

Supplementary Information

Origins of Reversal Diastereoselectivity of α,β -Dichloro- γ -butenolides and γ -Butyrolactams in Direct Vinylogous Aldol Addition: A Computational Study

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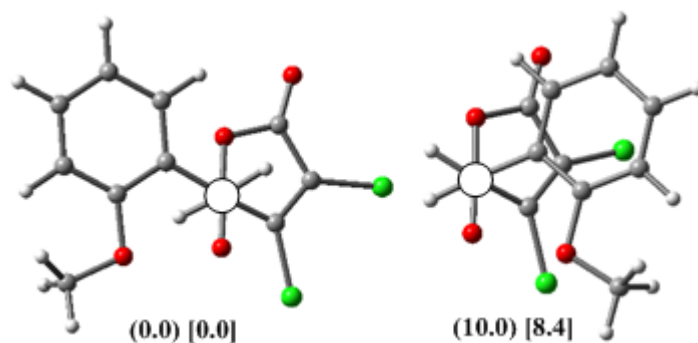


Figure S1 B3LYP/cc-pVDZ optimized transition state geometries of *syn* (left) and *anti* (right) aldol products of γ -butenolides in solvent phase (methanol) along with the corresponding Gibb's free energies () and electronic energies with ZPVE correction [].

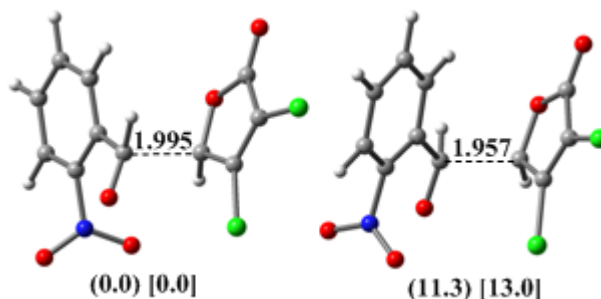


Figure S2 B3LYP/cc-pVDZ optimized transition state geometries of *syn* (left) and *anti* (right) aldol products of γ -butenolides in solvent phase (methanol) along with the corresponding Gibb's free energies () and electronic energies with ZPVE correction [].

Table S1 Difference of distortion energies between *syn* and *anti* transition state geometries studied (given in kJ/mol).

Difference between	Difference in distortion energies
1S & 1A	0.8
2S & 2A	1.3
3S & 3A	0.4
4S & 4A	16.8
5S & 5A	-11.9
6S & 6A	-13.9
7S & 7A	6.3

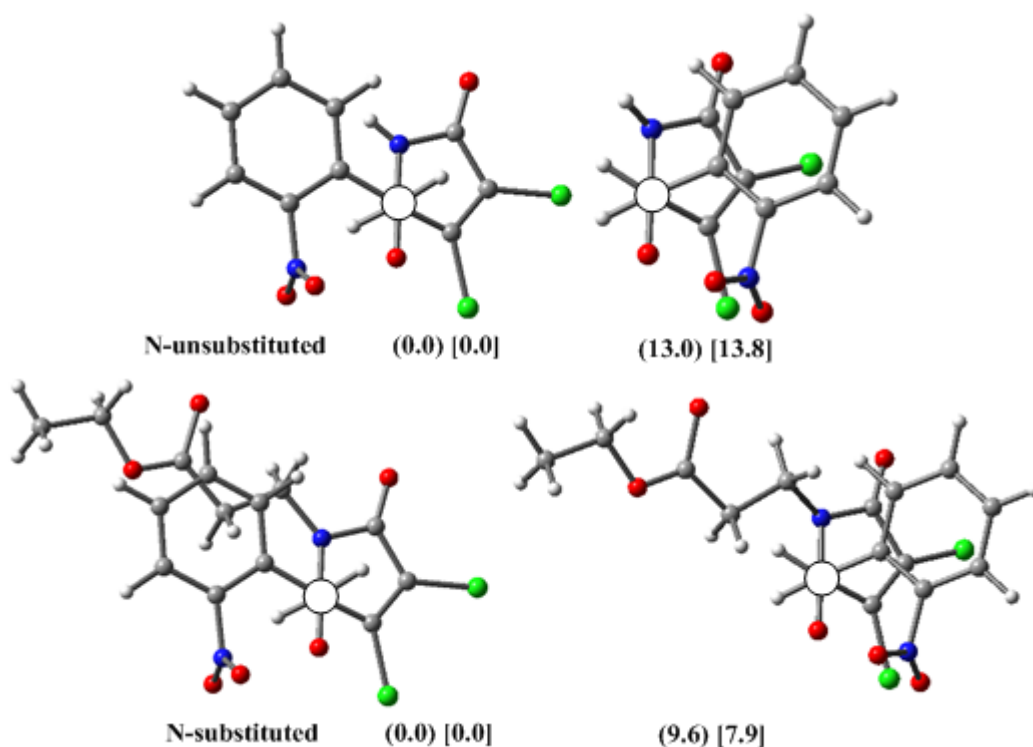


Figure S3 B3LYP/cc-pVDZ optimized transition state geometries of *syn* (left) and *anti* (right) aldol products of γ -butyrolactams in solvent phase (methanol) along with the corresponding Gibb's free energies () and electronic energies with ZPVE correction [].

Cartesian coordinates of all optimized stationary points, including all the thermodynamic data generated from frequency calculation at B3LYP/cc-pVDZ in methanol solvent phase and imaginary frequencies of all transition states geometries.

1A

Zero-point correction= 0.153306 (Hartree/Particle)
 Thermal correction to Energy= 0.166862
 Thermal correction to Enthalpy= 0.167807
 Thermal correction to Gibbs Free Energy= 0.111057
 Sum of electronic and zero-point Energies= -1569.460136
 Sum of electronic and thermal Energies= -1569.446579
 Sum of electronic and thermal Enthalpies= -1569.445635
 Sum of electronic and thermal Free Energies= -1569.502385
 1 Imaginary frequency = -228.3 cm^{-1}
 Charge = -1, Multiplicity = 1

C	1.29782600	0.83162300	-0.01852900
C	1.70543200	-0.47153100	-0.10159800
Cl	2.32875100	-1.33216100	-1.47204900
Cl	1.36253300	2.01819400	-1.27169600
C	1.50180700	-1.09064600	1.20019800
O	1.70802900	-2.22491900	1.59602500

O	0.97609300	-0.11419900	2.02160400
C	-1.13233800	1.48195200	1.25253200
O	-1.29950100	2.68874800	0.87633500
C	0.72449300	1.07851000	1.28118300
H	1.04476600	1.96840300	1.83114200
H	-1.22282000	1.23123900	2.34720400
C	-1.75444000	0.35597600	0.43578300
C	-1.89229300	-0.94669200	0.94010200
C	-2.24779600	0.63578900	-0.84764900
C	-2.49449200	-1.95083700	0.17298100
H	-1.53107600	-1.17377900	1.94644400
C	-2.84951600	-0.36288400	-1.61748400
H	-2.15805000	1.66097600	-1.21167100
C	-2.97301300	-1.66334500	-1.11050900
H	-2.59625300	-2.96023600	0.58049800
H	-3.23191400	-0.12845200	-2.61492100
H	-3.44746600	-2.44523400	-1.70878700

2A

Zero-point correction= 0.151923 (Hartree/Particle)
Thermal correction to Energy= 0.167332
Thermal correction to Enthalpy= 0.168276
Thermal correction to Gibbs Free Energy= 0.106863
Sum of electronic and zero-point Energies= -1661.718455
Sum of electronic and thermal Energies= -1661.703046
Sum of electronic and thermal Enthalpies= -1661.702102
Sum of electronic and thermal Free Energies= -1661.763515
1 Imaginary frequency = -230.3 cm⁻¹
Charge = -1, Multiplicity = 1

C	1.91125000	0.14484700	-0.38862600
C	1.65865800	-1.16963500	-0.10123500
Cl	1.43928500	-2.49946300	-1.19131500
Cl	2.15013800	0.83823400	-1.95162000
C	1.56383900	-1.30385700	1.34456200
O	1.34488400	-2.26899100	2.05512100
O	1.76706200	-0.04080800	1.87015300
C	0.45169700	2.22170000	0.89887300
O	0.74415500	3.21700300	0.16738100
C	1.88683700	0.91707100	0.82545300
H	2.69142100	1.63250000	1.01623400
H	0.56812200	2.29553700	2.01406900
C	-0.77945800	1.39440200	0.57188800
C	-1.31867200	0.46139900	1.47318300
C	-1.42364000	1.59949600	-0.65904000
C	-2.46268100	-0.26578100	1.15003500
H	-0.83941000	0.30751300	2.44213200
C	-2.56699100	0.88371900	-0.99859100
H	-1.00324300	2.34969500	-1.33015300
C	-3.09390300	-0.05951800	-0.09229600
H	-2.87701300	-0.98927200	1.85426600
H	-3.06496600	1.04963100	-1.95580000
C	-4.27568400	-0.79951800	-0.42896400
N	-5.23591900	-1.40118600	-0.70336300

3A

Zero-point correction= 0.185419 (Hartree/Particle)
Thermal correction to Energy= 0.201606
Thermal correction to Enthalpy= 0.202550
Thermal correction to Gibbs Free Energy= 0.139737
Sum of electronic and zero-point Energies= -1683.958359
Sum of electronic and thermal Energies= -1683.942172
Sum of electronic and thermal Enthalpies= -1683.941228
Sum of electronic and thermal Free Energies= -1684.004041
1 Imaginary frequency = -231.2 cm⁻¹
Charge = -1, Multiplicity =1

C	-1.53429800	-1.02207000	0.07968400
C	-2.02642100	-0.02445000	-0.71678500
Cl	-2.10573100	0.04763600	-2.44766700
Cl	-0.90886600	-2.54648600	-0.43788900
C	-2.47959200	1.05725200	0.14547400
O	-2.97651800	2.14055900	-0.11068600
O	-2.24048300	0.65140200	1.44289700
C	0.18525400	-0.39975300	2.23070700
O	0.64351400	-1.54999600	2.53482500
C	-1.54680300	-0.59360500	1.45541100
H	-1.95069900	-1.27313300	2.21151400
H	-0.23331700	0.25680000	3.04323400
C	0.94981000	0.46513700	1.23590100
C	0.69104100	1.83216400	1.07257800
C	1.97387400	-0.14151600	0.49116700
C	1.44511100	2.57982400	0.15733600
H	-0.09187500	2.31299100	1.66281200
C	2.72306100	0.60689200	-0.42307900
H	2.15672200	-1.19874300	0.67946800
C	2.45487400	1.97814000	-0.59223900
H	1.24632300	3.64713700	0.02866700
O	3.73876100	0.10303300	-1.19058000
C	4.04901300	-1.28014300	-1.06140300
H	4.87032700	-1.47319400	-1.76374700
H	4.37871200	-1.52981400	-0.03790000
H	3.18645100	-1.91679500	-1.32389500
H	3.05377100	2.54798400	-1.30585000

4A

Zero-point correction= 0.197718 (Hartree/Particle)
Thermal correction to Energy= 0.218694
Thermal correction to Enthalpy= 0.219638
Thermal correction to Gibbs Free Energy= 0.144941
Sum of electronic and zero-point Energies= -2001.825197
Sum of electronic and thermal Energies= -2001.804221
Sum of electronic and thermal Enthalpies= -2001.803277
Sum of electronic and thermal Free Energies= -2001.877974
1 Imaginary frequency = -229.6 cm⁻¹
Charge = -1, Multiplicity =1

C	-2.52061700	-0.13534100	0.52818200
C	-2.30104700	-1.48627500	0.48561900

Cl	-1.87236700	-2.55975900	1.77615200
Cl	-2.50834700	0.87103400	1.92980000
C	-2.47192000	-1.92760400	-0.89007900
O	-2.37026500	-3.02519200	-1.40764700
O	-2.78836200	-0.79935600	-1.62702200
C	-1.37336000	1.62070400	-1.47538900
O	-1.59245800	2.77041600	-0.99521500
C	-2.73297400	0.35928200	-0.80592900
H	-3.56787100	1.03879700	-0.99580700
H	-1.68375200	1.37403800	-2.52385400
C	-0.06412100	0.92641900	-1.16099200
C	0.29200700	-0.29799500	-1.75621000
C	0.86669600	1.48752500	-0.27340100
C	1.48476300	-0.94298400	-1.44416200
H	-0.39036000	-0.74391600	-2.48067700
C	2.06083400	0.85798600	0.06478300
C	2.37706700	-0.37500500	-0.52134600
H	1.74414300	-1.89442200	-1.90955700
H	2.75102400	1.32836000	0.76394100
N	0.67635000	2.83199000	0.32696700
O	1.04243600	3.79226100	-0.33768200
O	0.30418900	2.88379500	1.49255200
C	3.64082600	-1.10061200	-0.20924400
O	3.95896600	-2.16598300	-0.70606600
O	4.40062000	-0.44700600	0.69041300
C	5.64101600	-1.08501100	1.04886700
H	6.11659700	-0.41593800	1.77483400
H	5.45143100	-2.07018300	1.49928200
H	6.28044600	-1.21037000	0.16302000

5A

Zero-point correction= 0.294950 (Hartree/Particle)
Thermal correction to Energy= 0.320074
Thermal correction to Enthalpy= 0.321018
Thermal correction to Gibbs Free Energy= 0.234589
Sum of electronic and zero-point Energies= -2099.819195
Sum of electronic and thermal Energies= -2099.794070
Sum of electronic and thermal Enthalpies= -2099.793126
Sum of electronic and thermal Free Energies= -2099.879556
1 Imaginary frequency = -192.7 cm⁻¹
Charge = -1, Multiplicity = 1

C	-0.44744300	1.91889400	0.24034000
C	-0.52030400	1.69764400	-1.10234700
Cl	-1.53461700	2.47803300	-2.27448600
Cl	-1.31850500	3.12100400	1.13217200
C	0.43174900	0.63126900	-1.46309600
O	0.68318500	0.14770500	-2.57142300
C	-0.44942000	-0.13547400	2.11707700
O	-0.60049500	0.50338000	3.21402100
C	0.44890500	0.95277200	0.86511300
H	1.18099900	1.35108400	1.57731000
H	0.32906000	-0.94773000	2.06777000
C	-1.68706600	-0.61177800	1.37242200
C	-1.63014200	-1.55623600	0.33122900

C	-2.94172800	-0.11686700	1.76970100
C	-2.78828000	-1.97928500	-0.31701800
H	-0.66888800	-1.97816500	0.03176400
C	-4.11038600	-0.52589600	1.13669200
H	-2.96093200	0.58946300	2.60020000
C	-4.01928500	-1.45434000	0.09210600
H	-2.75711000	-2.70915300	-1.12457000
H	-5.08788500	-0.14941800	1.43549000
N	-5.24113800	-1.89543100	-0.58039100
O	-6.31547400	-1.42744800	-0.20254900
O	-5.14096900	-2.71301900	-1.49556400
N	1.01216100	0.26120300	-0.26199400
C	2.10898300	-0.68653200	-0.18786700
H	1.99471000	-1.30537700	0.71363700
H	2.02758400	-1.34830900	-1.06107500
C	3.47946400	0.00027800	-0.18176000
H	3.62840400	0.58421100	-1.10466100
H	3.56116300	0.71866000	0.65110500
C	4.61677700	-0.98905600	-0.05584500
O	4.48652100	-2.19229900	0.06261600
O	5.80908200	-0.36695000	-0.08777600
C	6.98496000	-1.21050200	0.03279800
H	6.99105400	-1.92725400	-0.80341000
H	6.91179500	-1.78554400	0.96901700
C	8.19770100	-0.30382100	0.01377500
H	8.17112900	0.40789600	0.85369800
H	9.11366200	-0.90860200	0.10188200
H	8.24946700	0.26684300	-0.92664300

6A

Zero-point correction= 0.305485 (Hartree/Particle)
Thermal correction to Energy= 0.329335
Thermal correction to Enthalpy= 0.330280
Thermal correction to Gibbs Free Energy= 0.246334
Sum of electronic and zero-point Energies= -2063.665318
Sum of electronic and thermal Energies= -2063.641468
Sum of electronic and thermal Enthalpies= -2063.640523
Sum of electronic and thermal Free Energies= -2063.724469
1 Imaginary frequency = -196.3 cm⁻¹
Charge = -1, Multiplicity = 1

C	-0.68676000	2.07328300	0.11956000
C	-0.70298300	1.74837900	-1.20431800
Cl	-1.77818000	2.31365200	-2.44438500
Cl	-1.71536100	3.22239500	0.90829400
C	0.37823700	0.78243100	-1.47126900
O	0.71614000	0.25748700	-2.53761100
C	-0.49205400	0.17754900	2.15017000
O	-0.75960500	0.88012600	3.18329800
C	0.30384700	1.26966300	0.82545300
H	0.96885700	1.80064400	1.51642600
H	0.38686200	-0.52533100	2.18589300
C	-1.63289500	-0.51688100	1.42377300
C	-1.42132000	-1.52028300	0.46067600
C	-2.95290100	-0.17092400	1.76266800

C	-2.49404800	-2.14797200	-0.16798700
H	-0.40388000	-1.82514500	0.20882000
C	-4.03853700	-0.78511100	1.14783000
H	-3.08822800	0.58660100	2.53526800
C	-3.79524300	-1.76956600	0.18189000
H	-2.34317400	-2.92648200	-0.91423400
H	-5.06553000	-0.52680700	1.40293800
N	-4.92784700	-2.42978900	-0.46693700
O	-6.06549600	-2.08530900	-0.14574500
O	-4.69332700	-3.29955800	-1.30637400
N	0.96795200	0.56815500	-0.23766300
C	2.18640900	-0.20715800	-0.08591800
H	2.18105000	-0.68490600	0.90527100
H	2.16889900	-1.00238800	-0.84614200
C	3.46574800	0.64194900	-0.25786200
H	3.43790800	1.10643600	-1.25631100
H	3.45739300	1.45569400	0.48510900
C	4.72285300	-0.18517500	-0.10561500
C	5.35282400	-0.31930300	1.14271300
C	5.26830600	-0.87083800	-1.20418800
C	6.49524600	-1.11273400	1.29046700
H	4.94638300	0.21046600	2.00883000
C	6.41003900	-1.66546800	-1.06112700
H	4.79513700	-0.77496700	-2.18552600
C	7.02818100	-1.78935300	0.18808500
H	6.97295100	-1.19907600	2.26947600
H	6.82106700	-2.18626300	-1.92942600
H	7.92236500	-2.40672900	0.30081000

7A

Zero-point correction= 0.168120 (Hartree/Particle)
Thermal correction to Energy= 0.184554
Thermal correction to Enthalpy= 0.185498
Thermal correction to Gibbs Free Energy= 0.121499
Sum of electronic and zero-point Energies= -1754.109467
Sum of electronic and thermal Energies= -1754.093033
Sum of electronic and thermal Enthalpies= -1754.092089
Sum of electronic and thermal Free Energies= -1754.156087
1 Imaginary frequency = -210.1 cm⁻¹
Charge = -1, Multiplicity = 1

C	-2.10607600	0.12406300	0.49629600
C	-1.89545000	-1.19661000	0.22543000
Cl	-1.52051600	-2.48212600	1.33016900
Cl	-2.15918900	0.85900100	2.06541500
C	-1.98823400	-1.40600700	-1.23423600
O	-1.82907500	-2.43944700	-1.88885200
C	-0.90337500	2.19797100	-1.00777300
O	-1.17671300	3.24310100	-0.33148200
C	-2.26244700	0.87852500	-0.73873200
H	-3.08969000	1.59576800	-0.77995900
H	-1.07603200	2.20413000	-2.12105600
C	0.38260400	1.44639800	-0.71083500
C	0.91467900	0.47786700	-1.58131000
C	1.08696900	1.75981200	0.46546600

C	2.10289700	-0.18295200	-1.27832100
H	0.39873900	0.24530900	-2.51484200
C	2.27471100	1.11254300	0.78704900
H	0.67107200	2.53675400	1.10770900
C	2.76979100	0.14040300	-0.09130800
H	2.52479300	-0.93456000	-1.94384300
H	2.82850100	1.34654500	1.69533100
N	4.02121400	-0.54417800	0.23267300
O	4.59341900	-0.24634300	1.28142500
O	4.44552300	-1.38871200	-0.55646900
N	-2.29306600	-0.15440000	-1.72844600
H	-2.32107400	0.02834400	-2.72520200

1S

Zero-point correction=	0.153028 (Hartree/Particle)
Thermal correction to Energy=	0.166705
Thermal correction to Enthalpy=	0.167649
Thermal correction to Gibbs Free Energy=	0.110055
Sum of electronic and zero-point Energies=	-1569.460595
Sum of electronic and thermal Energies=	-1569.446918
Sum of electronic and thermal Enthalpies=	-1569.445974
Sum of electronic and thermal Free Energies=	-1569.503568
1 Imaginary frequency =	-237.1 cm ⁻¹
Charge = -1, Multiplicity =	1

C	-1.63523300	0.60803200	-0.39865600
C	-2.35504100	-0.51802400	-0.09947400
Cl	-4.00889900	-0.64932600	0.40584900
Cl	-2.21508100	2.23240500	-0.40729500
C	-1.48198300	-1.66907700	-0.27081900
O	-1.67637300	-2.86278600	-0.11323600
O	-0.25991500	-1.17557000	-0.67883800
C	0.81864200	0.82054600	0.83052600
C	2.18148400	0.26245600	0.41480500
C	3.14331900	1.14849700	-0.09267800
C	2.52561300	-1.08969700	0.56572400
C	4.41316900	0.69558700	-0.46123600
H	2.86729200	2.20215400	-0.17258600
C	3.79807400	-1.54733300	0.20621700
H	1.78956900	-1.78910000	0.96930600
C	4.74588800	-0.65697700	-0.31319200
H	5.15140900	1.39859900	-0.85716800
H	4.05333700	-2.60280400	0.33390200
H	5.73983700	-1.01414400	-0.59420400
H	0.31870200	0.10599000	1.54575500
O	0.71995200	2.07473700	1.02319500
C	-0.26060500	0.24864800	-0.63936000
H	0.25824500	0.67996600	-1.50052100

2S

Zero-point correction=	0.151711 (Hartree/Particle)
Thermal correction to Energy=	0.167204
Thermal correction to Enthalpy=	0.168148
Thermal correction to Gibbs Free Energy=	0.106287

Sum of electronic and zero-point Energies= -1661.718807
Sum of electronic and thermal Energies= -1661.703315
Sum of electronic and thermal Enthalpies= -1661.702370
Sum of electronic and thermal Free Energies= -1661.764232
1 Imaginary frequency = -234.5 cm⁻¹
Charge = -1, Multiplicity =1

C	-2.20936900	0.51830800	-0.46538000
C	-2.87875900	-0.63232000	-0.13868800
Cl	-4.54475800	-0.83400800	0.29670400
Cl	-2.87199500	2.10551500	-0.58467600
C	-1.93539500	-1.73661700	-0.20635300
O	-2.06662700	-2.93002600	0.00598300
O	-0.72179200	-1.19096600	-0.58253400
C	0.14478900	0.94758100	0.92282700
C	1.56064100	0.50397800	0.56627800
C	2.46676200	1.47473300	0.11020000
C	2.00529500	-0.81929500	0.72229200
C	3.77958300	1.13980700	-0.20714600
H	2.10822300	2.50217500	0.02785100
C	3.31816000	-1.17211600	0.41780500
H	1.31452200	-1.58123100	1.08726200
C	4.21423900	-0.19235600	-0.05461900
H	4.47808900	1.89899900	-0.56409600
H	3.65955100	-2.20091600	0.54507900
H	-0.33777800	0.19734100	1.60769200
O	-0.07115100	2.18561100	1.08148000
C	-0.81131300	0.22670600	-0.62557300
H	-0.26187400	0.65217800	-1.46976000
C	5.56735200	-0.54847300	-0.37068700
N	6.66695900	-0.83724600	-0.62909600

3S

Zero-point correction= 0.185109 (Hartree/Particle)
Thermal correction to Energy= 0.201416
Thermal correction to Enthalpy= 0.202360
Thermal correction to Gibbs Free Energy= 0.138562
Sum of electronic and zero-point Energies= -1683.958638
Sum of electronic and thermal Energies= -1683.942331
Sum of electronic and thermal Enthalpies= -1683.941387
Sum of electronic and thermal Free Energies= -1684.005185
1 Imaginary frequency = -239.2 cm⁻¹
Charge = -1, Multiplicity =1

C	2.08198900	-0.73242500	-0.36735700
C	3.02043900	0.24772000	-0.18050000
Cl	4.69470500	0.08380000	0.24179100
Cl	2.33479200	-2.43615500	-0.28684400
C	2.37552300	1.53420200	-0.39340200
O	2.80330800	2.67473000	-0.33069200
O	1.05954100	1.26440600	-0.70949200
C	-0.27860300	-0.38592800	0.99895700
C	-1.55906700	0.34941300	0.59307400
C	-2.67219600	-0.43249000	0.24501400
C	-1.66902500	1.74559300	0.59907800

C	-3.88047800	0.17447900	-0.11600500
H	-2.54699100	-1.51393900	0.29252700
C	-2.88261100	2.35049600	0.24618900
H	-0.80920600	2.35809000	0.87640000
C	-3.98582900	1.57732500	-0.11511200
H	-2.97247800	3.44009800	0.25380500
H	0.37391300	0.29595600	1.61455700
O	-0.36757800	-1.61720600	1.30798300
C	0.79083900	-0.12709700	-0.56938900
H	0.14616700	-0.50126400	-1.36997400
H	-4.93812300	2.03471800	-0.39184400
O	-5.01375600	-0.50528700	-0.47474600
C	-4.95956100	-1.92735400	-0.49579700
H	-5.95411500	-2.26376200	-0.81642300
H	-4.20199400	-2.29515200	-1.20947700
H	-4.73927700	-2.34147900	0.50341100

4S

Zero-point correction=	0.197666 (Hartree/Particle)
Thermal correction to Energy=	0.218695
Thermal correction to Enthalpy=	0.219639
Thermal correction to Gibbs Free Energy=	0.144658
Sum of electronic and zero-point Energies=	-2001.829890
Sum of electronic and thermal Energies=	-2001.808861
Sum of electronic and thermal Enthalpies=	-2001.807917
Sum of electronic and thermal Free Energies=	-2001.882898
1 Imaginary frequency = -230.5 cm ⁻¹	
Charge = -1, Multiplicity =1	

C	-3.13803100	0.30694000	-0.39709900
C	-3.77964700	-0.89723000	-0.23084200
Cl	-5.43613900	-1.19530800	0.18843700
Cl	-3.83481100	1.88041300	-0.26823200
C	-2.81295900	-1.95547900	-0.45632900
O	-2.90842000	-3.17120100	-0.41321900
O	-1.61301600	-1.32909400	-0.75619500
C	-0.79614200	0.59633200	1.08797300
C	0.59526600	0.13126100	0.69734200
C	1.55574000	1.02250000	0.19271300
C	1.02687200	-1.18015100	0.95266100
C	2.88139900	0.66392800	-0.02655700
C	2.34114200	-1.57517900	0.71627400
H	0.30980800	-1.89368500	1.36258500
C	3.28215800	-0.65481800	0.22916700
H	2.66314200	-2.59698100	0.92003500
H	-1.32922200	-0.21511000	1.64787700
O	-0.96085200	1.80856500	1.38994500
C	-1.74518800	0.07253900	-0.61152700
H	-1.17131200	0.64670600	-1.34040100
H	3.59340100	1.39698000	-0.40209000
N	1.19056900	2.40381200	-0.18717000
O	1.79595900	3.31769100	0.36053500
O	0.38165300	2.54914200	-1.09607100
C	4.68294400	-1.11407200	0.00773400
O	5.07290100	-2.24755500	0.22171900

O	5.47740100	-0.13218800	-0.45872000
C	6.85084700	-0.49379800	-0.69834200
H	6.91285100	-1.29420400	-1.44984000
H	7.33470700	0.41777100	-1.06674800
H	7.32737900	-0.83446100	0.23231800

5S

Zero-point correction=	0.294872 (Hartree/Particle)
Thermal correction to Energy=	0.320057
Thermal correction to Enthalpy=	0.321001
Thermal correction to Gibbs Free Energy=	0.233428
Sum of electronic and zero-point Energies=	-2099.816077
Sum of electronic and thermal Energies=	-2099.790892
Sum of electronic and thermal Enthalpies=	-2099.789947
Sum of electronic and thermal Free Energies=	-2099.877520
1 Imaginary frequency = -187.3 cm ⁻¹	
Charge = -1, Multiplicity =1	

C	3.12866600	-0.02022400	-0.49968500
C	3.31028100	0.46013700	0.76072000
Cl	4.79394100	0.67702600	1.63356300
Cl	4.38223300	-0.51905600	-1.58552300
C	1.99474600	0.80483200	1.33452000
O	1.72971300	1.31628600	2.42679000
C	1.42824400	-1.99758700	-1.12873300
C	0.01699100	-2.25976900	-0.61298100
C	-1.03409700	-2.36223900	-1.53972300
C	-0.25590000	-2.47210200	0.75028200
C	-2.33471500	-2.63259000	-1.12457100
H	-0.78822400	-2.23713600	-2.59530800
C	-1.54786000	-2.75102600	1.18738300
H	0.55834700	-2.42444100	1.47729500
C	-2.57721700	-2.82186000	0.24104700
H	-3.15981800	-2.70942300	-1.83149400
H	-1.77348100	-2.91864500	2.23944100
H	2.14841400	-2.39819200	-0.36158800
O	1.65769100	-2.20915200	-2.37177700
C	1.69902400	-0.17259300	-0.78613400
H	1.34343800	0.21145400	-1.74953300
N	-3.93879300	-3.11673000	0.69064600
O	-4.12990200	-3.28997100	1.89420000
O	-4.83115500	-3.17613400	-0.15502500
N	1.08107800	0.43972900	0.36451300
C	-0.29922200	0.89507200	0.41275500
H	-0.64956400	0.80829000	1.45064800
H	-0.91461100	0.22798300	-0.20186200
C	-0.44954300	2.34418600	-0.06479100
H	0.13073000	3.02860300	0.57460500
H	-0.05416000	2.46737900	-1.08740500
C	-1.89163500	2.80009200	-0.06775000
O	-2.84719900	2.09890600	0.20431000
O	-1.99426100	4.09506400	-0.41926500
C	-3.33668400	4.64579400	-0.47417300
H	-3.80078200	4.54227200	0.51920700
H	-3.93167200	4.05317900	-1.18668000

C	-3.21725500	6.09443400	-0.89873900
H	-4.21912300	6.54829000	-0.95208000
H	-2.61550900	6.66915600	-0.17740500
H	-2.74697300	6.17741700	-1.89105600

6S

Zero-point correction= 0.305602 (Hartree/Particle)
Thermal correction to Energy= 0.329473
Thermal correction to Enthalpy= 0.330417
Thermal correction to Gibbs Free Energy= 0.245992
Sum of electronic and zero-point Energies= -2063.662020
Sum of electronic and thermal Energies= -2063.638149
Sum of electronic and thermal Enthalpies= -2063.637205
Sum of electronic and thermal Free Energies= -2063.721629
1 Imaginary frequency = -186.0 cm⁻¹
Charge = -1, Multiplicity = 1

C	3.26969200	0.09288100	-0.49946400
C	3.40286300	0.69803800	0.71194800
Cl	4.85218000	1.01006500	1.61347300
Cl	4.56397900	-0.50618200	-1.48271100
C	2.06476300	1.08639300	1.20126400
O	1.75916900	1.70179300	2.22727500
C	1.60353600	-1.94822000	-1.00987800
C	0.20028100	-2.18833800	-0.46378900
C	-0.84942100	-2.41295100	-1.37017000
C	-0.06551600	-2.26156300	0.91545100
C	-2.14222800	-2.67104500	-0.92370100
H	-0.60748700	-2.39262100	-2.43383200
C	-1.34950900	-2.52349800	1.38469300
H	0.74841200	-2.11776500	1.63000500
C	-2.37822200	-2.72023500	0.45519700
H	-2.96602200	-2.84294800	-1.61528000
H	-1.56935900	-2.58367700	2.44954600
H	2.33283100	-2.27810400	-0.21814600
O	1.83146300	-2.25543400	-2.23365100
C	1.85178300	-0.09898800	-0.82031000
H	1.52755200	0.18584500	-1.82801000
N	-3.73108300	-3.00022200	0.93860500
O	-3.91695300	-3.04791100	2.15451600
O	-4.62235600	-3.17330700	0.10739400
N	1.18843500	0.61626900	0.24218700
C	-0.19309500	1.06845000	0.19000500
H	-0.57540400	1.10142000	1.22082400
H	-0.78313700	0.32746600	-0.36499600
C	-0.34257800	2.46211500	-0.46056300
H	0.25796200	3.18076500	0.11895400
H	0.07507100	2.42690400	-1.47979400
C	-1.78610200	2.91100400	-0.50761800
C	-2.59619400	2.62249200	-1.61856300
C	-2.36333800	3.59000600	0.57875800
C	-3.94218200	3.00176200	-1.64568900
H	-2.16475500	2.09805500	-2.47581500
C	-3.70883500	3.97069500	0.55635400
H	-1.74814600	3.82770900	1.45120300

C	-4.50398200	3.67728400	-0.55697000
H	-4.55322500	2.77155100	-2.52193200
H	-4.13686500	4.50177500	1.41010600
H	-5.55448200	3.97645900	-0.57731700

7S

Zero-point correction= 0.168015 (Hartree/Particle)
Thermal correction to Energy= 0.184533
Thermal correction to Enthalpy= 0.185478
Thermal correction to Gibbs Free Energy= 0.120775
Sum of electronic and zero-point Energies= -1754.109622
Sum of electronic and thermal Energies= -1754.093103
Sum of electronic and thermal Enthalpies= -1754.092159
Sum of electronic and thermal Free Energies= -1754.156862
1 Imaginary frequency = -219.0 cm⁻¹
Charge = -1, Multiplicity = 1

C	2.62047900	-0.50084400	-0.39727300
C	3.16207800	0.73306900	-0.16686400
Cl	4.78411800	1.12786100	0.31237500
Cl	3.46642200	-2.01245900	-0.36380000
C	2.11818200	1.75660900	-0.36009000
O	2.17822500	2.98044000	-0.20472100
C	0.26459500	-1.20367100	0.84997100
C	-1.14871100	-0.71264100	0.56620400
C	-2.04631600	-1.58348500	-0.07683500
C	-1.60598800	0.55530000	0.96994900
C	-3.35459900	-1.19706500	-0.34664400
H	-1.68386800	-2.57772500	-0.34235200
C	-2.91514300	0.96009400	0.71589200
H	-0.93246200	1.22803300	1.50645200
C	-3.77458600	0.07789300	0.05258000
H	-4.05750000	-1.86048200	-0.84874700
H	-3.28263000	1.93658300	1.02769100
H	0.74970500	-0.53981800	1.61640100
O	0.46659500	-2.45781700	0.86734400
C	1.19448900	-0.38538900	-0.65381800
H	0.77589700	-0.98464400	-1.46993900
N	-5.15268400	0.49289200	-0.21649900
O	-5.50484200	1.61402800	0.14903200
O	-5.89486700	-0.29815800	-0.79785900
N	1.01317700	1.03033700	-0.75770000
H	0.10046400	1.46644400	-0.82466600