280700	-1.24172600	0.55262500
O	0.65251300	-1.07649400	-1.52033000
C	-3.60995000	0.82241600	-0.13665400
C	3.66897300	-0.12976600	0.00112000
C	-4.10912300	0.84377200	-1.44873400
C	-4.99303600	-0.16071300	-1.85233400
H	-5.38188300	-0.14901400	-2.86885500
C	-4.86421600	-1.19053400	0.30000000
H	-5.14850800	-1.99203700	0.97719600
C	-3.97686900	-0.21457400	0.74820600
C	4.07683500	-0.91941000	-1.09642700
C	4.75612800	-2.11352800	-0.85072400
H	5.08514700	-2.71016700	-1.69843800
C	-5.38346800	-1.18259900	-0.99545400
C	5.02666400	-2.56206100	0.44192600
C	3.87792300	-0.59266100	1.31438500
C	4.55604300	-1.79910500	1.50587700
H	4.73877100	-2.14762400	2.52079500
H	4.64922300	4.14037200	-2.41743400
H	2.67941700	5.23699100	-3.36455000
H	1.37756000	6.91144900	-1.99215300
H	0.49264100	4.64584700	-2.20410100
H	1.11140800	4.85236000	1.32419100
H	-0.60290600	6.57837200	1.77945100

H	-1.90970900	6.45032400	3.94769900
H	-3.43348300	4.55475000	3.18161400
C	3.41215300	0.17062500	2.54545600
H	2.90940500	1.08492200	2.21982900
C	4.59955800	0.59078200	3.42019100
H	5.13254400	-0.28203600	3.81071800
H	5.31280600	1.19292500	2.85058000
H	4.25440300	1.18064600	4.27481200
C	2.39872500	-0.65348400	3.34900000
H	2.03303800	-0.07807900	4.20513000
H	1.54219200	-0.92637600	2.72729400
H	2.85702400	-1.57013500	3.73582800
C	5.79726100	-3.84645100	0.68811900
H	6.02806000	-3.88410100	1.76025000
C	7.12415800	-3.87262200	-0.07743200
H	7.72676000	-2.98914400	0.14785300
H	7.70134400	-4.76342000	0.18753000
H	6.95466400	-3.89814300	-1.15847800
C	4.95099600	-5.07815800	0.34735800
H	4.04872400	-5.11533300	0.96472000
H	4.64301600	-5.05420900	-0.70381900
H	5.51807400	-5.99931800	0.51346800
C	3.80085600	-0.51811200	-2.53916400
H	3.06024900	0.28657100	-2.52852700
C	3.19735900	-1.67042400	-3.35044900
H	2.90898600	-1.31028500	-4.34263000
H	3.91620900	-2.48368100	-3.49552100
H	2.30601100	-2.05743300	-2.85465300
C	5.07655100	-0.00494200	-3.21980300
H	5.50146400	0.85579000	-2.69631400
H	5.84019300	-0.79025400	-3.24137900
H	4.86781800	0.29125600	-4.25246000
C	-3.43452400	-0.29120600	2.16914500
H	-2.46685700	0.22114900	2.18214000
C	-3.19911200	-1.73035700	2.64200900
H	-4.14264400	-2.23533100	2.87532800
H	-2.67119900	-2.31884200	1.88921100
H	-2.60192300	-1.72427400	3.55830500
C	-4.37608800	0.41647500	3.15409700
H	-5.36726800	-0.04906900	3.12718100
H	-3.99109000	0.33778300	4.17583000
H	-4.49532000	1.47571200	2.91633300
C	-3.71561200	1.91851100	-2.44996000
H	-3.02271800	2.60796600	-1.95842200

C	-2.98755800	1.31242200	-3.65532700
H	-2.66466000	2.10173700	-4.34141200
H	-2.10793400	0.75002600	-3.33335100
H	-3.64527700	0.63642100	-4.21173300
C	-4.93637800	2.73309400	-2.89348600
H	-4.63584700	3.53236100	-3.57787000
H	-5.66256800	2.10164800	-3.41558900
H	-5.44058100	3.18487300	-2.03454800
C	-6.33149500	-2.27387800	-1.45508400
H	-6.59858500	-2.05917200	-2.49740200
C	-7.62111900	-2.28163100	-0.62712600
H	-8.11565200	-1.30755500	-0.66165300
H	-8.31752100	-3.03826300	-1.00124200
H	-7.40678300	-2.51247700	0.42142100
C	-5.65209300	-3.64782500	-1.41332700
H	-4.75416200	-3.66054500	-2.03849100
H	-5.35449900	-3.89672100	-0.38871900
H	-6.33117500	-4.42991500	-1.76744600

B_3

Zero-point correction=	1.513094 (Hartree/Particle)
Thermal correction to Energy=	1.597813
Thermal correction to Enthalpy=	1.598757
Thermal correction to Gibbs Free Energy=	1.390517
Sum of electronic and zero-point Energies=	-3882.672108
Sum of electronic and thermal Energies=	-3882.587389
Sum of electronic and thermal Enthalpies=	-3882.586445
Sum of electronic and thermal Free Energies=	-3882.794685

SCF Done: E(RM062X) = -3885.13812370

H	-0.40850300	0.92279500	1.51519300
C	-2.93676500	-2.04205300	0.07752900
N	-2.97241400	-0.92231900	-0.85125900
H	-2.03413100	-0.66400300	-1.14434800
C	-3.91525100	-0.91066400	-1.87732700
C	-3.64192700	-0.20698100	-3.06028900
C	-5.16250400	-1.53338100	-1.72811300
C	-4.59008700	-0.14437900	-4.07321400
H	-2.67439700	0.27588600	-3.17599900
C	-6.10714100	-1.45167700	-2.74503300
H	-5.39747900	-2.05485400	-0.80587400
C	-5.82858700	-0.76530000	-3.92401100
H	-4.35829100	0.39694000	-4.98541300

H	-7.07563200	-1.92222600	-2.60727100
H	-6.57214800	-0.70431200	-4.71127000
C	-2.66109900	1.95569800	-0.46055900
C	-4.32579300	0.83409000	0.77570200
C	-2.85024200	1.17470700	0.77232600
O	-4.89906700	0.12506100	1.57804400
N	-3.79942400	2.16192800	-1.02606100
N	-4.81010700	1.51702200	-0.31334500
C	-6.11861300	1.49640900	-0.85577400
C	-7.16721500	0.90506300	-0.14459100
C	-6.34483600	2.06846900	-2.10809300
C	-8.43682100	0.87890800	-0.71058700
H	-6.98455100	0.46394300	0.82546300
C	-7.62356400	2.03483500	-2.65163900
H	-5.51847200	2.51150200	-2.64788500
C	-8.67501700	1.43861700	-1.96271700
H	-9.24808600	0.41532900	-0.15840300
H	-7.79205400	2.47436700	-3.62969500
H	-9.66984000	1.41303200	-2.39461200
C	-1.36901100	2.47336900	-0.98272700
H	-0.74315200	2.85229300	-0.16651900
H	-0.82060500	1.66455100	-1.47715000
H	-1.54341900	3.27641100	-1.70026800
N	-2.00996800	0.95775200	1.69967800
C	-2.44372500	0.37957800	2.93784900
O	-2.87063700	1.05263500	3.83577600
O	-2.16153200	-0.91224100	2.93110200
C	-2.48471700	-1.74225800	4.09598900
C	-2.08986600	-3.13431100	3.62241400
H	-2.70526000	-3.43833400	2.77028900
H	-1.04341200	-3.14433700	3.30771900
H	-2.22853900	-3.85695800	4.43164000
C	-3.97948800	-1.66350500	4.38492600
H	-4.23654000	-2.42242200	5.12948300
H	-4.26089000	-0.68158500	4.76529700
H	-4.54647400	-1.85849200	3.47078900
C	-1.62799900	-1.30451100	5.27856700
H	-1.88721800	-0.29448500	5.59770800
H	-1.79223400	-1.99090400	6.11403200
H	-0.56870400	-1.33872400	5.00705500
H	-3.06186300	-2.99939400	-0.44634500
H	-1.96585800	-2.03887500	0.57732700
H	-3.72000100	-1.94013600	0.83924200
C	3.91720600	-0.83482100	-0.83220400

C	3.47728600	-3.44636700	-1.67673800
C	2.61092200	-2.91334000	-0.72651400
C	2.86876100	-1.60275000	-0.32804600
H	3.32754500	-4.47612000	-1.99329800
C	4.43553000	3.13571000	0.65341000
C	3.18535000	2.75206500	0.17891700
C	3.07138700	1.44142100	-0.28570400
C	4.13089900	0.53252000	-0.26943100
H	4.57441300	4.16651800	0.96992200
C	4.70215600	-1.36563900	-1.87604300
C	4.49345800	-2.69491200	-2.27232100
C	5.35856800	-3.35933900	-3.32714400
C	6.08421400	-2.36458800	-4.22949200
C	6.74485000	-1.28091500	-3.38179200
C	5.68098800	-0.48399700	-2.63147300
H	6.10336600	-3.98513000	-2.81661800
H	6.82183000	-2.88897200	-4.84415700
H	7.43221500	-1.74808800	-2.66336700
H	6.14458400	0.24872300	-1.96800600
C	5.50337900	2.24212400	0.76368500
C	5.34711800	0.91711800	0.33291000
C	6.43186200	-0.10954700	0.61056100
C	7.80772700	0.51708800	0.82125700
C	7.71997500	1.63743900	1.85361100
C	6.81403200	2.75073200	1.33412000
H	6.14157200	-0.64958600	1.52319300
H	8.51807100	-0.25248300	1.13766800
H	7.31085300	1.23236100	2.78754400
H	7.34323900	3.30033100	0.54360000
P	0.95734900	0.02153500	0.08936300
O	2.04433500	-1.02988100	0.63759000
O	1.84783100	1.02683000	-0.80837900
O	0.59169500	0.77380000	1.40874600
O	-0.14882700	-0.52706300	-0.71897300
C	2.03363900	3.70621200	0.14602600
C	1.45543200	-3.68698900	-0.17996900
C	1.66688000	4.31322000	-1.06752300
C	0.61343000	5.23231500	-1.07326300
H	0.32248400	5.70000200	-2.01227700
C	0.29041900	4.93739500	1.27480600
H	-0.25489600	5.16953600	2.18624900
C	1.33491400	4.01482400	1.33421000
C	0.40638800	-4.08359100	-1.03561900
C	-0.63736800	-4.85222400	-0.51450900

H	-1.43567900	-5.16481300	-1.18346800
C	-0.08805500	5.55685400	0.08238600
C	-0.68507700	-5.22573600	0.82613600
C	1.41833400	-4.03655700	1.18485700
C	0.35285900	-4.80447800	1.65408000
H	0.33125300	-5.09384300	2.70396100
H	4.74192600	-4.04174500	-3.92126700
H	5.36772100	-1.89523900	-4.91516700
H	7.34068200	-0.60617000	-4.00359000
H	5.09792800	0.10343800	-3.35505400
H	6.47113300	-0.86632900	-0.17486200
H	8.17731400	0.92507900	-0.12941800
H	8.71068400	2.04029600	2.08400200
H	6.60413200	3.47887200	2.12454800
C	2.50872600	-3.64376400	2.17109700
H	3.24111600	-3.01961400	1.65344800
C	3.25098500	-4.88317600	2.68614300
H	2.57480300	-5.54735200	3.23410200
H	3.68371700	-5.45250500	1.85882500
H	4.05836800	-4.59221500	3.36518600
C	1.94127900	-2.82001900	3.33348000
H	2.75042200	-2.46700500	3.98035100
H	1.39196300	-1.94984300	2.96265000
H	1.26655900	-3.42381900	3.95137000
C	-1.77499100	-6.12736200	1.37664700
H	-1.78581000	-5.98883400	2.46635700
C	-1.42844700	-7.59495200	1.09035200
H	-0.44899900	-7.85425000	1.50090300
H	-2.17688300	-8.26572500	1.52348900
H	-1.39663900	-7.76975500	0.00971600
C	-3.17214300	-5.79587200	0.84898300
H	-3.43722300	-4.75176100	1.03700700
H	-3.24468400	-5.97190600	-0.22911000
H	-3.91932000	-6.43105600	1.33358600
C	0.35852700	-3.71573200	-2.51324400
H	1.16104400	-3.00123100	-2.71508900
C	-0.95733000	-3.02548100	-2.88838600
H	-0.94031800	-2.72564500	-3.94077000
H	-1.82202400	-3.68335800	-2.74955700
H	-1.09794800	-2.13356000	-2.27673600
C	0.58718400	-4.95332500	-3.39046000
H	1.53831200	-5.44271500	-3.16111900
H	-0.20876200	-5.68919900	-3.23390900
H	0.58742900	-4.67901100	-4.44982500

C	1.69490400	3.38391000	2.67263900
H	2.19895000	2.43492800	2.46762700
C	0.46358400	3.07862000	3.53580800
H	0.06298800	3.98652300	3.99883000
H	-0.34252800	2.61961800	2.95850400
H	0.73662000	2.39664700	4.34603300
C	2.65353900	4.28691700	3.46207900
H	2.19433300	5.26608700	3.63530700
H	2.88185400	3.84164200	4.43555700
H	3.59523500	4.44502900	2.93157800
C	2.37389400	4.00312500	-2.37836000
H	3.20291900	3.32084700	-2.16830300
C	1.42879300	3.29550100	-3.35629100
H	1.94712200	3.06576000	-4.29254000
H	1.06041800	2.36020400	-2.92706800
H	0.56847400	3.92988300	-3.59673200
C	2.97028500	5.26891200	-3.00472000
H	3.52873600	5.01810900	-3.91159000
H	2.18761600	5.98170000	-3.28307700
H	3.64888000	5.76969100	-2.30869600
C	-1.26118200	6.51753200	0.04587900
H	-1.32790300	6.91284400	-0.97564100
C	-1.05642300	7.70076300	0.99763500
H	-0.12239300	8.22528800	0.78022000
H	-1.88277100	8.41217600	0.90922600
H	-1.01911600	7.36311400	2.03827800
C	-2.57366900	5.78763600	0.35927700
H	-2.76380100	4.97960100	-0.35325900
H	-2.54084900	5.34880900	1.36243200
H	-3.42003600	6.48015100	0.32310400

B_3'

Zero-point correction= 1.513668 (Hartree/Particle)
Thermal correction to Energy= 1.598027
Thermal correction to Enthalpy= 1.598971
Thermal correction to Gibbs Free Energy= 1.393205
Sum of electronic and zero-point Energies= -3882.668259
Sum of electronic and thermal Energies= -3882.583900
Sum of electronic and thermal Enthalpies= -3882.582956
Sum of electronic and thermal Free Energies= -3882.788722
SCF Done: E(RM062X) = -3885.13143758

H	0.51016000	-0.93941300	-1.61810900

C	1.47375800	-4.23526900	1.71172800
N	1.57171400	-2.78190700	1.68330100
H	0.72564800	-2.32193900	1.34220200
C	2.09669400	-2.12069100	2.80326200
C	1.59298200	-0.85775400	3.15653700
C	3.15614300	-2.66701100	3.54125700
C	2.13436800	-0.17311200	4.23864100
H	0.77457000	-0.43976500	2.57630900
C	3.69478300	-1.96206800	4.61208600
H	3.56928600	-3.63245600	3.26850000
C	3.18767500	-0.71610400	4.97189900
H	1.72798800	0.79834400	4.50512400
H	4.52250700	-2.39242800	5.16702600
H	3.60981700	-0.17486700	5.81196600
C	3.47849200	-3.46773400	-0.61735400
C	2.93120100	-1.25499200	0.01322200
C	2.42117300	-2.45182500	-0.77421300
O	2.36877100	-0.20031900	0.17712300
N	4.44672800	-2.96627500	0.07877200
N	4.16324300	-1.68480800	0.48075900
C	5.12864500	-0.96650200	1.22630000
C	4.73613900	0.12684600	1.99472800
C	6.46631400	-1.36340400	1.17401500
C	5.70222300	0.83080600	2.70697000
H	3.69350800	0.41442100	2.03100400
C	7.41605600	-0.64781400	1.89324900
H	6.74607900	-2.22059100	0.57362100
C	7.04153300	0.45488700	2.65891300
H	5.39396900	1.67738300	3.31411300
H	8.45631100	-0.95387400	1.85002800
H	7.78715400	1.01041400	3.21777000
C	3.58179100	-4.84209700	-1.18773000
H	4.58075000	-5.22730800	-0.97931600
H	2.82511100	-5.50107000	-0.75851700
H	3.41674200	-4.82918400	-2.26852000
N	1.35640400	-2.33162000	-1.46920200
C	0.72465800	-3.43168100	-2.09288000
O	0.73972400	-4.56703600	-1.67381400
O	0.06050600	-2.97162000	-3.14029100
C	-0.85080900	-3.83599900	-3.89254400
C	-1.45318000	-2.87356200	-4.90768500
H	-1.97410800	-2.06123800	-4.39469700
H	-0.66930400	-2.44445000	-5.53696100
H	-2.16469600	-3.40537100	-5.54433400

C	-1.92547100	-4.38953100	-2.96158500
H	-2.71078800	-4.85422300	-3.56558200
H	-1.51794500	-5.13916000	-2.28350700
H	-2.37728200	-3.58358500	-2.37354100
C	-0.05387400	-4.93800200	-4.58173000
H	0.38988500	-5.61654600	-3.85212000
H	-0.72083800	-5.51013800	-5.23242200
H	0.73608800	-4.50119200	-5.19910800
H	0.93960200	-4.56185600	0.81626200
H	2.47104400	-4.68590000	1.68814000
H	0.95158700	-4.59797800	2.60678500
C	-2.78789800	2.46616700	0.50844400
C	-4.65562000	1.09225700	2.04023300
C	-3.91908200	0.37102500	1.10526600
C	-3.00403700	1.09891700	0.34748300
H	-5.41139100	0.56825100	2.62002000
C	0.15102400	4.35810400	-1.93749800
C	0.50515700	3.22141500	-1.21756200
C	-0.50202400	2.62915300	-0.45331400
C	-1.80313000	3.13326600	-0.39375500
H	0.92531800	4.87385000	-2.50036000
C	-3.46168800	3.14149800	1.54601500
C	-4.42888100	2.44852500	2.28887700
C	-5.25581100	3.13481700	3.35992900
C	-4.61562700	4.41626500	3.88779500
C	-4.15292600	5.28418400	2.72072300
C	-3.07008900	4.55857900	1.92625000
H	-6.23925900	3.37794300	2.93462000
H	-5.32661200	4.95442100	4.52184400
H	-5.00844900	5.50102300	2.06655900
H	-2.78397500	5.13798000	1.04621000
C	-1.15727700	4.84543100	-1.98082600
C	-2.15598100	4.21574000	-1.22609500
C	-3.61043700	4.62341700	-1.38789700
C	-3.77686600	6.03902800	-1.93467100
C	-2.92290900	6.22053500	-3.18638500
C	-1.44606200	6.06733800	-2.83231700
H	-4.07165500	3.91322000	-2.08907200
H	-4.83270400	6.22935000	-2.14959700
H	-3.20690200	5.46178300	-3.92638400
H	-1.11865600	6.95882400	-2.27984400
P	-0.74226100	0.08157700	-0.22745800
O	-2.26919900	0.43190800	-0.62375900
O	-0.18997800	1.50294400	0.30577800

O	-0.15911700	-0.17993600	-1.65175000
O	-0.58052800	-0.97304900	0.79408900
C	1.90802600	2.70298500	-1.22215700
C	-4.06948000	-1.10716300	0.94825700
C	2.74675000	2.98342700	-0.12835500
C	4.06471600	2.53215400	-0.15596700
H	4.71714300	2.73361700	0.69229100
C	3.72373000	1.53076600	-2.29697800
H	4.09863000	0.96090900	-3.14285900
C	2.39724700	1.96873500	-2.31888700
C	-3.65176700	-1.95946800	1.98959900
C	-3.89111800	-3.32996200	1.87016700
H	-3.59192700	-3.99174600	2.67982600
C	4.57306300	1.79730500	-1.22467400
C	-4.48643100	-3.88388500	0.74179800
C	-4.63239300	-1.64942700	-0.22398300
C	-4.82666600	-3.02820300	-0.30505800
H	-5.26844100	-3.44388800	-1.20945700
H	-5.44202000	2.43067600	4.17770400
H	-3.74955000	4.16667700	4.51348200
H	-3.76875500	6.24526800	3.07550500
H	-2.16046400	4.49077300	2.54013400
H	-4.16042000	4.50634200	-0.45222100
H	-3.46679400	6.76797900	-1.17351500
H	-3.09739700	7.19864600	-3.64468200
H	-0.83316700	6.02767400	-3.73887800
C	-5.04829700	-0.78817400	-1.40749800
H	-4.83377400	0.25696500	-1.16835300
C	-6.55461800	-0.89746700	-1.67238700
H	-6.83420400	-1.91926800	-1.94898300
H	-7.12960400	-0.62127600	-0.78425600
H	-6.84854400	-0.23663200	-2.49368700
C	-4.24016700	-1.14800500	-2.66051800
H	-4.50853700	-0.48838700	-3.49213400
H	-3.16870100	-1.04179800	-2.46786000
H	-4.44122400	-2.17883700	-2.97541400
C	-4.74021000	-5.37637100	0.64817600
H	-4.43508900	-5.81840800	1.60497900
C	-3.89248900	-6.01463000	-0.45694100
H	-2.82891500	-5.82010200	-0.29422100
H	-4.04774800	-7.09746100	-0.49194600
H	-4.16386500	-5.60362000	-1.43567100
C	-6.22708000	-5.68286900	0.43966900
H	-6.83534800	-5.23960100	1.23221100

H	-6.57675100	-5.28034500	-0.51664200
H	-6.40153800	-6.76312200	0.43092400
C	-2.92939200	-1.44714800	3.22917400
H	-2.58173900	-0.43107400	3.01811400
C	-1.68951200	-2.28810100	3.55930500
H	-1.09889000	-1.79666600	4.33847800
H	-1.96239300	-3.28124200	3.93176100
H	-1.06029300	-2.40262400	2.67472100
C	-3.86590200	-1.40213800	4.44342100
H	-4.72318000	-0.74530800	4.27482100
H	-4.25115900	-2.40384300	4.66323800
H	-3.32988100	-1.04489300	5.32827200
C	1.53150200	1.66669500	-3.53431200
H	0.48511600	1.72234000	-3.22075700
C	1.76666000	0.26128200	-4.10048300
H	2.71227700	0.20409700	-4.65069500
H	1.78696100	-0.49546400	-3.31328600
H	0.96541100	0.00197900	-4.79872800
C	1.76541200	2.70497100	-4.64072400
H	2.81833700	2.70541200	-4.94296100
H	1.15801400	2.47245000	-5.52152600
H	1.51108600	3.71446600	-4.30924400
C	2.25314500	3.73556900	1.09756500
H	1.22628000	4.06313400	0.91114100
C	2.22794400	2.80768300	2.31739300
H	1.75011100	3.30089600	3.17095600
H	1.68433000	1.88677200	2.08676900
H	3.24756800	2.53794800	2.61708400
C	3.08929300	4.98974300	1.37238700
H	2.68935900	5.53502200	2.23303600
H	4.12921000	4.73102300	1.59659200
H	3.08863900	5.66031700	0.50849600
C	6.02693700	1.36103400	-1.21027600
H	6.31206900	1.22551500	-0.15827500
C	6.91255900	2.46708000	-1.80041400
H	6.78307800	3.40573800	-1.25493900
H	7.96952800	2.18510200	-1.75946600
H	6.64545200	2.64727600	-2.84732000
C	6.27537700	0.03783600	-1.93703700
H	5.58498000	-0.74245100	-1.60027900
H	6.16005400	0.15001100	-3.02048700
H	7.29616700	-0.30798100	-1.74872200

TS-A_3

Zero-point correction= 1.510022 (Hartree/Particle)
Thermal correction to Energy= 1.593681
Thermal correction to Enthalpy= 1.594626
Thermal correction to Gibbs Free Energy= 1.388633
Sum of electronic and zero-point Energies= -3882.666376
Sum of electronic and thermal Energies= -3882.582717
Sum of electronic and thermal Enthalpies= -3882.581772
Sum of electronic and thermal Free Energies= -3882.787765
SCF Done: E(RM062X) = -3885.12811683
Number of Imaginary Frequencies = -453.70

H	0.94816500	-0.89831400	1.20663400
C	2.59356600	1.87264200	0.60811200
N	2.70784900	1.00043100	-0.56143700
H	1.75427300	0.83738900	-0.92757000
C	3.62560600	1.34886000	-1.57968000
C	3.35072500	0.93710100	-2.88945600
C	4.81754000	2.02191900	-1.29262000
C	4.26407900	1.20025100	-3.90262400
H	2.41208100	0.43063800	-3.10051600
C	5.72814000	2.26591600	-2.31534600
H	5.04169800	2.32824900	-0.27711800
C	5.45869500	1.85869700	-3.61910300
H	4.04209600	0.88360200	-4.91648200
H	6.66049400	2.77114700	-2.08609900
H	6.17816100	2.04805900	-4.40828000
C	2.71036900	-1.66715600	-0.95309700
C	4.45332000	-0.68797700	0.31042800
C	2.95250400	-0.93797000	0.30927400
O	5.09299100	-0.01729000	1.09071300
N	3.81728300	-1.84799400	-1.58123700
N	4.86532800	-1.26733200	-0.86791200
C	6.11750700	-1.11276700	-1.51264200
C	7.22301800	-0.62820000	-0.80728700
C	6.22635100	-1.43273600	-2.86764500
C	8.42704200	-0.44723500	-1.47995500
H	7.13480200	-0.38743200	0.24267300
C	7.44100900	-1.25031600	-3.51719900
H	5.35912100	-1.80426500	-3.39754500
C	8.54542700	-0.75124500	-2.83272700
H	9.28249600	-0.06705500	-0.93086300
H	7.51842400	-1.49731900	-4.57125100
H	9.49005900	-0.60745300	-3.34637200

C	1.39973500	-2.18482500	-1.42689500
H	0.81699900	-2.58397100	-0.58884700
H	0.81525000	-1.37864400	-1.88352700
H	1.55732400	-2.97446500	-2.16273500
N	2.16005500	-0.97231000	1.35145300
C	2.66688600	-0.79949800	2.66628100
O	3.63289800	-1.37529000	3.09196100
O	1.84940400	0.01824000	3.32300500
C	2.11834100	0.36142500	4.71889000
C	0.95680800	1.28553400	5.05906800
H	0.93520400	2.13742900	4.37234300
H	0.00770200	0.75027300	4.97078700
H	1.06256700	1.65562700	6.08216700
C	3.45083200	1.09877800	4.80446300
H	3.61206600	1.43376400	5.83284200
H	4.27855800	0.45364200	4.50778200
H	3.43331700	1.97973500	4.15582300
C	2.08822600	-0.89277000	5.58650600
H	2.93325500	-1.54622000	5.37073500
H	2.12822700	-0.59721200	6.63881300
H	1.15650500	-1.44051700	5.41854900
H	2.45119900	2.91015000	0.28840800
H	1.71713400	1.56532100	1.18247000
H	3.48798900	1.78689500	1.23300600
C	-3.86697700	0.77253500	-0.98931200
C	-3.53106800	3.48787500	-1.49494000
C	-2.68676800	2.88661900	-0.56716900
C	-2.88363700	1.52297300	-0.34563900
H	-3.42933600	4.55575300	-1.67636300
C	-4.32005200	-3.29217300	0.25337300
C	-3.05663500	-2.83514600	-0.10700300
C	-2.96675900	-1.51261500	-0.54629900
C	-4.06324200	-0.64440100	-0.55573500
H	-4.43143500	-4.33525400	0.54054500
C	-4.62250700	1.38595800	-2.00969800
C	-4.46700600	2.76087400	-2.23700000
C	-5.31282600	3.50247000	-3.25571400
C	-5.94314000	2.58686300	-4.30233700
C	-6.58381800	1.38045000	-3.62109100
C	-5.51303800	0.55332600	-2.91465800
H	-6.11238400	4.03200700	-2.71951200
H	-6.67816500	3.14436400	-4.89065600
H	-7.32731700	1.72633700	-2.88985700
H	-5.96243000	-0.27742000	-2.36661000

C	-5.43417300	-2.45243600	0.30214000
C	-5.29999800	-1.10235700	-0.05378400
C	-6.43754800	-0.13106500	0.21620000
C	-7.80095900	-0.81179200	0.30552300
C	-7.73758500	-1.98984100	1.27311000
C	-6.76139900	-3.03810600	0.74618300
H	-6.22067500	0.36041200	1.17575100
H	-8.55466700	-0.08457400	0.62233800
H	-7.40093400	-1.63029300	2.25356500
H	-7.21874500	-3.54838000	-0.11273200
P	-0.88580800	-0.01639100	-0.08646400
O	-2.06347800	0.88277100	0.57128100
O	-1.74407400	-1.04858800	-1.00700100
O	-0.28617400	-0.75107100	1.10321900
O	0.01891800	0.73879400	-0.99997700
C	-1.83605900	-3.69386500	0.00608500
C	-1.61020100	3.63211500	0.15294000
C	-1.36975600	-4.41275800	-1.10556000
C	-0.20196300	-5.17274000	-0.97966500
H	0.17197200	-5.72252200	-1.84153800
C	0.02183500	-4.51481500	1.30884100
H	0.57006300	-4.54866400	2.24605700
C	-1.14749300	-3.75985600	1.23921500
C	-0.54631200	4.21508700	-0.56956500
C	0.43030500	4.93052200	0.12558400
H	1.24010700	5.39099800	-0.43785900
C	0.51489500	-5.22418100	0.21067000
C	0.40293600	5.07082500	1.51225500
C	-1.64916100	3.74996600	1.55682200
C	-0.63997500	4.46520300	2.20513000
H	-0.67745600	4.56712000	3.28828600
H	-4.70409300	4.27562000	-3.73620600
H	-5.17188800	2.23508200	-4.99896800
H	-7.11387300	0.75672900	-4.34714500
H	-4.86473500	0.08891300	-3.67106900
H	-6.46074200	0.67208400	-0.52150100
H	-8.09935400	-1.17215200	-0.68845800
H	-8.72570600	-2.43759000	1.41567500
H	-6.58014300	-3.81126800	1.50015900
C	-2.76760300	3.16694700	2.40862600
H	-3.44683900	2.60796800	1.76133700
C	-3.58638400	4.28512400	3.06638200
H	-2.96688700	4.87927200	3.74607300
H	-4.00318200	4.96087300	2.31429600

H	-4.41231500	3.86346100	3.64763700
C	-2.22330400	2.19276100	3.45985000
H	-3.04945100	1.70528900	3.98733100
H	-1.60487900	1.42094300	2.99353900
H	-1.62070000	2.71965800	4.20812200
C	1.47324700	5.85692200	2.24600900
H	1.19204600	5.87490600	3.30659200
C	1.54747600	7.30590900	1.75321900
H	0.57678100	7.80057000	1.83960800
H	2.28009400	7.87430900	2.33410200
H	1.85226500	7.34505400	0.70248100
C	2.84189700	5.17584000	2.13646200
H	2.80083900	4.15107300	2.51854000
H	3.17270400	5.13501300	1.09233200
H	3.59779300	5.72591000	2.70525800
C	-0.41295800	4.10282800	-2.08261800
H	-1.16410200	3.39433900	-2.44055400
C	0.95220200	3.54076600	-2.49144900
H	1.00915100	3.43088700	-3.57915600
H	1.77897800	4.19085300	-2.18422300
H	1.09030400	2.55743200	-2.04169000
C	-0.66527800	5.45847200	-2.75434400
H	-1.64836000	5.86183300	-2.49441000
H	0.08531300	6.19159900	-2.43961700
H	-0.60815800	5.36506000	-3.84322800
C	-1.69186400	-3.08337200	2.49130700
H	-2.22117700	-2.17745400	2.17790500
C	-0.61212800	-2.65975500	3.49115900
H	-0.16242700	-3.52432600	3.99216300
H	0.17541800	-2.07713000	3.01204400
H	-1.06623800	-2.03518800	4.26754700
C	-2.68512700	-4.01544500	3.20291300
H	-2.18399800	-4.94445300	3.49551100
H	-3.07442700	-3.53846700	4.10803900
H	-3.53205100	-4.27494700	2.56502800
C	-2.08453900	-4.35692800	-2.44682400
H	-3.05578800	-3.87779100	-2.28893500
C	-1.29805200	-3.49469700	-3.44151700
H	-1.82895700	-3.42442700	-4.39628500
H	-1.15267000	-2.48473300	-3.04808800
H	-0.31389300	-3.93658500	-3.63632700
C	-2.34838900	-5.75274600	-3.02070200
H	-2.94566900	-5.67834900	-3.93437900
H	-1.41577200	-6.26368700	-3.27971700

H	-2.88817800	-6.37933400	-2.30554400
C	1.82649100	-5.98134600	0.30196900
H	1.90385500	-6.60866700	-0.59521100
C	1.89003200	-6.90144600	1.52477000
H	1.02999600	-7.57532000	1.55902900
H	2.80235700	-7.50439000	1.49945000
H	1.90536700	-6.32389800	2.45423900
C	3.00785800	-5.00112200	0.29611000
H	3.03982100	-4.42766700	-0.63469400
H	2.92603400	-4.29170100	1.12878800
H	3.95807600	-5.53428400	0.39876800

TS-A_3'

Zero-point correction= 1.513346 (Hartree/Particle)
Thermal correction to Energy= 1.596408
Thermal correction to Enthalpy= 1.597353
Thermal correction to Gibbs Free Energy= 1.395307
Sum of electronic and zero-point Energies= -3882.664911
Sum of electronic and thermal Energies= -3882.581849
Sum of electronic and thermal Enthalpies= -3882.580905
Sum of electronic and thermal Free Energies= -3882.782950
SCF Done: E(RM062X) = -3885.12734605
Number of Imaginary Frequencies = -99.41

H	0.70912200	0.68792700	1.57963800
C	1.10232800	3.94139300	-0.75153700
N	1.73832700	2.65217900	-1.05208400
H	0.99715900	1.92726100	-1.03761100
C	2.49942900	2.55260800	-2.24765900
C	2.30495000	1.43394900	-3.06610600
C	3.48147900	3.49365900	-2.56166300
C	3.09771400	1.26253100	-4.19337900
H	1.53545400	0.71298800	-2.79788400
C	4.26579600	3.31086800	-3.69683800
H	3.64200100	4.35216200	-1.91660500
C	4.08054600	2.19814100	-4.51211300
H	2.95055800	0.38956800	-4.82108400
H	5.03243700	4.03977300	-3.93782000
H	4.70121300	2.05835300	-5.39047200
C	3.92090300	2.70300400	0.59783600
C	2.98303000	0.63922300	-0.08371600
C	2.64479700	1.92113400	0.67280500
O	2.24279200	-0.29552800	-0.28932100

N	4.79609600	2.04282600	-0.07717200
N	4.27245900	0.83557000	-0.51349200
C	5.07808200	-0.01140500	-1.30926200
C	4.49180200	-1.01757200	-2.07859900
C	6.46279400	0.17012500	-1.30786100
C	5.30927200	-1.84390600	-2.84393500
H	3.41948300	-1.15981600	-2.05597100
C	7.26109200	-0.66730400	-2.07749900
H	6.89432000	0.96038700	-0.70629100
C	6.69124300	-1.67874300	-2.84804100
H	4.85387400	-2.62854400	-3.44160800
H	8.33720700	-0.52758400	-2.07098000
H	7.31916600	-2.33096500	-3.44558500
C	4.29674700	4.02698800	1.17514500
H	5.32153500	4.24673900	0.87195400
H	3.62215500	4.81541700	0.83790400
H	4.22406700	4.01194100	2.26417100
N	1.71747600	1.81508500	1.59646000
C	1.39620100	2.87251800	2.44211100
O	1.73321800	4.03359600	2.30712000
O	0.61080400	2.40124400	3.41060600
C	-0.04181500	3.31058200	4.34378600
C	-0.90320700	2.37045500	5.17843300
H	-1.61091500	1.83637400	4.53997300
H	-0.27478000	1.63772700	5.69096000
H	-1.45940400	2.94149900	5.92639700
C	-0.91060700	4.30409500	3.57536100
H	-1.58670600	4.80818700	4.27293000
H	-0.30329800	5.05542700	3.07038700
H	-1.51657300	3.77584100	2.83071200
C	1.00111800	4.00399500	5.21487400
H	1.62503800	4.67300700	4.62216200
H	0.49360100	4.58588900	5.98961700
H	1.63342300	3.25816800	5.70479900
H	0.46188000	3.80669600	0.12015800
H	1.84710000	4.70549900	-0.52758700
H	0.48463800	4.25853500	-1.59869500
C	-3.29110700	-1.90558600	-0.67355600
C	-4.77665700	-0.04738600	-2.11760600
C	-3.88718000	0.42896900	-1.15967400
C	-3.17889000	-0.53555300	-0.44314900
H	-5.37866500	0.66903300	-2.67127600
C	-0.83065800	-4.54304700	1.61599100
C	-0.24008100	-3.46881000	0.95888900

C	-1.09575600	-2.63143100	0.24142700
C	-2.47712600	-2.82872000	0.17408500
H	-0.18828000	-5.24819400	2.13775800
C	-4.10976400	-2.34677600	-1.73298900
C	-4.88579100	-1.40625700	-2.42723300
C	-5.85904800	-1.82242400	-3.51450800
C	-5.54366000	-3.18925900	-4.11679600
C	-5.29223400	-4.20167800	-3.00267800
C	-4.06442700	-3.79345700	-2.19278200
H	-6.86891300	-1.84967600	-3.08245200
H	-6.36570200	-3.51057400	-4.76350500
H	-6.17103400	-4.24526600	-2.34495200
H	-3.91537500	-4.47089900	-1.34979400
C	-2.21474100	-4.73304900	1.64969400
C	-3.05442600	-3.85375800	0.95197800
C	-4.56157100	-3.93728900	1.12308100
C	-5.03501200	-5.31424400	1.58135200
C	-4.23532800	-5.76152900	2.80184000
C	-2.76252600	-5.91323300	2.43027600
H	-4.84443300	-3.19273100	1.88091900
H	-6.10554200	-5.28075200	1.80529100
H	-4.34161000	-5.00958100	3.59378600
H	-2.64194900	-6.81789100	1.81844400
P	-0.74496600	-0.08723100	0.14106900
O	-2.31012200	-0.11232800	0.55058000
O	-0.53691500	-1.57106200	-0.46302500
O	-0.09473400	0.00987000	1.54166700
O	-0.40816600	0.92491300	-0.89013700
C	1.23807000	-3.23638700	0.97470100
C	-3.63586200	1.88523700	-0.93334300
C	2.00432600	-3.59663800	-0.14820400
C	3.38291800	-3.39411100	-0.11834900
H	3.98229300	-3.66649300	-0.98599100
C	3.24240400	-2.46313600	2.07548100
H	3.71825500	-2.01015900	2.94047900
C	1.85961700	-2.66009300	2.09908000
C	-3.01801600	2.65048500	-1.94286800
C	-2.80211400	4.01185200	-1.71691800
H	-2.34397300	4.61202400	-2.50040800
C	4.02285900	-2.81913600	0.97737600
C	-3.14495500	4.63069800	-0.51928000
C	-3.97365100	2.48660100	0.29592400
C	-3.72037700	3.84602800	0.47926600
H	-3.99124100	4.30664000	1.42821100

H	-5.88066100	-1.05279500	-4.29325500
H	-4.64687600	-3.11880200	-4.74510200
H	-5.14734900	-5.20615300	-3.41160500
H	-3.16859200	-3.90639300	-2.82018100
H	-5.08062300	-3.63527600	0.21144300
H	-4.89826300	-6.04151800	0.76938400
H	-4.61863700	-6.70562800	3.20060000
H	-2.15224100	-6.06714400	3.32633000
C	-4.62866100	1.71435600	1.43143300
H	-4.71324600	0.66602800	1.13402000
C	-6.04797100	2.23176200	1.69587100
H	-6.03105700	3.27938300	2.01407100
H	-6.66403300	2.16470800	0.79486400
H	-6.52835300	1.64821000	2.48733200
C	-3.77766700	1.76418200	2.70551500
H	-4.21343000	1.12569000	3.48089700
H	-2.76087400	1.41598600	2.50214900
H	-3.72775600	2.78273300	3.10802300
C	-2.91411700	6.11622100	-0.31717700
H	-2.41301300	6.49233000	-1.21838900
C	-2.00136700	6.39451900	0.88098300
H	-1.04636000	5.86965600	0.78380800
H	-1.79946600	7.46612100	0.97324000
H	-2.47073700	6.06239700	1.81326100
C	-4.24417400	6.86404000	-0.16904600
H	-4.89126400	6.68962400	-1.03247500
H	-4.77834000	6.52461100	0.72457600
H	-4.07612300	7.94105300	-0.07201600
C	-2.56510300	2.05375800	-3.26875500
H	-2.55923100	0.96517100	-3.16387400
C	-1.13816900	2.47669000	-3.63622500
H	-0.79399700	1.91956300	-4.51334100
H	-1.07871600	3.54162200	-3.88595100
H	-0.45984300	2.26529600	-2.80834700
C	-3.53181300	2.43099200	-4.39897900
H	-4.55107900	2.09357500	-4.19328200
H	-3.56222800	3.51865500	-4.52635700
H	-3.20847900	1.98871400	-5.34656500
C	1.07018300	-2.27351500	3.34203200
H	0.03660400	-2.08895700	3.03434900
C	1.58621000	-0.99237700	4.00684400
H	2.52055600	-1.17263900	4.55021700
H	1.75988000	-0.19723500	3.27930700
H	0.85139600	-0.63157400	4.73247500

C	1.07973700	-3.41591900	4.36790200
H	2.10884700	-3.65254900	4.65959800
H	0.52838300	-3.12756100	5.26884600
H	0.62647000	-4.32613100	3.96861100
C	1.37425300	-4.17175000	-1.40714800
H	0.30128300	-4.29226400	-1.23202100
C	1.54312800	-3.20385700	-2.58426800
H	0.99047200	-3.55818500	-3.46040500
H	1.17920900	-2.20786100	-2.31437100
H	2.59966900	-3.12697900	-2.86678800
C	1.94136300	-5.55483100	-1.74402300
H	1.44843400	-5.96673400	-2.63028600
H	3.01466300	-5.50122700	-1.95387100
H	1.79647100	-6.25130700	-0.91352100
C	5.53130600	-2.64569800	0.96239200
H	5.82976100	-2.50047700	-0.08471900
C	6.21112100	-3.92341500	1.47352300
H	5.91385600	-4.79116900	0.87843000
H	7.30106300	-3.83029600	1.43105100
H	5.92312600	-4.11445200	2.51289900
C	6.01554200	-1.43172600	1.75801600
H	5.47139700	-0.52380900	1.47872800
H	5.89011500	-1.58493500	2.83523400
H	7.08019900	-1.26169800	1.57174200

TS-P_3

Zero-point correction= 1.515441 (Hartree/Particle)
Thermal correction to Energy= 1.598145
Thermal correction to Enthalpy= 1.599089
Thermal correction to Gibbs Free Energy= 1.399838
Sum of electronic and zero-point Energies= -3882.638811
Sum of electronic and thermal Energies= -3882.556107
Sum of electronic and thermal Enthalpies= -3882.555163
Sum of electronic and thermal Free Energies= -3882.754413
SCF Done: E(RM062X) = -3885.10564860
Number of Imaginary Frequencies = -200.84

H	1.64363400	-1.48014700	0.94953500
C	2.56528500	3.24635600	-2.47016400
N	2.18520900	2.40850500	-1.34699400
H	1.24073000	1.98507800	-1.31404800
C	2.93330700	2.23589100	-0.27050100
C	2.49924600	1.26208400	0.70171600

C	4.18496300	2.90466400	-0.06645900
C	3.17494300	1.19452300	1.95596700
H	1.46716300	0.93008500	0.64802100
C	4.86110500	2.70266000	1.10037800
H	4.58036400	3.56495000	-0.82954700
C	4.34755400	1.86260200	2.14238900
H	2.76775500	0.53868600	2.71991700
H	5.81173300	3.20469700	1.25239600
H	4.90033400	1.77243300	3.07049200
C	2.54873900	-0.55655500	-1.53119900
C	4.52600300	-0.15733100	-0.34662900
C	3.09922800	-0.64363700	-0.19346500
O	5.41708400	-0.10271400	0.46557600
N	3.39906700	0.01567800	-2.33667900
N	4.54327800	0.32377300	-1.66571600
C	5.61188700	0.94221700	-2.35978300
C	6.77696600	1.32873700	-1.68902700
C	5.47212500	1.18808900	-3.72997000
C	7.79051200	1.96110500	-2.40322200
H	6.88693300	1.12668500	-0.63313200
C	6.49637700	1.82485800	-4.42028500
H	4.56665600	0.87625300	-4.23504400
C	7.66058800	2.21637300	-3.76442700
H	8.69463800	2.25472800	-1.87962400
H	6.38039400	2.01016800	-5.48321700
H	8.45750700	2.71080900	-4.30905200
C	1.26622400	-1.11950400	-2.03829000
H	0.80070400	-1.76281800	-1.28889600
H	0.56217200	-0.32379400	-2.29169000
H	1.46755600	-1.71330000	-2.93192900
N	2.65811900	-1.50844200	0.75911000
C	3.53353400	-2.18463800	1.61710200
O	4.59738600	-2.62746600	1.25982400
O	2.99378000	-2.26984100	2.83181700
C	3.72071600	-2.94883600	3.90529300
C	2.76668200	-2.83492100	5.08771400
H	2.53022100	-1.78599800	5.28439800
H	1.83518800	-3.36877300	4.88689800
H	3.23373000	-3.26262600	5.97850400
C	5.01805000	-2.19536200	4.18455800
H	5.51483200	-2.64335400	5.04963400
H	5.69074300	-2.23448500	3.32771400
H	4.79736900	-1.14967000	4.41964700
C	3.96298200	-4.41020700	3.54040500

H	4.70170400	-4.50597500	2.74460600
H	4.32428800	-4.94280500	4.42470300
H	3.02634100	-4.87919500	3.22102400
H	3.56151300	2.97208800	-2.82814700
H	1.84606000	3.09014900	-3.27232100
H	2.55715300	4.30569200	-2.19109000
C	-4.17989800	0.48591800	-0.34045000
C	-4.45911500	3.24795500	-0.22832100
C	-3.32675600	2.67916600	0.34509500
C	-3.22958100	1.28600600	0.29649700
H	-4.58151400	4.32805600	-0.17451000
C	-3.71469000	-3.75660400	-0.24578300
C	-2.62201200	-2.96974400	-0.59059700
C	-2.81102400	-1.58403000	-0.62902200
C	-4.02846800	-0.99641400	-0.26196300
H	-3.60355900	-4.83821100	-0.27015200
C	-5.23519000	1.10724100	-1.04264100
C	-5.39774400	2.49536800	-0.93789000
C	-6.57579500	3.21616500	-1.56683900
C	-7.23646900	2.42866100	-2.69553500
C	-7.46301500	0.98428300	-2.25741800
C	-6.12342600	0.30707500	-1.98030900
H	-7.32249900	3.40543700	-0.78322600
H	-8.17782800	2.90686200	-2.98317000
H	-8.07986800	0.97093500	-1.34807300
H	-6.27426000	-0.70936400	-1.61324000
C	-4.92236300	-3.20881600	0.18798800
C	-5.06551600	-1.81573700	0.23771700
C	-6.27803600	-1.20860500	0.92571700
C	-7.48185500	-2.14645000	0.95954500
C	-7.07090800	-3.50669700	1.51540500
C	-6.04051700	-4.15137000	0.59250100
H	-5.97919700	-0.97695600	1.95816700
H	-8.27853500	-1.70124800	1.56345500
H	-6.63806700	-3.36805500	2.51409100
H	-6.54829100	-4.49619400	-0.31897200
P	-0.93372100	0.15850200	-0.02133600
O	-2.16409000	0.67440100	0.92429700
O	-1.77573700	-0.78591600	-1.07655500
O	-0.03789700	-0.65474000	0.86532700
O	-0.34914800	1.27453100	-0.83734500
C	-1.26866200	-3.56479200	-0.80927000
C	-2.21062700	3.50576500	0.88914900
C	-0.81732300	-3.88742100	-2.09980500

C	0.47348200	-4.39551100	-2.25092000
H	0.83663800	-4.64368400	-3.24733000
C	0.84415000	-4.28719100	0.11098600
H	1.48389400	-4.45821500	0.97324700
C	-0.44962800	-3.79907500	0.31521900
C	-1.51408000	4.37207200	0.01776200
C	-0.44844600	5.11875200	0.51859800
H	0.08809700	5.78261200	-0.15691500
C	1.32826400	-4.58084500	-1.16488600
C	-0.04720500	5.03661300	1.85014000
C	-1.81613500	3.40208100	2.23644100
C	-0.74471800	4.17441700	2.68863600
H	-0.44313500	4.10136300	3.73190900
H	-6.25061500	4.20002400	-1.92173300
H	-6.58762300	2.43475900	-3.58044000
H	-8.00887400	0.42435000	-3.02300600
H	-5.57783700	0.19794000	-2.92842800
H	-6.55336500	-0.25122500	0.48266000
H	-7.88079400	-2.27266300	-0.05657300
H	-7.93681400	-4.16630400	1.62795600
H	-5.60935500	-5.04392500	1.05826000
C	-2.53124700	2.51008500	3.24023400
H	-3.30106500	1.94237200	2.71226800
C	-3.23571100	3.35857600	4.30676000
H	-2.51214700	3.94281700	4.88501600
H	-3.94256400	4.05712100	3.85005800
H	-3.78444900	2.71861500	5.00481100
C	-1.57239900	1.50281700	3.88635400
H	-2.12592400	0.82755600	4.54658600
H	-1.06464400	0.90277200	3.12748100
H	-0.81840500	2.01327700	4.49564500
C	1.15115700	5.81411700	2.35825300
H	1.16733300	5.71160700	3.45075200
C	1.07178200	7.30652600	2.02592800
H	0.14482400	7.74604400	2.40282600
H	1.91563300	7.84398500	2.46913400
H	1.10697300	7.47221000	0.94439500
C	2.44027600	5.19513500	1.80741000
H	2.50997500	4.13778600	2.07958600
H	2.45440000	5.25936300	0.71260700
H	3.32818300	5.71170200	2.18782200
C	-1.86654700	4.53452300	-1.45634500
H	-2.64322500	3.81195700	-1.71135200
C	-0.67458000	4.22437500	-2.36550700

H	-0.95769100	4.34768800	-3.41628800
H	0.16788300	4.89625900	-2.16806900
H	-0.36227000	3.19026800	-2.20409100
C	-2.41430900	5.94011700	-1.73218000
H	-3.28375000	6.16018800	-1.10558800
H	-1.65629100	6.70241600	-1.52187300
H	-2.71108600	6.04032400	-2.78102500
C	-1.00736100	-3.65086900	1.72683100
H	-1.80338300	-2.90024000	1.69812700
C	0.00355100	-3.19326000	2.77447500
H	0.82981300	-3.90451800	2.88094200
H	0.40588300	-2.20781400	2.54064400
H	-0.49263200	-3.12843200	3.74903400
C	-1.61133800	-4.99405800	2.16824200
H	-0.82645400	-5.75690800	2.22122200
H	-2.06659700	-4.90310100	3.15954100
H	-2.37436900	-5.34859400	1.47247100
C	-1.70130300	-3.67344300	-3.31876400
H	-2.72561000	-3.52798500	-2.96057800
C	-1.28931500	-2.40341800	-4.07259100
H	-1.95715300	-2.22551900	-4.92169800
H	-1.32107500	-1.53217000	-3.41255700
H	-0.27012800	-2.50757900	-4.46313200
C	-1.70799900	-4.88529300	-4.25550100
H	-2.43917900	-4.73764000	-5.05589300
H	-0.73236000	-5.03353700	-4.72906600
H	-1.96496200	-5.80215600	-3.71806700
C	2.74618500	-5.06785900	-1.41469100
H	2.68468300	-5.82156600	-2.21119600
C	3.40196400	-5.71577000	-0.19553700
H	2.76598400	-6.48994400	0.24367000
H	4.35492000	-6.17086700	-0.47936500
H	3.62080000	-4.96448000	0.57050800
C	3.62383300	-3.91538300	-1.92457100
H	3.18607700	-3.43646100	-2.80575400
H	3.74001300	-3.16289400	-1.13672700
H	4.62302000	-4.27587700	-2.18793700

C_3

Zero-point correction=	1.515226 (Hartree/Particle)
Thermal correction to Energy=	1.598430
Thermal correction to Enthalpy=	1.599374
Thermal correction to Gibbs Free Energy=	1.394734

Sum of electronic and zero-point Energies= -3882.690929
Sum of electronic and thermal Energies= -3882.607725
Sum of electronic and thermal Enthalpies= -3882.606781
Sum of electronic and thermal Free Energies= -3882.811421
SCF Done: E(RM062X) = -3885.15624113

H	1.68117500	-0.42213000	1.59372100
C	1.75214800	2.31416500	1.22613500
N	2.03161900	1.58081000	-0.03418400
H	0.64999600	1.22254800	-0.41165200
C	2.46801700	2.45139000	-1.12081500
C	2.15416800	2.09044800	-2.43014000
C	3.17496900	3.62837900	-0.87169700
C	2.55080700	2.90213100	-3.48815200
H	1.57371900	1.19337400	-2.61971500
C	3.55493000	4.44202500	-1.93436800
H	3.44416500	3.89886300	0.14295100
C	3.24724900	4.08136800	-3.24348400
H	2.29895600	2.61569900	-4.50360000
H	4.10428500	5.35606800	-1.73455400
H	3.54974600	4.71690600	-4.06895200
C	2.98090700	-0.48782700	-1.06116100
C	4.42597000	0.94474000	0.12481400
C	2.96729500	0.42167200	0.15331000
O	4.90583800	1.72488600	0.91733200
N	4.10447400	-0.46458200	-1.67024800
N	4.96298900	0.43170200	-1.02997800
C	6.26385900	0.61398500	-1.54915700
C	7.13394100	1.54727500	-0.97570600
C	6.66910300	-0.14093600	-2.65366400
C	8.40480500	1.71030300	-1.51680300
H	6.81737000	2.12508900	-0.11918100
C	7.94272400	0.04107400	-3.17797300
H	5.98474400	-0.85908600	-3.08517200
C	8.81925500	0.96507200	-2.61604600
H	9.07689400	2.43378400	-1.06624500
H	8.24984700	-0.55008300	-4.03489900
H	9.81295500	1.10133800	-3.02923000
C	1.83722600	-1.34609500	-1.47219300
H	1.53777400	-2.01481700	-0.65565100
H	0.96154300	-0.73756000	-1.72255100
H	2.10640000	-1.94249000	-2.34423300
N	2.66685400	-0.23693100	1.39182600
C	3.60106500	-1.10453300	1.90314700

O	4.66889300	-1.33449500	1.36886700
O	3.16663400	-1.61445200	3.06057400
C	4.00971800	-2.54041100	3.80886100
C	3.17140100	-2.83530000	5.04701000
H	2.96588200	-1.91070700	5.59215100
H	2.22004000	-3.29353100	4.76768300
H	3.71304600	-3.51897700	5.70575500
C	5.31808100	-1.86057100	4.20336400
H	5.87064000	-2.51765300	4.88117000
H	5.93446800	-1.64941300	3.33040100
H	5.10723500	-0.92476200	4.72849500
C	4.23848100	-3.80886200	2.99242700
H	4.87990900	-3.61468800	2.13193300
H	4.70912200	-4.56876100	3.62291300
H	3.27560800	-4.19768800	2.64454900
H	1.18949700	3.21088800	0.95598900
H	1.12403300	1.69284000	1.86613300
H	2.67075800	2.57033700	1.75989900
C	-4.18559200	0.19905500	-0.42934700
C	-4.54406500	2.95565600	-0.51209200
C	-3.45407600	2.46205000	0.19949400
C	-3.32464200	1.07302900	0.23531300
H	-4.70126200	4.03197700	-0.53580700
C	-3.54328300	-4.01913500	-0.14747500
C	-2.46618800	-3.19608000	-0.45654500
C	-2.72871000	-1.82833700	-0.53518200
C	-3.98379600	-1.27386000	-0.27076100
H	-3.38724000	-5.09512700	-0.13768800
C	-5.19271100	0.74357900	-1.25417300
C	-5.39503600	2.13161700	-1.25170800
C	-6.52777900	2.77757300	-2.02813500
C	-7.06613400	1.90250700	-3.15703200
C	-7.30051900	0.48331400	-2.64724300
C	-5.97691900	-0.13868100	-2.21024700
H	-7.34475700	2.99422900	-1.32627100
H	-7.98771500	2.33577400	-3.55691700
H	-7.99555200	0.51012400	-1.79674700
H	-6.13839200	-1.13299400	-1.79084500
C	-4.79776000	-3.51101100	0.19774400
C	-5.01335700	-2.12575600	0.18608900
C	-6.29939200	-1.55376600	0.75896200
C	-7.45625100	-2.54949900	0.74338300
C	-7.02138800	-3.86487700	1.38323500
C	-5.89504700	-4.49203400	0.56605900

H	-6.08955500	-1.26897100	1.79985300
H	-8.31551500	-2.12347500	1.26989000
H	-6.67223100	-3.66715800	2.40434300
H	-6.31493200	-4.90111700	-0.36313900
P	-1.01295700	-0.05669800	0.21560800
O	-2.29229800	0.53242000	0.99137600
O	-1.68791100	-0.98639400	-0.91764300
O	-0.11963100	-0.72551900	1.18886000
O	-0.38051700	1.06877800	-0.65142300
C	-1.08446800	-3.73806900	-0.64743500
C	-2.43879100	3.36888000	0.81773500
C	-0.57227000	-3.95987400	-1.93616500
C	0.71593900	-4.48685800	-2.07064100
H	1.11998700	-4.65623500	-3.06772100
C	0.97933400	-4.55024500	0.30242900
H	1.58605300	-4.77259200	1.17523300
C	-0.30120900	-4.02977200	0.48934300
C	-1.72126100	4.26568100	-0.00789500
C	-0.80122700	5.13482500	0.57906800
H	-0.25974200	5.82900000	-0.06094800
C	1.50904200	-4.78690200	-0.96707000
C	-0.55755100	5.14681300	1.95181500
C	-2.19340700	3.35066000	2.20529800
C	-1.25594600	4.23891600	2.74070100
H	-1.08080900	4.23609400	3.81470100
H	-6.19332400	3.74571500	-2.41542500
H	-6.34080800	1.87110600	-3.97965700
H	-7.76264800	-0.13872400	-3.41959500
H	-5.34670100	-0.29373800	-3.09751600
H	-6.58261900	-0.62809700	0.25602600
H	-7.77232900	-2.73339700	-0.29270000
H	-7.85992700	-4.56343300	1.45932400
H	-5.45532500	-5.33991600	1.10168700
C	-2.95244800	2.45071200	3.17000900
H	-3.62494600	1.81041800	2.59442100
C	-3.82355400	3.28959400	4.11465000
H	-3.20876700	3.93792100	4.74726100
H	-4.51360600	3.92501700	3.55249500
H	-4.40956000	2.63936500	4.77137900
C	-2.00607700	1.54116200	3.96200000
H	-2.58099100	0.87388300	4.61153600
H	-1.39753700	0.92610900	3.29450400
H	-1.33869200	2.12844800	4.60148300
C	0.41706400	6.13817700	2.56050800

H	0.42426700	5.96720300	3.64421300
C	-0.04307600	7.57974500	2.31293800
H	-1.05862800	7.73746200	2.68489100
H	0.62409600	8.28911200	2.81165700
H	-0.03769500	7.81017800	1.24256700
C	1.84383600	5.92950800	2.03990100
H	2.22135300	4.93918100	2.30925500
H	1.87772500	6.01935400	0.94803200
H	2.52218600	6.67772200	2.46078400
C	-1.89624800	4.34562500	-1.51998400
H	-2.58711700	3.56068600	-1.83419500
C	-0.57665400	4.08232400	-2.25042900
H	-0.72157100	4.14554300	-3.33399600
H	0.20447000	4.80090100	-1.97714900
H	-0.21601300	3.08197000	-2.01132200
C	-2.49629600	5.69586400	-1.93145400
H	-3.44879500	5.88479800	-1.42696400
H	-1.81997400	6.51858500	-1.67680300
H	-2.66664800	5.72528400	-3.01201500
C	-0.83003100	-3.81792300	1.90137800
H	-1.56352100	-3.00551200	1.86530100
C	0.26261800	-3.40418900	2.88885800
H	0.90802500	-4.25484300	3.13949100
H	0.88241000	-2.59783200	2.49323700
H	-0.19233300	-3.05839100	3.82215000
C	-1.52400500	-5.08592400	2.42046300
H	-0.81876000	-5.92411200	2.42375600
H	-1.87640500	-4.93413000	3.44561200
H	-2.38067900	-5.36810600	1.80516600
C	-1.37490200	-3.63149100	-3.18520800
H	-2.37979500	-3.33096200	-2.87207500
C	-0.75154200	-2.45030800	-3.93823800
H	-1.33882500	-2.20906700	-4.82988600
H	-0.71199500	-1.56392700	-3.29926800
H	0.26753400	-2.69038100	-4.26171900
C	-1.52333500	-4.85168800	-4.10061000
H	-2.16353200	-4.61117900	-4.95470700
H	-0.55425600	-5.17468000	-4.49378000
H	-1.96605400	-5.69513600	-3.56380700
C	2.93245300	-5.28543800	-1.14134600
H	3.01122400	-5.69154600	-2.15809500
C	3.29300100	-6.40475800	-0.16014300
H	2.55067200	-7.20726300	-0.17612500
H	4.26849800	-6.82876200	-0.41446700

H	3.36313000	-6.02522500	0.86466300
C	3.92822200	-4.12272300	-1.01436100
H	3.79531800	-3.38313200	-1.80814200
H	3.80301500	-3.60270900	-0.05727900
H	4.95894200	-4.48794500	-1.06481200

C_3'

Zero-point correction= 1.515934 (Hartree/Particle)
Thermal correction to Energy= 1.599054
Thermal correction to Enthalpy= 1.599998
Thermal correction to Gibbs Free Energy= 1.397492
Sum of electronic and zero-point Energies= -3882.688385
Sum of electronic and thermal Energies= -3882.605265
Sum of electronic and thermal Enthalpies= -3882.604321
Sum of electronic and thermal Free Energies= -3882.806827
SCF Done: E(RM062X) = -3885.15169833

H	1.88365900	0.59886100	1.41267100
C	0.93769700	3.37657700	0.03856900
N	1.71631700	2.39223900	-0.73598500
H	0.51268000	1.30738000	-0.89707600
C	2.06316300	2.81569600	-2.07688900
C	2.15131000	1.84979300	-3.08390200
C	2.26986800	4.15965600	-2.39232100
C	2.47723500	2.22644900	-4.38238100
H	1.92110000	0.81385300	-2.85550700
C	2.58001000	4.52969300	-3.69777200
H	2.17283600	4.92129800	-1.62622300
C	2.69455200	3.56546600	-4.69433100
H	2.54041500	1.46809300	-5.15563300
H	2.73394100	5.57780500	-3.93271300
H	2.93910200	3.85708700	-5.71012500
C	4.22578900	2.40640700	-0.21849100
C	3.12117700	0.37796500	-0.70937400
C	2.85831400	1.74234400	-0.02190200
O	2.30199500	-0.50712800	-0.83630200
N	5.04896100	1.62326300	-0.81049500
N	4.42671200	0.40958000	-1.10077200
C	5.16720200	-0.60803700	-1.74269100
C	4.51135500	-1.57468400	-2.50498500
C	6.55554900	-0.63193600	-1.59757600
C	5.26042900	-2.57805500	-3.11256500
H	3.43278800	-1.55322300	-2.59403100

C	7.28600100	-1.64185900	-2.21176200
H	7.03960700	0.13677100	-1.00727900
C	6.64415800	-2.62101700	-2.96817700
H	4.75052200	-3.33382100	-3.70330600
H	8.36454200	-1.66401100	-2.09476000
H	7.21928200	-3.40883000	-3.44269000
C	4.65673000	3.79519300	0.12449100
H	5.50332200	4.06057700	-0.51033800
H	3.84170800	4.50418900	-0.02731600
H	4.93588400	3.86156800	1.17625800
N	2.53889500	1.38680800	1.33046600
C	2.45534900	2.31051700	2.34503000
O	2.92005800	3.43338700	2.30891000
O	1.78312100	1.77276200	3.36670000
C	1.32261000	2.61298600	4.46538200
C	0.49724500	1.64321100	5.30146400
H	-0.30206900	1.20953200	4.69416100
H	1.12846800	0.83166100	5.67287200
H	0.05741300	2.16804200	6.15369300
C	0.44199100	3.73549600	3.91978700
H	-0.03398200	4.25892400	4.75464400
H	1.02768900	4.45423400	3.34486700
H	-0.34728000	3.31950100	3.28327500
C	2.51239100	3.14210600	5.25950300
H	3.09997200	3.84235600	4.66622000
H	2.14922500	3.65015900	6.15765800
H	3.15031800	2.31008500	5.57012900
H	0.46373400	2.86592600	0.88215400
H	1.53797700	4.20703300	0.42129000
H	0.13925800	3.74533600	-0.61052800
C	-3.51933100	-1.48049700	-0.67913600
C	-4.84130700	0.73476100	-1.72664100
C	-3.80923200	0.95826400	-0.82021300
C	-3.17858800	-0.17818900	-0.31272800
H	-5.38124900	1.59214500	-2.12274900
C	-1.40755300	-4.68967000	1.20423700
C	-0.68522000	-3.64403900	0.64114900
C	-1.42832900	-2.63751800	0.02392900
C	-2.82390200	-2.61347000	0.00435900
H	-0.86328700	-5.52291400	1.64128200
C	-4.48014200	-1.66197700	-1.69527100
C	-5.16863000	-0.54319300	-2.18779100
C	-6.28697400	-0.67775800	-3.20484900
C	-6.24384700	-1.98945700	-3.98489700

C	-6.04049000	-3.15925000	-3.02569200
C	-4.69129500	-3.02796100	-2.32423000
H	-7.24563400	-0.61350200	-2.67190400
H	-7.16474000	-2.10880400	-4.56359000
H	-6.84705000	-3.16463500	-2.27971700
H	-4.55587800	-3.82524700	-1.59106000
C	-2.80399800	-4.68550400	1.26416200
C	-3.52379800	-3.62018900	0.70425500
C	-5.01747000	-3.49692200	0.95484100
C	-5.68130100	-4.83216700	1.28108000
C	-4.91695500	-5.53591500	2.39874100
C	-3.49831100	-5.85609700	1.93523700
H	-5.14720100	-2.81718200	1.80926600
H	-6.72474200	-4.66531700	1.56515100
H	-4.88016800	-4.87766300	3.27578700
H	-3.53820900	-6.68851300	1.21915300
P	-0.64577500	-0.21189300	0.17532300
O	-2.17959700	0.00588800	0.62791900
O	-0.73411700	-1.61319400	-0.61420200
O	0.19912700	-0.13994900	1.38401600
O	-0.37124200	0.79624700	-0.98738500
C	0.80626600	-3.54866500	0.69569600
C	-3.34709200	2.32753800	-0.43841900
C	1.56788900	-3.84178300	-0.44607500
C	2.95503400	-3.70519400	-0.38700400
H	3.55332600	-3.93383400	-1.26700900
C	2.82308600	-2.96107300	1.87996900
H	3.31059000	-2.60663600	2.78351200
C	1.43633700	-3.10653900	1.87791100
C	-2.84041000	3.19553500	-1.42785500
C	-2.43146200	4.47978700	-1.05509000
H	-2.05703000	5.15709900	-1.82065900
C	3.60029400	-3.24661300	0.75704200
C	-2.46960100	4.91931900	0.26374500
C	-3.39343600	2.75382800	0.90756700
C	-2.94668400	4.03467500	1.22964300
H	-2.99161500	4.35667200	2.26849500
H	-6.25963600	0.17811900	-3.88747000
H	-5.41310200	-1.96716800	-4.70130000
H	-6.08898900	-4.11419100	-3.55752200
H	-3.89040700	-3.17104600	-3.06351000
H	-5.52296800	-3.01133200	0.11871400
H	-5.68896000	-5.46956700	0.38628200
H	-5.42502500	-6.45471600	2.70681200

H	-2.88731900	-6.20431800	2.77449000
C	-3.95741100	1.89727100	2.03265700
H	-4.21896600	0.91661100	1.62964500
C	-5.24627800	2.51887700	2.58645700
H	-5.05216200	3.50372000	3.02396500
H	-5.99291600	2.64344100	1.79716800
H	-5.67262300	1.88254400	3.36809500
C	-2.92904800	1.68115000	3.15005600
H	-3.32122300	0.98171700	3.89519100
H	-1.99753300	1.27029600	2.75021100
H	-2.70647600	2.62071700	3.66917600
C	-2.02882200	6.32159100	0.63674800
H	-1.61392800	6.78460300	-0.26781800
C	-0.93300600	6.30925600	1.70722100
H	-0.07391300	5.71149700	1.38888100
H	-0.58679400	7.32547200	1.91862400
H	-1.30482400	5.88244100	2.64479100
C	-3.22402600	7.16548600	1.09549100
H	-3.99847400	7.20125500	0.32504400
H	-3.66977700	6.73820500	1.99983100
H	-2.91261500	8.18935600	1.32390300
C	-2.70327100	2.80427200	-2.89389900
H	-2.92884100	1.73954200	-2.98872800
C	-1.27069100	2.99970000	-3.40212300
H	-1.18806900	2.66700800	-4.44169800
H	-0.95840600	4.04912500	-3.36752600
H	-0.57279700	2.41172300	-2.80403400
C	-3.69673100	3.58515000	-3.76343400
H	-4.72831100	3.43684000	-3.43098100
H	-3.48778100	4.65944200	-3.72020400
H	-3.62281100	3.27042900	-4.80894700
C	0.64472800	-2.83338900	3.14992500
H	-0.37676600	-2.56778500	2.85690700
C	1.19058100	-1.67185400	3.98385700
H	2.16022800	-1.91475100	4.43245200
H	1.28761800	-0.76200900	3.38989300
H	0.49967100	-1.46858000	4.80880300
C	0.59133100	-4.09925300	4.01855600
H	1.60451700	-4.39117000	4.31589400
H	0.00848600	-3.91877700	4.92759800
H	0.14460600	-4.94305400	3.48790400
C	0.92571900	-4.29323100	-1.74760900
H	-0.16057700	-4.27310600	-1.61955100
C	1.27010000	-3.33966200	-2.89646500

H	0.69173600	-3.58962000	-3.79156500
H	1.05684100	-2.30484200	-2.61240100
H	2.33163200	-3.41895800	-3.15802500
C	1.32423800	-5.73346100	-2.08815400
H	0.84228600	-6.06039100	-3.01508300
H	2.40794500	-5.81461800	-2.22446100
H	1.03511500	-6.41987200	-1.28727900
C	5.11096700	-3.10350200	0.77886200
H	5.44742100	-3.04105400	-0.26448700
C	5.75477300	-4.34552700	1.40871100
H	5.46617300	-5.25244600	0.87039500
H	6.84672800	-4.26765400	1.39747600
H	5.43030000	-4.45482000	2.44925200
C	5.57893900	-1.83560700	1.49943500
H	5.05367800	-0.94698200	1.13477000
H	5.40735200	-1.90507500	2.57875200
H	6.65250200	-1.68902600	1.34531500

Pro3

Zero-point correction= 0.458118 (Hartree/Particle)
Thermal correction to Energy= 0.485691
Thermal correction to Enthalpy= 0.486635
Thermal correction to Gibbs Free Energy= 0.398106
Sum of electronic and zero-point Energies= -1297.721661
Sum of electronic and thermal Energies= -1297.694089
Sum of electronic and thermal Enthalpies= -1297.693145
Sum of electronic and thermal Free Energies= -1297.781674
SCF Done: E(RM062X) = -1298.53792096

H	-2.04217900	-2.05819000	-0.54450800
C	0.23401700	-2.19694000	-2.30972300
N	0.37665900	-2.10223400	-0.84796800
C	1.74961400	-2.27888200	-0.43379400
C	2.06680300	-3.39519000	0.33756300
C	2.75962900	-1.38727700	-0.80858800
C	3.37550800	-3.60618700	0.76336200
H	1.27363600	-4.09274900	0.58821600
C	4.06461900	-1.59577700	-0.37397200
H	2.52916700	-0.53332700	-1.44032500
C	4.37416600	-2.70163200	0.41492400
H	3.61348900	-4.47655200	1.36618600
H	4.84110300	-0.89189800	-0.65492500
H	5.39367700	-2.86097000	0.75047900

C	0.10880200	-0.76053700	1.20756100
C	0.23190900	0.39894000	-0.82815900
C	-0.28712800	-0.94061700	-0.24851600
O	0.14706000	0.75908800	-1.98188100
N	0.78231500	0.30489600	1.40931100
N	0.92836400	0.98802800	0.20273700
C	1.76478000	2.12394700	0.15942500
C	1.76295900	2.97011700	-0.95456900
C	2.61208200	2.38305000	1.24129500
C	2.61787300	4.06778700	-0.97165800
H	1.10224800	2.76732600	-1.78549000
C	3.45198700	3.48875600	1.20428000
H	2.59779400	1.71894700	2.09566000
C	3.46382200	4.33656100	0.09960500
H	2.61243800	4.72250500	-1.83729800
H	4.10485400	3.68504000	2.04886100
H	4.12328900	5.19752200	0.07569000
C	-0.30866000	-1.67695800	2.30137800
H	-1.39624900	-1.63800900	2.42679900
H	-0.03545900	-2.70806700	2.06131500
H	0.16643000	-1.37909400	3.23616300
N	-1.70266500	-1.11071400	-0.45601100
C	-2.56795100	-0.12326400	-0.07270800
O	-2.19430800	0.96773600	0.30826800
O	-3.83361600	-0.54824700	-0.18865700
C	-4.93369400	0.34645100	0.15686100
C	-6.16237600	-0.51255100	-0.11668700
H	-6.18853400	-0.81583100	-1.16628000
H	-6.14691200	-1.41035400	0.50659900
H	-7.06931400	0.05432600	0.10768200
C	-4.91769200	1.57062800	-0.75319500
H	-5.82161900	2.16081100	-0.57765800
H	-4.04397900	2.19249300	-0.55978400
H	-4.91021800	1.25684800	-1.80073900
C	-4.85611800	0.72169700	1.63388600
H	-3.98383300	1.34291100	1.83620500
H	-5.75804200	1.27361300	1.91308900
H	-4.80596500	-0.18303700	2.24715300
H	0.53308500	-3.20552400	-2.60321300
H	-0.80816800	-2.03362200	-2.58734200
H	0.84374700	-1.46629500	-2.85229500