Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Mechanism and Stereoselectivity in NHC-Catalyzed β-Functionalization of Saturated Carboxylic Ester

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Fig. S1 Scan for different C4−Ha distance of process of **IM2 → IM3**.

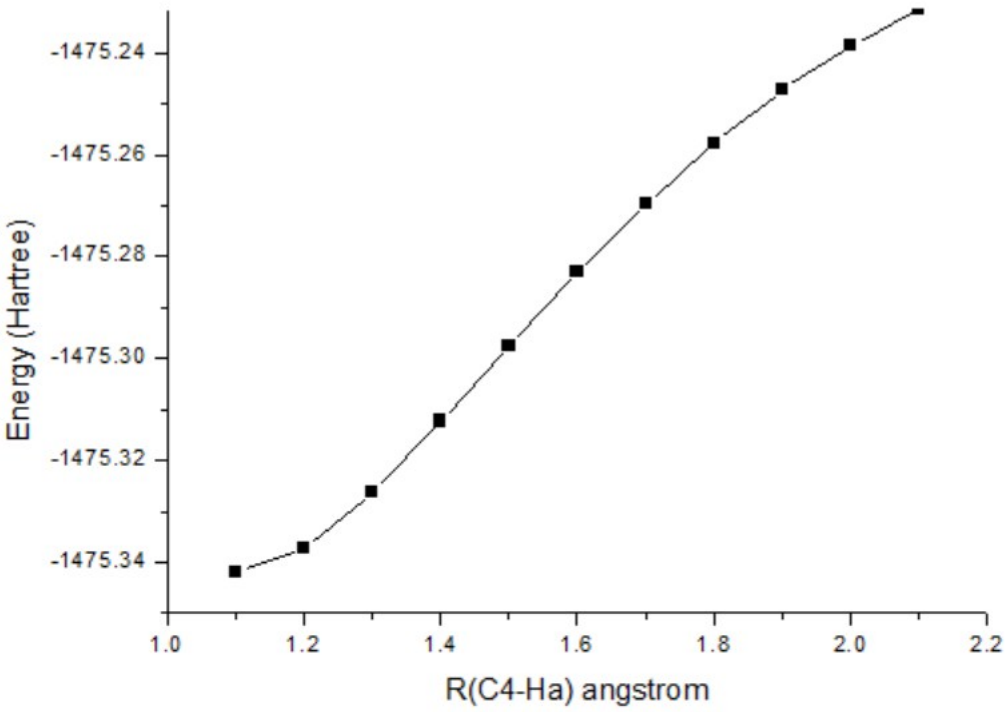

Fig. S2 Free energy profile for the C−C bond formation step. The solvation-corrected relative free energies at SMD(THF)/M06-2X/6-311++G(d,p) level are given in kcal/mol.

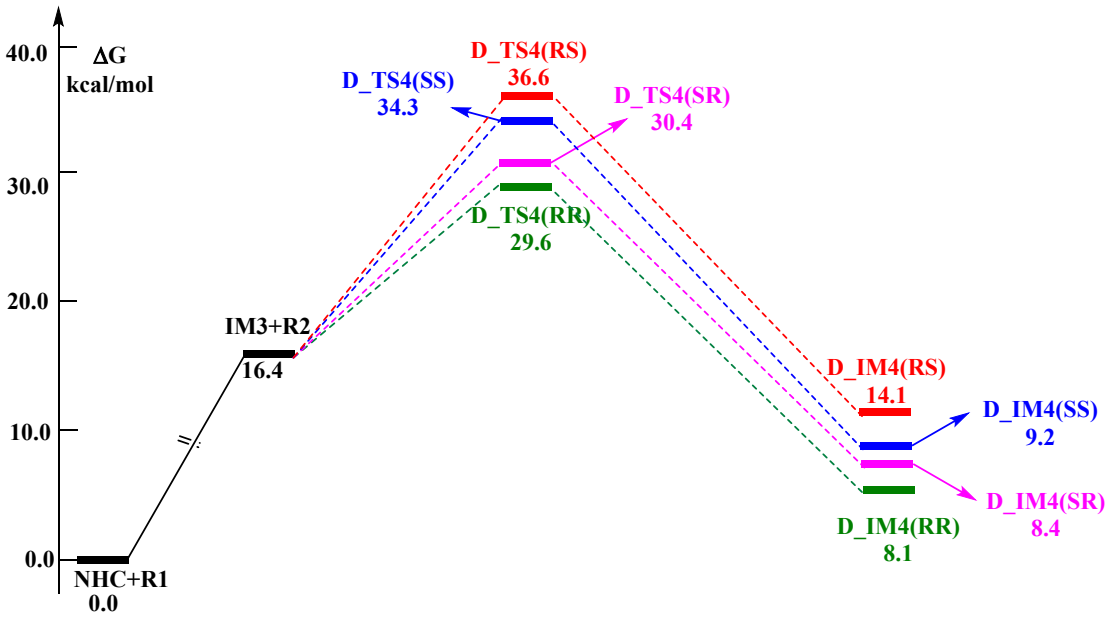

Fig. S3 Comparison between non and HOBt assisted transition states involved in the C－C bond formation step.

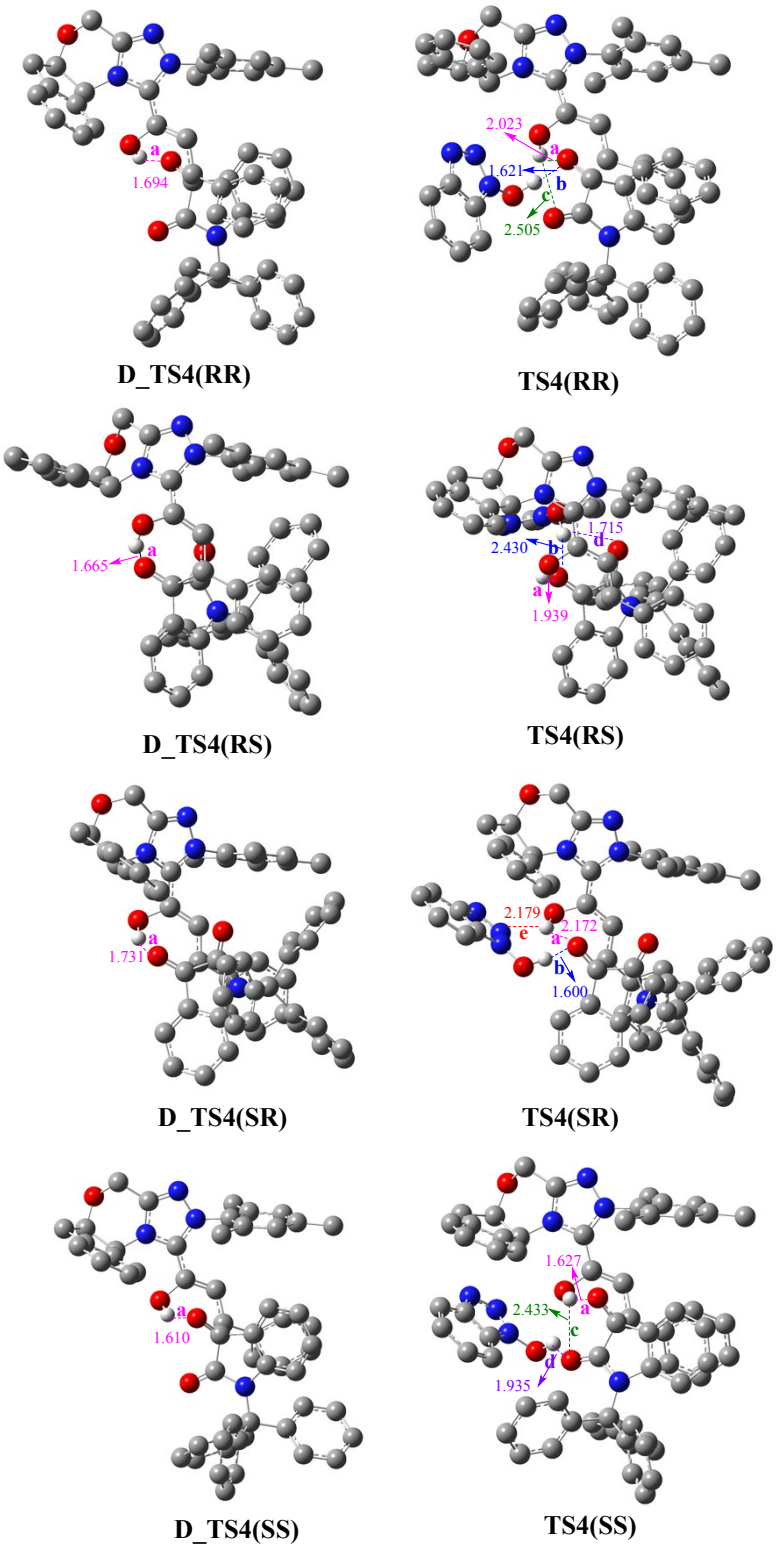

Fig. S4 Free energy profile of the *RR*-, *RS*- and *SS*-configurational pathways (steps IV−VI) obtained at SMD(THF)/M06-2X/6-311++G(d,p) level (kcal/mol).

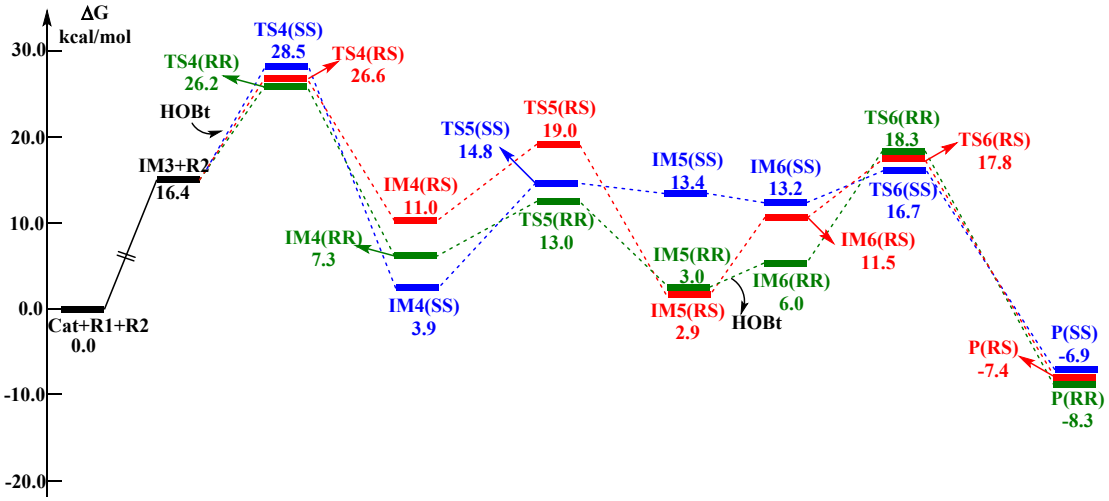

Table S1. Single point energies (a.u.), Gibbs free energies (a.u.) and Relative Gibbs Free Energies (kcal/mol) of the optimized structures at the SMD(THF)/M06-2X/6-311++G(d,p) level.

species	Esol	Gsol	ΔG (kcal/mol)
R+R2+NHC	-3191.493292	-3190.6082672	0.0
TS1-1	-3191.493684	-3190.5791041	18.3
TS1	-3191.496492	-3190.5833369	15.6
IM01-1	-3191.507428	-3190.5928141	9.7
IM01	-3191.513423	-3190.5982538	6.3
IM1	-3191.47376	-3190.5866506	13.6
B_TS2	-3191.484489	-3190.5745353	21.2
TS2	-3191.4955411	-3190.5828221	16.0
IM2	-3191.4786827	-3190.5879987	12.7
A-TS3	-3191.4738308	-3190.5682068	25.1
B-TS3	-3191.4548083	-3190.5448993	39.8
D_TS3	-3191.4236972	-3190.5384162	43.8
TS3	-3191.4498691	-3190.5440621	40.3
IM3	-3191.4695368	-3190.5820558	16.4
D_TS4(RR)	-3191.4803504	-3190.5610704	29.6
D_TS4(RS)	-3191.4707391	-3190.5498671	36.6
D_TS4(SR)	-3191.4809894	-3190.5598574	30.4
D_TS4(SS)	-3191.4747198	-3190.5536568	34.3
TS4(RR)	-3191.5091539	-3190.5665569	26.2

TS4(RS)	-3191.5086063	-3190.5659103	26.6
TS4(SR)	-3191.513926	-3190.5695127	24.3
TS4(SS)	-3191.5052965	-3190.5628455	28.5
IM4(RR)	-3191.5450410	-3190.5965850	7.3
IM4(RS)	-3191.5369255	-3190.5906995	11.0
IM4(SR)	-3191.5463082	-3190.6014312	4.3
IM4(SS)	-3191.5497800	-3190.6021220	3.9
TS5(RR)	-3191.5279227	-3190.5875197	13.0
TS5(RS)	-3191.5225848	-3190.5780668	19.0
TS5(SR)	-3191.5284772	-3190.5851732	14.5
TS5(SS)	-3191.5251831	-3190.5846401	14.8
IM5(RR)	-3191.5507886	-3190.6035066	3.0
IM5(RS)	-3191.5517740	-3190.6036230	2.9
IM5(SR)	-3191.5363459	-3190.5883439	12.5
IM5(SS)	-3191.5352298	-3190.5869168	13.4
TS6(RR)	-3191.5012640	-3190.5790330	18.3
TS6(RS)	-3191.5037868	-3190.5799748	17.8
TS6(SR)	-3191.5065049	-3190.5807479	17.3
TS6(SS)	-3191.5024355	-3190.5816955	16.7
IM6(RR)	-3191.5441895	-3190.5986835	6.0
IM6(RS)	-3191.5153270	-3190.5898870	11.5
IM6(SR)	-3191.5165551	-3190.5902621	11.3
IM6(SS)	-3191.5117108	-3190.5872108	13.2

P(RR)	-3191.5164718	-3190.6214948	-8.3
P(RS)	-3191.5165987	-3190.6200547	-7.4
P(SS)	-3191.5134398	-3190.6191858	-6.9
P(SR)	-3191.5194118	-3190.6246568	-10.3

The energies and Cartesian coordinates of all the optimized structures involved in the reaction.

NHC

NImag = 0

Sum of electronic and zero-point Energies= -1051.496568

Sum of electronic and thermal Energies= -1051.475492

Sum of electronic and thermal Enthalpies= -1051.474548

Sum of electronic and thermal Free Energies= -1051.548600

C	4.51439800	2.66120900	-0.22157900
C	4.98511900	1.38524700	0.07915100
C	4.17083900	0.28720100	-0.18670000
C	2.42975300	1.74663200	-1.04432200
C	3.24540200	2.84289600	-0.77852500
H	5.13755400	3.52583800	-0.01374300
H	5.96874400	1.25134800	0.52110000
H	1.43458500	1.86603700	-1.46630400
H	2.89389700	3.84567100	-1.00067300
C	2.91175600	0.47683600	-0.74711300
C	2.18582700	-0.83602900	-0.94201200
C	3.09167900	-1.89209600	-0.20695900
H	2.07490300	-1.08022700	-2.00202500
C	4.44430100	-1.17792200	0.04587700
H	3.22035500	-2.77691700	-0.83257800
H	4.79542800	-1.39983300	1.05934900

H	5.20820800	-1.54979100	-0.64662200
N	0.85224400	-0.79650700	-0.37663000
O	2.51959700	-2.39975100	0.98718600
C	0.65709500	-0.97928500	0.96628200
C	1.82260300	-1.44747100	1.77233300
H	2.47415900	-0.60433000	2.04845400
H	1.49199900	-1.95186200	2.68087600
N	-0.58060600	-0.77229700	1.28384000
C	-0.30772200	-0.41923000	-1.00184200
N	-1.14029900	-0.42411000	0.06556400
C	-2.53053200	-0.09109400	0.02291900
C	-2.96499900	1.06087500	0.68545700
C	-3.40699900	-0.92388800	-0.67610300
C	-4.32252300	1.36905500	0.63520700
C	-4.75590100	-0.57016300	-0.70469600
C	-5.23128900	0.56870100	-0.05752100
H	-4.67748600	2.26307000	1.14431200
H	-5.45325100	-1.20778000	-1.24397300
C	-1.98973000	1.94306200	1.41912200
H	-1.62147500	1.45318900	2.32535500
H	-1.11637600	2.16098200	0.79456800
H	-2.46182400	2.88798100	1.69860700
C	-2.91123500	-2.16116800	-1.37626200
H	-2.25681100	-1.89719900	-2.21187000
H	-2.32473900	-2.78705200	-0.69558700

H	-3.75049100	-2.75038400	-1.75354600
C	-6.68892500	0.94768400	-0.12707600
H	-6.85718200	1.71107900	-0.89495900
H	-7.31155300	0.08441700	-0.37632200
H	-7.03829200	1.35785700	0.82484700

R1

NImag=0

Sum of electronic and zero-point Energies= -893.421777

Sum of electronic and thermal Energies= -893.405712

Sum of electronic and thermal Enthalpies= -893.404768

Sum of electronic and thermal Free Energies= -893.470010

C	3.08653400	0.19245500	-0.34652000
C	4.17496200	-0.61551400	0.00556500
C	5.41654000	-0.03455000	0.30620400
C	5.50183000	1.34050400	0.24175600
C	4.38572400	2.13829100	-0.11419900
C	3.15699700	1.58866600	-0.41853100
H	6.26305700	-0.65541700	0.57802000
H	6.44239500	1.83164500	0.46773600
H	4.50438600	3.21663500	-0.14863900
H	2.30049600	2.19305300	-0.69426000
N	3.77490500	-1.93675100	-0.00838900
N	2.53656600	-1.98535000	-0.34111800
N	2.11781200	-0.73265100	-0.56946100

O	0.82169200	-0.50704700	-0.90045300
C	-0.00388700	-0.35574200	0.22058000
O	0.42096400	-0.34633400	1.33221800
C	-1.42724600	-0.21111000	-0.23945600
C	-2.38473600	-0.01775700	0.93827700
H	-1.68742900	-1.10337100	-0.82101800
H	-1.48189000	0.63066300	-0.94000000
H	-2.28189600	-0.86635500	1.62232200
H	-2.08825100	0.87394900	1.49977800
C	-3.81041500	0.10764000	0.45889400
C	-4.36997600	1.36006300	0.20044000
C	-4.57905000	-1.03340600	0.21902200
C	-5.67033800	1.47238700	-0.28420500
H	-3.78274000	2.25596900	0.39013100
C	-5.87886800	-0.92641900	-0.26611100
H	-4.15435700	-2.01462700	0.42070700
C	-6.42788200	0.32833600	-0.51917000
H	-6.09368600	2.45433100	-0.47296800
H	-6.46470400	-1.82324000	-0.44368800
H	-7.44275700	0.41401100	-0.89473900

R2

NImag=0

Sum of electronic and zero-point Energies= -1244.612344

Sum of electronic and thermal Energies= -1244.589679

Sum of electronic and thermal Enthalpies= -1244.588735

Sum of electronic and thermal Free Energies= -1244.664736

C	1.91342200	0.19130300	-0.46421000
C	2.92482300	-0.57987100	-1.05796900
C	4.25100100	-0.17532800	-1.08145700
C	4.58445500	1.03471000	-0.48179700
C	3.58505000	1.79371700	0.12792200
C	2.24658300	1.39400900	0.15095600
C	0.82689500	-1.73088100	-1.08502100
C	2.31175800	-1.82094700	-1.53604300
H	4.99435700	-0.81187800	-1.55191600
H	5.61119000	1.38386200	-0.47771100
H	3.84809700	2.73296200	0.60533100
H	1.50475200	2.02063900	0.62518800
O	2.78412100	-2.76175500	-2.11899000
O	0.04014100	-2.63995400	-1.12451900
N	0.63935600	-0.43143300	-0.60233400
C	-0.56832700	0.02060900	0.14048500
C	-0.29068600	-0.30016200	1.62040100
C	0.03879000	0.66162300	2.57491200
C	-0.25126600	-1.65201500	1.99377800
C	0.38320400	0.28743600	3.87445500
H	0.02657400	1.71601500	2.32018700
C	0.09199500	-2.02373000	3.28689200
H	-0.49536800	-2.41402100	1.25809200

C	0.40912100	-1.05279100	4.23606400
H	0.63402400	1.05459500	4.60077100
H	0.11201800	-3.07591200	3.55369900
H	0.67668800	-1.34217700	5.24759900
C	-1.83454100	-0.67855600	-0.40150300
C	-2.03879200	-0.75278800	-1.78242100
C	-2.85784000	-1.08411800	0.45097100
C	-3.22126100	-1.26033900	-2.29802500
H	-1.25828500	-0.41435200	-2.45874300
C	-4.05271300	-1.58519800	-0.06759000
H	-2.73180700	-1.01648200	1.52657900
C	-4.23719000	-1.68147800	-1.43979000
H	-3.35321900	-1.32594300	-3.37357500
H	-4.83698900	-1.90229800	0.61307300
H	-5.16460200	-2.07676900	-1.84220000
C	-0.86021800	1.50150700	-0.16670000
C	-1.77223100	2.20128600	0.62951800
C	-0.36679000	2.12225800	-1.31566900
C	-2.13925500	3.50503800	0.31434300
H	-2.21158000	1.71430800	1.49571900
C	-0.73626300	3.42672400	-1.63374900
H	0.31303700	1.58696200	-1.97090500
C	-1.61617700	4.12744600	-0.81628100
H	-2.84454100	4.03113000	0.95035500
H	-0.33320700	3.89130300	-2.52837400

H	-1.90202100	5.14497600	-1.06357500

HOBt

NImag=0

Sum of electronic and zero-point Energies= -470.724339

Sum of electronic and thermal Energies= -470.717245

Sum of electronic and thermal Enthalpies= -470.716301

Sum of electronic and thermal Free Energies= -470.755973

C	0.15400600	-0.39754300	-0.00460700
C	-0.29936400	0.92780300	0.00061300
C	-1.67705700	1.20214800	0.00968000
C	-2.53459100	0.12267200	0.01004500
C	-2.05217500	-1.21125000	0.00037900
C	-0.70434600	-1.50501100	-0.00741300
H	-2.03405800	2.22618900	0.01510700
H	-3.60671800	0.28870300	0.01591100
H	-2.76972000	-2.02576300	-0.00272700
H	-0.32538300	-2.52025600	-0.02082300
N	0.79069300	1.77208400	-0.00063000
N	1.85948500	1.05625800	-0.01651600
N	1.50166400	-0.23360400	-0.00510300
O	2.43553000	-1.21640900	-0.08604200
H	2.86989800	-1.23368900	0.78442300

OBt^-

NImag=0

Sum of electronic and zero-point Energies= -470.189965

Sum of electronic and thermal Energies= -470.183479

Sum of electronic and thermal Enthalpies= -470.182535

Sum of electronic and thermal Free Energies= -470.221080

C	-0.19861700	0.39237300	0.00000800
C	0.22475800	-0.95222500	-0.00002100
C	1.61131700	-1.22857700	-0.00000700
C	2.48590500	-0.16287200	-0.00000200
C	2.02915500	1.18694700	-0.00000200
C	0.68146400	1.48043800	0.00000800
H	1.96743100	-2.25558700	-0.00000100
H	3.55750900	-0.35015000	0.00000500
H	2.76050100	1.99140800	-0.00000600
H	0.29035300	2.49316700	0.00001200
N	-0.86572200	-1.75128900	-0.00001800
N	-1.93650600	-0.95705800	0.00000900
N	-1.56236000	0.32110400	0.00009000
O	-2.37844600	1.31692100	-0.00006000

HCO_3^-

NImag=0

Sum of electronic and zero-point Energies= -264.302157

Sum of electronic and thermal Energies= -264.298691

Sum of electronic and thermal Enthalpies= -264.297747

Sum of electronic and thermal Free Energies= -264.327892

H	1.70577200	-0.19230600	0.00002300
C	-0.15172900	0.07432200	-0.00000200
O	-1.24932900	-0.49122900	-0.00001400
O	0.18025000	1.27922700	0.00000100
O	0.96965400	-0.81970100	0.00001100

H_2CO_3

NImag=0

Sum of electronic and zero-point Energies= -264.835367

Sum of electronic and thermal Energies= -264.831386

Sum of electronic and thermal Enthalpies= -264.830442

Sum of electronic and thermal Free Energies= -264.861465

C	0.16924700	-0.00001900	0.00000200
O	1.35723800	-0.00035200	0.00001500
O	-0.55960100	1.14136800	0.03326100
H	-1.45721500	1.00603400	-0.30202900
O	-0.56021400	-1.14107700	-0.03331600
H	-1.45764900	-1.00542500	0.30233700

TS1

NImag= (-90.4830)

Sum of electronic and zero-point Energies= -1944.939745

Sum of electronic and thermal Energies= -1944.902246

Sum of electronic and thermal Enthalpies= -1944.901302

Sum of electronic and thermal Free Energies= -1945.013385

C	2.00599700	3.00133100	-0.73862300
C	3.13578400	2.73326200	-1.52225100
C	4.32211500	3.46383600	-1.32803600
C	4.30989200	4.43231200	-0.34898400
C	3.15435800	4.68182600	0.43868500
C	1.98338300	3.97660700	0.26830300
H	5.19843200	3.26303200	-1.93481200
H	5.20238500	5.02119300	-0.16482700
H	3.20224000	5.44882600	1.20503500
H	1.10342500	4.13735400	0.87919300
N	2.83496000	1.71782300	-2.40400800
N	1.61186800	1.35867400	-2.20881200
N	1.10222700	2.11284100	-1.22778700
O	-0.17633500	1.92021100	-0.84536200
C	-0.26732000	1.19669000	0.40443000
O	0.59718800	1.33350500	1.23698200
C	-1.73096700	0.93695900	0.65307300
C	-2.42524800	2.16640900	1.26152300
H	-1.80313400	0.08903300	1.34079000
H	-2.22143700	0.65720100	-0.28207700
H	-1.94454900	2.42592500	2.21034700
H	-2.30127400	3.02015000	0.58500300
C	-3.89217600	1.87612000	1.46931000
C	-4.75798200	1.82272700	0.37247700

C	-4.40173600	1.59655700	2.73768000
C	-6.10291900	1.51194400	0.54235600
H	-4.37084000	2.02909400	-0.62339000
C	-5.74670100	1.27696600	2.91179400
H	-3.73718900	1.63183200	3.59765600
C	-6.60169500	1.23514300	1.81449800
H	-6.76481300	1.48865200	-0.31854500
H	-6.12674900	1.06554800	3.90678700
H	-7.65189000	0.99435700	1.94871600
C	4.02091000	-2.14806700	3.80398100
C	4.85689600	-2.11484800	2.68954200
C	4.35183000	-1.63450100	1.48454200
C	2.19352500	-1.21424900	2.51776900
C	2.70088500	-1.69818900	3.72130300
H	4.40037600	-2.52599700	4.74856200
H	5.88369400	-2.46297700	2.76045300
H	1.17700600	-0.83732200	2.43858600
H	2.06832000	-1.72355500	4.60312100
C	3.03196500	-1.19798400	1.40923700
C	2.69395000	-0.73217900	0.01014400
C	3.90892500	-1.20959400	-0.86167000
H	2.58505600	0.35431000	-0.02403700
C	5.04576600	-1.47313200	0.15355300
H	4.16675600	-0.44215700	-1.59293900
H	5.62473700	-2.34965600	-0.15371200

H	5.73401700	-0.61992100	0.18033900
N	1.45316300	-1.31981000	-0.47205800
O	3.63145600	-2.36220900	-1.64677800
C	1.42711400	-2.61278600	-0.92326200
C	2.74251900	-3.30240700	-1.07379100
H	3.10840300	-3.66989600	-0.10399700
H	2.66008500	-4.14035400	-1.76646700
N	0.22313500	-2.96992400	-1.25125100
C	0.20236200	-0.79670700	-0.50035200
N	-0.50674400	-1.83385600	-0.97439300
C	-1.92590300	-1.80711300	-1.15969200
C	-2.73275900	-2.39194400	-0.18002500
C	-2.44401300	-1.10094600	-2.24568700
C	-4.11083300	-2.23842100	-0.30110500
C	-3.83225400	-0.97533100	-2.32570000
C	-4.67626600	-1.53032400	-1.36407800
H	-4.75936300	-2.66676000	0.45989100
H	-4.26172900	-0.42238700	-3.15830200
C	-2.11162600	-3.12454200	0.97928500
H	-1.56682300	-4.00926900	0.63566500
H	-1.38795500	-2.48781100	1.50226900
H	-2.87534100	-3.43861000	1.69392200
C	-1.52874800	-0.45739500	-3.25337400
H	-0.98370500	0.38352200	-2.80997600
H	-0.77685300	-1.16708300	-3.61184500

H	-2.09849700	-0.09043900	-4.11013000
C	-6.17300100	-1.39243700	-1.47201100
H	-6.44791000	-0.57570700	-2.14521600
H	-6.62176900	-2.31225700	-1.86312800
H	-6.61802600	-1.19373000	-0.49257100

TS1-1

NImag=1 (-139.7419)

Sum of electronic and zero-point Energies= -1944.935105

Sum of electronic and thermal Energies= -1944.897826

Sum of electronic and thermal Enthalpies= -1944.896882

Sum of electronic and thermal Free Energies= -1945.007735

C	2.03597000	1.73195700	-2.33733600
C	3.10580900	2.33412900	-1.66131900
C	4.35185500	2.48045500	-2.29817900
C	4.45887600	2.00734000	-3.58741100
C	3.36279100	1.39224500	-4.24896700
C	2.13453600	1.23673100	-3.64485500
H	5.18228700	2.94999900	-1.78150500
H	5.40186400	2.09846400	-4.11643600
H	3.50450400	1.02546700	-5.26057700
H	1.29841300	0.74391600	-4.12549900
N	2.69264000	2.68313000	-0.39427000
N	1.45550300	2.33987300	-0.26733300
N	1.04828900	1.77749700	-1.40636700

O	-0.23467400	1.38232600	-1.51933700
C	-0.37255300	-0.05487800	-1.41531600
O	0.53824900	-0.76915700	-1.79539500
C	-1.84150400	-0.33552000	-1.64431200
C	-2.17816900	-1.80139900	-1.37308600
H	-2.03367400	-0.09978700	-2.69945100
H	-2.44650300	0.34729000	-1.04440900
H	-1.52393500	-2.42109200	-1.99763200
H	-1.94100200	-2.04194500	-0.32863300
C	-3.62874200	-2.11604300	-1.65215100
C	-4.51816400	-2.41185100	-0.61768200
C	-4.11523000	-2.09779600	-2.96321600
C	-5.86068900	-2.67603400	-0.88145400
H	-4.15323500	-2.44246100	0.40637100
C	-5.45392000	-2.36133500	-3.23223900
H	-3.43245500	-1.88063500	-3.78192600
C	-6.33297100	-2.64954000	-2.18981000
H	-6.53580900	-2.90580500	-0.06262100
H	-5.81203600	-2.34555700	-4.25721400
H	-7.37806400	-2.85622700	-2.39828100
C	5.37232000	-1.67837300	0.58392800
C	4.80172700	-2.85343900	1.06989500
C	3.41585700	-2.98507800	1.05108900
C	3.18781200	-0.78106900	0.05768100
C	4.57287900	-0.64805000	0.08202900

H	6.45165700	-1.56074300	0.59952800
H	5.42865400	-3.64894100	1.46327500
H	2.55088100	0.00649100	-0.33034300
H	5.02826900	0.26324500	-0.29347900
C	2.62817500	-1.95433500	0.54765400
C	1.15803000	-2.29682400	0.63191500
C	1.11376600	-3.59212900	1.52106300
H	0.73397300	-2.47138200	-0.35816500
C	2.56097900	-4.14204400	1.50717900
H	0.40451500	-4.31100000	1.10735100
H	2.82232400	-4.51968500	2.50112700
H	2.64022600	-4.98434400	0.81003300
N	0.39505500	-1.21487900	1.25119900
O	0.64244200	-3.36672600	2.84155600
C	0.41143500	-1.05708800	2.61187500
C	1.04633200	-2.13879000	3.42015300
H	2.14084000	-2.03532300	3.42801800
H	0.67632500	-2.11872400	4.44545300
N	-0.24914400	-0.00006800	2.96800200
C	-0.29307800	-0.18879600	0.68535100
N	-0.66568200	0.51937500	1.76471300
C	-1.41627000	1.74117600	1.75439000
C	-0.75303600	2.92895700	2.08890000
C	-2.77992600	1.70230200	1.44982100
C	-1.48473900	4.11158700	2.01865200

C	-3.46374500	2.91745700	1.38709400
C	-2.83073200	4.12925700	1.65011600
H	-0.98556500	5.04758400	2.26031400
H	-4.52338100	2.90885000	1.13992500
C	0.67038500	2.94596600	2.58146200
H	0.68223100	2.90142100	3.67626400
H	1.25010000	2.10648500	2.19969500
H	1.17093500	3.86415800	2.26481800
C	-3.54553700	0.41211800	1.28653300
H	-4.23392100	0.45907600	0.43711400
H	-2.88840300	-0.44710600	1.14146000
H	-4.14476600	0.22311000	2.18423200
C	-3.57662000	5.43390400	1.53502600
H	-4.65557100	5.28458500	1.62724100
H	-3.26036700	6.14034000	2.30759600
H	-3.38752200	5.90322200	0.56332400

IM01

NImag=0

Sum of electronic and zero-point Energies= -1944.953492

Sum of electronic and thermal Energies= -1944.915739

Sum of electronic and thermal Enthalpies= -1944.914795

Sum of electronic and thermal Free Energies= -1945.026344

C	1.56537900	2.79095300	-1.19670800
C	2.78795300	2.64413000	-1.86616000

C	3.79958500	3.61271900	-1.71203000
C	3.52632300	4.67958600	-0.88674500
C	2.28215700	4.80076000	-0.20709200
C	1.28106900	3.86615100	-0.34071800
H	4.74643400	3.50966900	-2.23145400
H	4.27643800	5.44992100	-0.73929600
H	2.12714500	5.65403200	0.44562500
H	0.34212200	3.92009400	0.19676200
N	2.75535700	1.47980900	-2.59485900
N	1.59876800	0.92358100	-2.41401600
N	0.87116900	1.69596500	-1.59850200
O	-0.36191800	1.33499900	-1.23869800
C	-0.30535200	0.57089700	0.23198900
O	0.49874600	1.11499700	1.03209100
C	-1.80491900	0.59699200	0.54288000
C	-2.22287900	1.98353400	1.03731600
H	-2.00891300	-0.14374200	1.32717300
H	-2.40015200	0.32124000	-0.33145200
H	-1.59367800	2.26033200	1.88780400
H	-2.02937300	2.70665600	0.23675200
C	-3.68373800	1.99804700	1.41651300
C	-4.67190300	1.90853900	0.42984400
C	-4.08332100	2.05157900	2.75251900
C	-6.02040700	1.87814400	0.76946100
H	-4.37480500	1.86588800	-0.61623100

C	-5.43282600	2.02041300	3.09876800
H	-3.32576400	2.12161900	3.52939800
C	-6.40592400	1.93327500	2.10808400
H	-6.77346200	1.81825900	-0.01128600
H	-5.72304200	2.06735000	4.14427700
H	-7.45809200	1.91275300	2.37512500
C	4.07162400	-1.68920200	4.07661600
C	4.91029900	-1.68005300	2.96477100
C	4.40209500	-1.24844500	1.74209300
C	2.23545300	-0.81957900	2.75632600
C	2.74636900	-1.25772600	3.97506200
H	4.45380200	-2.02840700	5.03470000
H	5.94323800	-2.00589900	3.05028100
H	1.22224900	-0.44020000	2.65746100
H	2.11319000	-1.25615300	4.85682400
C	3.07594200	-0.83584200	1.64726000
C	2.73333300	-0.42640400	0.23253400
C	3.99424400	-0.83641300	-0.62004200
H	2.51965500	0.64005800	0.16212600
C	5.10922800	-1.11551700	0.41716100
H	4.24625600	-0.02685300	-1.30390000
H	5.67181200	-2.00898300	0.12603700
H	5.82048200	-0.28232800	0.44105200
N	1.53514500	-1.14408600	-0.23851800
O	3.78417300	-1.95065900	-1.47469600

C	1.63655200	-2.41376800	-0.73127500
C	3.00498100	-2.97999200	-0.91144300
H	3.41391300	-3.33111000	0.04767500
H	2.97694400	-3.81024500	-1.61758400
N	0.47606900	-2.89024100	-1.07246200
C	0.23366600	-0.80407800	-0.27080200
N	-0.38604600	-1.87364800	-0.77680300
C	-1.79371700	-2.03776400	-1.01588900
C	-2.56687100	-2.60323000	0.00015900
C	-2.31576400	-1.59218400	-2.22956000
C	-3.94203800	-2.65502800	-0.20216500
C	-3.70089700	-1.66892300	-2.38240700
C	-4.52574000	-2.17091600	-1.37593000
H	-4.57502200	-3.07085500	0.57809200
H	-4.14403100	-1.31733400	-3.31100500
C	-1.92549400	-3.12127700	1.26049100
H	-1.22377000	-3.93085200	1.03488000
H	-1.36023600	-2.33704700	1.77754900
H	-2.68245400	-3.50139500	1.94922100
C	-1.42269000	-1.03045100	-3.30239100
H	-0.99738200	-0.07085100	-2.99111300
H	-0.58456800	-1.70354400	-3.50854100
H	-1.98478800	-0.88344600	-4.22700100
C	-6.02406100	-2.17169400	-1.53356300
H	-6.31456000	-2.08341500	-2.58323100

H	-6.46575400	-3.08663200	-1.12910500
H	-6.46134900	-1.32632200	-0.99063100

IM01-1

NImag=0

Sum of electronic and zero-point Energies= -1944.945089

Sum of electronic and thermal Energies= -1944.907476

Sum of electronic and thermal Enthalpies= -1944.906532

Sum of electronic and thermal Free Energies= -1945.018621

C	1.09868600	3.36585000	-0.78551300
C	2.41670700	3.74795400	-0.50379800
C	3.06036200	4.70963900	-1.30408500
C	2.34193400	5.23989500	-2.35252100
C	1.00582500	4.83713900	-2.62046400
C	0.35697700	3.89883000	-1.84894200
H	4.08042500	5.01082800	-1.09120000
H	2.80058500	5.98332300	-2.99644700
H	0.48582700	5.28423600	-3.46197700
H	-0.66089800	3.58143100	-2.04273700
N	2.85621600	3.04118900	0.58968500
N	1.89087700	2.27152200	0.97743000
N	0.83069100	2.46538900	0.19146100
O	-0.28174000	1.74424900	0.34379800
C	-0.18881300	0.41924100	-0.58984200
O	0.76627900	0.45023400	-1.41214800

C	-1.61738700	0.36224700	-1.14042300
C	-1.79215000	-0.88766200	-2.00880800
H	-1.72743400	1.26191500	-1.75383400
H	-2.36316800	0.41845200	-0.34102200
H	-1.01377900	-0.85436300	-2.78065600
H	-1.60462500	-1.79120900	-1.41007200
C	-3.15755700	-0.99455700	-2.64560600
C	-3.99101300	-2.08684100	-2.39599500
C	-3.61618700	0.00520200	-3.51026500
C	-5.25109700	-2.17880600	-2.98445600
H	-3.64415100	-2.87966500	-1.73641100
C	-4.87191900	-0.08189600	-4.10071700
H	-2.97602100	0.85667500	-3.72835700
C	-5.69651600	-1.17462100	-3.83744000
H	-5.88193000	-3.03797400	-2.77682100
H	-5.20803100	0.70340000	-4.77114000
H	-6.67708500	-1.24268500	-4.29810400
C	5.90028800	-1.02976700	-0.05075900
C	5.50703100	-2.33388700	-0.34701800
C	4.15582900	-2.59638900	-0.55710500
C	3.61341200	-0.25386100	-0.20681400
C	4.96248500	0.00427500	0.01563800
H	6.95021600	-0.81506800	0.12476100
H	6.24244700	-3.13121900	-0.41027800
H	2.87171900	0.53464200	-0.18766900

H	5.27423300	1.01965400	0.23940700
C	3.22884500	-1.56201600	-0.47111700
C	1.82458900	-2.05858300	-0.71837500
C	1.96877600	-3.62768400	-0.78967900
H	1.39928100	-1.63208700	-1.62628300
C	3.48748000	-3.89741300	-0.92319700
H	1.41114100	-4.01168200	-1.64488000
H	3.76910000	-4.73801900	-0.27978900
H	3.73272500	-4.18611900	-1.95140900
N	0.91377000	-1.68205800	0.38123100
O	1.40825300	-4.31567900	0.31984000
C	0.86515200	-2.42046600	1.53059800
C	1.64710700	-3.68988000	1.56492300
H	2.71641800	-3.49565000	1.72805600
H	1.27123200	-4.34460300	2.35119600
N	-0.00846500	-1.94567400	2.36672600
C	0.03645900	-0.66838800	0.51817500
N	-0.51567900	-0.85272400	1.72164600
C	-1.59364700	-0.12617800	2.34693800
C	-1.26822900	0.86810900	3.27734800
C	-2.90497400	-0.51160400	2.07136900
C	-2.32351100	1.54437900	3.87750800
C	-3.92745800	0.20321800	2.70109200
C	-3.65708600	1.23944700	3.58842200
H	-2.09913600	2.32763000	4.59776600

H	-4.95934200	-0.07158300	2.49411200
C	0.16155800	1.15039200	3.63950000
H	0.62653200	0.26062800	4.07859800
H	0.74917900	1.43590000	2.76264700
H	0.21724900	1.95984500	4.37047400
C	-3.25186200	-1.65803600	1.15571400
H	-2.38134600	-2.26957100	0.90375100
H	-3.98586000	-2.30935000	1.63885400
H	-3.69732800	-1.29910600	0.22131000
C	-4.77224800	2.02050600	4.23394700
H	-5.73088600	1.50661700	4.12923100
H	-4.57975900	2.17573200	5.29944800
H	-4.86880800	3.00836500	3.77091600

IM1

NImag=0

Sum of electronic and zero-point Energies= -1474.592053

Sum of electronic and thermal Energies= -1474.561474

Sum of electronic and thermal Enthalpies= -1474.560530

Sum of electronic and thermal Free Energies= -1474.658233

C	-0.10125900	1.15840700	-0.11237800
O	0.55275900	2.14548200	0.12781500
C	-1.60054700	1.12943100	-0.21777100
C	-2.22294500	2.52814300	-0.18320400
H	-2.00110200	0.52039400	0.60400500

H	-1.88494600	0.59009800	-1.13254200
H	-1.92043700	3.03205400	0.74025600
H	-1.83271600	3.12607900	-1.01274600
C	-3.72720900	2.41652700	-0.26627900
C	-4.39100700	2.59037800	-1.48092600
C	-4.47006300	2.07895200	0.86799700
C	-5.77276800	2.43443600	-1.56218700
H	-3.82400700	2.86196600	-2.36836400
C	-5.85011400	1.92088500	0.79064600
H	-3.96371100	1.95390800	1.82340000
C	-6.50450400	2.09788300	-0.42694200
H	-6.27787600	2.58321800	-2.51125600
H	-6.41719900	1.67242600	1.68238100
H	-7.58189900	1.98322700	-0.48766900
C	5.61318700	1.13322700	2.49181600
C	6.08919600	0.95480500	1.19572000
C	5.17596600	0.88616300	0.14652600
C	3.32798100	1.18673000	1.69732600
C	4.24315900	1.24968700	2.74325900
H	6.31466100	1.18494000	3.31808600
H	7.15502300	0.86836700	1.00726100
H	2.26291300	1.29421900	1.88399600
H	3.89313500	1.39644700	3.75954200
C	3.81294400	1.00040300	0.40611400
C	3.01108100	0.88909800	-0.87042400

C	4.06202000	0.47023200	-1.97098900
H	2.49733700	1.81431900	-1.13082000
C	5.44560100	0.71742600	-1.32677200
H	3.91576700	1.07075700	-2.86876000
H	6.11667600	-0.11624700	-1.55832400
H	5.90310800	1.61942700	-1.74660800
N	1.97893700	-0.16146900	-0.73087400
O	3.89993500	-0.86353000	-2.42175900
C	2.30204600	-1.48118300	-0.86764400
C	3.66151400	-1.80498200	-1.39886000
H	4.41527600	-1.75710500	-0.60055100
H	3.66645200	-2.80048300	-1.84294300
N	1.27979500	-2.24977000	-0.60203900
C	0.68639100	-0.11654900	-0.36376500
N	0.28556800	-1.38668100	-0.28756200
C	-1.00249200	-1.86924500	0.14560000
C	-1.29437700	-1.80939300	1.50963700
C	-1.89208900	-2.33335900	-0.82565500
C	-2.57221200	-2.20880100	1.89555000
C	-3.15461200	-2.71819100	-0.38339100
C	-3.51656700	-2.64964300	0.96502700
H	-2.83643500	-2.17546600	2.94937200
H	-3.87770900	-3.07645200	-1.11142100
C	-0.29128600	-1.29822500	2.51254100
H	0.71385100	-1.68517400	2.31695400

H	-0.23666400	-0.20115000	2.50573100
H	-0.57691500	-1.59865200	3.52208500
C	-1.49939400	-2.40462300	-2.27766500
H	-1.12535200	-1.44135700	-2.64457700
H	-0.70716600	-3.14359900	-2.43291500
H	-2.35537100	-2.68665000	-2.89245600
C	-4.90874200	-3.02100600	1.39991600
H	-5.30426600	-3.84508800	0.80143400
H	-4.93312900	-3.31405500	2.45174100
H	-5.58233400	-2.16622300	1.27363400

TS2

NImag=1 (-975.9149)

Sum of electronic and zero-point Energies= -1944.936977

Sum of electronic and thermal Energies= -1944.900622

Sum of electronic and thermal Enthalpies= -1944.899678

Sum of electronic and thermal Free Energies= -1945.006171

C	0.24108900	0.50453600	-0.63373200
O	-0.65957900	0.28423000	-1.44965100
C	1.40817700	1.30634900	-0.83399000
C	1.80871600	1.43957900	-2.30055900
H	2.24904500	1.06573400	-0.18716000
H	1.06983200	2.52725000	-0.30766000
H	0.93577600	1.72416200	-2.89513100
H	2.56020200	2.22858200	-2.40683100
C	2.36341400	0.11561400	-2.77724200

C	3.68639400	-0.23967100	-2.49194400
C	1.53853500	-0.82917000	-3.39760200
C	4.17438300	-1.50288800	-2.81389500
H	4.33528900	0.48301700	-2.00038900
C	2.02296300	-2.09742300	-3.71412200
H	0.50784000	-0.56495300	-3.61630000
C	3.34154600	-2.43983800	-3.42337600
H	5.20752700	-1.75622400	-2.59085500
H	1.36770500	-2.81785500	-4.19634200
H	3.71956900	-3.42615900	-3.67547200
C	-3.01258300	-4.70860500	-1.21492300
C	-3.95001500	-4.11678600	-0.37136700
C	-3.69897200	-2.83976500	0.12402700
C	-1.59013600	-2.75337900	-1.08166200
C	-1.84213300	-4.03264700	-1.56887500
H	-3.19381900	-5.70624000	-1.60342800
H	-4.85920900	-4.64670200	-0.10109600
H	-0.69496500	-2.20722100	-1.36901100
H	-1.12568400	-4.50560100	-2.23351100
C	-2.52762000	-2.17590100	-0.23069700
C	-2.45892000	-0.81533300	0.42457100
C	-3.64534500	-0.80142500	1.45146000
H	-2.54565400	-0.00035600	-0.29021700
C	-4.55126800	-1.98582800	1.03148000
H	-4.14711300	0.16382100	1.39832900

H	-4.90909100	-2.51375300	1.92186100
H	-5.43589300	-1.61783200	0.49931300
N	-1.17237100	-0.65429400	1.11762200
O	-3.24334500	-0.90207200	2.80973500
C	-0.97922700	-1.20396400	2.34971000
C	-2.16761300	-1.77900300	3.04642100
H	-2.37361500	-2.79639900	2.68056900
H	-1.99044000	-1.81479900	4.12185900
N	0.25356900	-1.07184900	2.74591500
C	0.00612800	-0.13966700	0.72442100
N	0.85660800	-0.41550400	1.71527700
C	2.28139900	-0.21844800	1.74820100
C	3.07386400	-1.11484900	1.02902400
C	2.78338100	0.87071500	2.46044500
C	4.44961900	-0.89446900	1.04778700
C	4.16660400	1.03897100	2.45163500
C	5.00939600	0.17285600	1.75208700
H	5.09520100	-1.56826700	0.48882700
H	4.59493500	1.87840300	2.99449100
C	2.45937200	-2.21355800	0.20332600
H	1.67747200	-2.74729100	0.75448900
H	2.01501800	-1.80072400	-0.71408900
H	3.21968200	-2.93302400	-0.10758400
C	1.85796300	1.84755300	3.13316100
H	1.30537000	2.42773100	2.38267200

H	1.12201600	1.33582600	3.76034600
H	2.42522700	2.54209300	3.75644500
C	6.49755400	0.41131400	1.72820800
H	6.75914700	1.13867400	0.95154900
H	6.85031700	0.80962100	2.68325600
H	7.04445900	-0.51112100	1.51718100
C	-1.60734900	3.58473000	-0.64306500
C	-2.74643700	2.89821700	-0.20308700
C	-3.95356000	3.01063500	-0.92015700
C	-3.94510100	3.79838300	-2.04971200
C	-2.77357100	4.47880100	-2.48171700
C	-1.58552600	4.39000900	-1.79115100
H	-4.84897100	2.49512100	-0.58688100
H	-4.85477000	3.90849900	-2.63170100
H	-2.82298900	5.08401000	-3.38146700
H	-0.68041300	4.90117700	-2.09880500
N	-2.42049800	2.18859700	0.92314400
N	-1.16141000	2.40968900	1.18175600
N	-0.66565500	3.24967200	0.27455500
O	0.62524400	3.55318700	0.23946000

B_TS2

NImag=1 (-881.3271)

Sum of electronic and zero-point Energies= -1739.044147

Sum of electronic and thermal Energies= -1739.010260

Sum of electronic and thermal Enthalpies= -1739.009316

Sum of electronic and thermal Free Energies= -1739.111704

C	-0.08321300	0.16995000	-1.32755200
O	0.71397800	0.41697900	-2.22806100
C	-1.29763300	0.86582000	-1.02375400
C	-1.33980800	2.29577100	-1.55565800
H	-1.61446500	0.79679300	0.01784800
H	-2.30243400	0.29513100	-1.58161100
H	-1.06735600	2.30379000	-2.61480300
H	-2.37290100	2.64278000	-1.45930700
C	-0.40328500	3.17516400	-0.76315600
C	-0.73039500	3.51535000	0.55613200
C	0.82259200	3.60164600	-1.27838200
C	0.14211300	4.26435900	1.33780700
H	-1.68781800	3.18675300	0.95800800
C	1.69888900	4.35727300	-0.49859700
H	1.09099600	3.32971700	-2.29579200
C	1.36141500	4.69137600	0.81033200
H	-0.13147000	4.52748400	2.35571100
H	2.64752900	4.68421400	-0.91583300
H	2.03857400	5.28883100	1.41471700
C	5.12702000	1.50547300	1.32113500
C	5.63911700	0.31062500	0.82204100
C	4.82279200	-0.49157500	0.02872800
C	3.00235000	1.10641900	0.22901300

C	3.82127800	1.90351600	1.02427000
H	5.75174200	2.13755700	1.94480500
H	6.65764100	0.00884400	1.04994100
H	1.99353500	1.43444500	-0.01394600
H	3.43397900	2.84312500	1.40483400
C	3.51885900	-0.09349100	-0.25378300
C	2.80915100	-1.11881600	-1.10867300
C	3.82107400	-2.32133100	-1.22351200
H	2.52281200	-0.73045100	-2.08324200
C	5.15724400	-1.80178900	-0.63709800
H	3.92529000	-2.60467700	-2.27114600
H	5.57549000	-2.54622700	0.04951900
H	5.89334600	-1.66044700	-1.43563100
N	1.56292600	-1.55360600	-0.44599900
O	3.37930900	-3.51153300	-0.59278300
C	1.57648600	-2.52958200	0.50666000
C	2.83511800	-3.30986200	0.69189300
H	3.52978200	-2.76980500	1.35265600
H	2.61508000	-4.28576700	1.12575300
N	0.41259000	-2.65778000	1.07510700
C	0.32166200	-1.02223600	-0.45088200
N	-0.35376800	-1.70813100	0.47373900
C	-1.72798700	-1.53825500	0.87307300
C	-1.97256500	-0.72591200	1.98746000
C	-2.72578800	-2.12343000	0.10344000

C	-3.29963700	-0.46637800	2.29379500
C	-4.04462600	-1.84332600	0.46693100
C	-4.34410600	-0.98868300	1.52146800
H	-3.52979100	0.19541900	3.12543800
H	-4.84769000	-2.23160900	-0.15361600
C	-0.83648200	-0.09028600	2.74534100
H	-0.11604300	-0.83613100	3.09615800
H	-0.29539300	0.62661100	2.11198200
H	-1.21472600	0.45587600	3.61186900
C	-2.42350100	-2.93054200	-1.12837200
H	-2.42684500	-2.26359300	-1.99821200
H	-1.46205300	-3.44821200	-1.06359100
H	-3.20331300	-3.67836900	-1.28939200
C	-5.75823500	-0.54451400	1.77377200
H	-5.86362000	0.47751900	1.39118700
H	-6.47659800	-1.18522100	1.25642500
H	-5.99822900	-0.53617500	2.84110400
H	-6.23966600	0.48190300	-1.00994200
C	-4.40128800	0.46127500	-1.34702000
O	-3.50913400	-0.10690700	-2.05968700
O	-4.27137000	1.37385300	-0.52846700
O	-5.65144600	-0.07333300	-1.54387000

IM2

NImag=0

Sum of electronic and zero-point Energies= -1474.174900

Sum of electronic and thermal Energies= -1474.145065

Sum of electronic and thermal Enthalpies= -1474.144121

Sum of electronic and thermal Free Energies= -1474.237710

C	-0.16684300	0.24412500	-1.20253400
O	0.36955000	0.01146500	-2.33563200
C	-0.53993900	1.40340500	-0.58866900
C	-0.32988900	2.72596400	-1.25690400
H	-1.00021800	1.37067600	0.39587200
H	0.13365500	2.52504000	-2.23183100
H	-1.29188400	3.21445600	-1.47153200
C	0.53506300	3.71081100	-0.48847200
C	0.46135200	5.07836600	-0.77020500
C	1.44184100	3.28573200	0.48376900
C	1.27675600	5.99301500	-0.11210200
H	-0.24605800	5.42731300	-1.51973700
C	2.26400900	4.19698200	1.14397600
H	1.50084000	2.22579500	0.71560300
C	2.18586200	5.55477600	0.84921300
H	1.20192100	7.05094500	-0.34760900
H	2.96636600	3.83973900	1.89295600
H	2.82325400	6.26691100	1.36498100
C	4.73803300	0.45246500	0.85270700
C	4.58600400	-0.88595900	1.21309900
C	3.60818100	-1.64044900	0.57717400

C	2.95392300	0.26782500	-0.78190500
C	3.93415400	1.02138700	-0.13540800
H	5.49868400	1.05562600	1.33985900
H	5.22518000	-1.33117800	1.97061100
H	2.32148700	0.68514600	-1.56180700
H	4.06468300	2.06561200	-0.40302200
C	2.79714800	-1.06263600	-0.40459000
C	1.84470000	-2.09222900	-0.96954600
C	2.50015900	-3.42543700	-0.52302000
H	1.68859600	-1.99431200	-2.04400100
C	3.26241500	-3.09434300	0.77784200
H	3.22501800	-3.69459300	-1.29518600
H	2.62409900	-3.21828100	1.66222200
H	4.13273200	-3.74197800	0.91390800
N	0.49531500	-2.03410800	-0.36003400
O	1.60771300	-4.52026300	-0.46630400
C	-0.12111200	-3.06933000	0.28780200
C	0.57190400	-4.38354600	0.47653500
H	0.94095800	-4.47482300	1.50672900
H	-0.13732000	-5.19396200	0.29823500
N	-1.32840200	-2.75293300	0.65462900
C	-0.38550600	-1.01305300	-0.40987200
N	-1.47674100	-1.46590700	0.21117100
C	-2.75411900	-0.81351400	0.29084600
C	-3.18783200	-0.34812000	1.53230500

C	-3.49634900	-0.68356900	-0.88440900
C	-4.42908700	0.28081300	1.57895200
C	-4.72977900	-0.04205800	-0.78302500
C	-5.21003700	0.44288200	0.43345600
H	-4.79128300	0.66059100	2.53167100
H	-5.33052000	0.07996200	-1.68124600
C	-2.32877900	-0.51009900	2.75801900
H	-2.17406700	-1.56793700	2.99283500
H	-1.34088200	-0.06040900	2.60607000
H	-2.79366700	-0.02740300	3.62008700
C	-2.98672900	-1.21682400	-2.19851300
H	-2.09016600	-0.68588300	-2.54039200
H	-2.72650300	-2.27804900	-2.11047900
H	-3.75578200	-1.12049700	-2.96791000
C	-6.55889500	1.10986500	0.52004200
H	-6.53178500	1.96902100	1.19621200
H	-6.89378100	1.45692900	-0.46048900
H	-7.31253700	0.41307500	0.90316000

A_TS3

NImag=1 (-1251.4118)

Sum of electronic and zero-point Energies= -1944.914588

Sum of electronic and thermal Energies= -1944.877128

Sum of electronic and thermal Enthalpies= -1944.876184

Sum of electronic and thermal Free Energies= -1944.986401

C	-0.44932100	0.03868600	-0.17327600

O	-0.52094700	-1.32496300	-0.02249400
C	0.73692900	0.72291300	-0.06626900
C	1.98947200	0.07567700	0.16400500
H	0.73392800	1.78475600	-0.28273700
H	1.91850900	-0.76909800	0.86205300
H	0.18846700	-1.74089400	-0.57165400
C	3.23471900	0.86886600	0.31020900
C	3.38009200	2.16971500	-0.19328200
C	4.34717500	0.28294100	0.93170400
C	4.58156700	2.86010500	-0.06188300
H	2.55367800	2.65419800	-0.70849000
C	5.54913800	0.96972100	1.05778700
H	4.26455700	-0.73402600	1.30983100
C	5.67402700	2.26715400	0.56623500
H	4.66692300	3.86542600	-0.46623800
H	6.39248800	0.48485700	1.54086300
H	6.61182300	2.80524000	0.66289100
C	-4.96497000	-2.99565900	2.76493000
C	-5.60660400	-3.07164700	1.53155500
C	-4.97880700	-2.53015400	0.41281000
C	-3.07499800	-1.85835300	1.76394600
C	-3.70736500	-2.39774600	2.88051200
H	-5.44369600	-3.41209200	3.64581200
H	-6.58008100	-3.54588300	1.44432700
H	-2.08345600	-1.42015800	1.83447100

H	-3.21535200	-2.36241500	3.84712800
C	-3.73137800	-1.92564700	0.53844000
C	-3.24489400	-1.39374600	-0.79117700
C	-4.46344900	-1.59431800	-1.77155100
H	-2.36330800	-1.92433500	-1.14358500
C	-5.45275400	-2.51691800	-1.01824900
H	-4.11539200	-2.04861600	-2.69955300
H	-6.47446600	-2.14094300	-1.13953400
H	-5.43145000	-3.52572700	-1.44469500
N	-2.88931400	0.03018900	-0.69230900
O	-5.07438100	-0.38511000	-2.19070600
C	-3.86007100	0.99565200	-0.76638200
C	-5.23308000	0.56231000	-1.15636000
H	-5.77076800	0.13917100	-0.29512400
H	-5.79656000	1.40730400	-1.55244600
N	-3.38701800	2.18373700	-0.57166300
C	-1.71380900	0.66059400	-0.40230600
N	-2.05382700	1.97179000	-0.32821800
C	-1.19455700	3.06714900	0.00272500
C	-0.86996800	3.26989300	1.34618600
C	-0.64913400	3.82082700	-1.03805900
C	0.07746300	4.24914000	1.63308700
C	0.28827800	4.79519600	-0.69942300
C	0.68058800	5.00356700	0.62458800
H	0.36622500	4.41459700	2.66824800

H	0.73999400	5.38876300	-1.49075700
C	-1.47684800	2.41094200	2.42244700
H	-2.56023700	2.32129400	2.29601100
H	-1.05106000	1.40055300	2.39070100
H	-1.27595400	2.83090800	3.40999500
C	-1.02466300	3.53421000	-2.46734400
H	-0.71335600	2.52267300	-2.75423700
H	-2.10739100	3.59770000	-2.61151900
H	-0.54040500	4.24137600	-3.14357100
C	1.76960700	5.98857800	0.95915700
H	1.57186700	6.49370800	1.90830300
H	2.72798300	5.46561100	1.05558500
H	1.87661100	6.74668600	0.17943600
C	3.71199900	-2.87407900	-0.82195400
C	3.81425000	-3.93082900	0.09689100
C	5.08461200	-4.37735000	0.50917500
C	6.18360000	-3.73012400	-0.01226800
C	6.05363900	-2.65434000	-0.93298300
C	4.82320600	-2.20608800	-1.36007300
H	5.17845400	-5.19485400	1.21613000
H	7.17983100	-4.04173100	0.28557700
H	6.95275100	-2.17228800	-1.30405300
H	4.70427600	-1.37819400	-2.05005700
N	2.55239400	-4.32509000	0.45703000
N	1.70650400	-3.56914700	-0.17673000

N	2.37307000	-2.71942000	-0.95805300
O	1.73050900	-1.76269300	-1.63794100
H	1.99830400	-0.71689500	-0.90168900

B_TS3

NImag=1 (-1291.9485)

Sum of electronic and zero-point Energies= -1738.494725

Sum of electronic and thermal Energies= -1738.461301

Sum of electronic and thermal Enthalpies= -1738.460357

Sum of electronic and thermal Free Energies= -1738.560563

C	-0.00975600	0.30719700	-1.30914200
O	0.72359700	1.29958900	-1.72788000
C	-1.38031800	0.36753300	-1.13069400
C	-2.04435200	1.64750400	-1.20651200
H	-1.93994800	-0.50284000	-0.80699700
H	-1.45134000	2.13879300	-0.12563700
H	-1.63470000	2.30414400	-1.97981800
C	-3.51304300	1.70372200	-1.06995500
C	-4.27356100	2.63036100	-1.80090000
C	-4.20807700	0.86961200	-0.17601400
C	-5.65406900	2.71497200	-1.65955700
H	-3.75937800	3.29186300	-2.49427800
C	-5.58907100	0.94816900	-0.03882500
H	-3.64706200	0.16480200	0.43514500
C	-6.32714900	1.86944400	-0.78052600

H	-6.20956200	3.44480800	-2.24398400
H	-6.09505300	0.29179900	0.66594100
H	-7.40594600	1.93269800	-0.66822000
C	4.46825600	2.11946100	2.12951600
C	5.33943000	1.40256500	1.30944000
C	4.81727400	0.71025800	0.22003300
C	2.56991100	1.44003100	0.79548200
C	3.09394000	2.14680100	1.87563600
H	4.86690600	2.67603900	2.97355000
H	6.40787400	1.39330100	1.51278100
H	1.50600600	1.45768300	0.57748600
H	2.42017000	2.74812100	2.47986100
C	3.44732300	0.73530600	-0.02114400
C	3.08796500	-0.05116600	-1.25911700
C	4.42309900	-0.76342600	-1.67845300
H	2.68151500	0.60147900	-2.03060300
C	5.53957700	-0.08700300	-0.83973000
H	4.59319500	-0.63377200	-2.74848700
H	6.21152100	-0.85341400	-0.43517700
H	6.14918100	0.56514800	-1.47623300
N	2.04467600	-1.04061800	-0.96468100
O	4.41078100	-2.17749500	-1.50907100
C	2.36527100	-2.22200300	-0.35912100
C	3.80847200	-2.59602600	-0.30292800
H	4.28808500	-2.12416300	0.56860900

H	3.91967200	-3.67874500	-0.22638600
N	1.32765700	-2.86210700	0.06949400
C	0.68323700	-0.88125000	-0.87458400
N	0.27306200	-2.02926500	-0.25091700
C	-0.98035400	-2.27140300	0.39199300
C	-1.25354800	-1.61093600	1.59407200
C	-1.87829600	-3.15348800	-0.21101300
C	-2.49038500	-1.86483300	2.18932100
C	-3.09902400	-3.37433600	0.42162100
C	-3.42228800	-2.72973300	1.61656800
H	-2.73364900	-1.35608000	3.11988000
H	-3.81777100	-4.05239800	-0.03412300
C	-0.29263100	-0.62037900	2.19069200
H	0.74790300	-0.91403500	2.01645700
H	-0.44250100	0.37986800	1.75417600
H	-0.45122100	-0.54127800	3.26959000
C	-1.52596800	-3.79923900	-1.52409600
H	-1.35865900	-3.03255900	-2.28901500
H	-0.60384800	-4.38327300	-1.44099300
H	-2.33078600	-4.45637600	-1.86273300
C	-4.77391800	-2.93059100	2.25390200
H	-5.49979500	-2.21750000	1.84686100
H	-5.15875800	-3.93728800	2.06568900
H	-4.72930400	-2.77493600	3.33539200
H	0.49936400	2.82155800	-0.91276100

C	0.08358800	3.41092200	0.87799200
O	0.42825300	4.12838400	1.80780800
O	-0.73598700	2.40281400	0.96683100
O	0.59722200	3.64198000	-0.35856100

D_TS3

NImag=1 (-1640.8811)

Sum of electronic and zero-point Energies= -1474.124231

Sum of electronic and thermal Energies= -1474.094831

Sum of electronic and thermal Enthalpies= -1474.093887

Sum of electronic and thermal Free Energies= -1474.187256

C	-0.27669300	-0.00743300	-1.44738300
O	0.45422400	0.56861700	-2.40157200
C	-1.33368000	0.74558500	-0.97562500
C	-1.38296000	2.02794700	-1.64538500
H	-1.86951700	0.50798800	-0.05977100
H	-0.06825800	1.68767900	-2.18648000
H	-1.75980700	2.01437400	-2.67323300
C	-1.76136000	3.21607000	-0.86720600
C	-2.39502900	4.31787200	-1.46373700
C	-1.45093500	3.31501500	0.50095400
C	-2.70958200	5.45629800	-0.73154400
H	-2.64338900	4.27032000	-2.52143400
C	-1.77520000	4.44912700	1.23780900
H	-0.93096600	2.48970900	0.98458300

C	-2.40633100	5.53054200	0.62709200
H	-3.20099000	6.29118600	-1.22369200
H	-1.52479600	4.49200800	2.29478800
H	-2.65439100	6.41911800	1.19919800
C	3.59485500	2.65113300	1.73997000
C	4.49845300	1.62211800	1.48847800
C	4.16126200	0.63859200	0.56182700
C	2.03845700	1.73362600	0.12622600
C	2.37634800	2.70954200	1.05984000
H	3.84530600	3.42240600	2.46228600
H	5.45408500	1.58884700	2.00493000
H	1.10843700	1.81113100	-0.42828300
H	1.68540500	3.52702600	1.24447600
C	2.93685200	0.69080900	-0.10111100
C	2.76294500	-0.48786000	-1.03476800
C	4.11287700	-1.28779500	-0.92144900
H	2.53405200	-0.17530000	-2.05438900
C	4.99182700	-0.53492200	0.11001000
H	4.59045000	-1.29518200	-1.90177800
H	5.27471700	-1.20099400	0.93332900
H	5.92778000	-0.20679100	-0.35360400
N	1.64034000	-1.34053000	-0.61320600
O	3.95002200	-2.66381100	-0.61618000
C	1.77290700	-2.41440900	0.22428300
C	3.15115200	-2.90557900	0.51885800

H	3.54831800	-2.40207600	1.41272100
H	3.14073900	-3.98109900	0.70005700
N	0.62926100	-2.86961400	0.62696400
C	0.30897600	-1.07824800	-0.71433800
N	-0.28613100	-2.03265500	0.03223600
C	-1.68708000	-2.19356000	0.27821600
C	-2.18389600	-1.79321600	1.52299900
C	-2.49263300	-2.72928300	-0.72595500
C	-3.54713800	-1.94809900	1.74972200
C	-3.85456900	-2.85871600	-0.45212800
C	-4.39649300	-2.47544400	0.77270500
H	-3.96074200	-1.63835300	2.70710400
H	-4.50659100	-3.26960800	-1.21917700
C	-1.26530300	-1.19409200	2.55480100
H	-0.54056900	-1.93191600	2.91342800
H	-0.69577000	-0.35725000	2.13160900
H	-1.83531100	-0.82227600	3.40880600
C	-1.91205900	-3.12342000	-2.05654700
H	-1.62835400	-2.23404700	-2.63147200
H	-1.01402100	-3.73661900	-1.93028400
H	-2.63894300	-3.69081000	-2.64161600
C	-5.87296900	-2.60698700	1.04490400
H	-6.38365100	-3.12140800	0.22751400
H	-6.05494400	-3.16697300	1.96745100
H	-6.33454800	-1.62122100	1.16389600

TS3

NImag=1 (-1212.7998)

Sum of electronic and zero-point Energies= -1944.369139

Sum of electronic and thermal Energies= -1944.331557

Sum of electronic and thermal Enthalpies= -1944.330613

Sum of electronic and thermal Free Energies= -1944.443275

C	-0.41567500	0.28836200	1.12030300
O	0.62669500	0.61402400	1.81117700
C	-0.68321000	-0.95843000	0.55452600
C	0.25765300	-2.03390500	0.57380900
H	-1.56308700	-1.06954000	-0.07178200
H	1.10003100	-1.65096100	-0.46518800
H	0.98994800	-1.96689500	1.38389000
C	-0.17147300	-3.41134000	0.24663800
C	0.79907800	-4.41655600	0.07899100
C	-1.51367100	-3.77944300	0.05472200
C	0.44875300	-5.71562300	-0.26110400
H	1.84798200	-4.15267600	0.20339100
C	-1.86432100	-5.07997300	-0.29875900
H	-2.29841500	-3.04171300	0.20834400
C	-0.88939800	-6.06022400	-0.45845400
H	1.22721600	-6.46366500	-0.38769900
H	-2.91417500	-5.33065200	-0.43749300
H	-1.16412800	-7.07519700	-0.73211700
C	2.89181000	3.07993900	-2.58544400

C	2.53096400	4.28936000	-1.99322100
C	1.72388000	4.26788100	-0.85819800
C	1.67247100	1.83867400	-0.90100700
C	2.47127800	1.86367100	-2.04118500
H	3.51806700	3.08445100	-3.47347000
H	2.87834500	5.23308900	-2.40764200
H	1.38256600	0.88846100	-0.46554100
H	2.76057400	0.91564800	-2.48580900
C	1.29284000	3.05240900	-0.33318700
C	0.41731600	3.24454500	0.88266400
C	0.32506300	4.80433700	1.06226600
H	0.82534000	2.72152600	1.74840600
C	1.24395400	5.42821900	-0.02207600
H	0.66805400	5.06788500	2.06376600
H	0.68717100	6.17936500	-0.59610100
H	2.08315400	5.95493400	0.44623300
N	-0.92197200	2.67669700	0.67954800
O	-0.99685100	5.32933400	1.01279400
C	-1.93563200	3.38223300	0.09905800
C	-1.74352900	4.84964100	-0.08347500
H	-1.22786400	5.04873500	-1.03594200
H	-2.70577800	5.36421700	-0.08961900
N	-2.95771900	2.64748000	-0.19559700
C	-1.28999000	1.35161700	0.68763900
N	-2.57011700	1.37958400	0.19556900

C	-3.48325800	0.29754700	0.04705900
C	-3.76454200	-0.15674000	-1.24692400
C	-4.04322400	-0.29046100	1.18411900
C	-4.63998500	-1.22988100	-1.38458200
C	-4.90704900	-1.36914500	0.99633700
C	-5.21330600	-1.85297700	-0.27440600
H	-4.85814200	-1.60697000	-2.38185800
H	-5.34509900	-1.84719700	1.87006200
C	-3.08075300	0.47127400	-2.43153100
H	-3.37673500	1.51833100	-2.54928700
H	-1.99314300	0.45409300	-2.29350200
H	-3.32036200	-0.07204200	-3.34848200
C	-3.67764100	0.19212100	2.55939400
H	-2.65079500	-0.11096500	2.79711400
H	-3.71833500	1.28436500	2.61960600
H	-4.35204100	-0.22781900	3.30972700
C	-6.11176000	-3.05043300	-0.45273800
H	-5.52626500	-3.93515300	-0.72636300
H	-6.65308300	-3.28113900	0.46872400
H	-6.84503500	-2.88368000	-1.24811400
C	3.79294200	-1.42149400	0.19244300
C	4.97127000	-2.17086400	0.04741400
C	5.95873600	-2.12014000	1.05123200
C	5.70712600	-1.32475000	2.14751100
C	4.49836000	-0.58601500	2.27342300

C	3.51364300	-0.61269900	1.30895200
H	6.87582500	-2.69296800	0.95185500
H	6.44368400	-1.26123300	2.94428600
H	4.34192900	0.01210400	3.16680100
H	2.56610300	-0.08016700	1.41481100
N	4.91561800	-2.85395800	-1.13688400
N	3.77845400	-2.56561300	-1.70947000
N	3.10426400	-1.71293900	-0.94255000
O	1.91321600	-1.23582500	-1.31004200

IM3

NImag=0

Sum of electronic and zero-point Energies= -1944.920728

Sum of electronic and thermal Energies= -1944.881780

Sum of electronic and thermal Enthalpies= -1944.880836

Sum of electronic and thermal Free Energies= -1944.998692

C	-0.45509600	-0.24591300	-0.02135700
O	-0.57991800	-1.56184900	0.40635700
C	0.78761700	0.43145400	0.17900100
C	1.88421000	-0.10258600	0.78450400
H	0.86301300	1.43586200	-0.22830500
H	1.81654100	-1.10897500	1.19635000
H	0.06257200	-2.11324100	-0.08463400
C	3.17183900	0.57749900	0.94523500
C	3.36386700	1.94105700	0.65434200

C	4.27933100	-0.15440400	1.40291100
C	4.61329300	2.53020200	0.79431700
H	2.52424100	2.55265900	0.33148600
C	5.52889000	0.43822200	1.54490200
H	4.15467800	-1.21072300	1.63464300
C	5.70607600	1.78440100	1.23738100
H	4.73536400	3.58440900	0.56136400
H	6.36684200	-0.15922300	1.89257800
H	6.68018500	2.25066800	1.34680500
C	-5.35040600	-1.91517000	3.17362100
C	-5.93807000	-2.29096700	1.96839400
C	-5.20043900	-2.16994100	0.79323400
C	-3.29682000	-1.31696300	2.03599000
C	-4.03884200	-1.43433400	3.20829500
H	-5.91570200	-2.00009400	4.09675800
H	-6.95635700	-2.66953600	1.94610400
H	-2.26822100	-0.96748600	2.05098800
H	-3.59325000	-1.15590400	4.15818700
C	-3.89746400	-1.68209500	0.83404000
C	-3.29238600	-1.60035800	-0.55027500
C	-4.47235400	-1.98542300	-1.52240700
H	-2.45880500	-2.29052300	-0.66342800
C	-5.60812100	-2.52355300	-0.61478500
H	-4.13184300	-2.74587400	-2.22606300
H	-6.56411700	-2.08104200	-0.91602100

H	-5.70960500	-3.60808600	-0.73238800
N	-2.79743100	-0.25826300	-0.84624400
O	-4.90793100	-0.92344400	-2.35282400
C	-3.65667700	0.72849500	-1.26457400
C	-5.02815800	0.31016500	-1.67546000
H	-5.68602600	0.22221300	-0.79717300
H	-5.45493500	1.03653200	-2.36748900
N	-3.11830800	1.89630900	-1.29090000
C	-1.59135000	0.35155600	-0.52535100
N	-1.82654400	1.68197300	-0.82815000
C	-1.04489200	2.80422000	-0.43210500
C	-0.93985800	3.12250600	0.92809300
C	-0.37508600	3.52949100	-1.42117700
C	-0.09995200	4.17495500	1.28451200
C	0.44550800	4.58297900	-1.01834200
C	0.60616300	4.90889200	0.32879700
H	0.00688200	4.42877400	2.33720500
H	0.98052700	5.15338300	-1.77425800
C	-1.66992200	2.32073000	1.97148500
H	-2.66541400	2.02596400	1.62467800
H	-1.11686400	1.40281700	2.20457500
H	-1.77841900	2.89779400	2.89282900
C	-0.52442800	3.14558800	-2.86880200
H	-0.20733200	2.10901900	-3.02966400
H	-1.57041200	3.21126200	-3.18317300

H	0.07753400	3.79534800	-3.50790200
C	1.53868900	6.01342400	0.75663300
H	1.05097000	6.69094700	1.46394000
H	2.42238700	5.60103000	1.25630300
H	1.87911200	6.60102400	-0.09945900
C	3.86686800	-2.45831100	-1.03861200
C	3.67173300	-3.56973900	-0.20740300
C	4.77477100	-4.20335200	0.39466000
C	6.02009800	-3.67722400	0.13068100
C	6.19203300	-2.54838700	-0.71563400
C	5.12868300	-1.91605200	-1.32076100
H	4.63246100	-5.06288500	1.04027100
H	6.89886100	-4.13055100	0.57735400
H	7.19548300	-2.16937800	-0.88121200
H	5.24284600	-1.04114000	-1.94961000
N	2.32326500	-3.81877600	-0.10775600
N	1.70396000	-2.94070700	-0.82168100
N	2.60058400	-2.13322900	-1.39300400
O	2.20388800	-1.07504500	-2.13210800
H	1.96371000	-0.39987600	-1.45277300

TS4(RR)

NImag=1 (-169.9454)

Sum of electronic and zero-point Energies= -3189.565657

Sum of electronic and thermal Energies= -3189.504593

Sum of electronic and thermal Enthalpies= -3189.503649

Sum of electronic and thermal Free Energies= -3189.663758

C	2.07407900	0.78976900	-0.50306000
O	1.91045300	-0.56333000	-0.70041900
C	1.09327600	1.67271000	-0.87963000
C	-0.17630200	1.19626800	-1.27601200
H	1.23824100	2.74032100	-0.75919900
H	-0.17259300	0.18133000	-1.67118400
H	1.16814000	-0.83886200	-0.12224500
C	-1.16180400	2.09231000	-1.90315500
C	-1.37724800	3.40744300	-1.45993800
C	-1.92118300	1.63004500	-2.98753300
C	-2.32799000	4.21688800	-2.07014700
H	-0.80598900	3.79092400	-0.61806900
C	-2.85857500	2.44690300	-3.61262500
H	-1.75192100	0.62003000	-3.35360200
C	-3.07359100	3.74307900	-3.14975300
H	-2.48888200	5.22533100	-1.69994200
H	-3.42946200	2.06437300	-4.45401300
H	-3.81048000	4.38134400	-3.62815700
C	7.17122200	-2.33694700	-2.95785700
C	7.25847100	-2.86153100	-1.66849400
C	6.37280900	-2.40977700	-0.69592800
C	5.31515000	-0.92744700	-2.30501500
C	6.20733700	-1.37882300	-3.27640000

H	7.86179300	-2.67699400	-3.72354000
H	8.01172200	-3.60642400	-1.42744100
H	4.55509400	-0.18715000	-2.54419200
H	6.15193200	-0.98508700	-4.28634600
C	5.41694600	-1.44927300	-1.02233600
C	4.56751600	-1.12747100	0.18532700
C	5.36530100	-1.71894000	1.38992100
H	3.59288600	-1.59897800	0.12168300
C	6.23933600	-2.81807800	0.75238700
H	4.67558600	-2.11852900	2.13339500
H	7.19299300	-2.90569000	1.28128700
H	5.71017300	-3.77440300	0.83106500
N	4.36934100	0.31401700	0.35186000
O	6.14678600	-0.75165200	2.09147400
C	5.39523900	1.07455700	0.84583700
C	6.60549200	0.34551500	1.33335100
H	7.23631300	0.03276500	0.48951900
H	7.18481200	0.98981700	1.99566500
N	5.08698900	2.33167200	0.90069800
C	3.34147600	1.15435300	0.05918100
N	3.81057100	2.37835700	0.39925600
C	3.07434900	3.60482300	0.44589900
C	3.14372900	4.46877000	-0.64566800
C	2.26915300	3.83875200	1.56472400
C	2.34215000	5.60971500	-0.61204100

C	1.49361900	4.99578000	1.55400100
C	1.50658600	5.88087200	0.47187400
H	2.36141800	6.29282300	-1.45750200
H	0.85374600	5.20892500	2.40845400
C	4.00550600	4.12799300	-1.83162800
H	5.04146200	3.94970500	-1.52774000
H	3.64238800	3.21541400	-2.31994400
H	3.99085800	4.93494000	-2.56684300
C	2.20954800	2.83879800	2.68812900
H	1.68292600	3.25850000	3.54877300
H	1.67745200	1.93042300	2.36988400
H	3.21470200	2.54773000	3.00944700
C	0.61604300	7.09658700	0.48425600
H	-0.43499400	6.80263700	0.57765100
H	0.85087600	7.74687300	1.33289400
H	0.72541700	7.68045900	-0.43245000
C	-2.95510300	1.27436700	0.80898800
C	-1.65539400	1.66460400	1.16037900
C	-1.41315900	2.84184000	1.84697800
C	-2.48951500	3.66363000	2.17401900
C	-3.78296900	3.27180800	1.83310200
C	-4.03749100	2.07471000	1.15963300
C	-1.63341900	-0.47677900	0.16194800
C	-0.73779600	0.59783500	0.74265700
H	-0.39380400	3.10163000	2.11421000

H	-2.32671300	4.59477800	2.70816200
H	-4.62393000	3.90241500	2.10455200
H	-5.05570200	1.79149100	0.92931300
O	0.31881800	0.24401100	1.36057600
O	-1.22540800	-1.57884300	-0.14999000
N	-2.94043200	0.01457400	0.13422700
C	-4.14876100	-0.85670500	0.09131400
C	-4.50222300	-1.14163000	1.56492700
C	-5.67513100	-0.71529600	2.18404300
C	-3.53303300	-1.79196500	2.34396900
C	-5.88690900	-0.94980400	3.54430100
H	-6.43306700	-0.18699800	1.61561600
C	-3.74191500	-2.02279900	3.69632400
H	-2.60020900	-2.11851500	1.88950300
C	-4.92665600	-1.60500700	4.30326200
H	-6.80733000	-0.60613500	4.00650900
H	-2.97193100	-2.52417100	4.27450400
H	-5.09218800	-1.78312000	5.36130200
C	-3.86197600	-2.14904600	-0.70251800
C	-3.33156400	-2.03829500	-1.99248400
C	-4.24253700	-3.40368200	-0.23676900
C	-3.14373000	-3.16121100	-2.78032500
H	-3.05710300	-1.05389000	-2.36437700
C	-4.06948800	-4.53653400	-1.03814300
H	-4.67520800	-3.51231000	0.75216200

C	-3.51498200	-4.42115800	-2.30489200
H	-2.71110600	-3.05885000	-3.77066400
H	-4.37320200	-5.50828400	-0.65952700
H	-3.37621200	-5.30148900	-2.92556200
C	-5.27458400	-0.19308400	-0.72252400
C	-6.52389400	-0.82248900	-0.78568700
C	-5.05650600	0.93630500	-1.50974600
C	-7.54083200	-0.30818400	-1.58036900
H	-6.69238500	-1.73473300	-0.21905100
C	-6.07420300	1.44762700	-2.31419800
H	-4.09092500	1.42938900	-1.50035200
C	-7.32098200	0.83487600	-2.34802500
H	-8.50336800	-0.80951500	-1.61017300
H	-5.87529500	2.33146300	-2.91367600
H	-8.11364200	1.23445500	-2.97304500
C	0.59349400	-3.87556800	0.79511400
C	1.85612300	-4.35313000	0.41667200
C	1.97090500	-5.42217500	-0.49183600
C	0.80090600	-5.96312800	-0.97256600
C	-0.46950100	-5.45911200	-0.58176300
C	-0.60665100	-4.41109800	0.29971400
H	2.94670100	-5.79060500	-0.78954500
H	0.84044800	-6.78958100	-1.67501400
H	-1.36413300	-5.90422600	-1.00547600
H	-1.57231000	-3.99771000	0.56611300

N	2.81768800	-3.61824000	1.06477800
N	2.22042400	-2.74591100	1.81673100
N	0.90584000	-2.87510400	1.66081000
O	0.05346800	-2.14891900	2.41568000
H	0.12115500	-1.21392900	2.04113900

TS4(RS)

NImag=1 (-82.8859)

Sum of electronic and zero-point Energies= -3189.568738

Sum of electronic and thermal Energies= -3189.507340

Sum of electronic and thermal Enthalpies= -3189.506396

Sum of electronic and thermal Free Energies= -3189.666775

C	2.19706700	-1.30740600	0.81393700
O	2.73308800	-0.98081000	2.05411100
C	0.92509000	-1.85048100	0.69238100
C	0.01797000	-1.95883100	1.73655000
H	0.58603100	-2.09611200	-0.30749200
H	0.38218100	-1.76309300	2.74224600
H	2.20049000	-0.24102400	2.39507000
C	-1.21945900	-2.73123700	1.65556500
C	-1.68192500	-3.32915700	0.46634600
C	-1.96790400	-2.94875400	2.82702600
C	-2.79626100	-4.15919200	0.47262600
H	-1.15586600	-3.16752200	-0.47136800
C	-3.08245100	-3.78108500	2.82928400

H	-1.64496200	-2.47339500	3.75082800
C	-3.49541100	-4.40746100	1.65474000
H	-3.11956200	-4.62086900	-0.45731900
H	-3.62654400	-3.94445000	3.75535700
H	-4.35432400	-5.07184800	1.65591300
C	8.14276200	-0.40452000	2.84425400
C	8.05481600	0.79262700	2.13795400
C	6.88281300	1.08159500	1.44402100
C	5.89547700	-1.01241400	2.17535100
C	7.07116100	-1.30034400	2.86388600
H	9.05354200	-0.64463100	3.38447300
H	8.89010500	1.48733600	2.12404700
H	5.04850500	-1.69167500	2.19590100
H	7.15523800	-2.22733100	3.42248800
C	5.81898200	0.18300600	1.46692300
C	4.66059200	0.69462500	0.63807000
C	5.23229100	1.95695800	-0.11390100
H	3.80810300	0.99863600	1.24576500
C	6.54820700	2.30174400	0.62415300
H	4.50289000	2.76420900	-0.05389700
H	7.32340900	2.56457300	-0.10322700
H	6.40086200	3.17561100	1.26863500
N	4.18076500	-0.31175800	-0.30818500
O	5.44354500	1.77008700	-1.50532100
C	4.75411400	-0.44339900	-1.54360100

C	5.87898200	0.47802000	-1.86978800
H	6.79624800	0.18878100	-1.33582300
H	6.06750900	0.47566200	-2.94346100
N	4.10730100	-1.27090500	-2.30026600
C	3.08314100	-1.12034100	-0.27910100
N	3.08075200	-1.71102900	-1.50214700
C	2.13680300	-2.66510000	-1.99315000
C	2.23580700	-3.98910800	-1.55627100
C	1.10387200	-2.20429900	-2.81182200
C	1.23401900	-4.87056600	-1.95284300
C	0.12853300	-3.12786500	-3.18913600
C	0.17244600	-4.45475900	-2.76076500
H	1.27518300	-5.90285900	-1.61236100
H	-0.70077600	-2.78859300	-3.80381200
C	3.35505700	-4.41635900	-0.64551800
H	4.32226500	-4.06277500	-1.01597100
H	3.21148300	-4.00245900	0.35987800
H	3.39106000	-5.50469500	-0.56288500
C	1.03030200	-0.75637600	-3.21364400
H	0.10267200	-0.56153800	-3.75695100
H	1.04773900	-0.10521200	-2.33222200
H	1.88203800	-0.48298500	-3.84502300
C	-0.90919200	-5.42798500	-3.15400700
H	-1.25736900	-5.99658500	-2.28612000
H	-1.76584000	-4.90764800	-3.59056200

H	-0.54143700	-6.14821100	-3.89281900
C	-2.56539900	0.42577500	2.26778300
C	-1.26201500	0.44906200	2.80335600
C	-1.01848200	0.57415900	4.16414900
C	-2.10222700	0.67494000	5.02891000
C	-3.39335000	0.69967300	4.50187000
C	-3.64694800	0.59267900	3.13221700
C	-1.19088900	0.39749200	0.43427200
C	-0.33059600	0.48236700	1.68475400
H	0.00610300	0.60815200	4.52351700
H	-1.94713900	0.76644500	6.09855600
H	-4.24055700	0.81791500	5.17028800
H	-4.66608600	0.65735100	2.78107500
O	0.83505800	0.91116200	1.64280500
O	-0.74406600	0.47515400	-0.69160300
N	-2.51769500	0.30047000	0.84176400
C	-3.65213900	0.56796600	-0.08847800
C	-4.92426400	-0.06551500	0.52240100
C	-6.16831800	0.56712500	0.52223400
C	-4.82386300	-1.32308000	1.13144600
C	-7.28172000	-0.04663000	1.09727200
H	-6.28518200	1.55970000	0.10748200
C	-5.93233700	-1.93487200	1.70246600
H	-3.85532400	-1.80916000	1.19809600
C	-7.17214700	-1.29975000	1.68649500

H	-8.23547400	0.47215300	1.08898000
H	-5.81324600	-2.90467800	2.17498300
H	-8.03844800	-1.77199900	2.13946200
C	-3.38421700	-0.10684400	-1.47427500
C	-2.86484400	0.63556700	-2.54177100
C	-3.66897400	-1.45401400	-1.70235800
C	-2.66648200	0.06640700	-3.79303100
H	-2.59997600	1.67419400	-2.38745900
C	-3.45809500	-2.03431900	-2.95340400
H	-4.07471100	-2.07576800	-0.91607400
C	-2.96971200	-1.27641200	-4.01017500
H	-2.27149400	0.67737600	-4.60023600
H	-3.70376300	-3.08300500	-3.09745900
H	-2.82830900	-1.72181100	-4.99124700
C	-3.80071600	2.09319300	-0.26927000
C	-4.67990000	2.59524500	-1.24033500
C	-3.07352900	3.01039300	0.48988700
C	-4.84617200	3.96234000	-1.42378800
H	-5.22550500	1.90130000	-1.87424000
C	-3.23595500	4.38347700	0.30577100
H	-2.36340000	2.67606900	1.23751300
C	-4.12626400	4.86578100	-0.64383200
H	-5.53472700	4.32068200	-2.18311000
H	-2.64380600	5.07165600	0.90057300
H	-4.24758000	5.93495300	-0.78908500

C	0.64719900	3.49359400	-1.18508700
C	0.74998700	4.80060600	-0.68970700
C	-0.12064400	5.80282100	-1.15719800
C	-1.05706500	5.43484900	-2.09760200
C	-1.14753800	4.10129900	-2.57956900
C	-0.30117300	3.10470400	-2.14411300
H	-0.04168700	6.81824300	-0.78380000
H	-1.75325100	6.17378600	-2.48165900
H	-1.91497900	3.86467100	-3.31181300
H	-0.36109900	2.07940200	-2.49057000
N	1.77849200	4.85088100	0.22222300
N	2.29555900	3.67096900	0.30663000
N	1.64196700	2.85457500	-0.52147200
O	2.01680300	1.56109300	-0.64022000
H	1.47991300	1.09747500	0.06410800

TS4(SR)

NImag=1 (-61.2181)

Sum of electronic and zero-point Energies= -3189.572202

Sum of electronic and thermal Energies= -3189.511268

Sum of electronic and thermal Enthalpies= -3189.510324

Sum of electronic and thermal Free Energies= -3189.668249

C	-1.34447300	1.55838000	-1.35378900
O	-2.14137900	0.81695800	-2.20591500
C	0.03658600	1.52950800	-1.47109400

C	0.69367000	0.59688200	-2.26928200
H	0.62434900	2.18054000	-0.82988000
H	0.06950100	-0.03337900	-2.89701000
H	-2.15744500	-0.11449100	-1.91451900
C	2.08863400	0.71299000	-2.69548900
C	2.89052800	1.83136300	-2.39645500
C	2.64997800	-0.29271700	-3.50400300
C	4.19122600	1.93077900	-2.87558900
H	2.47898800	2.65019600	-1.80900700
C	3.94691800	-0.18433400	-3.99472400
H	2.04685300	-1.16079100	-3.76096100
C	4.72634600	0.92881400	-3.68573200
H	4.78499600	2.80730200	-2.63191800
H	4.34880300	-0.97562700	-4.62123200
H	5.73495500	1.02182300	-4.07728300
C	-5.17832700	-1.53135100	2.60525700
C	-6.19996900	-0.85840600	1.93627000
C	-5.86088200	0.06323600	0.95141100
C	-3.49400900	-0.36407900	1.30818400
C	-3.83841500	-1.28623400	2.29678200
H	-5.42864600	-2.25724300	3.37328600
H	-7.24099600	-1.05358100	2.17802300
H	-2.45022400	-0.17871400	1.06133900
H	-3.05484000	-1.81855400	2.82735400
C	-4.52208500	0.29215200	0.64008600

C	-4.40434300	1.31276600	-0.47252400
C	-5.82474400	1.96025500	-0.54859900
H	-4.15843900	0.85148800	-1.42652300
C	-6.75947800	0.90276400	0.07781500
H	-6.09048800	2.17556800	-1.58445600
H	-7.57909100	1.38951900	0.61526300
H	-7.19884100	0.28465400	-0.71504200
N	-3.39258000	2.32375200	-0.17383400
O	-5.91582100	3.22070000	0.10629400
C	-3.66651200	3.27604900	0.77153700
C	-5.08297300	3.38763800	1.23483200
H	-5.29233700	2.63889900	2.01197900
H	-5.26817200	4.38342900	1.63906900
N	-2.62418600	3.97247900	1.08398700
C	-2.05393700	2.39191300	-0.45153900
N	-1.61883400	3.42615900	0.31776100
C	-0.32191100	4.02630100	0.36510000
C	0.48908400	3.75423400	1.46760100
C	0.06503700	4.87211400	-0.68055000
C	1.73873700	4.37374200	1.51004600
C	1.32629900	5.45489100	-0.59821400
C	2.17045800	5.22244300	0.49208200
H	2.39292500	4.17258300	2.35447900
H	1.65287100	6.11788000	-1.39673500
C	0.02411400	2.82346200	2.55353200

H	-0.82258200	3.25525500	3.09736600
H	-0.28628200	1.86376500	2.12950500
H	0.83631900	2.62477500	3.25606300
C	-0.84753300	5.11877000	-1.85156000
H	-0.46404900	5.92942200	-2.47468700
H	-0.93369800	4.22017700	-2.47352900
H	-1.85461500	5.38651700	-1.51586100
C	3.52059600	5.89086600	0.55892500
H	4.05606800	5.61185700	1.47045900
H	4.14227000	5.61415900	-0.29980800
H	3.41797100	6.98080600	0.54745500
C	2.26502100	-2.22218700	-0.97098000
C	0.91851300	-2.13618800	-1.37325800
C	0.36977000	-2.97872800	-2.33180800
C	1.18761300	-3.93920900	-2.91662700
C	2.51922300	-4.04288900	-2.51209700
C	3.07423600	-3.20440500	-1.54244200
C	1.36092000	-0.57891800	0.35307900
C	0.27861500	-1.09587300	-0.57985800
H	-0.68009300	-2.88136800	-2.59529600
H	0.79251700	-4.61222700	-3.67000100
H	3.15493800	-4.80170800	-2.95805700
H	4.11071200	-3.33303100	-1.26609400
O	-0.93775200	-0.94799600	-0.32295100
O	1.18628700	0.19108900	1.27182600

N	2.55527200	-1.22775500	0.01043500
C	3.65244400	-1.33709400	1.01798200
C	3.15470300	-2.35959200	2.05125600
C	3.29963500	-3.73393900	1.83046200
C	2.39280100	-1.93863100	3.14792400
C	2.72672000	-4.66088900	2.69671500
H	3.86682000	-4.08882500	0.97658900
C	1.82178800	-2.86667300	4.01384600
H	2.23605000	-0.87822700	3.31225500
C	1.99013300	-4.23087700	3.79583900
H	2.85712300	-5.72182200	2.50688600
H	1.23902100	-2.51734700	4.86073300
H	1.54594400	-4.95338200	4.47367700
C	4.00226200	0.03713000	1.62138100
C	3.87594400	1.19701100	0.85845800
C	4.65686200	0.11126000	2.85134900
C	4.39250700	2.40305500	1.31139400
H	3.38293700	1.15141900	-0.10558800
C	5.15273500	1.32684200	3.31889700
H	4.79173200	-0.78592600	3.44843400
C	5.02826100	2.47878700	2.54918900
H	4.29467000	3.28611400	0.68652700
H	5.65251600	1.36435200	4.28211400
H	5.43197500	3.42274000	2.90460500
C	4.97398600	-1.70277300	0.32074600

C	5.94947800	-2.47315100	0.95228200
C	5.26504500	-1.12494600	-0.91866500
C	7.17624000	-2.70576900	0.33075600
H	5.75772900	-2.89662600	1.93314700
C	6.48392400	-1.36236300	-1.53932700
H	4.52017800	-0.50448900	-1.40960400
C	7.44485400	-2.16091900	-0.91985500
H	7.92152400	-3.31533800	0.83256400
H	6.67816800	-0.91693600	-2.51053700
H	8.39800100	-2.34795500	-1.40473900
C	-4.77184000	-3.10408500	-0.49662100
C	-5.65384700	-2.31842700	-1.25466400
C	-7.04456500	-2.50488800	-1.12561800
C	-7.47175200	-3.46151600	-0.23261700
C	-6.55660700	-4.24394600	0.52534300
C	-5.19416700	-4.08983500	0.40941200
H	-7.73907800	-1.92120400	-1.72104000
H	-8.53499400	-3.63817300	-0.10543700
H	-6.95073300	-4.98657300	1.21187200
H	-4.48161100	-4.67592000	0.97786000
N	-4.92425200	-1.45053400	-2.02249000
N	-3.66514000	-1.68244300	-1.79348200
N	-3.56375300	-2.64870000	-0.89183300
O	-2.36670700	-3.12230500	-0.48810700
H	-1.79532000	-2.29743000	-0.37018500

TS4(SS)

NImag=1 (-294.7256)

Sum of electronic and zero-point Energies= -3189.562121

Sum of electronic and thermal Energies= -3189.501275

Sum of electronic and thermal Enthalpies= -3189.500331

Sum of electronic and thermal Free Energies= -3189.660297

C	1.92468000	1.02636600	0.60830200
O	1.62527900	-0.31343100	0.62396400
C	0.97692300	1.97320600	0.80928000
C	-0.41606400	1.60884500	0.92909400
H	1.24959400	3.02209900	0.78644000
H	-0.54327300	0.71889900	1.54936000
H	1.04289100	-0.39562300	-0.20542100
C	-1.36340800	2.69018000	1.29985400
C	-1.22307200	3.99722400	0.81094900
C	-2.45273700	2.40910500	2.13186200
C	-2.13565300	4.98874400	1.15007700
H	-0.40013000	4.23727900	0.13988500
C	-3.36752600	3.40144300	2.47021700
H	-2.57442800	1.40246000	2.52682900
C	-3.21449700	4.69594300	1.98164700
H	-2.00792600	5.99357700	0.75658500
H	-4.19909200	3.15839500	3.12470800
H	-3.92791900	5.47046300	2.24648700

C	4.50220400	-3.50895700	-2.81525700
C	5.43925000	-3.59725000	-1.78838600
C	5.32409900	-2.74229800	-0.69598300
C	3.34942700	-1.71159800	-1.66898800
C	3.46357900	-2.57767300	-2.75397900
H	4.57815400	-4.17283000	-3.67127400
H	6.24479300	-4.32530700	-1.83679300
H	2.54089200	-0.98549800	-1.62939000
H	2.73599200	-2.52546600	-3.55739300
C	4.29082500	-1.80891500	-0.64782600
C	4.36483400	-0.99684300	0.62656600
C	5.73295800	-1.39887800	1.28203900
H	3.54127800	-1.20917400	1.30080000
C	6.17105100	-2.68665100	0.54930100
H	5.58767700	-1.57432200	2.34809500
H	7.24828700	-2.66227900	0.35265300
H	5.95860300	-3.55110300	1.18707200
N	4.33236000	0.44287000	0.33818800
O	6.72101200	-0.37445000	1.21937300
C	5.45903400	1.10767800	-0.05674300
C	6.74392600	0.34753400	0.00730800
H	6.84480700	-0.31573100	-0.86408200
H	7.58928200	1.03547500	0.03735200
N	5.21406200	2.35427800	-0.32554800
C	3.30864400	1.32438600	0.30460700

N	3.86749200	2.47803900	-0.11049100
C	3.19115100	3.69956400	-0.44204900
C	2.49499900	3.75916100	-1.65353700
C	3.20958400	4.73834600	0.48883800
C	1.77621000	4.92621000	-1.90741400
C	2.47056200	5.88156200	0.18729400
C	1.74236900	5.98659000	-0.99830300
H	1.22140800	5.00578000	-2.84030400
H	2.45315100	6.70075300	0.90160700
C	2.46790900	2.59413900	-2.60420500
H	3.44859100	2.11143700	-2.67143200
H	1.73334900	1.84422200	-2.27194000
H	2.18515200	2.92965900	-3.60510600
C	3.95840500	4.59136800	1.78656200
H	3.88853800	5.50624200	2.37801700
H	3.54517100	3.76945000	2.38307500
H	5.01512400	4.36959300	1.60932700
C	0.92378500	7.21487200	-1.30215400
H	1.33358200	7.75610700	-2.16124400
H	-0.10735200	6.94124300	-1.54847100
H	0.90113200	7.89872700	-0.45051700
C	-3.06384800	1.18282500	-1.06127300
C	-1.79444900	1.67455000	-1.40507500
C	-1.65263500	2.87537500	-2.07259800
C	-2.79216400	3.63200600	-2.35221300

C	-4.03884800	3.18489700	-1.92533200
C	-4.19737800	1.95644000	-1.27433300
C	-1.59439300	-0.36440700	-0.24214700
C	-0.76455400	0.77512300	-0.81688400
H	-0.65608900	3.22350700	-2.33583100
H	-2.70603800	4.58122000	-2.87197700
H	-4.91947300	3.79356300	-2.10535000
H	-5.18335000	1.62969000	-0.97037400
O	0.33187400	0.43669300	-1.40850800
O	-1.13288000	-1.34212100	0.33287600
N	-2.92633700	-0.12271300	-0.49227800
C	-3.97824100	-1.05863400	-0.01942900
C	-4.15540800	-0.76012500	1.47902900
C	-5.06152000	0.20984500	1.91733900
C	-3.29760300	-1.34548700	2.42074500
C	-5.15127600	0.54523200	3.26645900
H	-5.71018400	0.70917600	1.20473700
C	-3.37117100	-0.99039600	3.76505800
H	-2.55840900	-2.07092800	2.09940200
C	-4.30689500	-0.05285000	4.19664800
H	-5.87939600	1.28545000	3.58523100
H	-2.68987900	-1.45292000	4.47258500
H	-4.37132800	0.21455900	5.24685000
C	-3.56225100	-2.51869700	-0.32280900
C	-2.84742200	-2.82806800	-1.48360500

C	-4.05501500	-3.56599100	0.45506000
C	-2.61668500	-4.14908100	-1.84512200
H	-2.45573400	-2.03049400	-2.10770900
C	-3.81042300	-4.89218000	0.10139400
H	-4.63690000	-3.35128000	1.34607800
C	-3.09097100	-5.19136400	-1.04968300
H	-2.05566600	-4.36257200	-2.75034500
H	-4.19302100	-5.69066800	0.72953500
H	-2.90377600	-6.22418100	-1.32739800
C	-5.26511800	-0.93988000	-0.85929800
C	-6.51051900	-1.24483300	-0.30651200
C	-5.18820800	-0.71275300	-2.23772200
C	-7.65665500	-1.26657800	-1.09883500
H	-6.59167500	-1.47638100	0.75040800
C	-6.33119800	-0.72921000	-3.02758100
H	-4.22681300	-0.50963500	-2.69860800
C	-7.57465700	-0.99874300	-2.46025900
H	-8.61436800	-1.49983900	-0.64388800
H	-6.24676500	-0.53424800	-4.09209600
H	-8.46763600	-1.01177300	-3.07721800
C	1.26474800	-3.75690000	1.02424800
C	2.57974500	-4.23705900	0.97537800
C	2.94492200	-5.19266700	0.00979500
C	1.96031000	-5.61667000	-0.85439500
C	0.63091200	-5.12104700	-0.77667400

C	0.24708800	-4.18309300	0.15670400
H	3.96260600	-5.56442500	-0.04479100
H	2.19969900	-6.34829800	-1.61979000
H	-0.10889200	-5.49292900	-1.47866200
H	-0.75910300	-3.78077400	0.21329000
N	3.31435200	-3.61029900	1.95405300
N	2.53282900	-2.78198000	2.57735600
N	1.32132000	-2.86103800	2.04274400
O	0.31093700	-2.09978700	2.51855500
H	0.13257000	-1.45758500	1.79244800

IM4(RR)

NImag=0

Sum of electronic and zero-point Energies= -3189.590045

Sum of electronic and thermal Energies= -3189.529444

Sum of electronic and thermal Enthalpies= -3189.528500

Sum of electronic and thermal Free Energies= -3189.686512

C	2.16857000	-0.89756400	-1.44028900
O	1.92630400	-0.91316400	-2.68933700
C	1.36389000	-0.50992900	-0.40002200
C	0.00452900	0.04997800	-0.72180100
H	1.66352500	-0.69340600	0.63046800
H	0.08705900	0.56330400	-1.69250300
H	0.13334500	-1.52526100	-2.50517800
C	-0.46410100	1.06761500	0.29910900

C	-0.45213700	0.79545200	1.67279100
C	-0.91959100	2.31885800	-0.12857200
C	-0.87653900	1.75588900	2.58895500
H	-0.10860800	-0.17032200	2.03456000
C	-1.34063600	3.28183300	0.78658500
H	-0.95924700	2.52726600	-1.19650900
C	-1.31351800	3.00469300	2.15078900
H	-0.85184100	1.52616400	3.65019800
H	-1.69114000	4.24704700	0.43194900
H	-1.62474400	3.75733800	2.86953600
C	3.33185100	4.14455200	-1.67068000
C	4.66795100	3.74958600	-1.63096500
C	4.99510600	2.46231600	-2.03629200
C	2.66459400	1.97907700	-2.53126900
C	2.33921300	3.26848800	-2.11257500
H	3.06276900	5.15410400	-1.37181900
H	5.43904100	4.44027600	-1.30183900
H	1.91489100	1.28880500	-2.90578500
H	1.30522200	3.59768100	-2.14632400
C	3.99833300	1.58407500	-2.47242300
C	4.61786100	0.27218000	-2.90248500
C	6.09195700	0.68605500	-3.14305000
H	4.12900200	-0.19254500	-3.75891200
C	6.35402400	1.81621300	-2.12386700
H	6.14482600	1.10279800	-4.15171400

H	6.64630500	1.41603300	-1.14422700
H	7.14741400	2.49129400	-2.45470700
N	4.63607700	-0.74582100	-1.82091100
O	6.99872900	-0.39507100	-3.14378500
C	5.76083200	-1.37028000	-1.35412500
C	7.11695300	-1.06033800	-1.90972700
H	7.69160200	-0.47193200	-1.18191500
H	7.65541800	-1.99181900	-2.09473500
N	5.47527600	-2.22000100	-0.41246000
C	3.59460400	-1.24535200	-1.12545500
N	4.11956800	-2.12809800	-0.27911500
C	3.43957500	-2.95548400	0.68147800
C	3.75983000	-2.76509500	2.03218900
C	2.52704000	-3.91253600	0.23184400
C	3.10517400	-3.57122700	2.95727000
C	1.91841800	-4.70663300	1.20766600
C	2.18603100	-4.54728800	2.56447400
H	3.31727600	-3.42961300	4.01448500
H	1.19726800	-5.45574300	0.88747200
C	4.78432700	-1.75270700	2.47229500
H	5.79446100	-2.16168200	2.36537000
H	4.72122500	-0.83459100	1.88309100
H	4.61767100	-1.48207800	3.51684400
C	2.14279000	-4.07526500	-1.21500300
H	1.89607600	-5.11998300	-1.41960800

H	1.25814700	-3.46693300	-1.44831000
H	2.94120700	-3.77271500	-1.89840200
C	1.51102600	-5.41473200	3.59586800
H	1.10491800	-4.80851600	4.41155100
H	0.69294300	-5.99054100	3.15548600
H	2.22194700	-6.12229500	4.03591300
C	-2.84845300	-1.37576000	0.47438000
C	-1.53395900	-1.77114600	0.21641600
C	-0.86900200	-2.65357700	1.04400000
C	-1.53190400	-3.15474000	2.16546500
C	-2.84282700	-2.76191200	2.42218600
C	-3.52185100	-1.87117900	1.58568100
C	-2.32793400	-0.39618900	-1.53068200
C	-1.04134600	-1.07682400	-1.01076100
H	0.15494900	-2.93356100	0.81760400
H	-1.02701300	-3.84826900	2.83188600
H	-3.36100600	-3.15366400	3.29245200
H	-4.54017000	-1.58342800	1.81100600
O	-0.53699100	-1.98212800	-1.95329200
O	-2.42903800	0.10576300	-2.62568000
N	-3.29666600	-0.46857200	-0.52713400
C	-4.72368800	-0.08486600	-0.65714500
C	-5.48676500	-1.39361000	-0.93815800
C	-6.44717000	-1.94377600	-0.09178700
C	-5.12558900	-2.10652200	-2.09061600

C	-7.05092600	-3.16435800	-0.39643400
H	-6.72869200	-1.43266600	0.82245300
C	-5.72802500	-3.31927200	-2.39612000
H	-4.36889900	-1.69369300	-2.75462900
C	-6.69956800	-3.85316200	-1.54935700
H	-7.79361800	-3.57470800	0.28114300
H	-5.43544500	-3.85198900	-3.29574100
H	-7.17023300	-4.80270100	-1.78552600
C	-4.92569500	0.95991700	-1.77868800
C	-4.19908200	2.15439000	-1.71550300
C	-5.90210100	0.82167100	-2.75951300
C	-4.40938500	3.16267300	-2.64100100
H	-3.45894300	2.28185700	-0.92970600
C	-6.12341200	1.84394400	-3.68616200
H	-6.49952100	-0.08159700	-2.81539000
C	-5.37610300	3.01088600	-3.63751400
H	-3.82292600	4.07542400	-2.58513500
H	-6.88709700	1.71511200	-4.44730300
H	-5.54500700	3.80159800	-4.36219200
C	-5.18148000	0.67332400	0.60397200
C	-6.53327600	1.00852400	0.74430300
C	-4.27018000	1.17384900	1.53378600
C	-6.97048800	1.77272400	1.81907000
H	-7.24466400	0.68435000	-0.01105600
C	-4.70776200	1.94724000	2.60767100

H	-3.20931900	0.97250300	1.42083100
C	-6.05742800	2.24023800	2.76314200
H	-8.02487000	2.01559200	1.91087100
H	-3.97635800	2.32159500	3.31821400
H	-6.39615000	2.84048700	3.60216500
C	2.31798000	2.77356800	2.37663000
C	1.98340600	2.35884800	3.67217100
C	1.45166200	3.27854100	4.59240600
C	1.27475700	4.57413300	4.15704900
C	1.61429700	4.96953700	2.83618900
C	2.14424800	4.08656400	1.91994100
H	1.18933500	2.96445200	5.59721600
H	0.86474400	5.31651300	4.83430300
H	1.44788800	6.00157700	2.54291200
H	2.40296900	4.36653100	0.90548600
N	2.23354100	1.01092300	3.78585300
N	2.70774000	0.59551700	2.65956500
N	2.76591600	1.62569900	1.81201200
O	3.31707100	1.48571700	0.58307800
H	2.60987500	1.06343300	0.02481300

IM4(RS)

NImag=0

Sum of electronic and zero-point Energies= -3189.587521

Sum of electronic and thermal Energies= -3189.526878

Sum of electronic and thermal Enthalpies= -3189.525934

Sum of electronic and thermal Free Energies= -3189.684510

C	2.06374100	-0.92526900	-0.95000000
O	2.33839400	-0.94155100	-2.19260500
C	1.17453200	-0.11663900	-0.28779500
C	0.34457800	0.86923900	-1.07563900
H	0.88359800	-0.35501700	0.72878400
H	0.98187400	1.26901500	-1.87940200
H	0.60050000	-0.89209500	-2.67156000
C	-0.14446000	2.03711300	-0.23441700
C	-0.60631400	1.86440500	1.07623000
C	-0.14080900	3.32528900	-0.77545500
C	-1.02832700	2.95985300	1.82598500
H	-0.64671600	0.87125900	1.51792900
C	-0.57863900	4.41676200	-0.03160500
H	0.23170500	3.47783300	-1.78470900
C	-1.01736400	4.23844100	1.27656700
H	-1.36973600	2.80712100	2.84471500
H	-0.54863100	5.41066700	-0.46857400
H	-1.33129600	5.09288000	1.86908800
C	7.28535600	1.50317900	-1.16729100
C	7.84935700	0.23087400	-1.20633000
C	7.01258300	-0.86992600	-1.35832800
C	5.06556600	0.57851700	-1.45628700
C	5.90623800	1.67651400	-1.29440600

H	7.92698200	2.37145400	-1.04913700
H	8.92508700	0.09912800	-1.12546400
H	3.99791900	0.72050900	-1.59182300
H	5.47284300	2.67076700	-1.27971500
C	5.63346500	-0.69343300	-1.47080600
C	4.92240000	-2.01619300	-1.64245500
C	6.08944800	-3.05796000	-1.79618800
H	4.24042700	-2.01134100	-2.49168700
C	7.40536500	-2.31952500	-1.45452000
H	6.10074500	-3.37136800	-2.84112100
H	7.83877800	-2.69321400	-0.51949600
H	8.15652800	-2.49493300	-2.23055600
N	4.07406700	-2.37272700	-0.47609300
O	5.90885400	-4.26518900	-1.07687900
C	4.42065900	-3.30400100	0.46006100
C	5.68764500	-4.07531300	0.30032800
H	6.52181300	-3.55161500	0.78634100
H	5.57808000	-5.05807700	0.76059800
N	3.49683500	-3.44401300	1.36320200
C	2.85726800	-1.90004700	-0.12778500
N	2.52682900	-2.55989100	0.98772500
C	1.28992200	-2.56068600	1.73210000
C	1.28811000	-1.94618300	2.98870200
C	0.18424600	-3.21476000	1.19277500
C	0.11712400	-2.03249900	3.73384800

C	-0.96238000	-3.28210800	1.98695700
C	-1.00795000	-2.71375500	3.25560400
H	0.08364900	-1.56480900	4.71572100
H	-1.85091400	-3.76384800	1.58146000
C	2.50180200	-1.20856900	3.49015400
H	3.36882400	-1.87329500	3.55952100
H	2.77165400	-0.38239600	2.82037100
H	2.31169900	-0.78888200	4.48042500
C	0.18635300	-3.75460300	-0.20953500
H	-0.61580000	-4.48542400	-0.33288500
H	0.00647900	-2.93430900	-0.91800700
H	1.13565000	-4.23738600	-0.46549700
C	-2.24323700	-2.84802700	4.10971600
H	-2.46014800	-1.92184300	4.65093700
H	-3.11519100	-3.10405600	3.50081300
H	-2.11156000	-3.63841700	4.85740000
C	-3.04893800	0.95954000	-2.09504500
C	-1.73598600	1.08131400	-2.56971400
C	-1.42485400	1.96402900	-3.58496300
C	-2.43002000	2.78101400	-4.10751400
C	-3.71909100	2.69725600	-3.59417500
C	-4.05286100	1.78828800	-2.58516400
C	-1.80468800	-0.43075800	-0.76896300
C	-0.82804700	0.14990100	-1.80531800
H	-0.40561500	2.02453100	-3.95878300

H	-2.20461000	3.48541100	-4.90151500
H	-4.49710600	3.34572800	-3.98543800
H	-5.07155500	1.73976400	-2.22334000
O	-0.38082300	-0.92374100	-2.60276000
O	-1.50415200	-1.11537900	0.18598400
N	-3.09509800	-0.07416300	-1.11285600
C	-4.22017800	-0.51131800	-0.26053700
C	-4.16051700	0.35746400	1.00834900
C	-4.65055200	1.66743800	0.97233600
C	-3.50760700	-0.07533200	2.16689900
C	-4.56178700	2.49732000	2.08504400
H	-5.11654700	2.04433600	0.06709900
C	-3.42224700	0.75454900	3.28225700
H	-3.04790300	-1.05799600	2.18830400
C	-3.96716200	2.03438100	3.25477000
H	-4.95804700	3.50671900	2.03343800
H	-2.91633300	0.39797400	4.17561400
H	-3.90692600	2.67597400	4.12928600
C	-4.12264800	-2.03186000	0.01332200
C	-3.47419100	-2.90035000	-0.86876400
C	-4.84872100	-2.58057600	1.07188900
C	-3.53322800	-4.27749000	-0.67926600
H	-2.90764800	-2.50655400	-1.70814100
C	-4.89727900	-3.95903700	1.26984800
H	-5.39102200	-1.92553000	1.74817400

C	-4.23754500	-4.81653200	0.39511700
H	-3.02224000	-4.93164400	-1.38007800
H	-5.46561500	-4.35912200	2.10470800
H	-4.27959400	-5.89135000	0.54190600
C	-5.55045300	-0.41968000	-1.03199300
C	-6.74419300	-0.06496100	-0.40473000
C	-5.59383200	-0.84293000	-2.36518800
C	-7.94898300	-0.08904500	-1.10713900
H	-6.74227100	0.23419600	0.63825000
C	-6.79200300	-0.86130400	-3.06615400
H	-4.67582500	-1.14715900	-2.86051800
C	-7.97757800	-0.47769500	-2.44067400
H	-8.86605200	0.19767900	-0.60140300
H	-6.79975600	-1.17802800	-4.10452200
H	-8.91468700	-0.49118200	-2.98844900
C	2.52601800	3.86463700	1.34313700
C	2.53896800	4.92921700	0.43201300
C	2.18786400	6.22265500	0.85676100
C	1.84217400	6.37907400	2.18165000
C	1.83796900	5.28464400	3.08667900
C	2.17718100	4.00864800	2.69266600
H	2.19017700	7.05242000	0.15781000
H	1.56434600	7.36107900	2.55120100
H	1.55413400	5.46326200	4.11934900
H	2.16658500	3.15982300	3.36651000

N	2.90240800	4.45067200	-0.80367700
N	3.12509100	3.18173900	-0.69167900
N	2.90452800	2.81812600	0.57176500
O	3.15648400	1.55795600	0.99172300
H	2.46899600	0.97722500	0.54793100

IM4(SR)

NImag=0

Sum of electronic and zero-point Energies= -3189.598333

Sum of electronic and thermal Energies= -3189.537560

Sum of electronic and thermal Enthalpies= -3189.536616

Sum of electronic and thermal Free Energies= -3189.695641

C	-1.73694400	1.78148600	-1.50674200
O	-2.23835700	0.93062300	-2.34787800
C	-0.41939800	2.03284400	-1.30021100
C	0.63412100	1.30291200	-2.09653500
H	-0.10309300	2.73910600	-0.55175300
H	0.32647300	1.28502200	-3.15325100
H	-1.30516500	-0.12727100	-2.14180100
C	1.99998900	1.96121900	-1.99436800
C	2.42340300	2.58523700	-0.81616300
C	2.87983000	1.93526900	-3.08046800
C	3.67784600	3.18561800	-0.73389600
H	1.77687700	2.59087400	0.05823900
C	4.13617200	2.53177900	-3.00211900

H	2.57388200	1.43970700	-3.99836000
C	4.53739200	3.16744200	-1.82934800
H	3.98575500	3.65916900	0.19526100
H	4.79777700	2.50471000	-3.86265100
H	5.51301500	3.64066900	-1.76737600
C	-3.28267300	-2.01461900	2.70123700
C	-4.61733000	-1.81178800	2.35378900
C	-4.91398900	-1.00766500	1.25747700
C	-2.54710300	-0.61912500	0.86217600
C	-2.25574200	-1.42763000	1.95981600
H	-3.03983000	-2.64368000	3.55258200
H	-5.41267900	-2.28949500	2.92043100
H	-1.73458900	-0.18404700	0.28635500
H	-1.21723000	-1.58107500	2.23982900
C	-3.88298700	-0.41146800	0.53589900
C	-4.42049800	0.45809200	-0.57754600
C	-5.98080400	0.38294800	-0.42580700
H	-4.07472000	0.15716500	-1.56540600
C	-6.25136700	-0.71988300	0.62658400
H	-6.42617900	0.13355700	-1.38825500
H	-7.02283400	-0.39317100	1.33326200
H	-6.62413500	-1.61576500	0.11803900
N	-3.94841400	1.84751000	-0.34856200
O	-6.57818900	1.62644300	-0.07327500
C	-4.57449200	2.65779200	0.55580500

C	-5.94617200	2.27095000	1.00563500
H	-5.88064500	1.62108400	1.89132500
H	-6.52578400	3.15910900	1.26106800
N	-3.84341200	3.68287100	0.87827300
C	-2.73788800	2.39184800	-0.59347400
N	-2.69528500	3.50251900	0.15697800
C	-1.55033200	4.32933500	0.42302900
C	-0.71943300	3.94204700	1.47836100
C	-1.28879600	5.41911200	-0.40593300
C	0.42448400	4.70925700	1.69396400
C	-0.12956200	6.14795300	-0.15092700
C	0.73984300	5.80201800	0.88523600
H	1.09254200	4.43126600	2.50603100
H	0.10781500	6.99872600	-0.78552100
C	-0.98852900	2.69080100	2.27202200
H	-2.04261800	2.60787000	2.55438600
H	-0.71905300	1.80052400	1.68609200
H	-0.38243800	2.67438700	3.18080500
C	-2.20254700	5.74318500	-1.55660700
H	-1.93087800	6.69898700	-2.00916900
H	-2.13042000	4.96796500	-2.32837500
H	-3.24655700	5.79512000	-1.23303700
C	2.01755000	6.57282300	1.09321200
H	2.42305300	6.41063800	2.09507000
H	2.77447300	6.25382900	0.36768000

H	1.86132800	7.64637400	0.95500300
C	2.75450300	-1.36523000	-1.58272400
C	1.72480100	-0.99488000	-2.44845700
C	1.71843400	-1.39173300	-3.77274200
C	2.78258100	-2.16096400	-4.24737400
C	3.81301300	-2.52150500	-3.38366300
C	3.81547700	-2.13787700	-2.03971700
C	1.20876800	-0.33918600	-0.23836500
C	0.69103600	-0.21290800	-1.69194400
H	0.88442300	-1.12209800	-4.41639300
H	2.79998800	-2.48917500	-5.28139200
H	4.63551200	-3.12676000	-3.75232400
H	4.62371800	-2.44152300	-1.38708500
O	-0.57825300	-0.79806300	-1.78668600
O	0.56801600	-0.04244500	0.74811500
N	2.49529600	-0.86533500	-0.27224400
C	3.27332600	-1.31367200	0.91024100
C	3.01087200	-2.82817800	1.03586600
C	3.99035100	-3.81415400	0.93335600
C	1.67664600	-3.23100500	1.19396900
C	3.65140900	-5.16608000	1.01356300
H	5.02866400	-3.54189700	0.77782900
C	1.33932000	-4.57433200	1.28628100
H	0.89586500	-2.47647300	1.25404300
C	2.33054500	-5.55177400	1.19796300

H	4.43139800	-5.91600800	0.92345400
H	0.29863100	-4.85341900	1.42567200
H	2.07119700	-6.60396600	1.26459300
C	2.83807900	-0.53611700	2.17700400
C	2.97084500	0.85672100	2.16766900
C	2.42882600	-1.15938000	3.35124300
C	2.64619700	1.61148900	3.28292600
H	3.33813400	1.34303400	1.26903000
C	2.10972200	-0.39939900	4.48008500
H	2.35046700	-2.23947500	3.40240500
C	2.20449500	0.98433200	4.44992800
H	2.75702900	2.69232500	3.25012200
H	1.78817500	-0.90429200	5.38615400
H	1.95504500	1.57109100	5.32893700
C	4.75193500	-0.91806700	0.74159600
C	5.68113800	-1.35627500	1.69237000
C	5.17069200	-0.00753300	-0.22981100
C	7.00698900	-0.94389900	1.63699900
H	5.35322600	-2.00865800	2.49766300
C	6.49816300	0.41486000	-0.27804700
H	4.46431300	0.39148200	-0.95176300
C	7.42408000	-0.05938700	0.64407900
H	7.71181700	-1.30312100	2.38064600
H	6.79686000	1.12351100	-1.04520000
H	8.45853800	0.26755800	0.60202500

C	-2.84235700	-3.94178700	-0.98840100
C	-4.17206800	-3.62346300	-0.68716800
C	-4.85274500	-4.33542000	0.31619900
C	-4.15626300	-5.32706600	0.97294500
C	-2.80673700	-5.62974500	0.65056000
C	-2.12179700	-4.95170000	-0.33558300
H	-5.88591800	-4.10399800	0.55679800
H	-4.64603800	-5.89791300	1.75549300
H	-2.30667900	-6.42759100	1.19192900
H	-1.09614700	-5.17589200	-0.60687500
N	-4.57317700	-2.59820000	-1.51221400
N	-3.58147300	-2.29534500	-2.28973400
N	-2.54762800	-3.07638200	-1.98776100
O	-1.40390700	-3.05167600	-2.70370900
H	-0.92412600	-2.22746800	-2.37761000

IM4(SS)

NImag=0

Sum of electronic and zero-point Energies= -3189.599290

Sum of electronic and thermal Energies= -3189.538834

Sum of electronic and thermal Enthalpies= -3189.537890

Sum of electronic and thermal Free Energies= -3189.696520

C	2.01619500	0.93638700	0.59917100
O	2.00963700	-0.37488800	0.55107700
C	0.94477600	1.71966400	0.86410400
C	-0.35730500	1.02920200	1.16362900

H	1.02589500	2.79990400	0.89033500
H	-0.11135600	0.10009000	1.69773000
H	0.56919600	-0.51021400	-0.49470400
C	-1.31639300	1.82007200	2.03234300
C	-1.48433500	3.20107900	1.88973900
C	-2.07672300	1.14953600	2.99438300
C	-2.38282300	3.89513400	2.69299900
H	-0.91902800	3.74342700	1.13626600
C	-2.96608700	1.84593200	3.80867600
H	-1.96602900	0.07327700	3.10676500
C	-3.12414300	3.21975800	3.65916700
H	-2.50171700	4.96715700	2.56484700
H	-3.53472600	1.30746700	4.55910000
H	-3.81857800	3.76344700	4.29309300
C	5.42244100	-3.16087700	-2.49230300
C	6.36244100	-3.00221100	-1.47809100
C	6.09150300	-2.11237800	-0.44201300
C	3.94336300	-1.56207900	-1.43393100
C	4.21971600	-2.45080100	-2.46814300
H	5.61884500	-3.85626700	-3.30326000
H	7.28788500	-3.57093500	-1.48745100
H	2.99679000	-1.03293300	-1.38346100
H	3.48364000	-2.60712300	-3.25033300
C	4.89571500	-1.40043100	-0.42909800
C	4.82168100	-0.50773000	0.79203900

C	6.24802300	-0.59622300	1.44236000
H	4.06648100	-0.81745900	1.50709500
C	6.90781200	-1.83159800	0.79132000
H	6.15003900	-0.71483100	2.52158000
H	7.96740200	-1.63614700	0.59549600
H	6.83704800	-2.68948900	1.47017300
N	4.51151500	0.87780800	0.40331300
O	7.02383400	0.58931100	1.28945100
C	5.48879700	1.71033900	-0.06069500
C	6.89889900	1.22321600	0.03678200
H	7.12532400	0.54073600	-0.79541400
H	7.59249700	2.06446100	0.01126100
N	5.00004400	2.84889900	-0.45446500
C	3.33698100	1.52776400	0.28453400
N	3.65416200	2.71823700	-0.24336200
C	2.77125800	3.74342800	-0.72771100
C	2.08645400	3.51725700	-1.92202500
C	2.67119700	4.92804700	0.00745300
C	1.27320400	4.55335500	-2.38812300
C	1.83328400	5.91945400	-0.49245000
C	1.12801900	5.74887800	-1.68777100
H	0.72514200	4.40599400	-3.31649300
H	1.72998000	6.84995500	0.06126300
C	2.15250600	2.19921800	-2.64575500
H	3.14898100	1.74916000	-2.58646500

H	1.43127900	1.49001900	-2.21348700
H	1.90143400	2.33196300	-3.70056000
C	3.43219200	5.09882300	1.29524800
H	3.19780000	6.06009300	1.75658700
H	3.17717500	4.30688200	2.00889200
H	4.51192500	5.04985400	1.12278300
C	0.21080300	6.83466700	-2.18874100
H	0.69456000	7.81460400	-2.13941300
H	-0.09120600	6.65318000	-3.22323400
H	-0.69642600	6.88535900	-1.57667800
C	-3.22356900	1.10281400	-0.88698300
C	-1.88915800	1.52946800	-0.85709200
C	-1.51328400	2.75021300	-1.37867100
C	-2.49076700	3.59519100	-1.90683300
C	-3.82332000	3.19856900	-1.87802600
C	-4.21316100	1.95522000	-1.36995700
C	-2.10658600	-0.53233600	0.26323200
C	-1.04999500	0.51336900	-0.14248400
H	-0.46959300	3.04998200	-1.34528000
H	-2.21369000	4.56098000	-2.31980500
H	-4.59149700	3.86299900	-2.26207100
H	-5.26028300	1.68361200	-1.37164400
O	-0.14580000	-0.09928500	-1.03339000
O	-1.89076700	-1.49947900	0.96303200
N	-3.30698000	-0.21380600	-0.34857900

C	-4.49591200	-1.07059800	-0.13979600
C	-4.94637200	-0.82082100	1.30917400
C	-5.61590700	0.36751900	1.62554000
C	-4.59813000	-1.68534500	2.34913900
C	-6.00100100	0.64490900	2.93185400
H	-5.84739700	1.08220300	0.84055700
C	-4.97856500	-1.40486400	3.66058600
H	-4.01855500	-2.57579700	2.13429000
C	-5.70024000	-0.25281200	3.95360800
H	-6.52882500	1.56812900	3.15125100
H	-4.70748000	-2.09581900	4.45316300
H	-6.00682600	-0.04293100	4.97449000
C	-4.15731900	-2.54666200	-0.44983300
C	-3.09418800	-2.90906800	-1.27917700
C	-5.05302900	-3.53714000	-0.04081800
C	-2.92303400	-4.23462100	-1.66656800
H	-2.38719800	-2.16154800	-1.62771700
C	-4.87279800	-4.86410300	-0.41675400
H	-5.90768600	-3.26587500	0.57300000
C	-3.80374900	-5.22037700	-1.23286900
H	-2.09475300	-4.49537200	-2.31853900
H	-5.57749100	-5.61692000	-0.07677100
H	-3.66195600	-6.25388400	-1.53302000
C	-5.57512900	-0.77061500	-1.19777300
C	-6.93326700	-0.72769500	-0.88671800

C	-5.19238500	-0.67125200	-2.54069000
C	-7.88498300	-0.54232600	-1.89071800
H	-7.26171800	-0.83795900	0.14106600
C	-6.13774100	-0.47995300	-3.53833000
H	-4.13914100	-0.73439000	-2.80090100
C	-7.49292100	-0.40733300	-3.21598200
H	-8.93743500	-0.50671100	-1.62592700
H	-5.81606000	-0.39148300	-4.57143100
H	-8.23437400	-0.25889400	-3.99482600
C	2.40645100	-3.59442500	0.76772000
C	3.49894700	-4.41302800	0.44579900
C	3.41829200	-5.29331500	-0.64790900
C	2.24295400	-5.29638300	-1.36656400
C	1.15263700	-4.45216600	-1.02211700
C	1.20027300	-3.58522800	0.04827300
H	4.26021200	-5.92574600	-0.90924200
H	2.13909400	-5.95822300	-2.22085800
H	0.24726400	-4.49721300	-1.61884400
H	0.36748400	-2.94408900	0.32489100
N	4.52291400	-4.14767000	1.32203900
N	4.12608600	-3.21920000	2.13397900
N	2.87045000	-2.89181000	1.82781600
O	2.22135000	-1.94120900	2.53634900
H	2.03933100	-1.21960600	1.83835100

TS5(RR)

NImag=1 (-802.8793)

Sum of electronic and zero-point Energies= -3189.579521

Sum of electronic and thermal Energies= -3189.518819

Sum of electronic and thermal Enthalpies= -3189.517875

Sum of electronic and thermal Free Energies= -3189.677718

C	2.10046000	-1.37315000	-0.41198500
O	1.93556700	-1.95448300	-1.48301000
C	1.22662700	-0.42525500	0.22259500
C	-0.12601100	-0.25623000	-0.44947400
H	1.23363300	-0.43735000	1.31595300
H	0.03832400	-0.38096600	-1.52889300
H	-0.08235900	-2.66813900	-1.10283600
C	-0.70634400	1.12964400	-0.23917000
C	-0.81597800	1.69895100	1.03511700
C	-1.12957600	1.87384000	-1.34296700
C	-1.33869000	2.97981100	1.19503400
H	-0.47639800	1.15148300	1.91033300
C	-1.65494800	3.15558700	-1.18513800
H	-1.04461100	1.43878800	-2.33714700
C	-1.75958000	3.71222000	0.08567500
H	-1.38732700	3.41458100	2.18874200
H	-1.96912600	3.72182000	-2.05736700
H	-2.14313400	4.72042100	0.21046000
C	6.79969300	1.64617000	-3.57071300

C	7.19146500	0.35055700	-3.90400700
C	6.48587600	-0.72115800	-3.36747000
C	5.00411900	0.79944100	-2.17733200
C	5.71978200	1.86813600	-2.71436800
H	7.34578100	2.49236100	-3.97656700
H	8.03795900	0.18118500	-4.56363800
H	4.17401400	0.99451900	-1.49980200
H	5.43208700	2.88205100	-2.45472700
C	5.40413000	-0.48743900	-2.52071200
C	4.79552300	-1.79749400	-2.06701200
C	5.86776400	-2.87476300	-2.45602300
H	3.83142600	-2.00537400	-2.53042600
C	6.70762700	-2.20113300	-3.56337100
H	5.38413300	-3.78903600	-2.80278300
H	7.75411500	-2.50935300	-3.47542200
H	6.35470400	-2.52220300	-4.55051500
N	4.58475800	-1.80098400	-0.61285600
O	6.66769600	-3.30000800	-1.36026400
C	5.65395200	-1.92727000	0.22479700
C	6.95884200	-2.31398400	-0.39042200
H	7.46076200	-1.43848200	-0.82432200
H	7.60758500	-2.76728100	0.35972300
N	5.30201300	-1.77988700	1.46839700
C	3.50968900	-1.53441300	0.15389600
N	3.96709700	-1.52053300	1.40629000

C	3.24495600	-1.24900300	2.62328800
C	3.51360300	-0.03546800	3.26299200
C	2.33482400	-2.19778800	3.09257200
C	2.78112900	0.23777800	4.41513200
C	1.65959800	-1.88406600	4.27153700
C	1.85159900	-0.66754500	4.92843300
H	2.92965800	1.19536200	4.90704300
H	0.94477500	-2.60167500	4.67006800
C	4.54341200	0.92240100	2.73046100
H	5.55119900	0.51512400	2.86402800
H	4.37318600	1.11751200	1.66573200
H	4.46969500	1.87576400	3.25463200
C	2.03622300	-3.46636500	2.33612800
H	1.58085800	-4.20355300	3.00136800
H	1.32436300	-3.28216400	1.51772800
H	2.94125300	-3.90970100	1.90859400
C	1.03813700	-0.31749800	6.14704700
H	0.65419100	-1.21440800	6.64088200
H	1.62953800	0.24982800	6.87054300
H	0.18122900	0.30345800	5.86281400
C	-3.11135400	-0.92079500	1.08229100
C	-1.77335900	-1.28452600	1.25494000
C	-1.24388200	-1.48976500	2.51284300
C	-2.05775300	-1.30044500	3.63065900
C	-3.38628800	-0.92416600	3.45718500

C	-3.93590800	-0.73567600	2.18596000
C	-2.33199700	-1.27979800	-1.03496900
C	-1.12160500	-1.40105300	-0.08453600
H	-0.20894800	-1.79396200	2.61811000
H	-1.65672100	-1.45308100	4.62857000
H	-4.02274200	-0.77814600	4.32471500
H	-4.97423500	-0.45186500	2.07967400
O	-0.50545200	-2.65794100	-0.22561300
O	-2.28055500	-1.56506400	-2.20997600
N	-3.41955300	-0.81383900	-0.30357900
C	-4.81318700	-0.68003600	-0.79824700
C	-5.53391400	-1.97286500	-0.37035300
C	-6.58848000	-2.02602200	0.53855300
C	-5.02779700	-3.17843200	-0.87787600
C	-7.13986300	-3.25068100	0.91861600
H	-6.98751400	-1.11302000	0.96711200
C	-5.57745100	-4.39634500	-0.50262400
H	-4.19814100	-3.14978700	-1.58095600
C	-6.64144100	-4.43740100	0.39834700
H	-7.95979000	-3.26801700	1.63036000
H	-5.17195500	-5.31694900	-0.91107900
H	-7.07112900	-5.38926400	0.69547800
C	-4.83888300	-0.47200100	-2.32975400
C	-4.10415600	0.59129000	-2.86487800
C	-5.66817400	-1.20509700	-3.17216600

C	-4.15874200	0.88148000	-4.21793600
H	-3.48512200	1.19207100	-2.20407200
C	-5.73283200	-0.90496000	-4.53523200
H	-6.27130800	-2.01646700	-2.77982400
C	-4.97537300	0.12937100	-5.06462900
H	-3.56805400	1.70209900	-4.61531800
H	-6.38238600	-1.49174800	-5.17791100
H	-5.02316000	0.35787800	-6.12504200
C	-5.43315100	0.62414500	-0.26168800
C	-6.79363400	0.87192800	-0.47727000
C	-4.64858400	1.63803000	0.28918000
C	-7.36683000	2.07854600	-0.09415100
H	-7.40223100	0.11914700	-0.97186800
C	-5.22206400	2.85121500	0.66492600
H	-3.58023600	1.49551900	0.42197100
C	-6.58276800	3.07297500	0.48810800
H	-8.42566400	2.24752100	-0.26555200
H	-4.58573200	3.62125100	1.09128900
H	-7.02870100	4.01755600	0.78462100
C	1.81715100	3.83442200	0.19153000
C	1.37453800	4.51537700	1.33590000
C	0.81052900	5.79985000	1.20957800
C	0.71563300	6.32928600	-0.05904200
C	1.16611100	5.61691000	-1.20453200
C	1.72441700	4.36166100	-1.10506900

H	0.46432700	6.33899600	2.08581200
H	0.28504200	7.31654400	-0.19694300
H	1.05938200	6.07830500	-2.18173500
H	2.05971000	3.79420300	-1.96634600
N	1.57189000	3.71426700	2.42676300
N	2.11557900	2.60449900	2.00779000
N	2.28050800	2.66217600	0.68863800
O	2.81706200	1.65777100	0.00131900
H	1.93231700	0.62891600	0.04577000

TS5(RS)

NImag=1 (-926.7107)

Sum of electronic and zero-point Energies= -3189.580610

Sum of electronic and thermal Energies= -3189.520478

Sum of electronic and thermal Enthalpies= -3189.519534

Sum of electronic and thermal Free Energies= -3189.675002

C	1.81540700	-1.04103100	-1.20821500
O	1.97287300	-1.42362100	-2.37484000
C	1.02915400	0.04603000	-0.73100800
C	0.23476400	0.82528100	-1.77782000
H	0.51639500	-0.14844300	0.21821800
H	0.87410100	0.91076500	-2.66745200
H	0.23893300	-1.18649100	-3.09521700
C	-0.01485700	2.23497900	-1.27695300
C	-0.85903400	2.49709000	-0.19520300

C	0.63777100	3.30326400	-1.89575200
C	-1.04972600	3.80441700	0.24366100
H	-1.36265200	1.68187700	0.32269000
C	0.44906700	4.61036400	-1.45559200
H	1.30282400	3.10521300	-2.73382700
C	-0.39909700	4.86415500	-0.38345400
H	-1.69688600	3.98889300	1.09494200
H	0.97262000	5.42716100	-1.94426900
H	-0.53643600	5.87814500	-0.02063600
C	7.89788600	1.31280300	-0.96172300
C	8.16090900	0.12149200	-1.63649500
C	7.12123000	-0.78123200	-1.83037300
C	5.56711000	0.69891900	-0.68357700
C	6.61639200	1.59625700	-0.48762700
H	8.70115300	2.02408100	-0.79549700
H	9.16225600	-0.10203600	-1.99369300
H	4.57835400	0.92765800	-0.28952600
H	6.42956100	2.52204700	0.04739000
C	5.84248500	-0.48293300	-1.36183700
C	4.88803600	-1.61210500	-1.69428700
C	5.83374900	-2.80714200	-2.05832100
H	4.21466300	-1.37787900	-2.52094400
C	7.14311600	-2.12917500	-2.50992600
H	5.39121200	-3.42505600	-2.84127000
H	8.00025700	-2.75158200	-2.23690200

H	7.15161200	-2.01616700	-3.60084900
N	4.05314200	-1.97638000	-0.54872900
O	6.04785500	-3.70740200	-0.97725000
C	4.59682800	-2.64827600	0.50668500
C	5.98834300	-3.16211100	0.32813500
H	6.72589100	-2.36305900	0.47869100
H	6.18180800	-3.97271600	1.03098700
N	3.72038700	-2.83371700	1.44890600
C	2.77228900	-1.71129100	-0.23345900
N	2.59067000	-2.23136800	0.97727200
C	1.38743500	-2.27769100	1.77017000
C	1.39147900	-1.57257400	2.97646400
C	0.32974700	-3.07688500	1.33124400
C	0.24660700	-1.67806700	3.76086100
C	-0.79163600	-3.14240400	2.15661900
C	-0.84664900	-2.45543500	3.37022300
H	0.21145000	-1.13708900	4.70403700
H	-1.64277700	-3.74008600	1.83498800
C	2.58799100	-0.77782100	3.42563300
H	3.35642800	-1.44274200	3.83542100
H	3.02057200	-0.21114100	2.59489400
H	2.29049100	-0.06278200	4.19476400
C	0.38853700	-3.85131400	0.04134900
H	-0.42375100	-4.58130100	0.01308500
H	0.25262300	-3.18889200	-0.81921400

H	1.33933100	-4.38571600	-0.06599000
C	-2.07787300	-2.52348400	4.23591100
H	-2.72267500	-1.65579500	4.04916600
H	-2.65995400	-3.42311800	4.02064100
H	-1.81488600	-2.51989000	5.29759000
C	-3.27390000	0.84706900	-2.17549800
C	-2.07599200	1.01815500	-2.87816000
C	-1.95129400	1.97892700	-3.86188200
C	-3.03336100	2.81814600	-4.12967900
C	-4.20555700	2.68148700	-3.39482000
C	-4.34846900	1.69960700	-2.40976100
C	-1.81851700	-0.65249500	-1.24020300
C	-1.02891000	0.08586100	-2.33882700
H	-1.01156000	2.08460700	-4.39685500
H	-2.95470600	3.58381900	-4.89438300
H	-5.04081000	3.34845900	-3.58570700
H	-5.28150100	1.61708600	-1.86954600
O	-0.64777500	-0.85046100	-3.32445000
O	-1.34742800	-1.48173800	-0.48854800
N	-3.14630000	-0.25973800	-1.27979000
C	-4.09384900	-0.63136900	-0.19661800
C	-3.74328100	0.30829300	0.96730400
C	-4.29699700	1.58644500	1.07428700
C	-2.68540700	-0.03577900	1.81964200
C	-3.82215600	2.48634600	2.02836100

H	-5.09972500	1.89246700	0.41162300
C	-2.19507100	0.87134800	2.75224200
H	-2.20948500	-1.00476500	1.71332200
C	-2.76623600	2.13686500	2.86360900
H	-4.26851900	3.47452900	2.09596700
H	-1.33430600	0.60939500	3.36050300
H	-2.35766300	2.84796400	3.57476900
C	-3.97288000	-2.12730800	0.17145600
C	-3.60494000	-3.08983900	-0.77120300
C	-4.40896000	-2.55468500	1.42604800
C	-3.63971000	-4.44257100	-0.45347700
H	-3.27345300	-2.78057900	-1.75778200
C	-4.45719800	-3.91155500	1.74163400
H	-4.72161100	-1.82237600	2.16555400
C	-4.06521300	-4.86299000	0.80629400
H	-3.33603200	-5.17259700	-1.19824800
H	-4.80730300	-4.22012400	2.72261400
H	-4.09863900	-5.92053500	1.04983300
C	-5.54409100	-0.55472700	-0.70175800
C	-6.59482800	-0.24828400	0.16316800
C	-5.84346100	-0.94925200	-2.00940700
C	-7.91483900	-0.29117400	-0.28242200
H	-6.38582500	0.02395700	1.19296500
C	-7.15900700	-0.98987300	-2.45429500
H	-5.03586300	-1.21054400	-2.68736800

C	-8.20203000	-0.65414200	-1.59326800
H	-8.71848500	-0.04163800	0.40375300
H	-7.36921400	-1.28437400	-3.47792100
H	-9.22997900	-0.68336700	-1.94103900
C	2.05715800	3.44546900	1.61663800
C	1.07733400	3.71228300	2.58440600
C	0.82112000	5.04113100	2.97353300
C	1.56342900	6.03257200	2.37024300
C	2.55232400	5.73757600	1.39162600
C	2.82002200	4.44570700	0.99691300
H	0.06321000	5.26112300	3.71907500
H	1.39433000	7.07003500	2.64254600
H	3.10337900	6.55849500	0.94250800
H	3.55642100	4.20090100	0.23911800
N	0.50707800	2.53070600	2.96773800
N	1.08702200	1.57434400	2.29594000
N	2.01721600	2.09594800	1.49949500
O	2.77743200	1.33661300	0.71287500
H	1.94048500	0.78056600	-0.17437700

TS5(SR)

NImag=(-1025.7400)

Sum of electronic and zero-point Energies= -3189.589224

Sum of electronic and thermal Energies= -3189.529016

Sum of electronic and thermal Enthalpies= -3189.528072

Sum of electronic and thermal Free Energies= -3189.685553

C	2.13017100	0.21980300	1.58780800
O	2.26893500	-0.71018100	2.39635100
C	0.93766800	0.97344100	1.33916900
C	-0.30785100	0.38144700	1.98079300
H	0.80901600	1.28948800	0.30593400
H	-0.01870400	-0.00371300	2.96899500
H	0.84460800	-1.77128800	1.56692400
C	-1.41236800	1.40291100	2.19477500
C	-1.60319500	2.46968000	1.31125900
C	-2.27145800	1.28638300	3.29360100
C	-2.61972700	3.39845700	1.52615400
H	-0.95073900	2.58261500	0.44810700
C	-3.28511300	2.21649900	3.51338100
H	-2.13203400	0.46185900	3.98902900
C	-3.46139200	3.27833400	2.62864600
H	-2.74884800	4.22275400	0.83047000
H	-3.93362600	2.11183200	4.37828700
H	-4.24607300	4.00944200	2.79879300
C	5.77596100	-4.78926800	0.74354400
C	6.70879100	-4.10132000	1.51719500
C	6.40149200	-2.81736700	1.95825000
C	4.23441100	-2.92602900	0.86239400
C	4.54812200	-4.20804900	0.41792800
H	6.00645600	-5.78877200	0.38786100

H	7.66266700	-4.55828400	1.76535800
H	3.27758700	-2.46874400	0.62122500
H	3.83257700	-4.75984400	-0.18310400
C	5.17515100	-2.24575600	1.62795400
C	5.05988400	-0.85863000	2.21384600
C	6.50308500	-0.50975500	2.71431500
H	4.35206200	-0.80179100	3.03670800
C	7.22288900	-1.87714600	2.80809800
H	6.42648500	0.00438800	3.67227400
H	8.26050700	-1.77526800	2.47438800
H	7.24980200	-2.22006200	3.84874200
N	4.61822400	0.09984900	1.19159100
O	7.21059300	0.40124600	1.88331600
C	5.51379600	0.61074900	0.30220700
C	6.95530000	0.27879400	0.50300300
H	7.17484900	-0.73198000	0.12882600
H	7.58185000	1.00080000	-0.02125800
N	4.93653000	1.39842600	-0.55810500
C	3.41034000	0.59867800	0.86782700
N	3.62418900	1.37582700	-0.19630900
C	2.68308900	2.13551800	-0.98073000
C	1.88154000	1.44967300	-1.89423800
C	2.65570000	3.52028500	-0.79371900
C	0.98993600	2.21493700	-2.64830800
C	1.76965000	4.23519600	-1.59329200

C	0.94222000	3.60388700	-2.52584900
H	0.32278100	1.71071100	-3.34311500
H	1.72871100	5.31704900	-1.48852600
C	1.95339500	-0.04858300	-2.02663400
H	2.99246300	-0.38954100	-2.09767500
H	1.47028600	-0.54221000	-1.17393100
H	1.41881700	-0.37193000	-2.92161600
C	3.53555700	4.19219600	0.22504900
H	3.40014700	5.27497700	0.18276500
H	3.27868400	3.85345900	1.23488400
H	4.59127700	3.96791800	0.04466700
C	0.04757400	4.43479500	-3.40929400
H	-0.59910200	5.08934800	-2.81557200
H	0.64730100	5.07767000	-4.06244400
H	-0.58343700	3.80349000	-4.03780400
C	-3.11590300	-1.43488700	1.20891600
C	-1.92460000	-1.57872000	1.91967800
C	-1.87529800	-2.28522900	3.10684400
C	-3.04867500	-2.86511100	3.59340100
C	-4.23589600	-2.72138900	2.88085700
C	-4.29159300	-2.00760300	1.68107300
C	-1.52888100	-0.43839300	-0.11574400
C	-0.82234100	-0.86778500	1.18771800
H	-0.93551600	-2.38683600	3.64534100
H	-3.03553300	-3.42890700	4.52030900

H	-5.14732600	-3.17356500	3.25939300
H	-5.22950700	-1.90728500	1.15158100
O	0.23525400	-1.71926600	0.80899000
O	-0.95518600	0.00229000	-1.08784100
N	-2.89302100	-0.66662700	0.03002700
C	-3.91615800	-0.57298100	-1.04111100
C	-4.11062200	-2.01362400	-1.55368400
C	-5.29417100	-2.74111900	-1.44864200
C	-2.98210400	-2.64835200	-2.09273900
C	-5.35788900	-4.06420700	-1.88981000
H	-6.17823400	-2.28993600	-1.01159700
C	-3.04521500	-3.96278200	-2.53352800
H	-2.04864200	-2.09503900	-2.16923400
C	-4.23920200	-4.67767500	-2.43675300
H	-6.28992400	-4.61279800	-1.79428100
H	-2.15940800	-4.43251600	-2.94968400
H	-4.29045800	-5.70672200	-2.77868700
C	-3.47682900	0.39010900	-2.16737400
C	-3.14436600	1.70475900	-1.82193700
C	-3.55350900	0.04899400	-3.51363200
C	-2.86504200	2.64529300	-2.79783500
H	-3.11259800	1.98437700	-0.77269900
C	-3.27811300	0.99991300	-4.50053000
H	-3.83228900	-0.95591600	-3.81041500
C	-2.93240200	2.29659100	-4.14977400

H	-2.60786200	3.65954200	-2.50647500
H	-3.34660900	0.71630000	-5.54641600
H	-2.73323300	3.03799700	-4.91855000
C	-5.18309300	0.10807800	-0.48806400
C	-6.33891400	0.15166100	-1.27576500
C	-5.16151400	0.82767600	0.70751300
C	-7.46547800	0.84490500	-0.84844800
H	-6.34611800	-0.34184900	-2.24409800
C	-6.28798900	1.52991100	1.13084900
H	-4.26088400	0.85579000	1.31373200
C	-7.44754900	1.53204000	0.36388500
H	-8.35379400	0.86059000	-1.47245700
H	-6.24362800	2.07986600	2.06638900
H	-8.32550600	2.07713600	0.69642700
C	1.87746000	1.74785600	4.64936400
C	3.00054400	1.02587500	5.07281200
C	2.91202900	0.20169700	6.21237700
C	1.69310000	0.13630000	6.84983200
C	0.56353200	0.87158800	6.39311000
C	0.63084700	1.69613400	5.29190800
H	3.77365700	-0.35715200	6.56253900
H	1.58275100	-0.49131000	7.72858300
H	-0.37235100	0.78145900	6.93611700
H	-0.21182500	2.27185700	4.92391700
N	4.03244400	1.28100500	4.20799300

N	3.59233100	2.10187000	3.29329900
N	2.31912200	2.40720500	3.54874900
O	1.58247500	3.10933800	2.70360100
H	1.19676500	2.13240700	1.93808800

TS5(SS)

NImag=1 (-955.3066)

Sum of electronic and zero-point Energies= -3189.582582

Sum of electronic and thermal Energies= -3189.521933

Sum of electronic and thermal Enthalpies= -3189.520989

Sum of electronic and thermal Free Energies= -3189.681202

C	2.09298700	0.04632300	-0.37649800
O	1.96728300	-1.07008100	-0.88383900
C	1.16755000	0.75802500	0.45904400
C	-0.17258500	0.06958800	0.66090100
H	1.13578800	1.82817200	0.24671400
H	0.01804200	-1.01300300	0.65469300
H	0.07139900	-0.70825500	-1.67058500
C	-0.83247700	0.40043400	1.98989700
C	-0.61180200	1.62189200	2.63304500
C	-1.66995600	-0.53728900	2.60296600
C	-1.20378200	1.89707400	3.86202000
H	0.04661800	2.36070200	2.18453500
C	-2.25917800	-0.26501000	3.83533800
H	-1.84068300	-1.49866600	2.12481900

C	-2.02837000	0.95239600	4.46940200
H	-1.01144000	2.84784400	4.35000400
H	-2.89220700	-1.01424000	4.29918200
H	-2.48193500	1.16285600	5.43355500
C	5.60139600	-3.20465500	-4.56415800
C	6.43272600	-3.42716800	-3.46814400
C	6.11002800	-2.84013000	-2.24808300
C	4.12574300	-1.83114900	-3.22306700
C	4.45571500	-2.41481700	-4.44387600
H	5.84577500	-3.65194000	-5.52277000
H	7.32099500	-4.04479300	-3.56680800
H	3.22701400	-1.23174000	-3.10652000
H	3.81602000	-2.25926000	-5.30678300
C	4.96863500	-2.04920100	-2.13900300
C	4.82183400	-1.51893000	-0.73118800
C	6.19200300	-1.84050100	-0.03677300
H	4.00409200	-1.98677200	-0.18378300
C	6.82518000	-2.93868700	-0.92247700
H	6.00120700	-2.17058600	0.98434200
H	7.90691400	-2.78651900	-0.99158400
H	6.66247400	-3.92371400	-0.47044900
N	4.58334400	-0.07142900	-0.74020600
O	7.05486600	-0.71587100	0.09728700
C	5.61519600	0.80237600	-0.90438000
C	6.99257400	0.22646900	-0.94883800

H	7.19591000	-0.22497900	-1.93045500
H	7.73033500	1.00349600	-0.74738500
N	5.20434400	2.03762800	-0.86157800
C	3.47151200	0.65609400	-0.56501100
N	3.86175100	1.92914500	-0.65252000
C	3.06442600	3.12652500	-0.60179000
C	2.20006400	3.40273300	-1.66187400
C	3.21854200	3.95864600	0.51415400
C	1.46571200	4.58898200	-1.58564900
C	2.44934700	5.11817500	0.54169600
C	1.57412900	5.45087300	-0.49654300
H	0.77627700	4.82725500	-2.39237200
H	2.53633700	5.78085300	1.39957800
C	1.99342700	2.44370100	-2.80469400
H	2.92079500	1.93533300	-3.08752300
H	1.24603900	1.68253800	-2.53762700
H	1.61912100	2.97682400	-3.68143100
C	4.15872100	3.60001400	1.63328400
H	4.05852800	4.31655700	2.45112100
H	3.93950200	2.59890400	2.02416800
H	5.19646900	3.61466600	1.28622800
C	0.76551400	6.72087700	-0.42732300
H	1.41834700	7.59975100	-0.42971200
H	0.08310300	6.80441800	-1.27677300
H	0.17351700	6.75657900	0.49277600

C	-3.25482500	1.35703900	-0.56561400
C	-1.87342800	1.60539200	-0.54859700
C	-1.38552700	2.89711800	-0.49936100
C	-2.28047800	3.96607200	-0.42646400
C	-3.64606900	3.71330300	-0.38499200
C	-4.15532600	2.41308900	-0.45221600
C	-2.28971700	-0.71526600	-0.47779300
C	-1.13161100	0.29916800	-0.53647400
H	-0.31694000	3.08254200	-0.51297900
H	-1.90803000	4.98521600	-0.38557300
H	-4.34654100	4.53876100	-0.30281000
H	-5.22538100	2.25896000	-0.42529500
O	-0.46498100	0.10107100	-1.77343900
O	-2.15268000	-1.91047200	-0.33431900
N	-3.48211600	-0.04313300	-0.68559400
C	-4.76196000	-0.78878300	-0.69067600
C	-5.01405000	-1.19864500	0.77032500
C	-5.44027100	-0.23379600	1.69141100
C	-4.70213300	-2.47597400	1.24102100
C	-5.62343100	-0.55614700	3.03104500
H	-5.63807800	0.78067100	1.35770200
C	-4.88195700	-2.79897900	2.58522700
H	-4.30504500	-3.21705400	0.55708000
C	-5.36275100	-1.84887300	3.47984200
H	-5.96333000	0.20648400	3.72497700

H	-4.64268500	-3.80080400	2.92861600
H	-5.51300900	-2.10596100	4.52445700
C	-4.69303800	-1.98001000	-1.67271400
C	-3.77749400	-2.03272400	-2.72443900
C	-5.69648500	-2.95015700	-1.61059200
C	-3.84593900	-3.05241500	-3.66941400
H	-2.99586000	-1.28387900	-2.81032800
C	-5.76139100	-3.97217500	-2.55129900
H	-6.44054100	-2.90174900	-0.82011000
C	-4.83225800	-4.02990700	-3.58582500
H	-3.11670500	-3.08135700	-4.47320900
H	-6.54578300	-4.71917700	-2.47725500
H	-4.87982300	-4.82581600	-4.32242600
C	-5.88244100	0.06469900	-1.31449600
C	-7.17619000	0.09383600	-0.79720200
C	-5.62595700	0.73055900	-2.51934600
C	-8.18198700	0.81277500	-1.44561100
H	-7.40967100	-0.44257700	0.11610300
C	-6.62325400	1.45162200	-3.15962100
H	-4.62870200	0.68903400	-2.94907400
C	-7.90895900	1.50162300	-2.62023100
H	-9.18213300	0.82778200	-1.02339300
H	-6.39845500	1.97313900	-4.08476500
H	-8.69088100	2.06445100	-3.12038800
C	2.24291300	-1.29217600	3.49976000

C	2.92493500	-2.47628400	3.18382800
C	2.51716400	-3.69299600	3.76847500
C	1.44005500	-3.64925600	4.62449500
C	0.75627100	-2.43522400	4.91636100
C	1.14081800	-1.23356900	4.36723600
H	3.03407000	-4.61887300	3.53991400
H	1.09142700	-4.56578000	5.09025700
H	-0.09837100	-2.46270600	5.58540500
H	0.62670100	-0.29762200	4.56264700
N	3.91532200	-2.18166500	2.28781600
N	3.86909500	-0.89498600	2.05325100
N	2.89625100	-0.34948000	2.77458600
O	2.57366500	0.93070800	2.65971100
H	1.82000100	0.86902400	1.58723500

IM5(RR)

NImag=0

Sum of electronic and zero-point Energies= -3189.603735

Sum of electronic and thermal Energies= -3189.543418

Sum of electronic and thermal Enthalpies= -3189.542474

Sum of electronic and thermal Free Energies= -3189.701602

C	-2.01120400	-0.35867000	-0.51001300
O	-2.06970700	0.58903100	-1.41503400
C	-2.17943100	-1.81028900	-1.02503700
C	-0.73826200	-2.18023100	-1.36724400

H	-2.58260900	-2.46350400	-0.24231400
H	-0.46209500	-1.60150100	-2.25781400
H	-0.88591400	1.41493500	-1.25847500
C	-0.36955100	-3.62722300	-1.57909800
C	-1.16212500	-4.69026400	-1.14654200
C	0.85640400	-3.91093200	-2.19220300
C	-0.73702900	-6.00664500	-1.31425500
H	-2.12657800	-4.49952800	-0.68316100
C	1.28566100	-5.22345900	-2.35476200
H	1.46686900	-3.08649300	-2.55739200
C	0.48870700	-6.27782700	-1.91318000
H	-1.36894100	-6.82276900	-0.97658400
H	2.23879200	-5.42364600	-2.83515000
H	0.81871200	-7.30392400	-2.04275400
C	-1.15257100	5.36177000	2.35872200
C	-0.93436500	4.61648100	3.51868300
C	-1.11685300	3.23818000	3.47282000
C	-1.74472100	3.36555800	1.12300400
C	-1.55781200	4.74596900	1.17196300
H	-1.00824700	6.43783300	2.38039200
H	-0.63080500	5.10638200	4.44031900
H	-2.02821100	2.87962100	0.19336700
H	-1.71191300	5.32731000	0.26858300
C	-1.50238000	2.63450200	2.27837200
C	-1.53865400	1.13429100	2.44130300

C	-1.55176900	0.91489000	3.98829200
H	-0.67047300	0.66023600	1.98341700
C	-0.92090800	2.20461600	4.55680800
H	-0.98145600	0.02346400	4.25478600
H	-1.39069200	2.46321800	5.51106800
H	0.14743900	2.03832600	4.74242500
N	-2.74594900	0.56330700	1.83030200
O	-2.85280100	0.67151600	4.51607800
C	-3.95126200	0.74117200	2.45747300
C	-3.92002500	1.30624100	3.84060700
H	-3.80005500	2.39763700	3.81024600
H	-4.84140000	1.05767500	4.36837600
N	-4.93317200	0.27624200	1.74604700
C	-2.99269200	-0.03787800	0.65234700
N	-4.31816600	-0.19155400	0.61773000
C	-5.09270200	-0.80122900	-0.42933400
C	-5.43234100	-0.03193300	-1.54449800
C	-5.47946300	-2.13287100	-0.25961900
C	-6.14624600	-0.67818500	-2.55415800
C	-6.19016500	-2.72758100	-1.29812000
C	-6.51690800	-2.01929300	-2.45664600
H	-6.42255900	-0.11091400	-3.43964500
H	-6.49981700	-3.76536300	-1.19936200
C	-5.06032100	1.42179300	-1.64025600
H	-5.33957600	1.95476200	-0.72466600

H	-3.97812200	1.52268300	-1.77810200
H	-5.57622800	1.89201600	-2.47986500
C	-5.16976000	-2.87772900	1.01262100
H	-5.39763500	-3.94017800	0.90231800
H	-4.11584300	-2.78186700	1.29832500
H	-5.76164400	-2.48219000	1.84487400
C	-7.24874400	-2.69428000	-3.58790400
H	-6.53969900	-3.08043500	-4.32835100
H	-7.84593000	-3.53677600	-3.22956800
H	-7.91335700	-1.99498900	-4.10209300
C	1.77094400	-2.00313200	1.31300200
C	0.43023000	-2.27849100	1.02234600
C	-0.36706400	-2.97288200	1.91521800
C	0.18331000	-3.40940600	3.12078200
C	1.50978500	-3.11057300	3.41791400
C	2.32021900	-2.40257300	2.52793200
C	1.40475400	-0.96969300	-0.70163900
C	0.04865000	-1.52393800	-0.21744600
H	-1.41018200	-3.17140900	1.68083700
H	-0.42154500	-3.96782300	3.82764700
H	1.93402400	-3.43332400	4.36379500
H	3.34557800	-2.18161900	2.79052500
O	-0.72845100	-0.40292300	0.17979500
O	1.53135400	-0.34074600	-1.72388200
N	2.38349700	-1.29242100	0.23782500

C	3.63114500	-0.49937100	0.42148600
C	3.23641700	0.62585300	1.39830700
C	3.65965800	0.70240500	2.72392600
C	2.29249600	1.55831800	0.93893800
C	3.18240800	1.71277900	3.56288200
H	4.36636700	-0.02019200	3.11852100
C	1.81522500	2.56196900	1.77197200
H	1.92293000	1.51049100	-0.08230300
C	2.27058400	2.64872100	3.08944600
H	3.53433300	1.76215100	4.58930900
H	1.09274900	3.27542800	1.38400300
H	1.91080000	3.44567300	3.73540900
C	4.15314200	0.04095800	-0.92845700
C	4.28914200	-0.83922900	-2.00765900
C	4.63575200	1.33973600	-1.05719300
C	4.85818200	-0.41913000	-3.19866100
H	3.92886200	-1.86042900	-1.90985800
C	5.21918100	1.76208200	-2.25430900
H	4.55279800	2.03895300	-0.23204900
C	5.33008700	0.88916500	-3.32706400
H	4.93791300	-1.11216100	-4.03052300
H	5.57591800	2.78379600	-2.34122700
H	5.78199700	1.21876500	-4.25809900
C	4.78348700	-1.40877900	0.87785700
C	5.96272900	-0.83336200	1.36148300

C	4.74992900	-2.78936100	0.67065900
C	7.06067200	-1.62436500	1.68197000
H	6.02675800	0.24590600	1.47056100
C	5.85151700	-3.58102600	0.98655200
H	3.85461300	-3.25224200	0.26536900
C	7.00749200	-3.00428500	1.50200100
H	7.96414400	-1.15800900	2.06277700
H	5.80094800	-4.65365700	0.82613700
H	7.86478200	-3.62178800	1.75114300
C	0.77494100	3.23294300	-2.97105500
C	0.30723300	4.40348200	-3.58560100
C	1.00650100	4.94975700	-4.67783400
C	2.14396400	4.29072700	-5.08963800
C	2.59717100	3.10632100	-4.44744400
C	1.92980700	2.54574300	-3.37989600
H	0.65353300	5.85409000	-5.16241400
H	2.71433900	4.67898100	-5.92802400
H	3.49956900	2.62478200	-4.81246700
H	2.25685000	1.63400500	-2.88772500
N	-0.82986100	4.82006300	-2.93825700
N	-1.06679500	3.98527400	-1.97477500
N	-0.13192400	3.03597900	-1.98459300
O	-0.09417100	2.07432800	-1.04465100
H	-2.84649000	-1.83212000	-1.88847000

IM5(RS)

NImag=0

Sum of electronic and zero-point Energies= -3189.607553

Sum of electronic and thermal Energies= -3189.547162

Sum of electronic and thermal Enthalpies= -3189.546218

Sum of electronic and thermal Free Energies= -3189.703774

C	-2.03034900	2.42471900	0.72289600
O	-2.76270900	2.75849200	1.62868100
C	-0.61807000	2.92248000	0.55733100
C	0.26042700	2.36588400	1.70195100
H	-0.20381500	2.63998900	-0.41173600
H	-0.30657600	2.50470500	2.63251000
H	-1.00180500	-0.41458300	0.70058900
C	1.57877600	3.09426600	1.84972700
C	2.33672600	3.49023400	0.74369700
C	2.05303900	3.39164600	3.13046400
C	3.52688900	4.18982300	0.92240300
H	2.00134500	3.25074200	-0.26217100
C	3.25258900	4.07193500	3.30909700
H	1.47271000	3.08300300	3.99629300
C	3.99119800	4.47890800	2.20165500
H	4.09952100	4.49823700	0.05441200
H	3.60486700	4.29000100	4.31283200
H	4.92550400	5.01655200	2.33414300
C	-7.91529500	0.59218300	2.52857800

C	-7.30150300	-0.65758100	2.60103200
C	-5.98225400	-0.78403500	2.17904100
C	-5.89578400	1.58389800	1.63397000
C	-7.22002300	1.70448400	2.05103700
H	-8.94750000	0.70190600	2.84708200
H	-7.84816800	-1.51963600	2.97291100
H	-5.33477100	2.44331000	1.27683100
H	-7.71404800	2.67001600	2.00612400
C	-5.29865200	0.33160300	1.69853700
C	-3.89225800	-0.05440900	1.29968400
C	-3.93691700	-1.61611300	1.21054300
H	-3.13815300	0.25974600	2.02585100
C	-5.08517500	-1.99978300	2.16608300
H	-2.97417200	-2.04184900	1.50166200
H	-5.57284500	-2.91384200	1.81724200
H	-4.68985700	-2.19521600	3.17043100
N	-3.50970800	0.51925100	0.01280400
O	-4.18843700	-2.12679000	-0.09409800
C	-3.90275400	-0.05374000	-1.15817000
C	-4.76348600	-1.26957400	-1.05197700
H	-5.79084300	-0.98101700	-0.78623900
H	-4.77544200	-1.80799400	-2.00040100
N	-3.36149400	0.54044400	-2.18472500
C	-2.64404000	1.48835800	-0.29685700
N	-2.57589600	1.50285700	-1.62436900

C	-1.81934400	2.42587200	-2.42523900
C	-2.16732800	3.78060600	-2.38053200
C	-0.74483600	1.92410400	-3.16489000
C	-1.35677000	4.66735300	-3.08440500
C	0.03306200	2.86173800	-3.84419500
C	-0.24902100	4.22668000	-3.81065400
H	-1.59878800	5.72762200	-3.06662700
H	0.89133100	2.50678800	-4.40983800
C	-3.36797500	4.27991100	-1.61343300
H	-4.20501400	3.57673400	-1.67193300
H	-3.14682500	4.44655900	-0.55273900
H	-3.70217700	5.23414600	-2.02682500
C	-0.44065600	0.45510500	-3.24637000
H	0.61099900	0.30385600	-3.49793800
H	-0.63594100	-0.06557100	-2.30358800
H	-1.05664300	-0.01061400	-4.02526200
C	0.60215900	5.20662300	-4.57626200
H	0.66544100	6.16743000	-4.05837500
H	1.61581500	4.82296600	-4.71624100
H	0.17776400	5.39277100	-5.56906800
C	2.24189000	-0.49654400	2.19063000
C	1.12369000	0.18653600	2.67460400
C	0.82202700	0.22668000	4.02190100
C	1.68235800	-0.39608700	4.92631500
C	2.82224000	-1.03450800	4.45123300

C	3.12100200	-1.09956100	3.08766700
C	1.29588700	0.46361700	0.33204900
C	0.38688700	0.83252800	1.53563500
H	-0.07384700	0.74172100	4.36115600
H	1.46816000	-0.37864000	5.98988300
H	3.50367300	-1.50941600	5.15045200
H	4.00825900	-1.62742700	2.76802400
O	-0.92505500	0.35989800	1.38664700
O	1.17844800	0.89975700	-0.79815400
N	2.26475300	-0.41963800	0.76247400
C	3.37219800	-0.87064000	-0.12321000
C	4.35699300	0.30682100	-0.20506400
C	5.26461700	0.55601900	0.82937900
C	4.29469800	1.21712600	-1.26592800
C	6.13622700	1.64001200	0.77081200
H	5.30541000	-0.11084600	1.68442700
C	5.17698200	2.29142300	-1.33284300
H	3.55470900	1.07498300	-2.04604800
C	6.11214300	2.49882100	-0.32324600
H	6.84016100	1.80555400	1.58069300
H	5.12729700	2.97186700	-2.17854200
H	6.80358900	3.33491900	-0.37844000
C	2.87700200	-1.33579200	-1.51014500
C	1.58678100	-1.81864200	-1.70980100
C	3.81246200	-1.47690400	-2.54000600

C	1.23100100	-2.41283300	-2.91810800
H	0.84434500	-1.71572300	-0.92911900
C	3.45461600	-2.05609900	-3.75271500
H	4.83522800	-1.14238500	-2.39027800
C	2.15963800	-2.52873900	-3.94745900
H	0.21747700	-2.78146000	-3.04940900
H	4.19742000	-2.15135900	-4.53925300
H	1.87992200	-2.99211900	-4.88882400
C	3.95300300	-2.18774200	0.42842400
C	5.31398500	-2.48268800	0.38827100
C	3.05591600	-3.17370000	0.85792700
C	5.77649000	-3.72813000	0.81743400
H	6.02330200	-1.74830600	0.02027700
C	3.51779300	-4.41039000	1.28449300
H	1.98679100	-2.97351200	0.86960300
C	4.88446200	-4.69087700	1.27446800
H	6.84119600	-3.94010800	0.78744000
H	2.79821400	-5.15164200	1.61822400
H	5.24823800	-5.65714300	1.61053500
C	-1.59256000	-3.50367700	-1.11197400
C	-1.08393200	-4.65693100	-0.49200100
C	-1.28563400	-5.91380100	-1.10051100
C	-1.97232800	-5.94095900	-2.29349600
C	-2.46532900	-4.75388400	-2.90748800
C	-2.28879600	-3.51640300	-2.33141600

H	-0.90201500	-6.81802600	-0.63944800
H	-2.14136500	-6.89064700	-2.79148900
H	-2.98738700	-4.83559000	-3.85621200
H	-2.62814800	-2.59093500	-2.78802200
N	-0.44151800	-4.29062200	0.65457500
N	-0.53234600	-2.98685400	0.75486600
N	-1.21444600	-2.50932600	-0.28105200
O	-1.40308400	-1.21031700	-0.46247300
H	-0.65196300	4.01499500	0.63415600

IM5(SR)

NImag=0

Sum of electronic and zero-point Energies= -3189.586326

Sum of electronic and thermal Energies= -3189.525779

Sum of electronic and thermal Enthalpies= -3189.524835

Sum of electronic and thermal Free Energies= -3189.683397

C	1.88413700	0.54816800	-0.53711000
O	2.02691000	1.48062900	-1.30305200
C	0.77929100	-0.45624300	-0.57755500
C	-0.32045300	-0.07708000	-1.57168300
H	0.36246300	-0.58182600	0.42602600
H	0.15887000	0.32162600	-2.47522900
H	0.20720600	2.38646700	-1.01396600
C	-1.16100200	-1.27496400	-1.98261800
C	-1.42676000	-2.31731300	-1.08957000

C	-1.70095200	-1.34377200	-3.27024800
C	-2.20658300	-3.40387600	-1.47937800
H	-1.01931900	-2.28916100	-0.08142700
C	-2.47920400	-2.43035400	-3.66225100
H	-1.50030900	-0.54112100	-3.97560400
C	-2.73383400	-3.46574200	-2.76621900
H	-2.39481400	-4.20803600	-0.77368400
H	-2.87824000	-2.46985400	-4.67155400
H	-3.33262700	-4.31926700	-3.06978200
C	4.56546700	6.10702700	0.38383800
C	5.75067300	5.46462400	0.03426100
C	5.72253400	4.10041600	-0.24144000
C	3.33200900	4.03443300	0.17678100
C	3.36471000	5.39764900	0.45828500
H	4.57551700	7.16916400	0.60873300
H	6.68457100	6.01797000	-0.01169100
H	2.40175900	3.47559100	0.23671100
H	2.45117000	5.91223800	0.73880400
C	4.51958000	3.40116000	-0.17675300
C	4.73255500	1.93858300	-0.50243600
C	6.29458500	1.75368100	-0.51586800
H	4.31443000	1.64027400	-1.46357800
C	6.86126200	3.18974800	-0.62601100
H	6.55821000	1.12125000	-1.36072100
H	7.73949400	3.29481100	0.01947100

H	7.18973100	3.38913600	-1.65256000
N	4.10577500	1.09115100	0.51623800
O	6.82035000	1.06476400	0.60720400
C	4.76272700	0.78412200	1.66588400
C	6.15448900	1.29909000	1.82544300
H	6.14002300	2.36715600	2.09052100
H	6.67182100	0.74104800	2.60620400
N	4.05914100	-0.01352700	2.41844400
C	2.93529800	0.43580000	0.54601200
N	2.91669800	-0.21826100	1.70738800
C	1.89697700	-1.06576300	2.27880700
C	0.80787800	-0.45048100	2.90427200
C	2.07590400	-2.44807200	2.20410200
C	-0.13470000	-1.28551300	3.49936600
C	1.11819500	-3.23184300	2.84620400
C	0.02580000	-2.67292100	3.50773000
H	-1.01276900	-0.84212900	3.96211900
H	1.23530200	-4.31334000	2.82401400
C	0.64304100	1.04592500	2.88831400
H	1.56814700	1.55346300	3.18419100
H	0.34619900	1.39745600	1.89149000
H	-0.15052100	1.34338800	3.57648800
C	3.18446400	-3.09349700	1.41872200
H	3.56434300	-3.97238400	1.94627400
H	2.78415900	-3.41698400	0.44801500

H	4.02492100	-2.41926600	1.23061100
C	-0.93709900	-3.56071300	4.25201300
H	-1.83111400	-3.00979100	4.54976100
H	-1.24240400	-4.41670900	3.64178300
H	-0.46452800	-3.95863200	5.15690400
C	-3.46651100	1.30446800	-1.68217100
C	-2.15656700	1.60518600	-2.05363300
C	-1.87769300	2.28462600	-3.22499500
C	-2.93842800	2.68037800	-4.04195600
C	-4.24496100	2.38129700	-3.66673300
C	-4.53237300	1.69123400	-2.48672300
C	-2.18883100	0.56218200	0.07147500
C	-1.21505300	1.07338200	-1.01224400
H	-0.84903000	2.50795100	-3.50108600
H	-2.74597600	3.21870800	-4.96398900
H	-5.06957000	2.68858500	-4.30238300
H	-5.55730100	1.46755800	-2.22302100
O	-0.45675600	2.08265100	-0.37386100
O	-1.84358300	0.23319200	1.18548600
N	-3.47682600	0.59971800	-0.44452800
C	-4.73556000	0.38578600	0.31315400
C	-5.25876000	1.79718500	0.64596100
C	-6.46216300	2.32720400	0.18554500
C	-4.41887700	2.61655800	1.41402100
C	-6.83133000	3.63584900	0.50197000

H	-7.12327300	1.73102000	-0.43407000
C	-4.78631000	3.91684800	1.73129600
H	-3.47171700	2.21877000	1.77234600
C	-6.00049700	4.43251500	1.27795200
H	-7.77258700	4.02809500	0.12916800
H	-4.12274500	4.53122500	2.33205800
H	-6.28872100	5.44988300	1.52398400
C	-4.50535600	-0.45895700	1.58624800
C	-3.91741200	-1.72188400	1.45016900
C	-5.01002700	-0.08278100	2.82654400
C	-3.81113000	-2.57359100	2.53589400
H	-3.54819300	-2.03234800	0.47631800
C	-4.91291300	-0.94650100	3.92086900
H	-5.49027000	0.88083200	2.95490500
C	-4.31560200	-2.19041900	3.78189500
H	-3.34677100	-3.54780400	2.41058900
H	-5.31824400	-0.63778500	4.87981600
H	-4.25458100	-2.86723800	4.62958500
C	-5.69138700	-0.49442500	-0.51445600
C	-7.00181400	-0.69263500	-0.06516000
C	-5.24362400	-1.22750600	-1.61396100
C	-7.86286400	-1.55040300	-0.73902200
H	-7.34084600	-0.18775000	0.83584000
C	-6.10455100	-2.09459100	-2.28349500
H	-4.21527100	-1.13768400	-1.95138500

C	-7.41938900	-2.24977600	-1.85998700
H	-8.87768000	-1.68395000	-0.37691600
H	-5.73089200	-2.65096000	-3.13840100
H	-8.08996800	-2.92272100	-2.38557500
C	4.73536200	-3.14986700	-1.56288900
C	5.71470200	-2.18109800	-1.28319900
C	7.06699600	-2.57343300	-1.16216500
C	7.35448800	-3.90851200	-1.32364900
C	6.34196000	-4.87431800	-1.60027500
C	5.01978400	-4.51521400	-1.72247000
H	7.83571500	-1.83949600	-0.93977500
H	8.38237600	-4.24794600	-1.23523300
H	6.63004500	-5.91481300	-1.71410900
H	4.22541000	-5.22391600	-1.92967700
N	5.10895600	-0.97611400	-1.15220000
N	3.80917500	-1.17416900	-1.34919400
N	3.56397500	-2.45248500	-1.58374400
O	2.36820300	-2.93194000	-1.71022500
H	1.25336300	-1.41572600	-0.87678400

IM5(SS)

NImag=0

Sum of electronic and zero-point Energies= -3189.585039

Sum of electronic and thermal Energies= -3189.524173

Sum of electronic and thermal Enthalpies= -3189.523229

Sum of electronic and thermal Free Energies= -3189.681719

C	-1.75289000	-0.35352400	-0.27218800
O	-1.58591800	-0.85714100	-1.36129800
C	-0.90119200	0.69690300	0.37313300
C	0.44305900	0.91503200	-0.32137500
H	-0.81220700	0.46651900	1.43902500
H	0.27216100	0.83713300	-1.40357200
H	0.52818400	-1.50408600	-1.08170300
C	1.03554800	2.28635100	-0.04986200
C	0.89528800	2.91239900	1.19221300
C	1.76209000	2.93577500	-1.05181800
C	1.46373200	4.16008400	1.42704900
H	0.33487500	2.42529500	1.98579000
C	2.32149800	4.18925900	-0.82075200
H	1.88147900	2.45942800	-2.02161400
C	2.17780700	4.80325000	0.41963900
H	1.34037700	4.63242000	2.39694400
H	2.86870500	4.68335700	-1.61631100
H	2.61347000	5.78199600	0.59809300
C	-5.42031500	-4.57527100	-3.40375700
C	-6.36154600	-3.54911200	-3.36251200
C	-6.03796700	-2.36337400	-2.70945200
C	-3.83792800	-3.23297300	-2.15690200
C	-4.16714300	-4.42001000	-2.80660000
H	-5.66301200	-5.50677200	-3.90596600

H	-7.33515800	-3.67552800	-3.82779600
H	-2.86121900	-3.09154000	-1.70137100
H	-3.44447800	-5.22856700	-2.85395700
C	-4.78681000	-2.21766600	-2.11485800
C	-4.65787900	-0.85694800	-1.46676000
C	-6.11694500	-0.27322700	-1.47760400
H	-3.97421700	-0.19074600	-1.99481000
C	-6.86736300	-1.11514700	-2.53533900
H	-6.08898600	0.78701100	-1.73136200
H	-7.89136200	-1.30953500	-2.20031600
H	-6.93315000	-0.56007700	-3.47802600
N	-4.18381800	-0.98461700	-0.08650400
O	-6.75758800	-0.31941100	-0.20994600
C	-5.02474600	-1.39204700	0.90764200
C	-6.47840200	-1.46075000	0.57013900
H	-6.71537000	-2.39484400	0.04024600
H	-7.07665700	-1.39954300	1.47957000
N	-4.39099700	-1.56479000	2.03015400
C	-2.98618200	-0.80648900	0.48044000
N	-3.10483200	-1.22098500	1.73969600
C	-2.07908700	-1.43678000	2.72575700
C	-1.23600300	-2.54241500	2.55673500
C	-2.03548100	-0.59793100	3.84392800
C	-0.30072000	-2.78959500	3.55787000
C	-1.08229800	-0.90115200	4.81948100

C	-0.21448800	-1.98569500	4.69644900
H	0.37296800	-3.63634300	3.44908900
H	-1.02707600	-0.26903000	5.70270700
C	-1.34220700	-3.43835900	1.34985700
H	-2.38686600	-3.65639100	1.10258700
H	-0.86464400	-2.97228400	0.48155500
H	-0.83172700	-4.38511400	1.53782800
C	-2.96415000	0.57487500	3.99043400
H	-2.80852100	1.05626400	4.95853400
H	-2.81958900	1.30665000	3.18812200
H	-4.00861800	0.25780400	3.91772900
C	0.80945800	-2.29371700	5.75769500
H	0.64850300	-3.29123100	6.17900000
H	1.81903400	-2.27115000	5.33382400
H	0.76550700	-1.56946700	6.57520800
C	3.52165100	-0.01761800	1.15358600
C	2.13466100	-0.12206700	1.34452100
C	1.58710700	-0.08184000	2.61265400
C	2.42265800	0.12546800	3.71168600
C	3.78765400	0.29305300	3.51292500
C	4.35962300	0.22070700	2.23944500
C	2.65099000	-0.10343500	-0.95855800
C	1.45589300	-0.20776700	0.00715300
H	0.51927000	-0.20230200	2.76042900
H	1.99881400	0.17917600	4.71012300

H	4.43832800	0.48223700	4.36138600
H	5.42843300	0.34288400	2.12787700
O	0.87799900	-1.49269400	-0.17186600
O	2.54612600	-0.04109400	-2.16451500
N	3.82208400	-0.16854900	-0.23044600
C	5.13239500	-0.09912900	-0.92037200
C	5.28521800	1.35873400	-1.38556400
C	5.58165000	2.35139200	-0.44342800
C	5.01473900	1.74899800	-2.69899400
C	5.69256700	3.68449700	-0.81996000
H	5.73744200	2.08056200	0.59701300
C	5.12375900	3.08634800	-3.07701700
H	4.71063400	1.00711700	-3.42880700
C	5.48608600	4.05429200	-2.14685000
H	5.93293800	4.43493600	-0.07293100
H	4.92215400	3.36608800	-4.10669700
H	5.58141600	5.09401600	-2.44655700
C	5.19933600	-1.13474300	-2.06520100
C	4.37824800	-2.26249500	-2.10546600
C	6.23522500	-1.03047000	-2.99680600
C	4.56467200	-3.23915300	-3.07926900
H	3.57926100	-2.38632900	-1.38054900
C	6.41855500	-2.00354400	-3.97348500
H	6.91027900	-0.17992900	-2.95640000
C	5.57926400	-3.11236400	-4.02237700

H	3.90719300	-4.10294000	-3.09910900
H	7.22414800	-1.89461500	-4.69309800
H	5.71899300	-3.87333600	-4.78372400
C	6.25510000	-0.59183700	0.01265600
C	7.49734900	0.03462000	0.08941800
C	6.06225100	-1.78850700	0.71385500
C	8.51053300	-0.49901300	0.88806900
H	7.68533700	0.94442600	-0.47047100
C	7.06639100	-2.31530500	1.51253600
H	5.10805900	-2.30307200	0.63767700
C	8.29766800	-1.66687900	1.60886800
H	9.46962300	0.00736800	0.94004900
H	6.88952500	-3.23694900	2.05832500
H	9.08519300	-2.07749100	2.23310200
C	-5.24719100	2.86863200	0.05044600
C	-5.26241900	3.18003600	-1.32138300
C	-6.26749800	4.03442700	-1.82817300
C	-7.19322400	4.52451000	-0.93675200
C	-7.15611100	4.19314900	0.44951400
C	-6.18826700	3.36514900	0.96737800
H	-6.29308100	4.29019600	-2.88264200
H	-7.97802000	5.18632900	-1.29068400
H	-7.91346000	4.60970000	1.10660700
H	-6.13512000	3.09594300	2.01638100
N	-4.23684700	2.52784800	-1.93326300

N	-3.59607100	1.85663500	-0.99533300
N	-4.18041900	2.03936500	0.18539200
O	-3.73950600	1.46538300	1.27417900
H	-1.52198700	1.60210200	0.33093700

IM6(RR)

NImag=0

Sum of electronic and zero-point Energies= -3189.597569

Sum of electronic and thermal Energies= -3189.536935

Sum of electronic and thermal Enthalpies= -3189.535991

Sum of electronic and thermal Free Energies= -3189.695423

C	2.22179100	-0.35193500	0.31242400
O	2.38718600	-0.37470200	1.51160700
C	0.94248500	-0.04593700	-0.39115500
C	-0.22789000	0.12536500	0.57249400
H	1.11282200	0.85709800	-1.00144700
H	0.10051000	0.69888300	1.44538200
H	-0.16464600	2.47929200	-0.81993500
C	-0.70480900	-1.23260400	1.04679100
C	-1.16889800	-2.20219000	0.14700700
C	-0.63449300	-1.55982500	2.40317000
C	-1.56857300	-3.45762400	0.60051200
H	-1.22466800	-1.97166400	-0.91646100
C	-1.01975600	-2.82011100	2.85552400
H	-0.27131100	-0.81481700	3.10544800

C	-1.49647800	-3.77085500	1.95678400
H	-1.94025700	-4.19253800	-0.10908900
H	-0.95109100	-3.05634000	3.91358700
H	-1.80822500	-4.74943700	2.30858800
C	6.77476100	-3.00184200	3.74357300
C	7.53537900	-1.89620400	3.37056800
C	6.97427200	-0.94829100	2.51925600
C	4.89982100	-2.20841300	2.43373200
C	5.46691000	-3.15819000	3.27910000
H	7.20249000	-3.75012000	4.40376000
H	8.55194300	-1.77853100	3.73520800
H	3.87647200	-2.31133300	2.08385700
H	4.88657500	-4.02337500	3.58340500
C	5.66923100	-1.11090600	2.06049900
C	5.27345200	0.03466400	1.15627700
C	6.61046700	0.81482100	0.88831300
H	4.53103800	0.70329900	1.59104600
C	7.58298300	0.32496700	1.98687700
H	6.40386500	1.88253300	0.93241300
H	8.58380600	0.18879300	1.56433800
H	7.66813400	1.07567400	2.78076700
N	4.71385700	-0.46847000	-0.10495200
O	7.14701300	0.62195900	-0.41304900
C	5.52670200	-0.88796900	-1.11546200
C	6.99458100	-0.67343500	-0.94463000

H	7.42537100	-1.44620800	-0.29042400
H	7.49344600	-0.70258100	-1.91384000
N	4.83926100	-1.33902500	-2.12653700
C	3.45336800	-0.64909300	-0.52208800
N	3.54433800	-1.18788500	-1.73549800
C	2.47194500	-1.63320000	-2.58729900
C	1.79091600	-2.80133800	-2.22810800
C	2.13674800	-0.84682500	-3.69099000
C	0.72057800	-3.18305900	-3.03140100
C	1.06734700	-1.29070500	-4.47026600
C	0.34467100	-2.44005800	-4.15411600
H	0.16221900	-4.07945600	-2.77027600
H	0.78239500	-0.70251400	-5.33953300
C	2.13417800	-3.56582600	-0.97518600
H	3.21566100	-3.64012200	-0.82177900
H	1.69176500	-3.08647500	-0.08966700
H	1.72528000	-4.57730200	-1.02410900
C	2.82864600	0.45655600	-3.98424500
H	2.63942700	0.75634600	-5.01756000
H	2.43879000	1.24280800	-3.32199000
H	3.90881500	0.38951700	-3.83446900
C	-0.84443400	-2.86022700	-4.97603900
H	-1.77166000	-2.57389700	-4.46663000
H	-0.84028600	-2.37728100	-5.95660400
H	-0.86076500	-3.94374700	-5.12457800

C	-3.20514400	0.21290400	-1.21229700
C	-1.86690200	0.59444100	-1.38999400
C	-1.28115700	0.59381800	-2.64457900
C	-2.04096000	0.18060200	-3.74282200
C	-3.36597600	-0.20056600	-3.56474700
C	-3.97069800	-0.18437100	-2.30440600
C	-2.54686900	1.01513800	0.83310800
C	-1.30004200	1.05658300	-0.07180700
H	-0.25974600	0.94618400	-2.77532800
H	-1.60295500	0.17988500	-4.73679500
H	-3.95950500	-0.50498800	-4.42217700
H	-5.00580500	-0.47845600	-2.20173300
O	-0.82089700	2.37021200	-0.08468700
O	-2.60307900	1.47794000	1.94476300
N	-3.56595200	0.32939200	0.15651300
C	-4.95874300	0.26497800	0.67113900
C	-5.62253500	1.58993600	0.25992200
C	-6.41207500	1.71082700	-0.88561700
C	-5.30255000	2.75299200	0.97469600
C	-6.88952000	2.95450800	-1.29621700
H	-6.67032000	0.83221400	-1.46665300
C	-5.77909600	3.99212400	0.56389300
H	-4.66346300	2.68015900	1.84890900
C	-6.57870700	4.09881800	-0.57199700
H	-7.50344000	3.02117200	-2.18939800

H	-5.51763700	4.87886000	1.13303400
H	-6.94993900	5.06744100	-0.89266200
C	-4.95602900	0.01493500	2.19518500
C	-4.05862300	-0.91277800	2.73088800
C	-5.94059800	0.55104100	3.02066900
C	-4.11309900	-1.25716500	4.07245500
H	-3.30653000	-1.36436500	2.08951300
C	-6.00173000	0.19680200	4.36897900
H	-6.66525300	1.25307700	2.62057300
C	-5.08599400	-0.70076400	4.90261900
H	-3.39263100	-1.96773100	4.46770800
H	-6.77174600	0.63116200	4.99967700
H	-5.13072600	-0.97042700	5.95345900
C	-5.67192200	-1.00158000	0.16217700
C	-7.06666900	-1.07898700	0.19208600
C	-4.94791100	-2.14993900	-0.16600600
C	-7.72155300	-2.26048300	-0.14284600
H	-7.64614400	-0.21020800	0.49059900
C	-5.60186900	-3.33181700	-0.49812200
H	-3.86310700	-2.11808200	-0.16212400
C	-6.99230500	-3.39225000	-0.49597900
H	-8.80649200	-2.29555800	-0.11816700
H	-5.01760200	-4.21065000	-0.75553200
H	-7.50332100	-4.31421600	-0.75569000
C	2.44519500	4.04624300	-0.42851300

C	3.65623400	3.82927700	0.24888800
C	4.18510700	4.84685200	1.07271600
C	3.46661900	6.01439000	1.17458800
C	2.23410100	6.20599900	0.48494200
C	1.70093800	5.23311800	-0.32694200
H	5.12342100	4.70374300	1.59964500
H	3.84058300	6.81917300	1.80008200
H	1.70763800	7.14670200	0.61101500
H	0.76211300	5.34935900	-0.85646800
N	4.10612900	2.58105800	-0.05135400
N	3.23331700	2.04110800	-0.87947500
N	2.24380200	2.89208100	-1.11427800
O	1.22976400	2.58661800	-1.89552200
H	0.72261700	-0.83700200	-1.11458300

IM6(RS)

NImag=0

Sum of electronic and zero-point Energies= -2718.843236

Sum of electronic and thermal Energies= -2718.791407

Sum of electronic and thermal Enthalpies= -2718.790462

Sum of electronic and thermal Free Energies= -2718.929238

C	2.23489900	-0.34260900	1.60086300
O	3.22540600	-0.04828400	2.34845800
C	1.70741100	-1.82129700	1.55695000
C	0.29683200	-1.78974400	2.14673700

H	1.68707700	-2.21357300	0.53916900
H	0.37228600	-1.81226700	3.24057500
C	-0.68838300	-2.85248700	1.71287900
C	-0.72931800	-3.35117500	0.40507400
C	-1.63396900	-3.32451300	2.63054300
C	-1.67120200	-4.30873600	0.03748000
H	-0.03059500	-2.98564500	-0.34181700
C	-2.57632600	-4.28237900	2.26552600
H	-1.62447900	-2.93461300	3.64571900
C	-2.59482400	-4.78334700	0.96569300
H	-1.68100900	-4.68159100	-0.98304600
H	-3.29282500	-4.64058600	2.99925200
H	-3.32414800	-5.53494100	0.67764100
C	3.70634500	5.63210500	1.90256700
C	2.82462100	5.87261700	0.85086700
C	2.13418000	4.79754800	0.29786100
C	3.20803000	3.25740800	1.85498100
C	3.89611800	4.33947300	2.39957900
H	4.25502300	6.46055600	2.34113700
H	2.68463200	6.87946900	0.46669300
H	3.34071800	2.23809700	2.22567100
H	4.58920400	4.17671000	3.21914600
C	2.33409600	3.51658400	0.80275100
C	1.49063000	2.50496500	0.06707300
C	0.87029600	3.29388100	-1.14308400

H	0.71602300	2.09287900	0.71194700
C	1.12723100	4.78938800	-0.82681600
H	-0.19752300	3.07820900	-1.21352800
H	1.47446900	5.30423000	-1.72962400
H	0.19112300	5.27413700	-0.52480400
N	2.30719000	1.38090100	-0.39402100
O	1.38162900	2.91588800	-2.41215200
C	2.99431400	1.46182800	-1.57404500
C	2.77336900	2.66820300	-2.42215000
H	3.34052800	3.52998600	-2.04025100
H	3.07320700	2.46656000	-3.45095800
N	3.66203100	0.37793400	-1.81404700
C	2.55924800	0.17228600	0.14510900
N	3.39390400	-0.40979800	-0.72352400
C	3.94317800	-1.73853500	-0.68489000
C	5.10153600	-1.97144700	0.05726300
C	3.30621500	-2.72306000	-1.44844400
C	5.59183100	-3.27857000	0.06756800
C	3.83713900	-4.00860200	-1.40162600
C	4.96960800	-4.30545000	-0.63973200
H	6.48988600	-3.49384900	0.64179000
H	3.35579800	-4.79745600	-1.97556500
C	5.79631300	-0.85655600	0.78911900
H	6.04693900	-0.04467000	0.09682700
H	5.13546500	-0.45105200	1.56460000

H	6.72201500	-1.21828100	1.24256200
C	2.10794200	-2.39322900	-2.30029700
H	1.63231100	-3.30700000	-2.66671100
H	1.35891500	-1.80497700	-1.75845600
H	2.40684500	-1.79314800	-3.16747100
C	5.49820800	-5.71568700	-0.57701100
H	6.55895800	-5.73085900	-0.31354200
H	4.96001400	-6.29714800	0.17982800
H	5.37435200	-6.22793300	-1.53531200
C	-2.41355200	0.34475600	1.74797200
C	-1.33085000	0.14295100	2.60802900
C	-1.43659600	0.38221700	3.96564400
C	-2.65727000	0.82819900	4.47528100
C	-3.73375000	1.03032400	3.61538300
C	-3.63195200	0.79909600	2.24121200
C	-0.67632100	-0.23355400	0.37410900
C	-0.15580000	-0.33917800	1.81815600
H	-0.56983300	0.24236800	4.60604200
H	-2.76497600	1.02852500	5.53623700
H	-4.67963400	1.38525900	4.01277200
H	-4.47928800	0.98389500	1.59238000
O	0.99268100	0.43625600	1.98055300
O	0.04046800	-0.38272700	-0.59719900
N	-2.02057100	0.08528400	0.39738100
C	-2.91582000	0.23345300	-0.77955400

C	-4.23624500	-0.49627900	-0.42753900
C	-5.49378400	-0.02397500	-0.80510400
C	-4.17074300	-1.68672900	0.30933700
C	-6.65073000	-0.72796700	-0.47085200
H	-5.59489300	0.91262000	-1.33929100
C	-5.32303700	-2.38968200	0.63840500
H	-3.20791100	-2.06551100	0.64289900
C	-6.57265600	-1.91429700	0.24806400
H	-7.61664600	-0.33443500	-0.77290400
H	-5.23422500	-3.30751900	1.21213500
H	-7.47468100	-2.45812500	0.51113300
C	-2.25954600	-0.44146600	-2.01887300
C	-1.39378200	0.28992500	-2.84224700
C	-2.44999900	-1.79291700	-2.30124200
C	-0.72944600	-0.31206000	-3.90065200
H	-1.19683700	1.33654100	-2.63406400
C	-1.77887400	-2.40245900	-3.36244300
H	-3.11853300	-2.39387300	-1.69698400
C	-0.91626200	-1.66804300	-4.16567400
H	-0.05147200	0.28017100	-4.50787000
H	-1.94702400	-3.45717900	-3.56166900
H	-0.39584000	-2.14376400	-4.99187500
C	-3.13728700	1.72767600	-1.08307400
C	-3.76751100	2.09634900	-2.28037900
C	-2.69526800	2.74419700	-0.23568200

C	-3.97561400	3.43091000	-2.60348000
H	-4.07182400	1.32263400	-2.98025700
C	-2.90334100	4.08722800	-0.55893100
H	-2.17609100	2.50677400	0.68610600
C	-3.54690700	4.43688600	-1.73881100
H	-4.46361400	3.68555100	-3.53926300
H	-2.55569400	4.85673900	0.12442500
H	-3.70712200	5.48084600	-1.98945800
H	2.39582000	-2.42859500	2.14759200

IM6(SR)

NImag=0

Sum of electronic and zero-point Energies= -2718.841870

Sum of electronic and thermal Energies= -2718.789946

Sum of electronic and thermal Enthalpies= -2718.789002

Sum of electronic and thermal Free Energies= -2718.927920

C	2.22247500	0.63950700	1.39194400
O	2.85210300	0.41674900	2.48629700
C	1.34258900	1.90084000	1.30684400
C	0.09556200	1.40925000	2.02803900
H	1.82164600	2.74804700	1.80347000
H	0.37771700	1.19461300	3.06641600
H	1.09845200	2.15794200	0.27101000
C	-1.10834500	2.31964700	2.01818100
C	-1.13684000	3.49552200	1.26376600

C	-2.22716100	2.00209900	2.80000100
C	-2.25322800	4.33024800	1.28656700
H	-0.27973300	3.77172600	0.65705200
C	-3.35090100	2.82330800	2.80532900
H	-2.21151400	1.10190000	3.41146700
C	-3.36922100	3.99203300	2.04544000
H	-2.24892300	5.24662700	0.70308000
H	-4.21113900	2.55497500	3.41253100
H	-4.24279000	4.63646700	2.05459100
C	2.19118400	-5.40097000	-1.08938700
C	3.40779800	-5.42343700	-0.41120000
C	3.86477800	-4.25148300	0.18147900
C	1.89614400	-3.04887000	-0.58059800
C	1.44192100	-4.22576300	-1.17244100
H	1.82054700	-6.30812900	-1.55771100
H	3.99031200	-6.33871000	-0.34939300
H	1.31595400	-2.13092200	-0.62707600
H	0.49081100	-4.22608800	-1.69446600
C	3.11308200	-3.08067300	0.09271600
C	3.80487700	-1.95508300	0.82975100
C	5.25704200	-2.49258200	1.07167200
H	3.31330400	-1.68462600	1.77037400
C	5.12086100	-4.02625600	0.98752200
H	5.62727900	-2.15705300	2.04144000
H	6.02161700	-4.45834400	0.54120500

H	5.01531800	-4.45155700	1.99288100
N	3.86909500	-0.72104000	0.05461100
O	6.22361600	-2.00584200	0.14119600
C	4.78234900	-0.53975700	-0.94248100
C	5.75275400	-1.65521400	-1.14723500
H	5.27604200	-2.50313000	-1.65730600
H	6.61045900	-1.31573600	-1.72823600
N	4.73003900	0.66773900	-1.42249500
C	3.19886900	0.42992600	0.21145800
N	3.72251500	1.25509400	-0.69202300
C	3.44382400	2.65748800	-0.82969500
C	2.58342700	3.07462900	-1.84363800
C	4.01418500	3.51986100	0.10992800
C	2.29922900	4.43815100	-1.91017800
C	3.69529300	4.87134300	0.00122500
C	2.84555600	5.34534800	-1.00077300
H	1.62477400	4.79599900	-2.68452100
H	4.11610700	5.57056900	0.72015600
C	1.94568200	2.07452200	-2.76920000
H	2.69794900	1.41965600	-3.21988000
H	1.23209900	1.44732800	-2.21971600
H	1.40313000	2.58296300	-3.56901800
C	4.90171900	2.98883300	1.20618000
H	5.29524200	3.81024200	1.80882000
H	4.35860300	2.30059000	1.86902300

H	5.74953900	2.43716900	0.78446700
C	2.54326000	6.81821400	-1.10707300
H	1.61590600	6.99504700	-1.65779200
H	2.44773800	7.27435500	-0.11777200
H	3.34859200	7.34118600	-1.63444100
C	-2.08852400	-1.25116600	1.53616100
C	-0.86425900	-0.98490900	2.15728700
C	-0.47787000	-1.61598700	3.32284700
C	-1.34858600	-2.54371000	3.89828400
C	-2.56700300	-2.81476400	3.28301700
C	-2.95693400	-2.18285500	2.09769100
C	-0.96379100	0.11633600	0.08047500
C	-0.09362700	0.01143400	1.35057400
H	0.49964100	-1.39189900	3.74475500
H	-1.07409700	-3.06101600	4.81176800
H	-3.24202100	-3.54142000	3.72506700
H	-3.91410000	-2.42166300	1.65536600
O	1.19786300	-0.42671700	1.02766600
O	-0.61301800	0.61289800	-0.96838500
N	-2.20170400	-0.46875200	0.34498900
C	-3.22276100	-0.67167900	-0.71498000
C	-2.77572400	-1.90648300	-1.51620100
C	-3.19886300	-3.19565300	-1.18217000
C	-1.82673000	-1.76268500	-2.53818900
C	-2.73222700	-4.30672200	-1.88171000

H	-3.91767400	-3.34186600	-0.38366000
C	-1.36534600	-2.87110000	-3.24019900
H	-1.45515500	-0.77277700	-2.78105500
C	-1.82775900	-4.14775900	-2.92538200
H	-3.08654900	-5.29642500	-1.61027600
H	-0.63998000	-2.73489500	-4.03693000
H	-1.47593800	-5.01159800	-3.48250200
C	-3.37627900	0.59792000	-1.58143100
C	-3.27544800	1.86172200	-0.99695000
C	-3.80961000	0.50275600	-2.90375500
C	-3.55583500	3.00495300	-1.73331600
H	-2.97409800	1.95395300	0.04254900
C	-4.09347400	1.65027800	-3.64159400
H	-3.93107200	-0.47055600	-3.36889700
C	-3.96235600	2.90667200	-3.06252100
H	-3.45870900	3.97636900	-1.25777800
H	-4.42362100	1.55407200	-4.67167800
H	-4.18456600	3.80108700	-3.63663700
C	-4.62779800	-0.78426700	-0.09285100
C	-5.65616300	-1.44616000	-0.76666700
C	-4.93736400	-0.08097700	1.07457500
C	-6.95250500	-1.44912500	-0.25734700
H	-5.44814100	-1.96025300	-1.70009700
C	-6.23085500	-0.08503100	1.58352800
H	-4.15633900	0.46822700	1.59176200

C	-7.24444800	-0.77670200	0.92477400
H	-7.73580900	-1.97682400	-0.79293800
H	-6.44651000	0.45835400	2.49881600
H	-8.25418500	-0.78207300	1.32340800

IM6(SS)

NImag=0

Sum of electronic and zero-point Energies= -2718.833140

Sum of electronic and thermal Energies= -2718.781086

Sum of electronic and thermal Enthalpies= -2718.780142

Sum of electronic and thermal Free Energies= -2718.919506

C	-2.15011000	0.14193700	1.50606600
O	-2.26413400	0.59707400	2.68846300
C	-2.34861500	-1.37236900	1.25404300
C	-0.93082500	-1.92901500	1.34513000
H	-3.02161400	-1.78344500	2.00996700
H	-0.59620800	-1.84458000	2.38768200
H	-2.77195300	-1.57031100	0.26406300
C	-0.70220400	-3.33896500	0.84944200
C	-1.72980400	-4.10861200	0.30096500
C	0.58345400	-3.89287600	0.91759200
C	-1.48211800	-5.39373900	-0.17810500
H	-2.73962500	-3.70931600	0.24940900
C	0.83111500	-5.17356700	0.43703600
H	1.39744100	-3.32481900	1.36686000

C	-0.20081300	-5.92938000	-0.11603600
H	-2.29675900	-5.97623200	-0.59941300
H	1.83595200	-5.57977700	0.50166500
H	-0.00738100	-6.93054300	-0.48964000
C	1.13702100	4.40036900	-2.15637000
C	0.69675500	5.25554400	-1.14707000
C	-0.16365700	4.75933200	-0.17308300
C	-0.12914400	2.56313900	-1.20962400
C	0.72345200	3.06656500	-2.19164900
H	1.79835000	4.78033800	-2.92980100
H	1.01059900	6.29559600	-1.12988500
H	-0.45271300	1.52657400	-1.22509400
H	1.07259200	2.40699500	-2.98200600
C	-0.56225000	3.42400200	-0.20576100
C	-1.50971900	3.12675600	0.93888600
C	-1.92912800	4.54149400	1.46076800
H	-1.05817400	2.52303100	1.73174900
C	-0.78988600	5.47571000	0.99901500
H	-2.04150200	4.52729300	2.54563200
H	-1.19073500	6.46375000	0.75329500
H	-0.06036500	5.60844000	1.80725200
N	-2.68587300	2.39689100	0.48281700
O	-3.19848000	4.98261500	0.98471500
C	-3.70564400	3.01943400	-0.17449400
C	-3.60913100	4.50614100	-0.28255800

H	-2.90576200	4.79172400	-1.07740600
H	-4.58768100	4.93853800	-0.49296600
N	-4.64586500	2.18149900	-0.49754500
C	-2.98694100	1.09148500	0.58129800
N	-4.17339400	0.98101200	-0.01866500
C	-4.90585200	-0.23592400	-0.21227900
C	-4.87314900	-0.82291600	-1.47941900
C	-5.54010600	-0.81024000	0.89017500
C	-5.48358500	-2.06690000	-1.62037100
C	-6.13509000	-2.05720000	0.69464200
C	-6.10397100	-2.70256700	-0.54168900
H	-5.46782600	-2.55482100	-2.59242400
H	-6.63035600	-2.53807200	1.53486700
C	-4.20156700	-0.13118700	-2.63726600
H	-4.77253200	0.75054600	-2.94517800
H	-3.19361400	0.21035600	-2.37463400
H	-4.11901000	-0.80699200	-3.49200400
C	-5.56291000	-0.11259600	2.22552600
H	-6.14855200	-0.69060400	2.94374200
H	-4.55390000	0.03549000	2.63408400
H	-6.02122600	0.87791900	2.12891000
C	-6.70533100	-4.07483300	-0.70764300
H	-7.14114800	-4.20036000	-1.70245000
H	-5.93923000	-4.84829200	-0.58233700
H	-7.48519200	-4.25824600	0.03565400

C	1.41085400	-0.73835200	-1.21407400
C	0.07264500	-1.03027000	-0.90106900
C	-0.83388000	-1.36901100	-1.88988900
C	-0.41291700	-1.41464400	-3.22065900
C	0.91376800	-1.13820600	-3.52672000
C	1.84471800	-0.80502800	-2.53763400
C	1.31021100	-0.70813100	1.07656800
C	-0.13569200	-0.85287300	0.58281500
H	-1.85880000	-1.62527400	-1.63345900
H	-1.11207200	-1.68330700	-4.00621500
H	1.25174300	-1.18863700	-4.55744700
H	2.87006500	-0.61254100	-2.82183300
O	-0.77682100	0.37233200	0.87168600
O	1.67912800	-0.80850300	2.22174200
N	2.11993300	-0.41295500	-0.02056700
C	3.58943500	-0.35506500	0.17876500
C	4.01349600	-1.80086000	0.49015000
C	4.01836100	-2.74836400	-0.54159300
C	4.21962000	-2.24260200	1.79965800
C	4.26437000	-4.09135800	-0.27821300
H	3.82081000	-2.43619500	-1.56283600
C	4.46419400	-3.58899100	2.06383600
H	4.15553100	-1.53715800	2.61989300
C	4.49691500	-4.51654400	1.02799100
H	4.26562800	-4.80626300	-1.09568700

H	4.61964300	-3.91032800	3.08916800
H	4.69091100	-5.56470700	1.23661100
C	3.93981900	0.66039200	1.28575200
C	3.06615700	1.67880400	1.66856700
C	5.23896400	0.66257200	1.79785100
C	3.47702800	2.65687200	2.56904000
H	2.05561800	1.71139100	1.27056500
C	5.64703300	1.63650500	2.70263600
H	5.94123800	-0.10409200	1.48009500
C	4.76475100	2.63875200	3.09539000
H	2.77851700	3.43459900	2.86356300
H	6.65944600	1.61357700	3.09439800
H	5.08031400	3.40082600	3.80133800
C	4.27027700	0.26151200	-1.05374100
C	5.44608400	-0.24716700	-1.60055700
C	3.74091300	1.44701100	-1.57694000
C	6.05257800	0.38847600	-2.68590400
H	5.89611700	-1.14491700	-1.18998800
C	4.33858900	2.07358000	-2.66029000
H	2.84344000	1.87108400	-1.13383700
C	5.49712400	1.54057700	-3.22757000
H	6.96487000	-0.02602700	-3.10402900
H	3.90213600	2.98569900	-3.05797300
H	5.96785600	2.02918100	-4.07505000

TS6(RR)

NImag=1 (-199.1186)

Sum of electronic and zero-point Energies= -2718.826635

Sum of electronic and thermal Energies= -2718.774660

Sum of electronic and thermal Enthalpies= -2718.773716

Sum of electronic and thermal Free Energies= -2718.914292

C	2.03330300	-0.51256900	1.26760900
O	2.69912800	-0.23581400	2.26279300
C	1.62488700	-1.94803200	0.87987600
C	0.10766200	-1.88223500	1.04176200
H	1.90195200	-2.18569500	-0.15056100
H	-0.10704200	-1.79393300	2.11458200
C	-0.74802800	-2.98384300	0.47427400
C	-0.60204900	-3.46250200	-0.83235000
C	-1.75707600	-3.52942400	1.27350800
C	-1.44966400	-4.45272600	-1.32341200
H	0.17271200	-3.05544600	-1.47611500
C	-2.60850100	-4.51735800	0.78572700
H	-1.87555400	-3.16467000	2.29171800
C	-2.45514300	-4.98298600	-0.51725500
H	-1.32237300	-4.81153900	-2.34039200
H	-3.38930900	-4.92078400	1.42352700
H	-3.11313500	-5.75675400	-0.90175400
C	2.68164300	5.42951700	2.41727100
C	2.52621900	5.75752800	1.07182600

C	2.39785500	4.72906000	0.14323400
C	2.57457900	3.05981800	1.90610300
C	2.70452300	4.09546700	2.82969300
H	2.78864400	6.22061000	3.15359600
H	2.51173200	6.79675100	0.75432000
H	2.58854400	2.01672800	2.21982900
H	2.82398900	3.86078700	3.88280400
C	2.42455600	3.40205400	0.56577200
C	2.26623000	2.46188400	-0.60910900
C	2.44298200	3.38040400	-1.86928500
H	1.28685700	1.97970700	-0.60847200
C	2.20118200	4.81642100	-1.35076500
H	1.72799600	3.09801600	-2.64458800
H	2.88472900	5.51182100	-1.84867000
H	1.17968300	5.13628500	-1.58938600
N	3.27056800	1.40313700	-0.60350100
O	3.71000100	3.24978400	-2.50222100
C	4.55147900	1.66331100	-1.01589000
C	4.80214500	2.99791700	-1.63584200
H	4.89958700	3.77731700	-0.86716400
H	5.70688400	2.97575700	-2.24377200
N	5.30633200	0.61453900	-0.89687900
C	3.19324800	0.11994800	-0.17589900
N	4.44387100	-0.32069100	-0.36852900
C	4.90742100	-1.64697200	-0.08080300

C	5.59483700	-1.86873900	1.11503800
C	4.64561000	-2.66132400	-1.00497000
C	6.00065700	-3.17443500	1.38541100
C	5.06813800	-3.95052100	-0.68643500
C	5.74254000	-4.22425000	0.50336500
H	6.53013000	-3.37554900	2.31396400
H	4.87132700	-4.75810900	-1.38835900
C	5.86757100	-0.73574900	2.06579100
H	6.43117800	0.06032400	1.56854800
H	4.92009300	-0.31649800	2.42042800
H	6.44613200	-1.08627900	2.92352700
C	3.92822900	-2.37526800	-2.29893400
H	4.12505500	-3.16495400	-3.02791100
H	2.84172100	-2.32461500	-2.15428700
H	4.24833500	-1.42091700	-2.72810700
C	6.21808100	-5.62136600	0.81057600
H	6.30003800	-5.78372600	1.88849100
H	5.53566100	-6.37125700	0.40135000
H	7.20656100	-5.79962700	0.37265200
C	-1.75546300	-0.12327700	-1.22173400
C	-0.39087100	-0.33122400	-0.99377300
C	0.50405300	-0.36744600	-2.05113400
C	0.02628200	-0.21995400	-3.35545000
C	-1.33545500	-0.03576200	-3.57419800
C	-2.24433600	0.02144700	-2.51598100

C	-1.52823600	0.01525200	1.05356300
C	-0.17147400	-0.44878500	0.48839800
H	1.56545800	-0.49585000	-1.85990500
H	0.71591900	-0.24606200	-4.19299600
H	-1.70837400	0.07726000	-4.58750800
H	-3.29681000	0.17585300	-2.71126300
O	0.88999800	0.31724300	0.99949000
O	-1.72782600	0.33081300	2.19885800
N	-2.45696200	-0.06265100	0.01055000
C	-3.88082200	0.34801400	0.08914000
C	-3.92533200	1.80917600	-0.40012100
C	-4.58060800	2.24009200	-1.55197800
C	-3.17974800	2.74424300	0.33309400
C	-4.50661700	3.57405400	-1.95685900
H	-5.15023500	1.53982500	-2.15364100
C	-3.10564300	4.07084500	-0.06931700
H	-2.66232000	2.42170600	1.23384600
C	-3.77358300	4.49339500	-1.21863500
H	-5.02453600	3.88560300	-2.85900000
H	-2.52442400	4.77598800	0.51724600
H	-3.71859100	5.53069900	-1.53475500
C	-4.42035500	0.19335300	1.52860800
C	-4.29406600	-1.05161700	2.15386700
C	-5.14641600	1.19411300	2.16550900
C	-4.83820200	-1.27427100	3.40800700

H	-3.76268500	-1.84909600	1.64087500
C	-5.70708100	0.96554700	3.42439800
H	-5.28121200	2.16084700	1.69271400
C	-5.54884900	-0.26063400	4.05350800
H	-4.71566800	-2.24329500	3.88321600
H	-6.26667000	1.75976400	3.90930100
H	-5.98059700	-0.43312300	5.03458200
C	-4.74988500	-0.64068100	-0.71255400
C	-6.10636300	-0.35215900	-0.90114900
C	-4.27096800	-1.88750700	-1.11885100
C	-6.94732300	-1.25937900	-1.53440100
H	-6.50999000	0.58413100	-0.52460400
C	-5.11683900	-2.80051800	-1.74578500
H	-3.23539400	-2.16397500	-0.94235300
C	-6.45288700	-2.48804100	-1.96783800
H	-7.99501100	-1.01161800	-1.67535300
H	-4.71626600	-3.76172400	-2.05423200
H	-7.10985400	-3.19950200	-2.45877300
H	2.10990000	-2.65555300	1.55462200

TS6(RS)

NImag=1 (-178.7746)

Sum of electronic and zero-point Energies= -2718.836303

Sum of electronic and thermal Energies= -2718.784644

Sum of electronic and thermal Enthalpies= -2718.783700

Sum of electronic and thermal Free Energies= -2718.922217

C	2.17024100	-0.40562200	1.96131500
O	3.11524700	-0.08266500	2.66871500
C	1.75002800	-1.86672200	1.67667100
C	0.30505300	-1.92542100	2.17546100
H	1.81164700	-2.09720500	0.61392600
H	0.31650900	-2.01374800	3.26921700
C	-0.61564900	-2.99080000	1.62401100
C	-0.54088600	-3.44469300	0.30178200
C	-1.61971800	-3.50767200	2.44960600
C	-1.43915000	-4.39838900	-0.17148600
H	0.21180500	-3.04668000	-0.37179500
C	-2.51475400	-4.46519400	1.97969400
H	-1.69601000	-3.15282800	3.47477300
C	-2.42527300	-4.91620300	0.66474100
H	-1.36436300	-4.73575600	-1.20148400
H	-3.27985300	-4.85834200	2.64293400
H	-3.12013700	-5.66367600	0.29325300
C	3.53779300	5.57036600	2.09533500
C	2.71476200	5.84840800	1.00707800
C	2.04202900	4.79741300	0.38806600
C	3.01443100	3.20612500	1.95264400
C	3.68595800	4.26197500	2.56403300
H	4.07014700	6.37990200	2.58606400
H	2.60344100	6.86705900	0.64505600

H	3.11984500	2.18271600	2.31526900
H	4.32973700	4.06540600	3.41584000
C	2.19779900	3.49900800	0.86314100
C	1.39188800	2.51097800	0.05436600
C	0.73597500	3.36960300	-1.09292200
H	0.62950000	2.02691500	0.66815700
C	1.10221600	4.84586600	-0.79024300
H	-0.34589900	3.22850900	-1.06553900
H	1.55033500	5.30915300	-1.67710700
H	0.19709100	5.41965100	-0.56094200
N	2.23180500	1.44614600	-0.48417200
O	1.09853200	2.97707200	-2.40784400
C	2.80293000	1.53011900	-1.72414400
C	2.47968900	2.71610500	-2.56603600
H	3.08511400	3.58533700	-2.26750700
H	2.66284700	2.50090400	-3.61933800
N	3.50688100	0.47576800	-1.99208600
C	2.58209000	0.26950800	0.09207500
N	3.36667700	-0.27841900	-0.84672500
C	3.95144600	-1.58595300	-0.79520800
C	5.06138700	-1.80025900	0.02059600
C	3.35862200	-2.59932200	-1.55941100
C	5.56712700	-3.10120700	0.08295800
C	3.90213800	-3.87649700	-1.46304300
C	5.00022000	-4.14619600	-0.64160500

H	6.43063600	-3.29650800	0.71476300
H	3.45450400	-4.68362900	-2.03968200
C	5.68771400	-0.67504100	0.80019900
H	5.84569700	0.19926200	0.15995800
H	5.03865900	-0.37255500	1.62961300
H	6.65450000	-0.98648000	1.20324400
C	2.17446400	-2.30720200	-2.44388900
H	1.73499800	-3.23594200	-2.81905300
H	1.39814700	-1.74243000	-1.91508500
H	2.47318400	-1.69629400	-3.30268700
C	5.55069000	-5.54663500	-0.54750700
H	6.46887500	-5.57317800	0.04444800
H	4.82676000	-6.22052300	-0.07692200
H	5.77362200	-5.95005200	-1.54039200
C	-2.43462000	0.19585200	1.77586600
C	-1.38824700	-0.05282200	2.66744300
C	-1.55830400	0.08753400	4.03255500
C	-2.80846800	0.47576100	4.51657300
C	-3.85064200	0.71896900	3.62518800
C	-3.68360400	0.58895200	2.24454800
C	-0.64764300	-0.32659800	0.43663900
C	-0.17771000	-0.47351500	1.89785300
H	-0.72119100	-0.08711200	4.70322300
H	-2.96674700	0.59710300	5.58307900
H	-4.82055100	1.02601800	4.00406000

H	-4.50430200	0.80080800	1.57013500
O	0.94717400	0.33546800	2.14883400
O	0.08005900	-0.51461100	-0.51467500
N	-1.98492400	0.03603800	0.43158400
C	-2.84824600	0.24634200	-0.75998400
C	-4.14162900	-0.57427300	-0.52769400
C	-5.40764100	-0.13017100	-0.91293200
C	-4.04225500	-1.82421800	0.09806000
C	-6.53760300	-0.91822100	-0.69794900
H	-5.53823300	0.84637500	-1.36190300
C	-5.16826800	-2.61090700	0.30819300
H	-3.07367300	-2.18774600	0.43293900
C	-6.42504400	-2.16262500	-0.09051900
H	-7.51026800	-0.54523400	-1.00426400
H	-5.05419700	-3.57485300	0.79480000
H	-7.30659100	-2.77288300	0.08059600
C	-2.11001800	-0.26793200	-2.02773400
C	-1.24020700	0.58587000	-2.71613500
C	-2.21983700	-1.58852900	-2.45926600
C	-0.48792700	0.13138000	-3.78890700
H	-1.11412800	1.61431900	-2.39641800
C	-1.46658900	-2.04701800	-3.54066000
H	-2.88613000	-2.28071400	-1.95774100
C	-0.59836800	-1.19289600	-4.20919500
H	0.19406100	0.81680500	-4.28324300

H	-1.56937500	-3.08027000	-3.86030400
H	-0.01028400	-1.55381000	-5.04821600
C	-3.12997100	1.75191000	-0.93889200
C	-3.74936000	2.19087400	-2.11839600
C	-2.73454200	2.71521900	-0.01033100
C	-3.99607700	3.53851900	-2.34433700
H	-4.00743900	1.46417600	-2.88408300
C	-2.98061800	4.07208800	-0.23616500
H	-2.21717800	2.42786400	0.89802600
C	-3.61573100	4.48936000	-1.39832500
H	-4.47243900	3.84822900	-3.26949600
H	-2.66309300	4.79855200	0.50639000
H	-3.80360100	5.54385500	-1.57468400
H	2.42032100	-2.53142500	2.22500600

TS6(SR)

NImag=1 (-175.0852)

Sum of electronic and zero-point Energies= -2718.838859

Sum of electronic and thermal Energies= -2718.787260

Sum of electronic and thermal Enthalpies= -2718.786315

Sum of electronic and thermal Free Energies= -2718.922795

C	2.01415300	1.17525700	2.19967700
O	3.03275300	1.25190400	2.87230700
C	0.83805700	2.15366700	2.26021600
C	-0.32809700	1.27023300	2.69568400

H	0.64605500	2.56794000	1.27097600
H	-0.22672700	1.04046300	3.76499700
C	-1.71563900	1.81749800	2.44813000
C	-1.93306300	3.00919900	1.74970600
C	-2.82606200	1.12333500	2.94546600
C	-3.22661800	3.49069400	1.55282300
H	-1.09659000	3.57774100	1.35429200
C	-4.11828100	1.59310300	2.72954900
H	-2.67087700	0.20501400	3.50894400
C	-4.32406800	2.78040400	2.02890000
H	-3.37115500	4.42639400	1.01961300
H	-4.96609900	1.03519600	3.11727900
H	-5.33102800	3.15143500	1.86589800
C	2.93163300	-4.68968400	-0.22440000
C	4.27215600	-4.34062500	-0.06449800
C	4.59425700	-3.01670100	0.21868700
C	2.25100300	-2.39914800	0.14860700
C	1.92706800	-3.72620000	-0.11743400
H	2.66581100	-5.72047400	-0.44019700
H	5.05241000	-5.09126500	-0.15831100
H	1.48128600	-1.63810000	0.20840300
H	0.88515600	-4.00345800	-0.24877100
C	3.58594600	-2.06157500	0.33213300
C	4.16467100	-0.71742200	0.71675000
C	5.70057200	-0.87492000	0.45132900

H	3.97594000	-0.48761900	1.77000600
C	5.94927700	-2.40010900	0.47119200
H	6.27248400	-0.35901200	1.22442300
H	6.70223400	-2.66442700	-0.27785500
H	6.33882300	-2.70700400	1.44928500
N	3.62629400	0.39377900	-0.05409600
O	6.14677700	-0.28301300	-0.76539600
C	4.07658500	0.65457900	-1.32014000
C	5.19897200	-0.19544800	-1.81439700
H	4.83306900	-1.18864000	-2.11231400
H	5.69594000	0.27451800	-2.66343600
N	3.49241600	1.70017200	-1.82086900
C	2.68503500	1.30406800	0.28733000
N	2.63281300	2.07552000	-0.80801200
C	1.77723100	3.21656200	-0.93418300
C	0.71022300	3.19020400	-1.83220400
C	2.00700200	4.29512300	-0.06533000
C	-0.17901900	4.26898300	-1.80658200
C	1.09116400	5.34267400	-0.07783500
C	-0.01542600	5.33969100	-0.93382000
H	-1.03159600	4.24956800	-2.48256200
H	1.24401200	6.18286200	0.59641100
C	0.48653100	2.06877000	-2.80974200
H	0.68952700	2.41560700	-3.82892200
H	1.13376000	1.21622700	-2.60519300

H	-0.55269500	1.73393400	-2.75796100
C	3.19892500	4.31515000	0.85889500
H	3.29941500	5.29968000	1.32190900
H	3.12709500	3.56609000	1.65611800
H	4.11925700	4.10061000	0.30562000
C	-0.99398800	6.48700100	-0.92023900
H	-1.92765900	6.21506200	-1.42038800
H	-1.22951600	6.79406800	0.10349800
H	-0.58246400	7.36131900	-1.43642000
C	-1.47034200	-1.85015100	1.54726200
C	-0.58306700	-1.32379100	2.49263300
C	-0.31254400	-1.98105100	3.67716200
C	-0.95488100	-3.19420600	3.93280000
C	-1.83224300	-3.72128300	2.99031200
C	-2.10117000	-3.06657500	1.78433000
C	-0.51168200	-0.04942900	0.51239000
C	0.02661700	-0.06364300	1.96301300
H	0.40999500	-1.56286300	4.37230300
H	-0.75839100	-3.73246100	4.85388200
H	-2.32274200	-4.66994600	3.18511100
H	-2.79021100	-3.50332100	1.07445200
O	1.43298300	-0.12724900	2.03068300
O	-0.09723700	0.66335400	-0.37428100
N	-1.54011900	-0.98536500	0.41613700
C	-2.25286600	-1.30991600	-0.84796100

C	-1.39147600	-2.33754700	-1.60574300
C	-1.65560700	-3.70943300	-1.60381900
C	-0.25256300	-1.88153200	-2.28569600
C	-0.83920000	-4.59543900	-2.30834400
H	-2.51900800	-4.09948300	-1.07618500
C	0.56179100	-2.76497300	-2.98401500
H	-0.01911800	-0.82073400	-2.27112800
C	0.26400000	-4.12590200	-3.01111900
H	-1.07494200	-5.65533800	-2.30381500
H	1.43640000	-2.38707900	-3.50462500
H	0.89812500	-4.81445700	-3.56092200
C	-2.51484400	-0.03372200	-1.68164700
C	-2.87336700	1.15489100	-1.04202900
C	-2.58861600	-0.09570500	-3.07357700
C	-3.24237300	2.27151900	-1.77994500
H	-2.86435000	1.20903400	0.04251900
C	-2.97895000	1.01994500	-3.81387800
H	-2.33952000	-1.01541700	-3.59297000
C	-3.29762900	2.21123100	-3.17247200
H	-3.49434300	3.19002700	-1.25775100
H	-3.02597400	0.95137600	-4.89639500
H	-3.59409600	3.08265500	-3.74871600
C	-3.69498100	-1.76852300	-0.54635100
C	-4.42420200	-2.47322000	-1.50865500
C	-4.35738800	-1.33670400	0.60470900

C	-5.76366800	-2.78699400	-1.29916300
H	-3.94737000	-2.76919300	-2.43807000
C	-5.69735300	-1.64802100	0.81329400
H	-3.82438400	-0.74834100	1.34387000
C	-6.40558100	-2.38345900	-0.13202400
H	-6.30693600	-3.34164600	-2.05798500
H	-6.18801000	-1.30849600	1.72071900
H	-7.45017900	-2.62839800	0.03222500
H	1.06106800	2.95725700	2.96509700

TS6(SS)

NImag=1 (-197.9282)

Sum of electronic and zero-point Energies= -2718.829945

Sum of electronic and thermal Energies= -2718.777922

Sum of electronic and thermal Enthalpies= -2718.776978

Sum of electronic and thermal Free Energies= -2718.918225

C	-1.93478600	0.13353300	1.89980000
O	-2.23306500	0.77837000	2.91067300
C	-2.19385100	-1.38051900	1.74010800
C	-0.79939500	-1.98193200	1.57748300
H	-2.71807200	-1.74654000	2.62564400
H	-0.32362100	-2.04188800	2.56498800
H	-2.81136100	-1.57479800	0.86149000
C	-0.68054000	-3.32489900	0.88964800
C	-1.77789300	-3.98800400	0.33766200

C	0.58491400	-3.91697300	0.77574800
C	-1.61676500	-5.20555400	-0.32200300
H	-2.77565800	-3.56549600	0.42329300
C	0.74570400	-5.12934600	0.11487100
H	1.45395400	-3.43389600	1.22167700
C	-0.35576400	-5.77858500	-0.43955800
H	-2.48518700	-5.70516100	-0.74211700
H	1.73720300	-5.56516200	0.03768700
H	-0.23093500	-6.72766500	-0.95220400
C	1.01204300	4.52375400	-2.16336800
C	0.53367600	5.36772300	-1.16134900
C	-0.30137000	4.84123600	-0.18146100
C	-0.16891800	2.64041600	-1.20043100
C	0.66219900	3.17167200	-2.18646900
H	1.65165800	4.92735200	-2.94340200
H	0.79772200	6.42170200	-1.15642200
H	-0.45884100	1.59296200	-1.21999200
H	1.03941600	2.52206300	-2.97173200
C	-0.63790200	3.48900900	-0.20481300
C	-1.57383300	3.14973600	0.93464700
C	-2.05448300	4.54463600	1.45837800
H	-1.08728400	2.58656100	1.73456100
C	-0.96488000	5.53352600	0.98504200
H	-2.15142000	4.52565000	2.54479600
H	-1.41777900	6.49636700	0.72957100

H	-0.24279500	5.71347300	1.79073500
N	-2.70297300	2.35398300	0.47580500
O	-3.34698600	4.92515100	0.99907100
C	-3.75424300	2.94091700	-0.17035800
C	-3.73819300	4.43074700	-0.26812400
H	-3.05556600	4.76180900	-1.06387800
H	-4.73927700	4.81185700	-0.47203500
N	-4.65312500	2.06444900	-0.50109100
C	-2.91736100	1.02194600	0.56306000
N	-4.10902200	0.88527400	-0.03749700
C	-4.80158500	-0.35277900	-0.23274500
C	-4.80663800	-0.91423500	-1.51147900
C	-5.40277300	-0.96415900	0.87158400
C	-5.38413200	-2.17492700	-1.65813700
C	-5.96511500	-2.22473600	0.67261700
C	-5.95486500	-2.84739800	-0.57690600
H	-5.38540900	-2.64236100	-2.64040100
H	-6.42567200	-2.73189700	1.51745000
C	-4.23397700	-0.16748900	-2.68721100
H	-4.89901800	0.65254100	-2.97730900
H	-3.26082800	0.27667700	-2.45255800
H	-4.11466600	-0.83478900	-3.54481900
C	-5.44788900	-0.27673800	2.21146500
H	-5.97625200	-0.89805900	2.93825400
H	-4.45195000	-0.04751200	2.60860200

H	-5.98097700	0.67690800	2.12619600
C	-6.58232600	-4.20546500	-0.76318800
H	-6.52426800	-4.79774900	0.15374200
H	-7.64095300	-4.11098300	-1.02954000
H	-6.08866600	-4.76225300	-1.56426300
C	1.30568200	-0.58336100	-1.06835400
C	-0.00590300	-0.85857200	-0.64906100
C	-1.02328700	-1.06952400	-1.56175500
C	-0.73851400	-0.99532400	-2.92741100
C	0.56128100	-0.73049200	-3.34192800
C	1.60183300	-0.52936300	-2.42932100
C	1.44093700	-0.78867900	1.20842900
C	-0.05217000	-0.84249800	0.85409700
H	-2.02772300	-1.30567100	-1.21639700
H	-1.52234500	-1.15996600	-3.65948900
H	0.78968600	-0.68804300	-4.40271800
H	2.60057400	-0.34254100	-2.79946600
O	-0.60423600	0.35726700	1.37211100
O	1.91132200	-1.02128100	2.29596500
N	2.14510200	-0.40671100	0.07024600
C	3.62863300	-0.39215800	0.11411700
C	4.04390500	-1.87026500	0.21197300
C	3.92964600	-2.69306700	-0.91612200
C	4.35538500	-2.46267300	1.43854300
C	4.15509200	-4.06240200	-0.82756000

H	3.65603000	-2.26297100	-1.87497900
C	4.57846300	-3.83533000	1.52771700
H	4.39277400	-1.85211900	2.33298200
C	4.48686500	-4.63927200	0.39624000
H	4.06471000	-4.67909700	-1.71691400
H	4.81530400	-4.27478100	2.49184900
H	4.66390100	-5.70855700	0.46759300
C	4.12153000	0.48273400	1.28547700
C	3.32362300	1.47163200	1.86141700
C	5.46322300	0.39825100	1.66366500
C	3.85050700	2.33459800	2.81732900
H	2.28081000	1.57003800	1.57404400
C	5.98852100	1.25824300	2.62267300
H	6.10627100	-0.34482800	1.19872900
C	5.18205700	2.23037500	3.20661800
H	3.20885500	3.08864600	3.26279800
H	7.03279100	1.17013300	2.90681500
H	5.58882300	2.90369300	3.95468700
C	4.18742800	0.35915100	-1.10570700
C	5.30447800	-0.07932600	-1.81321200
C	3.61880700	1.59394600	-1.43844600
C	5.81811000	0.68354300	-2.86403300
H	5.77965800	-1.01908300	-1.55140700
C	4.12672900	2.34907500	-2.48487300
H	2.76008200	1.95776000	-0.87925600

C	5.22875500	1.89318000	-3.20929500
H	6.68568300	0.32415900	-3.40930200
H	3.66162700	3.30014400	-2.72849300
H	5.62876600	2.48314600	-4.02826400

P(RR)

NImag=0

Sum of electronic and zero-point Energies= -1667.327096

Sum of electronic and thermal Energies= -1667.296626

Sum of electronic and thermal Enthalpies= -1667.295682

Sum of electronic and thermal Free Energies= -1667.388169

C	-4.08048100	-1.87337300	1.42472500
O	-4.85097900	-2.70028800	1.80915500
C	-4.34539400	-0.41457500	1.07407100
C	-2.94616200	0.18956200	1.12928800
H	-4.78197800	-0.36195300	0.06964900
H	-2.67496500	0.30112900	2.18727300
C	-2.67528700	1.49582900	0.42942700
C	-3.05586500	1.73329100	-0.89551600
C	-1.99312800	2.50187500	1.11985300
C	-2.75403100	2.94467300	-1.51191800
H	-3.58334900	0.96791600	-1.45700600
C	-1.68840300	3.71419300	0.50587600
H	-1.69722100	2.32678500	2.15221800
C	-2.07193400	3.93895300	-0.81305900

H	-3.05560600	3.11170900	-2.54147400
H	-1.15379100	4.48081500	1.05825000
H	-1.84408300	4.88549800	-1.29424100
C	-0.60654100	-0.77369900	-1.13480400
C	-1.91097300	-1.16931700	-0.82984300
C	-2.77763400	-1.61649100	-1.81070000
C	-2.34141200	-1.62276800	-3.13691700
C	-1.05332600	-1.19249400	-3.44236700
C	-0.16295100	-0.77111500	-2.45194000
C	-0.66281300	-0.84996100	1.15521400
C	-2.10162700	-1.03144600	0.64629800
H	-3.77149500	-1.97274300	-1.55037200
H	-3.00030000	-1.97112400	-3.92513100
H	-0.71753000	-1.19772700	-4.47465300
H	0.83838500	-0.45801300	-2.71495000
O	-2.75521300	-2.14588000	1.23347100
O	-0.31996800	-0.97904800	2.30313600
N	0.09727100	-0.44594300	0.05793900
C	1.55958600	-0.18917100	0.06855800
C	2.22085900	-1.51014000	-0.37343300
C	2.95325300	-1.67266500	-1.54769500
C	1.99092900	-2.63548300	0.43131300
C	3.45807100	-2.92422200	-1.90432900
H	3.13220800	-0.82801600	-2.20436600
C	2.49432400	-3.87981800	0.07800500

H	1.41835500	-2.52513500	1.34952500
C	3.23446300	-4.02927500	-1.09457600
H	4.02237700	-3.02718900	-2.82625700
H	2.30441300	-4.73575700	0.71826800
H	3.62647500	-5.00224300	-1.37436900
C	2.02584800	0.26348800	1.47026700
C	1.40318800	1.36967600	2.05864800
C	3.12938300	-0.29968800	2.10257700
C	1.84336600	1.86724700	3.27475600
H	0.56815900	1.84311300	1.54731900
C	3.58135000	0.20965300	3.32183800
H	3.64795800	-1.14040100	1.65560100
C	2.93829900	1.28531400	3.91615300
H	1.33867700	2.71804000	3.72326000
H	4.44174700	-0.24627300	3.80211600
H	3.28780700	1.67674400	4.86647000
C	1.87849000	1.03114200	-0.81710500
C	3.21886600	1.35453700	-1.05947900
C	0.89003200	1.91558900	-1.25292600
C	3.56015800	2.49897800	-1.76981800
H	4.00230900	0.71265800	-0.66499900
C	1.23423500	3.06707900	-1.95954500
H	-0.15848200	1.72638200	-1.03887200
C	2.56546500	3.35867100	-2.23179800
H	4.60647200	2.72560000	-1.95041600

H	0.44518200	3.73544100	-2.29131600
H	2.82997600	4.25415400	-2.78551800
H	-5.05653200	0.01962700	1.77772200

P(RS)

NImag=0

Sum of electronic and zero-point Energies= -1667.330435

Sum of electronic and thermal Energies= -1667.300151

Sum of electronic and thermal Enthalpies= -1667.299206

Sum of electronic and thermal Free Energies= -1667.390401

C	3.58593900	-2.30598700	1.48989800
O	4.08610900	-3.17494900	2.13734100
C	3.86491800	-0.81263200	1.52188000
C	3.27711200	-0.32905800	0.19656400
H	3.34399800	-0.39412800	2.38717400
H	3.99990500	-0.54954200	-0.60001300
C	2.87136600	1.12038900	0.07196000
C	2.25955600	1.82131400	1.11739400
C	3.09346400	1.78159900	-1.14017700
C	1.89933600	3.15657500	0.95413600
H	2.04093300	1.32502800	2.05878200
C	2.73319800	3.11624400	-1.30361100
H	3.55667200	1.24085100	-1.96214100
C	2.13685100	3.80963400	-0.25277400
H	1.42261900	3.68131500	1.77667300

H	2.92151300	3.61345100	-2.25068000
H	1.85678900	4.85164400	-0.37476800
C	0.29903800	-1.02393900	-1.43274200
C	1.61598700	-1.49165700	-1.39796700
C	2.24373900	-1.97762600	-2.53009200
C	1.53350900	-2.00110900	-3.73072800
C	0.21746700	-1.54653300	-3.76223100
C	-0.42256800	-1.05690900	-2.62162500
C	0.87223300	-0.93800200	0.78351900
C	2.12867500	-1.35876500	-0.00576600
H	3.26162100	-2.35339200	-2.46961900
H	1.99828900	-2.38410000	-4.63297700
H	-0.33726900	-1.57494600	-4.69491800
H	-1.45143800	-0.72329100	-2.67230600
O	2.64066500	-2.56887800	0.53537500
O	0.84358400	-0.90776000	1.99199200
N	-0.11928900	-0.61733900	-0.13054400
C	-1.44953100	-0.01293800	0.15950000
C	-1.69145500	1.06081200	-0.93114000
C	-2.93050100	1.26994100	-1.53771000
C	-0.61748300	1.86902100	-1.32718900
C	-3.09416600	2.26476200	-2.50227700
H	-3.77992400	0.64627600	-1.28832500
C	-0.78176500	2.86327300	-2.28335300
H	0.36370600	1.71858300	-0.88500900

C	-2.02474400	3.06766700	-2.87832700
H	-4.06807900	2.40120300	-2.96257600
H	0.07294600	3.47132800	-2.56455400
H	-2.15459500	3.83854800	-3.63155400
C	-1.44511400	0.66671200	1.55820900
C	-1.70100600	-0.10292100	2.70051600
C	-1.21396500	2.03131100	1.72337800
C	-1.71260900	0.46927800	3.96345100
H	-1.86893800	-1.16991000	2.59855700
C	-1.22248700	2.60924400	2.99453500
H	-1.03130000	2.66923500	0.86729600
C	-1.47156100	1.83384300	4.11783300
H	-1.90519300	-0.15407000	4.83102100
H	-1.04781600	3.67692200	3.09415500
H	-1.48502900	2.28453400	5.10571900
C	-2.53427400	-1.10621200	0.15385700
C	-3.82566600	-0.78641400	0.59706700
C	-2.27536000	-2.42093200	-0.22959600
C	-4.83409900	-1.74050800	0.61507900
H	-4.03137300	0.21937600	0.95404400
C	-3.28630200	-3.38309200	-0.20462600
H	-1.27989900	-2.71886800	-0.53749400
C	-4.56861700	-3.04734900	0.20789900
H	-5.82545400	-1.46636500	0.96266800
H	-3.05701400	-4.40143000	-0.50287500

H	-5.35300100	-3.79762400	0.22952700
H	4.93478400	-0.63076300	1.63189600

P(SR)

NImag=0

Sum of electronic and zero-point Energies= -1667.332079

Sum of electronic and thermal Energies= -1667.301545

Sum of electronic and thermal Enthalpies= -1667.300601

Sum of electronic and thermal Free Energies= -1667.393497

C	3.70997000	-1.81239500	-1.72696800
O	4.24351900	-2.57308000	-2.47553000
C	3.91918100	-0.31229200	-1.58158400
C	3.33808900	-0.02834300	-0.19819600
H	4.97628300	-0.06572200	-1.68834600
H	4.07944900	-0.33175900	0.55315500
H	3.35792700	0.17480200	-2.38367200
C	2.86001200	1.36096200	0.14718200
C	2.34625200	2.23936100	-0.80981400
C	2.88484000	1.76646500	1.48634000
C	1.88011200	3.49829400	-0.43562400
H	2.28961200	1.93956500	-1.85280100
C	2.41794700	3.02289100	1.86165600
H	3.27204500	1.08371400	2.23934100
C	1.91473900	3.89460900	0.89837900
H	1.48413100	4.17001000	-1.19193500

H	2.44945700	3.32010900	2.90573300
H	1.55208700	4.87689200	1.18533800
C	0.40992800	-0.94886200	1.33590000
C	1.72469100	-1.41243200	1.24137000
C	2.37183300	-1.98736400	2.31945600
C	1.68151000	-2.10653100	3.52614600
C	0.37329600	-1.63882200	3.62197700
C	-0.28291300	-1.05421800	2.53633100
C	0.95219700	-0.65746600	-0.86629400
C	2.22837700	-1.11605600	-0.12759700
H	3.38854900	-2.35589900	2.21260700
H	2.15915900	-2.56602400	4.38489100
H	-0.16026700	-1.73091500	4.56289400
H	-1.29887200	-0.69765800	2.63955300
O	2.78643400	-2.23015100	-0.80662100
O	0.88560300	-0.55864500	-2.06989300
N	-0.02634500	-0.41806000	0.08667000
C	-1.45957700	-0.11560000	-0.17571900
C	-2.20257600	-1.45352800	0.00537800
C	-3.18235900	-1.69098300	0.96722900
C	-1.80342900	-2.51578500	-0.81815500
C	-3.76388800	-2.95368400	1.09380100
H	-3.49672900	-0.89939100	1.63871900
C	-2.38288600	-3.77115700	-0.69472600
H	-1.03636600	-2.34692100	-1.57106700

C	-3.37117400	-3.99490500	0.26397800
H	-4.52261600	-3.11610900	1.85320400
H	-2.05957100	-4.57761900	-1.34547800
H	-3.82339300	-4.97664200	0.36496500
C	-1.65910300	0.47309600	-1.59123200
C	-0.96388800	1.64008700	-1.92554900
C	-2.59763300	-0.02814400	-2.48727000
C	-1.16394800	2.26161200	-3.14654600
H	-0.25848800	2.05701300	-1.21234000
C	-2.81085100	0.60703800	-3.71365900
H	-3.17233900	-0.91470600	-2.24382000
C	-2.09249800	1.74408500	-4.05212900
H	-0.60201500	3.15795600	-3.39343100
H	-3.54488000	0.20009300	-4.40242100
H	-2.25589300	2.23169500	-5.00821600
C	-1.92073600	1.02355800	0.75155900
C	-3.27398900	1.38100600	0.77137100
C	-1.01063300	1.81746000	1.44985700
C	-3.71292900	2.46550000	1.52102400
H	-3.98413700	0.81682900	0.17229100
C	-1.44970900	2.91190600	2.19272500
H	0.05200100	1.59776800	1.40680000
C	-2.80088000	3.23317700	2.24343600
H	-4.76806700	2.72127800	1.52690500
H	-0.72013400	3.51369300	2.72724000

H	-3.14120400	4.08414400	2.82536600

P(SS)

NImag=0

Sum of electronic and zero-point Energies= -1667.325774

Sum of electronic and thermal Energies= -1667.295241

Sum of electronic and thermal Enthalpies= -1667.294297

Sum of electronic and thermal Free Energies= -1667.387378

C	2.90327800	3.39856800	-0.08560300
O	3.11104900	4.57205900	-0.00895200
C	3.86122800	2.28618400	-0.47236900
C	2.93225500	1.13357700	-0.83613500
H	4.51929900	2.61437400	-1.27800100
H	2.57249500	1.29985700	-1.86028100
H	4.48155100	2.07238300	0.40554200
C	3.44832700	-0.28266400	-0.72742600
C	4.70444500	-0.58507700	-0.20335800
C	2.62850300	-1.33443800	-1.15675700
C	5.13486000	-1.90665200	-0.09881000
H	5.37104100	0.20985300	0.11737100
C	3.05743800	-2.65256400	-1.05165100
H	1.65205000	-1.12479600	-1.59462500
C	4.31163500	-2.94425600	-0.51938500
H	6.11854500	-2.11933500	0.30900200
H	2.40693400	-3.45088600	-1.39381600

H	4.64646300	-3.97402900	-0.44082000
C	0.32478000	0.09978500	1.44410800
C	1.58230200	0.71549600	1.37072000
C	2.51141800	0.58018400	2.38522300
C	2.19535800	-0.20293400	3.49530600
C	0.96270100	-0.84256100	3.55059900
C	0.01240600	-0.70762200	2.53463900
C	0.38686500	1.04353900	-0.64089100
C	1.70033600	1.43158000	0.05910400
H	3.48095700	1.06459900	2.30953100
H	2.91221500	-0.32395400	4.30010100
H	0.71908600	-1.46740300	4.40425100
H	-0.93451400	-1.22152500	2.62200100
O	1.68789400	2.85703500	0.21087800
O	0.15359900	1.24130100	-1.80999200
N	-0.44272200	0.43360100	0.28542000
C	-1.71681000	-0.18067700	-0.17137600
C	-1.29730600	-1.41662600	-0.98504200
C	-0.86717700	-2.57077600	-0.31851700
C	-1.17327600	-1.36529700	-2.37664100
C	-0.36719800	-3.65906800	-1.02514300
H	-0.92735800	-2.62475300	0.76389400
C	-0.66544400	-2.45357800	-3.08349400
H	-1.45348200	-0.46226800	-2.90628800
C	-0.26937100	-3.60684700	-2.41385600

H	-0.04980300	-4.54696800	-0.48617200
H	-0.57768600	-2.39275900	-4.16388000
H	0.11888800	-4.45665800	-2.96778600
C	-2.55685000	0.83917100	-0.96836900
C	-2.39621500	2.21680500	-0.82003900
C	-3.62515400	0.36726000	-1.73428600
C	-3.26450800	3.10122900	-1.45269200
H	-1.58487700	2.61279100	-0.21694600
C	-4.49082800	1.25090300	-2.36969000
H	-3.78626000	-0.70328700	-1.83119500
C	-4.31170600	2.62427700	-2.23431000
H	-3.11367600	4.16976900	-1.33431500
H	-5.31015900	0.86192300	-2.96660900
H	-4.98584600	3.31658400	-2.72892900
C	-2.63077300	-0.48237400	1.02766300
C	-3.42425300	-1.62743800	1.07762500
C	-2.77766400	0.48298400	2.03060900
C	-4.31489700	-1.82593900	2.13267500
H	-3.35368800	-2.37395100	0.29338800
C	-3.65845500	0.28171800	3.08431600
H	-2.18415700	1.39271200	1.98801900
C	-4.42869400	-0.87974100	3.14344500
H	-4.92062400	-2.72659200	2.15640000
H	-3.74860800	1.03613900	3.85967300
H	-5.11940300	-1.03697900	3.96591400