Electronic Supplementary Information For

Mechanism and origin of stereoselectivity on cobalt-catalyzed hydroarylation reaction

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Content

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Part 1: Substituent effect

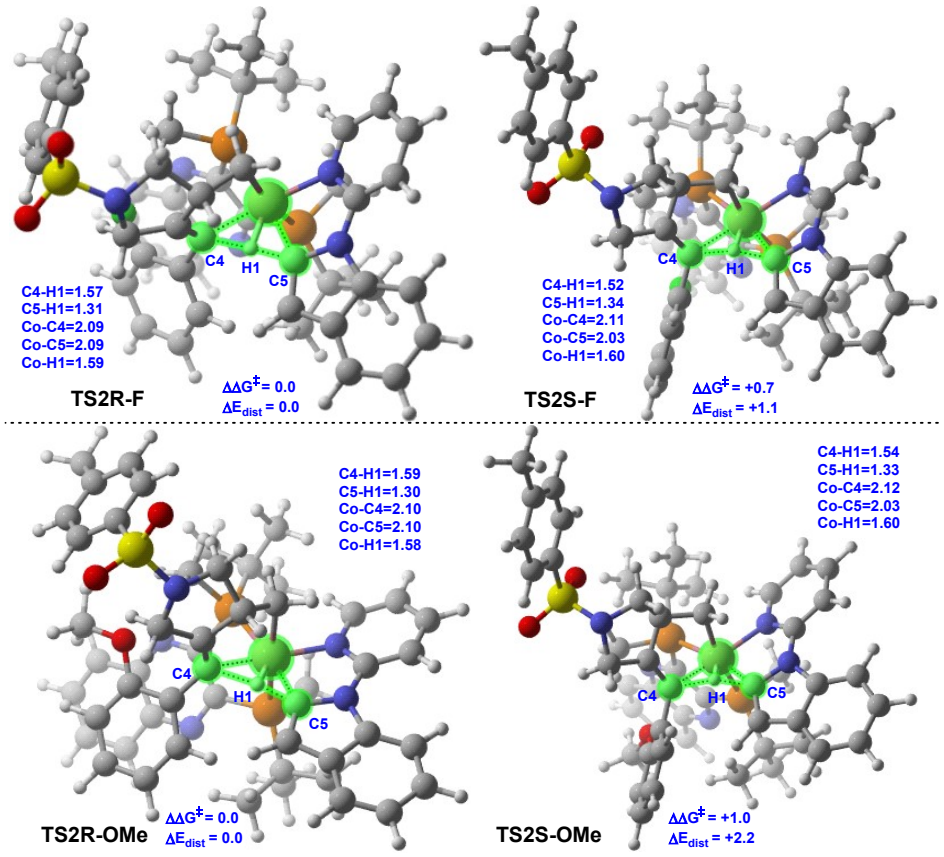

Fig. S1 Substituent effects on the stereoselectivity

Part 2: Cartesian Coordinates and energies for all the stationary points

R1

Zero-point correction=			0.336478 (Hartree/Particle)
Thermal correction to Energy=			0.358476
Thermal correction to Enthalpy=			0.359420
Thermal correction to Gibbs Free Energy=			0.282706
Sum of electronic and zero-point Energies=			-1338.296738
Sum of electronic and thermal Energies=			-1338.274740
Sum of electronic and thermal Enthalpies=			-1338.273796
Sum of electronic and thermal Free Energies=			-1338.350510
C	-6.27459600	1.68650500	-0.10318800
C	-4.88849200	1.59580700	-0.10622100
C	-4.25657400	0.39392300	-0.47448800
C	-5.04944600	-0.71034300	-0.83518800
C	-6.43508300	-0.61020500	-0.82484200
C	-7.05213900	0.58589300	-0.46118200
H	-6.75092300	2.62045200	0.18218900
H	-4.27961700	2.45032500	0.17450600
H	-4.56540200	-1.64006600	-1.12026500
H	-7.03670700	-1.47054600	-1.10371600
H	-8.13587200	0.66000700	-0.45621100
C	-2.83699100	0.30207200	-0.47942700
C	-1.62361500	0.23392600	-0.45734700
C	-0.17222600	0.18522600	-0.47732400
H	0.24341600	1.15809100	-0.16926400
H	0.16431200	0.00322500	-1.50347400
N	0.36756500	-0.89118200	0.38331500
C	0.50165800	-0.50882000	1.80303800
H	1.01152000	-1.33905100	2.30270100
H	1.12826800	0.39261900	1.90741500
C	-0.82928500	-0.28043000	2.43835200
C	-1.14259800	0.82832300	3.10634300
H	-1.54571100	-1.09676800	2.35057700
H	-2.10584900	0.94745700	3.59391800
H	-0.43995400	1.65535900	3.19384200
S	1.71898900	-1.68011700	-0.26521500
O	2.08893800	-2.69996900	0.71244000
O	1.35948400	-2.03804100	-1.63498400
C	3.02084100	-0.47434300	-0.33691400
C	3.77584000	-0.20870900	0.80637100

C	3.22679800	0.24605000	-1.51462400
C	4.74612900	0.78556700	0.75945900
H	3.61411500	-0.78415100	1.71354700
C	4.20678300	1.22927000	-1.54385000
H	2.63628600	0.02350900	-2.39834500
C	4.97965700	1.51711200	-0.41081800
H	5.34003700	0.99606200	1.64544400
H	4.37900600	1.78568600	-2.46218600
C	6.04749000	2.56228000	-0.46358900
H	5.71587900	3.45070300	-1.00889600
H	6.36246800	2.86920500	0.53670700
H	6.93567600	2.18747400	-0.98527500

R2

Zero-point correction=	0.199048 (Hartree/Particle)
Thermal correction to Energy=	0.208863
Thermal correction to Enthalpy=	0.209807
Thermal correction to Gibbs Free Energy=	0.163397
Sum of electronic and zero-point Energies=	-610.671882
Sum of electronic and thermal Energies=	-610.662067
Sum of electronic and thermal Enthalpies=	-610.661123
Sum of electronic and thermal Free Energies=	-610.707533

C	1.13913400	-0.11965800	0.00000100
C	2.17857400	0.85423400	-0.00003400
C	3.52014100	0.45731100	-0.00002600
C	3.82495400	-0.89518500	0.00004000
C	2.79813900	-1.84855200	0.00002800
C	1.45588900	-1.48239400	0.00003500
C	0.21783600	1.94782800	-0.00006000
C	1.56163000	2.14363700	0.00000300
H	4.30655000	1.20787800	0.00001400
H	4.86153000	-1.21997700	0.00012200
H	3.04708400	-2.90593900	-0.00001600
H	0.71256100	-2.26740600	0.00001000
H	-0.59743000	2.65228000	-0.00008900
H	2.06244500	3.10201000	0.00002600
N	-0.07682900	0.58269200	-0.00002400
C	-1.41151200	0.12447600	-0.00003600
C	-1.76154000	-1.23123000	-0.00004700
N	-2.33053500	1.09887500	0.00007500
C	-3.10873700	-1.56366700	-0.00002000
H	-1.02300500	-2.01733600	-0.00018300
C	-3.62026800	0.75412200	0.00008700
C	-4.07106200	-0.55933400	0.00000300

H	-3.39792000	-2.61037900	-0.00003600
H	-4.32731600	1.58248500	0.00005600
H	-5.13200900	-0.78411000	-0.00011200

Cat

Zero-point correction=			0.428186 (Hartree/Particle)
Thermal correction to Energy=			0.454374
Thermal correction to Enthalpy=			0.455318
Thermal correction to Gibbs Free Energy=			0.375083
Sum of electronic and zero-point Energies=			-1640.234676
Sum of electronic and thermal Energies=			-1640.208488
Sum of electronic and thermal Enthalpies=			-1640.207544
Sum of electronic and thermal Free Energies=			-1640.287779
C	5.25871400	-0.70894500	-0.35642000
C	4.07248800	-1.33974700	-0.65772600
C	2.84438700	-0.72397700	-0.33266600
C	2.84984200	0.55770800	0.30940200
C	4.08210900	1.17935200	0.60531900
C	5.26368800	0.55322800	0.27755500
H	6.20268400	-1.18516100	-0.60515500
H	4.04829000	-2.31111900	-1.14346400
H	4.06511500	2.15130000	1.09023000
H	6.21124400	1.03273800	0.50520700
C	0.57374300	0.56209700	0.29913800
C	0.56681100	-0.72269000	-0.30699500
N	1.68483800	1.19377400	0.62711400
N	1.67576800	-1.36712300	-0.62049100
P	-1.07191400	1.32907400	0.50899500
P	-1.09344500	-1.43886600	-0.59547600
C	-1.15935300	1.71198700	2.29258400
H	-0.25873000	2.24352100	2.61353500
H	-2.03658800	2.32799500	2.50677300
H	-1.24053500	0.78298000	2.86214400
C	-0.90452000	-2.33274000	-2.17413300
H	0.01849500	-2.91910900	-2.16777700
H	-1.75485200	-2.99732700	-2.34566000
H	-0.85498800	-1.61154200	-2.99341700
C	-1.28482900	-2.78410900	0.71330300
C	-1.14164800	-2.12209800	2.08203900
C	-2.69390500	-3.35633700	0.56368900
C	-0.24536500	-3.88765700	0.54170600
H	-0.15148700	-1.67344900	2.22449600
H	-1.89583100	-1.33915400	2.22673500
H	-1.28037600	-2.86941400	2.87163100

H	-2.84967300	-3.82204100	-0.41531600
H	-2.86161100	-4.12871100	1.32307800
H	-3.45965100	-2.58311900	0.70026900
H	-0.36217200	-4.62185800	1.34810800
H	-0.36723700	-4.42236900	-0.40555900
H	0.77867200	-3.50403300	0.58675500
C	-1.00911400	2.99204400	-0.36170300
C	-0.25561500	4.04877100	0.43828600
C	-0.35731300	2.79551800	-1.72956200
C	-2.47598800	3.38945600	-0.54707100
H	-0.74017700	4.26810500	1.39456500
H	0.77695000	3.74473400	0.63700600
H	-0.22636500	4.98264700	-0.13622500
H	-0.84972700	1.99729600	-2.29999000
H	-0.43985600	3.72152200	-2.30976100
H	0.70613300	2.54861400	-1.64654100
H	-2.54701100	4.34042000	-1.08747300
H	-3.01105200	2.63098800	-1.13677200
H	-2.99688700	3.51170400	0.40936700
Co	-2.50264500	0.13677800	-0.49246000

PR

Zero-point correction=	0.543300 (Hartree/Particle)
Thermal correction to Energy=	0.575050
Thermal correction to Enthalpy=	0.575994
Thermal correction to Gibbs Free Energy=	0.478410
Sum of electronic and zero-point Energies=	-1949.057925
Sum of electronic and thermal Energies=	-1949.026176
Sum of electronic and thermal Enthalpies=	-1949.025231
Sum of electronic and thermal Free Energies=	-1949.122815

C	-2.15178200	4.81113000	1.46385700
C	-1.73757400	3.74175100	0.67543500
C	-0.56589500	3.02825100	0.98989700
C	0.17127800	3.44540700	2.11459300
C	-0.24550700	4.50912900	2.90261200
C	-1.41415300	5.19812900	2.58156100
H	-3.05595300	5.35218200	1.19724300
H	-2.31827700	3.48442600	-0.20426800
H	1.08556800	2.91045400	2.36342000
H	0.34365200	4.80433500	3.76662700
H	-1.74283000	6.03529500	3.19102300
C	-0.04362700	1.89220900	0.24043800
C	-0.61721600	1.13303800	-0.70982600
C	-2.02457200	1.22938700	-1.22650400

H	-2.74312400	1.27558200	-0.38948900
H	-2.21069700	2.10339000	-1.86076200
N	-2.18488000	0.00015800	-2.03221300
C	-1.16709700	-0.97466300	-1.61780900
H	-1.00021200	-1.70718600	-2.40977100
H	-1.45650500	-1.50654700	-0.69422000
C	0.03479400	-0.07527600	-1.34888000
C	1.12550000	-0.77303500	-0.54318700
H	0.43653100	0.22333100	-2.32989400
H	1.18749300	-1.82399200	-0.86033400
H	0.83012800	-0.81359000	0.51185300
S	-3.74305700	-0.55374500	-2.27446000
O	-3.62232700	-1.71875700	-3.14749800
O	-4.52731500	0.61675500	-2.66142500
C	-4.32653200	-1.11314000	-0.69409400
C	-4.03564000	-2.41587900	-0.28090700
C	-5.00138400	-0.23086100	0.14953200
C	-4.43193600	-2.83061900	0.98273000
H	-3.52135100	-3.09601200	-0.95393600
C	-5.39306800	-0.66589200	1.41156400
H	-5.23341100	0.77489800	-0.18887800
C	-5.11550400	-1.96532400	1.84868000
H	-4.21389700	-3.84625100	1.30496400
H	-5.92721900	0.01435600	2.07058300
C	-5.54790700	-2.43243500	3.20191300
H	-5.95428300	-1.61425200	3.80107200
H	-4.71666600	-2.88062900	3.75525600
H	-6.32175800	-3.20434500	3.12559900
C	4.73072900	0.02484300	-0.47562200
C	4.26731000	1.10729300	-1.26591000
C	5.18757800	2.05417100	-1.73664000
C	6.52754700	1.91524000	-1.40300300
C	6.96229900	0.85230500	-0.59547000
C	6.07256100	-0.10404500	-0.11708600
C	2.47537400	-0.15411600	-0.68007700
C	2.85146300	0.96255600	-1.38019000
H	4.85040000	2.88855700	-2.34652800
H	7.25075600	2.64176400	-1.76305400
H	8.01356200	0.77361000	-0.33274800
H	6.41857100	-0.91296700	0.51912200
H	0.96874000	1.61105500	0.53059800
H	2.17597000	1.61489400	-1.91810800
N	3.62014900	-0.74452600	-0.12908400
C	3.65947900	-1.90489200	0.67577100

C	4.64566200	-2.87211000	0.45622700
N	2.73147100	-2.00090800	1.63215300
C	4.67545400	-3.97727300	1.29447800
H	5.35254000	-2.76289300	-0.35949200
C	2.76441800	-3.08895400	2.41150900
C	3.71741600	-4.09455900	2.29788100
H	5.42959800	-4.74579400	1.15357100
H	1.99046800	-3.14646100	3.17511500
H	3.70426400	-4.94493400	2.97135300

PS

Zero-point correction=	0.543301 (Hartree/Particle)
Thermal correction to Energy=	0.575050
Thermal correction to Enthalpy=	0.575994
Thermal correction to Gibbs Free Energy=	0.478412
Sum of electronic and zero-point Energies=	-1949.057925
Sum of electronic and thermal Energies=	-1949.026175
Sum of electronic and thermal Enthalpies=	-1949.025231
Sum of electronic and thermal Free Energies=	-1949.122814

C	2.15165600	4.81100900	1.46410700
C	1.73737800	3.74176500	0.67553800
C	0.56573600	3.02816400	0.98996100
C	-0.17131600	3.44514000	2.11480500
C	0.24554200	4.50872100	2.90297800
C	1.41414100	5.19781300	2.58194700
H	3.05578400	5.35212000	1.19745700
H	2.31808400	3.48467600	-0.20422700
H	-1.08557500	2.91014200	2.36364900
H	-0.34352900	4.80372700	3.76712400
H	1.74283500	6.03487500	3.19154300
C	0.04350000	1.89220500	0.24036400
C	0.61709300	1.13314600	-0.70999700
C	2.02443900	1.22961100	-1.22671700
H	2.74292300	1.27588300	-0.38967100
H	2.21047200	2.10365900	-1.86093600
N	2.18488000	0.00039600	-2.03246300
C	1.16713200	-0.97448200	-1.61801600
H	1.00031900	-1.70705300	-2.40995000
H	1.45656800	-1.50631200	-0.69440300
C	-0.03482300	-0.07516900	-1.34909500
C	-1.12547600	-0.77308000	-0.54345600
H	-0.43654200	0.22344500	-2.33012500
H	-1.18738400	-1.82397300	-0.86080900
H	-0.83018500	-0.81378000	0.51155700

S	3.74315500	-0.55355200	-2.27444400
O	3.62247200	-1.71857400	-3.14746800
O	4.52750200	0.61689700	-2.66137900
C	4.32650400	-1.11300000	-0.69404000
C	4.03546300	-2.41574500	-0.28091800
C	5.00142800	-0.23085700	0.14964600
C	4.43167300	-2.83057600	0.98271800
H	3.52109500	-3.09577900	-0.95397500
C	5.39297900	-0.66595700	1.41169300
H	5.23361400	0.77487800	-0.18872500
C	5.11527400	-1.96537200	1.84874100
H	4.21347400	-3.84617700	1.30493000
H	5.92716400	0.01420900	2.07076500
C	5.54764100	-2.43256800	3.20193200
H	5.95355300	-1.61434400	3.80135500
H	4.71652100	-2.88129200	3.75504200
H	6.32184800	-3.20412100	3.12557800
C	-4.73068800	0.02491000	-0.47549000
C	-4.26731800	1.10725400	-1.26595900
C	-5.18759100	2.05413400	-1.73667200
C	-6.52753400	1.91528600	-1.40289200
C	-6.96224900	0.85244100	-0.59521600
C	-6.07250000	-0.10388600	-0.11682600
C	-2.47536800	-0.15418900	-0.68024600
C	-2.85149800	0.96243000	-1.38041200
H	-4.85044600	2.88844200	-2.34668600
H	-7.25075300	2.64180300	-1.76294300
H	-8.01349100	0.77381700	-0.33239300
H	-6.41847300	-0.91272900	0.51950400
H	-0.96884400	1.61092400	0.53050700
H	-2.17607400	1.61461500	-1.91859600
N	-3.62008800	-0.74442600	-0.12892200
C	-3.65940200	-1.90488800	0.67578400
C	-4.64560800	-2.87208700	0.45623200
N	-2.73128300	-2.00104100	1.63205000
C	-4.67528300	-3.97736400	1.29433400
H	-5.35262800	-2.76278200	-0.35935700
C	-2.76411100	-3.08920700	2.41123500
C	-3.71711200	-4.09480300	2.29759400
H	-5.42946000	-4.74584800	1.15342000
H	-1.99004900	-3.14678500	3.17472200
H	-3.70385500	-4.94530200	2.97091500

M1R

Zero-point correction=			0.770958 (Hartree/Particle)
Thermal correction to Energy=			0.817956
Thermal correction to Enthalpy=			0.818901
Thermal correction to Gibbs Free Energy=			0.694442
Sum of electronic and zero-point Energies=			-2978.619038
Sum of electronic and thermal Energies=			-2978.572040
Sum of electronic and thermal Enthalpies=			-2978.571096
Sum of electronic and thermal Free Energies=			-2978.695554
C	6.15971900	-4.35130400	0.56225700
C	4.82688000	-4.11457800	0.80233200
C	4.25839100	-2.87581200	0.42920500
C	5.07672600	-1.88451300	-0.20536500
C	6.44380100	-2.15814500	-0.43672600
C	6.96975600	-3.37057100	-0.05765500
H	6.60129800	-5.30048000	0.85087700
H	4.18829500	-4.85259200	1.27903200
H	7.04845600	-1.39582100	-0.91948400
H	8.01923200	-3.58458300	-0.23654400
C	3.26586000	-0.50435400	-0.37591300
C	2.47087100	-1.46516700	0.30722800
N	4.55254800	-0.69473900	-0.60401700
N	2.94732500	-2.63323700	0.69379400
P	2.40481700	1.00484000	-0.96953800
P	0.73365400	-1.00573200	0.70345900
C	3.27206700	2.32103800	-0.04247000
H	4.34437800	2.10932100	-0.00629200
H	3.11911400	3.28563400	-0.53133400
H	2.88463300	2.39266100	0.97534200
C	-0.10691600	-2.61592100	0.67248900
H	0.49083900	-3.32536800	1.25050000
H	-1.10850300	-2.53789700	1.10204000
H	-0.18297600	-2.99742600	-0.34686300
C	0.77141000	-0.54574400	2.53982900
C	1.67571400	0.66643600	2.72874100
C	-0.64456800	-0.21785900	3.00630300
C	1.30974500	-1.72337800	3.35659100
H	2.70492600	0.47117000	2.40398300
H	1.29922000	1.53886000	2.18540000
H	1.71078600	0.92805100	3.79227800
H	-1.34595500	-1.04241800	2.84588600
H	-0.61801400	-0.01373900	4.08290200
H	-1.04158900	0.67373400	2.51349000
H	1.37156400	-1.40549900	4.40355200
H	0.64815400	-2.59306400	3.31993200

H	2.31003400	-2.03648800	3.04575900
C	3.01888900	1.25641300	-2.74783500
C	4.39365600	1.92572600	-2.78406800
C	3.12256600	-0.08352200	-3.47675400
C	1.99588200	2.17312800	-3.42142400
H	4.38083400	2.93893400	-2.37350400
H	5.14758400	1.34028900	-2.24986300
H	4.71185900	2.00255400	-3.83078400
H	2.22783500	-0.70252000	-3.38730600
H	3.28806300	0.10626600	-4.54345300
H	3.97207500	-0.66717900	-3.11123900
H	2.30234600	2.37337000	-4.45470400
H	0.99210800	1.73425000	-3.44680600
H	1.92377700	3.14008900	-2.90887900
Co	0.17282800	0.63430100	-0.61063100
C	0.24986900	5.19472600	2.51906900
C	-0.17183400	3.96236200	2.03409200
C	0.10329600	3.59035100	0.70554400
C	0.79424900	4.48975400	-0.12089400
C	1.19219900	5.73009600	0.36201400
C	0.92891000	6.08289700	1.68536800
H	0.03967000	5.46702800	3.54959600
H	-0.70861500	3.27011500	2.67951600
H	1.00648200	4.20228800	-1.14852000
H	1.71528300	6.42131000	-0.29306300
H	1.25112100	7.04821500	2.06527400
C	-0.33024600	2.30422300	0.20882700
C	-1.30889900	1.45554800	0.16526100
C	-2.69571900	1.01485700	0.36392800
H	-3.35065500	1.48204900	-0.39104300
H	-3.05749300	1.32136200	1.34985800
N	-2.72154300	-0.45212700	0.29353100
C	-2.37888500	-1.01700300	-1.02814900
H	-2.06160200	-2.05163800	-0.88399300
H	-3.26935100	-1.02963300	-1.67989900
C	-1.32263300	-0.20587000	-1.71941700
C	-0.08518000	-0.69334300	-2.17389300
H	-1.71065900	0.67052200	-2.24249600
H	0.34252900	-0.24447800	-3.06534400
H	0.20582500	-1.72856900	-2.00495900
S	-3.95554700	-1.24588000	1.11837500
O	-3.54366200	-2.64872300	1.14575400
O	-4.16768500	-0.49293700	2.35175400
C	-5.41564800	-1.13708200	0.11992800

C	-5.65614400	-2.13143200	-0.82908900
C	-6.26910800	-0.03909000	0.24226300
C	-6.76731100	-2.02488000	-1.65575000
H	-4.98708800	-2.98356100	-0.90236200
C	-7.37677000	0.04741300	-0.59128400
H	-6.07443000	0.72427300	0.99043600
C	-7.64387200	-0.93831300	-1.55162900
H	-6.96097600	-2.79902100	-2.39403300
H	-8.05219300	0.89430400	-0.49649200
C	-8.85532500	-0.84403900	-2.42253200
H	-9.09050300	0.19289300	-2.67719300
H	-8.73273000	-1.40977100	-3.34958300
H	-9.73560500	-1.25073900	-1.91115400

M1S

Zero-point correction=	0.771627 (Hartree/Particle)
Thermal correction to Energy=	0.818505
Thermal correction to Enthalpy=	0.819449
Thermal correction to Gibbs Free Energy=	0.694905
Sum of electronic and zero-point Energies=	-2978.621725
Sum of electronic and thermal Energies=	-2978.574847
Sum of electronic and thermal Enthalpies=	-2978.573903
Sum of electronic and thermal Free Energies=	-2978.698447

C	7.84983200	-1.70413300	-0.82512700
C	6.65439700	-2.16318900	-0.32435400
C	5.50450400	-1.34470800	-0.39848200
C	5.59804900	-0.04917900	-1.00674100
C	6.84230600	0.39490600	-1.50812600
C	7.94412800	-0.42195200	-1.41679900
H	8.73579500	-2.32914100	-0.76877100
H	6.56245700	-3.14273600	0.13551500
H	6.89400400	1.38038000	-1.96161300
H	8.90127500	-0.08352400	-1.80172400
C	3.37071900	0.28069600	-0.63791000
C	3.28926700	-0.98650300	-0.00268800
N	4.50729000	0.75489200	-1.11438200
N	4.32809700	-1.79229200	0.11424800
P	1.80959200	1.23970500	-0.74393800
P	1.66224200	-1.46257700	0.70341500
C	2.22350500	2.69291400	0.28614600
H	3.23648800	3.02993800	0.05021800
H	1.52223900	3.50825900	0.09497700
H	2.16856800	2.44310600	1.34742100
C	1.61213700	-3.24495200	0.34712600

H	2.58126000	-3.67201400	0.61793900
H	0.82274300	-3.73806100	0.91853400
H	1.44851900	-3.42277200	-0.71830200
C	1.86503800	-1.34966300	2.57386600
C	2.40453400	0.03355900	2.92340300
C	0.50019200	-1.56238600	3.22628000
C	2.84022100	-2.42979000	3.04786700
H	3.40606000	0.20582900	2.51269200
H	1.73785700	0.82402900	2.56408900
H	2.47332400	0.13079100	4.01266800
H	0.00818700	-2.47947500	2.88079500
H	0.63302600	-1.64730400	4.31045600
H	-0.17202700	-0.72111300	3.03534700
H	3.03619700	-2.26915500	4.11405200
H	2.42505800	-3.43536700	2.93886200
H	3.79862900	-2.39115800	2.52177500
C	1.75314300	1.96388000	-2.49353500
C	2.68498800	3.16917900	-2.63011600
C	2.17164100	0.91293800	-3.52000100
C	0.31022700	2.41489600	-2.72903900
H	2.37960700	4.01009000	-2.00176600
H	3.72179700	2.91428600	-2.39417500
H	2.65276000	3.51265700	-3.67089900
H	1.59245700	-0.00956300	-3.45829200
H	2.02481700	1.32556000	-4.52467200
H	3.23132700	0.65816100	-3.42374300
H	0.21905800	2.83777500	-3.73603600
H	-0.40790700	1.59144200	-2.64279900
H	0.01237600	3.19618600	-2.02036500
Co	0.11896500	-0.14250500	-0.09240600
C	-0.30717900	3.73793700	3.69295800
C	-0.36229900	2.48955900	3.08177800
C	-0.68242300	2.38409400	1.71844600
C	-0.95997800	3.55264300	0.99190500
C	-0.91790800	4.79459400	1.61491200
C	-0.58249600	4.89369100	2.96439200
H	-0.05328700	3.80547300	4.74727100
H	-0.15600600	1.58766600	3.65375800
H	-1.20957600	3.47572100	-0.06390100
H	-1.14358400	5.68939400	1.04147100
H	-0.54017000	5.86588600	3.44684000
C	-0.73652000	1.09091000	1.06940900
C	-1.46735200	0.03592800	0.85883900
C	-2.78458100	-0.57030700	1.07416300

H	-3.55161000	0.20594400	0.89901100
H	-2.88422100	-0.89287300	2.11605000
N	-2.98240200	-1.72989400	0.19323000
C	-2.35830500	-1.58146100	-1.12833900
H	-2.75024700	-2.38435300	-1.76151100
H	-2.61401700	-0.61954700	-1.60248500
C	-0.87885300	-1.76065700	-0.99491200
C	0.05591000	-1.19358500	-1.86703700
H	-0.62461900	-2.67367700	-0.46104800
H	0.98184000	-1.71703000	-2.09845700
H	-0.29159500	-0.51263900	-2.64299800
S	-4.53354000	-2.38431300	0.24469900
O	-4.51884400	-3.52729000	-0.66314800
O	-4.83566600	-2.53687500	1.66497400
C	-5.62001500	-1.15236100	-0.42378100
C	-5.84545400	-1.10752400	-1.80195200
C	-6.18262200	-0.19892300	0.42489800
C	-6.64792300	-0.10218700	-2.32287700
H	-5.41341200	-1.86450800	-2.45040900
C	-6.98128600	0.80258300	-0.11706000
H	-6.01313500	-0.25558600	1.49618800
C	-7.22652900	0.86891100	-1.49261400
H	-6.83915900	-0.07033100	-3.39301000
H	-7.42869800	1.54414800	0.54012700
C	-8.09922600	1.93688600	-2.06916500
H	-8.39185500	2.67034000	-1.31440200
H	-7.59759700	2.46778900	-2.88444700
H	-9.01545400	1.51170100	-2.49327500

TS1R

Zero-point correction=	0.768989 (Hartree/Particle)
Thermal correction to Energy=	0.815872
Thermal correction to Enthalpy=	0.816816
Thermal correction to Gibbs Free Energy=	0.691354
Sum of electronic and zero-point Energies=	-2978.604021
Sum of electronic and thermal Energies=	-2978.557138
Sum of electronic and thermal Enthalpies=	-2978.556194
Sum of electronic and thermal Free Energies=	-2978.681656

Imaginary frequency=-97.92 cm^{-1}

C	7.16725300	-3.38026500	-0.25199000
C	5.80670300	-3.51869600	-0.10663100
C	4.97815400	-2.37486400	-0.15071400
C	5.56607500	-1.08584700	-0.36126900
C	6.96784100	-0.97504500	-0.50055700

C	7.74932800	-2.10541000	-0.44609700
H	7.80712400	-4.25666100	-0.21563800
H	5.34112700	-4.48740300	0.04947900
H	7.39518500	0.01160600	-0.65409000
H	8.82663200	-2.02384400	-0.55416800
C	3.49023600	-0.13595000	-0.31070600
C	2.91150800	-1.40932600	-0.03746000
N	4.79295500	0.02960100	-0.44357000
N	3.63709500	-2.51070000	0.02905000
P	2.33594100	1.28037600	-0.52069400
P	1.10790100	-1.45370700	0.31975100
C	2.89462200	2.48627400	0.72756800
H	3.98593900	2.55065600	0.73930500
H	2.47796900	3.47073000	0.49394500
H	2.54484900	2.19203900	1.71912500
C	0.61059600	-3.10144800	-0.27518100
H	1.38424500	-3.83093900	-0.02117000
H	-0.33317200	-3.39930700	0.19084600
H	0.48120100	-3.09476000	-1.36011600
C	1.02729300	-1.58884100	2.20592400
C	1.77419500	-0.40392800	2.81334800
C	-0.44210500	-1.52360100	2.61822400
C	1.64570300	-2.90315300	2.67613500
H	2.83917900	-0.39669100	2.55301900
H	1.33595700	0.55024500	2.49630100
H	1.70350500	-0.45130600	3.90585300
H	-1.04506400	-2.31005300	2.15272900
H	-0.51571700	-1.64936500	3.70466300
H	-0.88918500	-0.55742400	2.36039700
H	1.63250600	-2.92441300	3.77226200
H	1.08094600	-3.77210400	2.32558900
H	2.68507800	-3.01752100	2.35424000
C	2.81540800	2.08250600	-2.15981800
C	4.11668900	2.87588400	-2.02840200
C	2.99266500	1.00256000	-3.22626200
C	1.67990400	3.03930000	-2.52619800
H	4.01484400	3.72547500	-1.34714000
H	4.94596700	2.25087700	-1.68533700
H	4.38122000	3.27698600	-3.01410300
H	2.12988000	0.33518400	-3.30829100
H	3.13481200	1.48018000	-4.20214600
H	3.87796200	0.38936200	-3.03064800
H	1.92687600	3.55912900	-3.45924800
H	0.72648600	2.51970800	-2.66957500

H	1.53297500	3.80403400	-1.75415600
Co	0.30633700	0.49326100	-0.34760500
C	-0.74371900	5.73526500	0.76906800
C	-0.85196500	4.48999900	0.16006300
C	-0.54258600	3.32043500	0.87563500
C	-0.12436700	3.43374800	2.21294500
C	-0.03425900	4.68244900	2.81781200
C	-0.33724500	5.83761900	2.09884000
H	-0.98259400	6.63051200	0.20157100
H	-1.16852500	4.41273300	-0.87744300
H	0.12194900	2.53261500	2.77150000
H	0.27920700	4.75253800	3.85586600
H	-0.25644200	6.81194500	2.57187300
C	-0.61724400	2.02671800	0.23319800
C	-1.50464900	1.04632500	0.06405500
C	-2.83004800	0.61079800	0.58850900
H	-3.65375700	1.12903100	0.06629500
H	-2.90875300	0.82104800	1.65819900
N	-2.82084000	-0.83038200	0.35035900
C	-2.32198700	-1.13535800	-0.99673900
H	-1.76998600	-2.07797600	-0.98048200
H	-3.14039700	-1.22985600	-1.72841400
C	-1.44557800	0.03421000	-1.39131700
C	-0.16542600	-0.19681200	-2.08593600
H	-2.01286300	0.81361000	-1.91319800
H	0.09291900	0.51499600	-2.87005300
H	0.05191100	-1.22754500	-2.36888700
S	-4.05825000	-1.76605400	0.97112600
O	-3.67684200	-3.14548900	0.68037400
O	-4.25642000	-1.29173000	2.33700900
C	-5.49926800	-1.36941700	0.02007900
C	-5.80200900	-2.11737400	-1.12004000
C	-6.27223600	-0.26471300	0.37898400
C	-6.89558100	-1.75486100	-1.89487800
H	-5.19645300	-2.98108300	-1.37817900
C	-7.36190500	0.08365600	-0.41145500
H	-6.03266000	0.30135100	1.27481800
C	-7.69098800	-0.65127300	-1.55653000
H	-7.14311300	-2.33996200	-2.77747900
H	-7.97338100	0.93848200	-0.13325600
C	-8.87013200	-0.28290900	-2.39885100
H	-9.33320900	0.64691800	-2.06181800
H	-8.58836600	-0.16231100	-3.44986000
H	-9.63517700	-1.06649300	-2.37158200

TS1S

Zero-point correction= 0.770552 (Hartree/Particle)
Thermal correction to Energy= 0.816957
Thermal correction to Enthalpy= 0.817901
Thermal correction to Gibbs Free Energy= 0.694122
Sum of electronic and zero-point Energies= -2978.601310
Sum of electronic and thermal Energies= -2978.554905
Sum of electronic and thermal Enthalpies= -2978.553961
Sum of electronic and thermal Free Energies= -2978.677740
Imaginary frequency=-179.49 cm^{-1}

C	8.01197400	0.60063300	-0.89192700
C	7.06315000	-0.38370500	-0.74447500
C	5.70462600	-0.02928800	-0.58469600
C	5.33249600	1.35588400	-0.58140800
C	6.33118200	2.34322200	-0.73698200
C	7.64484200	1.96695300	-0.88865100
H	9.05716800	0.33113400	-1.01128200
H	7.32429400	-1.43764200	-0.74276700
H	6.03018300	3.38646900	-0.73240800
H	8.41392200	2.72415100	-1.00690600
C	3.15099500	0.76237500	-0.30295000
C	3.52484400	-0.60690300	-0.27700100
N	4.03367800	1.73429700	-0.43423300
N	4.77413800	-1.00744100	-0.41948100
P	1.35528300	1.10191400	-0.15087700
P	2.17589600	-1.80413600	0.03631400
C	1.28220200	2.21331800	1.29007600
H	2.04731400	2.98921500	1.20009100
H	0.29844100	2.68472200	1.36211800
H	1.45903100	1.64819600	2.20817100
C	2.65037400	-3.24986100	-0.95831600
H	3.65827500	-3.56674000	-0.68015300
H	1.95326200	-4.07452400	-0.78705100
H	2.65768700	-3.00167000	-2.02066000
C	2.41058700	-2.36800800	1.82318400
C	2.45115800	-1.13468300	2.72012800
C	1.21711900	-3.25171600	2.18486900
C	3.70891600	-3.16201400	1.96709000
H	3.33253300	-0.51369800	2.52281300
H	1.55648700	-0.51656500	2.59187600
H	2.49436600	-1.44737200	3.76932400
H	1.12230700	-4.10824100	1.50733800
H	1.35254300	-3.64784800	3.19754300

H	0.27651500	-2.69120000	2.16576000
H	3.87622600	-3.36501800	3.03125900
H	3.66173800	-4.12722900	1.45544400
H	4.57975600	-2.61489300	1.59244600
C	0.89202900	2.19340900	-1.61924300
C	1.35697100	3.63232100	-1.39972400
C	1.54573300	1.63198800	-2.88027300
C	-0.63393600	2.15447000	-1.72735900
H	0.84487100	4.10991600	-0.55933400
H	2.43612900	3.69073200	-1.22988500
H	1.12679300	4.21553500	-2.29922500
H	1.37226200	0.55846800	-3.00217700
H	1.13351500	2.13876300	-3.76015500
H	2.62698100	1.80334500	-2.87925100
H	-0.96293400	2.81496100	-2.53823800
H	-1.00464300	1.14565700	-1.94435100
H	-1.11562500	2.50061800	-0.80392200
Co	0.28314900	-0.78347900	-0.16573800
C	-1.34411500	1.33256900	4.49906600
C	-0.93595800	0.42081000	3.53090400
C	-1.38567700	0.54559700	2.20792200
C	-2.25601600	1.60077400	1.88198300
C	-2.64742700	2.51608000	2.85272300
C	-2.18955000	2.38896200	4.16365500
H	-0.99359600	1.22008600	5.52144500
H	-0.27541700	-0.40059300	3.79734500
H	-2.61278100	1.69603300	0.85761200
H	-3.31556500	3.33059500	2.58291100
H	-2.49629900	3.10461700	4.92089400
C	-0.95477900	-0.36207100	1.16151100
C	-1.54872100	-1.30378500	0.45084100
C	-2.87188200	-1.96993700	0.58581000
H	-3.55462700	-1.30355200	1.12904300
H	-2.76862700	-2.88369100	1.18558700
N	-3.37741500	-2.31020400	-0.75415300
C	-2.39412500	-1.94033700	-1.77497900
H	-2.52413200	-2.57740300	-2.65271600
H	-2.48846900	-0.88900100	-2.09469400
C	-1.02084600	-2.15153600	-1.19419500
C	0.07154200	-1.56017900	-1.95221200
H	-0.85926800	-3.17822600	-0.85573500
H	0.80059000	-2.24527500	-2.37255300
H	-0.22033400	-0.77193700	-2.65044100
S	-4.97293700	-1.88410100	-1.07698200

O	-5.17978900	-2.22129800	-2.48182600
O	-5.76832300	-2.48209100	-0.01014500
C	-5.05613500	-0.12099200	-0.89739200
C	-4.62534400	0.70286000	-1.94255300
C	-5.49004300	0.42649900	0.31014000
C	-4.61012800	2.07892900	-1.75720800
H	-4.32846200	0.27048300	-2.89410400
C	-5.48521900	1.80793500	0.46923100
H	-5.84295300	-0.22524300	1.10387700
C	-5.03224600	2.65358300	-0.54926700
H	-4.27550000	2.72398400	-2.56675900
H	-5.83557100	2.23851100	1.40422600
C	-4.97569300	4.13447500	-0.35328300
H	-5.50903900	4.44530200	0.54829100
H	-3.93767400	4.47687100	-0.25894500
H	-5.40268900	4.67083500	-1.20601900

M2R

Zero-point correction=	0.771816 (Hartree/Particle)
Thermal correction to Energy=	0.818648
Thermal correction to Enthalpy=	0.819592
Thermal correction to Gibbs Free Energy=	0.693436
Sum of electronic and zero-point Energies=	-2978.607430
Sum of electronic and thermal Energies=	-2978.560598
Sum of electronic and thermal Enthalpies=	-2978.559654
Sum of electronic and thermal Free Energies=	-2978.685810

C	7.71762300	-2.50403500	-0.91764300
C	6.50367500	-2.80246400	-0.34577400
C	5.45145800	-1.86075900	-0.40612200
C	5.66498200	-0.60709100	-1.06736100
C	6.92462900	-0.32899000	-1.64446800
C	7.92905800	-1.26442600	-1.56728000
H	8.52864000	-3.22474800	-0.87173500
H	6.32302200	-3.74690100	0.15915300
H	7.06612500	0.62657400	-2.14114400
H	8.89834400	-1.05581100	-2.01019800
C	3.51078100	-0.00262200	-0.60825900
C	3.30838200	-1.23391000	0.08341200
N	4.66871400	0.31149900	-1.15710000
N	4.25752700	-2.14946600	0.17447200
P	2.08435700	1.16226700	-0.75708400
P	1.67990900	-1.49722400	0.88689700
C	2.61964200	2.65108300	0.14482200
H	3.64493500	2.91465600	-0.12966800

H	1.94943700	3.48055400	-0.10010200
H	2.57788500	2.48111900	1.22282100
C	1.34799800	-3.26210600	0.60851200
H	2.23136800	-3.85677300	0.85672300
H	0.50458600	-3.58931100	1.22170500
H	1.09801200	-3.43123400	-0.44204900
C	1.99100800	-1.28951100	2.72228700
C	2.46766700	0.15151600	2.89931100
C	0.63810600	-1.46390000	3.41515900
C	3.00528700	-2.27935200	3.27786100
H	3.45314000	0.32089100	2.44945700
H	1.76098600	0.85877400	2.43709100
H	2.53588200	0.40453600	3.96330900
H	0.22896000	-2.47118000	3.28615300
H	0.75412800	-1.29192700	4.49120500
H	-0.10463900	-0.74444500	3.04467500
H	3.15539500	-2.08512100	4.34668100
H	2.66059300	-3.31364600	3.17864600
H	3.97780700	-2.19552700	2.78434500
C	2.00769800	1.69668300	-2.55929700
C	3.16787000	2.64242800	-2.88602300
C	2.09290600	0.46480600	-3.45996500
C	0.69347200	2.45356300	-2.75990400
H	3.10414700	3.58254100	-2.33057300
H	4.14162700	2.18648900	-2.69271700
H	3.11436900	2.88967100	-3.95266500
H	1.34519000	-0.29625900	-3.21854200
H	1.92983700	0.76945900	-4.49954400
H	3.08120600	-0.00266900	-3.40589500
H	0.65502700	2.82834100	-3.78898500
H	-0.18892900	1.82910100	-2.59423300
H	0.62203100	3.32118100	-2.09349200
Co	0.39941900	0.27063700	0.26382000
C	-1.00610200	5.33755200	0.83355300
C	-1.17119000	4.08260400	0.25706800
C	-0.84215000	2.91710400	0.97219800
C	-0.35760400	3.05232000	2.28579900
C	-0.20637700	4.30943500	2.86170000
C	-0.52081600	5.45700900	2.13558600
H	-1.26284800	6.22717000	0.26483900
H	-1.54864400	3.99110300	-0.75910900
H	-0.11785500	2.15878400	2.86080400
H	0.15619600	4.39250800	3.88282300
H	-0.39620500	6.43825000	2.58421600

C	-0.92036200	1.61522300	0.32668900
C	-1.96609500	0.77189600	0.20011500
C	-3.24926800	0.68185000	0.97235100
H	-4.09632000	1.06549600	0.37943800
H	-3.22841300	1.21717700	1.92465600
N	-3.36106000	-0.78485100	1.19098200
C	-2.41458700	-1.53189400	0.31943700
H	-1.59415100	-1.93423800	0.93207800
H	-2.91272700	-2.37603400	-0.16615700
C	-1.89772800	-0.47943200	-0.65360900
C	-0.50408400	-0.63912100	-1.19925800
H	-2.64505700	-0.37222300	-1.46196800
H	-0.37500000	-0.10474200	-2.14090000
H	-0.16697300	-1.67425400	-1.31266700
S	-4.89912600	-1.41147600	1.38019200
O	-4.71625600	-2.83425400	1.65499100
O	-5.57251400	-0.52135400	2.32184700
C	-5.70429300	-1.25745400	-0.19381000
C	-5.55462900	-2.26893600	-1.14511900
C	-6.41369000	-0.09336000	-0.49669600
C	-6.11452800	-2.10333200	-2.40599300
H	-5.02282900	-3.18117500	-0.88971100
C	-6.97151300	0.05121500	-1.76144600
H	-6.54292300	0.67537500	0.25935000
C	-6.82893200	-0.94452500	-2.73597600
H	-6.00464900	-2.89042500	-3.14813200
H	-7.53165000	0.95244700	-1.99921500
C	-7.45793800	-0.78864500	-4.08356500
H	-7.47087100	0.25645500	-4.40424700
H	-6.93883000	-1.37813100	-4.84370500
H	-8.49988800	-1.12905000	-4.06917400

M2S

Zero-point correction=	0.771287 (Hartree/Particle)
Thermal correction to Energy=	0.818216
Thermal correction to Enthalpy=	0.819160
Thermal correction to Gibbs Free Energy=	0.692901
Sum of electronic and zero-point Energies=	-2978.621108
Sum of electronic and thermal Energies=	-2978.574180
Sum of electronic and thermal Enthalpies=	-2978.573236
Sum of electronic and thermal Free Energies=	-2978.699495

C	-7.61455600	-1.05845500	-2.33599200
C	-6.41834200	-0.40204000	-2.50230000
C	-5.43662900	-0.47272800	-1.48821900

C	-5.69178600	-1.24439900	-0.30757700
C	-6.93438900	-1.90304300	-0.16429100
C	-7.87493500	-1.80555800	-1.16263400
H	-8.37538100	-1.00105500	-3.10872000
H	-6.20226800	0.18480900	-3.39003700
H	-7.11365600	-2.47948100	0.73862400
H	-8.83056100	-2.31010700	-1.05593800
C	-3.60676400	-0.72897500	0.47870200
C	-3.39624700	0.11420100	-0.65184300
N	-4.74617300	-1.37385200	0.66017400
N	-4.27788900	0.22220900	-1.62756000
P	-2.17106600	-0.97602900	1.59925000
P	-1.87895700	1.15357700	-0.71871500
C	-2.72199900	-0.35394900	3.22833800
H	-3.74457000	-0.67130700	3.44876500
H	-2.05146300	-0.73922800	4.00209500
H	-2.67372800	0.73636100	3.25443700
C	-1.53330400	1.28007400	-2.49450100
H	-2.35885400	1.79665500	-2.99163500
H	-0.60677000	1.83324300	-2.65833500
H	-1.44165800	0.28266100	-2.92831000
C	-2.46108600	2.87254100	-0.20140400
C	-2.56867600	2.88249200	1.31997500
C	-1.42158500	3.88408400	-0.68091400
C	-3.82057800	3.20648700	-0.81150100
H	-3.28482500	2.13113600	1.67326400
H	-1.59854500	2.70187300	1.79812200
H	-2.92423100	3.86167200	1.66006600
H	-1.41186100	3.97082900	-1.77174500
H	-1.67465800	4.87000100	-0.27524300
H	-0.40939200	3.63923500	-0.34524900
H	-4.05008600	4.25410500	-0.58398500
H	-3.83727300	3.09540300	-1.89975400
H	-4.62395700	2.59453000	-0.39237100
C	-2.03645000	-2.84074700	1.85775900
C	-3.15306200	-3.37010200	2.75634500
C	-2.08392400	-3.54969500	0.50657200
C	-0.68230400	-3.08329900	2.52657400
H	-3.10644800	-2.94984900	3.76516800
H	-4.14419900	-3.16884800	2.34138700
H	-3.04012800	-4.45653500	2.85169100
H	-1.29878100	-3.20400500	-0.17217100
H	-1.93205600	-4.62383400	0.66191600
H	-3.05140200	-3.42449700	0.00966800

H	-0.56893200	-4.15243000	2.73944400
H	0.15354300	-2.78495600	1.88469700
H	-0.59153700	-2.54981000	3.47947900
Co	-0.45564100	0.27358200	0.61513200
C	2.55023900	4.52847400	1.48882800
C	2.20932600	3.52318400	0.58992200
C	1.44378100	2.41766300	1.00258900
C	1.03193400	2.36720700	2.34901300
C	1.36914800	3.37363300	3.24616300
C	2.13243100	4.45958500	2.81763800
H	3.14231400	5.37457800	1.14998600
H	2.51571200	3.59901400	-0.45125100
H	0.44784000	1.50856100	2.69082900
H	1.04338600	3.31072800	4.28097400
H	2.39953600	5.24815200	3.51540600
C	1.03538900	1.34212500	0.09915200
C	1.73643200	0.84143600	-0.94073700
C	3.14691400	1.08066000	-1.39368700
H	3.83918300	1.15129500	-0.53765000
H	3.27650900	1.99139300	-1.98916600
N	3.41015900	-0.10157300	-2.24822200
C	2.44918100	-1.16980100	-1.91438200
H	2.36921000	-1.87405400	-2.74414300
H	2.74760700	-1.72010500	-1.00457300
C	1.17873800	-0.35767900	-1.64226600
C	0.13449500	-0.98490600	-0.74179600
H	0.75357100	-0.07834400	-2.61619100
H	-0.67639000	-1.50101300	-1.26743900
H	0.60178300	-1.67376500	-0.01697600
S	5.00646000	-0.53438900	-2.49189000
O	4.97929600	-1.65733900	-3.42547800
O	5.71082900	0.70678200	-2.80314900
C	5.60721000	-1.13132900	-0.93275400
C	5.45457900	-2.48087100	-0.60918900
C	6.16235900	-0.23614800	-0.01627200
C	5.86944100	-2.93084300	0.63804500
H	5.03533500	-3.16891500	-1.33756800
C	6.56997400	-0.70457300	1.22716600
H	6.29324100	0.80761900	-0.28723000
C	6.43288400	-2.05436100	1.57451600
H	5.76233900	-3.98328200	0.89054800
H	7.00966100	-0.01302500	1.94170400
C	6.91051800	-2.55453300	2.90007700
H	6.87493400	-1.77324100	3.66376100

H	6.32169100	-3.40774600	3.24708700
H	7.95167400	-2.89201500	2.83778400

TS2R

Zero-point correction= 0.971204 (Hartree/Particle)
Thermal correction to Energy= 1.028367
Thermal correction to Enthalpy= 1.029311
Thermal correction to Gibbs Free Energy= 0.885734
Sum of electronic and zero-point Energies= -3589.277197
Sum of electronic and thermal Energies= -3589.220034
Sum of electronic and thermal Enthalpies= -3589.219089
Sum of electronic and thermal Free Energies= -3589.362666
Imaginary frequency=-1300.45 cm^{-1}

C	-3.74203100	5.45349800	-0.80184300
C	-3.55469000	4.36157800	0.01352400
C	-2.27333100	3.77402200	0.11025000
C	-1.18275000	4.33127900	-0.62646500
C	-1.40693200	5.44677100	-1.46307400
C	-2.66686400	5.99334900	-1.54584000
H	-4.72579000	5.90569400	-0.88439700
H	-4.36943900	3.92220100	0.58262700
H	-0.56897600	5.84546300	-2.02808800
H	-2.84396400	6.85096800	-2.18804600
C	0.21424200	2.72640700	0.21494800
C	-0.89705500	2.11980200	0.89189800
N	0.06539500	3.79716400	-0.53899400
N	-2.10264000	2.65159600	0.85733500
P	1.83948100	1.88659000	0.39034800
P	-0.67446700	0.45842800	1.68624900
C	2.33740800	2.45884100	2.05461700
H	2.25805200	3.54433200	2.14669200
H	3.36501000	2.15069600	2.26496000
H	1.69602800	2.00490800	2.80514700
C	-2.20702200	-0.41934600	1.21441400
H	-3.02968100	0.29786600	1.17424000
H	-2.43186100	-1.17830300	1.96674800
H	-2.10984800	-0.91281200	0.25147400
C	-1.11283200	0.71111200	3.56097000
C	-0.25748000	1.77754800	4.24259000
C	-0.98199100	-0.63182200	4.28376400
C	-2.57611900	1.16204200	3.67768100
H	-0.24015300	2.71874100	3.68231500
H	0.77245200	1.46456100	4.43126900
H	-0.69330400	1.99296800	5.22425000

H	-1.67899300	-1.37982300	3.89301000
H	-1.23658900	-0.48199700	5.33953200
H	0.02180600	-1.06179300	4.25000600
H	-2.77235000	1.36901900	4.73607300
H	-3.28158700	0.38707800	3.36918500
H	-2.78768500	2.07260300	3.11201400
C	3.12666900	2.74953800	-0.68612000
C	3.28654600	4.21891000	-0.29087100
C	2.76552200	2.64613500	-2.16190200
C	4.45122300	2.01775300	-0.44787400
H	3.69257100	4.33661400	0.71747900
H	2.34607000	4.77105500	-0.36175100
H	4.00093300	4.68277400	-0.98114100
H	2.70548600	1.60288300	-2.48317600
H	3.55330200	3.12870700	-2.75260800
H	1.81864800	3.14117800	-2.39162100
H	5.23917500	2.52470900	-1.01645700
H	4.41069000	0.98179500	-0.79455000
H	4.75778600	2.02196900	0.60358200
Co	1.21506200	-0.39592000	0.52382400
C	-2.24483200	1.95581800	-2.80817300
C	-1.76668800	0.99935400	-1.91839200
C	-0.49111300	0.42525600	-2.07712900
C	0.26048100	0.82396300	-3.19048500
C	-0.21389100	1.78377300	-4.08056900
C	-1.46367700	2.36530000	-3.88717700
H	-3.23433100	2.38167900	-2.65774700
H	-2.39843100	0.68606300	-1.09245200
H	1.23154900	0.37333500	-3.36659000
H	0.39946300	2.07380200	-4.92984400
H	-1.83252100	3.12005100	-4.57627600
C	-0.02031700	-0.62245100	-1.14153200
C	-0.49644500	-1.87958200	-1.22407100
C	-1.58958200	-2.42654500	-2.08676300
H	-2.43341500	-1.72501200	-2.15302400
H	-1.26829900	-2.63739900	-3.11381800
N	-1.95566100	-3.69179600	-1.40384800
C	-1.30150400	-3.76923600	-0.07705400
H	-1.11964600	-4.81295100	0.18526600
H	-1.92733300	-3.31392900	0.70966400
C	-0.03267400	-2.93578200	-0.27008600
C	0.57854000	-2.29380700	0.95910900
H	0.71073100	-3.56156300	-0.78959600
H	1.44455600	-2.84985700	1.33220400

H	-0.15019600	-2.22291300	1.77481800
S	-3.57060800	-4.12695300	-1.47236300
O	-3.67356200	-5.39355400	-0.75293700
O	-3.96272200	-4.00036300	-2.87330900
C	-4.44618500	-2.89036900	-0.54448700
C	-4.62139300	-3.05800000	0.82976200
C	-4.87525500	-1.72027200	-1.17976100
C	-5.21841300	-2.04134300	1.56870400
H	-4.30826300	-3.98224500	1.30696600
C	-5.46229100	-0.71405900	-0.42412000
H	-4.76445900	-1.61273700	-2.25510600
C	-5.63453300	-0.85177800	0.96074600
H	-5.35785700	-2.16801100	2.64018400
H	-5.79525800	0.19822000	-0.91508000
C	-6.22394100	0.26316000	1.76360700
H	-5.58430800	1.15400100	1.72562600
H	-6.34774700	-0.01388100	2.81344800
H	-7.20132600	0.56635700	1.37447600
C	4.94568300	-1.70762700	-0.65881400
C	4.56119400	-1.53746000	-2.01161000
C	5.50034300	-1.71195300	-3.03571100
C	6.80856100	-2.02149800	-2.69711800
C	7.18839800	-2.13510200	-1.35260400
C	6.27332400	-1.97461500	-0.31702100
C	2.74431300	-1.05911600	-0.72410500
C	3.19235100	-1.13277100	-2.01910600
H	5.20371800	-1.59005800	-4.07396100
H	7.55189000	-2.15924900	-3.47677000
H	8.22377700	-2.34877900	-1.10433700
H	6.61918400	-2.03744700	0.70637600
H	1.44899900	-1.05655700	-0.89526500
H	2.59075900	-0.94687400	-2.89783100
N	3.80287200	-1.46602000	0.12290500
C	3.69517300	-1.39699900	1.50055900
C	4.59122800	-2.00636300	2.38421300
N	2.60691200	-0.72592700	1.94163700
C	4.40104000	-1.84883100	3.74667000
H	5.38805600	-2.63329200	2.01127900
C	2.43949300	-0.59253600	3.26706800
C	3.31614500	-1.10550000	4.20495900
H	5.08733300	-2.31954700	4.44321700
H	1.55176500	-0.05414300	3.56542000
H	3.12750500	-0.95174200	5.26123600

TS2S

Zero-point correction= 0.970415 (Hartree/Particle)
Thermal correction to Energy= 1.028024
Thermal correction to Enthalpy= 1.028968
Thermal correction to Gibbs Free Energy= 0.882515
Sum of electronic and zero-point Energies= -3589.270916
Sum of electronic and thermal Energies= -3589.213307
Sum of electronic and thermal Enthalpies= -3589.212362
Sum of electronic and thermal Free Energies= -3589.358816
Imaginary frequency= -1120.79 cm^{-1}

C	-4.53945300	-6.17746400	-0.54871800
C	-3.45939900	-5.62213400	0.09702600
C	-3.32827300	-4.21646800	0.15400100
C	-4.32626800	-3.38838400	-0.44573200
C	-5.41742500	-3.98684600	-1.11448000
C	-5.51709900	-5.35811600	-1.16026200
H	-4.64389700	-7.25707500	-0.59834900
H	-2.69084500	-6.23378600	0.56105600
H	-6.16184000	-3.34122700	-1.57185100
H	-6.35636900	-5.82305700	-1.66888700
C	-3.19396100	-1.51996900	0.24147200
C	-2.14815800	-2.34607900	0.76080600
N	-4.24345800	-2.03397300	-0.36923100
N	-2.23083800	-3.66231900	0.73317200
P	-2.99133700	0.29297400	0.45939500
P	-0.53572600	-1.59090400	1.29116300
C	-3.68987900	0.42870600	2.15093000
H	-4.67572400	-0.04087900	2.19942400
H	-3.77590800	1.47592900	2.45161100
H	-3.03779800	-0.07833700	2.86542200
C	0.55030200	-2.69706200	0.30526600
H	0.20449000	-3.72160100	0.45311600
H	1.59736900	-2.62653700	0.60892800
H	0.47352200	-2.46256200	-0.75571800
C	-0.22318000	-2.27470200	3.05255200
C	-1.45672300	-2.10025100	3.93554500
C	0.98292200	-1.52239200	3.61678500
C	0.11421800	-3.76877400	3.02162800
H	-2.32604900	-2.62762700	3.52790800
H	-1.73955000	-1.05926900	4.10297100
H	-1.25071700	-2.52838800	4.92312100
H	1.86353900	-1.63224400	2.97125300
H	1.24609900	-1.94049500	4.59549700
H	0.79593000	-0.45302300	3.75260100

H	0.21445100	-4.11222400	4.05816600
H	1.06443200	-3.97243100	2.52228400
H	-0.66899200	-4.36362900	2.54414500
C	-4.30447900	1.16525700	-0.57736900
C	-5.72703600	0.72739900	-0.21727200
C	-4.02661700	0.89301600	-2.05404000
C	-4.19727300	2.66472600	-0.28365900
H	-6.00105100	1.02352700	0.79994000
H	-5.87858200	-0.34720800	-0.32557700
H	-6.41918200	1.23989700	-0.89645900
H	-3.00121400	1.15802200	-2.33593200
H	-4.70648900	1.49497300	-2.66852900
H	-4.19122100	-0.15905200	-2.30662600
H	-5.00497300	3.18157400	-0.81453800
H	-3.25509700	3.09276300	-0.62421800
H	-4.31820900	2.88949300	0.78221500
Co	-0.63061600	0.71454700	0.55242900
C	-1.95538000	-1.66493700	-3.77687000
C	-1.33945600	-1.34295100	-2.57149700
C	-0.41232600	-0.29423200	-2.48279300
C	-0.10110300	0.40342700	-3.66448800
C	-0.72107900	0.08823200	-4.86965000
C	-1.65796200	-0.94242900	-4.93021400
H	-2.67476000	-2.48024100	-3.80892600
H	-1.57070900	-1.92471100	-1.68558500
H	0.63005500	1.20829400	-3.62534200
H	-0.46990500	0.65012200	-5.76534600
H	-2.14666300	-1.18341600	-5.87012700
C	0.25915400	0.03879600	-1.20990700
C	1.58421300	-0.12287700	-1.02894400
C	2.65651300	-0.61660800	-1.95735800
H	2.57201100	-1.68426600	-2.19268500
H	2.65911700	-0.08433500	-2.91478000
N	3.93431800	-0.32953700	-1.24263200
C	3.61861500	0.60675600	-0.13139300
H	3.64272900	1.62849400	-0.52941400
H	4.37209000	0.52942100	0.65707600
C	2.20516300	0.20099600	0.28768400
C	1.30672500	1.11401700	1.06985400
H	2.31346000	-0.74908500	0.83564500
H	1.47369300	2.17045600	0.81736800
H	1.40645400	0.99785900	2.15289600
S	4.76373900	-1.71562900	-0.73250600
O	4.79371800	-2.60249900	-1.89658400

O	4.25913000	-2.24061700	0.54608400
C	6.37118800	-1.02881800	-0.43699600
C	7.05381400	-0.41233200	-1.48798100
C	6.94351400	-1.14117500	0.82625700
C	8.32082800	0.10041300	-1.25721500
H	6.59195400	-0.33089100	-2.46769200
C	8.21770900	-0.62274000	1.03790300
H	6.39354400	-1.62651300	1.62645600
C	8.92338300	0.00509500	0.00712600
H	8.85814300	0.58610600	-2.06819700
H	8.67321700	-0.70589100	2.02152000
C	10.28864300	0.56890900	0.23732400
H	10.64469500	0.36478700	1.24966100
H	10.29979000	1.65428200	0.08967900
H	11.01473800	0.15285000	-0.46848100
C	-1.11561200	4.73376000	-0.19860300
C	-1.18955300	4.40987100	-1.57744800
C	-1.44971000	5.40932900	-2.52326200
C	-1.65729500	6.70694600	-2.08381700
C	-1.62743900	7.00729200	-0.71457900
C	-1.36867700	6.03367400	0.24540700
C	-0.80667400	2.47012300	-0.44759300
C	-1.00433000	3.00079900	-1.70061800
H	-1.49748500	5.15907100	-3.57937700
H	-1.85782900	7.49726200	-2.80120600
H	-1.81553400	8.02528700	-0.38572900
H	-1.38488600	6.30901000	1.29160600
H	0.00885800	1.45545500	-0.71153900
H	-0.99978100	2.43798500	-2.62317200
N	-0.83468400	3.53853400	0.48174600
C	-0.83641700	3.27196600	1.84129800
C	-0.68489500	4.24654600	2.83189900
N	-0.95329800	1.95796600	2.14389700
C	-0.71313200	3.85952500	4.16083700
H	-0.49809100	5.27657100	2.56599300
C	-0.96816900	1.60722500	3.43960700
C	-0.87566300	2.51350500	4.47971200
H	-0.59140300	4.60517600	4.93992100
H	-1.05414600	0.54512000	3.62384700
H	-0.90463900	2.16530100	5.50546300

M3R

Zero-point correction= 0.973557 (Hartree/Particle)

Thermal correction to Energy= 1.032319

Thermal correction to Enthalpy=			1.033263
Thermal correction to Gibbs Free Energy=			0.881580
Sum of electronic and zero-point Energies=			-3589.334705
Sum of electronic and thermal Energies=			-3589.275943
Sum of electronic and thermal Enthalpies=			-3589.274999
Sum of electronic and thermal Free Energies=			-3589.426682
C	7.44124900	-3.08275600	2.64296600
C	6.07471300	-2.93745900	2.67931200
C	5.40857900	-2.31988600	1.59689200
C	6.16964800	-1.83066400	0.48501300
C	7.57236300	-2.00589800	0.47187700
C	8.19090300	-2.62142400	1.53447100
H	7.95618700	-3.56233500	3.46979900
H	5.48071500	-3.29482400	3.51536400
H	8.13233000	-1.63242000	-0.38063900
H	9.26876600	-2.75283200	1.53096800
C	4.25470200	-1.01942900	-0.46855600
C	3.49123100	-1.62790600	0.57168100
N	5.56706000	-1.15955500	-0.53118400
N	4.05268600	-2.23977500	1.59860800
P	3.36696400	0.10944200	-1.62748800
P	1.67433700	-1.68638300	0.36406300
C	3.75902900	-0.49722400	-3.30747100
H	4.79783700	-0.83190600	-3.37171300
H	3.60701500	0.32014900	-4.01884000
H	3.10242300	-1.32219600	-3.59087200
C	1.01607100	-1.88368100	2.04678900
H	1.16244600	-2.90989700	2.39513400
H	-0.05227700	-1.65199300	2.06182400
H	1.53588900	-1.21771800	2.73732600
C	1.41326400	-3.36912400	-0.48214300
C	1.68944300	-3.15950100	-1.96861600
C	-0.02801200	-3.83274000	-0.27042500
C	2.36242700	-4.42540400	0.07861300
H	2.74997300	-2.95545000	-2.15285400
H	1.09991800	-2.32430700	-2.37360600
H	1.42763700	-4.06075100	-2.53452500
H	-0.29236800	-3.90174200	0.78953900
H	-0.13413700	-4.83605000	-0.69826900
H	-0.75736100	-3.18962300	-0.76766200
H	2.12084500	-5.38984900	-0.38282600
H	2.26431600	-4.54720200	1.16208100
H	3.41007300	-4.20757300	-0.14688800
C	4.37598400	1.71188300	-1.51931500

C	5.70529400	1.58565800	-2.26432800
C	4.63950700	2.05353000	-0.05383000
C	3.54715400	2.82256400	-2.16348000
H	5.56694200	1.47137700	-3.34342000
H	6.31025300	0.75256600	-1.89808100
H	6.27290800	2.51051100	-2.10629600
H	3.71672200	2.09119400	0.53361800
H	5.11023400	3.04189000	0.00075800
H	5.32259900	1.34122700	0.41912800
H	4.17354500	3.71497200	-2.27499300
H	2.69314900	3.09910200	-1.54181000
H	3.18295700	2.55261100	-3.16185800
Co	1.06934500	-0.03449700	-1.01831100
C	-4.23750700	1.63636100	4.61650600
C	-3.86822600	1.39514700	3.29725100
C	-2.55280200	1.00847800	2.97505700
C	-1.63309200	0.88855900	4.03585500
C	-2.00224600	1.13269900	5.35172000
C	-3.31188500	1.50585300	5.65034800
H	-5.25916300	1.93390400	4.83789600
H	-4.61322400	1.52392200	2.51976200
H	-0.60700500	0.60730400	3.80294200
H	-1.26695300	1.03358500	6.14594800
H	-3.60704400	1.69969600	6.67783700
C	-2.06343500	0.72324400	1.63240900
C	-2.70333300	0.70235700	0.44910400
C	-4.16968800	0.90691500	0.19837500
H	-4.76513800	0.22434000	0.82959700
H	-4.52262100	1.92480900	0.39881400
N	-4.32676100	0.60254100	-1.23882600
C	-3.20739400	-0.25303300	-1.65245100
H	-3.07389200	-0.20772700	-2.73580000
H	-3.35830300	-1.30623500	-1.35362700
C	-2.04179600	0.35631400	-0.86687000
C	-0.83494000	-0.56312800	-0.80034600
H	-1.81223800	1.30211100	-1.37981400
H	-0.76938800	-1.15014400	-1.73956300
H	-0.99658800	-1.26950100	0.02003200
S	-5.86028100	0.18711900	-1.76449100
O	-5.73746800	-0.04601600	-3.20096500
O	-6.75649900	1.20727300	-1.22584400
C	-6.25428100	-1.35779000	-0.98652100
C	-5.90853000	-2.55588400	-1.61240300
C	-6.84807100	-1.35876100	0.27818500

C	-6.16737800	-3.75882200	-0.96455800
H	-5.46031400	-2.54317700	-2.60179000
C	-7.09581500	-2.56982200	0.91069100
H	-7.12956800	-0.41948000	0.74556300
C	-6.76199600	-3.78742000	0.30231000
H	-5.90959500	-4.69594800	-1.45265700
H	-7.56341700	-2.57477700	1.89254800
C	-7.05141100	-5.08385100	0.98911700
H	-6.72885900	-5.06397700	2.03449500
H	-6.55779600	-5.92327000	0.49371300
H	-8.12706400	-5.29289200	0.99851600
C	0.50808800	3.51088900	0.73188100
C	1.04850500	2.89293800	1.89122100
C	1.14841300	3.62732700	3.07828700
C	0.72531100	4.95066800	3.09230900
C	0.19756800	5.54534100	1.94035200
C	0.07871800	4.83635300	0.74629700
C	1.05169900	1.31903600	0.24910200
C	1.37583600	1.53558200	1.56179000
H	1.54918400	3.16182000	3.97565200
H	0.79721000	5.52982100	4.00879000
H	-0.13539300	6.57860100	1.97139800
H	-0.35466900	5.32579600	-0.11739800
H	-0.99808300	0.49633700	1.59408900
H	1.80755100	0.81164300	2.23938900
N	0.52087700	2.53064900	-0.27197600
C	0.26095700	2.58152700	-1.62438300
C	-0.18611400	3.68653600	-2.35357400
N	0.51479500	1.39875900	-2.23563600
C	-0.39030800	3.54334200	-3.71606700
H	-0.37110900	4.63340700	-1.86807200
C	0.30478800	1.27060600	-3.55552100
C	-0.15030000	2.31675200	-4.33710600
H	-0.73936800	4.39277400	-4.29459700
H	0.51755700	0.29045700	-3.97627400
H	-0.30776800	2.17401800	-5.39949900

M3S

Zero-point correction=	0.974247 (Hartree/Particle)
Thermal correction to Energy=	1.032462
Thermal correction to Enthalpy=	1.033406
Thermal correction to Gibbs Free Energy=	0.884653
Sum of electronic and zero-point Energies=	-3589.332075
Sum of electronic and thermal Energies=	-3589.273859

Sum of electronic and thermal Enthalpies= -3589.272915

Sum of electronic and thermal Free Energies= -3589.421668

C	7.13338800	3.47817400	-0.99031600
C	5.80759900	3.52001300	-0.62871200
C	5.01312000	2.35686400	-0.74791900
C	5.61028200	1.14115400	-1.21878800
C	6.97150000	1.13511400	-1.59931800
C	7.71430200	2.28585400	-1.48448100
H	7.74523600	4.37119500	-0.90564700
H	5.34145500	4.42991700	-0.26226000
H	7.40231100	0.20621100	-1.96141800
H	8.76224100	2.28377600	-1.76815400
C	3.63044500	0.04889700	-0.88551200
C	3.00346000	1.28876300	-0.56984700
N	4.89779700	-0.01516700	-1.25321900
N	3.68504500	2.41502500	-0.46830500
P	2.65762700	-1.47549800	-0.57476600
P	1.16806300	1.33065300	-0.48006700
C	2.82883500	-2.47104000	-2.09648800
H	3.84955300	-2.41768200	-2.48496400
H	2.58690900	-3.51499000	-1.87649300
H	2.14115700	-2.11129400	-2.86596400
C	0.85885400	2.83285300	0.48955400
H	1.38625500	3.66651500	0.01689400
H	-0.20971400	3.04555400	0.52246900
H	1.23331500	2.72817100	1.50892000
C	0.70184600	1.83821800	-2.25274200
C	0.59318500	0.54678900	-3.06078200
C	-0.62538500	2.60081700	-2.22521100
C	1.75867300	2.74181900	-2.88520500
H	1.57040700	0.05196200	-3.13412000
H	-0.12494500	-0.16252000	-2.62371000
H	0.26099200	0.76296800	-4.08304100
H	-0.50641800	3.58941500	-1.77140900
H	-0.96390300	2.75612400	-3.25648400
H	-1.42766600	2.08119600	-1.69167300
H	1.37650200	3.10886400	-3.84493900
H	1.98741400	3.61408100	-2.26454200
H	2.69497900	2.21231000	-3.08634200
C	3.72563800	-2.39433600	0.68979000
C	4.96014800	-3.00304500	0.02539900
C	4.15038000	-1.41365200	1.78200800
C	2.87940300	-3.51018200	1.30027400
H	4.69787900	-3.79739900	-0.67992000

H	5.56333300	-2.25601800	-0.49717700
H	5.58290300	-3.45460400	0.80675700
H	3.29252700	-0.89418700	2.22327100
H	4.65165200	-1.96735400	2.58380000
H	4.85662400	-0.66476900	1.40971000
H	3.52795100	-4.16748400	1.89053600
H	2.12138100	-3.10883600	1.97584100
H	2.38509300	-4.13007000	0.54251200
Co	0.43495200	-0.78985700	-0.12547300
C	-3.28340800	5.86741400	0.70935500
C	-3.05448600	4.49641700	0.65207400
C	-2.53036600	3.80579200	1.76036800
C	-2.20655400	4.55214900	2.90741900
C	-2.43784600	5.92096300	2.96400900
C	-2.98537300	6.58455500	1.86638800
H	-3.68736200	6.38006500	-0.15982400
H	-3.24991600	3.96521500	-0.27580800
H	-1.77565300	4.03644500	3.76339500
H	-2.18786500	6.47413000	3.86545400
H	-3.16436900	7.65539100	1.90721100
C	-2.26671000	2.36999100	1.75628500
C	-2.82440100	1.41822700	0.98859400
C	-3.96450300	1.55468200	0.02340000
H	-3.61055400	1.75999500	-1.00233300
H	-4.66667000	2.35083200	0.29014100
N	-4.62324700	0.23449200	0.09910500
C	-3.81289600	-0.71651000	0.89338300
H	-4.28472700	-0.85368900	1.87338200
H	-3.76352700	-1.69675300	0.40473700
C	-2.44399300	-0.03867700	1.01329900
C	-1.53470100	-0.37131200	-0.18440100
H	-1.97815600	-0.30320200	1.96694100
H	-1.87884000	-1.30279600	-0.65257900
H	-1.62377200	0.40763000	-0.94982400
S	-5.45915300	-0.31706800	-1.22482400
O	-6.19912900	-1.49533800	-0.78052400
O	-6.13004200	0.85343400	-1.78576400
C	-4.24896100	-0.86894300	-2.40092400
C	-3.85485000	-2.20663400	-2.40746500
C	-3.64772400	0.05670600	-3.25873500
C	-2.84615300	-2.61364400	-3.27536800
H	-4.34670900	-2.91962100	-1.75179800
C	-2.63969600	-0.36675500	-4.11462300
H	-3.98637500	1.08911800	-3.26717100

C	-2.21646600	-1.70419000	-4.13220800
H	-2.54781300	-3.65916900	-3.29656000
H	-2.17660100	0.34760500	-4.79211000
C	-1.11456500	-2.13980000	-5.04487800
H	-0.17806900	-1.61720000	-4.81328800
H	-0.92802600	-3.21451600	-4.97327600
H	-1.34356100	-1.90793700	-6.09002400
C	-0.10163900	-1.89185900	3.67805300
C	0.45485800	-0.62537700	3.99997100
C	0.57265500	-0.24787400	5.34222700
C	0.13724700	-1.12197600	6.33090300
C	-0.41566300	-2.36338600	5.99618700
C	-0.54436500	-2.76630300	4.66792600
C	0.46404800	-0.78675100	1.72913000
C	0.78659500	0.04033400	2.77088000
H	0.99592000	0.71914600	5.60191900
H	0.22097100	-0.83795400	7.37631100
H	-0.75988200	-3.02971300	6.78176700
H	-0.99484200	-3.72644600	4.44877100
H	-1.51898100	2.03127200	2.47714100
H	1.22537400	1.02570100	2.69259900
N	-0.08758700	-1.97771200	2.27757600
C	-0.38060100	-3.00524000	1.40853000
C	-0.85858600	-4.27703100	1.73643000
N	-0.10972700	-2.67387200	0.12414000
C	-1.06150300	-5.19182400	0.71549900
H	-1.06345400	-4.54882200	2.76151600
C	-0.31858200	-3.56491600	-0.85731500
C	-0.79209300	-4.84073000	-0.60809000
H	-1.43089000	-6.18391800	0.95574100
H	-0.08918900	-3.22133600	-1.86493800
H	-0.94347200	-5.53618000	-1.42529900

TS3R

Zero-point correction= 0.973410 (Hartree/Particle)
Thermal correction to Energy= 1.031250
Thermal correction to Enthalpy= 1.032194
Thermal correction to Gibbs Free Energy= 0.883055
Sum of electronic and zero-point Energies= -3589.316885
Sum of electronic and thermal Energies= -3589.259045
Sum of electronic and thermal Enthalpies= -3589.258100
Sum of electronic and thermal Free Energies= -3589.407239
Imaginary frequency=-339.79 cm^{-1}

C	7.96817700	-2.46960900	2.80406800

C	6.63782400	-2.18944200	3.00765800
C	5.82752100	-1.80581100	1.91567000
C	6.41116100	-1.68644700	0.61058300
C	7.77850200	-1.99619100	0.43151600
C	8.53825900	-2.37927900	1.51197200
H	8.59178400	-2.77035700	3.64050700
H	6.17843100	-2.26749500	3.98859900
H	8.20214400	-1.90719300	-0.56473000
H	9.59057700	-2.61159200	1.37777100
C	4.40676200	-0.97182900	-0.21336000
C	3.80298300	-1.23183900	1.04773400
N	5.67866500	-1.23975900	-0.44561400
N	4.49601300	-1.60783000	2.10596400
P	3.34679200	-0.11262100	-1.44752300
P	1.97887600	-1.17790200	1.08940400
C	3.70032700	-0.97579300	-3.01651400
H	4.77013700	-1.18296800	-3.10588700
H	3.38342800	-0.35873900	-3.86245400
H	3.15419100	-1.92173600	-3.05295200
C	1.59931500	-0.84315700	2.83459300
H	1.93821800	-1.67260100	3.46150400
H	0.52539600	-0.70172500	2.97931100
H	2.12306200	0.06234800	3.15026600
C	1.51926400	-3.00283400	0.81763900
C	1.56173300	-3.26214700	-0.68839700
C	0.11001100	-3.24043800	1.35977700
C	2.49334400	-3.94134200	1.52603900
H	2.56975800	-3.11605700	-1.09616800
H	0.87628000	-2.60087000	-1.23816500
H	1.27193100	-4.29849900	-0.89789500
H	0.05923600	-3.10252800	2.44442700
H	-0.17769900	-4.27675100	1.14867700
H	-0.64294100	-2.59492300	0.89657700
H	2.11821400	-4.96786400	1.43946100
H	2.59511900	-3.71674700	2.59277500
H	3.49119500	-3.91626500	1.07808700
C	4.23168600	1.55498400	-1.62932700
C	5.58882600	1.38627000	-2.31070800
C	4.40952000	2.15222600	-0.23449500
C	3.35939900	2.47797600	-2.47743200
H	5.48688300	1.06861400	-3.35305500
H	6.23552100	0.67175900	-1.79513700
H	6.09670100	2.35797400	-2.31554300
H	3.45739900	2.21398100	0.30736800

H	4.80507600	3.17045100	-0.32297100
H	5.11638900	1.57816000	0.37505800
H	3.93600700	3.37278100	-2.73832000
H	2.47595100	2.80792300	-1.92817200
H	3.03850300	2.01050000	-3.41587100
Co	1.22607600	-0.03101600	-0.66428100
C	-5.68746200	1.87066200	4.22110800
C	-4.96588200	1.48846900	3.09533500
C	-3.57391900	1.68884200	3.02813400
C	-2.94723200	2.28686400	4.13904900
C	-3.67018800	2.67230300	5.26037200
C	-5.04808100	2.46518700	5.30746200
H	-6.76056700	1.70058000	4.24946900
H	-5.49676100	1.01954100	2.27413000
H	-1.87093900	2.45221500	4.10237000
H	-3.15872500	3.13574900	6.09983300
H	-5.61838300	2.76168000	6.18320300
C	-2.72739700	1.31759200	1.90186600
C	-3.04199500	0.86059900	0.67699500
C	-4.40714700	0.57579400	0.12037200
H	-4.88629500	-0.24802600	0.67991900
H	-5.08929300	1.43226700	0.14897400
N	-4.13946400	0.19024400	-1.27905800
C	-2.79361100	-0.38862000	-1.33169200
H	-2.41942000	-0.39548000	-2.35816700
H	-2.77275100	-1.42016800	-0.93538400
C	-2.02169800	0.54946500	-0.40299400
C	-0.69426500	-0.02966700	0.07476200
H	-1.88405800	1.48046300	-0.96722600
H	-0.51676100	-0.98279500	-0.47983400
H	-0.73345500	-0.26826600	1.13829500
S	-5.36729100	-0.61134700	-2.09057800
O	-4.84493000	-0.88560800	-3.42642000
O	-6.56863100	0.19246700	-1.88425500
C	-5.58893000	-2.15880300	-1.25262800
C	-4.81984300	-3.26150400	-1.62654200
C	-6.47762000	-2.23890600	-0.17780900
C	-4.95298700	-4.45171400	-0.92056800
H	-4.14263300	-3.18945600	-2.47297200
C	-6.59665500	-3.43600600	0.51548400
H	-7.07983600	-1.37661900	0.09224700
C	-5.83875400	-4.55931700	0.15828800
H	-4.36378400	-5.31753600	-1.21300500
H	-7.29359600	-3.50543500	1.34739100

C	-5.99836900	-5.84877500	0.89767300
H	-6.04805200	-5.68908500	1.97880500
H	-5.17841000	-6.53994800	0.68866300
H	-6.92977000	-6.35064700	0.61158600
C	0.17498800	3.77369400	-0.26269100
C	0.41620000	3.58982200	1.12653700
C	0.41710900	4.70941100	1.96974400
C	0.21223400	5.97001400	1.42132500
C	0.02391900	6.13332100	0.04312100
C	0.00928000	5.03771700	-0.82004300
C	0.57769000	1.53105800	0.14266900
C	0.63724200	2.19698700	1.35485100
H	0.58839800	4.58800100	3.03649500
H	0.21216000	6.84349100	2.06726100
H	-0.11153000	7.12904500	-0.36839800
H	-0.11203600	5.19210100	-1.88648000
H	-1.66320500	1.45936400	2.09131100
H	0.79975100	1.73108200	2.31731000
N	0.24462200	2.50374500	-0.84503300
C	0.09939200	2.07116500	-2.14539800
C	-0.50780600	2.77446200	-3.18922700
N	0.55907000	0.80725200	-2.31451900
C	-0.61481600	2.15758600	-4.42506300
H	-0.92168800	3.76018800	-3.02240500
C	0.43254600	0.21660800	-3.51661700
C	-0.13706100	0.85756200	-4.60141400
H	-1.08988000	2.68443300	-5.24634200
H	0.81310700	-0.79980300	-3.58333300
H	-0.21572300	0.34685400	-5.55379700

TS3S

Zero-point correction=			0.973546 (Hartree/Particle)
Thermal correction to Energy=			1.030977
Thermal correction to Enthalpy=			1.031921
Thermal correction to Gibbs Free Energy=			0.885897
Sum of electronic and zero-point Energies=			-3589.311745
Sum of electronic and thermal Energies=			-3589.254315
Sum of electronic and thermal Enthalpies=			-3589.253371
Sum of electronic and thermal Free Energies=			-3589.399394
Imaginary frequency=-339.16 cm^{-1}			
C	7.10657300	3.67451500	-0.56523500
C	5.76927100	3.66776400	-0.24499000
C	5.00445600	2.49801400	-0.45445800
C	5.64258200	1.32237700	-0.97274600

C	7.01438100	1.36776900	-1.31066500
C	7.72835400	2.52478300	-1.10706000
H	7.69532900	4.57334600	-0.40772900
H	5.27182300	4.54540600	0.15749000
H	7.47798900	0.47016900	-1.70982900
H	8.78455400	2.55940300	-1.35662400
C	3.68363800	0.17555000	-0.75867000
C	3.02161500	1.37997700	-0.39687200
N	4.95979500	0.15219500	-1.09600700
N	3.66613400	2.51623900	-0.21302800
P	2.69647100	-1.35819400	-0.55999200
P	1.19276800	1.32414500	-0.39153000
C	3.14148200	-2.37740800	-2.00618600
H	4.20659500	-2.26647300	-2.22788500
H	2.92943200	-3.43058700	-1.80201300
H	2.56571800	-2.06681200	-2.88211300
C	0.75677300	2.77103200	0.61306800
H	1.21218300	3.66949000	0.18676300
H	-0.32581100	2.89232400	0.64961300
H	1.13427000	2.64558200	1.63075500
C	0.81086000	1.84125100	-2.18185200
C	0.92740900	0.58539500	-3.04712400
C	-0.61602200	2.38447400	-2.21980100
C	1.77010100	2.91198500	-2.69403000
H	1.95868000	0.21284400	-3.08483100
H	0.28040500	-0.22510700	-2.67507800
H	0.62596800	0.80896100	-4.07773600
H	-0.71196500	3.31362400	-1.64846000
H	-0.88933200	2.60671900	-3.25817600
H	-1.34972900	1.66669500	-1.83836500
H	1.42832500	3.24909900	-3.67986900
H	1.80718600	3.79107300	-2.04277300
H	2.78992700	2.53303300	-2.81261900
C	3.60261400	-2.19126200	0.88764600
C	4.99148300	-2.65954000	0.45565100
C	3.71458800	-1.17599500	2.02475200
C	2.79462200	-3.39981600	1.35628200
H	4.94264600	-3.47431800	-0.27344900
H	5.59795100	-1.85486300	0.03242900
H	5.51383700	-3.04393000	1.33973900
H	2.74247600	-0.73089700	2.27101300
H	4.08499100	-1.68156200	2.92386000
H	4.41598300	-0.36716900	1.79201400
H	3.41236300	-3.99280700	2.04033900

H	1.90198800	-3.09884000	1.90771200
H	2.49751400	-4.05868800	0.53144000
Co	0.52157000	-0.80880800	-0.17453000
C	-3.01578600	5.96231200	0.54762100
C	-2.83664200	4.58320400	0.58154400
C	-2.62318800	3.91365400	1.79973400
C	-2.56101000	4.68326300	2.97462500
C	-2.74510700	6.05992000	2.93986200
C	-2.97938700	6.70528800	1.72591400
H	-3.17333800	6.46019900	-0.40543600
H	-2.82303600	4.02451700	-0.35109300
H	-2.37654100	4.18178000	3.92248200
H	-2.70348800	6.63320200	3.86205200
H	-3.11829900	7.78237200	1.69708800
C	-2.43161100	2.46892000	1.88588100
C	-2.88962200	1.52135500	1.04870600
C	-3.85480900	1.69662100	-0.08817600
H	-3.34306300	1.80177300	-1.06034200
H	-4.50151200	2.57155000	0.03051500
N	-4.64829800	0.45366900	-0.03960000
C	-4.03704700	-0.52859500	0.88125400
H	-4.65468000	-0.60509000	1.78258300
H	-3.99189700	-1.52351100	0.42489200
C	-2.65343900	0.04191300	1.21605000
C	-1.57847400	-0.52474900	0.26191400
H	-2.40377400	-0.19848900	2.25248700
H	-1.89379100	-1.52176200	-0.05011100
H	-1.49859600	0.09429600	-0.64670400
S	-5.35965800	-0.09569200	-1.43649300
O	-6.25074500	-1.18190800	-1.03933600
O	-5.84760300	1.09385200	-2.12945400
C	-4.06038900	-0.80476000	-2.41635200
C	-3.76708800	-2.16398600	-2.30032400
C	-3.29611800	0.02269400	-3.24290200
C	-2.69853600	-2.69188700	-3.01829700
H	-4.38453900	-2.80098800	-1.67381500
C	-2.23164100	-0.52139100	-3.94935600
H	-3.55293900	1.07354100	-3.34681600
C	-1.91263800	-1.88315900	-3.84813400
H	-2.47667700	-3.75405200	-2.94585800
H	-1.63926300	0.11687700	-4.60139400
C	-0.77445900	-2.45325500	-4.63323700
H	0.14912200	-1.88329700	-4.47708900
H	-0.58323800	-3.49767100	-4.37325800

H	-0.97874900	-2.41470400	-5.70887900
C	-0.40498600	-2.31165200	3.38290700
C	-0.12900600	-0.99909700	3.85982300
C	-0.03702800	-0.78726300	5.24289400
C	-0.20382100	-1.86321100	6.10681500
C	-0.44529900	-3.15149900	5.61505300
C	-0.54390200	-3.39438600	4.24408300
C	-0.10254500	-0.89240500	1.57644600
C	0.03043900	-0.13882500	2.73023300
H	0.17022300	0.20763400	5.62874200
H	-0.13683900	-1.70552800	7.17987500
H	-0.55881000	-3.98073400	6.30705000
H	-0.71367900	-4.40405600	3.88818300
H	-1.85187900	2.12354300	2.74374200
H	0.20761800	0.92754400	2.76294700
N	-0.41698400	-2.22602100	1.98427400
C	-0.43188900	-3.19311600	1.00533200
C	-0.89241600	-4.50476400	1.14055500
N	0.05018400	-2.73166900	-0.17901300
C	-0.83178100	-5.34474700	0.03960600
H	-1.31601900	-4.84603700	2.07542100
C	0.07851000	-3.55229200	-1.24282900
C	-0.33622500	-4.87058500	-1.17603800
H	-1.18513400	-6.36741100	0.12700800
H	0.45709200	-3.11403000	-2.16329300
H	-0.28807700	-5.50030800	-2.05713900

M4R

Zero-point correction=	0.974847 (Hartree/Particle)
Thermal correction to Energy=	1.033452
Thermal correction to Enthalpy=	1.034397
Thermal correction to Gibbs Free Energy=	0.883758
Sum of electronic and zero-point Energies=	-3589.345499
Sum of electronic and thermal Energies=	-3589.286894
Sum of electronic and thermal Enthalpies=	-3589.285949
Sum of electronic and thermal Free Energies=	-3589.436588

C	7.96591300	-3.17673100	2.13004100
C	6.61400600	-3.03712400	2.34381400
C	5.84358000	-2.23806900	1.47026700
C	6.48610200	-1.56546000	0.38033100
C	7.87463800	-1.73471000	0.18213800
C	8.59686000	-2.52661200	1.04457600
H	8.55869700	-3.79546900	2.79706000
H	6.10864900	-3.53641600	3.16539100

H	8.34344900	-1.21993000	-0.65159900
H	9.66511400	-2.65382300	0.89630500
C	4.49139600	-0.63431000	-0.21035600
C	3.83740700	-1.38520300	0.80395100
N	5.78630300	-0.73818600	-0.44466500
N	4.49704700	-2.14758500	1.65563500
P	3.44505900	0.58264200	-1.09431100
P	2.00527700	-1.32896000	0.76490900
C	4.06628800	0.50270300	-2.80852400
H	5.15910700	0.46594500	-2.80389000
H	3.73938900	1.37483300	-3.38085500
H	3.69215500	-0.39983700	-3.29866600
C	1.54353200	-1.25546900	2.52793600
H	2.10446900	-1.99272900	3.10828200
H	0.47257700	-1.44158700	2.65243500
H	1.77138300	-0.25757700	2.91098400
C	1.57402700	-3.10037800	0.23290000
C	2.33278400	-3.40149400	-1.05948900
C	0.07048900	-3.17700600	-0.03067000
C	1.94677200	-4.11285900	1.31343400
H	3.41559400	-3.45784300	-0.90081700
H	2.13938400	-2.64117900	-1.82791300
H	2.00880500	-4.36963600	-1.45820100
H	-0.52401500	-2.80375800	0.81267500
H	-0.21528700	-4.22330200	-0.19363300
H	-0.21188200	-2.61905900	-0.92964600
H	1.75518900	-5.12297100	0.93175500
H	1.34332300	-3.98531100	2.21753100
H	3.00149400	-4.05475000	1.59628700
C	4.10449400	2.23532200	-0.43864600
C	5.55410100	2.47626900	-0.85037600
C	3.97943400	2.21475700	1.08411900
C	3.21729700	3.33589600	-1.01324500
H	5.65832000	2.59354800	-1.93353700
H	6.22355200	1.67345600	-0.52912100
H	5.90117900	3.40785000	-0.38705100
H	2.96057900	1.95862700	1.40372400
H	4.21292100	3.20741100	1.48663500
H	4.67253600	1.50114100	1.54433100
H	3.60087000	4.31635900	-0.70634900
H	2.19785800	3.24846900	-0.63464500
H	3.18368300	3.32145700	-2.10966400
Co	1.36447600	0.21120300	-0.64571500
C	-6.80017800	2.56641800	2.29797700

C	-5.79176900	1.90377200	1.60657100
C	-4.51964400	2.48660200	1.45108900
C	-4.30403900	3.74830900	2.03937900
C	-5.31359300	4.41011500	2.72601600
C	-6.57136100	3.82253600	2.85615100
H	-7.77224800	2.09279000	2.40621600
H	-6.00011600	0.91572700	1.21060200
H	-3.32211000	4.20971800	1.94203700
H	-5.11881600	5.38536800	3.16407900
H	-7.36378300	4.33535900	3.39369900
C	-3.40144000	1.87806300	0.73938100
C	-3.37346100	0.81487200	-0.08646200
C	-4.54309200	-0.02740500	-0.51663100
H	-4.88183000	-0.67989700	0.30927500
H	-5.40551300	0.55731000	-0.85125900
N	-4.00068200	-0.81965000	-1.63566400
C	-2.58681000	-1.05787500	-1.34132200
H	-2.05078200	-1.37283300	-2.23947800
H	-2.45746600	-1.82774600	-0.55928700
C	-2.14043100	0.29950100	-0.80672800
C	-0.84699900	0.15579800	0.01379600
H	-1.95315300	0.94666700	-1.67440800
H	-0.22113400	-0.52708400	-0.65232100
H	-1.03098700	-0.46283500	0.89844600
S	-4.90513700	-2.14372400	-2.13920300
O	-4.13272300	-2.76198700	-3.21282300
O	-6.25734900	-1.63865900	-2.35607500
C	-4.94283200	-3.25969400	-0.76272100
C	-3.92602000	-4.20221700	-0.60560600
C	-5.95222200	-3.12904900	0.19423200
C	-3.93196700	-5.02381700	0.51668100
H	-3.15604500	-4.30055100	-1.36601400
C	-5.94069200	-3.95726100	1.30851700
H	-6.74404600	-2.39961900	0.05040800
C	-4.93329400	-4.91493500	1.48925200
H	-3.14827500	-5.76756400	0.64060400
H	-6.72908700	-3.86531000	2.05175900
C	-4.94603200	-5.81430500	2.68348600
H	-5.12017900	-5.25395300	3.60710500
H	-4.00702100	-6.36332000	2.78693100
H	-5.75231100	-6.55282600	2.61118200
C	-0.02319200	3.71614800	0.43566900
C	0.07653300	3.27860100	1.78293200
C	0.26976300	4.23240700	2.79538000

C	0.37708600	5.57052500	2.44502600
C	0.31570700	5.97409100	1.10202300
C	0.12465200	5.05320200	0.07641500
C	-0.20098200	1.43107800	0.47457400
C	-0.05750200	1.86115100	1.78217700
H	0.33734400	3.92085200	3.83418800
H	0.52029400	6.31894900	3.21895000
H	0.41816200	7.02635100	0.85333100
H	0.09879300	5.37650000	-0.95891800
H	-2.46100700	2.40210200	0.89379300
H	-0.12885400	1.21808000	2.64968700
N	-0.21380100	2.58295300	-0.35679100
C	-0.03051300	2.46857300	-1.73344100
C	-0.57268600	3.35686900	-2.65990500
N	0.68205500	1.37794000	-2.10082900
C	-0.37131900	3.10371900	-4.00930200
H	-1.17132600	4.19496400	-2.32196300
C	0.82449200	1.11992900	-3.41559300
C	0.32728400	1.96038200	-4.39688500
H	-0.78312400	3.77826300	-4.75298400
H	1.37943600	0.21760300	-3.65738900
H	0.48109800	1.71799800	-5.44208300

M4S

Zero-point correction=	0.975083 (Hartree/Particle)
Thermal correction to Energy=	1.033255
Thermal correction to Enthalpy=	1.034199
Thermal correction to Gibbs Free Energy=	0.885844
Sum of electronic and zero-point Energies=	-3589.345840
Sum of electronic and thermal Energies=	-3589.287668
Sum of electronic and thermal Enthalpies=	-3589.286724
Sum of electronic and thermal Free Energies=	-3589.435078

C	-3.88481500	-6.86808300	0.69821800
C	-2.73132000	-6.11587300	0.69079300
C	-2.79425400	-4.73330200	0.41434300
C	-4.06391300	-4.12451800	0.14887400
C	-5.22843400	-4.92278900	0.16069700
C	-5.13610200	-6.26961000	0.43215000
H	-3.83660500	-7.93187800	0.91130300
H	-1.75841700	-6.55717600	0.88809400
H	-6.18241000	-4.44404700	-0.04189600
H	-6.03326500	-6.88122500	0.44470200
C	-3.03744600	-2.10686100	-0.11713300
C	-1.77252600	-2.72180700	0.10034300

N	-4.17035700	-2.78536700	-0.09287500
N	-1.64198400	-4.00191500	0.39054100
P	-2.97793400	-0.29068500	-0.37083700
P	-0.31962700	-1.63192700	-0.13724600
C	-4.39784400	0.05221600	-1.46102700
H	-5.29380400	-0.46442900	-1.10860100
H	-4.59317100	1.12822500	-1.49832900
H	-4.17438800	-0.29417000	-2.47341600
C	0.67201200	-1.91767100	1.37163800
H	0.80590300	-2.98910200	1.54634000
H	1.65278100	-1.44000800	1.27584000
H	0.16121500	-1.48336700	2.23490300
C	0.67788200	-2.44307600	-1.52066600
C	-0.27002400	-2.83503400	-2.65189000
C	1.64349500	-1.35944500	-2.00526900
C	1.44743200	-3.67023100	-1.04534700
H	-0.92999000	-3.66081300	-2.36660900
H	-0.89843800	-1.99276800	-2.96744100
H	0.31133200	-3.16311700	-3.52151800
H	2.32065100	-1.03181900	-1.20544600
H	2.26357100	-1.73932600	-2.82675000
H	1.10046400	-0.47727200	-2.37969700
H	1.95449000	-4.12947200	-1.90285400
H	2.21458100	-3.41657700	-0.30676800
H	0.78267100	-4.42263700	-0.60976600
C	-3.49207700	0.39572200	1.31614500
C	-4.94450600	0.04933100	1.63100000
C	-2.56388200	-0.19018500	2.37641800
C	-3.30331000	1.90993600	1.26458500
H	-5.64145500	0.53447100	0.94088200
H	-5.13160300	-1.02911800	1.60303000
H	-5.18546300	0.40219200	2.64109500
H	-1.51535300	0.06231100	2.17183700
H	-2.81741500	0.23075800	3.35647600
H	-2.64999100	-1.27981200	2.46017800
H	-3.61227600	2.36108500	2.21605800
H	-2.25020000	2.16811600	1.09554100
H	-3.90214900	2.37583600	0.47378600
Co	-1.03430900	0.22446300	-1.01124500
C	1.97094100	-0.71138800	5.30960100
C	2.13214000	-0.12607700	4.05764600
C	1.17194400	0.77145700	3.55451700
C	0.05150000	1.04938700	4.36016200
C	-0.10616200	0.46815200	5.61153700

C	0.85582900	-0.41794200	6.09319600
H	2.72205800	-1.40667600	5.67463200
H	2.99963300	-0.39597600	3.46408100
H	-0.70207500	1.73902400	3.98207300
H	-0.98144600	0.70535700	6.21042600
H	0.73705800	-0.87922000	7.06949900
C	1.23306500	1.43245400	2.25552500
C	2.26204400	1.58704100	1.40107700
C	3.64850700	1.02533900	1.53063600
H	3.62736900	-0.07552800	1.41188200
H	4.13522500	1.24099800	2.48746500
N	4.38003500	1.66991600	0.42815100
C	3.42513200	1.92313700	-0.65551000
H	3.82000600	2.67054400	-1.34577400
H	3.19510600	1.00404000	-1.22399100
C	2.19751100	2.39531100	0.11735500
C	0.90186300	2.28256100	-0.69067600
H	2.36117700	3.45269800	0.37035200
H	1.12017100	2.39418000	-1.76187500
H	0.56765100	1.22608400	-0.54842400
S	5.87409100	1.02793900	0.02351700
O	6.40675300	1.89366600	-1.02373200
O	6.57102200	0.83213000	1.29133100
C	5.56846600	-0.56760400	-0.69142800
C	5.43466300	-0.68724600	-2.07654300
C	5.43189600	-1.68210400	0.13873100
C	5.18283100	-1.93707100	-2.62719600
H	5.55150700	0.18732400	-2.70982000
C	5.16657500	-2.92286100	-0.43057300
H	5.56172600	-1.58078500	1.21248800
C	5.04462200	-3.07283400	-1.81759000
H	5.09192400	-2.03790200	-3.70630700
H	5.06541200	-3.79577800	0.21025000
C	4.79575800	-4.41472800	-2.42830900
H	4.42096900	-5.13231300	-1.69410500
H	4.07795900	-4.35574200	-3.25254400
H	5.71948300	-4.83000800	-2.84751100
C	-2.05857100	4.48666100	-0.51015100
C	-1.38291400	4.91246900	0.65728900
C	-1.96763200	5.89937300	1.46278400
C	-3.19759300	6.42344700	1.09145700
C	-3.85824900	5.97383900	-0.06332900
C	-3.30194900	4.99599700	-0.88057000
C	-0.15579100	3.25488100	-0.29470900

C	-0.18995200	4.13259200	0.75746100
H	-1.46706200	6.23813800	2.36588200
H	-3.66342300	7.18895200	1.70552500
H	-4.82541900	6.39356800	-0.32454500
H	-3.82568300	4.64105300	-1.76389100
H	0.29699100	1.91855500	1.97495900
H	0.56694900	4.21140500	1.52656100
N	-1.30049500	3.46309600	-1.08123600
C	-1.58667900	2.87027400	-2.31727500
C	-1.91691100	3.66444500	-3.41663900
N	-1.54519000	1.52238100	-2.39219200
C	-2.19861500	3.05822800	-4.63019800
H	-1.92145800	4.74323600	-3.30640200
C	-1.80219900	0.94784900	-3.59023700
C	-2.12833500	1.66907300	-4.72342200
H	-2.45350400	3.66169000	-5.49523900
H	-1.76356700	-0.13858400	-3.59455700
H	-2.33260000	1.14831800	-5.65194200

TS2R'

Zero-point correction= 0.972636 (Hartree/Particle)
Thermal correction to Energy= 1.029903
Thermal correction to Enthalpy= 1.030848
Thermal correction to Gibbs Free Energy= 0.885771
Sum of electronic and zero-point Energies= -3589.256571
Sum of electronic and thermal Energies= -3589.199303
Sum of electronic and thermal Enthalpies= -3589.198359
Sum of electronic and thermal Free Energies= -3589.343435
Imaginary frequency=-395.42 cm^{-1}

C	-5.11253000	4.97907400	-0.58739100
C	-4.68236400	3.85456500	0.07729800
C	-3.31172500	3.51253700	0.05781500
C	-2.38559400	4.34681800	-0.64498600
C	-2.85726700	5.49419900	-1.32086600
C	-4.19841100	5.79900500	-1.28981400
H	-6.16541000	5.24393800	-0.57869700
H	-5.36888000	3.20881300	0.61780200
H	-2.13985800	6.11180100	-1.85389200
H	-4.56501700	6.67938000	-1.80941600
C	-0.67874000	2.94207300	-0.06183600
C	-1.60413200	2.09636800	0.62735800
N	-1.06010100	4.04478700	-0.67547900
N	-2.89107800	2.38347200	0.68765800
P	1.09619800	2.46721600	-0.01589600

P	-1.01954800	0.49687200	1.35250000
C	1.55659100	3.43858500	1.46775800
H	1.32620900	4.49430600	1.30583900
H	2.61591800	3.32831700	1.71282500
H	0.95715500	3.09688900	2.31423300
C	-2.24399200	-0.65787100	0.63395700
H	-3.23931700	-0.21148300	0.69754700
H	-2.23504900	-1.59622600	1.19752500
H	-2.01456700	-0.88693200	-0.40420600
C	-1.64213500	0.54358200	3.16446900
C	-1.35077800	1.89540300	3.81344300
C	-0.93528700	-0.60280100	3.89066500
C	-3.15332100	0.31053400	3.25345600
H	-1.93812000	2.69445700	3.34954900
H	-0.30075600	2.19668300	3.77915000
H	-1.63456000	1.85246800	4.87107600
H	-1.17514000	-1.57120000	3.43301300
H	-1.27743200	-0.64425800	4.93138600
H	0.15362300	-0.49647300	3.90323900
H	-3.45405900	0.41855400	4.30290200
H	-3.44127000	-0.69588500	2.93620300
H	-3.71632500	1.04006900	2.66516900
C	2.00839400	3.35875700	-1.41869700
C	1.25143800	3.23074900	-2.73701500
C	3.37401600	2.67618300	-1.54033500
C	2.21202900	4.84162800	-1.10441400
H	0.30783100	3.78199100	-2.71576700
H	1.04411400	2.19208400	-2.99768700
H	1.87107200	3.65503800	-3.53614700
H	3.93184000	2.67807500	-0.59591600
H	3.98052100	3.21620300	-2.27623700
H	3.28764600	1.64018900	-1.88965000
H	2.68827000	5.31241500	-1.97249200
H	2.86986300	5.00374600	-0.24589900
H	1.26406400	5.35713900	-0.92523400
Co	1.24210900	0.21189000	0.39868500
C	-1.92572700	1.44665000	-3.59488300
C	-1.45622800	0.88261500	-2.41118300
C	-0.29484000	0.09331800	-2.38920300
C	0.35666900	-0.12678600	-3.62076200
C	-0.10961700	0.43622300	-4.80332400
C	-1.25040800	1.23771900	-4.79463200
H	-2.83175300	2.04790000	-3.57569700
H	-2.02904300	1.03401600	-1.50416800

H	1.25283700	-0.74442300	-3.62865600
H	0.41975700	0.24900400	-5.73405600
H	-1.61685300	1.68209900	-5.71570500
C	0.28443900	-0.56719000	-1.19998000
C	0.27472300	-1.91615500	-1.18987900
C	-0.63442600	-2.84048000	-1.95990900
H	-1.62354800	-2.38682700	-2.12435200
H	-0.25109200	-3.15222300	-2.93943000
N	-0.70107900	-4.03160900	-1.06844900
C	-0.03896500	-3.76392700	0.22478800
H	0.35275500	-4.69457800	0.64055700
H	-0.73188600	-3.31011700	0.95568200
C	1.02082100	-2.75886100	-0.20628300
C	1.67587900	-1.89482700	0.82497100
H	1.79369700	-3.32035100	-0.75657800
H	2.50070300	-2.35587900	1.36851800
H	0.95281600	-1.57708900	1.58743000
S	-2.09118200	-4.94784600	-1.04510300
O	-1.77757900	-6.12593100	-0.23972900
O	-2.52615400	-5.05830100	-2.43513000
C	-3.31218500	-4.00912500	-0.15988100
C	-3.38606900	-4.10911600	1.23055800
C	-4.15001100	-3.13550100	-0.85716800
C	-4.30463300	-3.32443500	1.92142400
H	-2.74284900	-4.80721200	1.75874400
C	-5.06260000	-2.36314600	-0.15116000
H	-4.09529600	-3.08056100	-1.94049700
C	-5.15317700	-2.43958600	1.24575200
H	-4.36808500	-3.40062700	3.00477700
H	-5.72002900	-1.68491400	-0.69081000
C	-6.13480500	-1.58859300	1.98687300
H	-5.99895200	-1.65755000	3.06907200
H	-7.16530900	-1.88473500	1.76155600
H	-6.04694900	-0.53519200	1.69844000
C	5.21090100	-1.00522700	0.03821700
C	4.82804100	-1.61262100	-1.19313700
C	5.81845600	-2.14762600	-2.03481600
C	7.14716700	-2.06312100	-1.64869700
C	7.50711300	-1.43628500	-0.44776700
C	6.54779000	-0.89556700	0.40834100
C	2.91127300	-0.82958600	-0.19542200
C	3.42787200	-1.49687100	-1.33224800
H	5.53703500	-2.61267900	-2.97543100
H	7.92166900	-2.47416600	-2.28992800

H	8.55518000	-1.35792800	-0.17489400
H	6.86691700	-0.38030000	1.30547400
H	2.46030300	0.18352500	-0.61831700
H	2.83189500	-1.78611800	-2.18624400
N	4.04044300	-0.53150300	0.63896300
C	3.80120100	0.00670300	1.88296800
C	4.72710000	-0.00188500	2.93410100
N	2.54148700	0.49017600	2.03331700
C	4.35341100	0.51767500	4.15952300
H	5.70069000	-0.45094400	2.80290400
C	2.20535100	0.96952700	3.24401900
C	3.06430200	1.02146500	4.32406400
H	5.05768100	0.50815700	4.98565400
H	1.18918600	1.32393000	3.32950600
H	2.72045300	1.42686300	5.26835700

TS2S'

Zero-point correction= 0.974358 (Hartree/Particle)
Thermal correction to Energy= 1.031078
Thermal correction to Enthalpy= 1.032022
Thermal correction to Gibbs Free Energy= 0.888506
Sum of electronic and zero-point Energies= -3589.255372
Sum of electronic and thermal Energies= -3589.198652
Sum of electronic and thermal Enthalpies= -3589.197708
Sum of electronic and thermal Free Energies= -3589.341224
Imaginary frequency=-369.52 cm^{-1}

C	7.08504600	-1.97842900	-0.62471300
C	6.15626100	-1.13354000	-0.06376000
C	4.79089400	-1.49781000	-0.06084200
C	4.39092000	-2.73931500	-0.65037300
C	5.36849200	-3.58812500	-1.21653700
C	6.69043700	-3.20910800	-1.20081200
H	8.13539700	-1.70349900	-0.62645100
H	6.43967600	-0.18650000	0.38677200
H	5.04529100	-4.52799400	-1.65481200
H	7.44437200	-3.85904500	-1.63492100
C	2.21146500	-2.27929900	-0.13383000
C	2.61075500	-1.05296600	0.48361900
N	3.08500800	-3.11458400	-0.66422800
N	3.87547100	-0.67288000	0.51253900
P	0.42855600	-2.72570900	-0.09320900
P	1.34959800	0.04369600	1.27626000
C	0.50192300	-3.95334100	1.26504000
H	1.18390200	-4.76196100	0.99178700

H	-0.48476800	-4.37105200	1.47940500
H	0.89289200	-3.48484700	2.16875200
C	1.88654800	1.68124300	0.64816100
H	2.97440900	1.75150700	0.72418600
H	1.43533600	2.47210300	1.25287600
H	1.58856400	1.82471600	-0.38895600
C	1.94068200	0.18127700	3.09173300
C	2.40834300	-1.17413500	3.61831500
C	0.74672400	0.72712000	3.87872100
C	3.10673300	1.15851400	3.25311700
H	3.36022400	-1.46534800	3.16266400
H	1.70429200	-1.99140400	3.44343000
H	2.56709200	-1.11031500	4.70083400
H	0.42958200	1.70419800	3.49082400
H	1.02977300	0.87330800	4.92794100
H	-0.12301200	0.06338500	3.85812700
H	3.43287400	1.13146300	4.30005100
H	2.82005100	2.18963300	3.02963500
H	3.96447800	0.88931200	2.62942400
C	-0.00555800	-3.80495400	-1.61451200
C	0.88120300	-3.49545900	-2.81696400
C	-1.46338800	-3.47733200	-1.94401200
C	0.11716900	-5.29593600	-1.30211000
H	1.89478800	-3.87696200	-2.67666600
H	0.94654500	-2.43042600	-3.02746600
H	0.45156400	-3.98331900	-3.70049900
H	-2.13114400	-3.63912200	-1.08786600
H	-1.80955900	-4.12668700	-2.75626500
H	-1.57621100	-2.44075200	-2.28120600
H	-0.15892600	-5.85508500	-2.20367900
H	-0.54788200	-5.62376400	-0.49828600
H	1.14246400	-5.57791000	-1.04481000
Co	-0.72936800	-0.81905800	0.46291100
C	2.29014800	-0.28823900	-3.82936100
C	1.71369600	-0.02082500	-2.59038800
C	0.31866700	-0.04265200	-2.41705400
C	-0.47480200	-0.32830600	-3.54380400
C	0.10090400	-0.59143100	-4.78339800
C	1.48728900	-0.57867100	-4.93086800
H	3.37208700	-0.26361200	-3.93339800
H	2.35781100	0.22888000	-1.75143700
H	-1.55819900	-0.33328200	-3.43629800
H	-0.53553200	-0.80782700	-5.63745500
H	1.93780000	-0.78635000	-5.89737100

C	-0.31865400	0.31520600	-1.13539500
C	-0.84697800	1.53921800	-0.99264500
C	-0.90804200	2.66390500	-1.99787200
H	0.07535000	3.10785600	-2.20763700
H	-1.31176000	2.33921700	-2.96477600
N	-1.81551600	3.66352800	-1.38731600
C	-2.50829500	3.04092200	-0.24165200
H	-3.43027800	2.56908800	-0.60811600
H	-2.79116700	3.80044200	0.49024400
C	-1.52915200	1.98600800	0.26740500
C	-2.08758000	0.82807800	1.05946700
H	-0.77919500	2.49911100	0.89601400
H	-3.13739800	0.95800100	1.32752400
H	-1.56499800	0.67104600	2.00684900
S	-1.20575000	5.21226200	-1.19892700
O	-2.24313600	5.96361100	-0.49599600
O	-0.73255800	5.60634500	-2.52319600
C	0.22376900	5.14013200	-0.13856700
C	0.06436400	5.17425100	1.24756700
C	1.49635300	5.04866500	-0.70638600
C	1.19061600	5.12010900	2.06296000
H	-0.92818700	5.26876500	1.67957800
C	2.60967900	4.99755100	0.12318100
H	1.60700600	5.04381700	-1.78663500
C	2.47840500	5.03805000	1.51716600
H	1.07132500	5.15673200	3.14361600
H	3.60214500	4.93185400	-0.31698700
C	3.68945400	5.00684100	2.39418900
H	3.43094800	4.82416100	3.44014500
H	4.22790600	5.96047200	2.35075200
H	4.39811600	4.23582300	2.07436300
C	-4.85974800	-1.44014500	0.21952900
C	-4.82452000	-0.63582900	-0.95806700
C	-5.99338800	-0.48633700	-1.72561900
C	-7.14704100	-1.14521300	-1.33156400
C	-7.15115600	-1.96732400	-0.19602400
C	-6.01054200	-2.13117100	0.58909400
C	-2.71151500	-0.62249800	-0.06366100
C	-3.50791100	-0.16036000	-1.13657100
H	-5.97795200	0.12922700	-2.62043000
H	-8.05625100	-1.03775400	-1.91626300
H	-8.05592900	-2.50100400	0.07886000
H	-6.04419900	-2.80879300	1.43263700
H	-1.87579500	-1.32324000	-0.52531900

H	-3.13764200	0.43945700	-1.95517700
N	-3.56867400	-1.42428900	0.75985800
C	-3.06062100	-1.91297800	1.94482800
C	-3.85160600	-2.42681000	2.98051200
N	-1.71242200	-1.79421400	2.05716800
C	-3.23916800	-2.84956100	4.14558400
H	-4.92734000	-2.44835500	2.88874100
C	-1.15146700	-2.19815000	3.21131900
C	-1.85502400	-2.74071000	4.26871300
H	-3.84251600	-3.24055900	4.95894700
H	-0.08111300	-2.06522800	3.26635300
H	-1.33071500	-3.04635000	5.16656200

M3R'

Zero-point correction=	0.974989 (Hartree/Particle)
Thermal correction to Energy=	1.032173
Thermal correction to Enthalpy=	1.033118
Thermal correction to Gibbs Free Energy=	0.888545
Sum of electronic and zero-point Energies=	-3589.292739
Sum of electronic and thermal Energies=	-3589.235554
Sum of electronic and thermal Enthalpies=	-3589.234610
Sum of electronic and thermal Free Energies=	-3589.379183

C	-3.77022300	6.14960800	-0.52137200
C	-3.66695700	4.91854900	0.08280300
C	-2.43539800	4.22710000	0.05322600
C	-1.31026100	4.81747600	-0.60641000
C	-1.44679000	6.08362500	-1.21815300
C	-2.65816000	6.73321800	-1.17254500
H	-4.71460500	6.68528800	-0.50085100
H	-4.50805000	4.45312900	0.58835300
H	-0.58217700	6.51435100	-1.71511600
H	-2.76814000	7.70604900	-1.64205700
C	-0.05291700	2.98236300	-0.08642500
C	-1.16952000	2.39363300	0.58396900
N	-0.11651500	4.16765500	-0.65835600
N	-2.33575500	3.00769100	0.64571500
P	1.53717100	2.05104400	-0.10407900
P	-1.00372000	0.70388100	1.31445800
C	2.38502600	2.87598200	1.29100900
H	2.43970800	3.94938700	1.09547200
H	3.39392200	2.47843600	1.43079500
H	1.81248700	2.73502300	2.20840700
C	-2.41907500	-0.17962100	0.56092000
H	-3.29749000	0.47027700	0.53337600

H	-2.64807800	-1.06056800	1.16772700
H	-2.18215200	-0.51838200	-0.44626100
C	-1.65977400	0.91434500	3.09937800
C	-1.10469800	2.18736400	3.73945000
C	-1.24562600	-0.34515800	3.86480100
C	-3.18788700	1.00783500	3.13641000
H	-1.55456500	3.07927600	3.29186000
H	-0.01943900	2.30146300	3.66682500
H	-1.35664900	2.19342000	4.80603000
H	-1.64249000	-1.24960900	3.38518900
H	-1.65899300	-0.30874700	4.87950600
H	-0.16202700	-0.46305400	3.95314600
H	-3.49613500	1.20442100	4.17057500
H	-3.66611000	0.07395500	2.82700100
H	-3.56662400	1.82078800	2.51103800
C	2.57357000	2.58305500	-1.60744600
C	1.73793400	2.70985100	-2.87743400
C	3.66858400	1.53285200	-1.80342300
C	3.23043500	3.94082000	-1.33043400
H	0.98217000	3.49505000	-2.79286500
H	1.25013400	1.77591100	-3.15194900
H	2.41170800	2.98267400	-3.69799100
H	4.22934600	1.33605200	-0.88126000
H	4.38080500	1.90470600	-2.54883300
H	3.26593300	0.58254000	-2.16788100
H	3.75166000	4.24794500	-2.24406400
H	3.97619400	3.89784800	-0.53256100
H	2.49599900	4.71550600	-1.09169700
Co	1.10370300	-0.01152600	0.39942700
C	-1.66213900	1.64785700	-3.59681400
C	-1.26694700	1.04298200	-2.40681400
C	-0.32115800	0.00443200	-2.39258200
C	0.18783000	-0.41516600	-3.63987300
C	-0.20499700	0.18693400	-4.82986200
C	-1.12826900	1.23099700	-4.81388100
H	-2.39835900	2.44782200	-3.56841400
H	-1.72928900	1.37631400	-1.48630700
H	0.92206000	-1.21858600	-3.65377500
H	0.21342200	-0.15854000	-5.77144300
H	-1.43430600	1.70914200	-5.74022900
C	0.18289600	-0.70184800	-1.19277900
C	-0.00222100	-2.04758400	-1.19157500
C	-1.10205700	-2.73102800	-1.98846900
H	-1.95988400	-2.06240200	-2.14874500

H	-0.78715200	-3.10196500	-2.97193000
N	-1.45603300	-3.89381900	-1.13004300
C	-0.73178300	-3.83814300	0.14616600
H	-0.57124600	-4.84668600	0.53487300
H	-1.26539400	-3.24265000	0.91035700
C	0.54032800	-3.13178000	-0.29809100
C	1.50593300	-2.72736300	0.79161900
H	1.05318900	-3.85486700	-0.95086800
H	1.57955100	-3.52431400	1.54691100
H	1.07332100	-1.89297500	1.37600100
S	-3.00997900	-4.48261100	-1.14128800
O	-2.96602800	-5.73363100	-0.38735400
O	-3.44530700	-4.43689800	-2.53460400
C	-4.01834400	-3.34857100	-0.21666300
C	-4.08746500	-3.46398500	1.17310700
C	-4.71723800	-2.34092000	-0.88459700
C	-4.86617700	-2.56207500	1.89204300
H	-3.55714400	-4.26629400	1.67818500
C	-5.49665500	-1.45578800	-0.15133100
H	-4.66709100	-2.27342500	-1.96738400
C	-5.58419300	-1.54899200	1.24466800
H	-4.92746200	-2.64972900	2.97472000
H	-6.05082400	-0.67562600	-0.66842300
C	-6.43172000	-0.58798800	2.01568800
H	-6.28366400	-0.69021200	3.09354400
H	-7.49606200	-0.74870100	1.81046800
H	-6.21509600	0.44901000	1.73760900
C	4.98804600	-1.59890600	0.24066300
C	4.81124300	-2.39275800	-0.91843500
C	5.86322000	-2.49295400	-1.83937200
C	7.04106300	-1.80177000	-1.59070000
C	7.18661000	-1.00668200	-0.44269200
C	6.16128700	-0.89029900	0.49011100
C	2.87044700	-2.43161200	0.25350400
C	3.47989400	-2.91177000	-0.87497800
H	5.75054700	-3.09497900	-2.73724900
H	7.86318000	-1.87042200	-2.29763200
H	8.11624300	-0.46973300	-0.27678100
H	6.27708500	-0.26490900	1.37064000
H	2.26953100	-0.22342300	-0.44800900
H	3.02873200	-3.57310700	-1.60190700
N	3.78910200	-1.63986100	0.95429700
C	3.51944600	-0.89086600	2.10227000
C	4.40726200	-0.93765200	3.17919800

N	2.38677600	-0.15161400	2.12064000
C	4.11961300	-0.21567700	4.32613300
H	5.28865900	-1.56549900	3.10919300
C	2.10742500	0.49487500	3.26782400
C	2.93145700	0.50770600	4.37835500
H	4.79613400	-0.24365600	5.17445400
H	1.17552500	1.04210900	3.26072600
H	2.63962900	1.06915500	5.25877700

M3S'

Zero-point correction=	0.975146 (Hartree/Particle)
Thermal correction to Energy=	1.032054
Thermal correction to Enthalpy=	1.032998
Thermal correction to Gibbs Free Energy=	0.889539
Sum of electronic and zero-point Energies=	-3589.277502
Sum of electronic and thermal Energies=	-3589.220595
Sum of electronic and thermal Enthalpies=	-3589.219650
Sum of electronic and thermal Free Energies=	-3589.363109

C	1.77156000	-7.08416000	-1.19392200
C	2.10375700	-5.94120300	-0.50401100
C	1.14371200	-4.91745500	-0.34279700
C	-0.16248000	-5.08229800	-0.90194500
C	-0.47697000	-6.26884000	-1.60094100
C	0.47862500	-7.24822300	-1.74385700
H	2.50746300	-7.87250400	-1.32064600
H	3.09058700	-5.79745300	-0.07348000
H	-1.47414800	-6.37437600	-2.01874700
H	0.24277100	-8.15901600	-2.28620300
C	-0.73991600	-2.99954800	-0.15664300
C	0.55000900	-2.84797600	0.44411400
N	-1.09733400	-4.10283200	-0.78281400
N	1.47062100	-3.78922700	0.34237900
P	-1.95648000	-1.62331200	-0.00066400
P	0.93516800	-1.30087500	1.38389600
C	-2.96396200	-2.30317100	1.36924400
H	-3.35995600	-3.27965300	1.07827300
H	-3.79206600	-1.64001700	1.63056300
H	-2.33117500	-2.44594900	2.24765600
C	2.59292300	-0.84700800	0.74987200
H	3.20650400	-1.73957100	0.59537400
H	3.08307900	-0.20480100	1.48717400
H	2.51211900	-0.28849900	-0.18321800
C	1.41395400	-1.94118900	3.11930900
C	0.37507900	-2.94067200	3.62266000

C	1.48878900	-0.70400400	4.01701700
C	2.77520600	-2.63926800	3.12991300
H	0.39080700	-3.86380000	3.03346100
H	-0.64954000	-2.55913500	3.60628500
H	0.60113400	-3.21028100	4.66070000
H	2.23393300	0.01292600	3.64855600
H	1.79269300	-0.99552800	5.02928700
H	0.53335900	-0.17498700	4.09488200
H	2.94453400	-3.05345200	4.13146800
H	3.59886800	-1.95146600	2.92230600
H	2.82114300	-3.46296000	2.41263300
C	-3.14005700	-1.64339800	-1.50046800
C	-2.49874500	-2.26768500	-2.74075200
C	-3.48598800	-0.17474700	-1.75378000
C	-4.42533700	-2.40932200	-1.18645400
H	-2.53306900	-3.35783900	-2.69549300
H	-1.45921300	-1.97551300	-2.88480900
H	-3.06099500	-1.94413600	-3.62493800
H	-3.95162000	0.29010800	-0.87544500
H	-4.20123100	-0.10055700	-2.58159800
H	-2.60093600	0.41215200	-2.01881400
H	-5.07238900	-2.36676800	-2.07047500
H	-4.98477500	-1.97820400	-0.35124000
H	-4.23396000	-3.46499300	-0.97250500
Co	-0.78591200	0.10531200	0.65200900
C	1.15971900	-2.05796200	-3.67623200
C	1.08851100	-1.41845300	-2.44015000
C	0.33740800	-0.24423600	-2.26975300
C	-0.30840900	0.28206400	-3.40622700
C	-0.22636900	-0.34630200	-4.64374100
C	0.49954200	-1.52860500	-4.78287200
H	1.74511000	-2.96954700	-3.77259400
H	1.64971700	-1.82735000	-1.60573500
H	-0.87881700	1.20390000	-3.30156300
H	-0.73636800	0.08563000	-5.50107900
H	0.55770500	-2.02681900	-5.74657500
C	0.24720500	0.49167900	-0.99050200
C	0.83765400	1.70447100	-0.92797200
C	1.69553000	2.31352800	-2.02805900
H	2.58902600	1.71505600	-2.25228000
H	1.14874800	2.41302600	-2.97315200
N	2.07482200	3.65338900	-1.54358600
C	1.18835900	4.01145700	-0.43037700
H	0.30207600	4.51568200	-0.83991700

H	1.67980700	4.71597500	0.24401400
C	0.79804900	2.68487800	0.22430100
C	-0.51481800	2.74846800	1.00815900
H	1.59325400	2.41834800	0.94177600
H	-0.65152300	3.75510200	1.41873500
H	-0.43420800	2.09928400	1.88797700
S	3.70963100	3.99079100	-1.41033900
O	3.78898400	5.32865500	-0.82880400
O	4.27959800	3.68523300	-2.71959400
C	4.42191700	2.84953100	-0.24649300
C	4.34040900	3.11910700	1.12154100
C	5.03300700	1.68346500	-0.70804900
C	4.86621700	2.20405700	2.02539700
H	3.88377900	4.04158100	1.47009300
C	5.56221800	0.78380300	0.21037700
H	5.10415200	1.49589800	-1.77539600
C	5.48440800	1.02462300	1.58714200
H	4.80602800	2.40946900	3.09207000
H	6.03735300	-0.12744500	-0.14620100
C	6.04726700	0.04672000	2.56811900
H	5.48124500	0.04295400	3.50460100
H	7.08274500	0.29819900	2.82554200
H	6.05770000	-0.96951600	2.16365800
C	-4.06838600	2.82202400	0.26554900
C	-3.54711200	3.32249700	-0.96844700
C	-4.44009200	3.85010900	-1.92386800
C	-5.79666900	3.84852900	-1.64910800
C	-6.29025000	3.31276000	-0.44808000
C	-5.43568900	2.78803900	0.52081200
C	-1.78554500	2.40807300	0.21497300
C	-2.15693400	3.14094400	-0.96508800
H	-4.05860500	4.23988500	-2.86317300
H	-6.49428200	4.25245000	-2.37696300
H	-7.36064300	3.30162400	-0.26583000
H	-5.84292600	2.36092400	1.43046700
H	-1.68688800	1.24400800	-0.16410800
H	-1.46190000	3.40791900	-1.75104400
N	-2.99257300	2.34989400	1.01567000
C	-3.02891900	1.59007600	2.17373700
C	-3.93771700	1.88776400	3.19574000
N	-2.12197400	0.58105900	2.27394000
C	-3.93714900	1.12057200	4.34633300
H	-4.59255800	2.74461200	3.09326300
C	-2.11830100	-0.11355900	3.42969700

C	-3.00358200	0.09335700	4.46995400
H	-4.63262800	1.34368400	5.14930300
H	-1.36355900	-0.88445400	3.49476200
H	-2.94566900	-0.52405000	5.35883500

M5

Zero-point correction=	0.629168 (Hartree/Particle)
Thermal correction to Energy=	0.666775
Thermal correction to Enthalpy=	0.667719
Thermal correction to Gibbs Free Energy=	0.562589
Sum of electronic and zero-point Energies=	-2250.973483
Sum of electronic and thermal Energies=	-2250.935876
Sum of electronic and thermal Enthalpies=	-2250.934932
Sum of electronic and thermal Free Energies=	-2251.040062

C	6.91775700	0.09023200	-1.48181200
C	5.85366500	-0.76745800	-1.32911000
C	4.62047400	-0.27679200	-0.84497100
C	4.49042600	1.11608800	-0.53216100
C	5.60504400	1.97006400	-0.69046000
C	6.79431700	1.46157100	-1.15846900
H	7.86660900	-0.28532900	-1.85266600
H	5.92997100	-1.82466900	-1.56633800
H	5.48841600	3.02174600	-0.44447000
H	7.65020900	2.11772000	-1.28579500
C	2.30223900	0.78359400	0.01284300
C	2.45298000	-0.61172900	-0.22340400
N	3.30335300	1.63424300	-0.11376300
N	3.57979200	-1.13695800	-0.66686800
P	0.60394300	1.34935300	0.41772500
P	0.99668800	-1.64864500	0.18892700
C	0.90180200	2.68622600	1.62338600
H	1.71733800	3.32784700	1.27933300
H	0.00078400	3.29015200	1.75988300
H	1.18445000	2.25480100	2.58747500
C	0.98618400	-2.88880700	-1.14323000
H	1.99075200	-3.29612100	-1.28684600
H	0.29830600	-3.70351900	-0.90206100
H	0.66299400	-2.42008100	-2.07626600
C	1.51267000	-2.57955300	1.74610500
C	1.89350900	-1.52844500	2.78943100
C	0.28422800	-3.35621800	2.22291700
C	2.67396000	-3.53391500	1.49405800
H	2.80358600	-0.98351500	2.51290400
H	1.08671000	-0.79341000	2.92398400

H	2.07614200	-2.00965900	3.75708300
H	-0.08369500	-4.05845100	1.46582900
H	0.54076000	-3.94024600	3.11461600
H	-0.53883200	-2.68058000	2.48795400
H	2.96957500	-3.99965200	2.44206800
H	2.39926900	-4.34008400	0.80656900
H	3.55128500	-3.02262900	1.08603400
C	0.05770500	2.23661500	-1.16220100
C	0.86693700	3.51069600	-1.38989300
C	0.24361700	1.27417100	-2.33413900
C	-1.42430200	2.57627900	-1.01159600
H	0.66279600	4.26973200	-0.62847000
H	1.94490000	3.32238400	-1.40545900
H	0.58710600	3.93795600	-2.36023500
H	-0.29594800	0.33268800	-2.17038900
H	-0.15352400	1.73177300	-3.24740800
H	1.29922200	1.04105000	-2.51669300
H	-1.75504500	3.15389300	-1.88259300
H	-2.03445000	1.66887200	-0.96021200
H	-1.62635400	3.18083900	-0.11934900
Co	-0.67026000	-0.37480200	0.79675800
C	-4.19923600	-0.44061000	-1.03720000
C	-3.61086600	-1.34494900	-1.96705000
C	-4.26177600	-1.58658500	-3.18802900
C	-5.44340000	-0.91501900	-3.46447700
C	-5.98172500	0.00544800	-2.55204100
C	-5.36653100	0.25997700	-1.32915400
C	-2.20138100	-1.18538500	-0.18466100
C	-2.39577900	-1.82260400	-1.40394000
H	-3.83476600	-2.28269800	-3.90468000
H	-5.95587200	-1.09236200	-4.40589000
H	-6.89683400	0.53496500	-2.80052500
H	-5.78962500	0.98629700	-0.64511000
H	-1.78924100	-1.74938000	0.72246900
H	-1.73535900	-2.56320300	-1.83323400
N	-3.35861000	-0.39348100	0.07188700
C	-3.35204500	0.43404500	1.17693100
C	-4.48047300	1.01877600	1.75440800
N	-2.10946000	0.59424400	1.69982800
C	-4.31433800	1.78100500	2.89961300
H	-5.46427600	0.84504300	1.33791700
C	-1.97444700	1.31092500	2.83422700
C	-3.04327900	1.92576900	3.45859400
H	-5.17770500	2.24324600	3.36758300

H	-0.96280800	1.38624100	3.22285000
H	-2.88242600	2.50054400	4.36323700

TS4

Zero-point correction= 0.625468 (Hartree/Particle)
Thermal correction to Energy= 0.662714
Thermal correction to Enthalpy= 0.663658
Thermal correction to Gibbs Free Energy= 0.559837
Sum of electronic and zero-point Energies= -2250.919365
Sum of electronic and thermal Energies= -2250.882119
Sum of electronic and thermal Enthalpies= -2250.881175
Sum of electronic and thermal Free Energies= -2250.984997
Imaginary frequency=-907.06 cm^{-1}

C	6.98997600	-1.14802300	-1.05261800
C	5.73235000	-1.70266600	-1.08372200
C	4.62663200	-0.95455500	-0.62080100
C	4.82908900	0.38001000	-0.13716900
C	6.13530900	0.91843200	-0.11004400
C	7.19218200	0.16339500	-0.56121700
H	7.84287700	-1.72108400	-1.40360900
H	5.55783600	-2.71075400	-1.44818200
H	6.26932900	1.93025500	0.26147300
H	8.19654100	0.57601100	-0.54653900
C	2.58554700	0.58406300	0.20558800
C	2.39888400	-0.77390500	-0.16875800
N	3.77720300	1.14859200	0.25146100
N	3.39063000	-1.52244300	-0.60924200
P	1.06180600	1.56335100	0.41997100
P	0.71754900	-1.49143900	0.06252500
C	1.47272600	2.78884200	1.69663100
H	2.52025100	3.08562700	1.59176400
H	0.83710500	3.67138900	1.59116800
H	1.32111400	2.35850200	2.68962800
C	0.57797600	-2.61769200	-1.36223000
H	1.57138100	-3.01245500	-1.59426100
H	-0.09380400	-3.44958800	-1.14204400
H	0.19451500	-2.07751800	-2.23072900
C	0.95107500	-2.59836100	1.58073200
C	1.27025700	-1.70061900	2.77503000
C	-0.33438400	-3.38088300	1.84351300
C	2.08780900	-3.59543900	1.35050600
H	2.19425600	-1.12861400	2.62959900
H	0.45663400	-0.99448500	2.97814400
H	1.40664900	-2.32133300	3.66771000

H	-0.59604200	-4.04019900	1.00910600
H	-0.17824500	-4.01541500	2.72304200
H	-1.19206000	-2.73555200	2.05453200
H	2.15130200	-4.24826300	2.22844600
H	1.90829600	-4.23456900	0.48027200
H	3.05926500	-3.11290700	1.22599300
C	1.00699200	2.51593700	-1.21597500
C	2.17163400	3.49495900	-1.32243200
C	1.05870300	1.49267400	-2.35143400
C	-0.31430200	3.27734400	-1.27689700
H	2.12332800	4.27280500	-0.55391600
H	3.14403400	3.00070600	-1.24551200
H	2.12439800	3.99362500	-2.29770900
H	0.26612800	0.73699300	-2.26044800
H	0.91231400	2.00544500	-3.30859600
H	2.02102100	0.97138300	-2.40375300
H	-0.35417800	3.85228300	-2.20906500
H	-1.17515100	2.59958800	-1.26227000
H	-0.42189900	3.98576000	-0.44829900
Co	-0.72564300	0.11805900	0.41953200
C	-4.56147100	-0.74841900	-0.43851600
C	-4.09057100	-2.06106500	-0.70696000
C	-4.98942800	-3.02802300	-1.18153200
C	-6.31557300	-2.67116600	-1.37764400
C	-6.75904700	-1.36631600	-1.10853700
C	-5.89298500	-0.38442700	-0.63864100
C	-2.30371100	-0.83567000	0.02824700
C	-2.69843800	-2.09002800	-0.39258500
H	-4.64789000	-4.03891300	-1.38900200
H	-7.02293100	-3.40869700	-1.74633100
H	-7.80328100	-1.11342900	-1.27004900
H	-6.23500700	0.62321100	-0.43789100
H	-1.28357400	-0.82188200	1.39379100
H	-2.05815300	-2.95828600	-0.46336700
N	-3.46909500	-0.02269100	0.03340600
C	-3.39449500	1.30753600	0.41214200
C	-2.28105200	1.71461900	1.17622000
N	-4.35352500	2.14467100	0.01214300
C	-2.17130800	3.06084600	1.51494800
H	-1.69158600	0.97726000	1.76229400
C	-4.22122800	3.43073400	0.35656200
C	-3.15187100	3.94670400	1.08429600
H	-1.34701700	3.39786800	2.13705300
H	-5.02574900	4.08694400	0.02928500

H	-3.11016100	5.00207200	1.32886500

M6

Zero-point correction=	0.628095 (Hartree/Particle)
Thermal correction to Energy=	0.665414
Thermal correction to Enthalpy=	0.666359
Thermal correction to Gibbs Free Energy=	0.561640
Sum of electronic and zero-point Energies=	-2250.969571
Sum of electronic and thermal Energies=	-2250.932251
Sum of electronic and thermal Enthalpies=	-2250.931307
Sum of electronic and thermal Free Energies=	-2251.036026

C	6.65761400	-2.36368100	-0.06925400
C	5.31956200	-2.67408800	-0.00341100
C	4.35874100	-1.63801800	-0.03064700
C	4.79360600	-0.27543900	-0.13381200
C	6.17588300	0.01023500	-0.20041300
C	7.08636700	-1.01896000	-0.16660800
H	7.39892800	-3.15699900	-0.04432400
H	4.97111700	-3.69979300	0.07418500
H	6.48456000	1.04864400	-0.27581200
H	8.14941100	-0.80247500	-0.21488500
C	2.62058300	0.41481400	-0.10134100
C	2.19096900	-0.93425900	0.03247200
N	3.89686900	0.74605700	-0.17053200
N	3.03666300	-1.94602000	0.05772800
P	1.30940100	1.68627200	-0.17273200
P	0.38277700	-1.24608700	0.21847600
C	1.81571900	2.81238900	1.17341100
H	2.87631800	3.06019900	1.07259100
H	1.23167200	3.73566500	1.14765800
H	1.66349900	2.32558400	2.14070900
C	0.15415700	-2.77687700	-0.72744600
H	0.96722100	-3.46576300	-0.48300700
H	-0.80705100	-3.23823500	-0.49367000
H	0.19029300	-2.55283000	-1.79533800
C	0.14112900	-1.71142000	2.02178700
C	0.61970000	-0.54283000	2.88104100
C	-1.35196700	-1.95272500	2.23969900
C	0.92641200	-2.97647400	2.36474900
H	1.69064800	-0.34758200	2.75029100
H	0.06896000	0.37722400	2.65462500
H	0.45477200	-0.77619000	3.93875200
H	-1.73937600	-2.75973300	1.60796000
H	-1.52131000	-2.24163400	3.28314500

H	-1.94127100	-1.05307400	2.04215300
H	0.78700900	-3.19150600	3.43070800
H	0.57061900	-3.84734800	1.80674200
H	1.99940300	-2.86786000	2.18425300
C	1.55662600	2.66747400	-1.76156300
C	2.60893900	3.76024700	-1.60661100
C	1.95876700	1.72958800	-2.89780300
C	0.17774000	3.27254900	-2.04515200
H	2.33524100	4.49810500	-0.84722200
H	3.58843400	3.34528200	-1.34759100
H	2.71437000	4.29260100	-2.55923500
H	1.24712400	0.90800400	-3.03031200
H	1.98568200	2.29708100	-3.83511900
H	2.95464500	1.30266400	-2.74234200
H	0.19480000	3.83949600	-2.98294500
H	-0.58451800	2.48438700	-2.13942200
H	-0.14232600	3.95558200	-1.24863100
Co	-0.62060400	0.52553000	-0.38249600
C	-4.47570100	-0.68352900	-0.58827900
C	-4.03684100	-1.50621500	-1.66219200
C	-4.95671800	-2.32088800	-2.33318200
C	-6.28452900	-2.31557300	-1.92741200
C	-6.69843500	-1.51411000	-0.85601800
C	-5.80591400	-0.69120200	-0.17206500
C	-2.19704400	-0.39277300	-0.87887000
C	-2.62690400	-1.30995900	-1.80819800
H	-4.62814100	-2.94978200	-3.15656200
H	-7.00956400	-2.94319500	-2.43803200
H	-7.73761500	-1.53344800	-0.54099800
H	-6.16303000	-0.10922200	0.66773700
H	0.02813900	0.01794700	-1.60406100
H	-1.99157800	-1.81079200	-2.52800700
N	-3.34085100	-0.00172100	-0.13004400
C	-3.18141600	0.99591900	0.80874100
C	-4.20995900	1.61002300	1.53130000
N	-1.88087800	1.36375900	0.97245100
C	-3.88611200	2.59136300	2.45204700
H	-5.24279100	1.34422900	1.36022700
C	-1.59351200	2.32033100	1.87633900
C	-2.55270100	2.95222700	2.64387400
H	-4.67714000	3.07758100	3.01436500
H	-0.54238000	2.56916900	1.97525800
H	-2.26232600	3.71260600	3.35908300

TS5

Zero-point correction=	0.966159 (Hartree/Particle)
Thermal correction to Energy=	1.025382
Thermal correction to Enthalpy=	1.026326
Thermal correction to Gibbs Free Energy=	0.875945
Sum of electronic and zero-point Energies=	-3589.271953
Sum of electronic and thermal Energies=	-3589.212730
Sum of electronic and thermal Enthalpies=	-3589.211785
Sum of electronic and thermal Free Energies=	-3589.362167

Imaginary frequency=-229.95 cm^{-1}

C	7.76913900	-2.52802900	-2.11847000
C	6.41188900	-2.61071600	-2.32117800
C	5.54690900	-1.74120700	-1.61816100
C	6.09844000	-0.77645600	-0.71564400
C	7.49737300	-0.71798100	-0.52524500
C	8.31280500	-1.58132000	-1.21747500
H	8.43740300	-3.19679200	-2.65269800
H	5.97729000	-3.33433000	-3.00450100
H	7.89500500	0.01977400	0.16545100
H	9.38877700	-1.53859400	-1.07777000
C	3.99370800	-0.01142400	-0.26839400
C	3.43690000	-1.02395600	-1.09655500
N	5.29349900	0.10275800	-0.06588500
N	4.20365300	-1.84533200	-1.78794900
P	2.84757200	1.23433800	0.41694200
P	1.59243800	-1.18377500	-1.15945500
C	3.59370100	1.61851600	2.03010900
H	4.67069300	1.75039400	1.90190700
H	3.16588600	2.53224100	2.45023500
H	3.42342000	0.79371800	2.72562600
C	1.25047100	-0.86617800	-2.91980500
H	1.90881200	-1.48466900	-3.53495100
H	0.20908600	-1.10268600	-3.15605100
H	1.44016100	0.18130200	-3.15550200
C	1.31832200	-3.06763100	-1.00227200
C	2.06892000	-3.55923000	0.23215600
C	-0.17178300	-3.39581100	-0.88312500
C	1.82764100	-3.79883100	-2.25090200
H	3.15406300	-3.48505100	0.10948500
H	1.78571600	-3.00650600	1.13380400
H	1.82898000	-4.61416500	0.40691700
H	-0.76434500	-2.91139800	-1.66700300
H	-0.29230000	-4.47689100	-1.01670700
H	-0.59066700	-3.13942700	0.08974700

H	1.74595600	-4.87501400	-2.05830100
H	1.21070100	-3.58164400	-3.12780400
H	2.86756200	-3.57244100	-2.48672800
C	3.22911000	2.76619800	-0.62885600
C	4.66537500	3.23548700	-0.39580300
C	3.02924800	2.41255700	-2.10008600
C	2.27125100	3.88511700	-0.22464400
H	4.81808500	3.61134900	0.62032000
H	5.40596700	2.45481500	-0.58836300
H	4.86650300	4.06528600	-1.08350600
H	2.00316100	2.08476600	-2.29681600
H	3.21212300	3.30351800	-2.71159000
H	3.72372800	1.63560800	-2.44154000
H	2.57516800	4.81040700	-0.72724000
H	1.24454000	3.66988600	-0.52560100
H	2.29212900	4.07996500	0.85417700
Co	0.80814100	0.25475000	0.45391600
C	-1.64728200	3.32545400	-0.69337900
C	-1.54278100	2.81101700	-2.00916100
C	-2.27711600	3.40548600	-3.04061200
C	-3.10562300	4.48207800	-2.74735000
C	-3.22441600	4.95659400	-1.43542200
C	-2.50489400	4.38194000	-0.38863300
C	-0.21582200	1.49194700	-0.68524600
C	-0.65858400	1.68174600	-1.96566200
H	-2.21126700	3.01408100	-4.05301900
H	-3.68163900	4.95195300	-3.54012100
H	-3.89675800	5.78213400	-1.21930400
H	-2.65091600	4.74972900	0.62007800
H	-0.42655100	1.06231700	-2.81859100
N	-0.81697700	2.52350800	0.09896900
C	-0.43821700	2.65782700	1.40752200
C	-0.70325500	3.75840700	2.23537800
N	0.29251800	1.61117300	1.85767700
C	-0.29161900	3.71361000	3.55455800
H	-1.19556000	4.63527100	1.83892300
C	0.65282600	1.56513400	3.15188300
C	0.36709700	2.58269100	4.04259800
H	-0.48823700	4.56053200	4.20498700
H	1.20725100	0.68020300	3.44888700
H	0.67900600	2.50221800	5.07724000
C	-1.09904500	-3.24189700	4.52783800
C	-1.17349100	-2.49642900	3.35901500
C	-0.02280900	-1.87311700	2.83527200

C	1.19278900	-2.01730800	3.52114200
C	1.26065000	-2.76783000	4.68879200
C	0.11667500	-3.38029100	5.19751100
H	-1.99487300	-3.71577600	4.91912700
H	-2.12040000	-2.38857700	2.83423700
H	2.08588400	-1.53740700	3.12250600
H	2.21049400	-2.87273100	5.20520200
H	0.17102000	-3.96206300	6.11288500
C	-0.18554600	-1.12795500	1.61393300
C	-0.94400700	-0.71241300	0.68557200
C	-2.16387600	-0.89490000	-0.12121400
H	-2.65341300	-1.82982000	0.21086400
H	-1.86972700	-1.02471500	-1.16798500
N	-3.11528900	0.22525800	-0.07970500
C	-3.91777400	0.28754300	1.16965000
H	-4.71516100	1.01508800	0.99803100
H	-4.38694600	-0.69691400	1.34940200
C	-3.13849800	0.69576000	2.37736500
C	-3.34003500	1.84941700	3.01302100
H	-2.42118200	-0.01856700	2.78091300
H	-2.80022700	2.09994100	3.92215000
H	-4.05524300	2.58413500	2.64623300
S	-4.12241600	0.26650400	-1.46531200
O	-4.92999800	1.47381200	-1.33191100
O	-3.25921800	0.04775800	-2.62267400
C	-5.19995700	-1.13993700	-1.32560500
C	-6.44387200	-1.00332800	-0.71125700
C	-4.76149200	-2.38424700	-1.78613600
C	-7.25626500	-2.12322600	-0.57086700
H	-6.77466800	-0.02853600	-0.36472100
C	-5.58510000	-3.49084600	-1.63455800
H	-3.79684900	-2.47456000	-2.27802900
C	-6.84327100	-3.38076200	-1.02448400
H	-8.23197300	-2.02044200	-0.10260100
H	-5.25217800	-4.45951500	-1.99987500
C	-7.72455600	-4.57966000	-0.87939200
H	-8.61680100	-4.35576000	-0.28994700
H	-8.05500900	-4.94763200	-1.85691800
H	-7.19676200	-5.40857000	-0.39731000
H	1.60418200	-0.59398700	1.42729900

M7

Zero-point correction=	0.972671 (Hartree/Particle)
Thermal correction to Energy=	1.031934

Thermal correction to Enthalpy= 1.032879
Thermal correction to Gibbs Free Energy= 0.882268
Sum of electronic and zero-point Energies= -3589.301086
Sum of electronic and thermal Energies= -3589.241823
Sum of electronic and thermal Enthalpies= -3589.240879
Sum of electronic and thermal Free Energies= -3589.391489

C	7.01885400	-3.26764700	-2.70067800
C	5.65062900	-3.13564500	-2.68449300
C	5.03654400	-2.34071000	-1.68989000
C	5.85248100	-1.65797800	-0.72802800
C	7.25557500	-1.82769900	-0.76146000
C	7.82216700	-2.61860700	-1.73274300
H	7.49444400	-3.88025500	-3.46081500
H	5.01640600	-3.63544700	-3.41086700
H	7.85671200	-1.30779900	-0.02105500
H	8.90018700	-2.74420000	-1.76725300
C	3.98307000	-0.68951000	0.15626000
C	3.17025500	-1.48400100	-0.69897500
N	5.29880600	-0.80880800	0.17667400
N	3.68144600	-2.26946400	-1.62861900
P	3.13843900	0.65638200	1.07137400
P	1.36371600	-1.53037600	-0.37192200
C	3.77985200	0.52427400	2.77434400
H	4.85611800	0.33089500	2.76828500
H	3.58792200	1.45287100	3.31947600
H	3.27863100	-0.29413100	3.29845200
C	0.70371300	-2.04611900	-1.98875400
H	0.90816300	-3.10968800	-2.14065300
H	-0.36659500	-1.86197100	-2.08406800
H	1.21532700	-1.49352000	-2.77908400
C	1.23036900	-3.05802700	0.73801100
C	1.64646000	-2.61242000	2.13844200
C	-0.22282600	-3.53263600	0.72169200
C	2.13753300	-4.19163500	0.26622200
H	2.70245200	-2.31755900	2.16689200
H	1.04327400	-1.76263500	2.48173200
H	1.51521600	-3.43205100	2.85444000
H	-0.53094700	-3.86774700	-0.27488200
H	-0.32487500	-4.38745700	1.40039000
H	-0.91888500	-2.76205300	1.06137600
H	1.92195400	-5.08225700	0.86775900
H	1.97458400	-4.45800800	-0.78294400
H	3.19773900	-3.95675800	0.39649900
C	3.98034700	2.19144700	0.34290700

C	5.39202600	2.35488600	0.90256100
C	4.03141200	2.04481900	-1.17842500
C	3.14235200	3.41698800	0.70231400
H	5.38744700	2.56429700	1.97655400
H	6.01390000	1.47389500	0.72238600
H	5.86566700	3.20954700	0.40473700
H	3.04313900	1.83217300	-1.60148400
H	4.38026400	2.98802200	-1.61398000
H	4.72487800	1.26043200	-1.49800500
H	3.69694400	4.32063000	0.42429300
H	2.20028200	3.43040100	0.14876100
H	2.92474400	3.48359900	1.77469700
Co	0.79652200	0.31741800	0.83899900
C	-0.62123000	3.36980500	-1.30433500
C	-0.23433900	2.60558800	-2.43589200
C	-0.53208500	3.07775200	-3.71822200
C	-1.21740300	4.27989000	-3.85159900
C	-1.61564200	5.00778300	-2.72416600
C	-1.32698700	4.56271500	-1.43424700
C	0.37743600	1.41561600	-0.60248100
C	0.37973000	1.39515800	-1.96689900
H	-0.24854800	2.49805600	-4.59290500
H	-1.46212000	4.65325300	-4.84242500
H	-2.17091200	5.93308000	-2.84914300
H	-1.68005700	5.12860300	-0.58010700
H	0.71989100	0.58594600	-2.59659400
N	-0.21094600	2.63818000	-0.18197900
C	-0.08708300	2.97581900	1.14298800
C	-0.39271600	4.21387600	1.72060200
N	0.43776800	1.97022800	1.88248200
C	-0.17554800	4.38473700	3.07619900
H	-0.77554400	5.02498100	1.11647900
C	0.64475600	2.15164500	3.19807900
C	0.34529200	3.33798000	3.84061000
H	-0.40619900	5.33969100	3.53855000
H	1.06961300	1.30576600	3.73309900
H	0.52612500	3.44041700	4.90402300
C	-4.51451700	-1.92631700	3.61326300
C	-3.61647400	-1.17614700	2.86010100
C	-2.23758900	-1.22698000	3.12183900
C	-1.80171900	-2.03701200	4.18696700
C	-2.69825100	-2.79187300	4.93339600
C	-4.06183400	-2.74423400	4.64610500
H	-5.57735500	-1.86188200	3.39556400

H	-3.99467200	-0.51908900	2.08411300
H	-0.73854300	-2.07063700	4.42002800
H	-2.33349900	-3.41511100	5.74574400
H	-4.76626000	-3.32842500	5.23141700
C	-1.21351200	-0.48169600	2.37228600
C	-1.07546500	-0.18736700	1.06020700
C	-2.08005500	-0.53322300	0.00223300
H	-2.88325200	-1.16510900	0.41937400
H	-1.56972700	-1.13419300	-0.75507500
N	-2.67692300	0.61398900	-0.72301100
C	-3.76604500	1.31192700	0.00372600
H	-4.30689500	1.92272200	-0.72267100
H	-4.47708200	0.56363500	0.40014600
C	-3.28856500	2.20055500	1.10483000
C	-3.63783100	3.48394800	1.19124100
H	-2.67126600	1.75082800	1.88299800
H	-3.33250900	4.10389300	2.03007300
H	-4.25577900	3.95697100	0.42958800
S	-3.15489900	0.18951600	-2.30280300
O	-3.76673700	1.38084000	-2.88317800
O	-2.00557100	-0.44807600	-2.94269700
C	-4.41203900	-1.05002200	-2.10457000
C	-5.74828500	-0.66829200	-1.99152500
C	-4.03990600	-2.39119200	-1.98498800
C	-6.71608700	-1.64317500	-1.77380700
H	-6.02552100	0.37726500	-2.09164500
C	-5.01965100	-3.35035100	-1.76598700
H	-2.99489100	-2.67708000	-2.07799100
C	-6.37122900	-2.99472400	-1.65759900
H	-7.76054300	-1.35120800	-1.69498200
H	-4.73468600	-4.39648300	-1.68101500
C	-7.41783100	-4.04187800	-1.44756500
H	-8.35837400	-3.61035200	-1.09688900
H	-7.63121200	-4.57500600	-2.38125500
H	-7.09336900	-4.79556300	-0.72424900
H	-0.35320900	-0.24237500	3.01176100

TS6R

Zero-point correction=	0.974223 (Hartree/Particle)
Thermal correction to Energy=	1.031711
Thermal correction to Enthalpy=	1.032656
Thermal correction to Gibbs Free Energy=	0.888679
Sum of electronic and zero-point Energies=	-3589.264446
Sum of electronic and thermal Energies=	-3589.206958

Sum of electronic and thermal Enthalpies= -3589.206014

Sum of electronic and thermal Free Energies= -3589.349991

Imaginary frequency=-284.73 cm^{-1}

C	-4.31530200	-3.98602600	-3.14118000
C	-3.00272800	-3.57477200	-3.17623600
C	-2.35461700	-3.21174600	-1.97430800
C	-3.07556900	-3.25731600	-0.74385500
C	-4.42057800	-3.68749100	-0.73533300
C	-5.02386600	-4.04756200	-1.91810700
H	-4.82078500	-4.26368900	-4.06142800
H	-2.44356900	-3.51620600	-4.10607200
H	-4.95115300	-3.71252700	0.21253300
H	-6.05883200	-4.37606000	-1.92010900
C	-1.23590400	-2.44176800	0.36126000
C	-0.50676500	-2.39807700	-0.87534700
N	-2.48846500	-2.85096500	0.41164000
N	-1.07085000	-2.77169100	-2.00637100
P	-0.45877000	-1.77298600	1.90026300
P	1.20399900	-1.67624000	-0.93547000
C	-1.85378700	-0.93025100	2.75005500
H	-2.80821100	-1.37625500	2.45708000
H	-1.73282300	-1.03342900	3.83032400
H	-1.87503600	0.13953800	2.53115700
C	2.27035700	-3.08458900	-0.45443500
H	1.96786400	-4.00462300	-0.96019100
H	3.30549800	-2.85733100	-0.72730700
H	2.23606400	-3.24015100	0.62360800
C	1.62261100	-1.48050700	-2.77226000
C	0.61701900	-0.54315600	-3.43344500
C	3.01422900	-0.85324900	-2.88082900
C	1.66084800	-2.83325700	-3.49028700
H	-0.38944000	-0.96620300	-3.46587100
H	0.57774900	0.42013000	-2.91448900
H	0.93428800	-0.34624700	-4.46447500
H	3.78441600	-1.42150300	-2.34840100
H	3.29855400	-0.83964800	-3.93925800
H	3.02658100	0.17760300	-2.52223100
H	1.86469800	-2.64463100	-4.55126400
H	2.46955500	-3.46950800	-3.11814500
H	0.71910400	-3.37854700	-3.41995700
C	-0.33117600	-3.35193100	3.01235900
C	-1.66845800	-4.09736800	3.02972800
C	0.73304400	-4.30135500	2.47139200
C	-0.01642300	-2.96293800	4.46137100

H	-2.50916300	-3.46130900	3.32054800
H	-1.90621100	-4.56305900	2.07171000
H	-1.58943100	-4.89636600	3.77702000
H	1.74683800	-3.89910100	2.55152000
H	0.70891400	-5.22887400	3.05493900
H	0.54645200	-4.57087300	1.42633800
H	0.20426100	-3.88043700	5.01878700
H	0.84329500	-2.30090300	4.59159700
H	-0.87128500	-2.49391100	4.95606100
Co	1.23749900	0.03172400	0.75032300
C	4.93885500	0.85461900	-0.73915900
C	4.39829400	2.05848700	-1.24415000
C	5.18983400	2.88693600	-2.04747300
C	6.48860700	2.49094500	-2.34458700
C	6.99510700	1.27482600	-1.86905000
C	6.22642600	0.43451600	-1.06556500
C	2.70045000	1.00194400	-0.11308100
C	3.02293600	2.12618000	-0.83450300
H	4.78665600	3.81597200	-2.44189100
H	7.11393100	3.12163100	-2.97019000
H	8.00092700	0.96795600	-2.14110400
H	6.62377400	-0.52505100	-0.75491300
H	2.37576000	2.95234600	-1.08773900
N	3.90909900	0.24097200	-0.01332600
C	4.00485900	-0.63893400	1.03648600
C	5.18727400	-1.21619800	1.51429100
N	2.81392600	-0.85188800	1.64157100
C	5.13582100	-1.99186000	2.65863000
H	6.12953400	-1.02227800	1.02232400
C	2.79889700	-1.56058800	2.78026500
C	3.92042700	-2.15912400	3.32150100
H	6.04608800	-2.43855800	3.04615200
H	1.83314900	-1.63162600	3.25830300
H	3.83656600	-2.73119500	4.23873100
C	-3.62783900	0.79142500	-3.47276400
C	-2.52003600	0.84438100	-2.63363200
C	-2.62575600	0.48400300	-1.27567200
C	-3.88068300	0.02930800	-0.81905400
C	-4.98725800	-0.01354900	-1.65603500
C	-4.86695900	0.37298800	-2.99027500
H	-3.51805700	1.07130900	-4.51696600
H	-1.56283100	1.13571800	-3.05218200
H	-3.97596300	-0.28076600	0.22137400
H	-5.94214500	-0.36186400	-1.27069800

H	-5.72702800	0.33311300	-3.65247100
C	-1.53828200	0.47780100	-0.30031500
C	-0.32793300	1.09180000	-0.25675600
C	-0.07316500	2.29161000	-1.12488500
H	-0.93103100	2.49397300	-1.76815000
H	0.79121000	2.16768200	-1.78210500
N	0.12818600	3.49640400	-0.29114700
C	0.66941900	3.19831100	1.03531700
H	1.76217200	3.21682700	0.99817700
H	0.37103700	3.98898200	1.73155800
C	0.21196500	1.87846300	1.58960100
C	1.14097700	1.17737500	2.39820200
H	-0.83928600	1.81618300	1.86319900
H	0.77830700	0.56896700	3.22550200
H	2.12737600	1.61587300	2.54023800
S	-1.08659000	4.67435600	-0.30875100
O	-0.48830600	5.84570300	0.32576000
O	-1.58725400	4.71561500	-1.67962100
C	-2.38426900	4.10042300	0.75680600
C	-2.32189500	4.37402900	2.12449900
C	-3.40727900	3.31018700	0.23154100
C	-3.27882800	3.82449600	2.97051200
H	-1.54170200	5.02093900	2.51522400
C	-4.35864000	2.77735300	1.09148900
H	-3.46092600	3.12489400	-0.83817900
C	-4.30294600	3.01046000	2.47262600
H	-3.23676500	4.03637500	4.03617200
H	-5.16150000	2.16666400	0.68417600
C	-5.31561100	2.39758700	3.38605800
H	-5.25258300	1.30325200	3.36697400
H	-5.17762900	2.72205400	4.42009400
H	-6.33590900	2.65412100	3.08357200
H	-1.78979200	-0.15865900	0.53604200

TS6S

Zero-point correction=	0.972110 (Hartree/Particle)
Thermal correction to Energy=	1.029950
Thermal correction to Enthalpy=	1.030894
Thermal correction to Gibbs Free Energy=	0.885540
Sum of electronic and zero-point Energies=	-3589.251789
Sum of electronic and thermal Energies=	-3589.193949
Sum of electronic and thermal Enthalpies=	-3589.193005
Sum of electronic and thermal Free Energies=	-3589.338360

Imaginary frequency=-344.19 cm^{-1}

C	-3.50705500	3.63333000	3.74531300
C	-2.36115500	2.87881000	3.63990000
C	-1.65099100	2.86186700	2.41800800
C	-2.13686600	3.61255400	1.30816800
C	-3.31989800	4.37315200	1.44127100
C	-3.98618400	4.38294400	2.64488400
H	-4.05592800	3.65594100	4.68224000
H	-1.97943400	2.29337100	4.47251000
H	-3.67457300	4.93496800	0.58155900
H	-4.89442700	4.96786600	2.75687800
C	-0.36083200	2.88467100	0.03317300
C	0.13452400	2.13213100	1.15890700
N	-1.47686900	3.58642900	0.12314300
N	-0.52557600	2.11341900	2.30012600
P	0.53060000	2.88922000	-1.58461400
P	1.66770400	1.06287700	1.08393100
C	-0.85986500	2.83000800	-2.78543300
H	-1.75286200	3.34051000	-2.41367300
H	-0.53409500	3.31077400	-3.71263600
H	-1.11361400	1.79707400	-3.03613300
C	3.03387400	2.24549000	0.79722000
H	2.95575600	3.11559100	1.45338800
H	3.98471400	1.74226400	0.99460900
H	3.03715600	2.56974100	-0.24409100
C	1.98785300	0.50735000	2.86764400
C	0.91042600	-0.49274600	3.28614300
C	3.34656700	-0.20112500	2.92687200
C	2.06171300	1.69665600	3.83008200
H	-0.09396400	-0.06263400	3.26838000
H	0.93253600	-1.37501000	2.63721700
H	1.11486900	-0.83445400	4.30767900
H	4.17415100	0.42236000	2.57460900
H	3.55353800	-0.44036400	3.97625200
H	3.35307500	-1.14130800	2.37600500
H	2.26570700	1.30536600	4.83395400
H	2.88764600	2.36894200	3.57705600
H	1.13879100	2.27395800	3.87823800
C	1.05161700	4.72452400	-1.75648700
C	-0.13603000	5.65123400	-2.00608500
C	1.78342200	5.19712200	-0.50320200
C	2.00780600	4.77049100	-2.94969200
H	-0.64097700	5.44382900	-2.95366500
H	-0.87808600	5.59375300	-1.20446600
H	0.22690500	6.68575400	-2.05346300

H	2.70990100	4.64606300	-0.32383200
H	2.05641400	6.25202600	-0.62614000
H	1.16007600	5.12705600	0.39567300
H	2.32438100	5.80413700	-3.13486300
H	2.90806400	4.17211400	-2.76733100
H	1.53856600	4.40548200	-3.87130000
Co	1.46470500	-0.41996300	-0.80525300
C	4.77971800	-2.30704800	0.46918000
C	3.87266400	-3.26005200	1.00309300
C	4.36554100	-4.36235900	1.71059700
C	5.73828000	-4.50159300	1.86918000
C	6.62036700	-3.55349100	1.33626900
C	6.15728700	-2.44366800	0.63322100
C	2.62280700	-1.65008100	0.00134200
C	2.53932300	-2.82965600	0.69058900
H	3.67816200	-5.09428100	2.12610000
H	6.13448300	-5.35335100	2.41513800
H	7.69055100	-3.67617000	1.47465100
H	6.87157600	-1.72583900	0.25051800
H	-0.81604200	0.42854100	-1.60107400
H	1.63191300	-3.34724500	0.97193600
N	3.99169100	-1.32526300	-0.15301300
C	4.30382600	-0.31398200	-1.03708000
C	5.59177000	0.10143800	-1.38840400
N	3.20079400	0.25985300	-1.57763400
C	5.73407500	1.07155700	-2.36576400
H	6.46059300	-0.33356100	-0.91696400
C	3.36007000	1.16483000	-2.55990200
C	4.60256900	1.59987300	-2.98503200
H	6.72812600	1.39893900	-2.65423200
H	2.44377600	1.54749900	-2.99312400
H	4.67505800	2.33254600	-3.78055800
C	-4.23257200	0.74867500	1.35162800
C	-2.96724300	0.28515400	1.01127300
C	-2.53665500	0.28841200	-0.32794300
C	-3.41485900	0.79125000	-1.30601300
C	-4.68313200	1.24428200	-0.96437000
C	-5.09608100	1.22770100	0.36781700
H	-4.53946800	0.74953700	2.39419300
H	-2.28698700	-0.03679200	1.79685100
H	-3.08998300	0.81348200	-2.34421500
H	-5.34888100	1.61959100	-1.73723100
H	-6.08244300	1.59492800	0.63967400
C	-1.20111400	-0.13584300	-0.74614300

C	-0.37971600	-1.09753200	-0.25167500
C	-0.91838200	-2.23978600	0.55356600
H	-1.86110400	-1.96274600	1.03842000
H	-0.24245500	-2.61221800	1.32766200
N	-1.15013800	-3.32148000	-0.44632300
C	-0.89951900	-2.88539700	-1.82299500
H	-0.77528300	-3.77730200	-2.44643900
H	-1.69444500	-2.25401000	-2.24714200
C	0.42902300	-2.18422800	-1.73741000
C	1.04504300	-1.25619000	-2.61257300
H	1.13455800	-2.87936000	-1.28538400
H	2.00772900	-1.52116600	-3.03998500
H	0.43054200	-0.58630900	-3.21911300
S	-2.39488500	-4.40094600	-0.16749200
O	-2.23884000	-5.44902900	-1.17288500
O	-2.34144800	-4.68927500	1.26285100
C	-3.91538200	-3.55270800	-0.50075600
C	-4.40320800	-3.50337500	-1.80894600
C	-4.58937000	-2.91229600	0.53878500
C	-5.57479400	-2.80482400	-2.06809400
H	-3.87927500	-4.02303400	-2.60610400
C	-5.76368500	-2.22270300	0.25974600
H	-4.20668200	-2.97143800	1.55400100
C	-6.27237500	-2.15307200	-1.04175400
H	-5.96043500	-2.76392800	-3.08417400
H	-6.29481200	-1.72369700	1.06656300
C	-7.53440200	-1.40620900	-1.33336100
H	-7.78194700	-0.70493300	-0.53209200
H	-7.46107500	-0.84662400	-2.27083200
H	-8.38328200	-2.09108000	-1.44208600

M8R

Zero-point correction=	0.976489 (Hartree/Particle)
Thermal correction to Energy=	1.033843
Thermal correction to Enthalpy=	1.034788
Thermal correction to Gibbs Free Energy=	0.890478
Sum of electronic and zero-point Energies=	-3589.317945
Sum of electronic and thermal Energies=	-3589.260591
Sum of electronic and thermal Enthalpies=	-3589.259647
Sum of electronic and thermal Free Energies=	-3589.403956

C	4.57449400	-4.44628100	2.63466600
C	3.20496600	-4.35159200	2.54986500
C	2.62013400	-3.62572500	1.48769500
C	3.45872500	-3.00414500	0.51044800

C	4.86282900	-3.11020300	0.62899700
C	5.40473200	-3.82233400	1.67384700
H	5.03012700	-5.00119100	3.44927000
H	2.54975100	-4.81315200	3.28319800
H	5.48528600	-2.63068200	-0.12099100
H	6.48292300	-3.91109500	1.76597400
C	1.59858900	-2.22572500	-0.58094400
C	0.75825700	-2.80678700	0.42761700
N	2.91680700	-2.30900400	-0.52564900
N	1.26964700	-3.50009600	1.42713100
P	0.81971200	-1.29905500	-1.97111300
P	-1.06292400	-2.47049800	0.37164900
C	2.01923100	0.04787700	-2.27713800
H	2.97103100	-0.33174100	-2.65198000
H	1.59981800	0.73966200	-3.01249400
H	2.21254900	0.59929900	-1.35497000
C	-1.74027600	-3.85077100	-0.62026900
H	-1.30510300	-4.81215400	-0.33599600
H	-2.82379100	-3.89223200	-0.47336000
H	-1.55823700	-3.67305600	-1.68002500
C	-1.74703400	-2.81360700	2.09433000
C	-1.03508000	-1.90975500	3.09826200
C	-3.23918700	-2.46176500	2.07241600
C	-1.61068000	-4.28595400	2.48685300
H	0.02252300	-2.16523500	3.21194900
H	-1.11066800	-0.85639700	2.80589400
H	-1.51085800	-2.01387400	4.08059800
H	-3.79344500	-3.00807100	1.30091500
H	-3.67470500	-2.74573100	3.03730100
H	-3.41034500	-1.39194200	1.93722300
H	-2.01173100	-4.41052500	3.50002000
H	-2.19439600	-4.93797800	1.82915300
H	-0.57389700	-4.62497000	2.48880000
C	1.13293900	-2.39935100	-3.50776500
C	2.58885200	-2.86384300	-3.57112300
C	0.26154100	-3.65168300	-3.49354700
C	0.82388200	-1.53889000	-4.73555200
H	3.31631100	-2.04898100	-3.54095000
H	2.83161100	-3.56703500	-2.77059100
H	2.72948000	-3.38686500	-4.52453800
H	-0.80783700	-3.44442700	-3.58252200
H	0.53333300	-4.27687300	-4.35145000
H	0.42695900	-4.24909900	-2.59059400
H	0.89760300	-2.16126200	-5.63434500

H	-0.18302000	-1.10683700	-4.71886300
H	1.53749100	-0.71751800	-4.84845900
Co	-1.21515800	-0.39824900	-0.80604800
C	-4.79057500	0.75253800	0.65941700
C	-4.04751100	1.32413300	1.72669700
C	-4.72568700	1.97793100	2.76160300
C	-6.11270100	2.05257000	2.71946200
C	-6.82943700	1.48054300	1.66161400
C	-6.18095700	0.82205600	0.61785600
C	-2.53766800	0.36939600	0.31332100
C	-2.65395400	1.07420900	1.48156400
H	-4.16974400	2.42135100	3.58381100
H	-6.64900600	2.55892100	3.51709300
H	-7.91340400	1.54603600	1.64758200
H	-6.76869100	0.38568200	-0.18063200
H	-1.83891400	1.35394600	2.13545600
N	-3.84215200	0.17628500	-0.19867000
C	-3.93980500	-0.47730800	-1.39909400
C	-5.11144600	-0.76955100	-2.10402600
N	-2.72188300	-0.84238000	-1.88784100
C	-5.01855400	-1.41904500	-3.32258800
H	-6.07396500	-0.48312300	-1.70490500
C	-2.64884300	-1.44847800	-3.08420900
C	-3.76656500	-1.76350400	-3.83214700
H	-5.92263300	-1.64761800	-3.87782000
H	-1.64639700	-1.67575700	-3.42349400
H	-3.64956300	-2.25800200	-4.78919800
C	1.09511600	1.14582200	4.71066800
C	0.63820800	1.45654700	3.43351200
C	1.18164200	0.81768000	2.30520200
C	2.19375200	-0.13840900	2.50931900
C	2.65842000	-0.43742100	3.78306400
C	2.10522100	0.20241000	4.89238500
H	0.65347200	1.64079700	5.57125800
H	-0.16883400	2.17556700	3.31990700
H	2.62089900	-0.63741300	1.63935700
H	3.44931900	-1.17234800	3.91167000
H	2.45630600	-0.03492900	5.89267900
C	0.75014800	1.06185000	0.93398800
C	0.17648200	2.15681600	0.38969200
C	-0.07362600	3.46033400	1.09642900
H	0.67581800	3.71123200	1.85369600
H	-1.05161700	3.46184500	1.59975300
N	-0.11929600	4.47922200	0.03087600

C	-0.66757600	3.78815900	-1.14550800
H	-1.76054700	3.79603200	-1.04463000
H	-0.41235900	4.32255000	-2.06274400
C	-0.14240100	2.33772900	-1.09029700
C	-1.08569800	1.34371100	-1.76555600
H	0.82649200	2.32180700	-1.60648000
H	-0.77377500	1.13893900	-2.79796200
H	-2.10114300	1.75493100	-1.80044200
S	1.28907500	5.38953900	-0.18476400
O	1.02032300	6.25544200	-1.32909800
O	1.59698700	5.93157600	1.13611700
C	2.59764100	4.27436900	-0.63163000
C	2.86637900	4.02979500	-1.97810300
C	3.27556700	3.57877500	0.37233800
C	3.81172300	3.06734400	-2.31581300
H	2.34101500	4.58940700	-2.74676000
C	4.21096800	2.61685500	0.01611600
H	3.07119600	3.79428100	1.41767900
C	4.48459200	2.33575800	-1.32965300
H	4.02608300	2.86949800	-3.36385400
H	4.73938400	2.06981400	0.79363900
C	5.45143900	1.25477100	-1.69193900
H	5.11518900	0.28607900	-1.30162300
H	5.56637600	1.15842200	-2.77429700
H	6.44094300	1.43812400	-1.26061800
H	1.01399400	0.24585900	0.25405100

M8S

Zero-point correction=	0.974387 (Hartree/Particle)
Thermal correction to Energy=	1.032012
Thermal correction to Enthalpy=	1.032956
Thermal correction to Gibbs Free Energy=	0.885282
Sum of electronic and zero-point Energies=	-3589.308576
Sum of electronic and thermal Energies=	-3589.250951
Sum of electronic and thermal Enthalpies=	-3589.250007
Sum of electronic and thermal Free Energies=	-3589.397680

C	4.83319200	-5.25403000	-2.30593600
C	4.64736700	-3.90154300	-2.47292100
C	4.09791500	-3.13849500	-1.41798500
C	3.74296000	-3.78188800	-0.19203500
C	3.94123000	-5.17386500	-0.05035200
C	4.47915000	-5.89137600	-1.09291300
H	5.25505500	-5.84583500	-3.11287800
H	4.90706100	-3.39453200	-3.39802500

H	3.65975000	-5.64528100	0.88698500
H	4.63459300	-6.96114800	-0.99046600
C	2.99708300	-1.77758300	0.63889300
C	3.35363000	-1.13233100	-0.59003900
N	3.19003200	-3.07095200	0.82443100
N	3.89378000	-1.80695900	-1.58738100
P	2.12191800	-0.81645000	1.95323600
P	2.96130300	0.66309900	-0.78822500
C	0.85672300	-2.03072200	2.48191500
H	1.28660600	-3.03481600	2.47817500
H	0.50329400	-1.79405400	3.48880400
H	-0.00573600	-2.01789900	1.81293500
C	4.47808400	1.44358000	-0.12925000
H	5.37311300	1.01965000	-0.59235000
H	4.45607600	2.52199000	-0.31207200
H	4.53511200	1.27944400	0.94796600
C	3.01095300	1.04839800	-2.62944200
C	1.96621100	0.17990000	-3.33003900
C	2.64528400	2.52808400	-2.79224500
C	4.39689900	0.83731900	-3.24082800
H	2.23766800	-0.87982500	-3.31738600
H	0.97640300	0.29054400	-2.87058300
H	1.88023200	0.49088000	-4.37774600
H	3.32010500	3.18875800	-2.23589800
H	2.73880700	2.79429600	-3.85152300
H	1.61773600	2.73810200	-2.49104600
H	4.33538600	1.05722200	-4.31351500
H	5.13549100	1.52421000	-2.81533000
H	4.75727600	-0.18544200	-3.12369900
C	3.29854800	-0.84643000	3.46391900
C	3.56450200	-2.28737500	3.90510800
C	4.64180800	-0.20078500	3.12667200
C	2.61095900	-0.10846900	4.61462600
H	2.65901900	-2.80306900	4.23346400
H	4.03919700	-2.88591700	3.12414400
H	4.24665800	-2.25484300	4.76293100
H	4.58318800	0.88129100	2.98398600
H	5.32958500	-0.36581000	3.96337200
H	5.10335800	-0.64125100	2.23555800
H	3.28499300	-0.09610500	5.47868600
H	2.35698200	0.92993600	4.38448000
H	1.69195800	-0.61168300	4.93039900
Co	1.05348300	1.01787100	0.64508300
C	-0.26644300	4.36904000	-1.19755600

C	-1.01503100	3.49052700	-2.02497000
C	-1.80812000	4.02132600	-3.04912500
C	-1.84620100	5.39832100	-3.22958600
C	-1.10642700	6.25056700	-2.40075700
C	-0.30718800	5.75045100	-1.37412700
C	0.11561000	2.18399000	-0.53600100
C	-0.76348200	2.14658800	-1.58801900
H	-2.38431300	3.36011900	-3.69130300
H	-2.45811800	5.82160700	-4.02162300
H	-1.15095700	7.32468000	-2.55525600
H	0.24882700	6.44096500	-0.75228100
H	0.22321500	-0.64444400	0.19984300
H	-1.18448900	1.25493300	-2.03347400
N	0.41873300	3.54536600	-0.29257600
C	1.31391100	3.80731700	0.71050800
C	1.76770600	5.06540200	1.12119100
N	1.76831700	2.67302100	1.31052100
C	2.67941500	5.14802800	2.15870000
H	1.40662600	5.96050800	0.63565500
C	2.64290900	2.77413700	2.32316100
C	3.13014000	3.98333000	2.77919700
H	3.03390000	6.12093400	2.48381300
H	2.95017400	1.83299300	2.75668100
H	3.83805000	4.00229900	3.59963300
C	-1.64724000	-2.36791500	-3.58059400
C	-1.68620300	-1.53504000	-2.46812400
C	-0.73757700	-1.66700600	-1.43984700
C	0.25610000	-2.65152700	-1.56981000
C	0.29159600	-3.48511000	-2.68122800
C	-0.65896700	-3.34378300	-3.69283300
H	-2.38538300	-2.24622800	-4.36830800
H	-2.43919800	-0.75321300	-2.40655400
H	0.99315000	-2.76674700	-0.77829600
H	1.06306800	-4.24733200	-2.76002600
H	-0.62733200	-3.98969200	-4.56546200
C	-0.76550200	-0.77712800	-0.28482400
C	-1.82650400	-0.19453000	0.29901200
C	-3.27032300	-0.50102400	0.06310200
H	-3.43346200	-1.55318800	-0.19942600
H	-3.70389500	0.11373100	-0.73828200
N	-3.92035300	-0.13218600	1.35399700
C	-2.89570700	0.37992200	2.30400200
H	-3.32116100	1.17762300	2.91618200
H	-2.52014200	-0.41060500	2.97174400

C	-1.77536200	0.84280400	1.37229700
C	-0.42604600	1.10880700	2.00333300
H	-2.11765300	1.76717400	0.87840500
H	-0.40674800	2.10047200	2.46691000
H	-0.21506600	0.37263300	2.78806800
S	-4.92045400	-1.31722300	2.01406900
O	-4.31226900	-2.64951000	1.91141800
O	-5.30717400	-0.80149500	3.32642200
C	-6.31017100	-1.26848500	0.91744700
C	-6.46330700	-2.25753800	-0.05267400
C	-7.24092400	-0.23930900	1.05131200
C	-7.56276500	-2.20588300	-0.90039200
H	-5.73146000	-3.05610100	-0.13026900
C	-8.33654300	-0.20714200	0.19840400
H	-7.10891800	0.51904100	1.81764500
C	-8.51655700	-1.18615900	-0.78731200
H	-7.68926800	-2.97316600	-1.66032500
H	-9.07030000	0.58909100	0.29775400
C	-9.70807400	-1.15941700	-1.69040500
H	-10.22629800	-0.19850900	-1.64912500
H	-9.42969700	-1.35695000	-2.72985500
H	-10.43055700	-1.93385400	-1.40877300

TS7R

Zero-point correction=	0.973654 (Hartree/Particle)
Thermal correction to Energy=	1.031309
Thermal correction to Enthalpy=	1.032253
Thermal correction to Gibbs Free Energy=	0.884715
Sum of electronic and zero-point Energies=	-3589.306472
Sum of electronic and thermal Energies=	-3589.248818
Sum of electronic and thermal Enthalpies=	-3589.247873
Sum of electronic and thermal Free Energies=	-3589.395411

Imaginary frequency=-296.24 cm^{-1}

C	-8.71279100	-2.15675600	1.83620000
C	-8.11805000	-1.32428200	0.91808200
C	-6.70964600	-1.29651900	0.80625600
C	-5.91819000	-2.15920000	1.63516900
C	-6.55952700	-2.99586500	2.57647900
C	-7.93143800	-2.99026700	2.67105500
H	-9.79445800	-2.17508400	1.92944700
H	-8.69969600	-0.66759800	0.27768000
H	-5.94444100	-3.63829200	3.19967700
H	-8.42620800	-3.63596300	3.39052000
C	-4.03297900	-1.39627900	0.60741400

C	-4.80496300	-0.44423100	-0.11159300
N	-4.56639100	-2.21703900	1.49294300
N	-6.12350100	-0.42045900	-0.05289000
P	-2.26451700	-1.53021100	0.13977200
P	-3.85666200	0.85267000	-0.99351300
C	-1.51530200	-2.14622200	1.68141200
H	-1.94461300	-3.11568300	1.94943300
H	-0.43163500	-2.24603500	1.59232200
H	-1.73794200	-1.44132300	2.48682000
C	-4.80394400	1.09823800	-2.53406700
H	-5.87547400	1.07743200	-2.31802500
H	-4.55006600	2.05840600	-2.99118500
H	-4.57296700	0.29994700	-3.24439800
C	-4.27169500	2.38116200	0.05603000
C	-3.99006600	2.04318200	1.51957200
C	-3.37154000	3.53375700	-0.38357000
C	-5.73442400	2.78389000	-0.12021700
H	-4.70041500	1.31162600	1.92030000
H	-2.97361000	1.65365100	1.65854800
H	-4.08131200	2.95274000	2.12405600
H	-3.38276000	3.69190900	-1.46872200
H	-3.72310800	4.45961000	0.08606300
H	-2.34015300	3.37644000	-0.06078800
H	-5.95219600	3.60857600	0.56894200
H	-5.94279700	3.14168300	-1.13321800
H	-6.42556500	1.96708200	0.10551800
C	-2.30408400	-3.00275000	-1.06320500
C	-3.23182400	-4.11595700	-0.58441400
C	-2.78825600	-2.45892200	-2.40883500
C	-0.88912100	-3.55326700	-1.22053700
H	-2.98086200	-4.47357500	0.41929400
H	-4.28179200	-3.81244600	-0.58345000
H	-3.13592900	-4.96714000	-1.26852300
H	-2.13058400	-1.65505200	-2.77147000
H	-2.78603500	-3.25992300	-3.15757900
H	-3.81102500	-2.06530500	-2.35112200
H	-0.91751500	-4.42386900	-1.88542300
H	-0.21819400	-2.82443200	-1.68052600
H	-0.45202600	-3.88025900	-0.27121100
Co	-1.66981700	0.28037500	-1.02967900
C	0.45216500	3.19221600	0.68473500
C	0.38930000	2.36696300	1.84193800
C	0.87508800	2.85880900	3.06005600
C	1.38968500	4.14871700	3.11157200

C	1.41278000	4.95818100	1.96944000
C	0.94106600	4.49341100	0.74061300
C	-0.47933800	1.14873400	0.11801300
C	-0.17871500	1.11263700	1.46311000
H	0.85486700	2.23072900	3.94737600
H	1.77532900	4.53722800	4.04997700
H	1.80725200	5.96815000	2.03240000
H	0.96714800	5.14652500	-0.12329000
H	-0.30366400	0.25427800	2.10776700
N	-0.07403300	2.43143200	-0.36658600
C	-0.43155200	2.74827800	-1.65681600
C	-0.01771000	3.86625100	-2.38679400
N	-1.25708600	1.81561200	-2.20321800
C	-0.46409200	4.00950900	-3.69019300
H	0.66119400	4.58826600	-1.95458100
C	-1.65240700	1.95363600	-3.48090600
C	-1.29059700	3.03853200	-4.25829700
H	-0.15333100	4.87304500	-4.26980500
H	-2.28818000	1.15938900	-3.86425000
H	-1.64164200	3.11483500	-5.28057700
C	5.47097500	1.66474900	2.85618600
C	4.38369000	1.27522000	2.07919700
C	3.61562200	0.15224100	2.43164000
C	3.94452300	-0.53356500	3.61342900
C	5.03422100	-0.14798100	4.38471900
C	5.80796000	0.94852700	4.00393900
H	6.05161100	2.53784300	2.57032500
H	4.09970600	1.86224600	1.20767900
H	3.34686000	-1.39438500	3.90611100
H	5.28175700	-0.70370800	5.28532300
H	6.65844700	1.25279900	4.60772700
C	2.51021500	-0.34564000	1.61771300
C	2.44435500	-0.37063600	0.27781000
C	3.56820100	-0.09196500	-0.66914700
H	4.53465600	0.08537200	-0.19300100
H	3.36844300	0.76128900	-1.33236500
N	3.60735900	-1.30606700	-1.52607800
C	2.18902200	-1.73472400	-1.66802500
H	1.84213700	-1.40775800	-2.65485800
H	2.11519100	-2.82552800	-1.64726100
C	1.36343100	-1.05441300	-0.52772800
C	0.34185200	-0.13244200	-1.19376100
H	0.85923000	-1.81236900	0.08038400
H	-0.22159900	-0.72067800	-1.95910600

H	0.87116900	0.64313600	-1.75540300
S	4.57538200	-2.56708100	-0.89316900
O	4.21971200	-2.91658800	0.48681200
O	4.53430200	-3.61400500	-1.91527300
C	6.16633000	-1.78911700	-0.87712200
C	6.71444600	-1.38537700	0.33791900
C	6.84270200	-1.58303400	-2.08048800
C	7.95580400	-0.75821200	0.34186300
H	6.16931200	-1.55415100	1.26277700
C	8.08101900	-0.95808900	-2.05560900
H	6.40415000	-1.91317100	-3.01787100
C	8.65447700	-0.53058500	-0.84838100
H	8.38778300	-0.43385500	1.28561400
H	8.61711300	-0.79407400	-2.98752500
C	9.98528200	0.15072800	-0.84306800
H	9.96802800	1.06169200	-1.45060200
H	10.29423100	0.42614000	0.16800800
H	10.76247100	-0.49171700	-1.27025900
H	1.69205400	-0.80964200	2.17021700

TS7S

Zero-point correction=	0.972487 (Hartree/Particle)
Thermal correction to Energy=	1.030545
Thermal correction to Enthalpy=	1.031489
Thermal correction to Gibbs Free Energy=	0.881931
Sum of electronic and zero-point Energies=	-3589.321347
Sum of electronic and thermal Energies=	-3589.263289
Sum of electronic and thermal Enthalpies=	-3589.262344
Sum of electronic and thermal Free Energies=	-3589.411903

Imaginary frequency=-323.09 cm^{-1}

C	-7.70522700	-4.00122900	-0.62332000
C	-6.95376700	-3.09679700	-1.33642600
C	-5.75083600	-2.59719100	-0.78796500
C	-5.31950600	-3.06078900	0.49860700
C	-6.11923100	-3.98239600	1.21118000
C	-7.28937100	-4.44231300	0.65536500
H	-8.63300700	-4.38128500	-1.04040500
H	-7.26473400	-2.73803700	-2.31346500
H	-5.77471400	-4.31858600	2.18472400
H	-7.90251400	-5.15645600	1.19707500
C	-3.43493800	-1.79595300	0.31020800
C	-3.92768700	-1.22924500	-0.89740800
N	-4.12834300	-2.66538300	1.02077000
N	-5.04448500	-1.64973300	-1.46306100

P	-1.71528800	-1.37382900	0.76229500
P	-3.01624300	0.24000300	-1.51525100
C	-1.70466100	-1.55531300	2.57176900
H	-1.93497800	-2.58879400	2.84595900
H	-0.72833700	-1.28621900	2.98441500
H	-2.46683600	-0.90250600	3.00466400
C	-3.05290300	0.04385500	-3.32768800
H	-4.03942600	-0.30018400	-3.65029700
H	-2.82916100	0.99566100	-3.81716100
H	-2.30672100	-0.69084000	-3.64099600
C	-4.26522900	1.62390100	-1.16614200
C	-4.65671800	1.54578900	0.30954200
C	-3.58804100	2.96500900	-1.44339300
C	-5.50501800	1.49038900	-2.04820600
H	-5.25692600	0.65682100	0.53325700
H	-3.77620400	1.54386300	0.96485100
H	-5.26113300	2.42173800	0.57110400
H	-3.11092500	3.00689200	-2.43026300
H	-4.34329700	3.75864500	-1.41173800
H	-2.84057400	3.19501500	-0.68156700
H	-6.22890500	2.25615400	-1.74464400
H	-5.27924000	1.65940600	-3.10576200
H	-5.98988800	0.51524100	-1.95086600
C	-0.74536500	-2.86969300	0.10788400
C	-1.54722100	-4.16346000	0.23073400
C	-0.44389500	-2.58924400	-1.36422600
C	0.54479500	-3.01115300	0.91519300
H	-1.91259200	-4.33682800	1.24841800
H	-2.40744000	-4.18588200	-0.44537400
H	-0.89645100	-5.00476900	-0.03510200
H	0.15783500	-1.68022900	-1.49514100
H	0.12605400	-3.42111800	-1.79551100
H	-1.36843700	-2.48506300	-1.94686400
H	1.14545400	-3.81496300	0.47416600
H	1.16468000	-2.11223500	0.90347600
H	0.34079100	-3.28594000	1.95537400
Co	-1.06016200	0.43521400	-0.37575400
C	-0.88797500	3.99302500	1.41385900
C	-1.24229800	3.29371300	2.60141900
C	-1.55620700	4.02668000	3.75420400
C	-1.53038700	5.41521800	3.70190100
C	-1.21246400	6.08477800	2.51430500
C	-0.89243200	5.38252500	1.35148400
C	-0.90190000	1.71766000	0.97849600

C	-1.21248100	1.89483000	2.31505100
H	-1.82362200	3.50932900	4.67212300
H	-1.77177400	5.99100800	4.59124300
H	-1.21444000	7.17054900	2.48965000
H	-0.67104600	5.92661200	0.44101200
H	-1.38799100	1.09887100	3.02622500
N	-0.64628500	3.01454200	0.44094000
C	-0.32724100	3.09979600	-0.89474100
C	0.13891500	4.23105000	-1.56935000
N	-0.47532900	1.90933300	-1.52985200
C	0.44497800	4.11759300	-2.91652600
H	0.29426500	5.16442600	-1.04532600
C	-0.15640400	1.81198800	-2.83241800
C	0.29978500	2.89143800	-3.56690600
H	0.81251500	4.98538900	-3.45549400
H	-0.27354500	0.82602000	-3.27211300
H	0.54533400	2.76871900	-4.61520500
C	5.83364300	-1.69770600	4.24800500
C	5.06869800	-0.84828100	3.45515900
C	3.68446700	-0.71407600	3.67150400
C	3.11186000	-1.44928300	4.72660700
C	3.87636400	-2.30044900	5.51391100
C	5.24386400	-2.43172200	5.27554200
H	6.90205100	-1.77980000	4.06613500
H	5.56156100	-0.26309900	2.68517200
H	2.04434300	-1.34677900	4.91526400
H	3.40535800	-2.86028200	6.31748600
H	5.84699000	-3.09241300	5.89183800
C	2.80266700	0.12982900	2.87559400
C	2.98078000	0.64481800	1.64507600
C	4.17204900	0.49653600	0.74128000
H	4.58174800	-0.51977200	0.72441900
H	4.99262600	1.16590600	1.03435700
N	3.71137500	0.90996700	-0.60006300
C	2.61045500	1.87062500	-0.37245700
H	3.07273000	2.85360400	-0.23029400
H	1.99019700	1.91868200	-1.26539400
C	1.89371700	1.42615000	0.91192900
C	0.68727100	0.50010000	0.72367100
H	0.55390600	-0.07413800	1.63848700
H	0.91271300	-0.21186300	-0.09723600
S	3.36304200	-0.37526600	-1.64862800
O	2.76410600	-1.52739100	-0.95965800
O	2.64619500	0.22360200	-2.77821400

C	4.99586300	-0.85831600	-2.14076500
C	5.48247800	-2.09779600	-1.73701200
C	5.75944100	-0.00882800	-2.94436100
C	6.75394300	-2.48959000	-2.14444700
H	4.86931300	-2.74324100	-1.11625700
C	7.02287600	-0.41860700	-3.34319900
H	5.36534100	0.95568500	-3.25240500
C	7.54160500	-1.66233100	-2.95011400
H	7.14106200	-3.45645000	-1.83226800
H	7.62395100	0.23383100	-3.97204000
C	8.90801900	-2.08270700	-3.38688600
H	9.67397500	-1.40333500	-2.99765100
H	9.14994900	-3.09183300	-3.04539900
H	9.00138600	-2.06213700	-4.47751300
H	1.83129300	0.31943500	3.33911600
H	1.60040600	2.30069700	1.50617000

TS5R'

Zero-point correction= 0.966653 (Hartree/Particle)
Thermal correction to Energy= 1.025953
Thermal correction to Enthalpy= 1.026897
Thermal correction to Gibbs Free Energy= 0.875138
Sum of electronic and zero-point Energies= -3589.209919
Sum of electronic and thermal Energies= -3589.150619
Sum of electronic and thermal Enthalpies= -3589.149674
Sum of electronic and thermal Free Energies= -3589.301434
Imaginary frequency=-299.29 cm^{-1}

C	-1.43503800	7.37997500	-1.66985200
C	-2.24227900	6.33362300	-1.29028700
C	-1.66493500	5.08182800	-0.97985600
C	-0.24097900	4.92762300	-1.03765300
C	0.56070600	6.01893100	-1.44169700
C	-0.03135900	7.22068600	-1.75147700
H	-1.87609300	8.34104800	-1.91712900
H	-3.32246900	6.43211200	-1.23597200
H	1.63711500	5.88116500	-1.48465300
H	0.58181000	8.06295200	-2.05726600
C	-0.45652500	2.77747600	-0.30860400
C	-1.87270500	2.88660700	-0.39334800
N	0.34866900	3.76145500	-0.66020800
N	-2.47020500	4.02798700	-0.67917700
P	0.20758100	1.24684900	0.45539800
P	-2.81388100	1.31162300	-0.32004700
C	1.80310700	1.00554900	-0.36475800

H	2.29519100	1.97299500	-0.50170200
H	2.43465400	0.32805200	0.21578000
H	1.62269300	0.54520700	-1.34036000
C	-4.38663300	1.73540400	0.48443700
H	-4.76010800	2.69307100	0.11251400
H	-5.12717300	0.95414600	0.29066000
H	-4.23922900	1.80562600	1.56520800
C	-3.20818400	1.11548300	-2.16377300
C	-1.90838100	1.24465800	-2.95877200
C	-3.80475300	-0.26745400	-2.37767600
C	-4.21113300	2.17367100	-2.62029500
H	-1.51240600	2.26580300	-2.95013800
H	-1.12752000	0.56708900	-2.58881000
H	-2.10262600	0.97903200	-4.00383200
H	-4.67173500	-0.44943000	-1.73473200
H	-4.13854500	-0.36317400	-3.41757100
H	-3.06391000	-1.04988600	-2.19254000
H	-4.34701500	2.07509500	-3.70363800
H	-5.19197100	2.03412500	-2.15601200
H	-3.87640400	3.19484200	-2.41853700
C	0.55272600	1.84108900	2.22529600
C	1.36047700	3.13629400	2.23522500
C	-0.81610800	2.05184600	2.87505900
C	1.32371400	0.77406000	3.00542900
H	2.32255400	3.02741400	1.72358200
H	0.82654500	3.97429600	1.78305900
H	1.57250000	3.40520500	3.27661800
H	-1.42356500	1.13477000	2.82620900
H	-0.69570600	2.30786700	3.93384700
H	-1.38502000	2.86067900	2.40236500
H	1.65248100	1.20787300	3.95622200
H	0.70302000	-0.09153300	3.25321100
H	2.22147300	0.42166200	2.48446900
Co	-1.44379100	-0.23511100	0.62906600
C	-5.15335500	-2.06710800	1.47822000
C	-4.88523900	-1.26219900	2.61549800
C	-5.88366100	-1.04397700	3.57859300
C	-7.12249500	-1.63730700	3.40282300
C	-7.37133800	-2.44731300	2.28291200
C	-6.40271800	-2.67304300	1.31006400
C	-2.97325500	-1.34652900	1.35564000
C	-3.53658400	-0.84546900	2.51930600
H	-5.67494300	-0.42521300	4.44766300
H	-7.90821000	-1.48031900	4.13670800

H	-8.34647000	-2.91167500	2.16558800
H	-6.61965100	-3.29088900	0.44966100
H	-3.00486000	-0.25071400	3.25277900
N	-3.97397800	-2.12723400	0.71470200
C	-3.85818400	-2.84794300	-0.49316400
C	-2.62925200	-3.34592700	-0.93454700
N	-4.98495200	-3.00189200	-1.19412300
C	-2.57075400	-3.99619700	-2.15820800
H	-1.73940000	-3.24189100	-0.33882200
C	-4.91495400	-3.65320100	-2.35951200
C	-3.73726900	-4.15549600	-2.90020500
H	-1.61861100	-4.37952100	-2.51657900
H	-5.85811100	-3.76410200	-2.89265900
H	-3.73857500	-4.65951900	-3.86067300
C	8.01881700	0.04273300	2.75843400
C	6.97689400	-0.82191100	2.44617000
C	5.76418900	-0.31688800	1.94471600
C	5.62756200	1.07056100	1.75550600
C	6.67740400	1.92592200	2.06634100
C	7.87351200	1.41692600	2.57131800
H	8.95090700	-0.35847600	3.14593300
H	7.08971400	-1.89417300	2.58062700
H	4.69651900	1.46125200	1.35157500
H	6.56200000	2.99540600	1.91383000
H	8.69165800	2.08880400	2.81458400
C	4.70345500	-1.19824100	1.59612600
C	3.81485800	-1.95568900	1.25544800
C	2.76594400	-2.84703600	0.79143000
H	2.09432500	-3.10156400	1.61957700
H	3.18672000	-3.80686800	0.45385700
N	1.93623400	-2.21764900	-0.26766200
C	0.49510700	-2.46622100	-0.10770900
H	0.01680700	-2.19447400	-1.05379800
H	0.30612800	-3.54502500	0.04518100
C	-0.05265300	-1.67382100	1.06171800
C	-1.23811600	-2.09318900	1.75747900
H	0.72898000	-1.26729000	1.69736900
H	-1.24524000	-1.82507800	2.81134600
H	-1.61184500	-3.10408700	1.59799900
S	2.44552000	-2.59257900	-1.85626400
O	2.38587100	-4.04006500	-2.08710400
O	1.68325200	-1.69373200	-2.72636000
C	4.14088000	-2.10009800	-1.80939100
C	5.12175500	-3.06476100	-1.58627000

C	4.46783600	-0.75025300	-1.93677500
C	6.44374000	-2.66048000	-1.45149500
H	4.84651300	-4.11220300	-1.50509700
C	5.79420100	-0.36673400	-1.80434900
H	3.69253400	-0.01563800	-2.13145500
C	6.79919000	-1.30919200	-1.54331000
H	7.21420900	-3.40344400	-1.26134800
H	6.05974000	0.68475600	-1.88662100
C	8.21837000	-0.87525700	-1.36890000
H	8.27812200	0.13128800	-0.94473400
H	8.77246900	-1.55797900	-0.71907600
H	8.74417200	-0.84908800	-2.33057800
H	-1.34258200	-0.64856100	-0.73337400

TS5S'

Zero-point correction=	0.969463 (Hartree/Particle)
Thermal correction to Energy=	1.027960
Thermal correction to Enthalpy=	1.028904
Thermal correction to Gibbs Free Energy=	0.881121
Sum of electronic and zero-point Energies=	-3589.212511
Sum of electronic and thermal Energies=	-3589.154014
Sum of electronic and thermal Enthalpies=	-3589.153070
Sum of electronic and thermal Free Energies=	-3589.300853

Imaginary frequency=-281.89 cm^{-1}

C	-8.76426700	-0.80378200	-1.21147900
C	-7.66864300	-1.38179600	-0.61467600
C	-6.45065800	-0.66787900	-0.54927700
C	-6.37649900	0.65082900	-1.10516800
C	-7.51843400	1.21685400	-1.71474600
C	-8.68902100	0.49740700	-1.76311300
H	-9.70198500	-1.34886000	-1.26333800
H	-7.70697200	-2.38045600	-0.18937200
H	-7.44085800	2.21721200	-2.13017400
H	-9.57071500	0.92920100	-2.22724600
C	-4.19224300	0.77807600	-0.46585100
C	-4.24923500	-0.54166400	0.05955800
N	-5.22551700	1.36839700	-1.03470100
N	-5.36669100	-1.24373600	0.03299900
P	-2.62668000	1.70239600	-0.26245200
P	-2.68200100	-1.22984100	0.75424300
C	-2.61429900	2.69852200	-1.78338800
H	-3.57270900	3.20825700	-1.90308600
H	-1.81049900	3.43688100	-1.78024100
H	-2.46993500	2.02234700	-2.63025700

C	-2.86280400	-1.01990800	2.56224400
H	-3.86526400	-1.29668500	2.89886600
H	-2.12365700	-1.64966100	3.06732800
H	-2.66991100	0.01740500	2.84568700
C	-2.82108300	-3.09679300	0.51689800
C	-3.14015200	-3.39240700	-0.94759400
C	-1.48519400	-3.73415100	0.89599000
C	-3.90200000	-3.68755500	1.42823600
H	-4.16367300	-3.11132300	-1.20824600
H	-2.45603900	-2.87923600	-1.63291500
H	-3.03532500	-4.46857300	-1.12635700
H	-1.10818600	-3.39351700	1.86736800
H	-1.62333100	-4.81921700	0.96264000
H	-0.72286400	-3.54905900	0.14136400
H	-3.98529200	-4.75612100	1.19686200
H	-3.63000500	-3.61025100	2.48522900
H	-4.88163900	-3.23193400	1.27874800
C	-2.94768900	2.87248400	1.22528100
C	-4.26133100	2.49468700	1.91385900
C	-1.80168500	2.73026200	2.22998300
C	-3.03645700	4.31729700	0.74187200
H	-5.12738900	2.64523900	1.26391200
H	-4.27451800	1.45776900	2.26692300
H	-4.38566500	3.13995500	2.79030600
H	-0.87106800	3.16985000	1.86398000
H	-2.06501200	3.25778100	3.15333300
H	-1.60620000	1.68528100	2.49774500
H	-3.18644700	4.96673200	1.61194200
H	-2.12289600	4.65138000	0.23915200
H	-3.88135700	4.47369700	0.06418700
Co	-1.01892200	0.18142900	-0.00503000
C	1.84139700	-2.58285700	1.56061700
C	1.42551200	-1.70749200	2.59969800
C	1.82485300	-1.95322900	3.92264800
C	2.61209800	-3.06347700	4.18991200
C	3.00342800	-3.92778700	3.15564200
C	2.62667200	-3.70588100	1.83455300
C	0.47773700	-0.98960100	0.65398600
C	0.61398000	-0.70491000	2.00048000
H	1.50888200	-1.28553500	4.72078000
H	2.92752100	-3.26959900	5.20914800
H	3.61686600	-4.79408400	3.38665100
H	2.94020400	-4.37711300	1.04632200
H	0.16138400	0.14585500	2.50438500

N	1.25561300	-2.12530800	0.36823200
C	1.36906500	-2.74876700	-0.89149200
C	0.39779100	-2.53958900	-1.87893800
N	2.43208600	-3.53323800	-1.07659300
C	0.56076000	-3.16033600	-3.10763600
H	-0.46415400	-1.91493500	-1.66793500
C	2.56181000	-4.13483500	-2.26408400
C	1.66761100	-3.97938300	-3.31588400
H	-0.18111300	-3.01564900	-3.88809700
H	3.44194400	-4.76663400	-2.37602600
H	1.82989500	-4.48764300	-4.26029100
C	6.41089600	-1.21633600	-3.51034000
C	5.56010000	-0.11774900	-3.53636300
C	4.56773600	0.03152300	-2.55070600
C	4.44886900	-0.95065500	-1.55046700
C	5.30954300	-2.04107200	-1.52859200
C	6.29215700	-2.17863000	-2.50710100
H	7.17384900	-1.32102300	-4.27650500
H	5.65698900	0.63570100	-4.31282700
H	3.67980800	-0.84706800	-0.78806000
H	5.19601000	-2.79179200	-0.75083600
H	6.96320300	-3.03284400	-2.48978100
C	3.70420700	1.16233200	-2.52516900
C	2.95738300	2.11855600	-2.42904100
C	2.11633400	3.29355100	-2.23185600
H	1.20010400	3.22904700	-2.83016200
H	2.63916600	4.18913200	-2.57919200
N	1.70268300	3.52901000	-0.84478000
C	0.54486700	2.81651900	-0.25940000
H	0.78034200	2.61618700	0.79147200
H	-0.31539500	3.49977900	-0.26103000
C	0.22122600	1.51668600	-0.94215300
C	1.05557800	0.39504700	-0.68783600
H	-0.20355000	1.59718300	-1.94196500
H	1.91646400	0.56121900	-0.04218300
H	1.23956200	-0.29570000	-1.50532000
S	2.81171400	4.16329500	0.23504900
O	3.79122100	4.88531300	-0.57237600
O	2.01876300	4.83121000	1.26608700
C	3.62261700	2.79285700	1.01812500
C	4.77558300	2.25017500	0.44751200
C	3.06324400	2.23076400	2.16685800
C	5.35048300	1.12500100	1.02224500
H	5.21485100	2.70961500	-0.43250600

C	3.64880400	1.09838500	2.72310200
H	2.18773400	2.68375400	2.62550700
C	4.79027400	0.52052500	2.15686800
H	6.24864400	0.69993800	0.57921800
H	3.21090500	0.64967300	3.61221000
C	5.40789000	-0.70400200	2.75097100
H	6.35265400	-0.46774200	3.25390000
H	4.74632500	-1.17130100	3.48546100
H	5.64278300	-1.44681800	1.98139400
H	-1.45872200	-0.26827000	-1.29443800

M7R'

Zero-point correction=	0.968904 (Hartree/Particle)
Thermal correction to Energy=	1.028032
Thermal correction to Enthalpy=	1.028976
Thermal correction to Gibbs Free Energy=	0.878230
Sum of electronic and zero-point Energies=	-3589.265831
Sum of electronic and thermal Energies=	-3589.206702
Sum of electronic and thermal Enthalpies=	-3589.205758
Sum of electronic and thermal Free Energies=	-3589.356504

C	3.97326900	5.27517200	-1.85219000
C	2.63483300	4.98570700	-1.97701100
C	2.02889900	4.07460000	-1.08262000
C	2.81442600	3.48244700	-0.04164000
C	4.18929500	3.79423500	0.05747600
C	4.75383300	4.67393200	-0.83672900
H	4.44287500	5.96912000	-2.54274400
H	2.02225100	5.42889700	-2.75690800
H	4.77044300	3.32214600	0.84500200
H	5.81035400	4.91490000	-0.76611300
C	0.98389600	2.31816900	0.66578500
C	0.21407200	2.86332000	-0.40186600
N	2.25768900	2.61266700	0.84354900
N	0.71788300	3.75004700	-1.24058900
P	0.14454900	1.15207900	1.82104900
P	-1.50429900	2.24096900	-0.60806000
C	1.50372100	0.03602600	2.27210900
H	2.40877200	0.62858000	2.42584200
H	1.27959900	-0.52115600	3.18466500
H	1.66421200	-0.67251300	1.45554400
C	-2.48493800	3.77197600	-0.41017300
H	-1.99412300	4.60052000	-0.92893000
H	-3.48261000	3.62930700	-0.83231800
H	-2.58935900	4.02872000	0.64606100

C	-1.67874900	1.83843500	-2.44256900
C	-0.46735000	1.03520300	-2.90507000
C	-2.94292100	0.98222200	-2.53754200
C	-1.83216700	3.08735200	-3.30781400
H	0.45282700	1.62893700	-2.87964800
H	-0.32161300	0.13078600	-2.30762800
H	-0.62337500	0.71440900	-3.94183100
H	-3.82435200	1.51119700	-2.15378500
H	-3.14397400	0.72418400	-3.58410700
H	-2.84301300	0.03974800	-1.98204900
H	-1.89405800	2.77974400	-4.35865800
H	-2.74560600	3.64484300	-3.07955800
H	-0.97889400	3.76418300	-3.20717100
C	-0.21252900	2.15630300	3.37486400
C	1.08914300	2.67301600	3.98350400
C	-1.12080000	3.32463000	3.00462600
C	-0.92432100	1.23302300	4.36125700
H	1.74519100	1.86057400	4.30904600
H	1.64946700	3.31005000	3.29274800
H	0.84852500	3.27412700	4.86837800
H	-2.06762800	2.97949800	2.57480100
H	-1.35767400	3.90440500	3.90371900
H	-0.64766000	4.00709900	2.28890400
H	-1.14871800	1.78622400	5.28020400
H	-1.87217400	0.86354700	3.95703700
H	-0.31250600	0.36834100	4.64030500
Co	-1.52142900	0.37490900	0.74824700
C	-5.14147900	-0.06055400	-0.00477000
C	-4.78953100	1.11015000	0.70433700
C	-5.42241700	2.31590900	0.37837600
C	-6.35015800	2.32754900	-0.65524000
C	-6.66304600	1.15476600	-1.36221200
C	-6.06654800	-0.05992500	-1.04616800
C	-3.67535600	-0.65848200	1.61631400
C	-3.81379200	0.72293600	1.68931600
H	-5.19106800	3.22457900	0.92833700
H	-6.84943400	3.25621800	-0.91774700
H	-7.39140700	1.19432300	-2.16706900
H	-6.31001500	-0.96794100	-1.58832700
H	-3.43812200	1.33140600	2.50389200
N	-4.44542700	-1.12890000	0.56573800
C	-4.45985700	-2.45753400	0.05495000
C	-4.77964900	-3.53421200	0.87922200
N	-4.14473400	-2.56932200	-1.23680100

C	-4.72407200	-4.80985100	0.32728200
H	-5.07512200	-3.37023500	1.91041200
C	-4.11293300	-3.80304100	-1.75259600
C	-4.37730500	-4.95166900	-1.01214800
H	-4.96133200	-5.67740400	0.93532700
H	-3.85112900	-3.86922500	-2.80647500
H	-4.32125700	-5.92902000	-1.47948700
C	7.31341300	-3.10581900	0.98875800
C	5.97732500	-3.48378500	1.04621800
C	4.97650500	-2.51771400	1.24947700
C	5.34885900	-1.16793300	1.39407800
C	6.68691300	-0.80028700	1.33205700
C	7.67291500	-1.76636800	1.13079000
H	8.07813100	-3.86113500	0.83219000
H	5.69381700	-4.52619400	0.93128500
H	4.57639300	-0.41620400	1.53815700
H	6.96180800	0.24601000	1.43782900
H	8.71843000	-1.47540700	1.08355000
C	3.60275900	-2.88476900	1.27596800
C	2.42049300	-3.16666200	1.25960500
C	0.99483600	-3.43627300	1.22359100
H	0.55877300	-3.23144600	2.20867500
H	0.80280700	-4.49783800	1.00867500
N	0.26382900	-2.56478000	0.27244100
C	-1.16294000	-2.42327700	0.62330400
H	-1.70544500	-2.14928300	-0.28885900
H	-1.56786800	-3.40694900	0.93312800
C	-1.36150900	-1.38707100	1.71801600
C	-2.71995700	-1.50262000	2.39566600
H	-0.56460200	-1.47010800	2.46328800
H	-2.67146200	-1.09293200	3.40903600
H	-3.06865500	-2.53965200	2.49011100
S	0.58060600	-2.93853900	-1.35872700
O	0.81686900	-4.37520000	-1.53200600
O	-0.47644500	-2.28500000	-2.13582800
C	2.11734200	-2.09985600	-1.65454600
C	3.16129200	-2.79451600	-2.26112300
C	2.25838800	-0.75973600	-1.30109600
C	4.36106000	-2.13509700	-2.50310400
H	3.03780100	-3.84302300	-2.51421300
C	3.46553500	-0.11908800	-1.54413200
H	1.44113800	-0.23303300	-0.81320400
C	4.53548000	-0.79262200	-2.14669600
H	5.18633300	-2.67741800	-2.95856700

H	3.59293000	0.91993500	-1.24712400
C	5.83711400	-0.09779400	-2.38779400
H	5.90984500	0.82957300	-1.81185700
H	6.68606500	-0.73539300	-2.12279100
H	5.95681400	0.16260200	-3.44582300
H	-0.35203700	0.00359100	-0.02930600

M7S'

Zero-point correction=	0.971325 (Hartree/Particle)
Thermal correction to Energy=	1.029925
Thermal correction to Enthalpy=	1.030870
Thermal correction to Gibbs Free Energy=	0.882485
Sum of electronic and zero-point Energies=	-3589.263710
Sum of electronic and thermal Energies=	-3589.205110
Sum of electronic and thermal Enthalpies=	-3589.204166
Sum of electronic and thermal Free Energies=	-3589.352550

C	8.71342700	-0.71602200	1.98603800
C	7.72557700	-1.29765200	1.22685400
C	6.50320300	-0.61714700	1.02650200
C	6.31885200	0.68178900	1.60266900
C	7.35098700	1.25157900	2.38134700
C	8.52411400	0.55967900	2.56826800
H	9.65158200	-1.23917000	2.14617100
H	7.84948100	-2.27858900	0.77747700
H	7.19030300	2.23523100	2.81278800
H	9.31989300	0.99534700	3.16511100
C	4.24085400	0.78343700	0.67384700
C	4.38784700	-0.53855400	0.16550700
N	5.17600200	1.38546300	1.38232100
N	5.51370000	-1.21325400	0.30871200
P	2.72931800	1.69205800	0.17784200
P	2.91927500	-1.28103300	-0.66564700
C	2.47218600	2.85641700	1.54272300
H	3.39655100	3.40474600	1.74293300
H	1.67712400	3.56476400	1.29863500
H	2.19158100	2.29776100	2.43892000
C	3.56047500	-1.74092800	-2.31347800
H	4.55222500	-2.19498200	-2.23642300
H	2.87445100	-2.45152600	-2.78403700
H	3.62652600	-0.85467800	-2.94990200
C	2.68433000	-2.93096700	0.22158600
C	2.66285600	-2.68947300	1.72952400
C	1.33099200	-3.46502000	-0.23858400
C	3.77927400	-3.93458700	-0.13136200

H	3.62991700	-2.34164800	2.10728200
H	1.90102200	-1.95541700	2.01716600
H	2.42835700	-3.62918800	2.24273400
H	1.30239200	-3.62862400	-1.32206200
H	1.12304200	-4.42669000	0.24602100
H	0.52537300	-2.77260900	0.02618000
H	3.60137500	-4.85928400	0.43090000
H	3.77025400	-4.19392800	-1.19418200
H	4.77582400	-3.56745200	0.12707700
C	3.23975000	2.69777300	-1.36816500
C	4.71828500	2.48355600	-1.68566000
C	2.38126900	2.19401800	-2.52958200
C	2.98445400	4.18345000	-1.13141900
H	5.36910200	2.82923600	-0.87668800
H	4.95572900	1.43300800	-1.88871000
H	4.96977500	3.05589100	-2.58582600
H	1.31693500	2.37121800	-2.34414600
H	2.64952000	2.72841800	-3.44839700
H	2.52985500	1.12267600	-2.71611600
H	3.24155700	4.73445500	-2.04329900
H	1.93564600	4.40044300	-0.90552000
H	3.59957900	4.58163200	-0.31909700
Co	1.24414900	0.24191000	-0.34195000
C	-1.27083200	-2.51255000	-2.00633500
C	-0.35270600	-1.65101800	-2.64714000
C	0.24851800	-2.05091700	-3.84567300
C	-0.06356300	-3.30209600	-4.36040800
C	-0.96335500	-4.15150100	-3.69648300
C	-1.58169000	-3.77346400	-2.50990700
C	-1.09096900	-0.65016000	-0.72724700
C	-0.23946300	-0.48243800	-1.82035500
H	0.95079000	-1.39450400	-4.35448000
H	0.39128800	-3.63116500	-5.29024400
H	-1.18767200	-5.12552700	-4.12155800
H	-2.28324400	-4.42889700	-2.00482200
H	0.17617200	0.47219600	-2.15318700
N	-1.68749300	-1.88921000	-0.82481300
C	-2.50372800	-2.51669100	0.15902700
C	-2.05925100	-2.62229300	1.47844600
N	-3.65358200	-3.01960100	-0.28678200
C	-2.88271700	-3.27014200	2.38966600
H	-1.08876400	-2.23090300	1.76968200
C	-4.42265100	-3.65824900	0.60451100
C	-4.09103900	-3.80103500	1.94705000

H	-2.57659800	-3.36984400	3.42707200
H	-5.35299500	-4.07011600	0.21748100
H	-4.76140900	-4.31817200	2.62609900
C	-4.28752600	-0.57113400	5.33346800
C	-3.61060700	0.44913600	4.67457700
C	-3.91057600	0.74725400	3.33325900
C	-4.88933900	-0.01575900	2.66940700
C	-5.56863300	-1.02430800	3.34086100
C	-5.27329400	-1.30483900	4.67451800
H	-4.04788500	-0.79040100	6.37017700
H	-2.85119900	1.02862500	5.19211700
H	-5.10437300	0.19380000	1.62454000
H	-6.32989700	-1.59752700	2.81739500
H	-5.80510500	-2.09558900	5.19641400
C	-3.24905600	1.80091300	2.64126300
C	-2.70174900	2.67882400	2.00050400
C	-2.06008200	3.70489900	1.18471300
H	-1.08634200	3.97516200	1.61307700
H	-2.65773400	4.62166400	1.19161900
N	-1.82307600	3.32412600	-0.20797800
C	-0.59177000	2.58836300	-0.56761200
H	-0.71177300	2.30179800	-1.61694800
H	0.24385400	3.30411300	-0.53673600
C	-0.28110700	1.39972400	0.31442600
C	-1.37860900	0.34029800	0.34436900
H	-0.06552800	1.75000800	1.32961800
H	-2.39688700	0.74577000	0.22079000
H	-1.38306800	-0.14930600	1.32193000
S	-2.98547800	3.63129900	-1.35983900
O	-3.78290800	4.74912700	-0.85787600
O	-2.28402400	3.71077400	-2.64065400
C	-4.04901000	2.21076700	-1.43465600
C	-5.20394300	2.18189600	-0.65327100
C	-3.68803200	1.11461200	-2.21924500
C	-5.99820500	1.04275300	-0.66294700
H	-5.47449000	3.04492400	-0.05234000
C	-4.48710800	-0.02418500	-2.20311500
H	-2.79503700	1.15510100	-2.83794400
C	-5.64860900	-0.08154300	-1.42339000
H	-6.90318700	1.01778200	-0.05977100
H	-4.20343600	-0.88821900	-2.80042600
C	-6.51243600	-1.30224700	-1.40605400
H	-6.01288200	-2.15745300	-1.86701500
H	-6.78986500	-1.57631000	-0.38212200

H	-7.44986500	-1.12975700	-1.94730700
H	1.41190800	-0.13319600	1.04002200

M05

Zero-point correction=	0.971603 (Hartree/Particle)
Thermal correction to Energy=	1.030825
Thermal correction to Enthalpy=	1.031769
Thermal correction to Gibbs Free Energy=	0.883367
Sum of electronic and zero-point Energies=	-3589.268154
Sum of electronic and thermal Energies=	-3589.208933
Sum of electronic and thermal Enthalpies=	-3589.207989
Sum of electronic and thermal Free Energies=	-3589.356391

C	6.71509000	-1.63910100	-1.97230700
C	5.40168600	-1.57679500	-2.37607200
C	4.36867100	-1.67103100	-1.41565800
C	4.70137900	-1.81334600	-0.03008800
C	6.06063600	-1.87720000	0.35331600
C	7.04499200	-1.78898400	-0.60395900
H	7.51142100	-1.57366000	-2.70782600
H	5.12600400	-1.46895000	-3.42149700
H	6.29585700	-1.98561500	1.40845600
H	8.08973600	-1.83243200	-0.31119000
C	2.47982500	-1.77679600	0.50618700
C	2.15611800	-1.74871400	-0.87449900
N	3.73042200	-1.85768100	0.92087800
N	3.07254900	-1.66895000	-1.82253900
P	1.06567200	-1.66906900	1.69068200
P	0.40732600	-2.04771600	-1.30307800
C	1.36477900	-3.14486700	2.75109200
H	2.41831200	-3.43321600	2.69355200
H	1.13373400	-2.92875000	3.79760300
H	0.74366600	-3.98248100	2.42567100
C	0.30797400	-1.20837100	-2.92138600
H	1.05923000	-1.61787000	-3.60184600
H	-0.68013700	-1.31453100	-3.37258400
H	0.52574300	-0.14416600	-2.78025800
C	0.45676900	-3.90811800	-1.75758700
C	0.44822600	-4.71504200	-0.46284400
C	-0.77627600	-4.24530900	-2.59475500
C	1.70901300	-4.26275000	-2.55854600
H	1.32525900	-4.49144700	0.15714200
H	-0.44836800	-4.51823200	0.13673700
H	0.47525000	-5.78588400	-0.69686100
H	-0.80672300	-3.68264800	-3.53395600

H	-0.74729500	-5.30996100	-2.85339900
H	-1.71186700	-4.07118000	-2.05650100
H	1.61227600	-5.29666400	-2.91058000
H	1.84911900	-3.62848800	-3.43895800
H	2.61805500	-4.20730000	-1.95396600
C	1.63354100	-0.23778100	2.83706200
C	2.92466300	-0.56660500	3.59157400
C	1.87346800	0.99695000	1.96903100
C	0.56128600	0.03061600	3.89497400
H	2.83181300	-1.46803300	4.20466100
H	3.78168300	-0.68982200	2.92876700
H	3.13771100	0.26609400	4.27350500
H	0.99209600	1.30914800	1.40018700
H	2.16466100	1.84085400	2.60704000
H	2.69030300	0.83288600	1.25723800
H	0.85393200	0.91475400	4.47375200
H	-0.43596900	0.22061400	3.49106100
H	0.48130100	-0.80141500	4.60396500
Co	-0.88557300	-1.55136300	0.46490700
C	-4.83436700	-1.32655400	-0.32751000
C	-4.51442000	-1.40898100	-1.71427000
C	-5.46346200	-0.99572200	-2.66574800
C	-6.68019200	-0.50481700	-2.22587100
C	-6.96383000	-0.40069600	-0.85252800
C	-6.05124500	-0.80365000	0.11432200
C	-2.66770100	-2.02722600	-0.54139500
C	-3.18074900	-1.87670200	-1.82420300
H	-5.23134500	-1.04869400	-3.72580700
H	-7.42209400	-0.17482800	-2.94712700
H	-7.91613500	0.01312600	-0.53440700
H	-6.28203100	-0.68240400	1.16665700
H	-1.95723400	-2.85273600	-0.22599600
H	-2.63996400	-2.06002900	-2.74326000
N	-3.71567300	-1.76150600	0.36929400
C	-3.47814600	-1.92899000	1.71823700
C	-4.49074300	-2.11501100	2.66134400
N	-2.15407800	-1.94414100	2.03193500
C	-4.13988900	-2.30227800	3.98637800
H	-5.52477900	-2.15280600	2.34359500
C	-1.84762500	-2.16307700	3.32879300
C	-2.78811000	-2.32544500	4.32779300
H	-4.90871000	-2.45238600	4.73708200
H	-0.79519400	-2.20745400	3.56595300
H	-2.45957800	-2.48613800	5.34840000

C	5.14757500	1.62658900	-0.75473600
C	3.93626900	1.70734300	-1.43171200
C	2.96693200	2.64821800	-1.03961600
C	3.24942400	3.50822000	0.03672100
C	4.46288700	3.41912100	0.70740200
C	5.41357200	2.47614800	0.31829400
H	5.88845600	0.89502600	-1.06749200
H	3.72545600	1.04506800	-2.26774100
H	2.50009200	4.23206900	0.34374700
H	4.66578200	4.08623400	1.54131100
H	6.36065700	2.40491800	0.84586500
C	1.70901000	2.69796500	-1.70332800
C	0.62521200	2.70883200	-2.25760800
C	-0.67902800	2.69079400	-2.91344900
H	-0.66550200	1.96266100	-3.73489200
H	-0.89448400	3.66142600	-3.37420600
N	-1.81578400	2.34024100	-2.05620600
C	-1.89268400	0.96831900	-1.52864000
H	-2.93374300	0.78108300	-1.25970700
H	-1.66335700	0.32232600	-2.38068200
C	-1.00829300	0.70846600	-0.34430300
C	-1.54152500	0.57472800	0.90047100
H	0.06091800	0.87518900	-0.46907000
H	-2.62342900	0.58743000	1.02572500
H	-0.95159400	0.69436700	1.79942800
S	-2.59869000	3.58308500	-1.24579000
O	-2.85832700	4.60847700	-2.25494400
O	-3.68375300	2.94046700	-0.50759600
C	-1.47221400	4.29875300	-0.07263000
C	-0.60226800	5.30535500	-0.48888700
C	-1.43047400	3.81415800	1.23494500
C	0.33247600	5.80682100	0.40934800
H	-0.65769600	5.69004800	-1.50298100
C	-0.48178300	4.31685600	2.11554600
H	-2.14173900	3.05972200	1.55448000
C	0.42242800	5.30982500	1.71515500
H	1.01826200	6.58786900	0.08895200
H	-0.43961000	3.93475000	3.13392500
C	1.46186000	5.81883300	2.66207100
H	1.98776700	4.99394600	3.15498300
H	2.20381200	6.43884300	2.15197500
H	1.01490900	6.42398300	3.45874900

M1R-F

Zero-point correction= 0.763169 (Hartree/Particle)
Thermal correction to Energy= 0.810888
Thermal correction to Enthalpy= 0.811832
Thermal correction to Gibbs Free Energy= 0.686265
Sum of electronic and zero-point Energies= -3077.852247
Sum of electronic and thermal Energies= -3077.804527
Sum of electronic and thermal Enthalpies= -3077.803583
Sum of electronic and thermal Free Energies= -3077.929150

C	-6.25190700	-4.29171700	-0.81870900
C	-4.90734900	-4.07527100	-1.00680200
C	-4.32456600	-2.86720800	-0.56206900
C	-5.14124600	-1.88670400	0.09098800
C	-6.52066600	-2.13827700	0.26775500
C	-7.06040400	-3.32037900	-0.18199000
H	-6.70442600	-5.21617300	-1.16469900
H	-4.27070000	-4.80558400	-1.49774600
H	-7.12395700	-1.38328800	0.76358800
H	-8.11996200	-3.51696900	-0.04781200
C	-3.30867500	-0.55374500	0.37031800
C	-2.51506100	-1.49728600	-0.33684000
N	-4.60430600	-0.72774800	0.55662700
N	-3.00311000	-2.63928600	-0.78398100
P	-2.43914000	0.91388300	1.04924000
P	-0.76632700	-1.04499500	-0.68746600
C	-3.28267500	2.27718500	0.16938400
H	-4.35312300	2.06599400	0.09349700
H	-3.14711800	3.21490000	0.71203200
H	-2.86707600	2.40131100	-0.83203100
C	0.04978600	-2.66764000	-0.70973700
H	-0.55589500	-3.34535100	-1.31675000
H	1.05538300	-2.59059500	-1.12979600
H	0.11282500	-3.08514000	0.29660200
C	-0.77583800	-0.50851200	-2.50423000
C	-1.64131400	0.73816000	-2.65011500
C	0.65281900	-0.20405500	-2.94612200
C	-1.33795100	-1.63673400	-3.37256400
H	-2.68350300	0.55768500	-2.35944200
H	-1.25152000	1.56871100	-2.05269100
H	-1.64274700	1.05555700	-3.69881700
H	1.33006400	-1.05108300	-2.80217000
H	0.64141100	0.03007500	-4.01689800
H	1.06417400	0.66549800	-2.42982800
H	-1.37216400	-1.27807000	-4.40758800
H	-0.70355300	-2.52728500	-3.35854700

H	-2.35230200	-1.92954800	-3.09003500
C	-3.08438200	1.08258100	2.82748500
C	-4.45685000	1.75632000	2.86907000
C	-3.20630400	-0.29241300	3.48579000
C	-2.07317200	1.95878000	3.56935200
H	-4.43182200	2.78668200	2.50422300
H	-5.20340100	1.20007500	2.29526200
H	-4.79349400	1.78820000	3.91228400
H	-2.30819000	-0.90603000	3.39006900
H	-3.39987700	-0.15636600	4.55604800
H	-4.04500000	-0.85771800	3.06995600
H	-2.40446800	2.10631700	4.60384500
H	-1.07208900	1.51434500	3.59773300
H	-1.98516800	2.95133100	3.11135300
Co	-0.20471400	0.53729900	0.70015700
C	0.00458400	5.33587300	-2.11504900
C	0.34111900	4.06849300	-1.67401800
C	-0.05193500	3.56861000	-0.42377600
C	-0.80417100	4.42432700	0.39673500
C	-1.13772900	5.70753400	-0.01570500
C	-0.74004400	6.15996900	-1.27381900
H	0.33037400	5.66285200	-3.09701900
H	-1.11016700	4.05736700	1.37393900
H	-1.71078500	6.35493100	0.64069100
H	-1.00702900	7.15911800	-1.60487500
C	0.33187100	2.24244900	-0.01279100
C	1.29155000	1.36896500	-0.02629300
C	2.67007600	0.91697100	-0.25207300
H	3.33858500	1.35443200	0.50896600
H	3.02238900	1.25332100	-1.23178500
N	2.68226300	-0.55121900	-0.22838100
C	2.32649500	-1.15729100	1.07114000
H	1.99874200	-2.18251300	0.88906100
H	3.21271700	-1.20084600	1.72720700
C	1.27397900	-0.35989000	1.78373300
C	0.02638200	-0.85059000	2.20836100
H	1.66753000	0.48984800	2.34480000
H	-0.40663800	-0.43063200	3.11126900
H	-0.27285200	-1.87552300	1.99699900
S	3.90660300	-1.33226200	-1.07932400
O	3.47961600	-2.72896100	-1.14995300
O	4.12589000	-0.54240200	-2.28795100
C	5.37248400	-1.27274500	-0.08504300
C	5.59349800	-2.28046500	0.85492900

C	6.26103400	-0.20426700	-0.21515500
C	6.72085800	-2.21626200	1.66433400
H	4.89877300	-3.11168100	0.93296000
C	7.38559600	-0.16147800	0.59904400
H	6.08082600	0.56884200	-0.95661200
C	7.63487500	-1.16208500	1.54848200
H	6.89991300	-3.00112900	2.39496600
H	8.08948500	0.66082900	0.49541400
C	8.86753900	-1.12009500	2.39348100
H	9.14680400	-0.09474900	2.65056000
H	8.74395400	-1.68834400	3.31889200
H	9.71999900	-1.55565100	1.85934800
F	1.06521400	3.26776400	-2.48328700

M1S-F

Zero-point correction=	0.762528 (Hartree/Particle)
Thermal correction to Energy=	0.809470
Thermal correction to Enthalpy=	0.810414
Thermal correction to Gibbs Free Energy=	0.686208
Sum of electronic and zero-point Energies=	-3077.855203
Sum of electronic and thermal Energies=	-3077.808262
Sum of electronic and thermal Enthalpies=	-3077.807318
Sum of electronic and thermal Free Energies=	-3077.931524

C	7.83663100	-1.81117000	-0.88017900
C	6.64729600	-2.24538900	-0.34438600
C	5.49996300	-1.42467800	-0.43189200
C	5.58786900	-0.15689500	-1.09734800
C	6.82724900	0.26427700	-1.62967800
C	7.92770600	-0.55186500	-1.51996300
H	8.72118800	-2.43706200	-0.81230500
H	6.55919600	-3.20474300	0.15704800
H	6.87561400	1.23009400	-2.12402800
H	8.88129400	-0.23139600	-1.92855200
C	3.36463800	0.18951600	-0.72003400
C	3.29611200	-1.03389900	-0.00395000
N	4.49433600	0.63841900	-1.23549300
N	4.33456700	-1.83729100	0.13230100
P	1.79465500	1.12214800	-0.90376800
P	1.69488700	-1.43981700	0.79555800
C	2.21114400	2.68710500	-0.05530400
H	3.24158000	2.96580500	-0.29305300
H	1.54523600	3.48756300	-0.38354300
H	2.10863400	2.58393400	1.02696900
C	1.63524400	-3.24876800	0.62955100

H	2.61181800	-3.65234600	0.90872100
H	0.86683300	-3.67610200	1.27751300
H	1.43356600	-3.53637500	-0.40477400
C	1.95017000	-1.12485800	2.63403700
C	2.39866000	0.32160900	2.81665500
C	0.62249500	-1.36357100	3.35029200
C	3.01100400	-2.08192800	3.18003000
H	3.37427600	0.51437000	2.35493700
H	1.66744600	1.01786400	2.39684500
H	2.48636300	0.54352600	3.88599200
H	0.23401900	-2.37351900	3.17749400
H	0.77723500	-1.25100800	4.42924200
H	-0.13669900	-0.63968000	3.04732400
H	3.19918100	-1.82204200	4.22795300
H	2.67909900	-3.12365300	3.15712800
H	3.96165000	-2.01016900	2.64372200
C	1.71248100	1.63104900	-2.72723500
C	2.66172000	2.79163500	-3.02967200
C	2.08539400	0.45300500	-3.62518600
C	0.27289800	2.07857000	-2.98187100
H	2.39218400	3.70583800	-2.49441900
H	3.70041100	2.54253400	-2.79661900
H	2.60190000	3.01365700	-4.10184200
H	1.47360100	-0.43353400	-3.45169000
H	1.94283100	0.74950600	-4.67065800
H	3.13678000	0.17262400	-3.50731700
H	0.15822500	2.36564700	-4.03342400
H	-0.45534500	1.28875300	-2.76630300
H	0.01364400	2.95454600	-2.37586100
Co	0.11223700	-0.19825800	-0.07472800
C	-0.52146100	4.14261800	3.22439800
C	-0.55017500	2.84539200	2.74341000
C	-0.71884800	2.54114900	1.38809000
C	-0.90039000	3.61987400	0.50929900
C	-0.89579700	4.93012200	0.97268500
C	-0.69319800	5.19366700	2.32663200
H	-0.37763500	4.31193500	4.28656300
H	-1.05232500	3.40711400	-0.54604400
H	-1.04492500	5.74686800	0.27316900
H	-0.67593700	6.21638500	2.69032100
C	-0.73122400	1.17044400	0.92917300
C	-1.45415500	0.08989000	0.88420700
C	-2.77619600	-0.46707500	1.18327900
H	-3.53066200	0.29234000	0.90959500

H	-2.87484400	-0.64600800	2.25898300
N	-2.99402000	-1.73096800	0.46528000
C	-2.38845600	-1.75492000	-0.87307400
H	-2.78057300	-2.63973100	-1.38677600
H	-2.66421100	-0.86745600	-1.46746900
C	-0.90555900	-1.90283700	-0.75253300
C	-0.00605800	-1.43112100	-1.71537600
H	-0.62872400	-2.74747000	-0.12635100
H	0.91401600	-1.97353400	-1.92412200
H	-0.38906900	-0.84165700	-2.54790400
S	-4.57185800	-2.32063000	0.57252200
O	-4.55420000	-3.63045100	-0.07096900
O	-4.94751400	-2.15796200	1.97384800
C	-5.56960000	-1.23238100	-0.40924900
C	-5.69117500	-1.46616000	-1.78170100
C	-6.15810600	-0.11417000	0.18118600
C	-6.41219700	-0.57063200	-2.55829900
H	-5.24057400	-2.34886400	-2.22664700
C	-6.87736000	0.77158800	-0.61445300
H	-6.06899500	0.04501400	1.25184100
C	-7.01502100	0.56177300	-1.99099700
H	-6.51752400	-0.75268800	-3.62529300
H	-7.34638900	1.64003400	-0.15829400
C	-7.80151500	1.50655500	-2.84167100
H	-8.08847500	2.40510900	-2.29065400
H	-7.23678500	1.81352600	-3.72752300
H	-8.71993500	1.03403700	-3.20735400
F	-0.40839500	1.81994800	3.61411400

M1R-OMe

Zero-point correction=	0.805228 (Hartree/Particle)
Thermal correction to Energy=	0.854268
Thermal correction to Enthalpy=	0.855212
Thermal correction to Gibbs Free Energy=	0.727160
Sum of electronic and zero-point Energies=	-3093.101897
Sum of electronic and thermal Energies=	-3093.052858
Sum of electronic and thermal Enthalpies=	-3093.051913
Sum of electronic and thermal Free Energies=	-3093.179966

C	-6.49855100	-3.97358500	-1.18687300
C	-5.14478800	-3.80256000	-1.35554700
C	-4.50940400	-2.66549200	-0.80725400
C	-5.28325000	-1.71088800	-0.06967500
C	-6.67466800	-1.91033700	0.07830700
C	-7.26552700	-3.02327100	-0.47222400

H	-6.99045200	-4.84473300	-1.60933700
H	-4.53993600	-4.51687300	-1.90647400
H	-7.24515700	-1.17382400	0.63687100
H	-8.33378100	-3.18109900	-0.35746400
C	-3.38874700	-0.50858000	0.35150800
C	-2.63743400	-1.41489800	-0.44565600
N	-4.69394700	-0.63115900	0.51022300
N	-3.17693400	-2.48165000	-1.00511800
P	-2.45089000	0.82666600	1.19216300
P	-0.86227600	-1.02014200	-0.73052400
C	-3.20462000	2.31551400	0.44240100
H	-4.28189800	2.16562300	0.32782400
H	-3.03399900	3.18902600	1.07356000
H	-2.76287800	2.51659000	-0.53455000
C	-0.13263800	-2.67237800	-0.93091400
H	-0.74350700	-3.23408200	-1.64189800
H	0.89403100	-2.60235300	-1.29834900
H	-0.14117300	-3.22085800	0.01246700
C	-0.79971800	-0.28672100	-2.47554900
C	-1.54176000	1.04475900	-2.48557500
C	0.66042400	-0.07632900	-2.86712600
C	-1.45559600	-1.24718800	-3.47039400
H	-2.59566400	0.93014200	-2.20288600
H	-1.07567400	1.77280500	-1.81470900
H	-1.51614200	1.46401600	-3.49831200
H	1.24481500	-1.00025900	-2.82705400
H	0.69161900	0.28815700	-3.90094600
H	1.14463400	0.67602400	-2.24111500
H	-1.43092000	-0.77456100	-4.45902200
H	-0.91771700	-2.19558000	-3.55356300
H	-2.50098100	-1.46079900	-3.23389800
C	-3.11723300	0.85518600	2.96938100
C	-4.43601600	1.62293500	3.06836400
C	-3.35046300	-0.56687500	3.48091800
C	-2.05274300	1.56637300	3.80718600
H	-4.32843700	2.68075800	2.81255500
H	-5.21127900	1.18734600	2.43121300
H	-4.78876100	1.57286700	4.10556800
H	-2.50620400	-1.23847700	3.31002100
H	-3.52819900	-0.52909600	4.56186900
H	-4.23422300	-1.01621900	3.01941700
H	-2.39115900	1.64058400	4.84710700
H	-1.09544600	1.03297200	3.80114600
H	-1.87136900	2.58694900	3.44873400

Co	-0.24223600	0.34169400	0.85727000
C	0.25683500	5.24561900	-1.64542400
C	0.59653700	3.95428000	-1.24027700
C	0.11957100	3.44620600	-0.00389100
C	-0.64632800	4.28711700	0.81225000
C	-0.95357200	5.58631800	0.42733100
C	-0.51262000	6.05266800	-0.80938600
H	0.59697500	5.62716400	-2.60220100
H	-0.99265100	3.89523400	1.76590000
H	-1.54104500	6.22547200	1.07891600
H	-0.76378800	7.05918700	-1.13270000
C	0.42033500	2.08546100	0.35576000
C	1.31852000	1.15378800	0.26300800
C	2.66771600	0.65454000	-0.01589000
H	3.36185800	0.95143800	0.78965100
H	3.03609600	1.09199900	-0.94950400
N	2.59599200	-0.80404400	-0.17596700
C	2.19568400	-1.53858300	1.04322000
H	1.84380100	-2.52666200	0.74357100
H	3.06566600	-1.68242100	1.70631000
C	1.15285800	-0.79037100	1.82388800
C	-0.13070200	-1.26243900	2.15537000
H	1.57199500	-0.05088900	2.50921600
H	-0.56037400	-0.94949700	3.10256900
H	-0.48246400	-2.22757400	1.79592300
S	3.83058100	-1.51515800	-1.07189500
O	3.42743700	-2.91098800	-1.23121500
O	4.03832900	-0.64687400	-2.22807800
C	5.29214000	-1.46739600	-0.06987700
C	5.60973700	-2.55521300	0.74283500
C	6.07711900	-0.31160300	-0.06305400
C	6.73173800	-2.48296400	1.56094500
H	4.99373100	-3.44914600	0.72002800
C	7.19254500	-0.25874100	0.76133800
H	5.82308200	0.52436200	-0.70865000
C	7.54039500	-1.34086700	1.58253800
H	6.99009000	-3.33045000	2.19097500
H	7.81281500	0.63422000	0.76547900
C	8.76156100	-1.27838500	2.44259100
H	8.85951000	-0.30605100	2.93424800
H	8.75539700	-2.05481100	3.21129400
H	9.66896700	-1.41832300	1.84399600
O	1.36123100	3.10458300	-1.96567200
C	1.75827000	3.51407600	-3.26771000

H	0.88748000	3.68187200	-3.91260900
H	2.36956700	4.42263200	-3.23758500
H	2.35629700	2.69528000	-3.66947800

M1S-OMe

Zero-point correction=	0.804190 (Hartree/Particle)
Thermal correction to Energy=	0.853619
Thermal correction to Enthalpy=	0.854563
Thermal correction to Gibbs Free Energy=	0.724501
Sum of electronic and zero-point Energies=	-3093.104870
Sum of electronic and thermal Energies=	-3093.055442
Sum of electronic and thermal Enthalpies=	-3093.054498
Sum of electronic and thermal Free Energies=	-3093.184560

C	-7.92438800	-1.91577800	-0.20127800
C	-6.70307300	-2.09619900	-0.80623700
C	-5.56398000	-1.43484100	-0.29312700
C	-5.69722400	-0.58589200	0.85454500
C	-6.96653800	-0.42179900	1.45380500
C	-8.05628100	-1.07588900	0.93036000
H	-8.80244400	-2.41964500	-0.59429400
H	-6.58121800	-2.73513200	-1.67594000
H	-7.04716600	0.22648300	2.32137300
H	-9.03321400	-0.95040700	1.38729500
C	-3.46134800	-0.13582100	0.77699800
C	-3.33651100	-0.95543100	-0.37430900
N	-4.62236500	0.06317400	1.37405700
N	-4.36088900	-1.60054000	-0.90213900
P	-1.92787900	0.68144400	1.37443900
P	-1.66844900	-1.08831700	-1.13180600
C	-2.36174800	2.42630300	1.04257300
H	-3.41306100	2.59793900	1.29045900
H	-1.74350100	3.09572500	1.64222800
H	-2.19723100	2.66366100	-0.01037600
C	-1.63838500	-2.85194500	-1.57988500
H	-2.59947700	-3.10429700	-2.03549500
H	-0.83219800	-3.07295200	-2.28253800
H	-1.51352200	-3.47127800	-0.68882800
C	-1.74996900	-0.17398400	-2.77405100
C	-2.11152800	1.28426500	-2.50482400
C	-0.37585600	-0.26325800	-3.43740100
C	-2.80106900	-0.81957800	-3.67904400
H	-3.10339800	1.38445600	-2.04829300
H	-1.37655200	1.76700500	-1.85332700
H	-2.12554900	1.83429700	-3.45292500

H	-0.03162900	-1.29672500	-3.55843800
H	-0.44199200	0.17820900	-4.43860000
H	0.37727900	0.29388900	-2.87685600
H	-2.86616600	-0.22962000	-4.60045100
H	-2.53023600	-1.84041600	-3.96360000
H	-3.79501600	-0.84061300	-3.22360300
C	-1.97617800	0.57482800	3.26407900
C	-2.98731200	1.55729200	3.85759800
C	-2.35046600	-0.83840200	3.70649300
C	-0.57404900	0.93929100	3.75391100
H	-2.72571400	2.59999800	3.65848600
H	-3.99975300	1.37521200	3.48759900
H	-2.99609300	1.42666600	4.94615500
H	-1.66863400	-1.60229000	3.32866300
H	-2.31626600	-0.88342400	4.80108900
H	-3.36803100	-1.10157500	3.40129400
H	-0.53743400	0.86394800	4.84671700
H	0.19749800	0.27795300	3.34443300
H	-0.31138300	1.97075800	3.49109000
Co	-0.17651100	-0.25892800	0.23797600
C	0.99370300	4.84232600	-1.57480600
C	0.93854800	3.45038100	-1.49880400
C	0.74837200	2.81092800	-0.24881700
C	0.66898300	3.60318200	0.90160800
C	0.76108100	4.98917900	0.83149200
C	0.90825000	5.60267200	-0.40979000
H	1.11986000	5.33491300	-2.53301900
H	0.54766800	3.10635300	1.86141700
H	0.71243900	5.58390700	1.73824500
H	0.96287200	6.68528800	-0.48035900
C	0.70524800	1.36800600	-0.20380700
C	1.39419900	0.31604500	-0.54877500
C	2.69996700	-0.13731000	-1.03226800
H	3.48032500	0.45767200	-0.52277500
H	2.79181700	0.06373100	-2.10545800
N	2.87783900	-1.57700400	-0.79139900
C	2.29181100	-2.03093500	0.48001900
H	2.67620400	-3.03931200	0.66935600
H	2.59215600	-1.38837000	1.32422000
C	0.80516800	-2.11213000	0.33943200
C	-0.09718800	-1.95793300	1.39787200
H	0.51371800	-2.71102800	-0.51913700
H	-1.02713000	-2.52404900	1.40913200
H	0.27663700	-1.66406600	2.37858800

S	4.42427900	-2.14669300	-1.14784100
O	4.37787200	-3.59278100	-0.95402600
O	4.76033300	-1.55722400	-2.44073400
C	5.50190300	-1.45577600	0.07819900
C	5.68137000	-2.12584200	1.29044300
C	6.10436400	-0.21874900	-0.15185600
C	6.47933400	-1.55047600	2.26928700
H	5.21472400	-3.09347300	1.45120900
C	6.89887100	0.34236500	0.84225200
H	5.96838500	0.28292100	-1.10553500
C	7.10024500	-0.30978100	2.06361900
H	6.63102200	-2.07287300	3.21106700
H	7.37875100	1.30186800	0.66541700
C	7.97612500	0.28311100	3.12031000
H	8.20571300	1.33141200	2.91594000
H	7.51261200	0.21818400	4.10918900
H	8.92808400	-0.25583800	3.18709200
O	1.04958300	2.62112200	-2.56527900
C	1.15797900	3.21278300	-3.85219100
H	0.28267200	3.83124200	-4.08233400
H	2.06542900	3.82071400	-3.94059900
H	1.21141000	2.38461300	-4.55942500

M2R-F

Zero-point correction= 0.762362 (Hartree/Particle)
Thermal correction to Energy= 0.810524
Thermal correction to Enthalpy= 0.811468
Thermal correction to Gibbs Free Energy= 0.682593
Sum of electronic and zero-point Energies= -3077.848360
Sum of electronic and thermal Energies= -3077.800198
Sum of electronic and thermal Enthalpies= -3077.799254
Sum of electronic and thermal Free Energies= -3077.928129

C	-7.23282800	-3.27856500	-0.01213900
C	-6.12556200	-3.01163200	-0.78148000
C	-5.15680000	-2.09406800	-0.31747600
C	-5.33475100	-1.45963400	0.95522100
C	-6.48464000	-1.75378900	1.72256200
C	-7.41315400	-2.64715700	1.24183400
H	-7.98167800	-3.98018400	-0.36693500
H	-5.96989100	-3.48242500	-1.74767500
H	-6.60413200	-1.26378000	2.68441800
H	-8.29702600	-2.87676500	1.82921800
C	-3.35002700	-0.36206900	0.67818700
C	-3.19933300	-0.95234500	-0.61055900

N	-4.40326000	-0.59636100	1.43894300
N	-4.07733800	-1.81380800	-1.09185500
P	-2.00066700	0.74286400	1.28785900
P	-1.76552300	-0.42826500	-1.62652500
C	-2.77221000	2.39545800	1.30068800
H	-3.72691800	2.35550200	1.83112400
H	-2.11079400	3.11178100	1.79614000
H	-2.95259000	2.73487100	0.28026000
C	-1.24025000	-1.97853200	-2.42891400
H	-2.12238000	-2.54324800	-2.74239800
H	-0.62554400	-1.75554300	-3.30455500
H	-0.65416400	-2.59656800	-1.74541800
C	-2.51530600	0.57311300	-3.03541800
C	-3.40806900	1.66359200	-2.44845000
C	-1.34286000	1.20530700	-3.78873800
C	-3.32659300	-0.31089500	-3.97966400
H	-4.25228000	1.24989600	-1.88482800
H	-2.84991000	2.34104500	-1.79604800
H	-3.82332900	2.26803800	-3.26280900
H	-0.65149800	0.45226700	-4.18355400
H	-1.72387700	1.77743800	-4.64234600
H	-0.77283400	1.89205900	-3.15450900
H	-3.77574600	0.32047800	-4.75535300
H	-2.70262300	-1.05473200	-4.48364500
H	-4.13729700	-0.83580600	-3.46494100
C	-1.75027300	0.31911800	3.11369400
C	-2.85376700	0.96726400	3.95758100
C	-1.80197400	-1.19389300	3.33455600
C	-0.39929600	0.89434400	3.54379700
H	-2.79317600	2.05878700	3.95619700
H	-3.85217300	0.66687000	3.62853300
H	-2.72728200	0.63410300	4.99411600
H	-1.13485300	-1.75976900	2.67970500
H	-1.50361200	-1.40486400	4.36741500
H	-2.81512700	-1.58221300	3.20066000
H	-0.28063100	0.74607800	4.62304000
H	0.44542000	0.41186800	3.04349800
H	-0.33392000	1.97108000	3.35000900
Co	-0.37586000	0.65438200	-0.15263200
C	2.14106400	5.17542100	1.12413000
C	2.20403800	3.78514300	1.15026100
C	1.22517700	3.01627700	0.49945000
C	0.22170600	3.72255800	-0.16524400
C	0.12778700	5.09438500	-0.22303400

C	1.11071700	5.82747600	0.44652000
H	2.90239300	5.75671300	1.63540200
H	3.00312900	3.27443500	1.68130500
H	-0.67767700	5.57213900	-0.77011200
H	1.06655900	6.91197200	0.43196600
C	1.14810200	1.57012800	0.47630400
C	2.10325400	0.68939000	0.10156400
C	3.37057600	0.91263300	-0.67087100
H	4.24873200	0.89431600	-0.00580800
H	3.38861700	1.85774300	-1.22018500
N	3.38278600	-0.24595800	-1.60440100
C	2.24174300	-1.15088700	-1.31330600
H	1.42356900	-0.92303300	-2.01270500
H	2.53069200	-2.19467700	-1.46142000
C	1.83702200	-0.79525100	0.11440300
C	0.40135400	-1.00723900	0.52797900
H	2.55210200	-1.29465300	0.79476500
H	0.32451500	-1.02298200	1.61548200
H	-0.06799300	-1.91253500	0.12874600
S	4.87590200	-0.94297200	-1.90328900
O	4.62437700	-2.05681900	-2.81405800
O	5.75762600	0.16422200	-2.26243900
C	5.44153800	-1.60519400	-0.35685800
C	5.00608300	-2.86489400	0.05759000
C	6.25513100	-0.82403400	0.46665300
C	5.39309100	-3.33752300	1.30608100
H	4.38729600	-3.47081600	-0.59811700
C	6.63310900	-1.31412700	1.70973200
H	6.60129600	0.14555900	0.12108900
C	6.20879600	-2.57445200	2.15107100
H	5.06424000	-4.32155500	1.63182700
H	7.27436400	-0.71227900	2.34924700
C	6.64286000	-3.09898000	3.48206300
H	6.50319300	-2.35548100	4.27268700
H	6.09421200	-4.00205100	3.75978900
H	7.70942100	-3.34982200	3.47599200
F	-0.70846900	2.94955500	-0.83011700

M2S-F

Zero-point correction=	0.764251 (Hartree/Particle)
Thermal correction to Energy=	0.811766
Thermal correction to Enthalpy=	0.812710
Thermal correction to Gibbs Free Energy=	0.686462
Sum of electronic and zero-point Energies=	-3077.841527

Sum of electronic and thermal Energies= -3077.794012
Sum of electronic and thermal Enthalpies= -3077.793068
Sum of electronic and thermal Free Energies= -3077.919315

C	-6.37877400	-2.16707200	-3.32849800
C	-5.31215300	-1.30245600	-3.25572000
C	-4.63542700	-1.12997800	-2.02733300
C	-5.05952900	-1.87242600	-0.87744800
C	-6.16021900	-2.75232400	-0.98383700
C	-6.80439100	-2.89247400	-2.19031200
H	-6.90535300	-2.29826700	-4.26910000
H	-4.97484800	-0.73297500	-4.11661500
H	-6.46634400	-3.30663300	-0.10146000
H	-7.64911200	-3.56927400	-2.27692300
C	-3.38036000	-0.92679400	0.35216800
C	-3.00865300	-0.13444400	-0.77348400
N	-4.40235500	-1.76268800	0.30670400
N	-3.60658900	-0.24543300	-1.94454700
P	-2.29551500	-0.83358800	1.82897800
P	-1.70431700	1.14620000	-0.55190500
C	-3.31975100	-0.10414200	3.15753100
H	-4.33662900	-0.50476900	3.14519000
H	-2.85545800	-0.33736700	4.12023100
H	-3.36166400	0.98100900	3.06010900
C	-0.89905400	1.26555100	-2.17263000
H	-1.57268300	1.70630500	-2.91152700
H	0.00324400	1.87439100	-2.08533500
H	-0.62335100	0.26508800	-2.51139500
C	-2.70084600	2.74763400	-0.36761600
C	-3.35070200	2.76450000	1.01126500
C	-1.76120100	3.94069900	-0.51315000
C	-3.79084600	2.82139600	-1.43841500
H	-4.02683100	1.91327000	1.15104000
H	-2.60684200	2.76227900	1.81679800
H	-3.94726300	3.67697600	1.12175700
H	-1.19269400	3.92677100	-1.44875200
H	-2.35951700	4.85851900	-0.50882600
H	-1.05984400	4.00554400	0.31974100
H	-4.26626900	3.80595600	-1.36185900
H	-3.40239100	2.72479400	-2.45641300
H	-4.56964500	2.06893900	-1.29569200
C	-2.06773800	-2.62292700	2.41240000
C	-3.28860200	-3.12175600	3.18641500
C	-1.83014900	-3.56202400	1.23065200
C	-0.85056700	-2.60649500	3.34086400

H	-3.44871400	-2.57653400	4.12051600
H	-4.20237100	-3.07095100	2.58871300
H	-3.12081300	-4.17243400	3.45136200
H	-1.01150800	-3.24727500	0.57836400
H	-1.57333200	-4.55402000	1.61943200
H	-2.72969100	-3.67279000	0.61919000
H	-0.70381400	-3.60412000	3.76988800
H	0.06996600	-2.33317700	2.81293300
H	-0.98501800	-1.90829600	4.17572500
Co	-0.49235100	0.48840500	1.10906100
C	1.57513700	5.33414700	0.51788700
C	1.49854100	3.99896900	0.16290800
C	1.16154600	2.97673600	1.06063300
C	0.86214700	3.38652400	2.37325900
C	0.92698500	4.72149700	2.75953500
C	1.29017000	5.69730300	1.83267600
H	1.84160600	6.06964600	-0.23445900
H	0.58691600	2.62213300	3.09907000
H	0.70032100	4.99970000	3.78443400
H	1.34607500	6.74150700	2.12487500
C	1.04701900	1.57173500	0.66564000
C	2.00809500	0.85079000	0.05792100
C	3.36200400	1.18675800	-0.48487800
H	4.15928700	0.89527400	0.21645500
H	3.50476000	2.23897200	-0.73470700
N	3.41340900	0.34929000	-1.71918500
C	2.24436200	-0.57316300	-1.77220300
H	1.50682600	-0.17258500	-2.47668900
H	2.54654200	-1.55966100	-2.13422300
C	1.72706200	-0.56290400	-0.33594600
C	0.29841700	-0.93178900	0.01063400
H	2.41122900	-1.21096600	0.24127200
H	-0.30798500	-1.24702900	-0.84757900
H	0.27996700	-1.73746400	0.75352900
S	4.90260600	-0.29616900	-2.12410500
O	4.71783900	-0.96400600	-3.41017100
O	5.86406800	0.78974300	-1.95063000
C	5.25476800	-1.54416700	-0.91145300
C	4.78293000	-2.84392200	-1.10323500
C	5.93472800	-1.19907000	0.25936200
C	4.98675500	-3.79445200	-0.10940900
H	4.28112400	-3.11026600	-2.02923200
C	6.13316000	-2.16385300	1.23872700
H	6.32186300	-0.19206000	0.38526600

C	5.66243900	-3.47359900	1.07387100
H	4.62656200	-4.80973000	-0.25801800
H	6.67291700	-1.90164200	2.14582000
C	5.90575800	-4.50824600	2.12586800
H	5.66913700	-4.13113600	3.12549600
H	5.31459700	-5.41010800	1.94996300
H	6.96003400	-4.80586800	2.14691800
F	1.71571100	3.67403000	-1.13584700

M2R-OMe

Zero-point correction=			0.805501 (Hartree/Particle)
Thermal correction to Energy=			0.854220
Thermal correction to Enthalpy=			0.855164
Thermal correction to Gibbs Free Energy=			0.727599
Sum of electronic and zero-point Energies=			-3093.110523
Sum of electronic and thermal Energies=			-3093.061805
Sum of electronic and thermal Enthalpies=			-3093.060861
Sum of electronic and thermal Free Energies=			-3093.188425
C	-6.20545500	-4.11498600	-0.10588300
C	-5.61838200	-3.19905800	-0.94628800
C	-4.59836000	-2.35274100	-0.45390500
C	-4.17266700	-2.48235300	0.90747300
C	-4.80446500	-3.42402500	1.75107700
C	-5.80290400	-4.22298700	1.24701400
H	-6.99292200	-4.76339700	-0.47839300
H	-5.92317700	-3.09348200	-1.98351200
H	-4.47303900	-3.50016300	2.78267100
H	-6.28846400	-4.95213400	1.88867300
C	-2.59236500	-0.86495900	0.56139300
C	-3.10201900	-0.64681100	-0.75085500
N	-3.14322800	-1.73636200	1.38346600
N	-4.06201800	-1.40017200	-1.25980900
P	-1.07843000	0.05358200	1.10950600
P	-2.50503600	0.83326000	-1.65018200
C	-1.65869100	1.02227600	2.54001300
H	-2.20806600	0.37746000	3.23097000
H	-0.80726100	1.47030600	3.06127300
H	-2.32174800	1.82079600	2.20178100
C	-2.40259500	0.27154600	-3.38281000
H	-3.32060500	-0.24949100	-3.66508700
H	-2.26022700	1.13336700	-4.04052300
H	-1.56166300	-0.40931800	-3.52248800
C	-4.03777300	1.93567100	-1.65292400
C	-4.50744800	2.06612300	-0.20129000

C	-3.60561400	3.27000800	-2.26700500
C	-5.18466600	1.37185900	-2.48927500
H	-5.04937600	1.16673200	0.11296000
H	-3.68492500	2.20803800	0.50765700
H	-5.19061500	2.91659400	-0.09727600
H	-3.40332900	3.15517300	-3.33727700
H	-4.40952100	4.00801000	-2.16396600
H	-2.70248000	3.68926300	-1.81353900
H	-6.05396400	2.03113400	-2.37638500
H	-4.94166800	1.33622700	-3.55515200
H	-5.48213700	0.36944400	-2.16870500
C	0.01542800	-1.29898200	1.86714400
C	-0.56731500	-1.77614500	3.20414600
C	0.09350800	-2.47539500	0.89396500
C	1.41274800	-0.74841200	2.15380000
H	-0.51060100	-1.00013600	3.97293300
H	-1.59948500	-2.11996300	3.12270800
H	0.04514800	-2.61771600	3.54911900
H	0.42075100	-2.17234700	-0.10582400
H	0.82033500	-3.20305300	1.27233400
H	-0.86702000	-2.99102000	0.79797800
H	1.93891900	-1.47028600	2.78970000
H	2.00572800	-0.60835300	1.24930100
H	1.38312400	0.20303600	2.69708100
Co	-0.50449900	1.36601700	-0.51619300
C	2.64000400	4.04154600	2.82349800
C	2.57869200	3.02905300	1.87176500
C	1.41351000	2.80690200	1.12144300
C	0.30156800	3.62701800	1.38509200
C	0.34291000	4.63890200	2.33766000
C	1.52454500	4.84175600	3.05277500
H	3.55254200	4.19907100	3.39082500
H	3.43820300	2.38234800	1.71631700
H	-0.51680900	5.26705100	2.53715400
H	1.55990400	5.63005400	3.79918400
C	1.24615400	1.75798000	0.13305100
C	2.22178200	1.09745300	-0.53014700
C	3.69505300	1.33898400	-0.67898000
H	4.26400100	0.96672500	0.18592300
H	3.95492500	2.39845100	-0.79049800
N	4.06622300	0.57936700	-1.90225400
C	2.83465200	0.05924700	-2.54296500
H	2.49705200	0.78910200	-3.28930000
H	3.04377800	-0.87824000	-3.06329600

C	1.82176500	-0.04692600	-1.39758400
C	0.35727300	0.09649800	-1.72667700
H	2.01801600	-0.99037600	-0.86065600
H	-0.16204100	-0.85204300	-1.90495000
H	0.23436600	0.74578600	-2.61181000
S	5.34774800	-0.49540900	-1.74678700
O	5.53683100	-1.08474300	-3.06972900
O	6.40879100	0.25225400	-1.07695200
C	4.80767000	-1.78171500	-0.64825400
C	4.08804500	-2.86276600	-1.16034700
C	5.02695500	-1.65745800	0.72572800
C	3.57584300	-3.81316800	-0.28427200
H	3.94319200	-2.96198600	-2.23244700
C	4.51575700	-2.62274200	1.58426600
H	5.60824200	-0.82362700	1.10902700
C	3.77705400	-3.70905200	1.09768000
H	3.01224800	-4.65630100	-0.67768100
H	4.69048300	-2.53415200	2.65432200
C	3.23163600	-4.73653600	2.03756800
H	2.73181300	-4.27198200	2.89442300
H	2.51883900	-5.40096000	1.54297100
H	4.03354100	-5.36065300	2.44793100
O	-0.81662800	3.33456700	0.61985100
C	-1.92742600	4.21895300	0.81212000
H	-2.31513100	4.14303000	1.83394700
H	-1.62878100	5.25082200	0.60636600
H	-2.69583800	3.92078200	0.10874900

M2S-OMe

Zero-point correction=	0.805456 (Hartree/Particle)
Thermal correction to Energy=	0.854480
Thermal correction to Enthalpy=	0.855424
Thermal correction to Gibbs Free Energy=	0.726216
Sum of electronic and zero-point Energies=	-3093.089444
Sum of electronic and thermal Energies=	-3093.040421
Sum of electronic and thermal Enthalpies=	-3093.039476
Sum of electronic and thermal Free Energies=	-3093.168685

C	-6.28678700	-2.08947300	-3.58678700
C	-5.18533200	-1.27976800	-3.43992300
C	-4.60713300	-1.11151200	-2.16165400
C	-5.16191000	-1.80799300	-1.03884500
C	-6.30047300	-2.62544300	-1.22022500
C	-6.85006300	-2.75762300	-2.47378800
H	-6.73816100	-2.21609200	-4.56614400

H	-4.74552500	-0.74964700	-4.27960100
H	-6.71036900	-3.14043000	-0.35614200
H	-7.72367700	-3.38612600	-2.61842800
C	-3.52579500	-0.94328400	0.30426200
C	-3.04826500	-0.16290900	-0.79134000
N	-4.58457400	-1.72438000	0.18883400
N	-3.55670400	-0.26264700	-2.00474900
P	-2.51425700	-0.93804000	1.83877700
P	-1.73455100	1.08586800	-0.46895200
C	-3.58049200	-0.21494800	3.13761600
H	-4.61083300	-0.57056100	3.05426500
H	-3.18157900	-0.50633800	4.11356300
H	-3.57111600	0.87398300	3.08270300
C	-0.84861700	1.24121800	-2.04350000
H	-1.47544100	1.72826800	-2.79468800
H	0.06440800	1.82098800	-1.88356400
H	-0.58591000	0.24733200	-2.41111000
C	-2.71947100	2.69712900	-0.29363000
C	-3.42377700	2.70191700	1.05842500
C	-1.76016800	3.88019200	-0.38611900
C	-3.76265400	2.79920000	-1.40761100
H	-4.12837400	1.86757600	1.15137800
H	-2.71377900	2.66018800	1.89285400
H	-4.00010600	3.62776200	1.16567300
H	-1.17984500	3.88259000	-1.31480700
H	-2.34603900	4.80600800	-0.36361200
H	-1.06831000	3.90892300	0.45704900
H	-4.23444900	3.78577700	-1.33487300
H	-3.33144500	2.71644600	-2.40953100
H	-4.55120500	2.04917600	-1.31209500
C	-2.38964100	-2.75369300	2.36973100
C	-3.67269800	-3.22755600	3.05406200
C	-2.12065900	-3.66293000	1.17219000
C	-1.22742000	-2.81330800	3.36467100
H	-3.87685800	-2.69578300	3.98726100
H	-4.54323700	-3.13229300	2.39896600
H	-3.55750600	-4.28872500	3.30565500
H	-1.24919100	-3.36469400	0.58403200
H	-1.93322200	-4.67856100	1.53875900
H	-2.98358100	-3.71167600	0.50233200
H	-1.14263800	-3.82835000	3.76932600
H	-0.26875200	-2.56060200	2.89742500
H	-1.38197700	-2.13512200	4.21270800
Co	-0.63149500	0.34181800	1.22885500

C	1.58287300	5.12873400	0.76378900
C	1.47949000	3.79659500	0.36393400
C	1.08144700	2.79287200	1.28291800
C	0.74906500	3.19970200	2.58289100
C	0.83714800	4.53039000	2.98585300
C	1.26369600	5.48976100	2.07308800
H	1.89942500	5.88997000	0.05845300
H	0.43020300	2.43663600	3.29261000
H	0.58571400	4.81096700	4.00430000
H	1.34647400	6.53164300	2.37032400
C	0.95504000	1.38858700	0.88865800
C	1.92829800	0.63710600	0.34221100
C	3.31939400	0.93599400	-0.11936800
H	4.06672600	0.51839800	0.57556500
H	3.53626000	1.99343300	-0.26935600
N	3.34310600	0.21331900	-1.42173300
C	2.21647300	-0.75676400	-1.51564800
H	1.49699800	-0.39901900	-2.26106500
H	2.57194000	-1.73961800	-1.84092800
C	1.62690500	-0.75689000	-0.10522300
C	0.16526400	-1.07932800	0.13362600
H	2.24702200	-1.44547200	0.49464400
H	-0.39273700	-1.33571800	-0.77553000
H	0.06269000	-1.91166600	0.83906300
S	4.83214500	-0.28530000	-1.98514600
O	4.59409900	-0.85694400	-3.30890300
O	5.73329500	0.84741700	-1.78605900
C	5.36050200	-1.60054600	-0.91457100
C	5.00554300	-2.91749100	-1.21084600
C	6.06184900	-1.29835100	0.25589600
C	5.35253000	-3.93088500	-0.32427400
H	4.48489900	-3.14518600	-2.13656800
C	6.40069800	-2.32411300	1.12859300
H	6.35481400	-0.27312700	0.46299200
C	6.05014100	-3.65373400	0.85694200
H	5.08537400	-4.95928500	-0.55532200
H	6.95457800	-2.09361900	2.03576000
C	6.43739100	-4.74931900	1.79813400
H	6.21398200	-4.48527900	2.83626000
H	5.92235200	-5.68417400	1.56396200
H	7.51441900	-4.94631300	1.75202100
O	1.70394200	3.37340300	-0.90874600
C	2.15744400	4.32764100	-1.85639200
H	3.10761100	4.77909800	-1.54804200

H	2.30776200	3.77572500	-2.78511300
H	1.41788700	5.12080000	-2.02076700

TS2R-F

Zero-point correction= 0.963863 (Hartree/Particle)
Thermal correction to Energy= 1.021709
Thermal correction to Enthalpy= 1.022654
Thermal correction to Gibbs Free Energy= 0.877830
Sum of electronic and zero-point Energies= -3688.507908
Sum of electronic and thermal Energies= -3688.450062
Sum of electronic and thermal Enthalpies= -3688.449117
Sum of electronic and thermal Free Energies= -3688.593940
Imaginary frequency= -1261.61 cm^{-1}

C	-3.51633800	5.51009900	-0.80269200
C	-3.38676600	4.37560200	-0.03532400
C	-2.11377200	3.78525000	0.12898200
C	-0.97362900	4.37631500	-0.49679400
C	-1.13642100	5.54016900	-1.27952600
C	-2.38874200	6.09215300	-1.42690300
H	-4.49270800	5.96608000	-0.93603500
H	-4.23971700	3.90470300	0.44586700
H	-0.25950600	5.97102400	-1.75497800
H	-2.51808400	6.98619500	-2.02974900
C	0.35562000	2.70901200	0.33474900
C	-0.79830600	2.09273100	0.93488500
N	0.26287100	3.82375000	-0.36261700
N	-1.99521200	2.63797400	0.84832900
P	1.95798300	1.82068100	0.49366600
P	-0.63407700	0.42529500	1.72783000
C	2.45640300	2.27328500	2.19388400
H	2.37152800	3.34807000	2.36847900
H	3.48655500	1.95741200	2.37758600
H	1.82599500	1.75892200	2.91075000
C	-2.18926200	-0.43165200	1.29368500
H	-2.99793700	0.29934000	1.24241200
H	-2.41483600	-1.16622000	2.06860700
H	-2.12087600	-0.93480900	0.33581600
C	-1.05533400	0.69740300	3.61113900
C	-0.15440300	1.71709600	4.30309100
C	-0.98816300	-0.64807100	4.33877500
C	-2.49668600	1.21626800	3.71943000
H	-0.08684500	2.66033200	3.75052800
H	0.85615600	1.34942500	4.49719600
H	-0.58558800	1.94608300	5.28377200

H	-1.71238400	-1.37008600	3.95063200
H	-1.24031500	-0.48088900	5.39247700
H	-0.00250200	-1.11882000	4.31294500
H	-2.68205800	1.45948600	4.77201100
H	-3.23570800	0.46488700	3.43264400
H	-2.67249100	2.11976000	3.13024400
C	3.31858600	2.70915700	-0.48549900
C	3.51200900	4.14159000	0.01642100
C	3.04628000	2.72850500	-1.98315800
C	4.60071500	1.90427700	-0.24586300
H	3.85419500	4.18181800	1.05363000
H	2.60034400	4.73656800	-0.07887000
H	4.28819600	4.61560700	-0.59595200
H	3.04583200	1.71645900	-2.39573900
H	3.85563600	3.27995100	-2.47610200
H	2.10217800	3.21673800	-2.23588500
H	5.42449900	2.39237800	-0.77896100
H	4.51570500	0.88526500	-0.63555200
H	4.88607600	1.85124900	0.80950000
Co	1.23362900	-0.44138700	0.51565600
C	-2.06299100	2.17596700	-2.92236600
C	-1.69229900	1.14006800	-2.08064300
C	-0.41102700	0.56851300	-2.05618400
C	0.48591100	1.09663000	-2.99487500
C	0.14585700	2.13042700	-3.86085500
C	-1.13016400	2.68446300	-3.82044100
H	-3.07640500	2.56099400	-2.86296000
H	1.48145600	0.67408300	-3.03879400
H	0.88555500	2.50326100	-4.56350700
H	-1.40429000	3.50312900	-4.47928500
C	-0.03631600	-0.53833700	-1.14741000
C	-0.57828600	-1.76767800	-1.26176800
C	-1.70538000	-2.25523600	-2.11893000
H	-2.54914300	-1.55211400	-2.09594600
H	-1.42421400	-2.39195300	-3.16976500
N	-2.04942400	-3.56759700	-1.51413900
C	-1.37675700	-3.72129900	-0.20542300
H	-1.18986600	-4.77811500	-0.00709900
H	-1.99022100	-3.31330700	0.61569500
C	-0.11369000	-2.87923800	-0.37207700
C	0.53017800	-2.32393200	0.87936300
H	0.61749900	-3.47298600	-0.94467600
H	1.37377800	-2.93365800	1.21697000
H	-0.18756300	-2.25840200	1.70484500

S	-3.66239400	-4.01494100	-1.57950600
O	-3.73754200	-5.32298500	-0.93450100
O	-4.08129400	-3.81252000	-2.96387700
C	-4.53109000	-2.84532900	-0.56353100
C	-4.65140700	-3.07698400	0.80808100
C	-4.99957700	-1.65555200	-1.12760500
C	-5.22915100	-2.10127200	1.61427500
H	-4.30811800	-4.01596700	1.23253600
C	-5.57098400	-0.69293900	-0.30657100
H	-4.92428300	-1.49519500	-2.19939800
C	-5.68338400	-0.89182500	1.07598900
H	-5.32254400	-2.27587800	2.68414500
H	-5.93038800	0.23657700	-0.74272400
C	-6.25413200	0.17962000	1.94879800
H	-5.64312700	1.08970000	1.90374800
H	-6.30985400	-0.13454700	2.99383800
H	-7.26092900	0.46613100	1.62764400
C	4.90752300	-1.85980900	-0.72150000
C	4.54243700	-1.61637200	-2.06759300
C	5.48171900	-1.78774000	-3.09219800
C	6.77246000	-2.16775700	-2.75861900
C	7.13564500	-2.35429500	-1.41769000
C	6.21974400	-2.19788400	-0.38230600
C	2.73433900	-1.11574100	-0.77349900
C	3.19110100	-1.15535500	-2.06754500
H	5.19935800	-1.60836100	-4.12597200
H	7.51582400	-2.30427900	-3.53842800
H	8.15888400	-2.62192900	-1.17149300
H	6.55472000	-2.31793600	0.63977000
H	1.44020900	-1.03296300	-0.94211000
H	2.60663400	-0.92074200	-2.94636200
N	3.76969600	-1.60231500	0.06241100
C	3.65991200	-1.59448400	1.44191700
C	4.51808700	-2.29390800	2.29577900
N	2.60415300	-0.89377400	1.91431000
C	4.32518900	-2.20147000	3.66361900
H	5.28360800	-2.94087300	1.89325200
C	2.43369500	-0.82329800	3.24474500
C	3.27593600	-1.43022200	4.15706500
H	4.98054900	-2.74516800	4.33652200
H	1.57309900	-0.25514000	3.56792800
H	3.08679700	-1.32601700	5.21928500
F	-2.64443400	0.65865000	-1.24718800

TS2S-F

Zero-point correction= 0.961082 (Hartree/Particle)
Thermal correction to Energy= 1.019930
Thermal correction to Enthalpy= 1.020874
Thermal correction to Gibbs Free Energy= 0.869165
Sum of electronic and zero-point Energies= -3688.504137
Sum of electronic and thermal Energies= -3688.445290
Sum of electronic and thermal Enthalpies= -3688.444346
Sum of electronic and thermal Free Energies= -3688.596054
Imaginary frequency= -1068.73 cm^{-1}

C	4.25461300	-6.46048800	0.25813500
C	3.12026600	-5.83069000	-0.19826200
C	3.07479400	-4.41890900	-0.23876200
C	4.20837800	-3.66232400	0.18698700
C	5.35722700	-4.33657400	0.65872200
C	5.37437300	-5.71150500	0.68937300
H	4.29521300	-7.54511000	0.29235000
H	2.24710100	-6.38793000	-0.52555800
H	6.20956800	-3.74546000	0.98132900
H	6.25706800	-6.23367500	1.04685700
C	3.10268100	-1.71728200	-0.30406100
C	1.94902000	-2.47130000	-0.67591700
N	4.19844200	-2.30420100	0.13192200
N	1.94452600	-3.78922500	-0.65340600
P	2.99406800	0.11232200	-0.49194500
P	0.34546200	-1.62454800	-1.05833600
C	3.67173100	0.20768500	-2.19424800
H	4.65014600	-0.27859100	-2.23854100
H	3.76728100	1.24213500	-2.53169000
H	3.00588800	-0.31766100	-2.88283800
C	-0.68974000	-2.57848700	0.12137800
H	-0.45193300	-3.63587000	-0.01039100
H	-1.75819900	-2.43095000	-0.05115700
H	-0.44879500	-2.29699200	1.14449800
C	-0.17494200	-2.39108300	-2.73807800
C	1.03322900	-2.47737600	-3.67116100
C	-1.28044900	-1.52410000	-3.34147900
C	-0.73511200	-3.80489600	-2.56318400
H	1.76603000	-3.20573400	-3.31107300
H	1.55602600	-1.52652000	-3.81150200
H	0.69912700	-2.80790000	-4.66137900
H	-2.14984100	-1.45676700	-2.67696400
H	-1.62423900	-1.98356200	-4.27572900
H	-0.95631700	-0.50713300	-3.57660700

H	-0.95903200	-4.20408300	-3.55983200
H	-1.66796600	-3.81417700	-1.99226800
H	-0.02185800	-4.47930000	-2.08311700
C	4.36571300	0.91907300	0.52760000
C	5.76365200	0.35749500	0.25906100
C	4.01790300	0.75942000	2.00508800
C	4.38883800	2.40077400	0.13849900
H	6.06075200	0.46721500	-0.78834000
H	5.85710500	-0.69162300	0.53675100
H	6.47686200	0.94073100	0.85464100
H	3.04900600	1.20931000	2.24843400
H	4.77803800	1.25940900	2.61676000
H	3.99278100	-0.29416300	2.30186600
H	5.11468400	2.91868600	0.77618000
H	3.42609800	2.89334800	0.27404700
H	4.71035200	2.54525600	-0.89853600
Co	0.63036200	0.71540000	-0.52226100
C	1.77274200	-0.96357900	4.26667400
C	1.23777100	-0.81160000	2.99836400
C	0.27998900	0.14738800	2.66515500
C	-0.13925200	0.97926400	3.72263300
C	0.37946500	0.85667200	5.00639300
C	1.33999300	-0.11639300	5.28123800
H	2.51522100	-1.73623900	4.43767000
H	-0.88173100	1.74465700	3.50758000
H	0.03351500	1.52105300	5.79255400
H	1.75174700	-0.21918100	6.28056600
C	-0.30876700	0.28767300	1.31916300
C	-1.63534700	0.14923600	1.12479200
C	-2.74668600	-0.22055000	2.06782000
H	-2.68591500	-1.25203000	2.43399600
H	-2.77276000	0.42329800	2.95360300
N	-4.00041200	-0.00495900	1.28583200
C	-3.63591800	0.83922900	0.11791200
H	-3.65592500	1.88739800	0.43936300
H	-4.36541500	0.71696900	-0.68699500
C	-2.21844900	0.38143700	-0.22667800
C	-1.28322400	1.21522400	-1.04801400
H	-2.33214200	-0.60227200	-0.70563200
H	-1.38739800	2.28754500	-0.83106500
H	-1.40482100	1.06543200	-2.12371400
S	-4.79226100	-1.44476300	0.85690800
O	-4.88634000	-2.21687400	2.09595000
O	-4.20734000	-2.07895200	-0.33598100

C	-6.38807200	-0.82389000	0.40278300
C	-7.24084900	-0.35125100	1.40190500
C	-6.78036400	-0.83976600	-0.93252100
C	-8.49894000	0.11101900	1.04750600
H	-6.92006700	-0.35221300	2.43958800
C	-8.04522100	-0.36798900	-1.26908800
H	-6.10235000	-1.22004900	-1.69040000
C	-8.92216400	0.11106200	-0.29086000
H	-9.17200500	0.47705600	1.81916800
H	-8.36009100	-0.37581300	-2.30953600
C	-10.28044600	0.61780800	-0.65545600
H	-10.37695700	1.68641400	-0.43439700
H	-11.06291100	0.11092800	-0.08179500
H	-10.49313400	0.47615900	-1.71763300
C	1.46102700	4.72506000	-0.15861300
C	1.55399000	4.52459100	1.24247700
C	1.94791300	5.57807600	2.07764200
C	2.26529800	6.80071100	1.50722800
C	2.21154600	6.97266600	0.11681900
C	1.81885600	5.94557200	-0.73520600
C	0.95998000	2.53149800	0.31160600
C	1.24379600	3.15652100	1.50383700
H	2.01230800	5.42605300	3.15154400
H	2.57231300	7.63011800	2.13754600
H	2.48639800	7.93068600	-0.31494900
H	1.81811300	6.12023500	-1.80313300
H	0.06292300	1.61232900	0.67712500
H	1.21810200	2.68752100	2.47770700
N	1.04548500	3.50487100	-0.71368900
C	0.98295000	3.11868900	-2.04168300
C	0.86252600	4.00799100	-3.11344700
N	1.00187100	1.77781100	-2.22710100
C	0.83386000	3.50278100	-4.40245300
H	0.74805900	5.06755900	-2.93714700
C	0.95713400	1.31144000	-3.48530400
C	0.90287600	2.12606700	-4.60108600
H	0.74057400	4.18259700	-5.24338400
H	0.95971800	0.23382800	-3.57827200
H	0.88443300	1.68632800	-5.59143400
F	1.68129500	-1.65127300	2.02844100

TS2R-OMe

Zero-point correction=	1.004097 (Hartree/Particle)
Thermal correction to Energy=	1.063890

Thermal correction to Enthalpy= 1.064834
Thermal correction to Gibbs Free Energy= 0.914787
Sum of electronic and zero-point Energies= -3703.755735
Sum of electronic and thermal Energies= -3703.695942
Sum of electronic and thermal Enthalpies= -3703.694997
Sum of electronic and thermal Free Energies= -3703.845045
Imaginary frequency= -1162.93 cm^{-1}

C	-2.81522000	6.02149900	-0.80666300
C	-2.80324100	4.89683400	-0.01336400
C	-1.62410600	4.12391200	0.08867500
C	-0.44939000	4.53765700	-0.60889000
C	-0.49381700	5.68724500	-1.42783100
C	-1.66025000	6.41092500	-1.52384700
H	-3.72001900	6.61615100	-0.88940600
H	-3.68251600	4.57492800	0.53827400
H	0.40490500	5.97361900	-1.96716800
H	-1.69715900	7.29604800	-2.15175400
C	0.69177300	2.74535000	0.24291900
C	-0.51246100	2.28583700	0.88769100
N	0.71085200	3.83657500	-0.49653500
N	-1.63295100	2.97672300	0.82021500
P	2.19925300	1.70718700	0.42204600
P	-0.51362700	0.64167900	1.74995500
C	2.77367300	2.20168200	2.09149500
H	2.73089100	3.28434400	2.22881500
H	3.80148000	1.86300300	2.24531800
H	2.16098200	1.73483300	2.85428200
C	-2.15463500	-0.09789700	1.40739000
H	-2.88771900	0.70051500	1.27544800
H	-2.44785800	-0.71284200	2.26098500
H	-2.14191700	-0.70912700	0.51063800
C	-0.85438200	1.07392300	3.62192600
C	0.17286000	2.02351000	4.23221300
C	-0.92308300	-0.21830000	4.43985100
C	-2.22209900	1.76629600	3.71997000
H	0.34248200	2.90973700	3.61229400
H	1.13565500	1.55162500	4.44197100
H	-0.21134700	2.37129300	5.19762800
H	-1.71378200	-0.89282700	4.09932300
H	-1.15749800	0.04681900	5.47725600
H	0.01085300	-0.78456100	4.45661200
H	-2.37759400	2.03790300	4.77065400
H	-3.05153100	1.11623900	3.43350400
H	-2.27849200	2.68138300	3.12611300

C	3.63108200	2.41680600	-0.60894500
C	3.98542800	3.82929300	-0.13451100
C	3.33960300	2.45328300	-2.10257100
C	4.82643500	1.48424700	-0.38098700
H	4.37240900	3.84632200	0.88718800
H	3.13308600	4.51103100	-0.20040600
H	4.77751500	4.21959200	-0.78418600
H	3.24651700	1.44629600	-2.51523900
H	4.18759700	2.93183400	-2.60685900
H	2.43915300	3.02179400	-2.34357300
H	5.69539000	1.89965100	-0.90449500
H	4.64666400	0.48438100	-0.78939700
H	5.10701900	1.38469500	0.67260600
Co	1.23345600	-0.45773800	0.57178700
C	-1.76433600	2.31450500	-3.05288700
C	-1.56770400	1.30383800	-2.10773800
C	-0.33283700	0.61139000	-2.02425600
C	0.65027800	0.97437000	-2.94650600
C	0.46249000	1.97025000	-3.90075000
C	-0.74880900	2.64867900	-3.94518700
H	-2.71236400	2.84071100	-3.09665100
H	1.59513300	0.44727100	-2.90488400
H	1.26331700	2.21190500	-4.59396500
H	-0.91607000	3.43675400	-4.67428800
C	-0.07873000	-0.48744100	-1.06518000
C	-0.70859800	-1.67754500	-1.13166200
C	-1.88886200	-2.11707400	-1.94569600
H	-2.72600400	-1.41403300	-1.80824600
H	-1.68880200	-2.18338900	-3.02059100
N	-2.18703900	-3.46585400	-1.39924200
C	-1.55686300	-3.60780600	-0.07047000
H	-1.39988100	-4.66330000	0.15760500
H	-2.17731700	-3.15936700	0.72450400
C	-0.27877300	-2.79627800	-0.23103700
C	0.37364700	-2.24969400	1.01581800
H	0.44380300	-3.40835400	-0.79611200
H	1.15846200	-2.91134500	1.39626100
H	-0.35767500	-2.09564900	1.81757200
S	-3.76756100	-4.00189900	-1.53535700
O	-3.78369000	-5.34464800	-0.96171000
O	-4.16526400	-3.75191100	-2.91837600
C	-4.72225800	-2.94094800	-0.48073300
C	-4.79090500	-3.21328700	0.88735200
C	-5.31537200	-1.79321100	-1.00969000

C	-5.43929700	-2.31475100	1.72722400
H	-4.35506100	-4.12618000	1.28278900
C	-5.97545100	-0.91747800	-0.15687600
H	-5.27482300	-1.60572700	-2.07909100
C	-6.02902300	-1.14960600	1.22402600
H	-5.49382900	-2.52213600	2.79338500
H	-6.45284200	-0.03035500	-0.56776600
C	-6.67961800	-0.15852600	2.13489800
H	-6.06784200	0.74819200	2.22299700
H	-6.81759400	-0.56097000	3.14118700
H	-7.65519000	0.16019700	1.75544300
C	4.72744100	-2.30316300	-0.66625600
C	4.33925700	-2.13085700	-2.01662700
C	5.20825600	-2.49524700	-3.05214100
C	6.46100600	-2.99290200	-2.72891300
C	6.85573700	-3.10772700	-1.38917300
C	6.00725900	-2.76028700	-0.34281200
C	2.64114900	-1.34256500	-0.71837500
C	3.04389100	-1.53129300	-2.01625000
H	4.90291100	-2.37207000	-4.08760800
H	7.15008700	-3.28061100	-3.51772500
H	7.85159800	-3.47070200	-1.15216800
H	6.36940400	-2.83530000	0.67367200
H	1.37419300	-1.11239800	-0.86090800
H	2.45053700	-1.30922400	-2.89237000
N	3.65308600	-1.86324100	0.12793800
C	3.57868400	-1.77097300	1.50766400
C	4.41299900	-2.47063400	2.38566800
N	2.58567800	-0.97378500	1.96073400
C	4.25481500	-2.29184300	3.74943000
H	5.13475300	-3.18010400	2.01044400
C	2.44390300	-0.82560400	3.28742100
C	3.26207500	-1.43556000	4.21864800
H	4.89303700	-2.83516500	4.43897300
H	1.62397000	-0.18976700	3.58865800
H	3.09883600	-1.26521300	5.27659600
O	-2.52732900	0.91717500	-1.22899000
C	-3.77457100	1.59016700	-1.27107700
H	-4.30941300	1.38508700	-2.20723700
H	-4.35178800	1.20434900	-0.42962200
H	-3.65686200	2.67269900	-1.15325700

TS2S-OMe

Zero-point correction= 1.001892 (Hartree/Particle)

Thermal correction to Energy= 1.061264
Thermal correction to Enthalpy= 1.062208
Thermal correction to Gibbs Free Energy= 0.912223
Sum of electronic and zero-point Energies= -3703.753432
Sum of electronic and thermal Energies= -3703.694059
Sum of electronic and thermal Enthalpies= -3703.693115
Sum of electronic and thermal Free Energies= -3703.843100
Imaginary frequency= -1109.77 cm^{-1}

C	4.48554200	-6.36429700	-0.15993600
C	3.27967100	-5.75776800	-0.42437700
C	3.18455700	-4.34841000	-0.38371300
C	4.34154000	-3.57087100	-0.07203800
C	5.56579900	-4.22179000	0.20069100
C	5.63031200	-5.59496800	0.15495100
H	4.56485500	-7.44681300	-0.19071800
H	2.38913800	-6.33138500	-0.66519200
H	6.43387800	-3.61396600	0.43959700
H	6.56907600	-6.10054300	0.36167800
C	3.11306700	-1.64752900	-0.28636800
C	1.95434600	-2.42351300	-0.59171000
N	4.27909800	-2.21368200	-0.04154300
N	1.99467700	-3.74209500	-0.63810100
P	2.95831300	0.18756900	-0.36963200
P	0.32767100	-1.61158200	-0.94224200
C	3.76390100	0.41603800	-2.00398600
H	4.81029600	0.09995400	-1.95805500
H	3.71756700	1.45839300	-2.32639400
H	3.26321900	-0.19684500	-2.75827500
C	-0.69825800	-2.55537500	0.24945500
H	-0.41060500	-3.60708700	0.17428400
H	-1.76501700	-2.46665100	0.03089900
H	-0.50131800	-2.20887900	1.26162700
C	-0.16449200	-2.41701700	-2.61327800
C	1.07461300	-2.55140800	-3.50456200
C	-1.23449700	-1.55196000	-3.28271900
C	-0.75921300	-3.81371100	-2.41953600
H	1.67761500	-3.41526900	-3.21138900
H	1.73984500	-1.68224400	-3.48112500
H	0.76475000	-2.70204300	-4.54492500
H	-2.12433900	-1.44398400	-2.65163300
H	-1.55569500	-2.04260200	-4.20909400
H	-0.88403600	-0.55162300	-3.54700000
H	-0.96037700	-4.23591400	-3.41185700
H	-1.70876200	-3.79038800	-1.87679200

H	-0.07188100	-4.48739900	-1.90244400
C	4.22962000	0.99288000	0.78411800
C	5.61571200	0.34557800	0.78928900
C	3.68368800	0.97743500	2.20678500
C	4.38728800	2.43246800	0.27554700
H	6.03421400	0.20874300	-0.21205500
H	5.61976400	-0.62355700	1.28937400
H	6.29186800	1.01591800	1.33524000
H	2.69090700	1.42891800	2.27817400
H	4.35713500	1.54094800	2.86366600
H	3.62312800	-0.04413100	2.59506600
H	4.91660000	3.02016900	1.03444900
H	3.43499300	2.93226000	0.08309800
H	4.98329600	2.46822400	-0.64151900
Co	0.58994400	0.74698800	-0.52592000
C	1.47363900	-0.54373900	4.50791300
C	1.03923900	-0.56432400	3.18037000
C	0.13732700	0.40627300	2.69831500
C	-0.31131300	1.37694000	3.60962500
C	0.11528800	1.40634900	4.93314300
C	1.01481700	0.44245600	5.37740400
H	2.17721100	-1.28835300	4.86425700
H	-1.01289800	2.12661900	3.24931100
H	-0.25382700	2.17259300	5.60824000
H	1.36459500	0.44846600	6.40594800
C	-0.39250200	0.41831400	1.32112400
C	-1.70694600	0.23781400	1.08732500
C	-2.83990000	-0.09599600	2.01928600
H	-2.76611400	-1.09487900	2.46381900
H	-2.91571900	0.61233500	2.85179400
N	-4.07128000	0.02361600	1.18421500
C	-3.69382000	0.80829000	-0.02056600
H	-3.75515300	1.87235500	0.23794100
H	-4.39103100	0.61648900	-0.84052700
C	-2.25214700	0.37735800	-0.29231600
C	-1.31459200	1.20286700	-1.11856800
H	-2.31773200	-0.63303900	-0.72125800
H	-1.44385900	2.27805900	-0.93112500
H	-1.40944900	1.02482500	-2.19224400
S	-4.81025600	-1.45915200	0.81927700
O	-4.88587700	-2.18000500	2.09036900
O	-4.20042200	-2.12456000	-0.34357500
C	-6.42472900	-0.91328900	0.33299200
C	-7.30219500	-0.43774100	1.30910300

C	-6.80335500	-0.98245000	-1.00433600
C	-8.57058100	-0.02653100	0.92903000
H	-6.99233700	-0.39664800	2.34928000
C	-8.07892200	-0.56063500	-1.36731400
H	-6.10710900	-1.36477800	-1.74434900
C	-8.97954600	-0.07818700	-0.41269800
H	-9.26227700	0.34229700	1.68266700
H	-8.38229000	-0.60868800	-2.41021000
C	-10.34782000	0.37949700	-0.80414600
H	-10.53766600	0.22333000	-1.86863600
H	-10.48419600	1.44543000	-0.59151900
H	-11.12272100	-0.14996800	-0.24041100
C	1.37169700	4.78273300	-0.44674800
C	1.46036400	4.68544800	0.96505000
C	1.83777500	5.79940200	1.72547500
C	2.14337700	6.98244600	1.07122100
C	2.09239300	7.05487300	-0.32789100
C	1.71705900	5.96411400	-1.10649900
C	0.89071700	2.62283300	0.18248500
C	1.16133900	3.33859700	1.32500400
H	1.89875300	5.72387300	2.80759200
H	2.43642900	7.85816700	1.64271600
H	2.35475200	7.98353300	-0.82658700
H	1.71950200	6.06150400	-2.18384100
H	0.00504800	1.72071300	0.59994400
H	1.12647500	2.94695900	2.33163900
N	0.97220200	3.52030600	-0.91376400
C	0.94916800	3.03360300	-2.21137900
C	0.85290700	3.84004800	-3.34961900
N	1.00417800	1.68466500	-2.29562300
C	0.89250700	3.24306500	-4.59829200
H	0.70567100	4.90632200	-3.25744100
C	1.04441100	1.12879000	-3.51779000
C	1.01753800	1.85934500	-4.69168100
H	0.81731800	3.85673100	-5.49027100
H	1.10895700	0.04894600	-3.53394700
H	1.06749900	1.34934200	-5.64668700
O	1.45150800	-1.49939700	2.27777000
C	2.17961200	-2.61158000	2.78338100
H	2.21455900	-3.34623600	1.97755300
H	3.20226400	-2.33376200	3.06944100
H	1.67129100	-3.06137000	3.64287300