Electronic Supplementary Information

Computational study on N-heterocyclic carbene-catalyzed C_{sp2}–C_{sp3} bond activation/[4 + 2] cycloaddition cascade reaction of cyclobutenones with imines: A new application of the conservation principle of molecular orbital symmetry

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Content

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Part 1: Single-point energies of all the stationary points

Table S1 The single-point energies of all the stationary points involved in the reaction calculated at M06-2X/6-311++G(2df,2pd)//IEF-PCM$_{THF}$

	Sing-point energy		Sing-point energy
R1	-920.62570823	**P*RR*&*SS***	-1798.98332
R2	-878.2786203	**P*RS*&*SR***	-1798.988297
Cat	-1016.33291	***E*-TS1^{D}**	-920.5695735
***Re*-TS1**	-1936.96713	***Z*-TS1^{D}**	-920.5827898
***Si*-TS1**	-1936.957173	***E*-M1^{D}**	-920.62265
***Re*-M1**	-1936.982733	***Z*-M1^{D}**	-920.617716
***Si*-M1**	-1936.972413	**TS2^{D}*RR***	-1798.882652
TS2	-1936.94772	**TS2^{D}*RS***	-1798.87269
M2	-1937.012953	**TS2^{D}*SR***	-1798.884337
TS3*RR*	-2815.287118	**TS2^{D}*SS***	-1798.869064
TS3*RS*	-2815.286813	**TS3$_{C=O}$*RR***	-2815.263799
TS3*SR*	-2815.29191	**TS3$_{C=O}$*RS***	-2815.263033
TS3*SS*	-2815.290985	**TS3$_{C=O}$*SR***	-2815.277918
M3*RR*	-2815.33405	**TS3$_{C=O}$*SS***	-2815.279695
M3*RS*	-2815.331375	**M3$_{C=O}$*RR***	-2815.299052
M3*SR*	-2815.339403	**M3$_{C=O}$*RS***	-2815.29045
M3*SS*	-2815.338189	**M3$_{C=O}$*SR***	-2815.28908
TS4*RR*	-2815.314664	**M3$_{C=O}$*SS***	-2815.292311
TS4*RS*	-2815.31693	**TS2$^{D}_{C=O}$*RR***	-1798.872568
TS4*SR*	-2815.322517	**TS2$^{D}_{C=O}$*RS***	-1798.872101
TS4*SS*	-2815.320558	**TS2$^{D}_{C=O}$*SR***	-1798.871677
M4*RR*	-2815.336109	**TS2$^{D}_{C=O}$*SS***	-1798.875537
M4*RS*	-2815.343197	**P$_{C=O}$*RR*&*SS***	-1798.943668
M4*SR*	-2815.342035	**P$_{C=O}$*RS*&*SR***	-1798.942863
M4*SS*	-2815.33734		

Part 2 : Structures of the catalytic approach

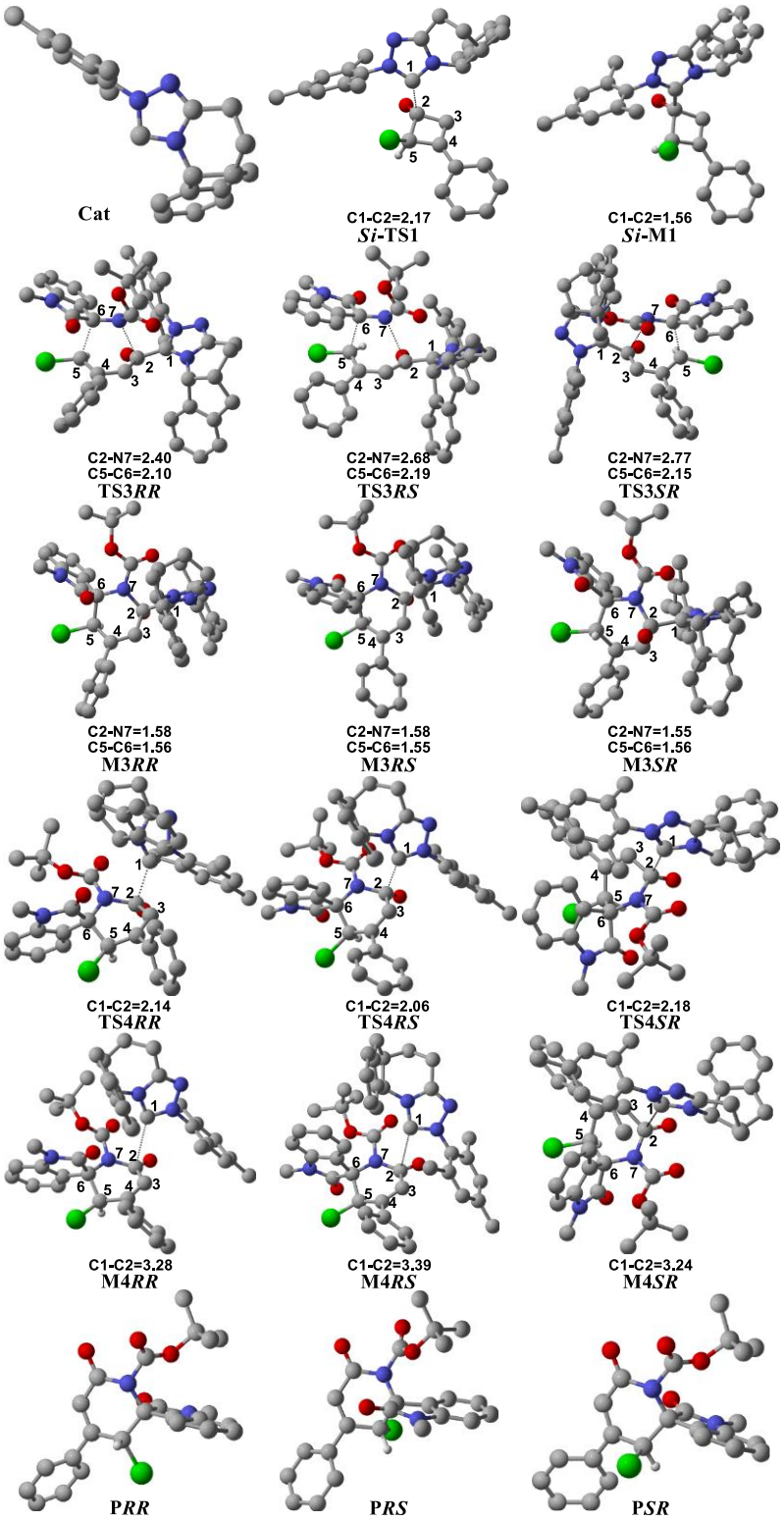


Fig. S1 Optimized geometries of the stationary points involved in the catalytic approach. Most of the hydrogen atoms are omitted for sake of clarify (Distances are given in Å).

Part 3: Structures and energy barriers of the regioselective approach

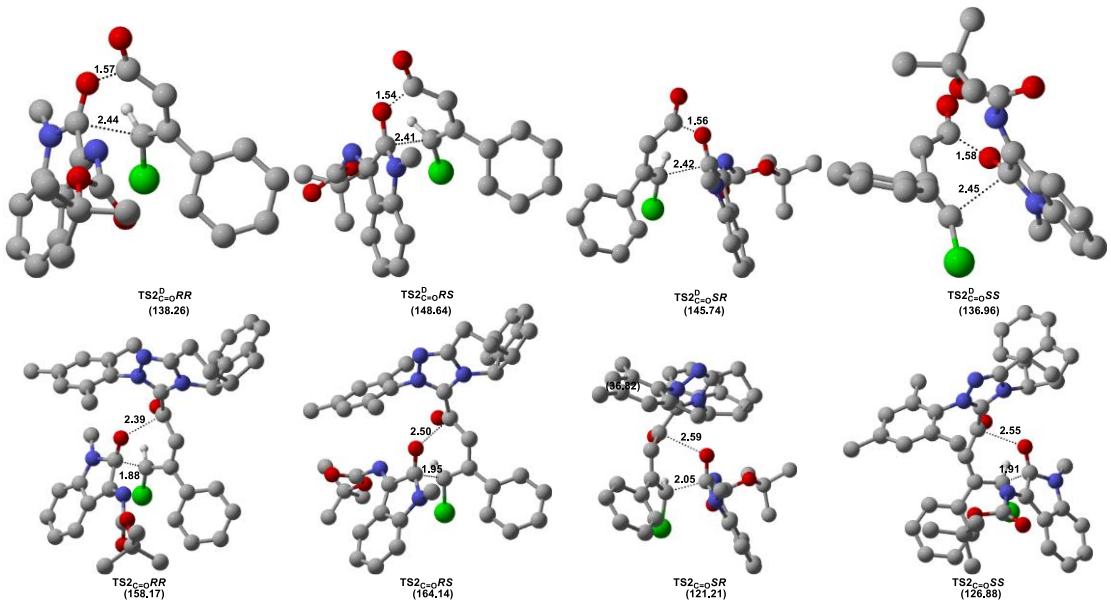


Fig. S2 The optimized structures and energy barriers involved in the regioselective [4 + 2] cycloaddition of **M2** with C=O bond of **R2**. Most of the hydrogen atoms are omitted for sake of clarify (Distances and energies are given in Å and kJ/mol, respectively).

Part 4: Structures of the direct approach

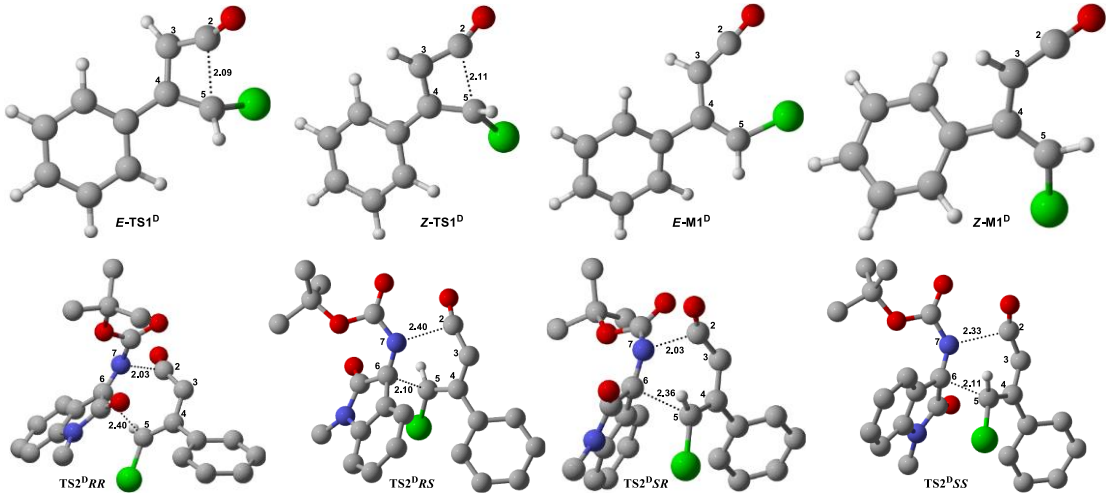
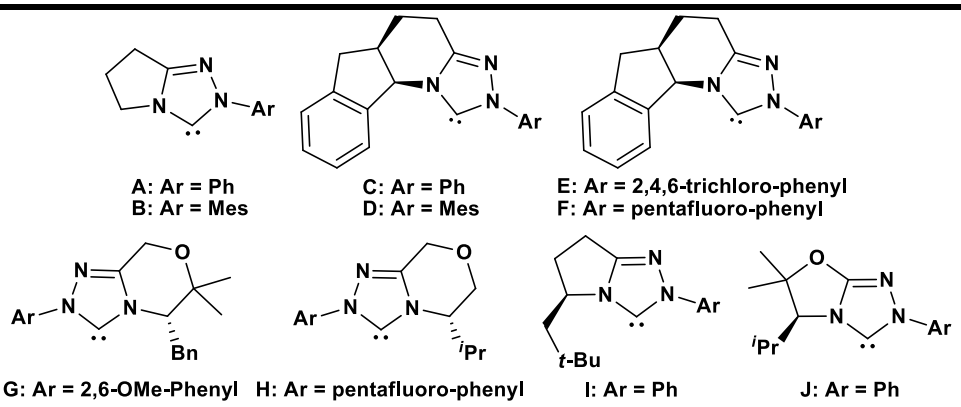


Fig. S3 The optimized structures of the direct C-C bond cleavage/[4 + 2] cycloaddition approach. Most of the hydrogen atoms are omitted for sake of clarify (Distances are given in Å).

Part 5: Relationship between the energy gap of FMO

Table S2 Relationship between the energy gap of FMO and the Gibbs free energy barrier with different NHC catalysts

Catalyst	HOMO energy (eV)		Energy gap (eV)	Energy barrier (kcal/mol)
	$HOMO_{M1}$	$HOMO_{M2}$		
Direct	–8.69	–7.25	1.44	26.08
A	–6.72	–5.82	0.90	19.55
B	–6.84	–5.83	1.01	19.68
C	–6.95	–6.02	0.93	17.52
D	–6.92	–5.95	0.97	18.47
E	–6.91	–5.97	0.94	22.13
F	–6.94	–6.02	0.92	21.04
G	–6.77	–5.83	0.94	20.13
H	–6.98	–6.06	0.92	21.74
I	–6.90	–5.97	0.93	20.57
J	–6.93	–5.93	1.00	18.05



Part 6: The second-order perturbation energy of TS3*RS* and TS3*SR*

Table S3 The second-order perturbation energy *E*(2) (kcal/mol) of the donor-acceptor interactions in terms of forming bonds in **TS3*RS*** and **TS3*SR***

TS3*RS*				**TS3*SR***			
Donor	Acceptor	Interaction	*E*(2)	Donor	Acceptor	Interaction	*E*(2)
LP(1)C5	BD*(2)C6-N7	n-π*	97.98	LP(2)N7	BD*(1)C5-C6	n-σ*	93.97
BD(2)C6-N7	LP(1)C5	π-n	19.27	BD*(1)C5-C6	BD*(2)C4-C3	σ*-π*	63.33
BD*(2)C6-N7	BD*(2)C2-O13	π*-π*	15.88	BD(1)C5-C6	BD*(2)C4-C3	σ-π*	35.28
BD*(2)C6-N7	BD*(2)C4-C5	π*-π*	12.92	BD(1)C5-C6	LP(2)N7	σ-n	32.21
BD(1)C6-C10	LP(1)C5	σ-n	6.60	BD(1)C5-C6	BD*(2)C10-O11	σ-π*	19.70
				BD(1)C5-C6	BD*(2)C8-C9	σ-π*	12.88
				BD(2)C8-C9	BD*(1)C5-C6	π-σ*	12.45
				LP(3)Cl12	BD*(1)C5-C6	n-σ*	11.79
				BD*(2)C16-C17	BD*(2)C4-C3	π*-π*	11.06

Note: The overall delocalization in **TS3*RS*** is 152.65 kcal/mol and that in **TS3*SR*** is 292.67 kcal/mol.

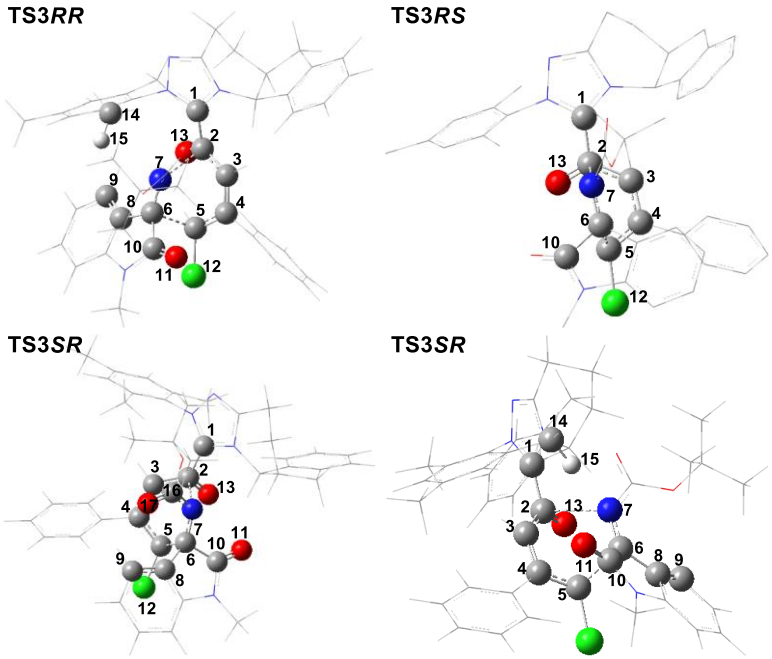


Fig. S4 Labels of the transition states **TS3*RR***, **TS3*RS***, **TS3*SR***, and **TS3*SS***.

Part 7: IRC points of TS2

Table S4 The distances of C2–C5 (unit: Å) and single-point energies *E* (unit: a.u.) of several IRC points in **TS2** at M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ level

	C2–C5	E
IRC-F-100	1.65	-1936.49540061
IRC-F-50	1.75	-1936.48454074
IRC-F-40	1.84	-1936.47951416
IRC-F-30	1.97	-1936.47434926
IRC-F-20	2.11	-1936.46998270
IRC-F-10	2.24	-1936.46640997
IRC-1	2.39	-1936.46360342
IRC-R-10	2.55	-1936.46832159
IRC-R-20	2.63	-1936.47371341
IRC-R-50	2.72	-1936.48535544
IRC-R-80	2.82	-1936.49334845
IRC-M2	2.95	-1936.53058423

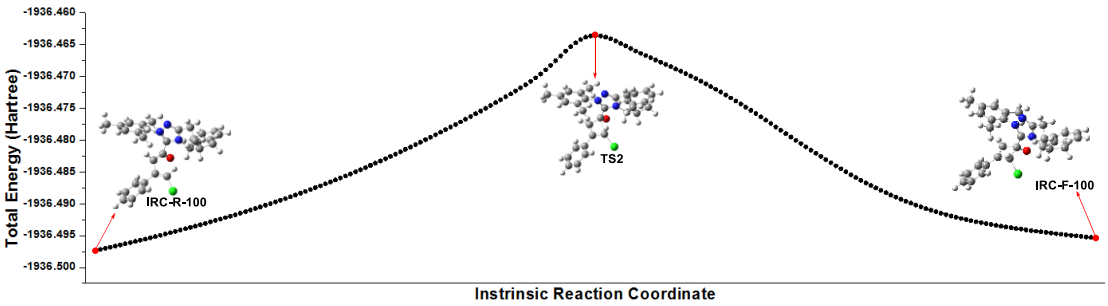


Fig. S5 IRC points of **TS2**

Part 8: IRC points of *Z*-TS1^{D}

Table S5 The distances of C2–C5 (unit: Å) and single-point energies *E* (unit: a.u.) of several IRC points in ***Z*-TS1^{D}** at M06-2X/6-31G(d, p)//IEF-PCM$_{THF}$ level

	C2–C5	E
IRC-R-46	1.56	-920.44134771
IRC-R-15	1.67	-920.42236633
IRC-R-13	1.71	-920.41959333
IRC-R-11	1.79	-920.41586485
IRC-R-10	1.98	-920.41362725
IRC-1	2.09	-920.39933771
IRC-F-5	2.19	-920.40141659
IRC-F-10	2.36	-920.40963177
IRC-F-15	2.49	-920.41521448
IRC-F-25	2.58	-920.42174136
IRC-F-40	2.69	-920.42837608
IRC-F-50	2.78	-920.43081851

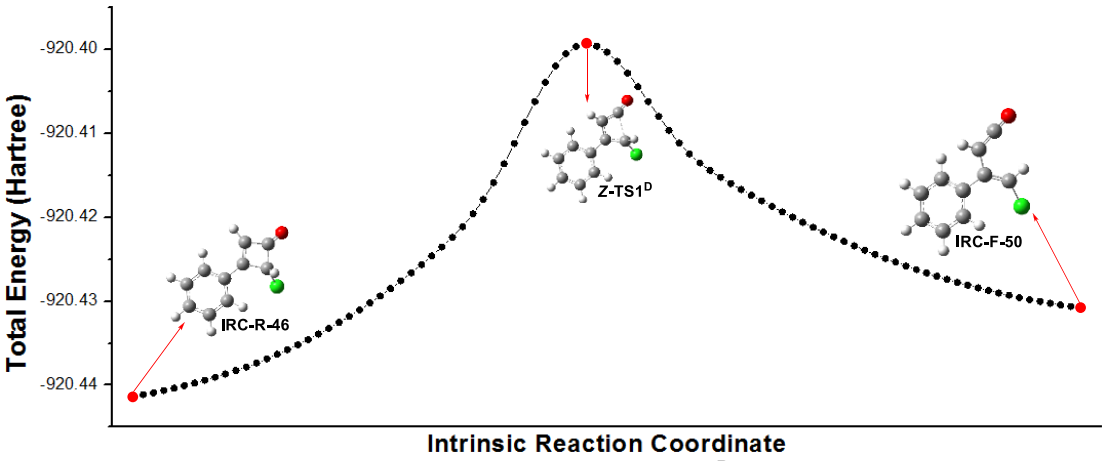


Fig. S6 IRC pictures of ***Z*-TS1^{D}**

Part 9: Coordinates of stationary points involved in the reaction

Coordinates of stationary points of all the stationary points involved in the reaction

R1

Total energy=−920.44408620
Sum of electronic and zero-point Energies= −920.301914
Sum of electronic and thermal Energies= −920.292098
Sum of electronic and thermal Enthalpies= −920.291154
Sum of electronic and thermal Free Energies= −920.338660

C	-0.45287000	-0.59244700	0.17004600
C	-1.59994100	0.33090000	0.53295500
C	-2.46693200	-0.91828500	0.22248900
C	-1.23402400	-1.68968600	-0.01073800
H	-1.62871600	0.70157600	1.55853600
H	-1.03080600	-2.73070700	-0.22957600
O	-3.65406700	-1.09567400	0.16276500
C	0.97014900	-0.31490200	0.09385600
C	1.45877400	0.94029700	0.47870400
C	1.86267400	-1.29938800	-0.35547700
C	2.82279700	1.20379300	0.42272600
H	0.76860400	1.70580500	0.82087900
C	3.22289100	-1.03144300	-0.41135000
H	1.48260000	-2.26901200	-0.66323900
C	3.70359600	0.21999800	-0.02169200
H	3.19831300	2.17563200	0.72420600
H	3.91107400	-1.79375700	-0.76036600
H	4.76764600	0.42775500	-0.06766100
Cl	-1.87993300	1.73265100	-0.55376500

R2

Total energy= −877.99334470
Sum of electronic and zero-point Energies= −877.707527
Sum of electronic and thermal Energies= −877.689625
Sum of electronic and thermal Enthalpies= −877.688681
Sum of electronic and thermal Free Energies= −877.753987

C	2.59576300	0.44890400	0.10624300
C	1.21631800	0.49829500	-0.16664900
C	0.57289700	1.72089700	-0.31572300
C	1.32200700	2.88980700	-0.17564300
C	2.68778000	2.82316400	0.10013700
C	3.35130000	1.60125700	0.24425100
C	2.00764300	-1.75830100	0.00544100
C	0.75982600	-0.89584400	-0.23263200
H	-0.48439000	1.76892100	-0.55302900
H	0.84149200	3.85460800	-0.28953600
H	3.25485500	3.74282700	0.20169900
H	4.41420000	1.56059200	0.45404700
N	3.03959000	-0.87629200	0.20444000
O	2.06676500	-2.96701900	0.02005300
N	-0.36538000	-1.45392800	-0.40857600
C	4.40600500	-1.27181900	0.46713600
H	4.43268700	-2.36096000	0.48417700

H	5.06988500	-0.90270400	-0.31921300
H	4.73784000	-0.88346200	1.43367200
C	-1.50058300	-0.65708600	-0.66128700
O	-1.73112300	-0.15721200	-1.73825100
O	-2.26953100	-0.63046600	0.41928300
C	-3.57386100	0.04301000	0.39384900
C	-3.38270800	1.53139400	0.12562900
C	-4.47902000	-0.62485800	-0.63469200
C	-4.09401200	-0.18854100	1.80629800
H	-2.66347900	1.95120600	0.83538100
H	-3.03665700	1.71051700	-0.89318200
H	-4.33819900	2.04432700	0.26456700
H	-4.54053700	-1.69877600	-0.43851300
H	-5.48367600	-0.20165000	-0.55073500
H	-4.11279600	-0.46399100	-1.64882100
H	-5.07824200	0.27262500	1.91748200
H	-4.18303100	-1.25888100	2.00803000
H	-3.41444000	0.25224000	2.54007800

NHC

Total energy= - 1016.03688327

Sum of electronic and zero-point Energies= −1015.628659

Sum of electronic and thermal Energies= −1015.607664

Sum of electronic and thermal Enthalpies= −1015.606720

Sum of electronic and thermal Free Energies= −1015.679329

C	-2.89624900	0.67857700	0.70169900
C	-3.88776200	0.57289100	-0.27316900
C	-4.56991900	1.70784700	-0.70255900
C	-4.24398500	2.94244600	-0.14406300
C	-3.24452000	3.04406500	0.82661800
C	-2.55909400	1.90886900	1.25606000
C	-2.28900500	-0.67590100	0.99947700
C	-3.28682100	-1.66808100	0.34307000
C	-4.03518800	-0.85398700	-0.73848300
H	-5.34565100	1.63208200	-1.45922800
H	-4.77271000	3.83476100	-0.46467700
H	-3.00324400	4.01339000	1.25114500
H	-1.77067900	1.97746800	1.99836400
H	-4.01244400	-1.91808700	1.12341400
H	-3.58033300	-0.97579600	-1.72937400
H	-2.18890300	-0.85762200	2.07281700
H	-5.07835200	-1.17033100	-0.82878300
C	-0.55744400	-1.68867900	-0.54409100
C	0.12044700	-0.01832500	0.82430000
N	0.70411300	-1.53767700	-0.82205900
N	-0.93868100	-0.79466800	0.42817500
N	1.08353700	-0.51410800	0.02212400
C	-1.49929900	-2.68125100	-1.14009400
H	-1.89585500	-2.28753000	-2.08183500
H	-0.94804200	-3.59172600	-1.38377600
C	2.44021200	-0.06270100	-0.01414200
C	2.71788200	1.19689000	-0.54878400
C	3.44354300	-0.90164000	0.48276500
C	4.05010300	1.61482500	-0.57348500
C	4.75899000	-0.44655100	0.43119900

C	5.08061100	0.80702300	-0.09472100
H	4.28553800	2.59405700	-0.98329000
H	5.55228500	-1.08272200	0.81743700
C	1.61287300	2.07110700	-1.08120300
H	1.05218600	1.55110100	-1.86454000
H	0.89846000	2.31910700	-0.29147700
H	2.01944700	2.99390300	-1.49887700
C	6.51667200	1.26317400	-0.15050800
H	6.58572800	2.32325600	-0.41053300
H	7.01501800	1.11107400	0.81311600
H	7.07707200	0.69326100	-0.90133900
C	3.09654500	-2.24380300	1.07004600
H	2.32123700	-2.13894900	1.83579000
H	2.69895000	-2.91440800	0.30342800
H	3.97528100	-2.70654300	1.52176900
C	-2.63548100	-2.96075100	-0.15038000
H	-2.23634000	-3.51380400	0.70723300
H	-3.39008700	-3.59702800	-0.62178700

***Re*-TS1**

Total energy= − 1936.48669487

Sum of electronic and zero-point Energies= −1935.935618

Sum of electronic and thermal Energies= −1935.904212

Sum of electronic and thermal Enthalpies= −1935.903267

Sum of electronic and thermal Free Energies= −1935.999586

C	3.87381000	-0.11205900	-0.58381400
C	5.14468600	-0.08255000	-0.02273800
C	6.15392100	0.66642300	-0.63078900
C	5.86120000	1.37170400	-1.79475200
C	4.57763600	1.33316700	-2.35350700
C	3.57049600	0.58524000	-1.74958500
C	2.92673200	-0.96035000	0.23741200
C	3.81055500	-1.54367700	1.38967300
C	5.22177300	-0.91267000	1.22935800
H	7.14919900	0.70257200	-0.20293300
H	6.63773500	1.95985000	-2.27747200
H	4.36933600	1.88387200	-3.26566200
H	2.57290000	0.51622400	-2.17842600
H	3.88286700	-2.62319000	1.22193400
H	5.48656800	-0.29415800	2.09644900
H	2.45950000	-1.74039900	-0.37070800
H	5.99028800	-1.68760000	1.15682200
C	1.78068900	0.46153700	1.98816900
C	0.71930900	0.22817700	0.04261500
N	0.71226200	1.19335200	2.10781900
N	1.81555300	-0.13849200	0.74915000
N	0.08083700	1.03849100	0.89767200
C	2.82703100	0.14571400	3.00061200
H	3.68797300	0.81040100	2.86244900
H	2.42460800	0.32948700	3.99658900
C	-1.12535400	1.75373900	0.61724700
C	-1.08397300	2.79516500	-0.31221800
C	-2.30778900	1.35467400	1.25518600
C	-2.28315900	3.44663400	-0.60418700
C	-3.47611200	2.04093400	0.93392000

C	-3.48204500	3.08662600	0.00792000
H	-2.27545900	4.25705900	-1.33303800
H	-4.41004900	1.73101900	1.39875700
C	0.19569500	3.16675100	-1.01456300
H	1.03537200	3.22333700	-0.31667500
H	0.45757400	2.42305800	-1.77433000
H	0.09027900	4.13445300	-1.50953300
C	-4.77091200	3.79805300	-0.31477500
H	-4.66517500	4.43264600	-1.20007800
H	-5.57428700	3.08171900	-0.50313900
H	-5.08623400	4.43259300	0.51891400
C	-2.31694200	0.20128200	2.22094400
H	-1.70449800	-0.62603500	1.84372600
H	-1.90582600	0.49729900	3.19212600
H	-3.33896300	-0.16658300	2.36006900
C	-1.92350500	-1.23307400	-1.00704400
C	-0.64686700	-1.97956800	-0.69560100
C	0.05040300	-0.85601400	-1.57946900
C	-1.33154300	-0.25761900	-1.72670700
H	-0.36566300	-2.07727800	0.35565300
H	-1.70138300	0.64524500	-2.20449500
O	0.96663800	-1.00859600	-2.38617400
C	-3.28767600	-1.48717200	-0.54547600
C	-3.57154600	-2.61682900	0.23173300
C	-4.31783600	-0.57916900	-0.83539300
C	-4.85989900	-2.83093600	0.71642400
H	-2.77914900	-3.32773700	0.45460100
C	-5.59956100	-0.79518500	-0.35173100
H	-4.09372400	0.31010200	-1.42461900
C	-5.87307000	-1.92076400	0.42767300
H	-5.07039000	-3.70522200	1.31890900
H	-6.38846800	-0.07846000	-0.57531900
H	-6.87556200	-2.08241500	0.81182000
Cl	-0.49663000	-3.62840800	-1.40910400
C	3.23030800	-1.31763000	2.79389400
H	2.34866000	-1.95492100	2.94653100
H	3.97229700	-1.61201500	3.54018300

_Si_-TS1

Total energy= −1936.47681220
Sum of electronic and zero-point Energies= −1935.925198
Sum of electronic and thermal Energies= −1935.893656
Sum of electronic and thermal Enthalpies= −1935.892712
Sum of electronic and thermal Free Energies= −1935.990432

C	-2.55069600	-1.94336700	-0.48463200
C	-3.61463400	-2.74528800	-0.08523700
C	-4.21964900	-3.60757600	-0.99728700
C	-3.73567400	-3.65678300	-2.30239600
C	-2.65407100	-2.86226900	-2.69204300
C	-2.04644000	-1.99816600	-1.78374500
C	-2.05073500	-1.08649900	0.66032600
C	-2.85130700	-1.57968100	1.91817400
C	-3.93791700	-2.54948300	1.37295100
H	-5.04890300	-4.23978500	-0.69318300
H	-4.19449600	-4.32803400	-3.02156400

H	-2.27959000	-2.92428200	-3.70866500
H	-1.18827200	-1.39798700	-2.08337800
H	-3.33210100	-0.71324300	2.37604100
H	-3.93006600	-3.50385500	1.91237200
H	-2.23292300	-0.02599700	0.47880700
H	-4.93898200	-2.12622100	1.50233300
C	-0.04039800	-2.26897000	1.50524500
C	0.37493900	-0.50141400	0.19035100
N	1.25198600	-2.25280000	1.38428300
N	-0.59982700	-1.22437000	0.81104500
N	1.48078800	-1.16843700	0.56512100
C	-0.90394500	-3.15161000	2.33532200
H	-1.38506300	-3.90982900	1.70458800
H	-0.29099500	-3.66765900	3.07573000
C	2.84576600	-0.86658600	0.24178000
C	3.61676800	-0.18018300	1.18347100
C	3.37782700	-1.36138600	-0.95205800
C	4.94499600	0.09117400	0.85776100
C	4.71208000	-1.06642200	-1.23277900
C	5.50254100	-0.32840500	-0.35089100
H	5.56022000	0.63617100	1.57003700
H	5.14711500	-1.43719900	-2.15785800
C	3.05094900	0.19899500	2.52585900
H	2.01643100	0.53920500	2.44206100
H	3.06168200	-0.66558800	3.19786700
H	3.64414700	0.99346700	2.98357900
C	6.92968000	0.01046900	-0.69687400
H	6.98402600	0.97961500	-1.20358200
H	7.55039000	0.07240500	0.20012000
H	7.36195200	-0.73631100	-1.36692100
C	2.55250100	-2.22292000	-1.86910700
H	2.08882300	-3.04184400	-1.30979500
H	1.75458400	-1.63403700	-2.32797200
H	3.17887200	-2.65135700	-2.65403600
C	-0.91777800	2.47047600	-0.85091400
C	0.56049800	2.21216700	-1.00223500
C	0.11322400	0.78813900	-1.53034300
C	-1.30378500	1.27134300	-1.33063100
H	1.05860600	2.77671000	-1.79323400
H	-2.26485800	0.86224500	-1.62856400
O	0.59055000	0.15081700	-2.46283500
C	-1.61891500	3.66854500	-0.40043200
C	-0.92139400	4.86586900	-0.20194100
C	-2.99950300	3.63139000	-0.15990300
C	-1.59511200	6.00782800	0.22077200
H	0.14917700	4.89940700	-0.38135300
C	-3.66926700	4.77210400	0.26203400
H	-3.54094300	2.69981700	-0.30040800
C	-2.96776700	5.96326600	0.45283200
H	-1.04819200	6.93287000	0.37062200
H	-4.73790600	4.73486600	0.44643000
H	-3.49171800	6.85384200	0.78464400
Cl	1.56356900	2.42465800	0.47212000
C	-1.95894900	-2.24113000	2.98002400
H	-1.44344600	-1.47447400	3.56766000
H	-2.58626800	-2.81115000	3.67036200

***Re*-M1**

Total energy= - 1936.50064372

Sum of electronic and zero-point Energies= -1935.947522

Sum of electronic and thermal Energies= -1935.916020

Sum of electronic and thermal Enthalpies= -1935.915075

Sum of electronic and thermal Free Energies= -1936.011639

C	3.76764100	-0.30375500	-0.49782800
C	5.01759000	-0.62734900	0.01766700
C	6.16594700	-0.06898300	-0.53967600
C	6.03279300	0.81075800	-1.61163100
C	4.77173600	1.12222600	-2.12819500
C	3.62082900	0.56242400	-1.57803200
C	2.66612800	-1.00506600	0.27141500
C	3.38933500	-1.64779000	1.50771000
C	4.90240100	-1.60523600	1.15749100
H	7.14752900	-0.31102500	-0.14249800
H	6.91868600	1.25805700	-2.05178400
H	4.69071000	1.80318800	-2.96954300
H	2.62565800	0.75144600	-1.97451200
H	3.05546200	-2.68157800	1.61416500
H	5.50912400	-1.31055100	2.02026200
H	2.14440100	-1.73565600	-0.35181500
H	5.25456000	-2.59438100	0.84676200
C	1.85804900	0.84964600	1.73488500
C	0.47699600	0.28112000	0.13044000
N	0.87308200	1.69826500	1.82860800
N	1.65141300	-0.02857100	0.70182700
N	0.02636800	1.32982800	0.81382300
C	3.01307500	0.61526400	2.64150800
H	3.93621900	0.99814800	2.19121000
H	2.84602500	1.14006200	3.58286300
C	-1.13725200	2.10987600	0.49772800
C	-1.04639600	2.99394200	-0.57880300
C	-2.30723400	1.90123300	1.22962200
C	-2.19555800	3.71160900	-0.90950000
C	-3.42775500	2.64321700	0.86128100
C	-3.38892300	3.54850200	-0.20324400
H	-2.15836000	4.40783300	-1.74331400
H	-4.35510300	2.50476000	1.41200100
C	0.22450500	3.10292800	-1.37922400
H	1.08669800	3.28639500	-0.72966700
H	0.41504600	2.16780500	-1.92283100
H	0.15458600	3.91798900	-2.10097800
C	-4.62695800	4.31077700	-0.59898600
H	-4.37384800	5.21001200	-1.16401100
H	-5.27320000	3.69143700	-1.22909200
H	-5.20677900	4.60343600	0.27939400
C	-2.35469800	0.87225500	2.32503400
H	-2.22178300	-0.13130900	1.90217500
H	-1.55932500	1.03244600	3.05794200
H	-3.31689300	0.89862300	2.83853500
C	-1.99488700	-1.37895000	-0.70724600
C	-0.60014700	-1.90093400	-0.51345200
C	-0.10204800	-0.44170700	-1.09778600
C	-1.62134300	-0.19834800	-1.22745300

H	-0.30879100	-2.21389700	0.49542100
H	-2.18625400	0.64793500	-1.61227900
O	0.72190000	-0.35091400	-2.10115500
C	-3.28556400	-1.96579300	-0.34093900
C	-3.39207800	-3.32635100	-0.03234800
C	-4.42802100	-1.15622100	-0.26495400
C	-4.62131400	-3.87107600	0.32881200
H	-2.50815300	-3.95552300	-0.08672400
C	-5.65368400	-1.70250100	0.09387900
H	-4.33984500	-0.09226600	-0.47261500
C	-5.75401200	-3.06262100	0.38956900
H	-4.69484500	-4.92838600	0.56246700
H	-6.53253600	-1.06804900	0.15016800
H	-6.71163400	-3.48799100	0.67230500
Cl	-0.11623100	-3.24407400	-1.60595900
C	3.08544400	-0.91173400	2.82734600
H	2.12718100	-1.25232600	3.23328600
H	3.85254500	-1.16491500	3.56288800

***Si*-M1**

Total energy= − 1936.49032817

Sum of electronic and zero-point Energies= -1935.936854

Sum of electronic and thermal Energies= -1935.905602

Sum of electronic and thermal Enthalpies= -1935.904658

Sum of electronic and thermal Free Energies= -1935.999792

C	-3.11928500	-1.08075900	-0.50887300
C	-4.33870100	-1.63121200	-0.12790500
C	-5.15535300	-2.23874100	-1.07909600
C	-4.72313000	-2.29235700	-2.40198700
C	-3.48471000	-1.75978600	-2.77014900
C	-2.66282600	-1.14890300	-1.82528800
C	-2.40679900	-0.46987000	0.67784900
C	-3.29158800	-0.82457200	1.92372200
C	-4.57120500	-1.49979300	1.35435300
H	-6.10822700	-2.67351800	-0.79142300
H	-5.34858500	-2.76509200	-3.15277400
H	-3.15605100	-1.82748100	-3.80215600
H	-1.68137200	-0.76467100	-2.10997200
H	-3.56272200	0.11338500	2.41127600
H	-4.74350100	-2.48129300	1.81219900
H	-2.30064500	0.61067500	0.58955600
H	-5.45795100	-0.89615800	1.56956700
C	-0.75488200	-2.18038400	1.42878800
C	0.08718300	-0.60124400	0.14151200
N	0.48897600	-2.51455200	1.25630300
N	-1.03572300	-1.00666300	0.77399000
N	0.99654700	-1.53646600	0.44838400
C	-1.79342600	-2.83150800	2.26999300
H	-2.45807600	-3.43362400	1.63830800
H	-1.30702200	-3.49972900	2.98169800
C	2.38669900	-1.62963200	0.07848800
C	3.34987200	-1.29548600	1.03633400
C	2.71349600	-2.19711200	-1.15865600
C	4.68787400	-1.38745400	0.65622900
C	4.06675100	-2.27032400	-1.48662500

C	5.06316900	-1.84413300	-0.60755400
H	5.45614400	-1.11656500	1.37715200
H	4.34882600	-2.68971800	-2.44895100
C	2.99861700	-0.96309400	2.46351500
H	1.98070300	-0.59012300	2.57161700
H	3.09303000	-1.86626400	3.07606600
H	3.68475000	-0.21228500	2.86132300
C	6.51836500	-1.90351100	-0.99165400
H	6.96079600	-0.89882500	-0.98476000
H	7.08765900	-2.51591100	-0.28092700
H	6.64904300	-2.32500700	-1.99344300
C	1.65788400	-2.78835200	-2.05013900
H	1.12970800	-3.58948900	-1.52113500
H	0.93870500	-2.01195300	-2.32500900
H	2.11272000	-3.21375800	-2.94679700
C	-0.04973000	2.59719500	-0.53924200
C	1.17570800	1.74056200	-0.47874200
C	0.23229700	0.50704300	-0.94648700
C	-0.86198800	1.59844600	-0.91961500
H	1.94338600	1.91444100	-1.23365800
H	-1.87138000	1.59273400	-1.32658700
O	0.47545700	-0.04311000	-2.10518500
C	-0.20165500	4.03719800	-0.33368900
C	0.92742900	4.85664100	-0.22163400
C	-1.47502400	4.61538700	-0.24705000
C	0.78596700	6.22848300	-0.03557700
H	1.91759500	4.41428100	-0.28469500
C	-1.61469700	5.98529500	-0.06358900
H	-2.35408000	3.98039100	-0.31671400
C	-0.48385000	6.79560300	0.04302900
H	1.66808700	6.85530300	0.04639000
H	-2.60536400	6.42359300	0.00263800
H	-0.59418200	7.86515600	0.19036800
Cl	2.01675500	1.76771800	1.13333200
C	-2.57431100	-1.70387300	2.95630300
H	-1.87645200	-1.10177100	3.54715500
H	-3.31154400	-2.11779500	3.64840300

TS2

Total energy= -1936.46452331
Sum of electronic and zero-point Energies= -1935.915223
Sum of electronic and thermal Energies= -1935.883029
Sum of electronic and thermal Enthalpies= -1935.882085
Sum of electronic and thermal Free Energies= -1935.981097

C	3.69251200	-0.35591600	-0.76060200
C	4.90063900	-0.99480700	-0.47331000
C	5.98655500	-0.85709800	-1.32898100
C	5.84917500	-0.06155200	-2.46700400
C	4.64384100	0.58538600	-2.74101900
C	3.54832400	0.43889200	-1.88939300
C	2.69379200	-0.69951100	0.32824200
C	3.60313700	-1.06790300	1.52425800
C	4.79680100	-1.75602200	0.82877900
H	6.93001300	-1.34827600	-1.10943400
H	6.69039700	0.06297900	-3.14156100

H	4.55685600	1.20698500	-3.62631900
H	2.60128500	0.91959700	-2.10926400
H	3.08094600	-1.73189600	2.22029700
H	5.70921600	-1.70821300	1.43009200
H	2.05888700	-1.54658100	0.03312800
H	4.57649700	-2.81325900	0.64119600
C	1.82739700	1.16393100	1.81004200
C	0.59141800	0.65606000	0.07565200
N	0.79112500	1.95327000	1.88741500
N	1.76265600	0.37777900	0.68431900
N	0.03143300	1.62128500	0.80203900
C	2.90865600	1.00781600	2.82464800
H	3.22757500	1.99507300	3.16531900
H	2.47320100	0.49172700	3.68753900
C	-1.17055700	2.32967400	0.47328600
C	-1.14546100	3.19220400	-0.62411400
C	-2.31728800	2.09062500	1.23896300
C	-2.33366400	3.85057700	-0.94519900
C	-3.47285300	2.77725200	0.88064200
C	-3.49959100	3.65713700	-0.20606100
H	-2.34292800	4.53283400	-1.79108100
H	-4.38069900	2.61370500	1.45616500
C	0.10352600	3.39330300	-1.44340600
H	0.99144200	3.47515700	-0.80976300
H	0.26209900	2.55503200	-2.13178800
H	0.02304800	4.30195000	-2.04173500
C	-4.77739900	4.36648800	-0.57062500
H	-5.21892400	4.84885300	0.30552700
H	-4.60634300	5.12707300	-1.33453300
H	-5.51411800	3.65604000	-0.95769700
C	-2.31145500	1.08401900	2.35665000
H	-1.47720600	1.24793800	3.04323300
H	-3.24390100	1.13388400	2.92065500
H	-2.21510800	0.07175400	1.94418400
C	-1.80579700	-1.53580700	-0.33400800
C	-0.72487300	-1.92597600	0.51783900
C	-0.03400800	-0.15739900	-1.03153800
C	-1.50683200	-0.36041000	-0.97082100
H	-0.47863500	-1.33808400	1.39356500
H	-2.22409000	0.39253600	-1.28989600
O	0.71147800	-0.55898300	-1.92221500
C	-3.11640000	-2.21529300	-0.47841800
C	-3.69450600	-2.90442800	0.59473000
C	-3.81998600	-2.12761500	-1.68405500
C	-4.95140000	-3.48552800	0.46473500
H	-3.15129900	-2.96637000	1.53327200
C	-5.08020300	-2.70431700	-1.81413500
H	-3.35763200	-1.61247200	-2.52127700
C	-5.64771100	-3.38609300	-0.73983700
H	-5.39309900	-4.01286700	1.30460000
H	-5.61550900	-2.62982200	-2.75562300
H	-6.62780900	-3.84168300	-0.84093800
Cl	-0.43356100	-3.65801600	0.85299600
C	4.07310000	0.19788100	2.25385800
H	4.74651500	-0.08356900	3.06698800
H	4.64820900	0.81834900	1.55673600

M2

Total energy= -1936.53058424
Sum of electronic and zero-point Energies= -1935.977009
Sum of electronic and thermal Energies= -1935.944814
Sum of electronic and thermal Enthalpies= -1935.943869
Sum of electronic and thermal Free Energies= -1936.043191

C	-2.52025800	-2.03743300	0.71484200
C	-3.60239400	-2.88158800	0.49591500
C	-4.43404300	-3.23377200	1.55741300
C	-4.16178300	-2.72310200	2.82358300
C	-3.07665200	-1.86639700	3.03165500
C	-2.24019100	-1.51369300	1.97564900
C	-1.75388500	-1.79208600	-0.56598300
C	-2.55885300	-2.54097200	-1.68290800
C	-3.70827800	-3.28914400	-0.94986700
H	-5.28312700	-3.89204700	1.39837800
H	-4.80167600	-2.98849300	3.65914400
H	-2.88460800	-1.47340800	4.02465000
H	-1.40115800	-0.83652000	2.13197200
H	-1.88783100	-3.26619200	-2.14616100
H	-4.68779700	-3.02398200	-1.36511900
H	-0.72104900	-2.13906100	-0.49538200
H	-3.60385400	-4.37189900	-1.06658800
C	-2.63706400	0.38046800	-1.47537600
C	-0.77538000	0.53227100	-0.33130100
N	-2.38190300	1.65777500	-1.40940400
N	-1.66586300	-0.34271900	-0.82882800
N	-1.22738700	1.73097300	-0.68244400
C	-3.71900100	-0.33944400	-2.19785600
H	-4.52507100	-0.59528900	-1.49963200
H	-4.13416600	0.31455900	-2.96569500
C	-0.59309600	2.99479100	-0.42324500
C	0.36274400	3.44826900	-1.33150000
C	-0.97115800	3.69985100	0.72052700
C	0.95366700	4.68349100	-1.06801100
C	-0.35281200	4.92837100	0.93831900
C	0.60919100	5.43210500	0.05836900
H	1.70038800	5.06671700	-1.75850600
H	-0.62443500	5.50444200	1.81934000
C	0.74289100	2.61971600	-2.52955400
H	1.23696300	1.69489400	-2.21117000
H	-0.13882800	2.34155000	-3.11496600
H	1.42843000	3.16900500	-3.17617900
C	1.28148600	6.75030900	0.34190500
H	2.07751200	6.62249900	1.08226000
H	1.72921500	7.16938900	-0.56145500
H	0.57090900	7.47522600	0.74613900
C	-1.98125500	3.12198600	1.67266400
H	-2.92729100	2.91122500	1.16422900
H	-1.59233600	2.18050700	2.07533800
H	-2.17550600	3.81166000	2.49525200
C	2.64845400	-0.91811500	0.57196300
C	2.96603300	-0.53014300	1.82347200
C	0.42972700	0.25961000	0.54410900
C	1.40122100	-0.50844200	-0.06001000

H	2.32865400	0.10986000	2.41370500
H	1.24774700	-0.81108500	-1.09152400
O	0.35989100	0.76541300	1.70071400
C	3.52839400	-1.80133600	-0.24890600
C	4.86450100	-1.47041800	-0.49635500
C	3.00583800	-2.96443400	-0.82431300
C	5.66135800	-2.28879100	-1.29171300
H	5.27334100	-0.56113500	-0.06695200
C	3.80390900	-3.78860300	-1.61320500
H	1.96761600	-3.22640300	-0.63822500
C	5.13468800	-3.45200200	-1.84983400
H	6.69508500	-2.01574100	-1.47954100
H	3.38643000	-4.69400900	-2.04255200
H	5.75743700	-4.09049100	-2.46834100
Cl	4.39916800	-1.06927600	2.67946700
C	-3.08493300	-1.60895700	-2.78576600
H	-2.26945000	-1.31685900	-3.45536400
H	-3.81884700	-2.15092800	-3.38705500

TS3*RR*

Total energy= -2814.52204318

Sum of electronic and zero-point Energies= -2813.681448

Sum of electronic and thermal Energies= -2813.632520

Sum of electronic and thermal Enthalpies= -2813.631575

Sum of electronic and thermal Free Energies= -2813.762381

C	-4.43582800	0.17930700	-0.69971200
C	-5.78498100	0.06391800	-0.36766700
C	-6.76650300	0.22550800	-1.34251500
C	-6.38155400	0.49503200	-2.65248700
C	-5.02983500	0.59889200	-2.98636500
C	-4.04660300	0.44151000	-2.01296200
C	-3.55897800	-0.04244900	0.51785200
C	-4.56626700	-0.17997300	1.70846200
C	-5.98083200	-0.26243000	1.08733000
H	-7.81738200	0.13874000	-1.08274300
H	-7.13676300	0.62430200	-3.42104400
H	-4.74104900	0.80809500	-4.01094500
H	-3.00060500	0.53033200	-2.28764700
H	-4.48724900	0.75798400	2.26256600
H	-6.42396500	-1.25878300	1.20339400
H	-2.87099600	0.76963700	0.74356000
H	-6.66242400	0.43837800	1.57746300
C	-2.93061900	-2.43841100	0.96887500
C	-1.50898500	-1.35509200	-0.29623000
N	-1.97733500	-3.28850000	0.71666600
N	-2.68538700	-1.23512200	0.35863100
N	-1.10748700	-2.61037800	-0.07555200
C	-4.08176500	-2.63606800	1.88531900
H	-4.98196900	-2.88010800	1.31149000
H	-3.85875400	-3.48507500	2.53276600
C	0.15668500	-3.26162400	-0.33695400
C	1.07140300	-3.30063100	0.71926400
C	0.34720500	-3.92919600	-1.54752500
C	2.26258000	-3.99083400	0.50134100
C	1.55902200	-4.59859700	-1.71518300

C	2.52729700	-4.63182400	-0.70858500
H	3.00373900	-4.01961300	1.29711500
H	1.74563200	-5.11464700	-2.65364300
C	0.79164400	-2.63648200	2.04123500
H	1.61370200	-1.96094200	2.29244500
H	-0.12965100	-2.05732300	2.05322100
H	0.73084700	-3.39403600	2.83010400
C	3.83164900	-5.35874000	-0.91020100
H	3.97473300	-5.63383900	-1.95750500
H	4.67305900	-4.73266700	-0.60027100
H	3.86382100	-6.27483500	-0.31221200
C	-0.71449900	-3.93581100	-2.61156600
H	-1.67864700	-4.24652000	-2.19686200
H	-0.83470200	-2.93270200	-3.02747000
H	-0.44850000	-4.62580700	-3.41396100
C	0.02879100	1.97842500	-1.42430000
C	1.30314100	1.54458400	-1.87434100
C	-0.71177700	-0.39447700	-1.18550800
C	-0.86843500	1.02672400	-0.98958900
H	1.35863300	0.64409300	-2.46511300
H	-1.72196800	1.38536100	-0.43678700
O	-0.06126500	-0.94818500	-2.06963700
C	-0.29673600	3.39882700	-1.11305300
C	-0.70092900	3.75294600	0.17967900
C	-0.27511000	4.37854900	-2.11009200
C	-1.07271300	5.06189100	0.46809900
H	-0.69500000	2.99493400	0.95889500
C	-0.65142400	5.68730000	-1.82107800
H	0.02610400	4.10924700	-3.11754500
C	-1.04953300	6.03250500	-0.53159600
H	-1.37413800	5.32634300	1.47691700
H	-0.63654700	6.43711100	-2.60590500
H	-1.33843100	7.05429100	-0.30616900
Cl	2.47428400	2.72520600	-2.47898200
C	-4.26070000	-1.33106400	2.66639000
H	-3.34399600	-1.12096300	3.22765700
H	-5.07659700	-1.42908400	3.38693000
C	4.30483300	0.56967700	-0.54676200
C	3.12286800	-0.15497300	-0.75185100
C	3.14049600	-1.35972700	-1.42789200
C	4.36882100	-1.84309300	-1.89449800
C	5.53992500	-1.11547600	-1.68799900
C	5.52846700	0.10986700	-1.00970400
C	2.67901100	1.86879300	0.42368900
C	2.01661200	0.61304500	-0.13467300
H	2.20895500	-1.89375500	-1.59831600
H	4.40484900	-2.78665600	-2.43105100
H	6.48325100	-1.49989700	-2.06322800
H	6.44265100	0.67263400	-0.85188900
N	4.02645400	1.74370400	0.16606100
O	2.14422000	2.81995900	0.96174200
N	0.98167700	0.01437800	0.45989600
C	4.98463700	2.79261000	0.42051500
H	4.46188400	3.59048500	0.94777900
H	5.80740100	2.42320700	1.03926600
H	5.38803700	3.18083100	-0.52033400
C	0.52225400	0.36032900	1.69228400

O	-0.64976900	0.25590200	2.05211200
O	1.53898600	0.66430300	2.53061300
C	1.38130700	0.93460900	3.94370100
C	0.15417500	1.78716800	4.25966000
C	1.38654800	-0.39786700	4.68858200
C	2.64689200	1.72647100	4.26761700
H	0.11933500	2.64399000	3.57993600
H	-0.77166300	1.22396400	4.16417300
H	0.24770100	2.16257300	5.28320000
H	2.34082700	-0.90708600	4.52101400
H	1.27364900	-0.22894400	5.76365400
H	0.59118200	-1.06762500	4.35099900
H	2.68907100	1.95662900	5.33561800
H	3.53323600	1.14598200	3.99666000
H	2.65310400	2.65696100	3.69391600

TS3*RS*

Total energy= -2814.52077583

Sum of electronic and zero-point Energies=	-2813.680511
Sum of electronic and thermal Energies=	-2813.630153
Sum of electronic and thermal Enthalpies=	-2813.629209
Sum of electronic and thermal Free Energies=	-2813.765791

C	-2.15551600	3.27960400	-0.33662100
C	-2.48869600	4.48345100	0.27610000
C	-2.96930000	5.54707300	-0.48424300
C	-3.12265600	5.38299700	-1.85781900
C	-2.81545900	4.16368900	-2.46621500
C	-2.33425400	3.10045300	-1.70777400
C	-1.64375800	2.27679900	0.67767900
C	-1.81239300	2.97740700	2.07126100
C	-2.29713100	4.42162300	1.76775400
H	-3.23002000	6.48836800	-0.00922700
H	-3.49685100	6.20434600	-2.46044200
H	-2.95817700	4.04115300	-3.53476800
H	-2.11754000	2.14682600	-2.18281100
H	-0.82033000	3.01241700	2.52284200
H	-3.23469100	4.64948500	2.28959200
H	-0.59835200	2.00521500	0.54736900
H	-1.56433900	5.15931300	2.10869200
C	-3.53592600	0.78186500	1.27562900
C	-2.13018500	-0.10573900	-0.14424700
N	-4.00300000	-0.41076300	1.03344200
N	-2.39202700	1.01078800	0.56623900
N	-3.12899800	-0.94624100	0.14392300
C	-4.00442300	1.76249200	2.28768300
H	-4.50813300	2.60534300	1.79877700
H	-4.72213600	1.26860500	2.94383400
C	-3.41769300	-2.28593900	-0.31840500
C	-2.73471100	-3.36239800	0.24019900
C	-4.44790400	-2.42171200	-1.25229200
C	-3.13311200	-4.63701600	-0.16952300
C	-4.79925200	-3.71302000	-1.63098600
C	-4.15624200	-4.83167900	-1.09391000
H	-2.61700600	-5.49879300	0.24629900
H	-5.59195800	-3.85003600	-2.36253300

C	-1.57855500	-3.18108100	1.18144300
H	-0.64228400	-3.15252300	0.61207900
H	-1.63596800	-2.24349400	1.74196100
H	-1.53103700	-4.01205200	1.88898100
C	-4.57801900	-6.21853800	-1.50620300
H	-5.57653400	-6.45077100	-1.12240800
H	-4.61761200	-6.30877200	-2.59521100
H	-3.88634500	-6.97212700	-1.12470800
C	-5.13237500	-1.21286100	-1.83341100
H	-5.66916400	-0.65320900	-1.06181000
H	-4.40460800	-0.53253700	-2.28874700
H	-5.84615900	-1.51106200	-2.60279300
C	1.24042300	0.24052500	-1.97190600
C	1.73908900	-1.07928700	-1.91527700
C	-0.98626300	-0.49308700	-1.08155100
C	0.00477600	0.50333400	-1.39170000
H	1.02627000	-1.88858400	-1.86560700
H	-0.23629100	1.54107900	-1.21863900
O	-1.07274500	-1.62730000	-1.53614200
C	2.02135100	1.40551600	-2.47256900
C	3.41070200	1.52187400	-2.32450500
C	1.33267900	2.44889500	-3.10977300
C	4.07766000	2.65573700	-2.77714000
H	3.97262500	0.73656600	-1.83493900
C	2.00211600	3.57736300	-3.56914300
H	0.26121400	2.36138500	-3.26423800
C	3.37979500	3.68741200	-3.39955000
H	5.15144300	2.73021800	-2.63603500
H	1.44702000	4.36766700	-4.06439100
H	3.90620200	4.56776000	-3.75468200
Cl	3.12961800	-1.55784000	-2.88232900
C	-2.74409800	2.23136700	3.02905500
H	-2.22531400	1.35727800	3.43439800
H	-3.01197000	2.88822900	3.86083400
C	4.38322200	-1.40395800	0.20557100
C	3.31713400	-0.52144200	0.42750000
C	3.55497900	0.80289300	0.75267500
C	4.87724400	1.24704000	0.83401400
C	5.93039900	0.36676300	0.58137300
C	5.70246500	-0.97609700	0.26198600
C	2.51274000	-2.71038300	-0.03675100
C	2.06631800	-1.28129000	0.23595200
H	2.72104900	1.48140000	0.91497700
H	5.08746700	2.28267800	1.07921000
H	6.95263100	0.72737100	0.63745700
H	6.52645200	-1.65721500	0.07708100
N	3.89331100	-2.69039300	-0.03378500
O	1.81989100	-3.69147600	-0.22458900
N	0.87626000	-1.03431300	0.76513000
C	4.70358400	-3.82372200	-0.40961300
H	4.03071800	-4.67044300	-0.54618100
H	5.23226100	-3.62290500	-1.34739400
H	5.43062700	-4.05566900	0.37389400
C	0.68728800	-0.36316600	1.92172800
O	-0.35709100	0.20849100	2.24073700
O	1.73545300	-0.48658700	2.77653500
C	1.72883300	0.10948500	4.09407800

C	1.53101400	1.62085400	4.01351300
C	0.66956400	-0.55750400	4.96666100
C	3.13119300	-0.20634700	4.60587600
H	2.24387400	2.05222000	3.30362800
H	0.51547700	1.85798800	3.69809800
H	1.71338000	2.06570300	4.99606200
H	0.84268600	-1.63670100	5.00392200
H	0.72883800	-0.16236900	5.98525900
H	-0.32813500	-0.37070300	4.56748000
H	3.26520300	0.19292900	5.61492900
H	3.28986800	-1.28746300	4.62962700
H	3.87935800	0.23910900	3.94329100

TS3*SR*

Total energy= -2814.52785028

Sum of electronic and zero-point Energies=	-2813.685584
Sum of electronic and thermal Energies=	-2813.636126
Sum of electronic and thermal Enthalpies=	-2813.635182
Sum of electronic and thermal Free Energies=	-2813.766809

C	3.27796000	-2.49317900	-0.91912500
C	3.81874100	-3.68007700	-0.43597600
C	4.88700900	-4.28331800	-1.09424000
C	5.39768800	-3.67961700	-2.24081000
C	4.83908900	-2.49586900	-2.73196200
C	3.76831000	-1.89453800	-2.07431000
C	2.13945900	-2.02699800	-0.03790100
C	2.22936100	-2.92708000	1.23463800
C	3.07732200	-4.14917300	0.79059000
H	5.31496600	-5.20881500	-0.72093600
H	6.23460200	-4.13366300	-2.76106400
H	5.24058400	-2.04358200	-3.63443400
H	3.30426300	-0.98769900	-2.45832800
H	1.21273100	-3.23126100	1.49943400
H	3.75010500	-4.49224500	1.58617800
H	1.16869700	-2.12105600	-0.52517900
H	2.42792800	-4.99391200	0.53355500
C	3.25172600	-0.16155100	1.19307800
C	1.74785900	0.47582400	-0.23579400
N	3.30833800	1.14443400	1.20930300
N	2.32158000	-0.60379500	0.29406000
N	2.36156300	1.52823800	0.29885600
C	3.92221400	-1.17007600	2.05682500
H	4.73511300	-1.65532500	1.50337300
H	4.35209300	-0.67177100	2.92865800
C	2.32039700	2.87566300	-0.21045900
C	1.59066500	3.85346100	0.45927100
C	3.03645300	3.12779600	-1.38949700
C	1.60503000	5.14240400	-0.07452300
C	3.01932100	4.42773200	-1.88051300
C	2.31064800	5.44869100	-1.23566400
H	1.03717300	5.92287800	0.42642200
H	3.57004700	4.65489100	-2.79111000
C	0.79298300	3.53666800	1.69140600
H	0.66898200	2.45919700	1.81713900
H	1.28326100	3.92363500	2.59106200

H	-0.19880200	3.99464900	1.62729500
C	2.29745500	6.84032800	-1.81179000
H	3.30573300	7.15466500	-2.09954700
H	1.66947000	6.87637200	-2.70975400
H	1.90232200	7.56263700	-1.09221100
C	3.76364600	2.02322700	-2.10833200
H	4.33095200	1.39356700	-1.41789500
H	3.05499600	1.38180300	-2.64255000
H	4.45912400	2.43661800	-2.84249400
C	-1.80928200	0.94505700	-1.33960900
C	-2.09091300	-0.35267400	-1.84531200
C	0.61532400	0.40309600	-1.22983500
C	-0.52085200	1.23015700	-0.92981500
H	-1.30364500	-0.86098000	-2.37939200
H	-0.34921300	2.11543800	-0.32572800
O	0.78442700	-0.39435800	-2.14715000
C	-2.86596000	1.94673600	-1.02140800
C	-3.67742400	2.46652700	-2.03274900
C	-2.99624000	2.44824700	0.28061000
C	-4.60081600	3.46748800	-1.75253700
H	-3.57232300	2.09433300	-3.04578100
C	-3.93125400	3.44207100	0.56182800
H	-2.39540700	2.02248300	1.08056600
C	-4.73397300	3.95747100	-0.45354900
H	-5.22198400	3.86665000	-2.54984700
H	-4.03352600	3.81178100	1.57804700
H	-5.46065600	4.73263100	-0.23520600
Cl	-3.64763000	-0.69156600	-2.58938400
C	2.83126700	-2.19188200	2.44488500
H	2.02367200	-1.64776300	2.93924700
H	3.23492900	-2.91574700	3.15581300
C	-3.74336000	-2.86728600	-0.25947800
C	-3.32362900	-1.65128600	0.31109200
C	-4.29515500	-0.84178000	0.89060800
C	-5.62036000	-1.27972100	0.94738500
C	-5.99313100	-2.51248600	0.42175900
C	-5.05024200	-3.32765200	-0.20442900
C	-1.53495400	-2.76519900	-0.82183900
C	-1.87060500	-1.49447600	-0.03666500
H	-4.02586600	0.12100900	1.29623400
H	-6.36740300	-0.64269200	1.41040700
H	-7.02659100	-2.84153700	0.48005800
H	-5.32994300	-4.27668800	-0.64917600
N	-2.68094800	-3.50643500	-0.90371600
O	-0.45912900	-3.09755600	-1.28865700
N	-0.80755200	-1.03641900	0.65996100
C	-2.78708100	-4.73722600	-1.64909000
H	-1.80310300	-4.94790900	-2.06670500
H	-3.09134700	-5.56040400	-0.99601000
H	-3.51645300	-4.63078800	-2.45875500
C	-1.02712000	-0.27825700	1.76920000
O	-2.09170600	0.05400100	2.27195500
O	0.15876100	0.08639700	2.37899700
C	0.10582300	0.45333800	3.79065200
C	-0.83788900	1.62661700	4.10378200
C	-0.29819200	-0.77868100	4.59938100
C	1.53874700	0.86514200	4.12645100

H	-0.82854200	2.36330600	3.29866300
H	-1.86386000	1.29184700	4.24207100
H	-0.49097200	2.11700200	5.02044600
H	0.41532700	-1.59695800	4.45481100
H	-0.32343800	-0.53064400	5.66522500
H	-1.29473400	-1.11461600	4.30039400
H	1.60629500	1.10044500	5.19067600
H	2.24739600	0.06556600	3.91084700
H	1.84067600	1.74727500	3.55721500

TS3*SS*

Total energy= -2814.52605517

Sum of electronic and zero-point Energies= -2813.685712

Sum of electronic and thermal Energies= -2813.635661

Sum of electronic and thermal Enthalpies= -2813.634717

Sum of electronic and thermal Free Energies= -2813.769866

C	-4.26405600	-0.01905700	1.69665800
C	-5.63824800	-0.24578200	1.69693100
C	-6.43215000	0.24938600	2.72941900
C	-5.83359600	0.97759700	3.75341000
C	-4.45505800	1.20567100	3.74895300
C	-3.65873900	0.70745400	2.72145600
C	-3.60898000	-0.63077300	0.47394600
C	-4.77000800	-1.36887100	-0.27154100
C	-6.07763900	-1.03158100	0.49155300
H	-7.50368500	0.07214700	2.73225900
H	-6.44125700	1.36952400	4.56293400
H	-3.99927500	1.76962600	4.55632500
H	-2.58611800	0.86741500	2.72717300
H	-4.56792800	-2.43650300	-0.15973400
H	-6.77159900	-0.44667400	-0.12445500
H	-2.79260000	-1.30665700	0.71474500
H	-6.61076200	-1.94387000	0.77399000
C	-3.58844500	0.99071400	-1.44824400
C	-1.76757800	1.00444200	-0.24505200
N	-2.83288400	1.91245200	-1.98379800
N	-2.98370600	0.43190500	-0.35952100
N	-1.71459900	1.91818200	-1.22010800
C	-4.87515700	0.46960200	-1.97580200
H	-5.71506000	0.93222700	-1.44584600
H	-4.95149300	0.74647000	-3.02817300
C	-0.70304700	2.90890600	-1.48655500
C	0.29898000	2.61078400	-2.40935200
C	-0.75054800	4.09085700	-0.74277400
C	1.32207000	3.54912600	-2.54718800
C	0.29289500	4.99548800	-0.92212500
C	1.34495300	4.72960900	-1.80315300
H	2.13193000	3.33961900	-3.24115900
H	0.29436600	5.91819800	-0.34717400
C	0.31724900	1.29925200	-3.14062600
H	0.67580200	0.51101700	-2.46522000
H	-0.68204500	1.02009300	-3.48474200
H	0.98501900	1.35544900	-4.00217600
C	2.50880800	5.67821900	-1.91265100
H	2.21424500	6.70047400	-1.66522600

H	3.29751100	5.37723100	-1.21382400
H	2.93484600	5.67002500	-2.91833400
C	-1.83957700	4.32684700	0.26996900
H	-2.83007200	4.13466800	-0.15241600
H	-1.71463700	3.66295200	1.13442200
H	-1.81034900	5.35543900	0.63173200
C	1.75172400	0.88241500	1.26825000
C	1.92395400	-0.49623800	1.59996100
C	-0.68160000	0.54973500	0.72977800
C	0.55266800	1.27984000	0.70774800
H	1.02508200	-1.02191400	1.88738900
H	0.56619700	2.22018700	0.18344400
O	-1.00542800	-0.36997900	1.48256900
C	2.83422000	1.90305800	1.31272300
C	4.18996100	1.60255700	1.11740100
C	2.48110900	3.24413100	1.52836900
C	5.14850200	2.60972800	1.11435100
H	4.50042800	0.57916500	0.95041600
C	3.43946500	4.25173900	1.52485100
H	1.44213600	3.49820200	1.71580300
C	4.77997000	3.93840500	1.31300200
H	6.18989100	2.35309900	0.94740000
H	3.13700900	5.28058800	1.69507800
H	5.53179800	4.72140800	1.30969000
Cl	3.22379100	-0.95179800	2.71651100
C	-4.85676600	-1.04917300	-1.76420400
H	-3.99210100	-1.47330800	-2.28747400
H	-5.76085600	-1.49965100	-2.18176400
C	3.80949700	-2.82098900	0.21156900
C	2.41222100	-2.77888400	0.33184300
C	1.75170700	-3.80106200	0.99572200
C	2.49011400	-4.87945200	1.48827600
C	3.87523000	-4.92207000	1.32653900
C	4.56018100	-3.88632700	0.68777800
C	3.23713600	-0.83323800	-0.76615400
C	1.96368600	-1.46900700	-0.22198100
H	0.67419000	-3.76103000	1.12161000
H	1.98220300	-5.69042800	1.99960700
H	4.43478300	-5.76924600	1.71037100
H	5.63952100	-3.90840000	0.57972700
N	4.28034500	-1.66069400	-0.41247300
O	3.33342100	0.19886000	-1.40211800
N	0.84772600	-1.10730500	-0.86281500
C	5.66586800	-1.38687900	-0.71414100
H	5.70637700	-0.40719700	-1.19210000
H	6.26170600	-1.37177600	0.20380700
H	6.07438200	-2.14015100	-1.39444600
C	-0.19505900	-1.90196800	-1.17940200
O	-1.31833200	-1.46753400	-1.44160500
O	0.11017900	-3.22077500	-1.29852900
C	-0.88613600	-4.19430400	-1.69502200
C	-2.05509700	-4.21067100	-0.71272700
C	-1.34754700	-3.92901700	-3.12568300
C	-0.12146000	-5.51313200	-1.62285800
H	-1.68427500	-4.31781600	0.31176600
H	-2.63286600	-3.28954800	-0.78854600
H	-2.70406400	-5.06333100	-0.93350100

H	-0.48274300	-3.89742900	-3.79479500
H	-2.00711700	-4.73813900	-3.45324600
H	-1.88276600	-2.98168400	-3.19059500
H	-0.76952900	-6.34022200	-1.92488400
H	0.74613400	-5.48412200	-2.28746400
H	0.23226500	-5.69443400	-0.60395700

M3*RR*

Total energy= -2814.56929848

Sum of electronic and zero-point Energies= -2813.725997

Sum of electronic and thermal Energies= -2813.676451

Sum of electronic and thermal Enthalpies= -2813.675507

Sum of electronic and thermal Free Energies= -2813.809276

C	-1.13100300	3.10992400	1.45818500
C	-0.63042700	3.87620100	2.50936100
C	-0.91158100	5.23623700	2.57660800
C	-1.70829300	5.81073400	1.58556700
C	-2.22540100	5.03428100	0.54806400
C	-1.94130000	3.67031900	0.47784900
C	-0.64581900	1.68031400	1.59591900
C	-0.24300900	1.56841200	3.09694700
C	0.18094100	3.01593700	3.44847400
H	-0.52944900	5.84007200	3.39436800
H	-1.94135700	6.86975500	1.62984300
H	-2.85938200	5.49101500	-0.20462700
H	-2.37121800	3.06293200	-0.31416100
H	0.60650400	0.88696700	3.18652400
H	0.01129600	3.25526200	4.50208900
H	0.21650300	1.49420100	0.94775400
H	1.25063800	3.15212800	3.25068900
C	-2.79020600	0.54662700	2.04821600
C	-1.75847200	-0.20115900	0.27280200
N	-3.57876400	-0.36720000	1.55674400
N	-1.68834500	0.71231200	1.25284200
N	-2.92853000	-0.80641300	0.42981700
C	-2.80810300	1.23899200	3.36464700
H	-3.02710300	2.30355100	3.23592300
H	-3.58325000	0.79813300	3.99263700
C	-3.63212000	-1.70429900	-0.45460600
C	-3.45219400	-3.07847800	-0.33123200
C	-4.52488700	-1.12603900	-1.36010000
C	-4.22714000	-3.89733500	-1.15362600
C	-5.27391800	-1.98416800	-2.16062700
C	-5.14121000	-3.37177000	-2.06644300
H	-4.10499800	-4.97517000	-1.08033000
H	-5.97501400	-1.56031000	-2.87570500
C	-2.41601600	-3.63815900	0.59824900
H	-1.42719400	-3.36995200	0.21257000
H	-2.49079200	-3.20272100	1.59793600
H	-2.50417000	-4.72388700	0.66911300
C	-5.96924800	-4.27308200	-2.94604000
H	-5.76753600	-4.07662800	-4.00312600
H	-5.75513500	-5.32515100	-2.74835100
H	-7.03760800	-4.10471400	-2.78162100
C	-4.63085400	0.37054800	-1.48742100

H	-4.81934800	0.84419500	-0.51916500
H	-3.69681800	0.78394900	-1.88518700
H	-5.43700900	0.64455000	-2.16934300
C	0.67912200	1.08679700	-2.16309400
C	1.60103200	-0.11111300	-2.17808900
C	-0.69723200	-0.49319200	-0.81521700
C	-0.45447100	0.86492700	-1.49850600
H	1.11348800	-0.92510000	-2.71575500
H	-1.22636700	1.62974800	-1.46095500
O	-0.97800800	-1.49616800	-1.57608900
C	0.96237700	2.39608900	-2.79817800
C	0.87481700	3.55157400	-2.01393500
C	1.24513400	2.52076600	-4.16348300
C	1.05630500	4.80921100	-2.58332200
H	0.67665000	3.45176700	-0.95026700
C	1.42702900	3.77779700	-4.73055700
H	1.30433100	1.63127600	-4.78287000
C	1.33280800	4.92476100	-3.94290600
H	0.98618200	5.69642900	-1.96175900
H	1.63698900	3.86316100	-5.79198600
H	1.47632300	5.90368600	-4.38917200
Cl	3.16379200	0.18334400	-3.01910800
C	-1.40041800	1.02537400	3.96919400
H	-1.26191700	-0.05298000	4.09596800
H	-1.35739900	1.47856800	4.96262000
C	3.92768800	-1.74281800	-0.37362300
C	2.61853500	-1.94555500	-0.81437100
C	2.18999300	-3.17766900	-1.25863200
C	3.11055400	-4.23517300	-1.25861900
C	4.41731000	-4.02783000	-0.82280600
C	4.85313100	-2.77408600	-0.37071700
C	2.91430900	0.28331300	-0.03848900
C	1.87516000	-0.63748300	-0.72955700
H	1.15790000	-3.29944900	-1.58149300
H	2.80540900	-5.21916200	-1.59749700
H	5.11978200	-4.85509100	-0.83003300
H	5.87177500	-2.62392400	-0.02794900
N	4.08824500	-0.41741900	0.05679300
O	2.71708500	1.42594600	0.32705200
N	0.62568800	-0.68704200	0.02324300
C	5.30982600	0.12792600	0.60269300
H	5.11595100	1.16757200	0.86587700
H	5.61352700	-0.42373700	1.49780800
H	6.11232300	0.08124200	-0.13859300
C	0.61525400	-1.27060900	1.25829700
O	-0.39034000	-1.65163100	1.84261400
O	1.84752600	-1.30245000	1.80230400
C	2.15784000	-2.19855200	2.91315600
C	1.36838100	-1.83052500	4.16660400
C	1.91001900	-3.63582900	2.47058000
C	3.64441400	-1.95151000	3.14188700
H	1.51966200	-0.77482400	4.41281600
H	0.30480800	-2.02337200	4.03736700
H	1.74120200	-2.42691200	5.00448600
H	2.49162800	-3.85243400	1.56835400
H	2.22358200	-4.32091500	3.26333500
H	0.85043400	-3.80270000	2.26438700

H	3.98799800	-2.53619000	3.99903600
H	4.21971500	-2.24944500	2.26122300
H	3.82390600	-0.89123600	3.34432800

M3*RS*

Total energy= -2814.56476683

Sum of electronic and zero-point Energies= -2813.721144

Sum of electronic and thermal Energies= -2813.671701

Sum of electronic and thermal Enthalpies= -2813.670756

Sum of electronic and thermal Free Energies= -2813.804090

C	0.42631100	1.38802500	2.99778900
C	1.21031500	1.17637000	4.13049900
C	1.65654000	2.25764200	4.88221700
C	1.30089300	3.54711800	4.48579400
C	0.51154300	3.75283800	3.35374600
C	0.06731100	2.66919000	2.59578500
C	0.11329300	0.05953900	2.34030700
C	0.38327400	-0.99132000	3.46123800
C	1.45947500	-0.29840000	4.33215500
H	2.26248700	2.10106200	5.76985700
H	1.63406400	4.39998900	5.06838900
H	0.23723700	4.76138300	3.06302000
H	-0.55713000	2.83007100	1.72172600
H	0.78391400	-1.89955900	3.00683500
H	1.40820200	-0.60433100	5.38079700
H	0.77593400	-0.10937700	1.49129600
H	2.46068900	-0.55665400	3.96640600
C	-2.31229900	-0.14462600	2.70403300
C	-1.74176400	-0.11925000	0.58738800
N	-3.43218300	-0.25889800	2.05116500
N	-1.25782000	-0.01857700	1.83914500
N	-3.05997400	-0.21676500	0.73058500
C	-2.02367900	-0.31206900	4.15203400
H	-1.70680700	0.63952700	4.59093800
H	-2.92784400	-0.64580600	4.66248600
C	-4.12155100	-0.20811900	-0.24939500
C	-4.52725100	-1.41484700	-0.81945000
C	-4.75240900	1.00800500	-0.50163500
C	-5.62252700	-1.37494100	-1.67788900
C	-5.84453100	0.99636700	-1.37052200
C	-6.29545900	-0.18320800	-1.96039700
H	-5.95565100	-2.29922500	-2.14413400
H	-6.35145900	1.93315400	-1.58855400
C	-3.75561800	-2.67563700	-0.56298400
H	-2.76294600	-2.56431600	-1.01015400
H	-3.60715500	-2.84608300	0.50749300
H	-4.26647100	-3.53862900	-0.99390000
C	-7.49891100	-0.18199600	-2.86775400
H	-8.40181900	-0.45773000	-2.31315700
H	-7.66484300	0.80548100	-3.30381800
H	-7.37951100	-0.90333500	-3.67966400
C	-4.24564100	2.29389300	0.09678300
H	-4.01382500	2.18419800	1.16006300
H	-3.33245600	2.61614100	-0.41603700
H	-4.98639400	3.08741600	-0.01441200

C	0.48210500	1.73337800	-1.72069600
C	1.04974900	0.52713800	-2.44064700
C	-1.01965300	-0.02809200	-0.79154100
C	-0.50911900	1.41910100	-0.88373600
H	0.25935800	0.08274000	-3.05070800
H	-1.03368800	2.19647900	-0.33362800
O	-1.76585600	-0.41395200	-1.76502700
C	0.91799600	3.13694900	-1.92148000
C	2.25749700	3.52273900	-1.78027200
C	-0.04427400	4.11851700	-2.18614600
C	2.61926300	4.86059200	-1.89850700
H	3.01283700	2.77348800	-1.56437500
C	0.32076900	5.45639000	-2.30658600
H	-1.08117900	3.82033200	-2.31189800
C	1.65409600	5.83077900	-2.16328400
H	3.65945800	5.14677500	-1.77980700
H	-0.43686300	6.20450800	-2.51701500
H	1.94134600	6.87301700	-2.25849300
Cl	2.39269000	0.89730200	-3.57396400
C	-0.90030100	-1.36819400	4.23915000
H	-1.29870700	-2.30130800	3.82877300
H	-0.65532000	-1.55579800	5.28727200
C	3.77223100	-0.96284200	-1.05217700
C	2.70150500	-0.17171900	-0.62041400
C	2.89680200	0.79069400	0.35442500
C	4.17461600	0.94153600	0.91013500
C	5.22807600	0.14379600	0.47289600
C	5.04632000	-0.82247100	-0.52346600
C	1.99768400	-1.75975400	-2.25784200
C	1.47163600	-0.56125100	-1.41388500
H	2.07979000	1.43456200	0.67149000
H	4.33963900	1.68861900	1.67900700
H	6.21406600	0.27249800	0.90763500
H	5.87300000	-1.43514900	-0.86674900
N	3.34640600	-1.85779800	-2.03886500
O	1.33940600	-2.42761100	-3.02687800
N	0.29221200	-0.88869900	-0.61097200
C	4.21981300	-2.73937900	-2.77832900
H	3.59530600	-3.34395000	-3.43639700
H	4.92739200	-2.15934200	-3.37828700
H	4.77377900	-3.39395100	-2.09902800
C	0.19565400	-2.10153500	0.00819600
O	-0.79940200	-2.49324800	0.60416200
O	1.35420300	-2.78033400	-0.03965700
C	1.39202300	-4.20867200	0.26561000
C	1.25205500	-4.41549300	1.76869200
C	0.32392800	-4.95310000	-0.53081200
C	2.77991800	-4.61435300	-0.21481300
H	2.03735600	-3.86770200	2.29904700
H	0.27376300	-4.07735900	2.11364900
H	1.36028500	-5.47895300	2.00069500
H	0.36689300	-4.64009600	-1.57826900
H	0.52790000	-6.02629700	-0.47906900
H	-0.67560700	-4.76236800	-0.14048000
H	2.98387400	-5.65030800	0.06740400
H	2.83575500	-4.53012300	-1.30355100
H	3.54212400	-3.96745900	0.23121800

M3*SR*

Total energy= -2814.57630451
Sum of electronic and zero-point Energies= -2813.731484
Sum of electronic and thermal Energies= -2813.682768
Sum of electronic and thermal Enthalpies= -2813.681824
Sum of electronic and thermal Free Energies= -2813.811828

C	-4.57312200	-0.52733300	-1.14610000
C	-5.94006100	-0.27229700	-1.12969600
C	-6.82760700	-1.17706900	-1.71034500
C	-6.32226500	-2.33249400	-2.30052700
C	-4.94600400	-2.57848300	-2.32026400
C	-4.05672800	-1.67385900	-1.74606200
C	-3.79823500	0.58004100	-0.46644500
C	-4.89156200	1.55834400	0.09490700
C	-6.25092100	1.03532100	-0.45118200
H	-7.89669800	-0.98465200	-1.70136800
H	-7.00300200	-3.04698900	-2.75306200
H	-4.56818700	-3.47901400	-2.79418100
H	-2.98056800	-1.81561800	-1.78293100
H	-4.68370200	2.54945700	-0.31261700
H	-6.98540100	0.90603400	0.35281300
H	-3.10246600	1.06599800	-1.14566900
H	-6.68603900	1.74837200	-1.15825900
C	-3.40329700	-0.17989500	1.88261400
C	-1.63370900	-0.27194400	0.59868600
N	-2.45258200	-0.61174500	2.66140900
N	-2.94389400	0.02615200	0.61035100
N	-1.35799700	-0.67709700	1.84182900
C	-4.76645400	0.27217400	2.25964300
H	-5.52584400	-0.41417300	1.86730500
H	-4.84570100	0.29143500	3.34707700
C	-0.12553600	-1.12584000	2.43963600
C	0.71323600	-0.18062400	3.03723100
C	0.10402200	-2.50534900	2.53994800
C	1.83893600	-0.65263800	3.71523300
C	1.25994600	-2.91961900	3.19832000
C	2.13977100	-2.00984200	3.79037300
H	2.50675200	0.07074700	4.17697300
H	1.46431800	-3.98630200	3.26977200
C	0.47286800	1.30028900	2.94503500
H	1.16674600	1.73664500	2.21653500
H	-0.54353600	1.54375600	2.62987400
H	0.66255900	1.77568900	3.91055100
C	3.38446700	-2.49628000	4.48508700
H	3.14962000	-3.28426200	5.20565900
H	4.08884300	-2.91662200	3.76017000
H	3.88633100	-1.68312300	5.01321400
C	-0.84579800	-3.54317600	1.99752800
H	-1.19080100	-4.19029800	2.80810900
H	-1.72578600	-3.10744000	1.52132200
H	-0.33550100	-4.17884700	1.26563000
C	1.18242200	-1.66757300	-1.41436400
C	1.56170400	-0.38953400	-2.13028000
C	-0.72365500	-0.25489100	-0.68051800

C	0.08428200	-1.55462100	-0.66467500
H	0.80767500	-0.14872000	-2.88318900
H	-0.34712000	-2.42897200	-0.18816100
O	-1.42008500	-0.10014000	-1.76569000
C	1.89415800	-2.96176800	-1.54438800
C	2.20360400	-3.52153600	-2.79023100
C	2.19939300	-3.68546600	-0.38569900
C	2.80012800	-4.77560400	-2.86973500
H	1.96030500	-2.97890400	-3.69792900
C	2.79553400	-4.94110000	-0.46649000
H	1.97677700	-3.24785200	0.58455600
C	3.09897300	-5.48913000	-1.70966800
H	3.02645200	-5.20078100	-3.84241200
H	3.02932900	-5.48573700	0.44312800
H	3.56634500	-6.46627900	-1.77742800
Cl	3.13476100	-0.47908000	-3.00307900
C	-4.90807900	1.66468500	1.62474500
H	-4.08064400	2.29262500	1.97201700
H	-5.83872700	2.13954200	1.94544100
C	3.67385000	1.79192200	-0.59954800
C	2.79894400	0.77002600	-0.21635300
C	3.13538900	-0.08740400	0.81170800
C	4.35393300	0.10563700	1.47662200
C	5.21268400	1.13039600	1.08946700
C	4.88851500	1.99340700	0.03595500
C	1.88891600	2.05972500	-2.00433300
C	1.59382300	0.80482500	-1.12686100
H	2.46192600	-0.88897400	1.10074700
H	4.62816700	-0.55155800	2.29610900
H	6.15617900	1.26535000	1.60862600
H	5.56480700	2.78416600	-0.27064400
N	3.13519400	2.51476700	-1.67072500
O	1.16725100	2.49406400	-2.87820500
N	0.30486900	0.87290200	-0.42907800
C	3.83558600	3.54985000	-2.39494800
H	3.14895700	3.95275100	-3.13976300
H	4.15061000	4.34908900	-1.71759100
H	4.71600200	3.13484300	-2.89508000
C	-0.18873600	2.08306200	-0.02574700
O	-1.35084800	2.27888300	0.30112500
O	0.77685400	3.01266800	0.04172900
C	0.44786500	4.41688600	0.27174100
C	-0.59147700	4.89732300	-0.73709900
C	-0.00459300	4.60518500	1.71489800
C	1.77980200	5.11414400	0.02310900
H	-0.29069000	4.59147800	-1.74336200
H	-1.57886900	4.49027600	-0.52111400
H	-0.63837900	5.98954700	-0.70273300
H	0.76870900	4.25297400	2.40416900
H	-0.17446000	5.66917700	1.90327400
H	-0.93109000	4.06164900	1.90389300
H	1.70400900	6.16965200	0.29620600
H	2.57135000	4.64767400	0.61798100
H	2.04552000	5.04466000	-1.03506700

M3*SS*

Total energy= -2814.57678988

Sum of electronic and zero-point Energies=	-2813.731428
Sum of electronic and thermal Energies=	-2813.682725
Sum of electronic and thermal Enthalpies=	-2813.681781
Sum of electronic and thermal Free Energies=	-2813.811344

C	-4.39762500	-0.32647700	-1.36290700
C	-5.75965100	-0.04783200	-1.32947600
C	-6.62860400	-0.70217400	-2.20064900
C	-6.10975100	-1.63369800	-3.09648100
C	-4.73800000	-1.90327900	-3.12921700
C	-3.86660600	-1.24785200	-2.26352600
C	-3.64367400	0.49353800	-0.33935800
C	-4.74843600	1.29157300	0.43965300
C	-6.08746400	0.99333200	-0.29275000
H	-7.69387700	-0.49043800	-2.18046000
H	-6.77577100	-2.15261400	-3.77903500
H	-4.34980300	-2.62445200	-3.84153800
H	-2.79200500	-1.40540300	-2.28949000
H	-4.50591500	2.35251200	0.35403000
H	-6.85575200	0.63688100	0.40409400
H	-2.90143200	1.13913700	-0.80337900
H	-6.48760000	1.89920400	-0.75864900
C	-3.38257100	-0.94801400	1.69201700
C	-1.55811200	-0.69700100	0.51423100
N	-2.47364100	-1.61662800	2.34504700
N	-2.86269300	-0.38832200	0.55643300
N	-1.34390600	-1.45913100	1.59303200
C	-4.75259900	-0.58086700	2.13066700
H	-5.50657700	-1.09531700	1.52342400
H	-4.88451500	-0.87855400	3.17143100
C	-0.14619000	-2.17245700	1.95867300
C	0.89613300	-1.51120900	2.59985500
C	-0.08937300	-3.53280500	1.61071100
C	2.08132000	-2.23079200	2.79406900
C	1.10377000	-4.20337600	1.83608000
C	2.21067300	-3.55803500	2.40406700
H	2.92030700	-1.72415300	3.26431900
H	1.18185100	-5.25061500	1.55411300
C	0.78792100	-0.10319900	3.11532500
H	1.51932200	0.53664100	2.61497100
H	-0.20954200	0.31657800	2.96875000
H	1.00440100	-0.09231400	4.18798500
C	3.50715300	-4.30282700	2.58197300
H	3.34241700	-5.26734900	3.07020900
H	3.96514500	-4.49983600	1.60723000
H	4.21622600	-3.72750600	3.18045000
C	-1.27936300	-4.22653300	1.00002800
H	-2.09001900	-4.31759900	1.72903600
H	-1.68424600	-3.67201300	0.14512900
H	-1.00553100	-5.22575600	0.65861900
C	1.55378700	-1.34937200	-1.39311800
C	1.82515200	0.06209700	-1.85637300
C	-0.56294400	-0.28969700	-0.63344000
C	0.34515900	-1.50347300	-0.85756500
H	1.11287500	0.27794000	-2.65428100
H	-0.00929800	-2.49364600	-0.59900000
O	-1.17536300	0.14345500	-1.69935400

C	2.48800300	-2.49027100	-1.55078100
C	3.73838900	-2.46436300	-0.92036000
C	2.09644600	-3.63953900	-2.24272500
C	4.58185500	-3.56805200	-0.99484100
H	4.02770700	-1.58396500	-0.35328400
C	2.94103200	-4.74594700	-2.31000300
H	1.12689800	-3.65849100	-2.73223700
C	4.18605100	-4.71214700	-1.68841800
H	5.54804300	-3.53985600	-0.49979200
H	2.62685800	-5.63168600	-2.85324400
H	4.84623400	-5.57197900	-1.74256300
Cl	3.44758600	0.30063600	-2.59910700
C	-4.83513100	0.94182800	1.92997300
H	-4.01067500	1.41133100	2.47664300
H	-5.76998100	1.33216900	2.33986600
C	2.64277900	3.21644100	-1.02074700
C	1.50827000	2.49431300	-1.39513000
C	0.55476500	3.03664600	-2.23006300
C	0.76056200	4.33877700	-2.70838900
C	1.90055600	5.05044500	-2.34248800
C	2.86639800	4.50218100	-1.48653400
C	2.83417400	1.24914300	0.13906300
C	1.56825700	1.12952900	-0.75134600
H	-0.32836400	2.45179600	-2.47872300
H	0.02937000	4.79493100	-3.36698700
H	2.04838500	6.05555300	-2.72436100
H	3.74791600	5.06623500	-1.19969000
N	3.41686800	2.45956100	-0.13038200
O	3.25943900	0.40021700	0.89945500
N	0.37416300	0.76111900	0.01945500
C	4.66729300	2.89432600	0.44765400
H	5.00949600	2.10697200	1.11896700
H	5.41367300	3.05843400	-0.33475300
H	4.52944200	3.82074200	1.01364600
C	-0.16382100	1.73214500	0.82539800
O	-1.33904700	1.79959500	1.15644100
O	0.78989200	2.56468600	1.26942800
C	0.45767100	3.78491100	1.99654200
C	-0.41531900	4.67597500	1.11964500
C	-0.19364700	3.44671100	3.33362300
C	1.82347900	4.42421000	2.21937500
H	0.07051600	4.82908100	0.14982900
H	-1.39831100	4.22963900	0.96225000
H	-0.54141600	5.64827200	1.60425800
H	0.45152600	2.77239000	3.90529700
H	-0.32098000	4.36783300	3.90983900
H	-1.16638000	2.97710100	3.19110000
H	1.71586500	5.32673300	2.82634000
H	2.48696100	3.72591700	2.73905000
H	2.27368800	4.69789900	1.26094700

TS4*RR*

Total energy= -2814.54994919

Sum of electronic and zero-point Energies= -2813.707395

Sum of electronic and thermal Energies= -2813.658189

Sum of electronic and thermal Enthalpies= -2813.657245

Sum of electronic and thermal Free Energies= -2813.789834

C	-1.00004600	2.04150400	2.47995400
C	-0.57597300	2.51526200	3.71699500
C	-0.95015300	3.78737800	4.14068200
C	-1.75559500	4.56625200	3.30997900
C	-2.18815500	4.08014400	2.07393400
C	-1.81492800	2.80457100	1.65168800
C	-0.46859700	0.64645400	2.22537600
C	0.04933200	0.17190000	3.62032100
C	0.27350600	1.48481400	4.41863000
H	-0.62837300	4.16591500	5.10656400
H	-2.05857200	5.55771400	3.63123200
H	-2.82243800	4.69490100	1.44329400
H	-2.15650300	2.40823300	0.69758800
H	1.00233600	-0.34437000	3.47932200
H	0.01090100	1.37428900	5.47575600
H	0.33275200	0.67682100	1.48353900
H	1.32857300	1.77820400	4.37960400
C	-2.53878900	-0.67313000	2.49368100
C	-1.77422000	-0.51375900	0.40323000
N	-3.45043800	-1.25561200	1.77153300
N	-1.51776500	-0.21655000	1.69900800
N	-2.95688000	-1.13520200	0.48661800
C	-2.40846500	-0.52503200	3.96995800
H	-2.69269400	0.49063400	4.26999400
H	-3.07706900	-1.22674800	4.47105200
C	-3.79601500	-1.52730100	-0.61014200
C	-3.75555400	-2.84804800	-1.06603800
C	-4.65705500	-0.57042900	-1.14784900
C	-4.60613300	-3.19391600	-2.11170600
C	-5.49306200	-0.96364000	-2.19547600
C	-5.47761500	-2.26586500	-2.69003900
H	-4.59122200	-4.21564300	-2.48464400
H	-6.17468600	-0.23483600	-2.62698600
C	-2.80941300	-3.83566500	-0.44637000
H	-1.78014900	-3.50515300	-0.60545600
H	-2.96304100	-3.89618600	0.63591300
H	-2.95171700	-4.82892700	-0.87659100
C	-6.37799600	-2.67924900	-3.82596200
H	-5.78993600	-2.99347800	-4.69378400
H	-7.00803100	-3.52599600	-3.53831400
H	-7.02792700	-1.85842400	-4.13539300
C	-4.68356900	0.83987400	-0.61781200
H	-4.63794700	0.85672900	0.47494900
H	-3.83036000	1.41708200	-0.99087200
H	-5.59264800	1.35318600	-0.93605800
C	0.40448200	1.53521800	-2.06761700
C	1.65933100	0.71237000	-2.28203400
C	-0.50602500	-0.62231100	-1.31799200
C	-0.65087200	0.83684400	-1.64720000
H	1.51269500	0.04523000	-3.13547600
H	-1.63855900	1.27589300	-1.57483600
O	-0.95958400	-1.52172100	-2.01113900
C	0.32105000	2.99015500	-2.34766500
C	0.00653000	3.85680100	-1.29797100
C	0.51447800	3.51028200	-3.63215700

C	-0.12987300	5.22356700	-1.52891100
H	-0.10909500	3.44954200	-0.29825000
C	0.37781800	4.87528500	-3.86084300
H	0.75964500	2.84243400	-4.45292200
C	0.05381200	5.73454700	-2.81079100
H	-0.37525100	5.88541700	-0.70402700
H	0.52029800	5.27057700	-4.86148000
H	-0.05171600	6.79915300	-2.99371800
Cl	3.09725600	1.69973700	-2.71877800
C	-0.93154700	-0.80250800	4.30743000
H	-0.70889700	-1.82456400	3.98370600
H	-0.78021400	-0.76827900	5.38958700
C	4.26162900	-0.78552700	-0.75166500
C	3.09896300	-1.14828400	-1.43460900
C	3.09549400	-2.20597200	-2.32042100
C	4.29080400	-2.90989500	-2.52099400
C	5.44696100	-2.53869300	-1.83930400
C	5.45412000	-1.46611900	-0.93816400
C	2.69067200	0.68092100	0.03677700
C	1.99711800	-0.18549700	-1.05319800
H	2.18057300	-2.49193500	-2.83368400
H	4.31455200	-3.74934800	-3.20684500
H	6.36625800	-3.09078100	-2.00535400
H	6.35706400	-1.18437700	-0.40652900
N	4.00085800	0.29450900	0.10204200
O	2.16823300	1.56940100	0.68150700
N	0.77089700	-0.83089300	-0.57256300
C	4.98178900	0.92662900	0.95535600
H	4.47818500	1.72887900	1.49385800
H	5.39134700	0.20766500	1.67112500
H	5.79564100	1.34279200	0.35529800
C	0.85984400	-1.84752900	0.35650400
O	0.01021600	-2.69280300	0.54416300
O	1.98825700	-1.71922900	1.08139100
C	2.53173300	-2.85627400	1.82833800
C	1.60464000	-3.27288400	2.96572400
C	2.80486800	-4.00263100	0.86153400
C	3.83385800	-2.30335400	2.39501600
H	1.45826700	-2.44342600	3.66304600
H	0.63854500	-3.60717400	2.59091100
H	2.07720800	-4.09114400	3.51664300
H	3.47030400	-3.66760000	0.05988600
H	3.29211400	-4.81972100	1.40056300
H	1.87616500	-4.37891900	0.42750100
H	4.29974300	-3.05148600	3.04150400
H	4.52950800	-2.05744400	1.58860500
H	3.63823600	-1.40336500	2.98648600

TS4*RS*

Total energy= -2814.55102143

Sum of electronic and zero-point Energies= -2813.709250

Sum of electronic and thermal Energies= -2813.660842

Sum of electronic and thermal Enthalpies= -2813.659898

Sum of electronic and thermal Free Energies= -2813.790239

C	0.26030700	-1.13725800	3.00168200

C	0.94740400	-1.85697900	3.97287000
C	1.03196700	-1.36356400	5.27343400
C	0.41614000	-0.15041400	5.57796600
C	-0.28470100	0.56088200	4.60057700
C	-0.37270900	0.06581100	3.30165300
C	0.31212800	-1.84330600	1.66174200
C	0.87486400	-3.26893800	1.98995000
C	1.50791300	-3.13655500	3.40267800
H	1.56333400	-1.91751300	6.04474000
H	0.47429200	0.24489800	6.58768600
H	-0.76802800	1.49927400	4.85553300
H	-0.91796400	0.60927500	2.53001100
H	1.64807800	-3.51277000	1.26086100
H	1.27917200	-4.00091900	4.03460100
H	0.96300800	-1.31021500	0.96267500
H	2.60156300	-3.07522900	3.33076600
C	-1.97647900	-2.75741400	1.49999900
C	-1.56458800	-1.01177500	0.17244700
N	-3.12014700	-2.49963300	0.93848300
N	-1.01809400	-1.88070900	1.05890000
N	-2.83896800	-1.41630700	0.13361500
C	-1.57861400	-3.86991300	2.40837100
H	-1.50975100	-3.50648100	3.44037000
H	-2.33518700	-4.65545400	2.37366100
C	-3.92897600	-0.79091300	-0.56128600
C	-4.24556900	-1.22466100	-1.85019000
C	-4.65056800	0.19955000	0.10752800
C	-5.32193700	-0.60983200	-2.48681100
C	-5.71224300	0.79603300	-0.57493400
C	-6.05620800	0.40767000	-1.87016800
H	-5.59013700	-0.92710000	-3.49038200
H	-6.28696600	1.57405700	-0.07902100
C	-3.43960400	-2.31374500	-2.50106700
H	-2.39483600	-1.99990500	-2.57983100
H	-3.46936800	-3.22910900	-1.89738100
H	-3.83365600	-2.54225900	-3.49235600
C	-7.18627600	1.08408200	-2.60103900
H	-7.67185000	0.39853900	-3.30073300
H	-7.93913400	1.46040400	-1.90346500
H	-6.81400200	1.93711600	-3.17928300
C	-4.34001100	0.57140600	1.53333800
H	-4.76126800	-0.17130500	2.22081800
H	-3.26325000	0.60517500	1.72572800
H	-4.76776900	1.54339100	1.78123600
C	-0.12386500	2.55703500	-0.47862200
C	0.97411300	2.29052700	-1.49396900
C	-0.89337400	0.34377100	-1.23264500
C	-1.02175700	1.57689700	-0.37844000
H	0.53698500	2.27682200	-2.49694600
H	-1.91246000	1.67031300	0.23326600
O	-1.61020200	0.19212400	-2.22102200
C	-0.27503000	3.82602600	0.28239900
C	0.72127000	4.28893300	1.14835100
C	-1.47635000	4.53758500	0.18268300
C	0.51740800	5.44246200	1.89755300
H	1.65159700	3.73503500	1.24345200
C	-1.67670100	5.69335500	0.93126000

H	-2.24717100	4.18089500	-0.49496200
C	-0.67817000	6.14909500	1.79041300
H	1.29465200	5.79004800	2.57164900
H	-2.61176500	6.23868800	0.84133500
H	-0.83257800	7.05267700	2.37194400
Cl	2.24073500	3.56020600	-1.56497200
C	-0.20862600	-4.36179700	1.91324400
H	-0.32125500	-4.69044800	0.87416000
H	0.11361900	-5.23080100	2.49021200
C	3.84418700	0.74830900	-0.50028000
C	2.51896200	0.84596000	-0.06597700
C	2.23059700	0.92485600	1.28198200
C	3.28086500	0.86596800	2.20742000
C	4.59543500	0.75552400	1.75954100
C	4.90232200	0.70329900	0.39557500
C	2.63545300	0.71070900	-2.44246700
C	1.61605000	0.89486200	-1.27451300
H	1.20516400	1.03101100	1.61892900
H	3.06263400	0.90365300	3.26861600
H	5.40577500	0.71179400	2.48097500
H	5.92912600	0.63033300	0.05315400
N	3.89013400	0.70882200	-1.89826500
O	2.35415800	0.66554300	-3.62084400
N	0.53269300	-0.09625200	-1.30706200
C	5.10969400	0.74197300	-2.67658200
H	4.82846800	0.69514000	-3.72846500
H	5.65519700	1.66942300	-2.48417300
H	5.74630200	-0.10933800	-2.42766500
C	0.77259200	-1.40801500	-1.64883700
O	-0.09102300	-2.24556700	-1.81098800
O	2.09405100	-1.64815200	-1.70143800
C	2.59748200	-2.84700200	-2.37588200
C	2.35589000	-4.06384700	-1.49334100
C	1.96314400	-2.98915600	-3.75716500
C	4.08557900	-2.55830000	-2.51254100
H	2.89329000	-3.95438900	-0.54519700
H	1.29069100	-4.19088600	-1.29898400
H	2.73388400	-4.95867400	-1.99704200
H	2.02762800	-2.03554300	-4.28849600
H	2.52034600	-3.74237000	-4.32317900
H	0.92082900	-3.29635700	-3.69350100
H	4.60464900	-3.44792400	-2.87400400
H	4.24757400	-1.74473200	-3.22563500
H	4.50637900	-2.26996700	-1.54392200

TS4*SR*

Total energy= -2814.55797808
Sum of electronic and zero-point Energies= -2813.714529
Sum of electronic and thermal Energies= -2813.665617
Sum of electronic and thermal Enthalpies= -2813.664673
Sum of electronic and thermal Free Energies= -2813.795837

C	4.56700000	0.51726800	-1.19351200
C	5.93753700	0.29053100	-1.25275800
C	6.78285600	1.25396700	-1.80130200
C	6.23297400	2.43930500	-2.28306300

C	4.85379000	2.66061600	-2.22337500
C	4.00891600	1.69749800	-1.67803200
C	3.83717100	-0.64121500	-0.54981800
C	4.96862500	-1.64363700	-0.12590500
C	6.29974800	-1.05074400	-0.67102800
H	7.85501900	1.08534500	-1.84869900
H	6.88120800	3.19866800	-2.70933500
H	4.44086600	3.58750300	-2.60862000
H	2.93265800	1.84187200	-1.64523300
H	4.76559900	-2.59854800	-0.61485300
H	7.05184500	-0.95170400	0.12126500
H	3.12152600	-1.09982100	-1.22931500
H	6.73590200	-1.70511300	-1.43231700
C	3.56547400	-0.03318900	1.85368000
C	1.74874600	0.24763400	0.58536200
N	2.67979800	0.45961700	2.66848200
N	3.04179700	-0.17205000	0.59444700
N	1.57795300	0.63277700	1.85781800
C	4.92120800	-0.56421700	2.15732000
H	5.69230400	0.14112800	1.82359000
H	5.02510100	-0.69436800	3.23557800
C	0.40388500	1.18679900	2.45990200
C	-0.43365900	0.32721900	3.17821300
C	0.18224700	2.56562500	2.38978300
C	-1.50811100	0.88901800	3.86446400
C	-0.93773300	3.07418800	3.05162700
C	-1.78410500	2.25573800	3.80083800
H	-2.16497000	0.23711500	4.43530600
H	-1.13773700	4.14299800	2.99639100
C	-0.23151900	-1.16254100	3.13391300
H	-0.63768100	-1.55720000	2.19275000
H	0.82541900	-1.43605800	3.18453800
H	-0.76266100	-1.65067900	3.95374400
C	-2.98773200	2.83755100	4.49656200
H	-2.71990100	3.72634200	5.07388900
H	-3.74502100	3.13990500	3.76524000
H	-3.44334200	2.11079700	5.17245700
C	1.11531100	3.50083100	1.66409700
H	1.65969100	4.12283300	2.38086100
H	1.85071000	2.96704200	1.05926800
H	0.54953400	4.17264300	1.01048000
C	-1.32522000	1.59865500	-1.62320700
C	-1.91871800	0.32430000	-2.20154800
C	0.57062900	0.11039400	-1.24686400
C	-0.09382400	1.45011300	-1.12671100
H	-1.37960800	0.02765600	-3.10633800
H	0.48727800	2.28936300	-0.76090900
O	1.40927400	-0.10642000	-2.11461400
C	-2.00366900	2.91677200	-1.63332200
C	-2.50748500	3.47589100	-2.81380900
C	-2.08324500	3.65163700	-0.44582300
C	-3.07440100	4.74552100	-2.80216300
H	-2.44076300	2.92172100	-3.74486700
C	-2.65351000	4.92175200	-0.43562200
H	-1.70580300	3.21428700	0.47492200
C	-3.15131100	5.47139000	-1.61392000
H	-3.45435900	5.17150500	-3.72509900

H	-2.71223700	5.47672000	0.49576400
H	-3.59792900	6.46045700	-1.60837900
Cl	-3.63533500	0.48017200	-2.70222400
C	5.03465700	-1.88826300	1.38732800
H	4.21563500	-2.54544000	1.69955700
H	5.97218800	-2.39543000	1.63086400
C	-3.73382300	-1.73195700	-0.21942200
C	-2.75587700	-0.74541600	-0.04310600
C	-2.86242900	0.16315200	0.99040000
C	-3.95833000	0.06542300	1.85895100
C	-4.91758600	-0.92533000	1.67780900
C	-4.82200500	-1.84741000	0.62919700
C	-2.27696800	-2.11760600	-1.93792300
C	-1.77096800	-0.84888600	-1.18507100
H	-2.10895800	0.93374200	1.12941400
H	-4.05911800	0.77216600	2.67567000
H	-5.76206500	-0.98480200	2.35679100
H	-5.57736600	-2.61180600	0.48209300
N	-3.44167500	-2.51270300	-1.34468000
O	-1.75134800	-2.60738800	-2.91597400
N	-0.35083000	-0.96164100	-0.83061600
C	-4.29514000	-3.55793800	-1.86144500
H	-3.77524900	-4.02518800	-2.69791600
H	-4.49204400	-4.30730100	-1.08962300
H	-5.24486300	-3.13962500	-2.20781200
C	0.17393700	-2.15433100	-0.38205300
O	1.35946700	-2.39013200	-0.26985800
O	-0.81389100	-2.99181800	-0.02853300
C	-0.52514200	-4.38765000	0.29409600
C	0.25838200	-5.04240800	-0.83966000
C	0.20146100	-4.46128500	1.63170600
C	-1.91644500	-5.00062700	0.39385100
H	-0.22469100	-4.81390200	-1.79455900
H	1.29061800	-4.69511300	-0.86903100
H	0.24930000	-6.12640400	-0.69550000
H	-0.41571100	-4.02634100	2.42334600
H	0.39192000	-5.50921700	1.88016200
H	1.15349700	-3.93100100	1.58329700
H	-1.84585900	-6.02059600	0.78005900
H	-2.54569800	-4.40739900	1.06457400
H	-2.38440300	-5.03242900	-0.59380700

TS4*SS*

Total energy= -2814.55680707

Sum of electronic and zero-point Energies=	-2813.714150
Sum of electronic and thermal Energies=	-2813.665124
Sum of electronic and thermal Enthalpies=	-2813.664180
Sum of electronic and thermal Free Energies=	-2813.795402

C	4.54701700	-0.32214900	-1.24375100
C	5.87034500	-0.74846100	-1.23846100
C	6.80567000	-0.13655200	-2.07106800
C	6.39220100	0.90305000	-2.90071300
C	5.05932000	1.32508600	-2.90409300
C	4.12389800	0.71205700	-2.07457800
C	3.70641500	-1.10669300	-0.25983800

C	4.73123000	-2.02236800	0.50088800
C	6.07704700	-1.88109900	-0.26681000
H	7.84240900	-0.46125300	-2.07030700
H	7.11141600	1.39058300	-3.55156900
H	4.75304200	2.13362700	-3.56021500
H	3.07825600	1.00845400	-2.08249700
H	4.37619500	-3.05337300	0.44463700
H	6.91125400	-1.68065000	0.41577400
H	2.92566300	-1.68290700	-0.75605700
H	6.32324000	-2.80665300	-0.79719500
C	3.61523900	0.38321900	1.73230100
C	1.75232700	0.31305900	0.50431300
N	2.82308900	1.24253300	2.30411500
N	3.00322900	-0.19320000	0.64805200
N	1.69081700	1.18644100	1.52002400
C	4.94142300	-0.12658500	2.17449800
H	5.74177000	0.30641800	1.56139800
H	5.11534400	0.15940700	3.21288400
C	0.58894800	2.04883200	1.83147400
C	-0.42120100	1.56534100	2.66840700
C	0.56521200	3.33751600	1.29136000
C	-1.48057900	2.41944800	2.96107600
C	-0.53411800	4.14453200	1.58787700
C	-1.55890600	3.70460100	2.42249800
H	-2.28061000	2.05951800	3.60396400
H	-0.59588800	5.13490400	1.14099500
C	-0.38517000	0.16279300	3.21242700
H	-0.81936100	-0.53773000	2.49045200
H	0.63532900	-0.16019800	3.43546300
H	-0.97876600	0.09786100	4.12759600
C	-2.73651400	4.58900600	2.74059800
H	-2.76244100	4.83805600	3.80612500
H	-2.69590900	5.51972200	2.17038300
H	-3.67672500	4.08345600	2.49900900
C	1.67699900	3.87139100	0.42435700
H	2.30120000	4.57125000	0.98865000
H	2.33078200	3.07969400	0.05002000
H	1.25759200	4.41342000	-0.42903100
C	-1.31922000	1.50258000	-1.51220800
C	-2.11440000	0.26200500	-1.88501200
C	0.46691300	-0.15740200	-1.21782300
C	-0.02634200	1.25649900	-1.29402200
H	-1.72941500	-0.09803300	-2.84238400
H	0.68891200	2.05445000	-1.13955700
O	1.21798300	-0.66768600	-2.03897000
C	-1.85071200	2.88596400	-1.47388300
C	-2.96081700	3.21133600	-0.68521900
C	-1.17042000	3.90780400	-2.14540400
C	-3.38674400	4.53189700	-0.58750800
H	-3.46267600	2.42860500	-0.12506600
C	-1.58869200	5.23109900	-2.03179300
H	-0.31376500	3.65710600	-2.76473600
C	-2.70204600	5.54565000	-1.25602200
H	-4.25028200	4.77356600	0.02426300
H	-1.05194400	6.01335300	-2.55918100
H	-3.03683900	6.57497300	-1.17451800
Cl	-3.85710300	0.54802800	-2.20750400

C	4.88490200	-1.65148900	1.98445700
H	4.03708300	-2.04022500	2.55878500
H	5.78910800	-2.12076900	2.38123800
C	-3.63519200	-2.53938200	-0.72229900
C	-2.48839500	-2.18910400	-1.43821400
C	-2.02360600	-2.98327800	-2.46606400
C	-2.74169000	-4.14361700	-2.78835900
C	-3.89269600	-4.47675600	-2.07891800
C	-4.36135400	-3.67941200	-1.02702900
C	-2.88991900	-0.65001500	0.33599000
C	-1.93759900	-0.90055300	-0.86709200
H	-1.11232400	-2.71838100	-2.99670000
H	-2.39804800	-4.78525100	-3.59203800
H	-4.44037300	-5.37633300	-2.34026100
H	-5.25285300	-3.95014200	-0.47088900
N	-3.86401200	-1.61285000	0.30133600
O	-2.82139200	0.27457400	1.11890000
N	-0.52128800	-0.98570300	-0.49406400
C	-4.97920200	-1.65549200	1.21897000
H	-4.86268400	-0.82408300	1.91379600
H	-5.92407000	-1.55215800	0.67810300
H	-4.98392100	-2.59695100	1.77637100
C	-0.08545100	-2.05547400	0.25696500
O	1.05898300	-2.45589500	0.30882700
O	-1.10864900	-2.55203600	0.97096500
C	-0.98507900	-3.82351300	1.67761500
C	-0.67123100	-4.92517700	0.67158900
C	0.05484000	-3.71496900	2.78831400
C	-2.37601200	-4.01578600	2.27028100
H	-1.41589300	-4.91225200	-0.13217600
H	0.32325400	-4.79410400	0.24240400
H	-0.71536300	-5.89651300	1.17204000
H	-0.19265300	-2.87975000	3.45047200
H	0.04320600	-4.63541800	3.37885900
H	1.05316000	-3.56423200	2.37989900
H	-2.38974200	-4.90969100	2.89890300
H	-2.64759700	-3.14953700	2.88172700
H	-3.11540500	-4.13714600	1.47329900

M4*RR*

Total energy= -2814.56994035

Sum of electronic and zero-point Energies=	-2813.728372
Sum of electronic and thermal Energies=	-2813.677971
Sum of electronic and thermal Enthalpies=	-2813.677027
Sum of electronic and thermal Free Energies=	-2813.813637

C	0.34035700	2.53130100	2.27621800
C	0.09063300	3.67639500	3.02233900
C	0.36561700	3.69578300	4.38953800
C	0.89752000	2.55527900	4.98574000
C	1.15367900	1.40792000	4.22736100
C	0.87829500	1.38860900	2.86342800
C	-0.00315300	2.73118600	0.81385700
C	-0.35735900	4.25789000	0.69898000
C	-0.46573000	4.77968900	2.16009300
H	0.17595800	4.58877300	4.97857000

H	1.12116000	2.55781500	6.04815000
H	1.57110400	0.52669000	4.70514700
H	1.05480000	0.50203700	2.26114400
H	-1.32547000	4.36199500	0.20155700
H	0.08620000	5.71712900	2.29503300
H	-0.83057000	2.08155500	0.51105700
H	-1.50788200	4.99090700	2.42217200
C	2.21752500	3.17735200	-0.18335900
C	1.39418700	1.09556200	-0.51120300
N	3.18677400	2.54526200	-0.77345800
N	1.13264900	2.35088200	-0.02328700
N	2.65531000	1.28021000	-0.95137700
C	2.11315300	4.61066300	0.20946500
H	2.30970700	4.72533400	1.28310400
H	2.85816800	5.19580100	-0.33231500
C	3.49867600	0.25924500	-1.49307700
C	3.58848900	0.11627500	-2.87954400
C	4.20089000	-0.55748100	-0.60625300
C	4.42067400	-0.88330800	-3.37578100
C	5.01388400	-1.55683900	-1.14654600
C	5.13639400	-1.72978600	-2.52457000
H	4.50280000	-1.01584200	-4.45245600
H	5.56936400	-2.20662800	-0.47408900
C	2.75685800	0.98854800	-3.77762400
H	1.69563800	0.78706400	-3.59382600
H	2.94037100	2.04837700	-3.57648500
H	2.97817000	0.78754300	-4.82771700
C	6.01532700	-2.81279400	-3.09733100
H	5.41604700	-3.55488500	-3.63942700
H	6.73787300	-2.39649100	-3.80977200
H	6.56943700	-3.33173800	-2.30936400
C	4.06316300	-0.36964900	0.88221900
H	4.25438500	0.67035000	1.16548600
H	3.04590000	-0.60652600	1.21405200
H	4.76156600	-1.01247900	1.42132400
C	0.14008400	-2.74649500	0.60377100
C	-1.31663900	-2.86061400	0.18543600
C	0.42557900	-1.61748100	-1.56399200
C	0.94602300	-2.21053300	-0.31394600
H	-1.40346100	-3.64114000	-0.57544600
H	2.02459300	-2.16146400	-0.20021600
O	1.08537300	-1.53636200	-2.57170100
C	0.67470800	-3.25193500	1.89223800
C	0.30592600	-2.63536900	3.09466800
C	1.61584300	-4.28368900	1.90606900
C	0.87240100	-3.05705800	4.29283000
H	-0.40224500	-1.81157300	3.07355100
C	2.17460100	-4.70703500	3.11001600
H	1.90372200	-4.75468600	0.97086900
C	1.80291700	-4.09593900	4.30398800
H	0.58993800	-2.56958100	5.22066200
H	2.90060900	-5.51371000	3.11241200
H	2.23917500	-4.42501300	5.24170300
Cl	-2.40954000	-3.39838200	1.50314200
C	0.67826600	5.04849400	-0.11939500
H	0.50826600	4.89230600	-1.19057800
H	0.54800700	6.11668600	0.07414600

C	-4.11752100	-0.95613400	-0.18152700
C	-3.23764800	-1.68699200	-0.98454500
C	-3.69477000	-2.36845900	-2.09374000
C	-5.06517100	-2.32599200	-2.38519600
C	-5.93585900	-1.60795700	-1.57015600
C	-5.47579500	-0.90458500	-0.44980100
C	-2.06614300	-0.53609200	0.74152300
C	-1.83806100	-1.53598300	-0.42961500
H	-3.00626100	-2.91667100	-2.73095200
H	-5.44799400	-2.85390000	-3.25145500
H	-6.99457100	-1.58576300	-1.80688500
H	-6.15553200	-0.33784700	0.17782300
N	-3.41235000	-0.30936600	0.83845400
O	-1.21796600	-0.11249600	1.49847000
N	-0.89572300	-1.10633700	-1.47089400
C	-4.01167500	0.47796300	1.89254300
H	-3.20353300	0.83748200	2.52978700
H	-4.55557700	1.33181200	1.47781800
H	-4.69846900	-0.13616400	2.48152700
C	-1.19579600	0.03992300	-2.22885800
O	-0.74576600	0.28349700	-3.31955900
O	-2.04843400	0.80814300	-1.54472600
C	-2.72969600	1.92348600	-2.20071600
C	-1.71164500	2.97095900	-2.63953200
C	-3.57096800	1.38579000	-3.35253600
C	-3.62540500	2.46711300	-1.09470700
H	-1.02349800	3.18369500	-1.81505700
H	-1.13148200	2.63118700	-3.49639400
H	-2.23526300	3.89467200	-2.90190600
H	-4.23453900	0.59387900	-2.98724400
H	-4.18384600	2.19468700	-3.75984100
H	-2.94053300	0.98893300	-4.14952900
H	-4.14596900	3.36144100	-1.44555200
H	-4.36976400	1.71755600	-0.81064400
H	-3.03238300	2.72870600	-0.21193800

M4*RS*

Total energy= -2814.57629600
Sum of electronic and zero-point Energies= -2813.733552
Sum of electronic and thermal Energies= -2813.683319
Sum of electronic and thermal Enthalpies= -2813.682375
Sum of electronic and thermal Free Energies= -2813.819396

C	-0.96715700	3.39262000	1.70721800
C	-1.64631500	4.57490200	1.97768000
C	-1.46811800	5.21715500	3.20238800
C	-0.59957500	4.66082100	4.13823500
C	0.09460200	3.48086700	3.85387500
C	-0.08056200	2.84055500	2.62980200
C	-1.28433300	2.86816800	0.32209000
C	-2.25807600	3.93167200	-0.29283700
C	-2.49125500	5.00565200	0.80730100
H	-1.99179100	6.14334700	3.42119300
H	-0.45145400	5.15250000	5.09452300
H	0.77876500	3.06748000	4.58786800
H	0.47227100	1.93587500	2.38507600

H	-3.20596900	3.43259700	-0.50729200
H	-2.20006300	6.00504100	0.46172900
H	-1.74830200	1.87877500	0.36708500
H	-3.54991900	5.06751400	1.07739100
C	0.51894700	3.71382700	-1.17496600
C	0.79051400	1.62721400	-0.35166400
N	1.70258200	3.36615500	-1.57995400
N	-0.05365800	2.69990000	-0.44777400
N	1.84334100	2.09562300	-1.05460800
C	-0.25712900	4.95108100	-1.46930300
H	-0.13368500	5.67669200	-0.65548400
H	0.12414900	5.41099400	-2.38260200
C	3.06065200	1.38378900	-1.28115600
C	3.42541000	1.07489100	-2.59685800
C	3.82244600	0.97034400	-0.17911900
C	4.58601600	0.32532500	-2.79188500
C	4.97530000	0.22553700	-0.42888900
C	5.37270200	-0.10754400	-1.72452600
H	4.87124400	0.05937600	-3.80708300
H	5.56854000	-0.11535700	0.41675500
C	2.57724800	1.50122800	-3.76536800
H	1.51926800	1.32583100	-3.55548800
H	2.70773200	2.56603800	-3.97608200
H	2.85087300	0.93030200	-4.65471500
C	6.62949300	-0.90544800	-1.95890800
H	7.50885700	-0.25325300	-1.96801700
H	6.77864300	-1.64564500	-1.16811500
H	6.59350200	-1.42728100	-2.91782800
C	3.38814200	1.22847200	1.23957200
H	3.01546200	2.24832200	1.37141900
H	2.57191200	0.54980000	1.51349300
H	4.22057600	1.06103200	1.92662400
C	1.46685500	-2.42728300	0.29490200
C	0.23820100	-3.29621800	0.14110700
C	0.72348900	-1.42732300	-1.83189000
C	1.70200200	-1.62261300	-0.74576000
H	0.42909900	-4.02912500	-0.64832900
H	2.61137800	-1.03980800	-0.83386400
O	1.03606300	-1.02834300	-2.92970100
C	2.41247400	-2.46814000	1.43424100
C	1.96590500	-2.22917100	2.74069700
C	3.78351400	-2.60461300	1.19380300
C	2.87993300	-2.13309400	3.78460300
H	0.90551200	-2.09055300	2.92982300
C	4.69415100	-2.51579100	2.24302800
H	4.13128400	-2.77948500	0.17955900
C	4.24457100	-2.27981200	3.53976600
H	2.52541100	-1.93683400	4.79123800
H	5.75532300	-2.62993300	2.04453700
H	4.95453800	-2.20761900	4.35724700
Cl	-0.15903900	-4.29785600	1.57489500
C	-1.72974900	4.53735700	-1.60113200
H	-1.81659300	3.80628000	-2.41269400
H	-2.34476400	5.40009600	-1.87177400
C	-2.87413400	-2.34533600	1.10757200
C	-1.66830200	-1.70661300	0.79704900
C	-1.27799000	-0.56010700	1.46209700

C	-2.11976900	-0.06389800	2.47054600
C	-3.31042400	-0.71536700	2.78251600
C	-3.71321300	-1.87131300	2.10263300
C	-2.07451200	-3.55676300	-0.65757400
C	-1.00130700	-2.48046300	-0.31244200
H	-0.36465500	-0.04247100	1.16443600
H	-1.84206100	0.83735300	3.00772400
H	-3.94797800	-0.31810900	3.56573700
H	-4.64688100	-2.36934700	2.34262800
N	-3.07725700	-3.44475100	0.26444900
O	-1.96969600	-4.39208100	-1.52896800
N	-0.63047200	-1.67961500	-1.48905600
C	-4.19320100	-4.36002500	0.34892300
H	-4.06125600	-5.10866000	-0.43185600
H	-4.20793100	-4.84840300	1.32717600
H	-5.14028900	-3.83542000	0.19259400
C	-1.61014000	-0.84229100	-2.06348000
O	-1.37385300	0.17277700	-2.66873200
O	-2.81917100	-1.34085600	-1.80554800
C	-4.02008200	-0.53413300	-2.03318100
C	-3.92340900	0.74894500	-1.21555400
C	-4.19866700	-0.27659400	-3.52465900
C	-5.13354400	-1.42630000	-1.50072700
H	-3.70275900	0.50631200	-0.16837500
H	-3.14424600	1.40396200	-1.61010400
H	-4.88129200	1.27527500	-1.25645600
H	-4.19516800	-1.22451600	-4.06955800
H	-5.16378700	0.21081200	-3.68760700
H	-3.40711400	0.36357400	-3.91260000
H	-6.10334500	-0.96667700	-1.70598700
H	-5.09742100	-2.40705400	-1.98424200
H	-5.03006900	-1.55424800	-0.41932800

M4*SR*

Total energy= -2814.57513658

Sum of electronic and zero-point Energies=	-2813.732807
Sum of electronic and thermal Energies=	-2813.682160
Sum of electronic and thermal Enthalpies=	-2813.681215
Sum of electronic and thermal Free Energies=	-2813.820342

C	4.38904900	-0.36074100	-1.38910400
C	5.66312700	-0.90356400	-1.50830600
C	6.58055600	-0.34341100	-2.39601800
C	6.19939700	0.76281000	-3.15219300
C	4.91719300	1.30625800	-3.02496300
C	4.00070700	0.74472000	-2.13980300
C	3.55010300	-1.11311100	-0.38243700
C	4.52144400	-2.18421600	0.22736800
C	5.84404500	-2.08267300	-0.58727100
H	7.57928200	-0.75946200	-2.49509200
H	6.90511300	1.20891100	-3.84612800
H	4.63718000	2.16896200	-3.62115100
H	2.99934000	1.15105600	-2.02496700
H	4.07201700	-3.16818300	0.07587800
H	6.71134100	-1.94426700	0.07024500
H	2.69082200	-1.58161400	-0.85825000

H	6.02744200	-3.00136100	-1.15346300
C	3.72630200	0.19021500	1.72358100
C	1.83478100	0.51256700	0.52587400
N	3.09252500	1.11238400	2.38282700
N	3.00472300	-0.19726900	0.62203600
N	1.95036900	1.29127900	1.62443500
C	4.98963800	-0.51704300	2.07086700
H	5.82325400	-0.11525400	1.48049600
H	5.21867700	-0.35892300	3.12604000
C	1.01888200	2.28500600	2.05541800
C	0.24413900	2.02880600	3.18958500
C	0.95560100	3.50085200	1.36612600
C	-0.62990500	3.02765200	3.62309700
C	0.06718900	4.46830100	1.83492100
C	-0.73719800	4.24743000	2.95502700
H	-1.23917100	2.84663500	4.50630000
H	0.01544300	5.42709900	1.32334600
C	0.35793300	0.70875200	3.90435200
H	0.19165400	-0.11958500	3.20624700
H	1.35820500	0.58178800	4.32688700
H	-0.37682800	0.63685700	4.70897700
C	-1.71026700	5.30259500	3.41367000
H	-1.26669100	6.29971800	3.35277800
H	-2.60423300	5.30236900	2.78150100
H	-2.02908000	5.12813300	4.44345300
C	1.82196200	3.74872300	0.16014500
H	2.87933600	3.59913900	0.40065900
H	1.57766200	3.04533200	-0.64195900
H	1.68480600	4.76560600	-0.21246100
C	-1.60718500	1.01703700	-2.13061500
C	-2.56320900	-0.15489400	-2.19605700
C	0.12193300	-0.72335300	-1.93342000
C	-0.31656500	0.68368200	-2.02606100
H	-2.50285300	-0.65138600	-3.16960800
H	0.48280800	1.41315100	-2.07133500
O	1.18081200	-1.10460700	-2.37497200
C	-2.02760100	2.43351800	-2.21085900
C	-2.84508900	2.91044900	-3.24173500
C	-1.55131500	3.32489600	-1.24373200
C	-3.16761800	4.26137500	-3.30756700
H	-3.21577700	2.22623700	-3.99875200
C	-1.88433200	4.67450600	-1.30758300
H	-0.93600100	2.95023600	-0.42916900
C	-2.69043800	5.14555800	-2.34029100
H	-3.79354900	4.62500300	-4.11585100
H	-1.51871800	5.35416300	-0.54427600
H	-2.95080900	6.19782500	-2.39121200
Cl	-4.28569300	0.31616800	-2.01825600
C	4.76369900	-1.99730400	1.73211000
H	3.89962100	-2.35731300	2.30111100
H	5.62602700	-2.59704900	2.03660500
C	-3.71288700	-1.58244000	0.64516600
C	-2.59420300	-0.82313500	0.28170200
C	-2.05597800	0.10290600	1.15515600
C	-2.68269000	0.28153600	2.39702700
C	-3.80585600	-0.46537800	2.74037300
C	-4.34038500	-1.42157200	1.86941100

C	-3.16266100	-2.41103800	-1.41310300
C	-2.20184200	-1.21961900	-1.12081200
H	-1.15599200	0.65929800	0.89480500
H	-2.29017300	1.01604900	3.09052700
H	-4.27716800	-0.30979800	3.70538900
H	-5.20915900	-2.01099100	2.14316300
N	-4.04045900	-2.49052000	-0.36980100
O	-3.16988600	-3.06777800	-2.43147600
N	-0.79229600	-1.60158400	-1.29319400
C	-5.16769800	-3.39479200	-0.33844600
H	-5.13536700	-3.99003700	-1.25054100
H	-5.10770700	-4.05722900	0.52993300
H	-6.10506700	-2.83285700	-0.29990200
C	-0.26256100	-2.62775400	-0.48634700
O	0.91384600	-2.80497100	-0.28859300
O	-1.25502200	-3.34289900	0.03986100
C	-1.01229200	-4.19684400	1.20831700
C	-0.05366900	-5.32899100	0.85611300
C	-0.51545100	-3.32054700	2.35278900
C	-2.39765400	-4.74981700	1.51646400
H	-0.40593200	-5.85125700	-0.03778200
H	0.95541900	-4.95990400	0.68030000
H	-0.03426700	-6.04225800	1.68471100
H	-1.22630200	-2.50437700	2.52611600
H	-0.44540100	-3.92159100	3.26341800
H	0.46877800	-2.90140000	2.13342300
H	-2.33008900	-5.46544900	2.33955600
H	-3.07386400	-3.94228500	1.81112800
H	-2.80607800	-5.26005400	0.63898600

M4*SS*

Total energy= -2814.57117001

Sum of electronic and zero-point Energies=	-2813.727492
Sum of electronic and thermal Energies=	-2813.677875
Sum of electronic and thermal Enthalpies=	-2813.676930
Sum of electronic and thermal Free Energies=	-2813.809228

C	-4.49261400	-0.38291900	-1.25368100
C	-5.87222900	-0.21457700	-1.26806500
C	-6.66833300	-1.03689700	-2.06455900
C	-6.05878600	-2.02165200	-2.83809100
C	-4.66988200	-2.18245000	-2.82207200
C	-3.87404100	-1.36123400	-2.02724100
C	-3.81653200	0.59057900	-0.31050000
C	-4.99918300	1.37361000	0.36483500
C	-6.29772900	0.90419400	-0.35335700
H	-7.74785000	-0.91542100	-2.07877200
H	-6.66768800	-2.67033300	-3.46029100
H	-4.21089400	-2.95157200	-3.43539500
H	-2.79130600	-1.45402600	-2.01759600
H	-4.85101500	2.44147200	0.18677400
H	-7.05470800	0.56783300	0.36561500
H	-3.13479900	1.25213000	-0.84929600
H	-6.75023800	1.72419100	-0.92014900
C	-3.51563900	-0.69759500	1.79442600
C	-1.68768500	-0.51502100	0.47792900
N	-2.62570700	-1.43568500	2.38693200

N	-2.99096000	-0.13106000	0.65969900
N	-1.52794700	-1.31282400	1.55464400
C	-4.89221400	-0.33500600	2.23149600
H	-5.63214900	-0.94741500	1.70018800
H	-5.00212200	-0.52894400	3.29977600
C	-0.35168900	-2.06322600	1.87299600
C	0.43759200	-1.63290200	2.94483900
C	-0.03088600	-3.19521200	1.12192400
C	1.55925800	-2.38365100	3.27752400
C	1.12679500	-3.89801200	1.46790400
C	1.92068100	-3.51900100	2.54705600
H	2.18461500	-2.05971900	4.10709300
H	1.41050900	-4.76550300	0.87497200
C	0.10147600	-0.34960900	3.65249200
H	0.04597200	0.46065000	2.91607600
H	-0.86972400	-0.40684300	4.15244500
H	0.86619000	-0.09988800	4.39116300
C	3.15321700	-4.30235200	2.91954700
H	3.06581300	-4.71363100	3.93003600
H	3.31762200	-5.13024200	2.22628900
H	4.04261100	-3.66394600	2.90451900
C	-0.91091600	-3.70004300	0.00751400
H	-1.64508400	-4.41573300	0.39305900
H	-1.46186300	-2.88960100	-0.47285800
H	-0.30812900	-4.21580100	-0.74589700
C	2.02444800	-1.17463100	-1.73887900
C	2.68342600	0.19262300	-1.85445900
C	-0.06489000	0.10359700	-2.01250900
C	0.69739500	-1.15715400	-1.89129600
H	2.61910300	0.52165700	-2.89544000
H	0.10362200	-2.06350900	-1.92771500
O	-1.11748700	0.18215600	-2.60195900
C	2.75380900	-2.45491200	-1.58219900
C	3.62101800	-2.67578800	-0.50501300
C	2.50124900	-3.49829500	-2.48028000
C	4.24266600	-3.91080400	-0.35286200
H	3.77578400	-1.89083900	0.22785500
C	3.11455500	-4.73724800	-2.31597100
H	1.83102600	-3.32737600	-3.31761800
C	3.99288500	-4.94350000	-1.25539300
H	4.91619600	-4.07177700	0.48281400
H	2.91387700	-5.53547000	-3.02313800
H	4.48029700	-5.90524500	-1.13090800
Cl	4.43995700	0.21221800	-1.49456500
C	-5.08096900	1.14829800	1.88286800
H	-4.30298500	1.72731900	2.39303900
H	-6.04632700	1.50984800	2.24784500
C	3.14328100	3.01659700	0.02367800
C	2.51367200	2.63243900	-1.16349300
C	2.45013000	3.49186300	-2.24101300
C	3.05191200	4.75256800	-2.12570200
C	3.68963300	5.12054300	-0.94424800
C	3.74520000	4.25757300	0.15741500
C	2.29499600	0.94456900	0.50926800
C	1.94919700	1.24049900	-0.98299300
H	1.93633700	3.19940000	-3.15262000
H	3.01737300	5.44438900	-2.95972900

H	4.15167500	6.09947400	-0.86787200
H	4.23570500	4.55269400	1.07904400
N	3.02818300	2.00346300	0.97968900
O	2.05160900	-0.07750100	1.11228700
N	0.52432000	1.20422700	-1.34175100
C	3.61818800	2.03807900	2.29848200
H	3.34838300	1.10862100	2.80060600
H	4.70675200	2.11445500	2.22606600
H	3.23473400	2.88646500	2.87319100
C	-0.34165700	2.14661900	-0.75573100
O	-1.37574500	2.52726100	-1.24505800
O	0.16787300	2.53837300	0.41081900
C	-0.47772400	3.59401800	1.18927700
C	-0.54399100	4.87554500	0.36536800
C	-1.84410000	3.10514400	1.65928800
C	0.47199900	3.77131500	2.36704800
H	0.44909000	5.10110200	-0.03880800
H	-1.25540200	4.78792100	-0.45542300
H	-0.84933200	5.70189600	1.01299300
H	-1.74061500	2.14142300	2.17025500
H	-2.26605100	3.82991700	2.36143400
H	-2.52802700	2.98721300	0.81681100
H	0.05691000	4.49733100	3.07029900
H	0.61918800	2.82020800	2.88799500
H	1.44048800	4.13886400	2.01428500

PRR

Total energy= -1798.51915092

Sum of electronic and zero-point Energies= -1798.086538

Sum of electronic and thermal Energies= -1798.058752

Sum of electronic and thermal Enthalpies= -1798.057807

Sum of electronic and thermal Free Energies= -1798.144477

C	-1.54274700	-1.85742500	0.09873400
C	-1.02977200	-1.00193100	-0.88164400
C	-1.41096700	-1.12546800	-2.20234000
C	-2.32297800	-2.13433000	-2.54046300
C	-2.82323900	-2.98588300	-1.55945900
C	-2.44273100	-2.86227800	-0.21699400
C	-0.19501800	-0.43543500	1.28118000
C	-0.05837700	-0.05180300	-0.22262500
H	-1.02019900	-0.45031500	-2.95863300
H	-2.64143300	-2.25001200	-3.57030900
H	-3.52657600	-3.76451300	-1.83592800
H	-2.83885500	-3.52793300	0.54244000
N	-1.03039500	-1.51694000	1.35615400
O	0.36106200	0.11997800	2.20454000
N	-0.38441600	1.35628400	-0.46627700
C	-1.35111300	-2.19638400	2.59210800
H	-0.80612300	-1.69495200	3.39133800
H	-1.04472000	-3.24455700	2.53892000
H	-2.42452400	-2.14273100	2.79601100
C	-1.76430900	1.72823200	-0.49362700
O	-2.20985800	2.53121900	-1.26749900
O	-2.41788000	1.05780500	0.44596900
C	-3.88545300	1.08272900	0.51002100

C	-4.45877100	0.55626300	-0.79975200
C	-4.35601900	2.49311300	0.84288600
C	-4.18480300	0.12181400	1.65249400
H	-4.03768300	-0.42996300	-1.02146600
H	-4.25063900	1.23392900	-1.62842300
H	-5.54255700	0.45508800	-0.69497200
H	-3.87279600	2.84423400	1.75868800
H	-5.43676300	2.47640300	1.00743800
H	-4.13257600	3.18545100	0.03122900
H	-5.25862900	0.11383000	1.85459900
H	-3.65652600	0.42968500	2.55911100
H	-3.87414300	-0.89168600	1.38263800
C	2.37422900	0.72316900	-0.21603100
C	1.38183100	-0.30625700	-0.71947900
C	0.52770500	2.37949700	-0.18289200
C	1.93605600	1.96839100	-0.01504700
H	1.37476600	-0.27298100	-1.81389700
H	2.60762500	2.76657700	0.28078700
O	0.18038600	3.53860600	-0.08508600
C	3.81990800	0.40217700	-0.08376600
C	4.72916800	0.91719700	-1.01145800
C	4.28590300	-0.36323200	0.99038200
C	6.09069500	0.65555900	-0.87642600
H	4.36485000	1.51925000	-1.83872100
C	5.64665300	-0.61491800	1.12648300
H	3.57928100	-0.74250800	1.72244100
C	6.55019100	-0.11131900	0.19047500
H	6.79047100	1.05529800	-1.60326300
H	6.00277500	-1.20206100	1.96680000
H	7.61114300	-0.31238300	0.29811400
Cl	1.85479900	-1.99401700	-0.31494400

PRS

Total energy= -1798.52428579

Sum of electronic and zero-point Energies= -1798.091210

Sum of electronic and thermal Energies= -1798.063504

Sum of electronic and thermal Enthalpies= -1798.062560

Sum of electronic and thermal Free Energies= -1798.149062

C	1.45865900	-1.95347000	0.26988200
C	1.01894800	-1.10736100	-0.75409700
C	1.49696800	-1.26065900	-2.04253900
C	2.40237800	-2.29768400	-2.30157300
C	2.81168800	-3.14898100	-1.27914700
C	2.35022100	-2.98733500	0.03229700
C	0.17570200	-0.41428700	1.37065000
C	0.04616400	-0.11265700	-0.16060000
H	1.18447300	-0.58534900	-2.83192300
H	2.78960500	-2.43342800	-3.30503300
H	3.51157400	-3.94940400	-1.49553200
H	2.68577300	-3.63977100	0.83121700
N	0.91204600	-1.56032400	1.49856600
O	-0.32146400	0.23356400	2.26542800
N	0.35508300	1.27959700	-0.46892000
C	1.23177700	-2.16669200	2.77366400
H	0.68525100	-1.62143900	3.54241600

H	0.92783900	-3.21615700	2.77985900
H	2.30508600	-2.09957300	2.97528600
C	1.73151200	1.66319400	-0.47785300
O	2.19008400	2.45671000	-1.25339600
O	2.36772700	1.01340600	0.48996900
C	3.83108700	1.05339700	0.60209000
C	4.45118600	0.49479800	-0.67225700
C	4.28016000	2.47634900	0.90996700
C	4.09634300	0.12676600	1.78067700
H	4.06656500	-0.51220700	-0.86392900
H	4.23940100	1.13267800	-1.53177300
H	5.53509900	0.43414600	-0.54123000
H	3.75798800	2.85134900	1.79441200
H	5.35330000	2.47187400	1.11856000
H	4.08551000	3.14235500	0.06940700
H	5.16348300	0.12430400	2.01539000
H	3.54051200	0.46072300	2.66133500
H	3.79238000	-0.89416500	1.53033000
C	-2.38423000	0.60655600	-0.05700500
C	-1.41001300	-0.43419400	-0.53877300
C	-0.56992900	2.29626700	-0.19362700
C	-1.95844100	1.86830400	0.07202300
H	-1.64735900	-1.42789700	-0.15590500
H	-2.61672600	2.66743700	0.39440600
O	-0.24463100	3.46623400	-0.16098300
C	-3.79027200	0.20743800	0.16733800
C	-4.83202700	1.03504300	-0.26817800
C	-4.09929100	-0.98544800	0.83167400
C	-6.15616300	0.67948300	-0.03734600
H	-4.59779600	1.94603300	-0.81030900
C	-5.42465000	-1.33561300	1.06685400
H	-3.30524200	-1.62940400	1.19890500
C	-6.45535000	-0.50568700	0.63149400
H	-6.95526100	1.32447500	-0.38741700
H	-5.65193200	-2.25594000	1.59436700
H	-7.48894300	-0.78306300	0.81068600
Cl	-1.64581100	-0.56982100	-2.33428700

PSR

Total energy= -1798.52428579
Sum of electronic and zero-point Energies= -1798.091210
Sum of electronic and thermal Energies= -1798.063504
Sum of electronic and thermal Enthalpies= -1798.062560
Sum of electronic and thermal Free Energies= -1798.149062

C	-1.45865900	-1.95347000	0.26988200
C	-1.01894800	-1.10736100	-0.75409700
C	-1.49696800	-1.26065900	-2.04253900
C	-2.40237800	-2.29768400	-2.30157300
C	-2.81168800	-3.14898100	-1.27914700
C	-2.35022100	-2.98733500	0.03229700
C	-0.17570200	-0.41428700	1.37065000
C	-0.04616400	-0.11265700	-0.16060000
H	-1.18447300	-0.58534900	-2.83192300
H	-2.78960500	-2.43342800	-3.30503300
H	-3.51157400	-3.94940400	-1.49553200

H	-2.68577300	-3.63977100	0.83121700
N	-0.91204600	-1.56032400	1.49856600
O	0.32146400	0.23356400	2.26542800
N	-0.35508300	1.27959700	-0.46892000
C	-1.23177700	-2.16669200	2.77366500
H	-0.68525100	-1.62143900	3.54241600
H	-0.92783900	-3.21615700	2.77985900
H	-2.30508600	-2.09957300	2.97528600
C	-1.73151200	1.66319400	-0.47785300
O	-2.19008400	2.45671000	-1.25339600
O	-2.36772700	1.01340600	0.48996900
C	-3.83108700	1.05339700	0.60209000
C	-4.45118600	0.49479800	-0.67225700
C	-4.28016000	2.47634900	0.90996600
C	-4.09634300	0.12676600	1.78067700
H	-4.06656500	-0.51220700	-0.86392900
H	-4.23940100	1.13267800	-1.53177300
H	-5.53509900	0.43414600	-0.54123000
H	-3.75798800	2.85134900	1.79441100
H	-5.35330000	2.47187400	1.11855900
H	-4.08551000	3.14235500	0.06940700
H	-5.16348300	0.12430400	2.01539000
H	-3.54051200	0.46072300	2.66133500
H	-3.79238000	-0.89416500	1.53033000
C	2.38423000	0.60655600	-0.05700500
C	1.41001300	-0.43419400	-0.53877300
C	0.56992900	2.29626700	-0.19362700
C	1.95844100	1.86830400	0.07202300
H	1.64735900	-1.42789700	-0.15590500
H	2.61672600	2.66743700	0.39440600
O	0.24463100	3.46623400	-0.16098300
C	3.79027200	0.20743800	0.16733800
C	4.83202700	1.03504300	-0.26817800
C	4.09929100	-0.98544800	0.83167400
C	6.15616300	0.67948300	-0.03734600
H	4.59779600	1.94603300	-0.81030900
C	5.42465000	-1.33561300	1.06685400
H	3.30524200	-1.62940400	1.19890500
C	6.45535000	-0.50568700	0.63149400
H	6.95526100	1.32447500	-0.38741700
H	5.65193200	-2.25594000	1.59436700
H	7.48894300	-0.78306300	0.81068600
Cl	1.64581100	-0.56982100	-2.33428700

PSS

Total energy= -1798.51915092
Sum of electronic and zero-point Energies= -1798.086538
Sum of electronic and thermal Energies= -1798.058752
Sum of electronic and thermal Enthalpies= -1798.057807
Sum of electronic and thermal Free Energies= -1798.144477

C	1.54274700	-1.85742500	0.09873400
C	1.02977200	-1.00193100	-0.88164400
C	1.41096700	-1.12546800	-2.20234000
C	2.32297800	-2.13433000	-2.54046300
C	2.82323900	-2.98588300	-1.55945900

C	2.44273100	-2.86227800	-0.21699400
C	0.19501800	-0.43543500	1.28118000
C	0.05837700	-0.05180300	-0.22262500
H	1.02019900	-0.45031500	-2.95863300
H	2.64143300	-2.25001200	-3.57030900
H	3.52657600	-3.76451300	-1.83592800
H	2.83885500	-3.52793300	0.54244000
N	1.03039500	-1.51694000	1.35615400
O	-0.36106200	0.11997800	2.20454000
N	0.38441600	1.35628400	-0.46627700
C	1.35111300	-2.19638400	2.59210700
H	0.80612300	-1.69495200	3.39133800
H	1.04472000	-3.24455800	2.53892000
H	2.42452400	-2.14273100	2.79601100
C	1.76430900	1.72823200	-0.49362700
O	2.20985800	2.53121900	-1.26749900
O	2.41788000	1.05780500	0.44596900
C	3.88545300	1.08272900	0.51002100
C	4.45877100	0.55626300	-0.79975200
C	4.35601900	2.49311300	0.84288600
C	4.18480300	0.12181400	1.65249400
H	4.03768300	-0.42996300	-1.02146600
H	4.25063900	1.23392900	-1.62842300
H	5.54255700	0.45508800	-0.69497200
H	3.87279600	2.84423400	1.75868800
H	5.43676300	2.47640300	1.00743800
H	4.13257600	3.18545100	0.03122900
H	5.25862900	0.11383000	1.85459900
H	3.65652700	0.42968500	2.55911100
H	3.87414300	-0.89168600	1.38263800
C	-2.37422900	0.72316900	-0.21603100
C	-1.38183100	-0.30625700	-0.71947900
C	-0.52770500	2.37949700	-0.18289200
C	-1.93605600	1.96839100	-0.01504700
H	-1.37476600	-0.27298100	-1.81389700
H	-2.60762500	2.76657700	0.28078700
O	-0.18038600	3.53860600	-0.08508600
C	-3.81990800	0.40217700	-0.08376600
C	-4.72916800	0.91719700	-1.01145800
C	-4.28590300	-0.36323200	0.99038200
C	-6.09069500	0.65555900	-0.87642600
H	-4.36485000	1.51925000	-1.83872000
C	-5.64665300	-0.61491800	1.12648300
H	-3.57928100	-0.74250800	1.72244100
C	-6.55019100	-0.11131900	0.19047500
H	-6.79047100	1.05529800	-1.60326300
H	-6.00277500	-1.20206100	1.96680000
H	-7.61114300	-0.31238300	0.29811400
Cl	-1.85479900	-1.99401700	-0.31494400

***E*-TS1^{D}**

Total energy= -920.38577374

Sum of electronic and zero-point Energies= -920.246533

Sum of electronic and thermal Energies= -920.236669

Sum of electronic and thermal Enthalpies= -920.235724

Sum of electronic and thermal Free Energies= -920.283227

C	-0.42206400	-0.19679700	-0.16988700
C	-1.36161900	0.63071300	0.48822600
C	-2.17725100	-1.29026900	0.17923200
C	-1.12950800	-1.28921300	-0.71207600
H	-1.07000400	1.20459600	1.36292600
H	-0.95739200	-1.95122400	-1.55067000
O	-3.03706600	-1.73414900	0.84127400
C	1.03187900	-0.07944600	-0.05748800
C	1.61517800	1.16389300	0.22076600
C	1.85095700	-1.20051700	-0.25095700
C	2.99736300	1.28196100	0.30632100
H	0.97995000	2.03610500	0.34321700
C	3.23204700	-1.07663100	-0.17679700
H	1.39408800	-2.16838000	-0.43595700
C	3.80518700	0.16369700	0.10539300
H	3.44642300	2.24643600	0.51818800
H	3.86313900	-1.94633600	-0.32603800
H	4.88441600	0.25814100	0.16935900
Cl	-2.64100700	1.50291200	-0.37691800

***Z*-TS1^{D}**

Total energy= -920.39933772
Sum of electronic and zero-point Energies= -920.260085
Sum of electronic and thermal Energies= -920.250242
Sum of electronic and thermal Enthalpies= -920.249297
Sum of electronic and thermal Free Energies= -920.296611

C	-0.60784100	-0.38935800	0.48214200
C	-1.60812700	0.59993400	0.50123800
C	-2.51443000	-1.23095700	0.07944100
C	-1.30685500	-1.60995700	0.61872800
H	-2.26604000	0.71699800	1.34973700
H	-1.03686300	-2.55597400	1.07162300
O	-3.50914100	-1.35039000	-0.53309700
C	0.82517500	-0.26322600	0.20429100
C	1.51398300	0.91595800	0.52049700
C	1.52789800	-1.35115900	-0.32875600
C	2.88351000	1.00077400	0.30504000
H	0.97320000	1.75264100	0.95077200
C	2.89903300	-1.26363600	-0.54049100
H	0.98689200	-2.25466600	-0.59381800
C	3.57655900	-0.08717300	-0.22599100
H	3.41394800	1.91334700	0.55514000
H	3.43715700	-2.10810100	-0.95787100
H	4.64605900	-0.01622300	-0.39582000
Cl	-1.48321500	2.08399400	-0.43599000

***E*-M1^{D}**

Total energy= -920.43721708
Sum of electronic and zero-point Energies= -920.297126
Sum of electronic and thermal Energies= -920.286598
Sum of electronic and thermal Enthalpies= -920.285654
Sum of electronic and thermal Free Energies= -920.334775

C	-0.40718800	-0.06545400	0.05928800
C	-0.99995400	-1.22117100	-0.27662600
C	-2.37539100	1.45983300	0.28242900
C	-1.09156400	1.16839800	0.44048500
H	-0.45554300	-2.09422800	-0.60764300
H	-0.52712200	1.96706300	0.91059800
O	-3.47801400	1.80573100	0.17122300
C	1.08142300	-0.00664300	0.03558900
C	1.84917400	-1.08369000	0.49266100
C	1.73449700	1.13013000	-0.45444300
C	3.23864200	-1.03215800	0.44145800
H	1.35342300	-1.95350000	0.91267000
C	3.12393500	1.18095700	-0.50252500
H	1.14879200	1.97002400	-0.81655400
C	3.88036400	0.09935700	-0.05675900
H	3.82063100	-1.87343200	0.80375800
H	3.61560400	2.06619800	-0.89276400
H	4.96408500	0.14094100	-0.09108600
Cl	-2.72349300	-1.43801600	-0.25635900

_Z_-M1^{D}

Total energy= -920.43225474

Sum of electronic and zero-point Energies=	-920.291886
Sum of electronic and thermal Energies=	-920.281311
Sum of electronic and thermal Enthalpies=	-920.280366
Sum of electronic and thermal Free Energies=	-920.329841

C	-0.79741500	-0.02876300	0.32382200
C	-1.41675000	1.15103700	0.16676000
C	-2.81127600	-1.40733500	0.17004200
C	-1.60321100	-1.21648100	0.67092000
H	-2.47086000	1.28783100	0.37331300
H	-1.21520800	-1.99095800	1.32255500
O	-3.86909600	-1.58175100	-0.27988600
C	0.66027600	-0.26330200	0.15381300
C	1.60588200	0.60957100	0.70397500
C	1.10242600	-1.40209000	-0.52825900
C	2.96554200	0.35675300	0.55535800
H	1.27277000	1.47778400	1.26276600
C	2.46283700	-1.64838200	-0.68447900
H	0.37113100	-2.08962000	-0.94275900
C	3.39784900	-0.76879000	-0.14338200
H	3.68899500	1.03798400	0.99137500
H	2.79163300	-2.52941600	-1.22608900
H	4.45921000	-0.96289500	-0.25974500
Cl	-0.66716800	2.59588100	-0.44786800

TS2^{D}*RR*

Total energy= -1798.41562708

Sum of electronic and zero-point Energies=	-1797.988973
Sum of electronic and thermal Energies=	-1797.960102
Sum of electronic and thermal Enthalpies=	-1797.959157
Sum of electronic and thermal Free Energies=	-1798.050074

C	-1.63188100	2.29917600	-0.82902600

C	-1.70278300	1.72870700	0.45232400
C	-2.33712000	2.39307300	1.49068700
C	-2.89145900	3.64850800	1.23261500
C	-2.80822400	4.20968800	-0.04267900
C	-2.17934300	3.54274000	-1.09919300
C	-0.57898700	0.27962600	-1.06883200
C	-1.03352500	0.42944000	0.37276200
H	-2.39524600	1.93947100	2.47604000
H	-3.39229300	4.19061500	2.02691300
H	-3.24439800	5.18667500	-0.22351700
H	-2.12292100	3.98396600	-2.08837400
N	-0.96760100	1.43144500	-1.70669700
O	0.04033800	-0.64934200	-1.55698400
N	-1.10213500	-0.54529700	1.24955200
C	-0.64175100	1.74037200	-3.08099800
H	0.00950900	2.61815800	-3.12997900
H	-1.55097500	1.93005700	-3.65739100
H	-0.12246600	0.87649900	-3.49602900
C	-1.15729900	-1.89384400	0.86877800
O	-0.61109500	-2.78511300	1.48641900
O	-2.00513900	-2.05050000	-0.14613300
C	-2.17354300	-3.35634800	-0.78434700
C	-2.87975100	-4.30607000	0.17581300
C	-0.82630200	-3.89273000	-1.25654700
C	-3.06257600	-3.02246700	-1.97575700
H	-3.81566000	-3.86143900	0.52585100
H	-2.24711500	-4.53336800	1.03408000
H	-3.11518900	-5.23722800	-0.34736900
H	-0.30472800	-3.11955500	-1.82591500
H	-0.99762900	-4.75876000	-1.90220400
H	-0.20363000	-4.19819000	-0.41569200
H	-3.28454800	-3.93118300	-2.54048000
H	-2.55540000	-2.31143000	-2.63352300
H	-4.00344200	-2.58087200	-1.63676400
C	1.80171000	0.26613700	1.11043600
C	1.06141600	1.43041000	0.98739900
C	0.21959100	-0.55983800	2.79663700
C	1.37987800	-0.68732000	2.05085000
H	0.42861100	1.76510400	1.79831000
H	1.80444800	-1.68537400	2.07276500
O	-0.38783600	-0.48154300	3.78278900
C	3.00086800	-0.06450900	0.29517500
C	4.12707400	-0.58422000	0.94429400
C	3.03556400	0.11506600	-1.09187100
C	5.27021600	-0.91260700	0.22252100
H	4.11155100	-0.71308300	2.02257500
C	4.17871700	-0.22065600	-1.81033100
H	2.15821900	0.48144900	-1.61136400
C	5.29858800	-0.73091900	-1.15777100
H	6.13825300	-1.30742200	0.74017500
H	4.19043300	-0.08771100	-2.88721400
H	6.18848400	-0.98778100	-1.72309100
Cl	1.51233300	2.75069800	-0.04259700

TS2^{D}*RS*

Total energy= -1798.40503487

Sum of electronic and zero-point Energies= -1797.977921

Sum of electronic and thermal Energies= -1797.949355
Sum of electronic and thermal Enthalpies= -1797.948411
Sum of electronic and thermal Free Energies= -1798.036660

C	-0.21930200	2.24064800	0.22212400
C	-0.35560600	1.00237200	0.86580800
C	-1.13591500	0.87481400	2.00078600
C	-1.83815900	1.99670900	2.45253700
C	-1.73678100	3.21129900	1.77537600
C	-0.91500000	3.35991700	0.65130800
C	1.16908300	0.85658800	-0.96640900
C	0.49251500	0.03422100	0.14287600
H	-1.20877300	-0.08278500	2.50801200
H	-2.47121900	1.92194700	3.32982400
H	-2.29442200	4.07061900	2.13360900
H	-0.81789400	4.31662900	0.14938000
N	0.70319900	2.13803500	-0.82944200
O	1.89990700	0.44275900	-1.84567800
N	1.02821700	-1.03538800	0.72983800
C	0.98959500	3.19415400	-1.77449100
H	1.71700000	2.80615600	-2.48690900
H	1.40607200	4.06475400	-1.26139500
H	0.07839300	3.48552600	-2.30595400
C	2.38447000	-1.25990900	0.70789400
O	2.90335600	-2.35281000	0.84522200
O	3.07648700	-0.09635200	0.66801600
C	4.50867200	-0.08649400	0.42236000
C	4.84734700	-0.88549400	-0.83337600
C	5.24852200	-0.59964900	1.65298100
C	4.78980800	1.39448600	0.19104900
H	4.19890700	-0.56282400	-1.65228700
H	4.71462300	-1.95468100	-0.66936800
H	5.88879700	-0.69483000	-1.10825800
H	4.96212200	-0.01706400	2.53335800
H	6.32708900	-0.49227100	1.50390100
H	5.01611800	-1.65037100	1.82815400
H	5.85558400	1.55190600	0.00598600
H	4.49496100	1.97933100	1.06664100
H	4.22197900	1.74543900	-0.67577500
C	-1.71894900	-1.46208800	-0.44092700
C	-0.83144200	-0.75709000	-1.28260100
C	0.03316600	-3.06469300	-0.01190200
C	-1.22671900	-2.57688700	0.24000200
H	0.01497300	-1.27957300	-1.71737500
H	-1.73583000	-3.02488600	1.08663800
O	0.89545500	-3.75150600	-0.32904400
C	-3.11636600	-1.06023600	-0.15347000
C	-4.07228200	-2.06826500	0.04057900
C	-3.51343000	0.28031400	-0.04180900
C	-5.39018000	-1.74744100	0.34451500
H	-3.78531800	-3.10871700	-0.07693600
C	-4.82933500	0.59474800	0.27761800
H	-2.79419700	1.07985000	-0.17347600
C	-5.77099300	-0.41383700	0.46961200
H	-6.11880900	-2.53945100	0.47995800
H	-5.11553400	1.63631200	0.38010300
H	-6.79828900	-0.16144100	0.71142100

Cl	-1.46083500	0.40623700	-2.43028200

TS2^{D}*SR*

Total energy= -1798.41547400
Sum of electronic and zero-point Energies= -1797.988280
Sum of electronic and thermal Energies= -1797.959700
Sum of electronic and thermal Enthalpies= -1797.958756
Sum of electronic and thermal Free Energies= -1798.047331

C	0.18856700	-2.26035000	-1.00088000
C	-0.24857000	-0.95129300	-0.73897300
C	-0.26973600	0.00171900	-1.74700100
C	0.14985300	-0.37013500	-3.02532800
C	0.59188100	-1.67153200	-3.27094500
C	0.62249100	-2.64008900	-2.26239900
C	-0.31425600	-2.28530400	1.23303300
C	-0.55348400	-0.88852000	0.69218200
H	-0.57938600	1.02159200	-1.53639500
H	0.14593400	0.35861800	-3.82838900
H	0.92096200	-1.94291000	-4.26872800
H	0.96720600	-3.64885700	-2.46237400
N	0.10686300	-3.03631000	0.15966600
O	-0.44683400	-2.67324300	2.37857200
N	-1.26030300	-0.00222300	1.36772700
C	0.56351700	-4.40366000	0.26887800
H	0.41465800	-4.71520400	1.30245200
H	-0.01069700	-5.05444900	-0.39529500
H	1.62611600	-4.47051000	0.01614900
C	-2.15173900	0.88692600	0.76150200
O	-2.30080800	2.03539800	1.13256500
O	-2.87636800	0.27127700	-0.17256800
C	-3.95674100	0.96547800	-0.87650200
C	-5.03694700	1.37655600	0.11749800
C	-3.40474300	2.15143400	-1.65969200
C	-4.47117500	-0.10927900	-1.82569400
H	-5.34508600	0.51180700	0.71173900
H	-4.68262700	2.16227000	0.78475300
H	-5.90759600	1.74343100	-0.43298900
H	-2.64866100	1.81394600	-2.37464400
H	-4.21957800	2.61427300	-2.22329700
H	-2.97104400	2.89822100	-0.99430000
H	-5.28189400	0.29386400	-2.43755500
H	-3.66558900	-0.44632300	-2.48391600
H	-4.84755300	-0.96712400	-1.26273700
C	1.58242200	0.90256700	1.24686400
C	1.57741600	-0.44209800	1.59745900
C	-0.34727700	1.22138100	2.70205400
C	0.61480000	1.72627400	1.83663200
H	1.10758300	-0.77569400	2.51554200
H	0.41666600	2.73186900	1.48198900
O	-0.89384200	1.13133700	3.71975600
C	2.47692600	1.50800000	0.22599300
C	3.00093700	2.78637400	0.45419400
C	2.78078700	0.85334500	-0.97429500
C	3.81132600	3.39852000	-0.49635600
H	2.78810500	3.29306500	1.39086900

C	3.58233400	1.47368000	-1.92670300
H	2.37382800	-0.13095700	-1.17575600
C	4.10133400	2.74457700	-1.69152600
H	4.21784000	4.38540000	-0.30119100
H	3.79628700	0.95985800	-2.85832100
H	4.73056700	3.22260700	-2.43524100
Cl	2.79595900	-1.56203700	1.07466400

TS2^{D}SS

Total energy= -1798.40081894

Sum of electronic and zero-point Energies= -1797.973831

Sum of electronic and thermal Energies= -1797.945226

Sum of electronic and thermal Enthalpies= -1797.944282

Sum of electronic and thermal Free Energies= -1798.033242

C	-0.39494700	2.31928400	0.25848400
C	-0.99670100	1.19977900	-0.33360700
C	-1.92403700	1.36555900	-1.35085500
C	-2.26813500	2.65982700	-1.74320000
C	-1.68137800	3.76516200	-1.12366100
C	-0.73061100	3.61345600	-0.11240100
C	0.58442500	0.54931700	1.32844600
C	-0.36399600	-0.00023100	0.26469500
H	-2.37878400	0.49976100	-1.82302100
H	-2.99917700	2.80840300	-2.53030700
H	-1.96374200	4.76528700	-1.43600800
H	-0.26666700	4.47396400	0.35746400
N	0.54822400	1.91983800	1.21341100
O	1.24629400	-0.08824000	2.12257000
N	-0.82925500	-1.24023500	0.44670300
C	1.32148400	2.81947500	2.04026800
H	1.95075700	2.20658700	2.68645900
H	1.95089500	3.46364700	1.41903500
H	0.66586300	3.44193100	2.65555500
C	-2.15161000	-1.60061200	0.37351100
O	-2.52353900	-2.75541500	0.25510600
O	-2.99161300	-0.55945400	0.56323700
C	-4.43339000	-0.74555600	0.55909400
C	-4.89767700	-1.29816600	-0.78573100
C	-4.85708100	-1.63675400	1.72310300
C	-4.94954300	0.67578800	0.75659800
H	-4.56151100	-0.64503400	-1.59719600
H	-4.51105100	-2.30400300	-0.94891500
H	-5.99087500	-1.32760200	-0.80559800
H	-4.44365800	-1.24768000	2.65807000
H	-5.94808500	-1.63362500	1.80245600
H	-4.51264500	-2.66027400	1.57797300
H	-6.04260100	0.68203000	0.75612300
H	-4.59494800	1.07829500	1.70924200
H	-4.58931500	1.32270100	-0.04871100
C	1.99233400	-1.16545800	-0.63070500
C	1.10416600	-0.23825700	-1.22637600
C	0.27283700	-2.83347000	-0.83993400
C	1.51590500	-2.45087700	-0.38542500
H	0.31299400	-0.62450700	-1.85972500
H	2.00000800	-3.14036300	0.29764600

O	-0.53427400	-3.38964700	-1.43940700
C	3.36726000	-0.85370900	-0.17736900
C	4.35145300	-1.84275200	-0.30927500
C	3.71826600	0.37978500	0.38797200
C	5.65380800	-1.60895100	0.11786400
H	4.09899300	-2.79044300	-0.77510500
C	5.01856200	0.60592200	0.82214700
H	2.97340200	1.15694700	0.50664200
C	5.98977600	-0.38471800	0.68877500
H	6.40506000	-2.38229200	-0.00108000
H	5.27197900	1.56063000	1.27115200
H	7.00474900	-0.20056800	1.02544300
Cl	1.71256500	1.25399800	-1.90264400

TS3$_{C=O}$*RR*

Total energy= -2814.50077753

Sum of electronic and zero-point Energies= -2813.661904

Sum of electronic and thermal Energies= -2813.612339

Sum of electronic and thermal Enthalpies= -2813.611395

Sum of electronic and thermal Free Energies= -2813.746586

C	4.82690000	-1.56690500	-0.75927100
C	5.88502300	-2.42569900	-0.48740000
C	7.11508800	-2.22808500	-1.11187000
C	7.25659400	-1.16595200	-2.00108500
C	6.18576700	-0.30789300	-2.26964000
C	4.95547500	-0.50264500	-1.64772800
C	3.59861200	-1.95192600	0.03599900
C	4.06779800	-3.10191500	0.99175100
C	5.48958000	-3.49359700	0.49845300
H	7.95171900	-2.88832200	-0.90394600
H	8.21093900	-0.99965200	-2.49027200
H	6.31412900	0.51346400	-2.96655900
H	4.11917100	0.16309900	-1.85349300
H	3.38513600	-3.94483500	0.87532500
H	6.19869700	-3.56183700	1.33069600
H	2.78184800	-2.27138700	-0.61139700
H	5.47433100	-4.47625600	0.01700400
C	3.74518200	-0.34622000	1.93557800
C	2.32576100	0.23643700	0.37579200
N	3.36971100	0.86169700	2.24481600
N	3.12095700	-0.76828800	0.78780100
N	2.49935100	1.21894500	1.25583700
C	4.64444000	-1.28000200	2.66371900
H	5.65825000	-1.21462100	2.24977600
H	4.68869300	-0.98498300	3.71290900
C	1.98935300	2.56835400	1.23715100
C	0.96554700	2.90659400	2.12650100
C	2.62341500	3.48766400	0.40060000
C	0.51298000	4.22196100	2.09032000
C	2.12932100	4.79411000	0.40637300
C	1.06836900	5.17135300	1.22723300
H	-0.29182700	4.51630100	2.75933800
H	2.59820200	5.53345500	-0.23816400
C	0.39270000	1.89738000	3.08284900
H	-0.08152100	1.08945600	2.51909700

H	1.17653700	1.47514700	3.71902400
H	-0.35418000	2.36772300	3.72487600
C	0.52248100	6.57488900	1.18682300
H	-0.35233100	6.62715900	0.52961700
H	0.20516600	6.90411200	2.17908500
H	1.26517800	7.27948500	0.80674100
C	3.80372700	3.11034900	-0.45561700
H	4.48834000	2.44402100	0.07927700
H	3.46767600	2.59285900	-1.35786400
H	4.35897100	4.00378100	-0.74613300
C	-0.58487200	-0.89000700	-1.74172700
C	-1.13345900	0.41666300	-2.02970800
C	1.45898100	0.26127200	-0.88166500
C	0.59969200	-0.89484100	-1.04435100
H	-0.36995600	1.12677200	-2.31917300
H	0.82462000	-1.76559200	-0.43665900
O	1.68111200	1.17869000	-1.66651400
C	-1.30045600	-2.17460700	-1.92410400
C	-2.69529400	-2.29176400	-1.85482700
C	-0.54485600	-3.33551500	-2.14853100
C	-3.30482600	-3.53785300	-1.95691100
H	-3.31824400	-1.42409800	-1.68265600
C	-1.15673000	-4.57916100	-2.26105400
H	0.53306200	-3.25193700	-2.25267500
C	-2.54179400	-4.68621600	-2.15436600
H	-4.38479700	-3.60293800	-1.87014100
H	-0.55208900	-5.46320400	-2.43717400
H	-3.02285400	-5.65614000	-2.23318200
Cl	-2.42869700	0.56473900	-3.24920300
C	4.06277400	-2.68737400	2.47162100
H	3.04060000	-2.70099000	2.86260000
H	4.63947800	-3.41535500	3.04650400
C	-3.22923500	2.61644800	-0.85073000
C	-3.86069200	1.44297900	-0.34809600
C	-5.25927300	1.37895000	-0.29589400
C	-6.00994700	2.45425400	-0.74778500
C	-5.37150000	3.59534800	-1.26036200
C	-3.99107200	3.69547300	-1.32554100
C	-1.47234600	1.20220600	-0.35497400
C	-2.79245400	0.54254600	0.06761700
H	-5.74109200	0.48370500	0.07521800
H	-7.09285100	2.40989600	-0.71996400
H	-5.97570300	4.42289400	-1.62131400
H	-3.50947400	4.57916400	-1.72957000
N	-1.87788300	2.53952000	-0.77246200
O	-0.42579500	1.06824900	0.34478600
N	-2.70773800	-0.56879200	0.71569000
C	-0.92794700	3.48274600	-1.29666100
H	0.06471700	3.15348000	-0.97209800
H	-0.95929100	3.53740300	-2.39422800
H	-1.10914800	4.48271100	-0.88861200
C	-3.82120500	-1.35570200	0.97171400
O	-4.79888200	-1.49316900	0.25520500
O	-3.61622900	-2.04691700	2.10158300
C	-4.55000900	-3.08295300	2.51746300
C	-5.91013300	-2.47368900	2.84370800
C	-4.64526100	-4.17161600	1.45036500

C	-3.89760400	-3.63658200	3.77983100
H	-5.79498000	-1.67244900	3.57934800
H	-6.38486600	-2.07319200	1.94817800
H	-6.55681800	-3.24426600	3.27313100
H	-3.64197500	-4.48155300	1.14105900
H	-5.16301200	-5.03911800	1.86982500
H	-5.19057500	-3.82196800	0.57469600
H	-4.52101300	-4.42648600	4.20610600
H	-2.91366100	-4.05228200	3.54687100
H	-3.77536500	-2.84513000	4.52381000

TS3$_{C=O}$*RS*

Total energy= -2814.49719063

Sum of electronic and zero-point Energies= -2813.656707

Sum of electronic and thermal Energies= -2813.606687

Sum of electronic and thermal Enthalpies= -2813.605743

Sum of electronic and thermal Free Energies= -2813.741513

C	5.09924700	-0.42510200	1.09553400
C	6.48753200	-0.45148000	1.03954900
C	7.20342400	-1.21639000	1.95877600
C	6.50568400	-1.94642500	2.91737700
C	5.10870000	-1.91569500	2.96484800
C	4.39055000	-1.14938600	2.05134400
C	4.52734400	0.44806400	-0.00008000
C	5.75853500	0.89846900	-0.85767000
C	7.01328700	0.40316400	-0.08366500
H	8.28822900	-1.24861400	1.92352200
H	7.05218300	-2.54913900	3.63557600
H	4.58087500	-2.49010600	3.71870400
H	3.30299800	-1.12692900	2.08729200
H	5.75781700	1.98852000	-0.90266800
H	7.68959000	-0.16273200	-0.73450200
H	3.98246300	1.30084500	0.40495500
H	7.58798900	1.24938300	0.30457600
C	3.96314700	-1.22749700	-1.76537500
C	2.27824000	-0.63862300	-0.50109800
N	2.99378500	-2.03701400	-2.08386600
N	3.55911400	-0.34490300	-0.79345400
N	1.95683200	-1.67162500	-1.27673400
C	5.33426300	-1.12108700	-2.33139100
H	6.02813500	-1.71759600	-1.72641500
H	5.33454800	-1.53093700	-3.34228200
C	0.75305500	-2.46736500	-1.27234100
C	-0.14100900	-2.33310600	-2.33732800
C	0.57963200	-3.38219100	-0.23111200
C	-1.30105500	-3.10164200	-2.28883200
C	-0.59549100	-4.13370600	-0.23972900
C	-1.55148700	-3.99440400	-1.24528600
H	-2.02938100	-3.00044600	-3.08904000
H	-0.76050400	-4.85251100	0.55981700
C	0.14874000	-1.41716800	-3.49400900
H	0.29962000	-0.39851700	-3.13074800
H	1.04590200	-1.74132400	-4.03093100
H	-0.68898200	-1.41833500	-4.19390800
C	-2.80350200	-4.83136800	-1.22398200

H	-3.26204700	-4.81318500	-0.23217100
H	-3.53816400	-4.45853600	-1.93939300
H	-2.57506200	-5.87408000	-1.46891800
C	1.60936300	-3.59913800	0.84694400
H	2.61862200	-3.34640600	0.50800600
H	1.38410800	-2.97884900	1.71709700
H	1.61125000	-4.64757200	1.15261300
C	0.28238800	2.23244500	0.93195100
C	-0.97328100	1.57106400	1.09644700
C	1.36628000	0.02405900	0.52501400
C	1.34318700	1.46283900	0.48900600
H	-0.93460100	0.55984100	1.47706200
H	2.13423100	1.96275400	-0.06041800
O	0.80179200	-0.74276400	1.29761100
C	0.45829400	3.70787500	0.94602500
C	-0.52847400	4.60229000	0.50411400
C	1.67580200	4.23025600	1.40500400
C	-0.28939400	5.97259500	0.50638600
H	-1.47251800	4.21488400	0.13599400
C	1.90819300	5.60202000	1.41699600
H	2.43487000	3.54841700	1.77701100
C	0.92590100	6.47887500	0.96446800
H	-1.05880000	6.64934700	0.14838400
H	2.85478900	5.98476300	1.78499400
H	1.10394400	7.54943200	0.97075400
Cl	-2.30663100	2.42086200	1.91554100
C	5.71773400	0.36378300	-2.29713400
H	4.99148000	0.92974700	-2.88920900
H	6.69691000	0.51058400	-2.75846600
C	-3.21150400	2.29908200	-1.46612600
C	-3.79288800	1.14685700	-0.88924900
C	-5.17758900	0.98449600	-0.85812500
C	-5.98700700	1.96851800	-1.41118600
C	-5.40534300	3.10487500	-1.98898200
C	-4.02873600	3.29096000	-2.02370700
C	-1.39679700	1.05156200	-0.73288900
C	-2.69980200	0.30375700	-0.41001600
H	-5.61773300	0.09179600	-0.42568900
H	-7.06539700	1.85905200	-1.39873800
H	-6.04742300	3.86862300	-2.41822700
H	-3.60195700	4.18854900	-2.45819200
N	-1.83887700	2.28554500	-1.38371500
O	-0.39805900	0.44742400	-1.19908300
N	-2.66237900	-0.82700100	0.17653000
C	-0.96520300	2.90441400	-2.36055900
H	-0.43280700	2.12150400	-2.91540700
H	-1.56385000	3.49883200	-3.05771900
H	-0.22837900	3.55893800	-1.87820000
C	-3.82303700	-1.56329600	0.39233600
O	-4.40343000	-2.19808300	-0.46516400
O	-4.14130100	-1.53870600	1.69134600
C	-5.27221800	-2.30829000	2.19796600
C	-6.57119500	-1.78284800	1.59532400
C	-5.07129100	-3.79605300	1.92468600
C	-5.22327100	-2.02888800	3.69536300
H	-6.65885600	-0.70671700	1.77332000
H	-6.61183700	-1.97865000	0.52277800

H	-7.41952300	-2.27984400	2.07430900
H	-4.06826500	-4.09979500	2.24018700
H	-5.80163300	-4.36880200	2.50339300
H	-5.19919600	-4.02454900	0.86655200
H	-6.05112400	-2.53690800	4.19628300
H	-4.28175700	-2.38913200	4.11811500
H	-5.30304900	-0.95524700	3.88322500

TS3$_{C=O}$*SR*

Total energy= -2814.51218596

Sum of electronic and zero-point Energies= -2813.673408

Sum of electronic and thermal Energies= -2813.624332

Sum of electronic and thermal Enthalpies= -2813.623388

Sum of electronic and thermal Free Energies= -2813.757908

C	-1.78839800	-3.37669500	-0.69743300
C	-3.02900600	-3.78988800	-0.22269400
C	-3.69074900	-4.85051200	-0.83740000
C	-3.08740800	-5.48270600	-1.92332800
C	-1.84259200	-5.05887700	-2.39605800
C	-1.18220800	-3.99487000	-1.78595100
C	-1.26522000	-2.21476600	0.11253100
C	-2.22067500	-2.10732100	1.34468400
C	-3.47057800	-2.93539100	0.93880200
H	-4.65805900	-5.18488400	-0.47370200
H	-3.58935000	-6.31440900	-2.40758400
H	-1.38952600	-5.56061400	-3.24490100
H	-0.22046400	-3.64385100	-2.14942400
H	-2.49077300	-1.05442800	1.45498500
H	-3.86396100	-3.52793600	1.77186000
H	-1.26410400	-1.27704800	-0.44120500
H	-4.26850500	-2.25532200	0.61926800
C	0.46358800	-3.25288400	1.58421100
C	1.26586300	-1.96132700	0.02257000
N	1.75834900	-3.27508200	1.76027600
N	0.12832600	-2.46139200	0.51987500
N	2.24144800	-2.46790900	0.77125200
C	-0.62561200	-3.77828600	2.44732600
H	-1.13976200	-4.60813300	1.94945200
H	-0.20022300	-4.14297200	3.38284500
C	3.64224300	-2.16748000	0.67387400
C	4.14307500	-1.18420200	1.53503600
C	4.40118900	-2.80027300	-0.30680800
C	5.47987300	-0.83377900	1.38139900
C	5.73913700	-2.41537700	-0.41637900
C	6.28876900	-1.43727000	0.41139700
H	5.89944800	-0.06112700	2.02119400
H	6.36022500	-2.88682000	-1.17334200
C	3.23409600	-0.50537400	2.52409800
H	2.34873500	-0.09773600	2.01766800
H	2.88175300	-1.21308100	3.28106200
H	3.75601500	0.31009100	3.02762300
C	7.72949300	-1.02128700	0.26982000
H	8.20847700	-1.52609400	-0.57083500
H	7.80502700	0.05856200	0.11244200
H	8.29201500	-1.25918500	1.17711700

C	3.79184800	-3.82864700	-1.22342100
H	3.20248800	-4.55927500	-0.66242800
H	3.12596500	-3.35867000	-1.95578500
H	4.57042800	-4.35897400	-1.77321200
C	1.87371200	1.45496400	-1.28801800
C	0.49842600	1.78843200	-1.47533900
C	1.27825000	-0.95032300	-1.10657600
C	2.19978800	0.14741400	-0.97917400
H	-0.11829300	1.03202800	-1.93972300
H	3.14037300	-0.04089400	-0.47643600
O	0.43664400	-1.14430400	-1.97947200
C	2.96279700	2.46174500	-1.15684600
C	2.77333100	3.72632600	-0.58180400
C	4.24778900	2.11534300	-1.59887900
C	3.84193700	4.60716700	-0.44609700
H	1.78951400	4.00749400	-0.22142100
C	5.31294700	3.00058100	-1.46976500
H	4.40365400	1.14541200	-2.06202000
C	5.11367700	4.25153200	-0.89086100
H	3.67896000	5.57845400	0.01061200
H	6.29710300	2.71324400	-1.82658500
H	5.94150900	4.94600800	-0.78933000
Cl	0.07467900	3.36699200	-2.17031600
C	-1.58120700	-2.58749600	2.65947100
H	-1.00720400	-1.76867900	3.10579500
H	-2.36511200	-2.85996100	3.37043700
C	-0.93218300	3.59483700	1.11736400
C	-2.05677800	3.08840900	0.42508300
C	-3.20749800	3.85957500	0.26329700
C	-3.25093400	5.12890000	0.82536300
C	-2.14382000	5.61519800	1.53433200
C	-0.97887700	4.87291400	1.68612000
C	-0.26730500	1.50172800	0.39945500
C	-1.72081000	1.73709100	-0.00681700
H	-4.04865600	3.48243100	-0.30958100
H	-4.13428600	5.74678000	0.71118800
H	-2.19059600	6.60861800	1.97048000
H	-0.12928900	5.28308500	2.22058300
N	0.11681000	2.70270500	1.10652700
O	0.13204900	0.38058600	0.79634600
N	-2.39956200	0.79785900	-0.54418400
C	1.14528800	2.61487900	2.12068600
H	0.90878500	1.82387000	2.84507300
H	2.11349700	2.39064100	1.65841800
H	1.22358500	3.57330200	2.64007700
C	-3.74978800	0.97724700	-0.84480700
O	-4.16856300	1.42952400	-1.88773100
O	-4.49930700	0.49000900	0.15429000
C	-5.95907400	0.48117200	0.05576600
C	-6.48852400	1.90392200	-0.09736900
C	-6.39404100	-0.42559400	-1.09033900
C	-6.38701300	-0.09723700	1.39929400
H	-6.09321400	2.53793600	0.70237100
H	-6.21432300	2.32656600	-1.06440900
H	-7.57872700	1.89008300	-0.01417600
H	-5.94969300	-1.41915400	-0.97595700
H	-7.48222500	-0.53232600	-1.07172300

H	-6.09563500	-0.01073100	-2.05315100
H	-7.47770400	-0.13958300	1.45320500
H	-5.99340600	-1.10894900	1.52940200
H	-6.01909000	0.52850900	2.21656800

TS3$_{C=O}$*SS*

Total energy= -2814.51337086

Sum of electronic and zero-point Energies=	-2813.673000
Sum of electronic and thermal Energies=	-2813.623806
Sum of electronic and thermal Enthalpies=	-2813.622862
Sum of electronic and thermal Free Energies=	-2813.755164

C	5.04763700	-0.72859000	-0.17494500
C	6.00775800	-1.46383200	0.51213200
C	7.34608400	-1.38302700	0.13445300
C	7.69717800	-0.55655800	-0.93097900
C	6.72584800	0.17801200	-1.61686100
C	5.38660300	0.09508000	-1.24390300
C	3.67183000	-0.96533000	0.40557600
C	3.91762600	-1.77237900	1.72446300
C	5.38297500	-2.27930800	1.61532100
H	8.10593300	-1.94849100	0.66590200
H	8.73749300	-0.48013400	-1.23103900
H	7.01767900	0.81417800	-2.44597100
H	4.61778600	0.65036000	-1.77428000
H	3.21872500	-2.61056100	1.74021000
H	5.92179300	-2.17085300	2.56274300
H	3.00489300	-1.49595800	-0.27159900
H	5.40439000	-3.34402200	1.36066400
C	3.32381400	1.09596200	1.76750200
C	2.09884700	0.99151600	-0.03145400
N	2.65503300	2.21741200	1.74885900
N	3.01593400	0.32534400	0.67769100
N	1.90029100	2.13726700	0.61625900
C	4.17531600	0.51072100	2.83479100
H	5.23038200	0.53341100	2.53856100
H	4.05841700	1.09551000	3.74776200
C	1.07214600	3.23781100	0.20492200
C	-0.14936700	3.42007400	0.86160100
C	1.50938800	4.03161000	-0.85564000
C	-0.95266800	4.46514000	0.41452900
C	0.66320400	5.06256900	-1.26566700
C	-0.56627500	5.28920700	-0.64727300
H	-1.91089300	4.63413100	0.89867500
H	0.97581500	5.70138200	-2.08751700
C	-0.58937000	2.47206200	1.94266500
H	-0.70653800	1.45675200	1.53961000
H	0.14028300	2.43392000	2.75641500
H	-1.55442000	2.77987500	2.34841200
C	-1.48298400	6.38074000	-1.13372900
H	-2.05739200	6.80964300	-0.30981600
H	-0.92372300	7.18049900	-1.62344200
H	-2.19741500	5.98007000	-1.86047500
C	2.82379300	3.77305800	-1.54583500
H	3.61681100	3.54196500	-0.82872500
H	2.74566100	2.92862600	-2.24037600

H	3.12681800	4.64749000	-2.12328100
C	-0.92967900	-0.17212800	-1.81695300
C	-0.54242200	-1.56863500	-1.87185000
C	1.43191200	0.44765700	-1.28078400
C	0.01120600	0.72295900	-1.38353200
H	0.48935100	-1.70880800	-2.17278800
H	-0.33826000	1.64994100	-0.94616600
O	2.16442600	-0.13860500	-2.06743600
C	-2.32848700	0.31228800	-1.94739300
C	-3.44874200	-0.48811200	-1.68231500
C	-2.54339100	1.63968000	-2.34799200
C	-4.73454000	0.02581200	-1.81001400
H	-3.32124100	-1.51603200	-1.36608600
C	-3.82903200	2.15539400	-2.46790700
H	-1.69048700	2.26721700	-2.58940100
C	-4.93272400	1.34847700	-2.20064600
H	-5.58615700	-0.61467800	-1.60109700
H	-3.96798600	3.18474300	-2.78339800
H	-5.93819700	1.74543200	-2.30133600
Cl	-1.50980600	-2.67191200	-2.89361500
C	3.68035100	-0.93868200	2.99567300
H	2.60976200	-0.91323200	3.22255400
H	4.18185800	-1.41607200	3.84063700
C	-1.39126600	-4.08500700	-0.07998600
C	-2.31062800	-3.13202500	0.42724000
C	-3.64191500	-3.49602300	0.65409900
C	-4.04788700	-4.79338300	0.37399900
C	-3.12530100	-5.72851600	-0.12193700
C	-1.79941900	-5.39669200	-0.35769500
C	-0.20496300	-2.10745600	-0.06554500
C	-1.56957800	-1.88263800	0.58209200
H	-4.34417600	-2.77004800	1.04796400
H	-5.07771600	-5.08837600	0.54082600
H	-3.45880000	-6.74032300	-0.33343300
H	-1.10217700	-6.12403200	-0.75899400
N	-0.14327900	-3.55269000	-0.23143900
O	0.81869600	-1.45789700	0.29691400
N	-1.81953500	-0.72774600	1.08482200
C	0.93958100	-4.18738900	-0.93586400
H	1.81454200	-3.54051200	-0.84064700
H	1.17395200	-5.15476900	-0.48264100
H	0.71384000	-4.33851000	-2.00052100
C	-3.00346200	-0.46519900	1.76492500
O	-3.52068100	-1.18248500	2.60127500
O	-3.43036100	0.76275000	1.44279100
C	-4.61634500	1.32461600	2.07403900
C	-5.84447700	0.48446600	1.73658400
C	-4.40544000	1.45927800	3.57984300
C	-4.72394600	2.69943800	1.42511100
H	-5.93700400	0.39057800	0.65102000
H	-5.77704900	-0.50812300	2.18263300
H	-6.73930800	0.98328400	2.11966500
H	-3.46614800	1.98341500	3.78149700
H	-5.22368600	2.04779300	4.00499900
H	-4.37949200	0.48405900	4.06540300
H	-5.62228700	3.21087400	1.78043800
H	-3.85241700	3.30949700	1.67942200

H	-4.77502700	2.59785000	0.33761800

M3$_{C=O}$*RR*

Total energy= -2814.53728986

Sum of electronic and zero-point Energies= -2813.693929

Sum of electronic and thermal Energies= -2813.644827

Sum of electronic and thermal Enthalpies= -2813.643882

Sum of electronic and thermal Free Energies= -2813.776565

C	-5.28276500	-0.03787200	-0.31378000
C	-6.57046500	0.31595400	0.07458700
C	-7.66927700	-0.32755500	-0.48971700
C	-7.44985600	-1.32338100	-1.43912500
C	-6.15186100	-1.66642000	-1.82838700
C	-5.04974400	-1.02161300	-1.27109400
C	-4.25117700	0.77714000	0.44073300
C	-5.06709600	1.52058900	1.55596500
C	-6.54836500	1.41774700	1.10121300
H	-8.67912700	-0.06243500	-0.19060100
H	-8.29646500	-1.83778000	-1.88309800
H	-6.00304600	-2.43958400	-2.57528100
H	-4.02878900	-1.24124000	-1.57424800
H	-4.75320800	2.56552900	1.58793600
H	-7.21625600	1.21254800	1.94443400
H	-3.71955400	1.45828400	-0.22617600
H	-6.88220400	2.36071900	0.65561100
C	-3.49872900	-0.89446000	2.12682900
C	-2.01550600	-0.44438400	0.57835300
N	-2.50427900	-1.70086200	2.36797400
N	-3.23435000	-0.11192100	1.03157000
N	-1.59080200	-1.41144700	1.38899400
C	-4.72564600	-0.61688500	2.91906500
H	-5.60062400	-1.06985100	2.43874800
H	-4.61670200	-1.04902400	3.91438800
C	-0.37025100	-2.17395100	1.29995600
C	0.74979500	-1.70861900	1.97727200
C	-0.35438800	-3.25899900	0.42322100
C	1.94552100	-2.39907700	1.77326300
C	0.85834700	-3.91841000	0.25416900
C	2.01574000	-3.50072000	0.92106300
H	2.84676600	-2.03626800	2.26119500
H	0.91125500	-4.76070200	-0.43220700
C	0.67982500	-0.45371100	2.80059300
H	0.62596000	0.41180300	2.12815100
H	-0.20059900	-0.44814900	3.44932600
H	1.57775500	-0.34193300	3.40864600
C	3.31330700	-4.23496100	0.70872500
H	3.47520600	-4.43337900	-0.35445300
H	4.16164100	-3.65224300	1.07549500
H	3.30618200	-5.19606700	1.23352100
C	-1.58285800	-3.60488700	-0.37338400
H	-2.45560900	-3.74500700	0.27241500
H	-1.80997900	-2.78514300	-1.06800500
H	-1.42779700	-4.51737700	-0.95199700
C	-0.04404900	2.19250400	-1.14709300
C	0.52586100	1.25682400	-2.20063100

C	-1.39120600	0.18542000	-0.69544900
C	-1.00696000	1.63767400	-0.40550800
H	-0.25718300	1.06402500	-2.93687800
H	-1.50913700	2.19972500	0.37979600
O	-2.16306600	-0.00033900	-1.72189600
C	0.36104200	3.61014600	-0.98022000
C	1.68760000	3.97465500	-0.71184200
C	-0.61783500	4.60860800	-1.03105700
C	2.01725800	5.30935600	-0.49976500
H	2.45461000	3.20908800	-0.64981800
C	-0.28399000	5.94409000	-0.82066600
H	-1.64423100	4.32915800	-1.25051500
C	1.03584100	6.29812900	-0.55559200
H	3.04697500	5.57730800	-0.28456700
H	-1.05493400	6.70668400	-0.87096900
H	1.29952400	7.33839900	-0.39296800
Cl	1.91836100	1.90132800	-3.13210400
C	-4.85317100	0.91678600	2.95757900
H	-3.94034900	1.32433800	3.40391000
H	-5.68441300	1.20930300	3.60308100
C	2.41911700	-1.65283600	-2.42863200
C	3.14034400	-1.00953200	-1.40191600
C	4.44166400	-1.39895700	-1.08656300
C	5.02362700	-2.43732500	-1.80278000
C	4.29152200	-3.09062800	-2.80473100
C	2.98988300	-2.72289200	-3.12806000
C	0.89921500	-0.11272600	-1.57655800
C	2.23872000	-0.03446100	-0.80320700
H	4.99622800	-0.89647200	-0.30066300
H	6.03743600	-2.75085200	-1.58140400
H	4.75409300	-3.91019100	-3.34686100
H	2.43963900	-3.23720200	-3.90814500
N	1.17672100	-1.10333400	-2.61412500
O	-0.10392200	-0.55731500	-0.72543700
N	2.36185500	0.77784100	0.17009400
C	0.08928800	-1.84149000	-3.22565300
H	-0.84527000	-1.31575600	-3.00741700
H	0.23058000	-1.91258900	-4.30824300
H	0.02236200	-2.85499100	-2.80629100
C	3.60701300	0.99015300	0.76343000
O	4.49990500	1.61575100	0.23004600
O	3.62596000	0.50980600	2.00854100
C	4.79208500	0.72301300	2.86740300
C	6.00405000	0.01106800	2.27653200
C	5.03086300	2.21599800	3.07055100
C	4.37437300	0.07115400	4.17968700
H	5.76816100	-1.04334400	2.09755800
H	6.31722600	0.47709800	1.34120900
H	6.83330800	0.05900400	2.98748300
H	4.11008200	2.69574200	3.41463400
H	5.79696600	2.35274400	3.83866700
H	5.36211800	2.69495300	2.14982900
H	5.18537000	0.15479300	4.90744600
H	3.48886300	0.56609100	4.58778800
H	4.14975700	-0.98905100	4.03104200

M3$_{C=O}$*RS*

Total energy= -2814.51812370
Sum of electronic and zero-point Energies= -2813.674575
Sum of electronic and thermal Energies= -2813.625245
Sum of electronic and thermal Enthalpies= -2813.624301
Sum of electronic and thermal Free Energies= -2813.757269

C	-4.39877000	-1.63678800	-1.11344300
C	-5.74739700	-1.87542100	-1.35285900
C	-6.14346200	-3.05736500	-1.97704200
C	-5.16459900	-3.97889300	-2.34550300
C	-3.81172400	-3.72519600	-2.10427600
C	-3.41238600	-2.54203200	-1.48825800
C	-4.20864100	-0.30596300	-0.40937900
C	-5.65373600	0.11861900	0.02396800
C	-6.59480800	-0.72609400	-0.87604400
H	-7.19379300	-3.25756100	-2.16420300
H	-5.45946700	-4.90767100	-2.82427500
H	-3.06725900	-4.45205000	-2.40835900
H	-2.36623100	-2.30131400	-1.31415900
H	-5.79451100	1.18321800	-0.17309300
H	-7.48847900	-1.05315500	-0.33459000
H	-3.72450500	0.42400700	-1.06126000
H	-6.94429100	-0.13194000	-1.73110200
C	-3.75817800	-1.14881000	1.88355500
C	-2.01640800	-0.26259700	0.89559700
N	-2.76600100	-1.37051100	2.69400700
N	-3.33601000	-0.47596000	0.76581500
N	-1.67983100	-0.82240400	2.05560100
C	-5.21613100	-1.38748200	2.06002700
H	-5.52389400	-2.27339100	1.49446300
H	-5.42946400	-1.56198100	3.11282500
C	-0.37209700	-0.97163200	2.65345600
C	-0.03654700	-0.13811900	3.71290400
C	0.50535800	-1.90307500	2.08865900
C	1.25227600	-0.24982900	4.23108700
C	1.78396600	-1.96900200	2.63511700
C	2.17519800	-1.15773700	3.70344400
H	1.54749600	0.39304500	5.05688200
H	2.50407500	-2.65295600	2.18634300
C	-1.02170400	0.87655800	4.24023100
H	-1.35147100	1.54357800	3.43833200
H	-1.91035600	0.38976100	4.65247800
H	-0.56309600	1.48475400	5.02231900
C	3.55422200	-1.27827500	4.29697100
H	4.25685300	-1.68347100	3.56813600
H	3.92546800	-0.30391700	4.62408400
H	3.54006000	-1.94353800	5.16838300
C	0.10864800	-2.73076800	0.90064400
H	-0.85354800	-3.22834100	1.06967800
H	0.01021100	-2.09343300	0.01124100
H	0.86938900	-3.48681800	0.69505900
C	-0.56224900	2.53460500	-1.15160800
C	0.72386600	1.76751500	-1.43175200
C	-1.15311900	0.34018500	-0.25024200
C	-1.49826700	1.80187300	-0.53639400
H	0.49277800	0.95666400	-2.12596000

H	-2.45327100	2.23512700	-0.24009000
O	-1.19027300	-0.44935300	-1.26426100
C	-0.77939900	3.96304700	-1.48899300
C	0.10779300	4.95968700	-1.06695900
C	-1.93917100	4.33376200	-2.17832700
C	-0.16523700	6.29783300	-1.32793000
H	1.00717900	4.68056600	-0.52494500
C	-2.20936200	5.67334300	-2.44025100
H	-2.62001900	3.56223500	-2.52198600
C	-1.32279500	6.66080700	-2.01594300
H	0.52752300	7.06311200	-0.98900800
H	-3.10895800	5.94800200	-2.98358400
H	-1.52991200	7.70547900	-2.22183400
Cl	2.05338000	2.70121100	-2.18776200
C	-5.91595600	-0.12591400	1.52583600
H	-5.55829700	0.73246200	2.10740700
H	-6.99367200	-0.19457500	1.69196000
C	3.07836900	1.46248800	1.20018800
C	3.43510200	0.31679700	0.46903100
C	4.64471500	-0.33721500	0.70278000
C	5.49922000	0.16168600	1.67981600
C	5.12418200	1.28725100	2.42641000
C	3.91935700	1.94799500	2.21042200
C	1.21637100	1.07800000	-0.13914100
C	2.31946000	0.03079200	-0.43235300
H	4.90727100	-1.23316700	0.14937100
H	6.44314100	-0.33187500	1.88095700
H	5.79355700	1.65455300	3.19793000
H	3.64822000	2.81749300	2.79582500
N	1.86703600	1.98522200	0.80757100
O	0.15367000	0.43431000	0.48821500
N	2.10876900	-0.87794400	-1.29026000
C	1.09047000	2.77371600	1.74719300
H	0.08670700	2.90958400	1.35207800
H	1.02587900	2.27541800	2.72043100
H	1.54694300	3.75959600	1.88126400
C	3.01490100	-1.92957400	-1.44958500
O	3.09719500	-2.86761300	-0.68482800
O	3.68769800	-1.78462200	-2.59191300
C	4.60714200	-2.82288500	-3.05037100
C	5.74909900	-2.99609400	-2.05207200
C	3.84375800	-4.12348500	-3.28822800
C	5.12887700	-2.25563700	-4.36690300
H	6.23137600	-2.03031800	-1.86677900
H	5.38626700	-3.40960000	-1.10783800
H	6.49510200	-3.67276400	-2.47628300
H	2.99565100	-3.93601500	-3.95228300
H	4.50626600	-4.84666600	-3.77216900
H	3.48044500	-4.54381000	-2.35168200
H	5.84096900	-2.95291100	-4.81280800
H	4.30301200	-2.09304400	-5.06210100
H	5.62988700	-1.29762800	-4.19282000

M3$_{C=O}$*SR*

Total energy= -2814.51812370

Sum of electronic and zero-point Energies= -2813.682266

Sum of electronic and thermal Energies= -2813.632823

Sum of electronic and thermal Enthalpies= -2813.631879
Sum of electronic and thermal Free Energies= -2813.766002

C	-2.21021300	-3.11713200	-0.95124200
C	-3.46746400	-3.65911400	-0.70745100
C	-3.96720300	-4.66592900	-1.53084100
C	-3.18555300	-5.11656200	-2.59215300
C	-1.92415300	-4.56489200	-2.83263300
C	-1.42411900	-3.55549100	-2.01360400
C	-1.86583800	-2.05921500	0.07689200
C	-2.99674000	-2.16910800	1.15863400
C	-4.11939400	-3.00393600	0.48176500
H	-4.94692400	-5.09695000	-1.34561800
H	-3.55959000	-5.90396100	-3.23911800
H	-1.33120800	-4.92392200	-3.66785700
H	-0.45962400	-3.09014900	-2.19294500
H	-3.35506700	-1.16106200	1.37981600
H	-4.55710100	-3.73348700	1.17171500
H	-1.79262900	-1.06120200	-0.36089000
H	-4.93794800	-2.35572200	0.14861900
C	-0.34348500	-3.34280900	1.58592600
C	0.66431700	-1.84640200	0.35086100
N	0.92365300	-3.47952900	1.86406200
N	-0.53872800	-2.35444800	0.65746800
N	1.53499800	-2.54133500	1.07508000
C	-1.53164600	-3.96618300	2.22594500
H	-1.97072400	-4.71868300	1.56075800
H	-1.22542600	-4.45873700	3.14961200
C	2.95977900	-2.37652900	1.10165000
C	3.51334000	-1.60813900	2.12629200
C	3.70434800	-2.93073400	0.05980400
C	4.88785500	-1.38264500	2.07618400
C	5.07507000	-2.67991200	0.05592200
C	5.67785500	-1.90064200	1.04709700
H	5.35061700	-0.77908100	2.85306200
H	5.68236700	-3.08737400	-0.74812700
C	2.64420100	-1.04548400	3.21852600
H	1.74605800	-0.57847400	2.80127600
H	2.31515100	-1.83771100	3.89819800
H	3.18819300	-0.29683700	3.79669000
C	7.14831500	-1.58279200	0.97717300
H	7.70267700	-2.38404300	0.47973700
H	7.30676700	-0.65976400	0.40379900
H	7.57023900	-1.43046600	1.97554100
C	3.02401300	-3.68608700	-1.05161600
H	2.36042100	-4.46167500	-0.65862300
H	2.41122200	-3.00714400	-1.65890600
H	3.76037800	-4.15349800	-1.70648300
C	2.24877000	1.16599600	-1.30805900
C	0.88898200	1.81777200	-1.45894100
C	0.80236400	-0.69392300	-0.67028500
C	2.18746000	-0.10268100	-0.88093000
H	0.31592500	1.25057000	-2.19292600
H	3.09669100	-0.66368100	-0.69690000
O	0.12994900	-0.95591400	-1.72582200
C	3.55206100	1.83994800	-1.51249100
C	3.82575800	3.09031300	-0.94295200

C	4.57381800	1.17659700	-2.20359300
C	5.08945700	3.66005900	-1.06461500
H	3.04665800	3.61040600	-0.39463700
C	5.83730200	1.74761800	-2.32364600
H	4.36511700	0.21172900	-2.65716200
C	6.09901200	2.99231900	-1.75509200
H	5.28667100	4.62694900	-0.61254000
H	6.61645900	1.22277400	-2.86740800
H	7.08264700	3.44022300	-1.85208800
Cl	0.87425200	3.51419500	-2.03692100
C	-2.51923400	-2.81156600	2.47382400
H	-2.02073900	-2.06196000	3.09722100
H	-3.38475100	-3.17174600	3.03505700
C	-0.32444700	3.45983700	1.33093100
C	-1.52662300	3.30688400	0.61278800
C	-2.61889600	4.13837900	0.85179200
C	-2.51744100	5.10938500	1.84153700
C	-1.33383700	5.22821100	2.58216100
C	-0.22845100	4.41759600	2.34617600
C	0.11615400	1.68221400	-0.11687100
C	-1.34339500	2.16209800	-0.27165800
H	-3.52618200	4.04215800	0.26396300
H	-3.35016000	5.77401500	2.04103200
H	-1.27105800	5.98215600	3.36118300
H	0.68183000	4.53332000	2.92389500
N	0.64976400	2.58605900	0.91140600
O	0.13516000	0.36323300	0.30720700
N	-2.14106100	1.50855200	-1.01593000
C	1.73904400	2.20895100	1.79089400
H	1.36787600	1.89610400	2.77580400
H	2.28724000	1.38103900	1.34158400
H	2.43058000	3.04607100	1.92874400
C	-3.49183900	1.86493200	-1.08201200
O	-3.97316700	2.54627600	-1.95858200
O	-4.16379200	1.27033000	-0.08723300
C	-5.62199900	1.37031100	-0.00824600
C	-6.04961100	2.82239400	0.18085600
C	-6.24948000	0.73579800	-1.24456100
C	-5.95216800	0.56294100	1.24104700
H	-5.56963700	3.24426500	1.06919400
H	-5.80011200	3.42715900	-0.69138000
H	-7.13201500	2.85664600	0.33260600
H	-5.85737500	-0.27602900	-1.38424500
H	-7.33199300	0.67011600	-1.10494900
H	-6.04299600	1.32417100	-2.13862500
H	-7.02834300	0.59429300	1.42821300
H	-5.65248300	-0.48099200	1.11635300
H	-5.43184800	0.97650400	2.10913100

M3$_{C=O}$*SS*

Total energy= -2814.53000132

Sum of electronic and zero-point Energies=	-2813.687347
Sum of electronic and thermal Energies=	-2813.637598
Sum of electronic and thermal Enthalpies=	-2813.636654
Sum of electronic and thermal Free Energies=	-2813.773379

C	1.64991500	-3.49148800	0.26275600
C	1.79387900	-4.77199100	0.78532400
C	2.08798500	-5.84004400	-0.06066800
C	2.24539800	-5.59695500	-1.42261300
C	2.12248800	-4.30178300	-1.93546200
C	1.82304800	-3.23181800	-1.09577900
C	1.32069900	-2.49352600	1.34990200
C	1.38097600	-3.30468400	2.69047000
C	1.61805000	-4.78605500	2.28102600
H	2.20195100	-6.84403000	0.33770200
H	2.47798700	-6.41947300	-2.09179600
H	2.26681700	-4.12782500	-2.99741200
H	1.74505200	-2.21679600	-1.48122100
H	0.40313300	-3.21314000	3.16611400
H	2.50197900	-5.20373100	2.77807500
H	0.34401500	-2.04173700	1.20514000
H	0.77009900	-5.41036700	2.57786600
C	3.48586200	-1.41385600	1.98999700
C	2.29924100	-0.25030000	0.55831100
N	4.21486600	-0.37033900	1.71951000
N	2.29159500	-1.37142000	1.30847600
N	3.46845300	0.33487200	0.82240100
C	3.75887000	-2.50617900	2.95944000
H	4.11226200	-3.39615500	2.42420000
H	4.54900900	-2.18447400	3.63919000
C	4.00687800	1.54832400	0.26358300
C	3.83254000	2.74713100	0.95659900
C	4.74678100	1.44608700	-0.91914200
C	4.37504900	3.89899200	0.38516000
C	5.27600700	2.62336800	-1.44103300
C	5.08655900	3.85736200	-0.81330700
H	4.24380500	4.84949300	0.89706300
H	5.85324900	2.57598000	-2.36056400
C	3.13232800	2.82334800	2.28935300
H	2.53607300	1.93437700	2.50523900
H	3.86718000	2.92904400	3.09302800
H	2.47349600	3.69525300	2.32536100
C	5.63091700	5.12322900	-1.42146000
H	4.83328400	5.67273300	-1.93771100
H	6.04312000	5.78573700	-0.65337500
H	6.41349800	4.90663700	-2.15509300
C	4.96915800	0.11192800	-1.57512400
H	5.43185000	-0.59147700	-0.87500900
H	4.00282200	-0.29551600	-1.88933000
H	5.62385500	0.21583600	-2.44199300
C	-0.38546100	2.04105600	-0.67964400
C	-0.92003500	1.06813600	-1.71246600
C	1.32922700	0.29116400	-0.54453300
C	0.76132800	1.64460500	-0.12128600
H	-0.22524100	1.06954000	-2.55312700
H	1.25925300	2.25960700	0.62056800
O	1.88421100	0.23704700	-1.71080800
C	-1.00031500	3.34766200	-0.34105900
C	-2.31921000	3.44853100	0.12165500
C	-0.21402300	4.50413500	-0.40665600
C	-2.83189900	4.68401800	0.50498900
H	-2.93041800	2.55475800	0.20524100

C	-0.73211900	5.73870100	-0.02431000
H	0.80793300	4.42571800	-0.76719200
C	-2.04435900	5.83223000	0.43075800
H	-3.85161000	4.75134500	0.87244800
H	-0.11077800	6.62674100	-0.08464800
H	-2.45147600	6.79312000	0.72927500
Cl	-2.51752600	1.48235900	-2.42546800
C	2.43775300	-2.79830600	3.67976500
H	2.09262300	-1.88260200	4.17068200
H	2.58838100	-3.54826100	4.46012700
C	-2.31172000	-2.01518400	-2.10682600
C	-3.01379000	-1.63633300	-0.94193800
C	-4.22562900	-2.23673200	-0.60524900
C	-4.75564300	-3.19931000	-1.45643600
C	-4.06795200	-3.54769800	-2.62818500
C	-2.85076700	-2.97318400	-2.97434200
C	-0.95149400	-0.38557500	-1.15221800
C	-2.21198700	-0.61244800	-0.28771600
H	-4.74272500	-1.96398500	0.30972600
H	-5.69854100	-3.67834400	-1.21975300
H	-4.49760600	-4.29478400	-3.28894900
H	-2.33496000	-3.25910700	-3.88396400
N	-1.12523400	-1.35195300	-2.22526200
O	0.17540400	-0.64944500	-0.37362700
N	-2.37283100	0.07108000	0.77395800
C	-0.24315100	-1.45066300	-3.36476600
H	0.68660600	-0.93061000	-3.11461800
H	-0.01300300	-2.50243100	-3.56739400
H	-0.68879600	-1.00738500	-4.26507600
C	-3.55321900	-0.03850800	1.51357800
O	-3.66781500	-0.69579900	2.52386900
O	-4.48308000	0.76305100	0.98226100
C	-5.74714100	1.01893000	1.67268000
C	-6.55934600	-0.26768400	1.77082200
C	-5.47161300	1.64263900	3.03632600
C	-6.43276900	2.01862000	0.75033400
H	-6.70439400	-0.69644300	0.77461700
H	-6.06423700	-0.99751600	2.41277300
H	-7.54362400	-0.04048600	2.18971000
H	-4.81611000	2.51127000	2.92109700
H	-6.41539500	1.97900400	3.47418800
H	-5.00370100	0.92682200	3.71247200
H	-7.41291700	2.28480700	1.15385500
H	-5.83143600	2.92742800	0.65970000
H	-6.56591200	1.58746900	-0.24507100

TS2$^{D}_{C=O}$*RR*

Total energy= -1798.40407055

Sum of electronic and zero-point Energies= -1797.976704

Sum of electronic and thermal Energies= -1797.948050

Sum of electronic and thermal Enthalpies= -1797.947106

Sum of electronic and thermal Free Energies= -1798.038592

C	-1.63188100	2.29917600	-0.82902600
C	-1.70278300	1.72870700	0.45232400
C	-2.33712000	2.39307300	1.49068700

C	-2.89145900	3.64850800	1.23261500
C	-2.80822400	4.20968800	-0.04267900
C	-2.17934300	3.54274000	-1.09919300
C	-0.57898700	0.27962600	-1.06883200
C	-1.03352500	0.42944000	0.37276200
H	-2.39524600	1.93947100	2.47604000
H	-3.39229300	4.19061500	2.02691300
H	-3.24439800	5.18667500	-0.22351700
H	-2.12292100	3.98396600	-2.08837400
N	-0.96760100	1.43144500	-1.70669700
O	0.04033800	-0.64934200	-1.55698400
N	-1.10213500	-0.54529700	1.24955200
C	-0.64175100	1.74037200	-3.08099800
H	0.00950900	2.61815800	-3.12997900
H	-1.55097500	1.93005700	-3.65739100
H	-0.12246600	0.87649900	-3.49602900
C	-1.15729900	-1.89384400	0.86877800
O	-0.61109500	-2.78511300	1.48641900
O	-2.00513900	-2.05050000	-0.14613300
C	-2.17354300	-3.35634800	-0.78434700
C	-2.87975100	-4.30607000	0.17581300
C	-0.82630200	-3.89273000	-1.25654700
C	-3.06257600	-3.02246700	-1.97575700
H	-3.81566000	-3.86143900	0.52585100
H	-2.24711500	-4.53336800	1.03408000
H	-3.11518900	-5.23722800	-0.34736900
H	-0.30472800	-3.11955500	-1.82591500
H	-0.99762900	-4.75876000	-1.90220400
H	-0.20363000	-4.19819000	-0.41569200
H	-3.28454800	-3.93118300	-2.54048000
H	-2.55540000	-2.31143000	-2.63352300
H	-4.00344200	-2.58087200	-1.63676400
C	1.80171000	0.26613700	1.11043600
C	1.06141600	1.43041000	0.98739900
C	0.21959100	-0.55983800	2.79663700
C	1.37987800	-0.68732000	2.05085000
H	0.42861100	1.76510400	1.79831000
H	1.80444800	-1.68537400	2.07276500
O	-0.38783600	-0.48154300	3.78278900
C	3.00086800	-0.06450900	0.29517500
C	4.12707400	-0.58422000	0.94429400
C	3.03556400	0.11506600	-1.09187100
C	5.27021600	-0.91260700	0.22252100
H	4.11155100	-0.71308300	2.02257500
C	4.17871700	-0.22065600	-1.81033100
H	2.15821900	0.48144900	-1.61136400
C	5.29858800	-0.73091900	-1.15777100
H	6.13825300	-1.30742200	0.74017500
H	4.19043300	-0.08771100	-2.88721400
H	6.18848400	-0.98778100	-1.72309100
Cl	1.51233300	2.75069800	-0.04259700

TS2$^{D}_{C=O}$*RS*

Total energy= -1798.40323101

Sum of electronic and zero-point Energies= -1797.975724

Sum of electronic and thermal Energies= -1797.948135

Sum of electronic and thermal Enthalpies= -1797.947191

Sum of electronic and thermal Free Energies= -1798.034435

C	-0.21930200	2.24064800	0.22212400
C	-0.35560600	1.00237200	0.86580800
C	-1.13591500	0.87481400	2.00078600
C	-1.83815900	1.99670900	2.45253700
C	-1.73678100	3.21129900	1.77537600
C	-0.91500000	3.35991700	0.65130800
C	1.16908300	0.85658800	-0.96640900
C	0.49251500	0.03422100	0.14287600
H	-1.20877300	-0.08278500	2.50801200
H	-2.47121900	1.92194700	3.32982400
H	-2.29442200	4.07061900	2.13360900
H	-0.81789400	4.31662900	0.14938000
N	0.70319900	2.13803500	-0.82944200
O	1.89990700	0.44275900	-1.84567800
N	1.02821700	-1.03538800	0.72983800
C	0.98959500	3.19415400	-1.77449100
H	1.71700000	2.80615600	-2.48690900
H	1.40607200	4.06475400	-1.26139500
H	0.07839300	3.48552600	-2.30595400
C	2.38447000	-1.25990900	0.70789400
O	2.90335600	-2.35281000	0.84522200
O	3.07648700	-0.09635200	0.66801600
C	4.50867200	-0.08649400	0.42236000
C	4.84734700	-0.88549400	-0.83337600
C	5.24852200	-0.59964900	1.65298100
C	4.78980800	1.39448600	0.19104900
H	4.19890700	-0.56282400	-1.65228700
H	4.71462300	-1.95468100	-0.66936800
H	5.88879700	-0.69483000	-1.10825800
H	4.96212200	-0.01706400	2.53335800
H	6.32708900	-0.49227100	1.50390100
H	5.01611800	-1.65037100	1.82815400
H	5.85558400	1.55190600	0.00598600
H	4.49496100	1.97933100	1.06664100
H	4.22197900	1.74543900	-0.67577500
C	-1.71894900	-1.46208800	-0.44092700
C	-0.83144200	-0.75709000	-1.28260100
C	0.03316600	-3.06469300	-0.01190200
C	-1.22671900	-2.57688700	0.24000200
H	0.01497300	-1.27957300	-1.71737500
H	-1.73583000	-3.02488600	1.08663800
O	0.89545500	-3.75150600	-0.32904400
C	-3.11636600	-1.06023600	-0.15347000
C	-4.07228200	-2.06826500	0.04057900
C	-3.51343000	0.28031400	-0.04180900
C	-5.39018000	-1.74744100	0.34451500
H	-3.78531800	-3.10871700	-0.07693600
C	-4.82933500	0.59474800	0.27761800
H	-2.79419700	1.07985000	-0.17347600
C	-5.77099300	-0.41383700	0.46961200
H	-6.11880900	-2.53945100	0.47995800
H	-5.11553400	1.63631200	0.38010300
H	-6.79828900	-0.16144100	0.71142100
Cl	-1.46083500	0.40623700	-2.43028200

TS2$^{D}_{C=O}$*SR*

Total energy= -1798.40279496

Sum of electronic and zero-point Energies=	-1797.975125
Sum of electronic and thermal Energies=	-1797.946710
Sum of electronic and thermal Enthalpies=	-1797.945766
Sum of electronic and thermal Free Energies=	-1798.035367

C	0.18856700	-2.26035000	-1.00088000
C	-0.24857000	-0.95129300	-0.73897300
C	-0.26973600	0.00171900	-1.74700100
C	0.14985300	-0.37013500	-3.02532800
C	0.59188100	-1.67153200	-3.27094500
C	0.62249100	-2.64008900	-2.26239900
C	-0.31425600	-2.28530400	1.23303300
C	-0.55348400	-0.88852000	0.69218200
H	-0.57938600	1.02159200	-1.53639500
H	0.14593400	0.35861800	-3.82838900
H	0.92096200	-1.94291000	-4.26872800
H	0.96720600	-3.64885700	-2.46237400
N	0.10686300	-3.03631000	0.15966600
O	-0.44683400	-2.67324300	2.37857200
N	-1.26030300	-0.00222300	1.36772700
C	0.56351700	-4.40366000	0.26887800
H	0.41465800	-4.71520400	1.30245200
H	-0.01069700	-5.05444900	-0.39529500
H	1.62611600	-4.47051000	0.01614900
C	-2.15173900	0.88692600	0.76150200
O	-2.30080800	2.03539800	1.13256500
O	-2.87636800	0.27127700	-0.17256800
C	-3.95674100	0.96547800	-0.87650200
C	-5.03694700	1.37655600	0.11749800
C	-3.40474300	2.15143400	-1.65969200
C	-4.47117500	-0.10927900	-1.82569400
H	-5.34508600	0.51180700	0.71173900
H	-4.68262700	2.16227000	0.78475300
H	-5.90759600	1.74343100	-0.43298900
H	-2.64866100	1.81394600	-2.37464400
H	-4.21957800	2.61427300	-2.22329700
H	-2.97104400	2.89822100	-0.99430000
H	-5.28189400	0.29386400	-2.43755500
H	-3.66558900	-0.44632300	-2.48391600
H	-4.84755300	-0.96712400	-1.26273700
C	1.58242200	0.90256700	1.24686400
C	1.57741600	-0.44209800	1.59745900
C	-0.34727700	1.22138100	2.70205400
C	0.61480000	1.72627400	1.83663200
H	1.10758300	-0.77569400	2.51554200
H	0.41666600	2.73186900	1.48198900
O	-0.89384200	1.13133700	3.71975600
C	2.47692600	1.50800000	0.22599300
C	3.00093700	2.78637400	0.45419400
C	2.78078700	0.85334500	-0.97429500
C	3.81132600	3.39852000	-0.49635600
H	2.78810500	3.29306500	1.39086900
C	3.58233400	1.47368000	-1.92670300

H	2.37382800	-0.13095700	-1.17575600
C	4.10133400	2.74457700	-1.69152600
H	4.21784000	4.38540000	-0.30119100
H	3.79628700	0.95985800	-2.85832100
H	4.73056700	3.22260700	-2.43524100
Cl	2.79595900	-1.56203700	1.07466400

TS2$^{D}_{C=O}$*SS*

Total energy= -1798.40693649

Sum of electronic and zero-point Energies= -1797.979991

Sum of electronic and thermal Energies= -1797.951413

Sum of electronic and thermal Enthalpies= -1797.950469

Sum of electronic and thermal Free Energies= -1798.038975

C	-0.39494700	2.31928400	0.25848400
C	-0.99670100	1.19977900	-0.33360700
C	-1.92403700	1.36555900	-1.35085500
C	-2.26813500	2.65982700	-1.74320000
C	-1.68137800	3.76516200	-1.12366100
C	-0.73061100	3.61345600	-0.11240100
C	0.58442500	0.54931700	1.32844600
C	-0.36399600	-0.00023100	0.26469500
H	-2.37878400	0.49976100	-1.82302100
H	-2.99917700	2.80840300	-2.53030700
H	-1.96374200	4.76528700	-1.43600800
H	-0.26666700	4.47396400	0.35746400
N	0.54822400	1.91983800	1.21341100
O	1.24629400	-0.08824000	2.12257000
N	-0.82925500	-1.24023500	0.44670300
C	1.32148400	2.81947500	2.04026800
H	1.95075700	2.20658700	2.68645900
H	1.95089500	3.46364700	1.41903500
H	0.66586300	3.44193100	2.65555500
C	-2.15161000	-1.60061200	0.37351100
O	-2.52353900	-2.75541500	0.25510600
O	-2.99161300	-0.55945400	0.56323700
C	-4.43339000	-0.74555600	0.55909400
C	-4.89767700	-1.29816600	-0.78573100
C	-4.85708100	-1.63675400	1.72310300
C	-4.94954300	0.67578800	0.75659800
H	-4.56151100	-0.64503400	-1.59719600
H	-4.51105100	-2.30400300	-0.94891500
H	-5.99087500	-1.32760200	-0.80559800
H	-4.44365800	-1.24768000	2.65807000
H	-5.94808500	-1.63362500	1.80245600
H	-4.51264500	-2.66027400	1.57797300
H	-6.04260100	0.68203000	0.75612300
H	-4.59494800	1.07829500	1.70924200
H	-4.58931500	1.32270100	-0.04871100
C	1.99233400	-1.16545800	-0.63070500
C	1.10416600	-0.23825700	-1.22637600
C	0.27283700	-2.83347000	-0.83993400
C	1.51590500	-2.45087700	-0.38542500
H	0.31299400	-0.62450700	-1.85972500
H	2.00000800	-3.14036300	0.29764600
O	-0.53427400	-3.38964700	-1.43940700

C	3.36726000	-0.85370900	-0.17736900
C	4.35145300	-1.84275200	-0.30927500
C	3.71826600	0.37978500	0.38797200
C	5.65380800	-1.60895100	0.11786400
H	4.09899300	-2.79044300	-0.77510500
C	5.01856200	0.60592200	0.82214700
H	2.97340200	1.15694700	0.50664200
C	5.98977600	-0.38471800	0.68877500
H	6.40506000	-2.38229200	-0.00108000
H	5.27197900	1.56063000	1.27115200
H	7.00474900	-0.20056800	1.02544300
Cl	1.71256500	1.25399800	-1.90264400

$P_{C=O}RR$

Total energy= -1798.47913177

Sum of electronic and zero-point Energies= -1798.047927

Sum of electronic and thermal Energies= -1798.020606

Sum of electronic and thermal Enthalpies= -1798.019662

Sum of electronic and thermal Free Energies= -1798.106735

C	2.40259700	-0.14987700	0.72480700
C	1.85362900	1.20009100	0.30141000
C	1.17001400	0.16854200	2.83259200
C	2.08443600	-0.57944700	1.94855700
H	2.52551200	1.97830800	0.67704000
H	2.47391300	-1.50684600	2.35141100
O	1.00439600	-0.08608700	3.99746500
C	3.30323800	-0.93351200	-0.15732600
C	2.76997200	-1.62435700	-1.25121000
C	4.66655100	-1.02674100	0.12704900
C	3.60283900	-2.39405700	-2.05578500
H	1.70304000	-1.57123800	-1.45175300
C	5.49758300	-1.79316400	-0.68741900
H	5.07236500	-0.49638800	0.98329600
C	4.96731000	-2.47448700	-1.77919200
H	3.18471100	-2.93532800	-2.89817000
H	6.55752600	-1.85913000	-0.46486000
H	5.61393900	-3.07407000	-2.41158600
Cl	1.80153000	1.44977300	-1.47213500
C	-1.08813500	2.76295700	-0.22437400
C	-1.50884300	1.45216700	-0.51478200
C	-2.57773900	1.21361200	-1.37542300
C	-3.22497000	2.30215600	-1.94938900
C	-2.79357200	3.60262500	-1.66224800
C	-1.72341900	3.85834900	-0.80858100
C	0.45036200	1.43853000	0.89128200
C	-0.63429700	0.55323100	0.23030000
H	-2.87865300	0.20032500	-1.62040000
H	-4.05185500	2.14486000	-2.63190400
H	-3.30151200	4.44196600	-2.12689100
H	-1.39805200	4.87340800	-0.61277900
N	-0.03289400	2.77010000	0.66621200
O	0.50149100	1.23232200	2.30246100
N	-0.64363600	-0.69990300	0.43388700
C	0.77558700	3.93704700	0.94561700
H	1.37860600	3.74101200	1.83414700

H	1.42945800	4.20654800	0.10587700
H	0.12234100	4.78184800	1.17255600
C	-1.60961400	-1.50820700	-0.18757000
O	-1.43745500	-2.02240800	-1.27002900
O	-2.65308000	-1.66800400	0.61853800
C	-3.73799800	-2.59349900	0.27320300
C	-4.44462200	-2.11635500	-0.99037100
C	-3.18659400	-4.00811300	0.13469300
C	-4.66203900	-2.49011400	1.47937000
H	-4.78457000	-1.08387600	-0.86422900
H	-3.78809400	-2.18134300	-1.85938600
H	-5.32266800	-2.74336500	-1.16775100
H	-2.61993900	-4.27775700	1.03019000
H	-4.02174300	-4.70651600	0.03378100
H	-2.54294300	-4.10055000	-0.74007300
H	-5.52787200	-3.14099100	1.33552700
H	-4.13830600	-2.79687600	2.38814400
H	-5.01200100	-1.46235200	1.60468600

$P_{C=O}RS$

Total energy= -1798.47785439

Sum of electronic and zero-point Energies= -1798.045790

Sum of electronic and thermal Energies= -1798.017767

Sum of electronic and thermal Enthalpies= -1798.016822

Sum of electronic and thermal Free Energies= -1798.106154

C	-2.73073500	-0.22655600	0.58916100
C	-1.29171200	-0.29595600	0.12952900
C	-1.88178400	0.87961800	2.63136600
C	-2.95793200	0.32659900	1.78846800
H	-0.85157300	-1.22397200	0.50958600
H	-3.94985900	0.35329700	2.22506600
O	-2.03681800	1.20908200	3.77948700
C	-3.83269000	-0.89750600	-0.14774600
C	-4.25620200	-0.47245900	-1.41258900
C	-4.50153200	-1.95561900	0.47810400
C	-5.33003100	-1.09908100	-2.03598900
H	-3.75915800	0.35743900	-1.90266800
C	-5.56723700	-2.58846100	-0.15518100
H	-4.17298200	-2.28625800	1.45859100
C	-5.98324300	-2.16087700	-1.41287600
H	-5.65874900	-0.75433400	-3.01067700
H	-6.07177900	-3.41330800	0.33676400
H	-6.81625700	-2.65070900	-1.90624400
Cl	-1.07089600	-0.36590800	-1.64749200
C	0.63788100	2.54634900	-0.49820800
C	1.67645600	1.64273300	-0.19609000
C	2.99137200	1.89602300	-0.58647400
C	3.26368200	3.05434700	-1.30171900
C	2.22419200	3.93922600	-1.61375900
C	0.90887000	3.70792900	-1.22491000
C	-0.42904700	0.85529500	0.67681900
C	1.07106200	0.52406900	0.51244100
H	3.78826600	1.20873000	-0.32423200
H	4.27682900	3.27581300	-1.61567600
H	2.44845100	4.84067100	-2.17548600

H	0.13083800	4.41577100	-1.48362900
N	-0.57349100	2.11042900	0.00127700
O	-0.64119000	0.99222300	2.08501100
N	1.49543500	-0.58716400	0.95589800
C	-1.84694900	2.76963300	-0.17477300
H	-2.34720500	2.91373700	0.78754900
H	-1.68402600	3.75134500	-0.61646300
H	-2.51007200	2.19707000	-0.83432800
C	2.86262000	-0.90391700	0.88503900
O	3.69869600	-0.43086800	1.62114000
O	3.05169900	-1.84101800	-0.03810000
C	4.38126600	-2.42226800	-0.25101000
C	5.35921700	-1.33910000	-0.69313500
C	4.83697200	-3.13992800	1.01431900
C	4.13519200	-3.41581600	-1.37879500
H	4.95004100	-0.79217800	-1.54815300
H	5.57250000	-0.64100000	0.11696500
H	6.29569800	-1.80918700	-1.00562900
H	4.08241900	-3.86805200	1.32474700
H	5.76673000	-3.67595400	0.80523400
H	5.01232100	-2.43466000	1.82682200
H	5.06773400	-3.92731300	-1.62910300
H	3.39608400	-4.16130800	-1.07486800
H	3.76814100	-2.89906800	-2.26927700

$P_{C=O}SR$

Total energy= -1798.47777101

Sum of electronic and zero-point Energies=	-1798.045451
Sum of electronic and thermal Energies=	-1798.017405
Sum of electronic and thermal Enthalpies=	-1798.016460
Sum of electronic and thermal Free Energies=	-1798.105923

C	-0.57575000	2.42250200	0.36555900
C	-1.55097100	1.51734300	-0.09693800
C	-2.75948400	1.96277700	-0.63003300
C	-2.99349500	3.32983700	-0.69891400
C	-2.01736900	4.22501200	-0.24410600
C	-0.80309600	3.79781900	0.28447800
C	0.39118000	0.34279400	0.71760800
C	-1.01288700	0.17897900	0.09522100
H	-3.49462500	1.25715200	-1.00240400
H	-3.92287100	3.70474800	-1.11094900
H	-2.20781100	5.29180200	-0.30869400
H	-0.06828500	4.52009500	0.61867100
N	0.53100600	1.76255100	0.86462100
O	0.33937600	-0.30713500	1.98908600
N	-1.44444600	-0.99172100	-0.13554000
C	1.75683800	2.39560500	1.29457300
H	2.11400600	1.94775700	2.22556700
H	2.54727900	2.31489600	0.53765300
H	1.56479100	3.45028100	1.48759600
C	-2.70587700	-1.17318500	-0.72843600
O	-2.88068600	-1.16934500	-1.92529400
O	-3.61336600	-1.42077500	0.21090400
C	-4.98708600	-1.78454600	-0.15303400
C	-5.65226600	-0.62874300	-0.89212900

C	-4.98315100	-3.07261800	-0.96856700
C	-5.64456100	-2.00733900	1.20268500
H	-5.59592000	0.28405200	-0.29113900
H	-5.18328200	-0.45752800	-1.86222100
H	-6.70771400	-0.86618600	-1.05061500
H	-4.42991300	-3.85100000	-0.43584500
H	-6.01377400	-3.41320200	-1.09995500
H	-4.53586600	-2.92076800	-1.95065600
H	-6.69239500	-2.28379200	1.06210900
H	-5.13855600	-2.81092000	1.74349200
H	-5.59935400	-1.09570900	1.80365600
C	2.76311200	-0.56686700	0.51998600
C	1.44048200	-0.34386600	-0.17815000
C	1.46809300	-0.72704100	2.62068600
C	2.72226700	-0.75727000	1.84585800
H	1.02708100	-1.32157000	-0.44890800
H	3.61308500	-0.99740600	2.41492200
O	1.38610700	-1.07971800	3.76961100
C	4.03319200	-0.76216900	-0.22585000
C	4.63807600	0.26429600	-0.96103400
C	4.66951600	-2.00526600	-0.13523100
C	5.85684000	0.04390900	-1.59409100
H	4.16797700	1.23949300	-1.02434500
C	5.88330700	-2.22481400	-0.77995700
H	4.20008400	-2.80177100	0.43395400
C	6.47879900	-1.20031100	-1.51021800
H	6.32371300	0.84926800	-2.15136200
H	6.36197900	-3.19578700	-0.70797500
H	7.42739200	-1.36798800	-2.00960900
Cl	1.54655000	0.56370700	-1.71945700

$P_{C=O}SS$

Total energy= -1798.47958980

Sum of electronic and zero-point Energies= -1798.048157

Sum of electronic and thermal Energies= -1798.020936

Sum of electronic and thermal Enthalpies= -1798.019992

Sum of electronic and thermal Free Energies= -1798.106039

C	-2.82154100	-1.39955400	-0.55791500
C	-2.41255300	-0.10587600	-0.18242400
C	-3.17177000	1.01302600	-0.52217600
C	-4.32920000	0.82987000	-1.26933700
C	-4.71252700	-0.45841900	-1.66173100
C	-3.97446500	-1.58831000	-1.31972300
C	-0.79793200	-1.76225600	0.50730100
C	-1.15702200	-0.25516900	0.54527700
H	-2.86904800	2.00658600	-0.20937900
H	-4.93389600	1.68352300	-1.55189800
H	-5.61534000	-0.58446200	-2.25141300
H	-4.28881800	-2.57534300	-1.63813300
N	-1.96008800	-2.36391900	-0.07648700
O	-0.64291500	-2.30221900	1.82016100
N	-0.37799400	0.55996900	1.12997400
C	-1.98272600	-3.74691200	-0.49971300
H	-1.36941300	-4.33442400	0.18582400
H	-3.00367600	-4.12810500	-0.43372000

H	-1.61813400	-3.87839400	-1.52692300
C	-0.66563200	1.93313000	1.15567600
O	-1.46190500	2.44930100	1.90562200
O	0.13862000	2.55267700	0.29364900
C	0.15468700	4.01430500	0.18921400
C	-1.20622600	4.51255600	-0.28261000
C	0.56990900	4.62402000	1.52316800
C	1.22149000	4.25624500	-0.87104400
H	-1.49649800	3.99577100	-1.20237600
H	-1.96903600	4.35368100	0.48075700
H	-1.14251000	5.58285800	-0.49647000
H	1.51003900	4.17976800	1.86183600
H	0.72569400	5.69813300	1.39024000
H	-0.19482200	4.47088300	2.28442500
H	1.32830400	5.32848100	-1.05196000
H	2.18371100	3.85937800	-0.53560100
H	0.94514600	3.76642600	-1.80861700
C	1.71744600	-1.55766800	0.44453000
C	0.48572800	-2.03450700	-0.30146100
C	0.52524400	-2.16472000	2.51054100
C	1.71007200	-1.68599700	1.77328300
H	0.57500800	-3.11392400	-0.45970200
H	2.56682000	-1.42068900	2.38113500
O	0.53436000	-2.45932800	3.67783800
C	2.89679200	-1.00986100	-0.27273000
C	2.85247100	0.30498600	-0.75066900
C	4.05617900	-1.77000300	-0.42880600
C	3.96478300	0.84664900	-1.38531700
H	1.95324400	0.89918800	-0.60297100
C	5.16525200	-1.22299600	-1.07116700
H	4.08686400	-2.78627600	-0.04764600
C	5.11986400	0.08301600	-1.55062200
H	3.93113400	1.86842800	-1.74986500
H	6.06509400	-1.81738000	-1.19179800
H	5.98523400	0.50893900	-2.04800200
Cl	0.30683800	-1.34071600	-1.94468100

Coordinates of stationary points of IRC points involved in TS2

IRC-F-100

C	-0.21435800	-0.51973500	-0.77566800
C	-0.91175300	-1.69237900	0.14510900
C	-2.19828400	-1.27700600	-0.51183600
C	-1.68392800	-0.18106800	-1.09387900
O	0.58023500	-0.85537500	-1.75748900
C	3.67367300	-0.49665400	-0.65895300
C	4.96358300	-0.78782700	-0.22973600
C	6.05858900	-0.39872800	-0.99952800
C	5.83356600	0.28212400	-2.19346000
C	4.53232100	0.56301200	-2.62098500
C	3.43485300	0.16965100	-1.85861900
C	2.64341800	-1.01180600	0.32467000
C	3.47453100	-1.52155900	1.55372500
C	4.95332800	-1.54048300	1.07484300
H	7.07059900	-0.62051800	-0.67305500
H	6.67787600	0.59388400	-2.80062400
H	4.37741200	1.08332100	-3.56092800
H	2.40765700	0.32943600	-2.17669400
H	3.14668900	-2.53469500	1.79432200
H	5.62240700	-1.08582600	1.81420200
H	2.01900300	-1.78186300	-0.12997400
H	5.30043900	-2.56847500	0.92926700
C	2.05179600	1.04261100	1.63046300
C	0.51455500	0.38341000	0.21768800
N	1.11349000	1.94415100	1.71566700
N	1.72346000	0.07637800	0.71561100
N	0.16375900	1.51397500	0.82122500
C	3.26786800	0.84761400	2.46345100
H	4.16518000	1.12992600	1.90013100
H	3.20487200	1.48069400	3.34924900
C	-0.98180000	2.33083900	0.53192100
C	-0.92182500	3.14585700	-0.60305500
C	-2.08168900	2.28312200	1.38558800
C	-2.01959900	3.96207200	-0.85935600
C	-3.15492600	3.12426300	1.08940400
C	-3.13852800	3.96939300	-0.02006900
H	-2.00217100	4.60903000	-1.73284200
H	-4.02534300	3.11340500	1.74000000
C	0.27414600	3.09920300	-1.51751700
H	1.20275700	3.28110900	-0.96734100
H	0.36249500	2.11327900	-1.99061700
H	0.18550600	3.84921600	-2.30401600
C	-4.31154400	4.86284300	-0.32945800
H	-3.98124400	5.88487400	-0.53301600
H	-4.84274700	4.50829100	-1.21812100
H	-5.02021900	4.88773500	0.50039000
C	-2.12255500	1.32294400	2.54284200
H	-2.27109900	0.30064900	2.17326600
H	-1.19086200	1.34082500	3.11405200
H	-2.94958800	1.56094700	3.21327200
H	-0.87056200	-1.56906300	1.23287400
H	-2.12655800	0.61817000	-1.68421500
C	-3.50286500	-1.94046700	-0.48995900
C	-3.79925000	-2.87014400	0.51361300
C	-4.44365200	-1.70496600	-1.50105100

C	-5.01786100	-3.54133800	0.51501400
H	-3.06457200	-3.06946500	1.28917400
C	-5.65718500	-2.38240400	-1.50285700
H	-4.20476900	-1.00495400	-2.29667700
C	-5.94737200	-3.30222100	-0.49483900
H	-5.23740600	-4.25969500	1.29839500
H	-6.37572800	-2.20189400	-2.29599300
H	-6.89209100	-3.83625400	-0.50180400
Cl	-0.30789900	-3.35020300	-0.17590200
C	3.29304400	-0.65244000	2.80955100
H	2.35427100	-0.90641300	3.31315000
H	4.10220300	-0.86338300	3.51279100

IRC-F-50

C	-0.20822300	-0.44778400	-0.83044300
C	-0.82646800	-1.69253200	0.23381200
C	-2.13001900	-1.34264600	-0.41425200
C	-1.70622900	-0.22116900	-1.01389400
O	0.51413400	-0.70188800	-1.87593700
C	3.67162500	-0.46764900	-0.75053000
C	4.93987900	-0.80895900	-0.29376900
C	6.06785800	-0.45091700	-1.03045900
C	5.89963400	0.25302600	-2.21993200
C	4.62062100	0.58973900	-2.67437900
C	3.49005400	0.22625800	-1.94546500
C	2.60104600	-0.97036700	0.19717300
C	3.37806000	-1.57846500	1.41270800
C	4.87744500	-1.56806500	1.00553700
H	7.06177600	-0.71506200	-0.68091700
H	6.76966400	0.54049400	-2.80214400
H	4.50901900	1.13009200	-3.60910500
H	2.48013800	0.43810700	-2.28706600
H	3.03595100	-2.60569700	1.55306300
H	5.49885500	-1.09622100	1.77596900
H	1.94377600	-1.68691300	-0.29804900
H	5.25544600	-2.58751400	0.88195600
C	2.03444600	1.02467400	1.62612200
C	0.52468900	0.46612900	0.14594300
N	1.10098500	1.92887500	1.74553900
N	1.72675800	0.13408600	0.63158100
N	0.16912800	1.56857000	0.79958700
C	3.19318200	0.71346200	2.50524800
H	4.13380100	1.00078400	2.02072500
H	3.10121900	1.27253100	3.43708100
C	-0.97326600	2.40088800	0.53306500
C	-0.92170300	3.25070200	-0.57740800
C	-2.07364600	2.32331000	1.38535900
C	-2.03664800	4.04910800	-0.82176900
C	-3.16400600	3.14523000	1.10035900
C	-3.16455100	4.00745400	0.00363500
H	-2.02582700	4.71761500	-1.67900100
H	-4.03605400	3.10315100	1.74751900
C	0.28292500	3.26764600	-1.48147600
H	1.20458400	3.42168700	-0.91132800
H	0.38170800	2.31240700	-2.01170400
H	0.19603500	4.06373600	-2.22203900
C	-4.36572200	4.86326300	-0.30529800

H	-4.07134000	5.89826100	-0.49793500
H	-4.87766400	4.49726200	-1.20061100
H	-5.08059600	4.85467400	0.51959200
C	-2.08783900	1.35594700	2.53662000
H	-2.09597500	0.32599000	2.16087500
H	-1.20359500	1.47393000	3.16859500
H	-2.97914600	1.49800100	3.14918000
H	-0.76595300	-1.43669200	1.29791000
H	-2.23070000	0.56363900	-1.55050000
C	-3.41935800	-2.02965400	-0.44399200
C	-3.82689500	-2.93186300	0.54380300
C	-4.25201400	-1.79388800	-1.54533900
C	-5.06722600	-3.55765800	0.44213300
H	-3.17367800	-3.13619200	1.38764400
C	-5.48615800	-2.41835500	-1.64499400
H	-3.90841400	-1.12783700	-2.33094300
C	-5.89856000	-3.29980300	-0.64637400
H	-5.38572500	-4.25190700	1.21322700
H	-6.12252800	-2.22754300	-2.50321300
H	-6.86173000	-3.79413700	-0.72268500
Cl	-0.35197100	-3.44836600	0.19515500
C	3.13695900	-0.81201600	2.72336600
H	2.15586900	-1.06836400	3.13794700
H	3.88671500	-1.11466200	3.45857100

IRC-F-40

C	-0.19943700	-0.40128700	-0.86449600
C	-0.80509300	-1.73088600	0.25333100
C	-2.10107500	-1.36848000	-0.39678700
C	-1.70432400	-0.23512500	-0.99093100
O	0.49848700	-0.62039600	-1.92111900
C	3.67107600	-0.46549000	-0.76241800
C	4.93676300	-0.81020600	-0.30100900
C	6.06860500	-0.45402300	-1.03270300
C	5.90732500	0.25121200	-2.22224300
C	4.63116500	0.59264400	-2.68080400
C	3.49700100	0.23243000	-1.95633200
C	2.59550400	-0.96143800	0.18379800
C	3.36751900	-1.57915900	1.39872200
C	4.86890200	-1.56611600	0.99965000
H	7.06034100	-0.72040600	-0.67873100
H	6.78044900	0.53698700	-2.80060200
H	4.52449200	1.13563400	-3.61455100
H	2.49063100	0.45417700	-2.30117600
H	3.02438100	-2.60742500	1.52798900
H	5.48450600	-1.08932400	1.77176300
H	1.93017600	-1.67412800	-0.30757900
H	5.25066000	-2.58481800	0.88219000
C	2.03014600	1.02451500	1.62927700
C	0.53063500	0.48500800	0.13258600
N	1.09520900	1.92633500	1.75475800
N	1.73008300	0.14760200	0.62025400
N	0.17088200	1.57980600	0.79661800
C	3.18246400	0.70236100	2.51234200
H	4.12655000	0.99219700	2.03610800
H	3.08604700	1.25275400	3.44884200
C	-0.97078500	2.41300000	0.53132400

C	-0.92189700	3.26476700	-0.57785100
C	-2.07083900	2.32996600	1.38373400
C	-2.04062800	4.05841200	-0.82130100
C	-3.16428400	3.14788800	1.10006700
C	-3.16839500	4.01084900	0.00377200
H	-2.03248400	4.72827900	-1.67751300
H	-4.03625700	3.10145900	1.74703000
C	0.28261100	3.29075800	-1.48197700
H	1.20573800	3.42583000	-0.90949200
H	0.37338300	2.34621400	-2.03222600
H	0.20152000	4.10276000	-2.20578400
C	-4.37333000	4.86150600	-0.30463400
H	-4.08387400	5.89856900	-0.49363300
H	-4.88179200	4.49562200	-1.20196100
H	-5.08957000	4.84678100	0.51897300
C	-2.07949300	1.36029400	2.53307200
H	-2.05743100	0.33125500	2.15543600
H	-1.20747200	1.49784700	3.17794500
H	-2.98263700	1.48046600	3.13274300
H	-0.74296100	-1.46088100	1.31299100
H	-2.25991700	0.54805800	-1.49939500
C	-3.39564900	-2.04799000	-0.43780900
C	-3.82171700	-2.94665000	0.54505700
C	-4.21764500	-1.80059300	-1.54493700
C	-5.06927600	-3.55612800	0.43343800
H	-3.17811100	-3.15954700	1.39392700
C	-5.46030400	-2.40649600	-1.65321400
H	-3.85926500	-1.13933900	-2.32786000
C	-5.89087600	-3.28410500	-0.65905300
H	-5.40191000	-4.24786000	1.20083100
H	-6.08857400	-2.20471700	-2.51489400
H	-6.86038700	-3.76481400	-0.74204800
Cl	-0.38712100	-3.50981000	0.24888300
C	3.12079400	-0.82489600	2.71538100
H	2.13682300	-1.08272600	3.12214700
H	3.86592200	-1.13710400	3.45126500

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C	-0.19201500	-0.33431700	-0.90707300
C	-0.79316600	-1.77987100	0.29030000
C	-2.06883200	-1.39587600	-0.37960200
C	-1.70029500	-0.24949600	-0.96791900
O	0.48045100	-0.54810900	-1.96190500
C	3.67008100	-0.46509700	-0.77288900
C	4.93379800	-0.81132600	-0.30724600
C	6.06858600	-0.45578500	-1.03467700
C	5.91280800	0.25032800	-2.22433300
C	4.63893800	0.59468700	-2.68654400
C	3.50226800	0.23612100	-1.96579300
C	2.59049800	-0.95349700	0.17279100
C	3.35855200	-1.57877500	1.38749700
C	4.86153500	-1.56399000	0.99486200
H	7.05867500	-0.72302400	-0.67680700
H	6.78837000	0.53540900	-2.79927500
H	4.53585500	1.13989500	-3.61936000
H	2.49965100	0.46662200	-2.31447000
H	3.01446300	-2.60777900	1.50733100

H	5.47282000	-1.08320400	1.76797900
H	1.91602000	-1.66367800	-0.31121100
H	5.24587400	-2.58226100	0.88262500
C	2.02636400	1.02436600	1.63207200
C	0.53847800	0.50660000	0.11740400
N	1.09022900	1.92399200	1.76395100
N	1.73454300	0.16153600	0.60845700
N	0.17390800	1.59254000	0.79363000
C	3.17307800	0.69328500	2.51851900
H	4.11996100	0.98534500	2.04922200
H	3.07255900	1.23671300	3.45860600
C	-0.96738800	2.42571900	0.52975300
C	-0.92208900	3.27821000	-0.57902200
C	-2.06702400	2.33698900	1.38247600
C	-2.04477900	4.06661400	-0.82179000
C	-3.16373800	3.15055200	1.09991100
C	-3.17187300	4.01372600	0.00366200
H	-2.03983200	4.73717700	-1.67748200
H	-4.03544400	3.09993500	1.74692100
C	0.28213900	3.31318800	-1.48339300
H	1.20690600	3.42779400	-0.90925400
H	0.36431100	2.38093300	-2.05515700
H	0.20746400	4.14154100	-2.18913300
C	-4.38039400	4.85951300	-0.30388400
H	-4.09555200	5.89853900	-0.48912200
H	-4.88564200	4.49408700	-1.20319200
H	-5.09779300	4.83877200	0.51856300
C	-2.07072100	1.36461700	2.52950600
H	-2.02558000	0.33741800	2.14883500
H	-1.20807900	1.51597100	3.18378600
H	-2.98211700	1.46736200	3.11977300
H	-0.74709700	-1.50356900	1.34859100
H	-2.29341000	0.52680600	-1.44443300
C	-3.37196300	-2.06469300	-0.43642900
C	-3.81472800	-2.95988800	0.54224400
C	-4.18685400	-1.80567700	-1.54647900
C	-5.06884700	-3.55418500	0.42430000
H	-3.17823200	-3.18068400	1.39421800
C	-5.43788900	-2.39419400	-1.66009900
H	-3.81714900	-1.14875600	-2.32774900
C	-5.88347100	-3.26881700	-0.67011500
H	-5.41271900	-4.24362600	1.18882800
H	-6.06048500	-2.18165100	-2.52333400
H	-6.85873300	-3.73695700	-0.75777900
Cl	-0.42071500	-3.57294200	0.29719500
C	3.10718000	-0.83513100	2.70911800
H	2.12089600	-1.09425400	3.10930000
H	3.84855100	-1.15517500	3.44539900

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C	-0.18908800	-0.26282700	-0.94666500
C	-0.78299500	-1.83515700	0.32705400
C	-2.03461200	-1.42530900	-0.36286100
C	-1.69487900	-0.26037100	-0.93607800
O	0.45955300	-0.49037800	-1.99518500
C	3.66839400	-0.46438400	-0.78304400
C	4.93032700	-0.81178100	-0.31335800

C	6.06779400	-0.45666000	-1.03676700
C	5.91699500	0.25032500	-2.22649200
C	4.64521000	0.59676800	-2.69245300
C	3.50625300	0.23918800	-1.97530600
C	2.58515000	-0.94465200	0.16242000
C	3.34912400	-1.57767300	1.37642900
C	4.85361500	-1.56175300	0.98990100
H	7.05639900	-0.72452200	-0.67532000
H	6.79477200	0.53508600	-2.79814400
H	4.54546600	1.14373500	-3.62456200
H	2.50725100	0.47714400	-2.32820200
H	3.00365700	-2.60724200	1.48650400
H	5.46116500	-1.07798200	1.76413100
H	1.89911400	-1.65083400	-0.31305500
H	5.23975500	-2.57977200	0.88204400
C	2.02367100	1.02569500	1.63494300
C	0.54768600	0.53124900	0.10209300
N	1.08738400	1.92450200	1.77223100
N	1.74002100	0.17752400	0.59681500
N	0.17922700	1.60901300	0.79026700
C	3.16389100	0.68453200	2.52549900
H	4.11403400	0.97865000	2.06416200
H	3.05863300	1.22052600	3.46929400
C	-0.96241100	2.44121700	0.52852500
C	-0.92233000	3.29322000	-0.58085100
C	-2.06161900	2.34547100	1.38156400
C	-2.04984400	4.07501500	-0.82308400
C	-3.16241400	3.15350500	1.09993900
C	-3.17567000	4.01654700	0.00346000
H	-2.04926600	4.74551800	-1.67883800
H	-4.03371200	3.09794500	1.74709200
C	0.28070800	3.33747400	-1.48670400
H	1.20797300	3.42738600	-0.91239200
H	0.35168100	2.42059900	-2.08384600
H	0.21363000	4.18445400	-2.17083700
C	-4.38817700	4.85698100	-0.30282700
H	-4.10839300	5.89820500	-0.48341900
H	-4.88986800	4.49252600	-1.20449300
H	-5.10682900	4.82927900	0.51829900
C	-2.06050800	1.36959200	2.52564100
H	-1.99554900	0.34478300	2.14131400
H	-1.20620400	1.53195500	3.18811300
H	-2.97863700	1.45660200	3.10788100
H	-0.75555600	-1.55269700	1.38457000
H	-2.32812700	0.51085500	-1.36781700
C	-3.34696500	-2.08300100	-0.43928100
C	-3.80577700	-2.97482000	0.53532100
C	-4.15675300	-1.81000500	-1.54988800
C	-5.06697300	-3.55244200	0.41341800
H	-3.17468300	-3.20452200	1.38870600
C	-5.41679500	-2.38015400	-1.66690400
H	-3.77685700	-1.15640700	-2.32910600
C	-5.87623800	-3.25215900	-0.68120600
H	-5.42130800	-4.23949000	1.17534700
H	-6.03519400	-2.15539100	-2.53008800
H	-6.85770700	-3.70656700	-0.77206800
Cl	-0.45344400	-3.63890400	0.34285600

C	3.09330600	-0.84499600	2.70302600
H	2.10454900	-1.10515500	3.09623800
H	3.83066600	-1.17321600	3.43969600

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C	-0.19207000	-0.19513600	-0.97851900
C	-0.77904100	-1.90103000	0.34520100
C	-2.00127500	-1.45548200	-0.34895900
C	-1.68832200	-0.25662400	-0.88021200
O	0.43640100	-0.46578600	-2.01589100
C	3.66669400	-0.46286000	-0.79245100
C	4.92677000	-0.81158100	-0.31883600
C	6.06664600	-0.45671500	-1.03845500
C	5.92000100	0.25119000	-2.22813900
C	4.65009000	0.59937100	-2.69772400
C	3.50906000	0.24236900	-1.98404600
C	2.57946500	-0.93407000	0.15186300
C	3.33885800	-1.57542800	1.36555800
C	4.84500400	-1.55975000	0.98491600
H	7.05397600	-0.72515100	-0.67401200
H	6.79967700	0.53579800	-2.79687600
H	4.55354200	1.14767100	-3.62933400
H	2.51285700	0.48542700	-2.34099700
H	2.99115000	-2.60523700	1.46546200
H	5.44938400	-1.07441300	1.76065500
H	1.88206000	-1.63458100	-0.31743000
H	5.23170300	-2.57788600	0.88054100
C	2.01933300	1.02594000	1.63940000
C	0.56182600	0.56886200	0.07869700
N	1.08451000	1.92541000	1.78308300
N	1.74565100	0.19774100	0.58266000
N	0.18827100	1.63316600	0.78574100
C	3.15416800	0.67561800	2.53200000
H	4.10594100	0.97246100	2.07570100
H	3.04605600	1.20527100	3.47899900
C	-0.95523500	2.46228700	0.52955900
C	-0.92276800	3.31012200	-0.58298800
C	-2.05443800	2.35572800	1.38214600
C	-2.05641100	4.08248800	-0.82603300
C	-3.16054500	3.15619200	1.10026800
C	-3.17979500	4.01859200	0.00301200
H	-2.06206600	4.75108000	-1.68324800
H	-4.03186900	3.09440400	1.74683300
C	0.27783800	3.36130300	-1.49209300
H	1.20858100	3.42308200	-0.92007900
H	0.33386900	2.46161700	-2.11600200
H	0.21976500	4.22716300	-2.15301700
C	-4.39561500	4.85457900	-0.30161800
H	-4.11952400	5.89764300	-0.47727500
H	-4.89426800	4.49207500	-1.20571700
H	-5.11536700	4.82070100	0.51827000
C	-2.05041000	1.37285300	2.52057000
H	-1.97061100	0.35146000	2.12966100
H	-1.20357400	1.54052300	3.19114100
H	-2.97416900	1.44598000	3.09576900
H	-0.71969100	-1.58098300	1.38665100
H	-2.36126400	0.52947200	-1.21908100

C	-3.32170800	-2.10306600	-0.45034100
C	-3.79472300	-2.98992900	0.52262100
C	-4.13021300	-1.81318300	-1.55728200
C	-5.06317900	-3.54992900	0.40220600
H	-3.16674300	-3.22667700	1.37617100
C	-5.39975900	-2.36564800	-1.67317200
H	-3.74302200	-1.15971600	-2.33329700
C	-5.86980000	-3.23534600	-0.69080400
H	-5.42619800	-4.23269000	1.16395000
H	-6.01749000	-2.12795400	-2.53342200
H	-6.85781200	-3.67545600	-0.78163000
Cl	-0.48229800	-3.70461400	0.38577800
C	3.08159000	-0.85437500	2.69788400
H	2.09211500	-1.11668100	3.08775200
H	3.81802000	-1.18931800	3.43241900

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C	-0.19923800	-0.15748400	-1.02928300
C	-0.82814700	-2.01109700	0.34589600
C	-1.97156800	-1.51331900	-0.34688600
C	-1.66880400	-0.27046200	-0.84581300
O	0.44339000	-0.51918400	-2.02103100
C	3.67155600	-0.49557400	-0.80531600
C	4.93086200	-0.84455500	-0.33052400
C	6.07148700	-0.48959500	-1.04911300
C	5.92553500	0.21815800	-2.23864700
C	4.65628100	0.56660300	-2.70942300
C	3.51493300	0.21054500	-1.99641000
C	2.58190000	-0.96341100	0.13662700
C	3.33986300	-1.60773300	1.35212300
C	4.84694600	-1.59257100	0.97290800
H	7.05848200	-0.75817200	-0.68399200
H	6.80556800	0.50200900	-2.80749100
H	4.56013300	1.11496000	-3.64103500
H	2.52044500	0.45574300	-2.35586500
H	2.99188200	-2.63769900	1.44798400
H	5.45067100	-1.10784100	1.74947700
H	1.88717800	-1.66495400	-0.33557000
H	5.23314000	-2.61103800	0.86887100
C	2.01817000	0.98759100	1.63122200
C	0.57539200	0.57353900	0.04056700
N	1.08758500	1.89002700	1.78059300
N	1.74663500	0.17187300	0.56225900
N	0.19848400	1.61782500	0.77509700
C	3.15449600	0.63812600	2.52132100
H	4.10431600	0.93655100	2.06177400
H	3.04799400	1.16792300	3.46818300
C	-0.94591700	2.44215300	0.52346600
C	-0.91854000	3.28255800	-0.59378700
C	-2.04573300	2.32718400	1.37491900
C	-2.05472000	4.05078700	-0.83745400
C	-3.15490700	3.12282800	1.09166000
C	-3.17599100	3.98504500	-0.00626900
H	-2.06377600	4.71765400	-1.69558400
H	-4.02684900	3.05787800	1.73675900
C	0.28137200	3.33693700	-1.50420500
H	1.21338100	3.38852300	-0.93374000

H	0.33256400	2.44600600	-2.14092900
H	0.22568100	4.20985800	-2.15552600
C	-4.39321500	4.81964500	-0.31079600
H	-4.11535000	5.86584100	-0.48351600
H	-4.89009600	4.45609000	-1.21917700
H	-5.11492800	4.78133500	0.51121300
C	-2.04152700	1.33814500	2.50850900
H	-1.95122500	0.31885400	2.11299000
H	-1.20116200	1.51003400	3.18651900
H	-2.96964900	1.40226700	3.07788300
H	-0.47937100	-1.54072900	1.25682100
H	-2.36072900	0.56035000	-0.97214600
C	-3.29996600	-2.15411800	-0.47581000
C	-3.78493900	-3.02918500	0.50410400
C	-4.11427900	-1.84872600	-1.57213600
C	-5.05607100	-3.58166100	0.38940400
H	-3.15910900	-3.26108300	1.36070600
C	-5.38999200	-2.39345700	-1.68336500
H	-3.72529900	-1.18919200	-2.34273000
C	-5.86259800	-3.26451600	-0.70376900
H	-5.42262500	-4.25850900	1.15520700
H	-6.01097900	-2.14724700	-2.53901100
H	-6.85385000	-3.69788900	-0.79267600
Cl	-0.48602400	-3.76413800	0.39457200
C	3.08421900	-0.89075200	2.68668500
H	2.09583900	-1.15486700	3.07828000
H	3.82290500	-1.22667400	3.41877000

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C	-0.21926200	-0.05942100	-1.05723800
C	-0.90422200	-2.04264600	0.38350500
C	-1.95764000	-1.50049100	-0.33187800
C	-1.65079300	-0.21395100	-0.81670800
O	0.44429400	-0.51174500	-1.99337800
C	3.66750700	-0.45966400	-0.79636500
C	4.92586000	-0.81067400	-0.32053100
C	6.06673700	-0.45661800	-1.03883500
C	5.92151400	0.25130300	-2.22862700
C	4.65274600	0.60093400	-2.70005600
C	3.51128200	0.24556100	-1.98743600
C	2.57695100	-0.92662000	0.14283100
C	3.33288300	-1.57297200	1.36046800
C	4.84057800	-1.55854900	0.98277700
H	7.05352200	-0.72553200	-0.67348800
H	6.80192300	0.53512400	-2.79649700
H	4.55765500	1.14942200	-3.63157300
H	2.51782000	0.49316900	-2.34783300
H	2.98404000	-2.60305000	1.45430400
H	5.44297300	-1.07323100	1.75992800
H	1.89367800	-1.63287100	-0.33710900
H	5.22629100	-2.57712500	0.87981800
C	2.00736700	1.01738200	1.64197400
C	0.57461000	0.64367000	0.02609300
N	1.08265300	1.92383000	1.79495000
N	1.73384000	0.20974300	0.56407400
N	0.19830300	1.66863300	0.78431400
C	3.14507200	0.66886500	2.53092000

H	4.09361500	0.96993300	2.07035500
H	3.03764600	1.19942800	3.47745000
C	-0.94733900	2.48826600	0.53759100
C	-0.92297800	3.32158400	-0.58389100
C	-2.04832400	2.36533000	1.38660100
C	-2.06108900	4.08561300	-0.82930700
C	-3.15948400	3.15665200	1.10069400
C	-3.18154400	4.01895500	0.00238600
H	-2.07230700	4.75093000	-1.68895900
H	-4.03283400	3.08858200	1.74393000
C	0.27621300	3.37684200	-1.49566800
H	1.21006400	3.41690400	-0.92719300
H	0.32061600	2.49551200	-2.14499100
H	0.22489200	4.25812800	-2.13658200
C	-4.39830000	4.85350900	-0.30126600
H	-4.12272800	5.89702500	-0.47520800
H	-4.89626900	4.49198400	-1.20609400
H	-5.11826000	4.81808800	0.51836000
C	-2.04331700	1.37218400	2.51693100
H	-1.94153000	0.35498500	2.11809800
H	-1.20854100	1.54802000	3.20057600
H	-2.97526600	1.42814400	3.08093700
H	-0.21450700	-1.46783600	0.98166500
H	-2.31749600	0.63992800	-0.71547600
C	-3.29311600	-2.13183100	-0.47676900
C	-3.78854800	-2.99747600	0.50825600
C	-4.11257300	-1.81503300	-1.56494800
C	-5.06066500	-3.54674300	0.39609500
H	-3.16786000	-3.22185800	1.37057300
C	-5.39120300	-2.35671500	-1.67446500
H	-3.72475200	-1.14551300	-2.32771900
C	-5.86691500	-3.22812700	-0.69714600
H	-5.42996300	-4.21719300	1.16603800
H	-6.01375000	-2.10367000	-2.52715500
H	-6.86095100	-3.65548000	-0.78455800
Cl	-0.49439300	-3.74922500	0.41316100
C	3.07829700	-0.85894200	2.69661900
H	2.09181500	-1.12516600	3.09125200
H	3.81916200	-1.19452900	3.42624900

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C	-0.22262000	-0.02219700	-1.06933300
C	-0.91958400	-2.10660200	0.37489400
C	-1.94080900	-1.52832400	-0.33087500
C	-1.61804700	-0.19961100	-0.76977400
O	0.44944800	-0.55865300	-1.96027800
C	3.66883900	-0.45206700	-0.80029100
C	4.92494600	-0.80794300	-0.32243300
C	6.06744100	-0.45704500	-1.03962200
C	5.92433600	0.25104100	-2.22970800
C	4.65696200	0.60283500	-2.70365700
C	3.51406500	0.25080100	-1.99212600
C	2.57293800	-0.91313200	0.13281500
C	3.32372800	-1.56855700	1.35196300
C	4.83368100	-1.55606900	0.98011800
H	7.05345500	-0.72819100	-0.67385100
H	6.80587400	0.53298500	-2.79676600

H	4.56472300	1.15022900	-3.63609600
H	2.51996700	0.49722800	-2.35273900
H	2.97262600	-2.59881100	1.43573700
H	5.43345200	-1.07164000	1.75987600
H	1.89448400	-1.61621900	-0.35615000
H	5.21819100	-2.57527100	0.87880300
C	1.99675700	1.01429700	1.64301800
C	0.58053100	0.69890400	-0.00365400
N	1.08196100	1.92745400	1.80638900
N	1.72647000	0.22957300	0.54642500
N	0.21001600	1.70727600	0.77893600
C	3.13292000	0.66092200	2.53112500
H	4.08083800	0.96500500	2.07090000
H	3.02457400	1.19055000	3.47811100
C	-0.93787200	2.52253300	0.54621000
C	-0.92318500	3.34336500	-0.58359900
C	-2.03967000	2.38349200	1.39270400
C	-2.06824500	4.09423400	-0.83297000
C	-3.15866900	3.16144000	1.10132700
C	-3.18570300	4.02208200	0.00134300
H	-2.08752700	4.75421100	-1.69657900
H	-4.03402700	3.08488600	1.74093500
C	0.27243400	3.39880600	-1.50042100
H	1.20991600	3.42231800	-0.93760600
H	0.30367200	2.52624800	-2.16200700
H	0.22586700	4.28907300	-2.12920800
C	-4.40477900	4.85261300	-0.30203400
H	-4.13099200	5.89670400	-0.47542900
H	-4.90225800	4.49080000	-1.20700300
H	-5.12444500	4.81594700	0.51778700
C	-2.03237500	1.38076900	2.51563400
H	-1.90542400	0.36870200	2.11099700
H	-1.21119400	1.56527900	3.21321600
H	-2.97363300	1.41549500	3.06582700
H	-0.10528900	-1.53133000	0.78729500
H	-2.24342500	0.63982300	-0.48441900
C	-3.28289700	-2.14037100	-0.48372200
C	-3.78644100	-3.00264800	0.50101800
C	-4.10180200	-1.81271100	-1.56895900
C	-5.06089800	-3.54518500	0.38858400
H	-3.17222600	-3.22758000	1.36755000
C	-5.38215400	-2.35085900	-1.68020600
H	-3.71511300	-1.13470500	-2.32467000
C	-5.86369900	-3.22219000	-0.70545600
H	-5.43474400	-4.21101000	1.16025600
H	-6.00412500	-2.09081000	-2.53113400
H	-6.86088800	-3.64190300	-0.79341500
Cl	-0.51600200	-3.80782800	0.43182500
C	3.07015100	-0.86556700	2.69336700
H	2.08503700	-1.13607900	3.08866800
H	3.81394900	-1.20295700	3.41919200

IRC-R-50

C	-0.19874000	-0.02880600	-1.03747600
C	-0.86178800	-2.31007600	0.29029900
C	-1.87551000	-1.64583700	-0.31346200
C	-1.52412300	-0.26099800	-0.62383900

O	0.48081800	-0.61121400	-1.90797500
C	3.66923500	-0.41175700	-0.81450800
C	4.91791700	-0.78528500	-0.33128900
C	6.06713500	-0.45432900	-1.04702300
C	5.93672200	0.24956500	-2.24134700
C	4.67557400	0.61414600	-2.72294900
C	3.52558000	0.28204900	-2.01278400
C	2.56414600	-0.86423400	0.10976400
C	3.29457700	-1.54710100	1.32190700
C	4.80939500	-1.53343000	0.97072800
H	7.04844800	-0.73875300	-0.67859000
H	6.82369200	0.51630000	-2.80735200
H	4.59435300	1.15466400	-3.66047400
H	2.53300900	0.53132900	-2.37727200
H	2.93998900	-2.57845000	1.37662700
H	5.39875800	-1.04910100	1.75864300
H	1.88900400	-1.54953300	-0.40288600
H	5.19577100	-2.55244600	0.87500700
C	1.99196400	1.04765600	1.64352600
C	0.58983100	0.77072400	-0.02450800
N	1.09612500	1.97886200	1.80216200
N	1.72567500	0.28267400	0.53199400
N	0.23846400	1.79469900	0.75145100
C	3.10194300	0.65426700	2.54925200
H	4.06483200	0.95739100	2.12064700
H	2.97810200	1.16186200	3.50640700
C	-0.91569200	2.60929900	0.54067200
C	-0.93027200	3.42878200	-0.59041200
C	-2.00558200	2.45889800	1.40204200
C	-2.09372300	4.15340000	-0.83316900
C	-3.14550900	3.20823000	1.11500400
C	-3.20428600	4.05724600	0.00756900
H	-2.13545600	4.80640900	-1.70141200
H	-4.01341900	3.11391700	1.76244600
C	0.25182200	3.49938100	-1.52252400
H	1.19605100	3.53400900	-0.97204400
H	0.28371700	2.62375200	-2.18021900
H	0.18584500	4.38728200	-2.15302700
C	-4.44933900	4.84731300	-0.29943800
H	-4.21064500	5.90113800	-0.46610300
H	-4.92774200	4.47322800	-1.20965000
H	-5.17295300	4.78213000	0.51510800
C	-1.96668500	1.46866200	2.53660700
H	-1.74516000	0.46469800	2.15450200
H	-1.18982700	1.72190700	3.26295800
H	-2.92923600	1.43688400	3.04905300
H	0.03384100	-1.79850000	0.60644200
H	-2.08969500	0.52351500	-0.13306200
C	-3.24439400	-2.18984300	-0.48296300
C	-3.78862900	-3.04594300	0.48460700
C	-4.04171600	-1.81120200	-1.56818300
C	-5.07957100	-3.54226300	0.35139500
H	-3.19583800	-3.30772600	1.35484600
C	-5.33481000	-2.31149900	-1.70480000
H	-3.63120200	-1.12637000	-2.30487900
C	-5.85530600	-3.18262300	-0.74963500
H	-5.48429300	-4.20382000	1.11089200

H	-5.93814100	-2.01958200	-2.55865600
H	-6.86313600	-3.57101000	-0.85685100
Cl	-0.65003100	-4.02956300	0.48327300
C	3.02047800	-0.87504800	2.67381800
H	2.02482200	-1.14554100	3.04150700
H	3.74587400	-1.23631800	3.40681000

IRC-R-80

C	-0.18034100	-0.07132400	-0.99398000
C	-0.83406600	-2.52983600	0.22818100
C	-1.82733500	-1.77783600	-0.28577000
C	-1.44578500	-0.37195800	-0.49297400
O	0.49878300	-0.62647400	-1.88924900
C	3.68045300	-0.37186400	-0.81501800
C	4.92591500	-0.75329200	-0.33008100
C	6.07685500	-0.44162800	-1.05167800
C	5.95129600	0.25265300	-2.25229600
C	4.69312600	0.62711800	-2.73442400
C	3.54102700	0.31276900	-2.01919800
C	2.57279900	-0.81972400	0.10837600
C	3.29475000	-1.50339900	1.32127500
C	4.81121100	-1.49139200	0.97787800
H	7.05591900	-0.73426800	-0.68366100
H	6.83984000	0.50392500	-2.82291200
H	4.61576800	1.15951600	-3.67693600
H	2.54942600	0.56485200	-2.38487500
H	2.94041400	-2.53503000	1.37480200
H	5.39648500	-1.00048000	1.76486500
H	1.90058400	-1.49971600	-0.41282800
H	5.19887700	-2.51079800	0.89244100
C	2.00649700	1.10616400	1.62749800
C	0.59267400	0.79385700	-0.02383800
N	1.11464800	2.04379500	1.77062600
N	1.73673100	0.32679500	0.52853600
N	0.25223300	1.84459900	0.72268600
C	3.10204200	0.70151500	2.54746600
H	4.07417000	0.99687500	2.13497600
H	2.96886000	1.20715700	3.50444900
C	-0.90836500	2.65660900	0.52173000
C	-0.94391100	3.47869700	-0.60793600
C	-1.97588300	2.52582400	1.41345400
C	-2.11430300	4.19747400	-0.83487400
C	-3.12595900	3.26503900	1.13851600
C	-3.21369300	4.09632300	0.02076600
H	-2.17231700	4.84644700	-1.70529500
H	-3.97838800	3.17691300	1.80700100
C	0.22872900	3.56092600	-1.55026300
H	1.17314700	3.64526100	-1.00522500
H	0.28929200	2.66575200	-2.17912500
H	0.12881800	4.42584800	-2.20763000
C	-4.47638300	4.86060400	-0.28064000
H	-4.26292800	5.92088500	-0.44112700
H	-4.94585900	4.48080700	-1.19306900
H	-5.19818400	4.77345600	0.53347300
C	-1.89699100	1.59318500	2.59427300
H	-1.55008600	0.60016300	2.28583200
H	-1.19246600	1.96603500	3.34392300

H	-2.87791200	1.48614100	3.06044700
H	0.12357000	-2.09707800	0.47857700
H	-1.97975100	0.36572500	0.09620100
C	-3.22232900	-2.24847800	-0.46729300
C	-3.82009400	-3.09195300	0.47807700
C	-3.98031500	-1.82061000	-1.56215700
C	-5.12820800	-3.53102100	0.31202200
H	-3.25673500	-3.39081500	1.35549900
C	-5.28838100	-2.26655100	-1.73338800
H	-3.52800500	-1.14225000	-2.27998800
C	-5.86375200	-3.12779400	-0.80077800
H	-5.57596500	-4.18375300	1.05481500
H	-5.86107500	-1.94010700	-2.59581700
H	-6.88377900	-3.47378500	-0.93458300
Cl	-0.80006500	-4.25544600	0.48074800
C	3.00669600	-0.82868300	2.66873600
H	2.00363400	-1.09161400	3.02163000
H	3.71848000	-1.19480100	3.41263200

Coordinates of stationary points of IRC points involved in *Z*-TS1[D]

IRC-R-46

C	-0.44047700	-0.58667700	0.41593300
C	-1.56990700	0.41470400	0.57822000
C	-2.43829300	-0.80556800	0.15685700
C	-1.25540700	-1.66608700	0.28997000
H	-1.73093900	0.78841200	1.58968100
H	-1.08920300	-2.73224700	0.21283400
O	-3.55395200	-0.90783700	-0.28077700
C	0.99217400	-0.39195700	0.28394100
C	1.59502400	0.83243100	0.59760700
C	1.76455200	-1.42949800	-0.25788200
C	2.95535900	1.01142800	0.36908800
H	0.99638900	1.63972100	1.00891900
C	3.11925900	-1.24511600	-0.48779900
H	1.28853500	-2.36878300	-0.52242200
C	3.71423600	-0.02148400	-0.17839000
H	3.42272700	1.96081200	0.60733800
H	3.71005700	-2.04630700	-0.91864500
H	4.77179600	0.12877300	-0.36939200
Cl	-1.59535600	1.82585600	-0.52493100

IRC-R-15

C	-0.50331300	-0.48882200	0.49140400
C	-1.67216100	0.45340300	0.48014900
C	-2.43279100	-0.98155100	0.10616600
C	-1.22573000	-1.63228800	0.59085900
H	-1.97301000	0.77676400	1.47453100
H	-0.97448600	-2.66422900	0.80000200
O	-3.41334800	-1.34590100	-0.48215500
C	0.91433400	-0.30113200	0.26012200
C	1.58389500	0.89230500	0.54807800
C	1.61046700	-1.38018100	-0.30388800
C	2.95192200	0.97981900	0.31802300
H	1.03997100	1.73028200	0.97109700
C	2.97372900	-1.28644700	-0.53197900
H	1.06860700	-2.28165700	-0.57122100
C	3.64543500	-0.10693500	-0.21277000
H	3.48113800	1.89629800	0.55541100
H	3.51161700	-2.12359700	-0.96365100
H	4.71340200	-0.02971300	-0.38885900
Cl	-1.44411700	2.01519900	-0.43278400

IRC-R-13

C	-0.50902300	-0.48000200	0.49168300
C	-1.66279600	0.46715200	0.48092000
C	-2.43813300	-1.01557300	0.10485000
C	-1.22345800	-1.63146100	0.60377200
H	-1.97498800	0.78225200	1.47405800
H	-0.95818900	-2.65190100	0.85005000
O	-3.41739400	-1.36750400	-0.49146000
C	0.90876900	-0.29841500	0.25243900
C	1.58161000	0.89267800	0.54360500
C	1.60500000	-1.37932200	-0.30791800
C	2.95027600	0.97838200	0.31792800
H	1.03873100	1.73065000	0.96786300

C	2.96973800	-1.28779200	-0.53110200
H	1.06275100	-2.28036700	-0.57619300
C	3.64314600	-0.10919400	-0.21211300
H	3.48018700	1.89360100	0.55853000
H	3.50754600	-2.12672200	-0.95940700
H	4.71163500	-0.03419300	-0.38599600
Cl	-1.43511100	2.02886600	-0.42928400

IRC-R-11

C	-0.51501500	-0.46960700	0.49270500
C	-1.64593900	0.48624300	0.48521600
C	-2.44209700	-1.05730600	0.10252700
C	-1.22258100	-1.63178900	0.61343100
H	-1.98739700	0.78342900	1.47406100
H	-0.94690900	-2.63849200	0.90206400
O	-3.42433800	-1.37928500	-0.50025100
C	0.90382900	-0.29625500	0.24499800
C	1.58015500	0.89248600	0.54036400
C	1.60112400	-1.37877400	-0.31067700
C	2.94923700	0.97738200	0.31811000
H	1.03793000	1.73023700	0.96594500
C	2.96728400	-1.28860200	-0.53010500
H	1.05892500	-2.27987100	-0.57926300
C	3.64187400	-0.11051900	-0.21193800
H	3.47943100	1.89170200	0.56146100
H	3.50519600	-2.12894800	-0.95550700
H	4.71065600	-0.03684200	-0.38467900
Cl	-1.42915400	2.03855800	-0.42703900

IRC-R-10

C	-0.51814300	-0.46401400	0.49323200
C	-1.63584100	0.49652800	0.48796700
C	-2.44340500	-1.07941900	0.10121800
C	-1.22302100	-1.63220800	0.61714600
H	-1.99990000	0.78079900	1.47236200
H	-0.94438800	-2.63174200	0.92734700
O	-3.42782900	-1.38222200	-0.50397800
C	0.90164300	-0.29531200	0.24144500
C	1.57967700	0.89229100	0.53914900
C	1.59964300	-1.37855400	-0.31166900
C	2.94889500	0.97701000	0.31823100
H	1.03763900	1.72990300	0.96530800
C	2.96647200	-1.28886400	-0.52964300
H	1.05751800	-2.27977500	-0.58021400
C	3.64150400	-0.11096700	-0.21195000
H	3.47916400	1.89098700	0.56271200
H	3.50445200	-2.12979000	-0.95382700
H	4.71038300	-0.03773200	-0.38434100
Cl	-1.42704600	2.04217700	-0.42623000

IRC-1

C	-0.60784100	-0.38935800	0.48214200
C	-1.60812700	0.59993400	0.50123800
C	-2.51443000	-1.23095700	0.07944100
C	-1.30685500	-1.60995700	0.61872800
H	-2.26604000	0.71699800	1.34973700
H	-1.03686300	-2.55597400	1.07162300

O	-3.50914100	-1.35039000	-0.53309700
C	0.82517500	-0.26322600	0.20429100
C	1.51398300	0.91595800	0.52049700
C	1.52789800	-1.35115900	-0.32875600
C	2.88351000	1.00077400	0.30504000
H	0.97320000	1.75264100	0.95077200
C	2.89903300	-1.26363600	-0.54049100
H	0.98689200	-2.25466600	-0.59381800
C	3.57655900	-0.08717300	-0.22599100
H	3.41394800	1.91334700	0.55514000
H	3.43715700	-2.10810100	-0.95787100
H	4.64605900	-0.01622300	-0.39582000
Cl	-1.48321500	2.08399400	-0.43599000

IRC-F-5

C	-0.55131800	-0.39705900	0.49729900
C	-1.51128100	0.60148400	0.52504900
C	-2.45123900	-1.32297700	0.08670400
C	-1.25225400	-1.63626800	0.63878500
H	-2.28468500	0.64580600	1.28086500
H	-0.98325800	-2.56843700	1.11905700
O	-3.44865000	-1.36979200	-0.52132800
C	0.88579400	-0.28627000	0.21004300
C	1.57853700	0.88943800	0.53247200
C	1.58995900	-1.37573600	-0.31669000
C	2.94813200	0.97436900	0.31827500
H	1.03930200	1.72529100	0.96646000
C	2.96243700	-1.28888000	-0.52664000
H	1.05010500	-2.28099700	-0.57858300
C	3.64137500	-0.11325600	-0.21301700
H	3.47856400	1.88633000	0.57110500
H	3.50029400	-2.13478400	-0.94178100
H	4.71121200	-0.04357700	-0.38119900
Cl	-1.41603400	2.06362100	-0.42155700

IRC-F-10

C	-0.56277900	-0.37145000	0.50103600
C	-1.46839800	0.64559200	0.54099900
C	-2.45975100	-1.44167700	0.07569300
C	-1.26730100	-1.63566300	0.65004700
H	-2.37927500	0.58475000	1.12230100
H	-0.98111400	-2.54796100	1.15568800
O	-3.45456700	-1.36457300	-0.52172900
C	0.87894300	-0.28213200	0.20176400
C	1.57874300	0.88836600	0.52990400
C	1.58479300	-1.37339100	-0.31882200
C	2.94844400	0.97294400	0.31699200
H	1.04323300	1.72284100	0.97114500
C	2.95911200	-1.28806800	-0.52633800
H	1.04740100	-2.28205400	-0.57422400
C	3.64171400	-0.11450300	-0.21379500
H	3.47888900	1.88382600	0.57430100
H	3.49588000	-2.13711300	-0.93692900
H	4.71236500	-0.04817300	-0.37798600
Cl	-1.40870900	2.07795400	-0.42039700

IRC-F-15

C	-0.57934700	-0.35431700	0.50197000
C	-1.45519500	0.67900400	0.53976000
C	-2.46353800	-1.55255300	0.06384500
C	-1.27712400	-1.64014300	0.66478200
H	-2.42406000	0.57266200	1.00995000
H	-0.93655000	-2.53484100	1.16696700
O	-3.45807500	-1.39299600	-0.51632800
C	0.86772500	-0.27754500	0.20054400
C	1.57699700	0.88839000	0.52804500
C	1.57349300	-1.36914600	-0.32081700
C	2.94724000	0.97032000	0.31427800
H	1.04812500	1.72401300	0.97502800
C	2.94925700	-1.28790600	-0.52731700
H	1.03717400	-2.27932100	-0.57303900
C	3.63877000	-0.11831600	-0.21538800
H	3.47874900	1.87976200	0.57467100
H	3.48214500	-2.14088700	-0.93496300
H	4.71023700	-0.05764400	-0.37627800
Cl	-1.38761700	2.11259400	-0.41764200

IRC-F-25

C	-0.61164900	-0.32837100	0.47803500
C	-1.48210100	0.70505600	0.47118200
C	-2.45532300	-1.65140200	0.07252400
C	-1.27285700	-1.63494600	0.67720200
H	-2.48464300	0.59452400	0.86326200
H	-0.87840600	-2.49097900	1.20611400
O	-3.46092900	-1.54861400	-0.50143400
C	0.84302800	-0.26151100	0.20179900
C	1.56601500	0.89458700	0.53192200
C	1.53721600	-1.35906700	-0.32280100
C	2.93694800	0.96174600	0.31461300
H	1.05037700	1.73654700	0.98144800
C	2.91303400	-1.29283800	-0.53253500
H	0.99155700	-2.26281400	-0.57730500
C	3.61619800	-0.13177500	-0.22011500
H	3.47818400	1.86503900	0.57639300
H	3.43478700	-2.15094000	-0.94380000
H	4.68768300	-0.08169300	-0.38438600
Cl	-1.31826300	2.19515300	-0.39411100

IRC-F-40

C	-0.65240700	-0.28173100	0.42992900
C	-1.51430400	0.75156600	0.36116100
C	-2.45285300	-1.75983100	0.09083400
C	-1.27825500	-1.59830300	0.68090400
H	-2.54729200	0.64696200	0.66534500
H	-0.83789400	-2.39246100	1.26769000
O	-3.47071200	-1.81641100	-0.46849300
C	0.81158800	-0.23043800	0.19627300
C	1.55724600	0.90434400	0.54628100
C	1.48352700	-1.33659200	-0.33880400
C	2.92998400	0.94336000	0.33129200
H	1.06215400	1.75221400	1.00597000
C	2.85958200	-1.29790100	-0.54754800
H	0.91886200	-2.22470600	-0.60557800
C	3.58594500	-0.15546700	-0.22065000

H	3.49050300	1.83075000	0.60663000
H	3.36297300	-2.16137000	-0.97018100
H	4.65796800	-0.12439900	-0.38610100
Cl	-1.22029700	2.30113300	-0.35716100

IRC-F-50

C	-0.67773700	-0.24581300	0.39621200
C	-1.52697500	0.79304200	0.30049800
C	-2.45265400	-1.82147800	0.10307100
C	-1.28875100	-1.56379600	0.67499800
H	-2.57403000	0.69803200	0.55947900
H	-0.82367200	-2.32000400	1.29376700
O	-3.46986700	-2.00176300	-0.43087200
C	0.79130800	-0.20732700	0.18602800
C	1.55486500	0.90492800	0.56651800
C	1.44579900	-1.31405200	-0.36886800
C	2.92994900	0.92119100	0.36164000
H	1.07270400	1.75231100	1.04017600
C	2.82290400	-1.29741800	-0.56957600
H	0.86587500	-2.18544300	-0.65693900
C	3.56839800	-0.17677100	-0.21192700
H	3.50575000	1.79109400	0.66037200
H	3.31223300	-2.16048200	-1.00913900
H	4.64180000	-0.16205400	-0.37050100
Cl	-1.16283800	2.36455400	-0.34237900