

# DFT Visualization and Experimental Evidence of BHT-Mg-Catalyzed Copolymerization of Lactides, Lactones and Ethylene Phosphates

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## SUPPORTING INFORMATION

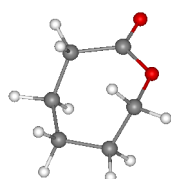
S1. DFT calculations	2
S1.1. Monomers	2
S1.2. LC sequence, binuclear mechanism	5
S1.3. CC sequence, mononuclear mechanism	23
S1.4. PP sequence, mononuclear mechanism	38
S1.5. CP sequence, mononuclear mechanism	49
S1.6. PC sequence, mononuclear mechanism	62
S1.7. LL sequence, mononuclear mechanism	73
S1.8. LP sequence, mononuclear mechanism	84
S1.9. PL sequence, mononuclear mechanism	95
S1.10. Transesterification of PP	110
S2. Polymerization experiments	123

## S1. DFT calculations data: molecular structures, energies and cartesian coordinates

The data for all stationary points and transition states mentioned in the manuscript. Note that the data for monomers (S1.1),  $\epsilon$ -CL and MeOEP homopolymerization (S1.3. and S1.4, respectively) have been published previously [26,46,81].

### S1.1. Monomers

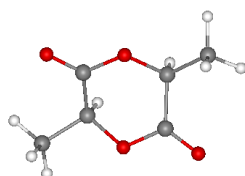
#### $\epsilon$ -CL



Zero-point vibrational energy	413924.6 (Joules/Mol)
	98.93035 (Kcal/Mol)
Zero-point correction=	0.157656 (Hartree/Particle)
Thermal correction to Energy=	0.164853
Thermal correction to Enthalpy=	0.165798
Thermal correction to Gibbs Free Energy=	0.126149
Sum of electronic and zero-point Energies=	-384.860246
Sum of electronic and thermal Energies=	-384.853048
Sum of electronic and thermal Enthalpies=	-384.852104
Sum of electronic and thermal Free Energies=	-384.891753

				cartesian			
8	-2.49640012	0.09650000	-0.41440001	1	0.34410000	1.60000002	-1.28910005
6	-1.36909997	-0.02400000	0.01080000	1	-0.27320001	0.89160001	1.62860000
8	-0.77679998	-1.24290001	-0.07160000	1	-1.30460000	1.95330000	0.67290002
6	-0.58899999	1.13250005	0.60570002	6	1.86199999	0.67570001	-0.04630000
6	0.55019999	-1.48150003	0.42449999	1	0.60909998	-1.21550000	1.48740005
6	0.62889999	1.55929995	-0.23090000	1	1.42149997	-0.92960000	-1.44739997
6	1.64820004	-0.79979998	-0.38229999	1	2.58159995	-1.34459996	-0.19520000
1	0.65160000	-2.56620002	0.35339999	1	2.20040011	0.75480002	0.99610001
1	0.88940001	2.58470011	0.05370000	1	2.67910004	1.06920004	-0.66170001

## L-LA

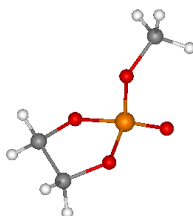


Zero-point vibrational energy	370616.7 (Joules/Mol) 88.57951 (Kcal/Mol)
Zero-point correction=	0.141160 (Hartree/Particle)
Thermal correction to Energy=	0.150579
Thermal correction to Enthalpy=	0.151523
Thermal correction to Gibbs Free Energy=	0.106579
Sum of electronic and zero-point Energies=	-534.087278
Sum of electronic and thermal Energies=	-534.077859
Sum of electronic and thermal Enthalpies=	-534.076915
Sum of electronic and thermal Free Energies=	-534.121860

### cartesian

8	-0.25319999	-1.35280001	-0.11950000	1	-3.39499998	-0.39100000	0.48490000
6	-1.25360000	-0.46730000	0.42940000	1	-2.73480010	-1.02769995	-1.02980006
6	1.03890002	-0.96079999	-0.06110000	1	-2.71370006	-2.03559995	0.43599999
6	-1.03890002	0.96079999	-0.06120000	1	1.14250004	0.46200001	1.52349997
6	-2.61220002	-1.01740003	0.05490000	1	2.71329999	2.03600001	0.43540001
1	-1.14269996	-0.46180001	1.52359998	1	3.39499998	0.39160001	0.48590001
6	1.25360000	0.46730000	0.42940000	1	2.73539996	1.02680004	-1.02960002
6	2.61220002	1.01740003	0.05500000	8	1.92960000	-1.71019995	-0.37459999
8	0.25319999	1.35270000	-0.11990000	8	-1.92960000	1.71029997	-0.37439999

## MeOEP



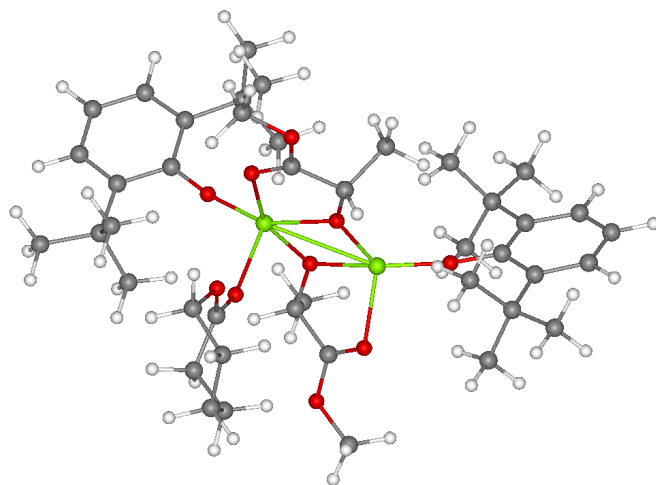
Zero-point vibrational energy	303039.1 (Joules/Mol) 72.42807 (Kcal/Mol)
Zero-point correction=	0.115421 (Hartree/Particle)
Thermal correction to Energy=	0.123826
Thermal correction to Enthalpy=	0.124770
Thermal correction to Gibbs Free Energy=	0.081434

Sum of electronic and zero-point Energies=	-760.559526
Sum of electronic and thermal Energies=	-760.551121
Sum of electronic and thermal Enthalpies=	-760.550177
Sum of electronic and thermal Free Energies=	-760.593513

cartesian						
8	1.01199996	1.91747999	-0.66900665	1	-2.53900003	-0.69611996 -1.28200662
15	0.33869994	0.72608006	-0.13230667	1	-1.50830007	-1.59751987 -0.13230667
8	-0.78800011	0.88518006	1.01729333	8	1.31199992	-0.35001999 0.54839331
8	-0.57990009	-0.08291996	-1.20180666	6	2.68899989	-0.42441994 0.12929332
6	-2.06210017	0.40018004	0.56029332	1	3.11589980	0.57578003 0.03799333
6	-1.74150014	-0.60941994	-0.54280668	1	2.76249981	-0.95062000 -0.82600665
1	-2.57720017	-0.05011997	1.40999329	1	3.20859981	-0.98942000 0.90299332
1	-2.64270020	1.24588001	0.17999333			

## S1.2. LC sequence, binuclear mechanism

### I-1\_LC



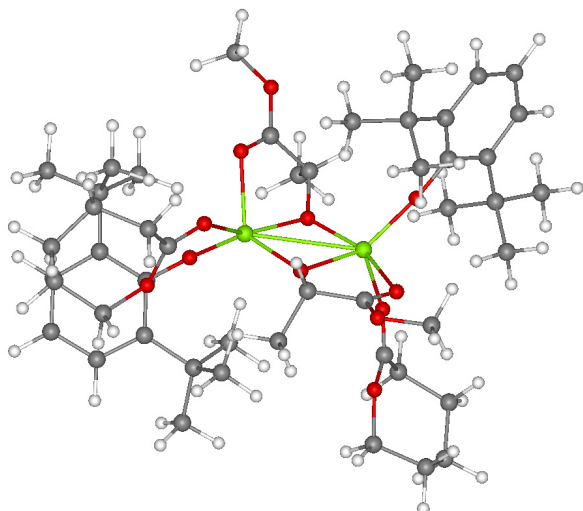
Zero-point vibrational energy	2702940.5 (Joules/Mol)
	646.01829 (Kcal/Mol)
Zero-point correction=	1.029496 (Hartree/Particle)
Thermal correction to Energy=	1.093004
Thermal correction to Enthalpy=	1.093948
Thermal correction to Gibbs Free Energy=	0.926001
Sum of electronic and zero-point Energies=	-2791.161249
Sum of electronic and thermal Energies=	-2791.097741
Sum of electronic and thermal Enthalpies=	-2791.096796
Sum of electronic and thermal Free Energies=	-2791.264744

cartesian											
12	-1.29932415	-0.08807253	0.27690756	1	6.19297600	3.72722745	1.21070755				
12	1.67837584	0.03872747	-0.43909246	1	6.84967566	2.37932754	2.14260745				
8	-2.88052416	-1.08357251	-0.04679247	6	4.92237568	2.38472748	-0.72739244				
8	3.49627590	-0.26527253	-0.19529246	1	5.76547575	2.31842756	-1.42409241				
8	-0.05022418	-0.47627252	-1.28979242	1	4.08747578	1.83242750	-1.15959239				
8	1.68627584	1.25552750	-2.20109248	1	4.63807583	3.44222760	-0.64449245				
8	0.66347581	1.46302748	-4.18579245	6	4.18777561	2.02972746	1.66990757				
6	-0.25562420	-0.12067255	-2.61529255	1	3.29257584	1.47602749	1.38370752				
6	-0.17412420	-1.31647253	-3.57279253	1	4.49407578	1.68292749	2.66320753				
1	-1.23572421	0.36192748	-2.75829268	1	3.92997575	3.09382749	1.74900758				
6	0.78507584	0.92992753	-2.98069263	6	4.83037567	-4.45317268	-0.75949246				
6	1.67627585	2.41482759	-4.57479239	1	5.67487574	-4.44207287	-1.45669246				
1	1.40827584	2.72262740	-5.58369255	1	5.18137598	-4.84357262	0.20150754				
1	2.65957570	1.94262755	-4.56239271	1	4.09417582	-5.16497278	-1.14959240				

6	-3.93402410	-1.88177252	-0.10859247	6	2.98617578	-3.25327253	0.34820756
6	-5.21152401	-1.35957253	-0.50549245	1	2.45847583	-2.31757259	0.53970754
6	-6.30742407	-2.22457242	-0.57029247	1	2.26637578	-3.97747254	-0.05089247
1	-7.27852440	-1.84467244	-0.86999243	1	3.34147573	-3.62687254	1.31490755
6	-6.20202398	-3.57577252	-0.26129246	6	3.67507577	-2.68547249	-2.03049254
6	-4.96482420	-4.08047295	0.12350753	1	4.51347589	-2.66987252	-2.73549247
1	-4.89862442	-5.13707256	0.36070755	1	2.94057584	-3.41497254	-2.39299250
6	-3.82342410	-3.27817249	0.20930754	1	3.22037578	-1.69317245	-2.04549265
6	-5.39882421	0.12762748	-0.85649246	1	-7.07102442	-4.22677279	-0.32049245
6	-2.48612428	-3.91127253	0.63570756	1	8.39237595	-1.72547245	0.94900757
6	-6.84272432	0.46312749	-1.27149248	1	1.67427576	3.26872754	-3.89549255
1	-7.15812397	-0.09197253	-2.16119266	1	-0.34592420	-1.01427245	-4.60979271
1	-7.56272411	0.26662749	-0.47009245	1	-0.94012421	-2.03737259	-3.28149247
1	-6.90952396	1.53082752	-1.51389241	1	0.80167580	-1.80437243	-3.49699259
6	-5.08052397	1.00202751	0.37250754	8	0.53277582	0.24012746	1.13790751
1	-5.17872429	2.06832743	0.12170753	8	-1.75272417	0.29522747	2.38000751
1	-5.78632402	0.78602749	1.18250751	8	-0.83182418	0.74212754	4.37730742
1	-4.07492399	0.81562752	0.74930757	6	0.65077579	0.44322747	2.50670743
6	-4.50152397	0.51032752	-2.04989266	6	1.48687577	-0.63387251	3.20590734
1	-4.78872442	-0.06237253	-2.93879247	1	1.10067582	1.42502749	2.72960734
1	-4.61112404	1.57712746	-2.28959250	6	-0.75922418	0.48712748	3.07700753
1	-3.45322418	0.30292749	-1.83609247	6	-2.15512419	0.73782754	4.95080757
6	-2.60442424	-5.42187262	0.90720755	1	-2.77602410	1.49882746	4.47530746
1	-3.30572414	-5.64677286	1.71800756	1	-2.61892414	-0.24087255	4.81900740
1	-2.91582417	-5.97977257	0.01770753	1	-2.01192403	0.95832753	6.00710726
1	-1.62442422	-5.80997276	1.20790756	1	1.57417583	-0.43837252	4.27830744
6	-1.99052417	-3.27487254	1.94950759	1	2.48747587	-0.64187247	2.76790738
1	-1.94262421	-2.18777251	1.87990761	1	1.03957582	-1.62087250	3.05840755
1	-2.67602420	-3.51627254	2.76990747	8	-1.67612422	1.88772750	-0.42379245
1	-0.99712420	-3.65827250	2.21500754	6	-2.02112412	3.02252746	-0.11489246
6	-1.43522418	-3.75307250	-0.48029244	6	-2.35272408	4.05212736	-1.16509247
1	-1.25542414	-2.70957255	-0.73909247	8	-2.07042408	3.33622742	1.17680752
1	-0.48152420	-4.20107269	-0.17449246	6	-1.39252424	5.25542736	-1.18559241
1	-1.77092421	-4.26887274	-1.38739240	1	-3.38452411	4.39502716	-1.02109241
6	4.74117565	-0.63677251	0.07610753	1	-2.32252407	3.51982760	-2.11619258
6	5.14377594	-2.00097251	-0.08949247	6	-2.53562427	4.62742710	1.63860750
6	6.45717573	-2.35337257	0.23460753	1	-0.35792419	4.89832735	-1.12049246
1	6.78337574	-3.38217258	0.12360753	1	-1.48932421	5.73482704	-2.16509247
6	7.37837601	-1.42157245	0.70050758	1	-3.54062414	4.81082726	1.24420750
6	6.98787594	-0.09347253	0.83380753	1	-2.62252426	4.48152733	2.71570754
1	7.72397566	0.62182748	1.18590760	6	-1.66392422	6.29822731	-0.10239246

6	5.69247580	0.33382750	0.52690756	1	-2.66202426	6.72672749	-0.26449245
6	4.17087603	-3.06917238	-0.62099242	1	-0.95502418	7.12492704	-0.21899246
6	5.32697582	1.82522750	0.65160757	6	-1.58002424	5.76892710	1.32880759
6	6.50817585	2.67922759	1.14610755	1	-0.56072420	5.44392729	1.56870759
1	7.36277580	2.63892746	0.46280757	1	-1.81512415	6.58342743	2.02390742

### I-1c\_LC



Zero-point vibrational energy	3121106.5 (Joules/Mol)
	745.96236 (Kcal/Mol)
Zero-point correction=	1.188767 (Hartree/Particle)
Thermal correction to Energy=	1.260893
Thermal correction to Enthalpy=	1.261838
Thermal correction to Gibbs Free Energy=	1.076890
Sum of electronic and zero-point Energies=	-3176.031992
Sum of electronic and thermal Energies=	-3175.959865
Sum of electronic and thermal Enthalpies=	-3175.958921
Sum of electronic and thermal Free Energies=	-3176.143869

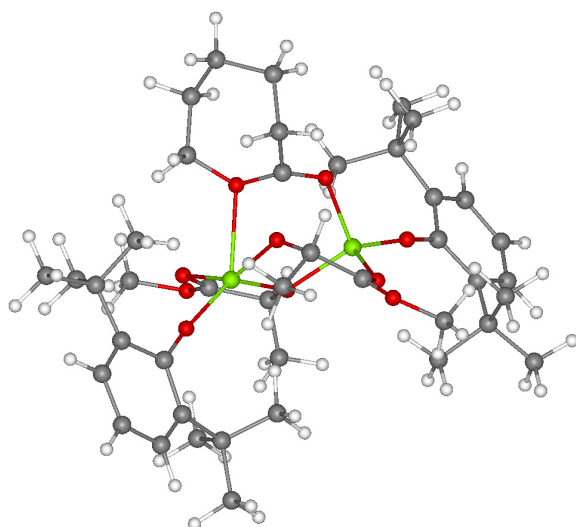
cartesian							
12	-1.12493479	-0.62537104	-0.02796813	1	6.87866497	1.21532893	-2.77986813
12	1.88406515	0.12092903	0.35233185	1	7.75796509	-0.00697098	-1.85756803
8	-2.57043457	0.16362903	-1.05466807	6	4.38136530	0.27232900	-2.51996803
8	3.42436504	-1.00177097	0.13943186	1	4.36896515	-0.42497095	-3.36526799
8	0.61606514	-0.45347098	-1.08866799	1	3.42936516	0.18942903	-1.99726796
8	-0.92373478	-2.57457089	-0.94016814	1	4.46046495	1.28962898	-2.92636800
8	0.15176520	-3.63957095	-2.59706807	6	5.64456511	0.98212898	-0.43596816
8	0.12746519	0.10702901	1.39893198	1	4.78506517	0.89902896	0.22933185
8	2.49246550	0.70662898	2.36933208	1	6.54976511	0.81282896	0.15823185
8	1.79416513	0.62772900	4.50123167	1	5.68946505	2.00622916	-0.83066815

6	0.86076522	-1.40207100	-2.07086802	6	3.61686516	-5.04387093	1.97563195
6	0.66026521	-0.85107100	-3.48876810	1	3.51756525	-5.78757095	1.17733192
1	1.88486516	-1.80297101	-1.99696803	1	4.60286522	-5.16417074	2.43663192
6	-0.05823481	-2.58837080	-1.81756806	1	2.86776543	-5.28427076	2.73923206
6	-0.68433475	-4.78827095	-2.36536813	6	3.48506546	-2.68527079	2.70223188
1	-0.55203485	-5.14977074	-1.34406805	1	3.39056540	-1.63847101	2.41293192
1	-1.73183489	-4.53207111	-2.53036809	1	2.70606518	-2.92837095	3.43773198
6	0.16336519	0.21562903	2.77763200	1	4.45886517	-2.81497097	3.18843198
1	-0.07423481	-0.74587101	3.26603198	6	1.95336521	-3.58037090	0.89613187
6	1.59386516	0.54272896	3.18913198	1	1.87796521	-4.26487112	0.04333187
6	3.14866543	0.89162898	4.91753197	1	1.22016513	-3.89607096	1.64893198
1	3.11916542	0.90212899	6.00593185	1	1.67846513	-2.58357096	0.55183184
1	3.48116541	1.85722899	4.53183174	1	-7.38053465	2.19562912	-1.48136806
6	-3.75413465	0.70062900	-1.27866805	1	7.18136501	-4.42417097	-1.15986800
6	-4.84553480	-0.09107098	-1.78646803	1	3.81356525	0.10622901	4.55543184
6	-6.12633467	0.46992901	-1.82086802	1	-0.35213482	-5.53607082	-3.08376813
1	-6.96543503	-0.12697098	-2.16416812	1	0.84456515	-1.61517107	-4.24946833
6	-6.37243462	1.78862894	-1.45056808	1	1.36456513	-0.02967098	-3.63826799
6	-5.28853464	2.59802914	-1.12426805	1	-0.35293481	-0.45847097	-3.60666800
1	-5.47793484	3.64832902	-0.92686814	6	-0.78323483	1.28022897	3.34863186
6	-3.98073483	2.10612917	-1.06796801	1	-0.73893476	1.30422902	4.44163179
6	-4.63453484	-1.51337099	-2.34176803	1	-1.80533481	1.05482900	3.03913188
6	-2.81723452	3.08632898	-0.82606816	1	-0.52853477	2.26882911	2.95803189
6	-5.88273478	-2.05227089	-3.06456804	8	1.71316516	3.78922915	0.87113184
1	-6.73213482	-2.19937086	-2.38806796	6	2.14686537	3.27112913	-0.27836815
1	-6.20363474	-1.39617097	-3.88056803	6	2.53006506	4.17012930	-1.42726803
1	-5.64953470	-3.03057098	-3.50066805	1	1.66086519	4.76972914	-1.72426808
6	-3.50013494	-1.49607098	-3.38516808	6	1.51196516	5.21092892	1.04243195
1	-3.33293486	-2.50357080	-3.78776813	1	0.99796522	5.26882887	2.00253201
1	-3.76293468	-0.84037101	-4.22286844	6	2.80306530	6.01452923	1.07733202
1	-2.57173491	-1.13097107	-2.94716811	1	0.82246518	5.57512903	0.27323186
6	-4.30923462	-2.51227093	-1.21886802	1	3.52556515	5.48252916	1.70763195
1	-5.15083504	-2.57947087	-0.51886815	6	3.39706516	6.32012892	-0.29696813
1	-4.14263487	-3.51647091	-1.62976801	1	2.58166504	6.95872927	1.58883202
1	-3.41703463	-2.22447085	-0.66696817	1	2.75746536	3.49822903	-2.25496793
6	-3.27433491	4.55612898	-0.87086815	6	3.73176527	5.08652925	-1.13386798
1	-3.75893450	4.80992889	-1.81956804	1	4.52536535	4.50232887	-0.65466815
1	-3.96093464	4.80872917	-0.05536813	1	4.13506508	5.41462898	-2.09736800
1	-2.39853477	5.20792913	-0.76406813	1	2.69116545	6.94902897	-0.85596812
6	-1.75423479	2.92162919	-1.93086803	1	4.30466509	6.92022896	-0.16876814
1	-1.34663486	1.91062903	-1.95366812	8	2.24286509	2.05592918	-0.36586815



1	-2.18813467	3.13972902	-2.91306806	8	-3.93443489	-0.21407098	1.81663203
1	-0.92823482	3.62762904	-1.76766801	6	-3.29003477	-1.32057106	2.15543199
6	-2.18493462	2.86102915	0.55503184	6	-3.81803465	-2.21857095	3.24633193
1	-1.77333486	1.85822904	0.65363187	1	-3.93753481	-1.63307106	4.16693163
1	-1.36723483	3.57252908	0.72913188	6	-5.19763470	0.18552904	2.40143204
1	-2.92783451	3.00272918	1.34833193	1	-5.38333464	1.14502895	1.91883194
6	4.39496517	-1.84977102	-0.15226814	6	-6.34333467	-0.77237099	2.12213206
6	4.41276503	-3.17017078	0.41713184	1	-5.05413485	0.35582903	3.47563195
6	5.41596508	-4.06177092	0.02713187	1	-6.31883478	-1.03107095	1.05843198
1	5.43026495	-5.06747103	0.43443185	6	-6.37473488	-2.01817107	3.00673199
6	6.41706514	-3.70687079	-0.87036812	1	-7.26893473	-0.20527098	2.27523208
6	6.43536520	-2.41017079	-1.37186801	1	-3.03563452	-2.95777082	3.42373204
1	7.23786497	-2.13647079	-2.04866815	6	-5.14373493	-2.91707087	2.89803195
6	5.46446514	-1.46427107	-1.03126800	1	-5.07103491	-3.34887099	1.89403200
6	3.38016510	-3.60897088	1.47213197	1	-5.26043463	-3.76017094	3.58723187
6	5.57266521	-0.03467098	-1.59276807	1	-6.49633503	-1.70857108	4.05413151
6	6.84486532	0.17512903	-2.43436813	1	-7.26473475	-2.60767078	2.75953197
1	6.86776495	-0.46127096	-3.32556796	8	-2.24503469	-1.58527100	1.56383193

## TS-12\_LC



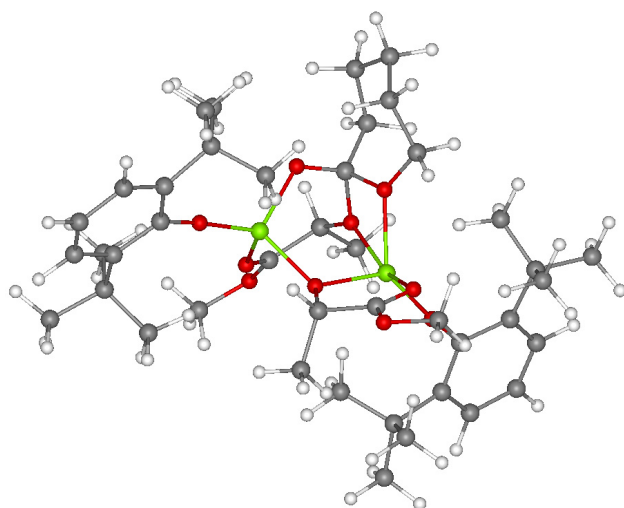
Zero-point vibrational energy	2702706.9 (Joules/Mol)
	645.96245 (Kcal/Mol)
Zero-point correction=	1.029407 (Hartree/Particle)
Thermal correction to Energy=	1.091539
Thermal correction to Enthalpy=	1.092483
Thermal correction to Gibbs Free Energy=	0.929877
Sum of electronic and zero-point Energies=	-2791.136244
Sum of electronic and thermal Energies=	-2791.074112
Sum of electronic and thermal Enthalpies=	-2791.073167

Sum of electronic and thermal Free Energies= -2791.235774

cartesian							
12	1.71657324	-0.04279250	-0.57503676	1	-6.79682684	3.04540753	-0.01013676
12	-1.43102682	0.35830751	0.34796324	1	-7.30182695	1.71920753	-1.05573678
8	3.54487324	-0.27829251	-0.30373675	6	-4.94552660	1.85910749	1.46476328
8	-3.15132689	-0.38309249	0.59086323	1	-5.62112665	1.55390751	2.27166319
8	0.41207317	-0.27179250	0.89276320	1	-3.95522690	1.46590745	1.69456327
8	-1.27572680	1.18320751	2.31186318	1	-4.90332699	2.95650744	1.46326327
8	-0.01552683	1.08120751	4.16436338	6	-4.60312700	1.87600756	-1.04673672
6	0.75107312	-0.13379250	2.24496317	1	-3.58682680	1.47900748	-1.01103675
6	0.83517313	-1.47649252	2.97816324	1	-5.03602695	1.58550751	-2.01073670
1	1.71957314	0.37500751	2.36546326	1	-4.55972672	2.97330761	-1.02003670
6	-0.27602684	0.77270752	2.90556335	6	-3.68892670	-4.75629234	1.17276323
6	-0.98302692	1.91170752	4.83996344	1	-4.53852701	-4.89559269	1.84906328
1	-0.61192685	2.01380754	5.85776329	1	-3.93822670	-5.21149254	0.20816323
1	-1.96282685	1.43250751	4.82916307	1	-2.84532690	-5.31909227	1.58826327
6	4.77327299	-0.46189249	0.17036323	6	-2.06762671	-3.24519253	0.10206324
6	5.54307318	0.65360749	0.63486320	1	-1.66532683	-2.23799253	-0.01083677
6	6.79867315	0.40960750	1.20036328	1	-1.26402676	-3.87969255	0.49516323
1	7.39177322	1.23690748	1.57496333	1	-2.33792686	-3.62089252	-0.89123678
6	7.33077335	-0.87109250	1.29626322	6	-2.90402675	-2.79359245	2.45016336
6	6.60927296	-1.94019246	0.77746320	1	-3.75722671	-2.89339256	3.13006330
1	7.05517340	-2.92789245	0.82736319	1	-2.08252692	-3.39969254	2.85256338
6	5.34787321	-1.77399254	0.19796324	1	-2.60362673	-1.74429250	2.44316316
6	5.04377317	2.10480762	0.49286327	1	8.30687332	-1.03099251	1.74766326
6	4.63277340	-2.98669243	-0.42763674	1	-7.71632671	-2.74429250	-0.43583676
6	6.08127308	3.13160753	0.98266321	1	-1.04472685	2.88680744	4.35396338
1	6.29877329	3.02960753	2.05136323	1	1.10957313	-1.33659256	4.02726316
1	7.02387333	3.06080747	0.43026325	1	1.59997320	-2.08749247	2.49626327
1	5.68727303	4.14240742	0.82656324	1	-0.11812682	-2.00609255	2.92246318
6	4.77537298	2.42600751	-0.99173677	8	-1.07622683	0.60030752	-1.61673677
1	4.40187311	3.45210743	-1.10003674	8	0.91757315	-1.27339256	-2.01073670
1	5.70307302	2.34310746	-1.56863678	8	-0.15942682	-2.10129261	-3.77653670
1	4.04287338	1.74690747	-1.42823672	6	-1.13682687	-0.16899250	-2.76903677
6	3.77477312	2.34110761	1.33316326	6	-2.52582693	-0.77259248	-3.00253677
1	3.96667314	2.12580752	2.39026332	1	-0.90022689	0.45470750	-3.65033674
1	3.44707322	3.38510752	1.25256324	6	-0.03442683	-1.22979248	-2.79193664
1	2.95087314	1.70910752	1.00016332	6	0.87947315	-3.09829259	-3.90243673
6	5.47627306	-4.27189255	-0.35163677	1	1.83937323	-2.61719251	-4.09343672
1	6.43377304	-4.17099237	-0.87323678	1	0.94087315	-3.69039249	-2.98903680

1	5.67697334	-4.57879257	0.68026322	1	0.57937312	-3.71599245	-4.74643660
1	4.92827320	-5.09079266	-0.83163679	1	-2.55472684	-1.35999250	-3.92323661
6	4.37407303	-2.71949244	-1.92423677	1	-3.24752688	0.04160750	-3.08143663
1	3.76957321	-1.82379246	-2.07243681	1	-2.82612681	-1.40359247	-2.16403675
1	5.32287312	-2.57939243	-2.45363665	8	1.22317314	1.69040751	-1.45193672
1	3.85757327	-3.57439256	-2.37973666	6	0.07177316	2.18160748	-1.47063673
6	3.31297326	-3.29319239	0.30446324	6	-0.36612684	2.99220753	-2.66583681
1	2.62667322	-2.44639254	0.27896324	8	-0.47642687	2.47390747	-0.22923677
1	2.80717325	-4.15379238	-0.15113677	6	0.23677316	4.40840769	-2.64813662
1	3.50757313	-3.53679252	1.35476327	1	-1.45582676	3.02870750	-2.74063683
6	-4.32192659	-0.97569251	0.39376324	1	0.01377317	2.45670748	-3.53833675
6	-4.44342661	-2.40099239	0.50646323	6	-1.33742678	3.62790751	-0.05513677
6	-5.66732693	-2.99769258	0.18826324	1	1.29267323	4.34370756	-2.36333680
1	-5.77142668	-4.07609272	0.24256323	1	0.21647316	4.79700756	-3.67193675
6	-6.77892685	-2.25239253	-0.18823677	1	-2.22542691	3.52880740	-0.68693680
6	-6.68222666	-0.86579251	-0.20403677	1	-1.65712678	3.53670740	0.98396319
1	-7.57102680	-0.29629251	-0.45393676	6	-0.51072687	5.38540745	-1.74133670
6	-5.49022675	-0.19869250	0.09386324	1	-1.52322686	5.53570747	-2.13953662
6	-3.29052687	-3.27529240	1.03736329	1	-0.01792683	6.36320734	-1.78743672
6	-5.46882677	1.34160745	0.10906324	6	-0.62092686	4.95310736	-0.27833676
6	-6.86932659	1.95360756	-0.07743676	1	0.36807317	4.89620733	0.19116323
1	-7.56972694	1.62370753	0.69676322	1	-1.18222678	5.71780729	0.27206326

## I-2\_LC



Zero-point vibrational energy

2706139.2 (Joules/Mol)

646.78280 (Kcal/Mol)

Zero-point correction=

1.030714 (Hartree/Particle)

Thermal correction to Energy=

1.092950

Thermal correction to Enthalpy=

1.093894

Thermal correction to Gibbs Free Energy=	0.932805
Sum of electronic and zero-point Energies=	-2791.141338
Sum of electronic and thermal Energies=	-2791.079102
Sum of electronic and thermal Enthalpies=	-2791.078157
Sum of electronic and thermal Free Energies=	-2791.239246

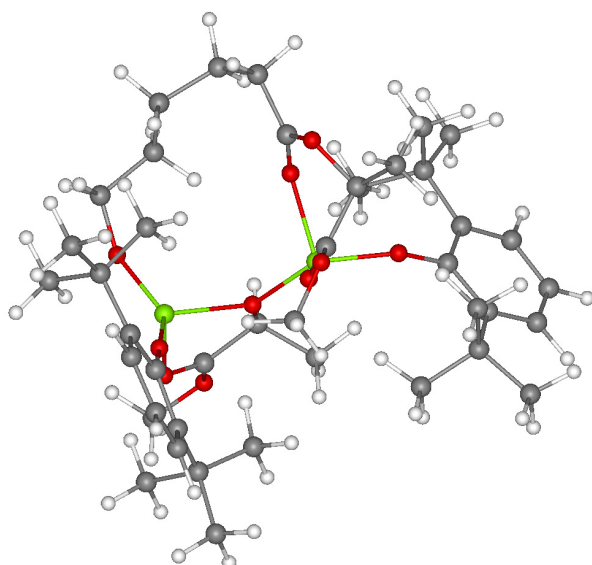
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8	-3.47919083	0.28642592	-0.28138500	6	4.75140905	-2.19807410	1.53451502				
8	3.16860914	0.21312591	0.67711502	1	5.48440933	-1.96077418	2.31361508				
8	-0.38359100	0.30502594	0.91441500	1	3.81860924	-1.69837415	1.79661500				
8	1.10980904	-1.22967410	2.46311498	1	4.58740902	-3.28327417	1.54991496				
8	-0.22469100	-0.95467407	4.24431515	6	4.33190918	-2.21587420	-0.96718502				
6	-0.76729101	0.28062594	2.26001501	1	3.36130905	-1.72187412	-0.91168499				
6	-0.68279099	1.65832591	2.92781496	1	4.76260900	-1.98397410	-1.94788504				
1	-1.79729092	-0.08777409	2.37671494	1	4.17590904	-3.30157423	-0.91858500				
6	0.12550899	-0.70807409	2.99481511	6	4.17310905	4.50142574	1.19891500				
6	0.62380898	-1.85447419	4.98881531	1	5.05370903	4.55802584	1.84671497				
1	0.19010898	-1.89747417	5.98581505	1	4.43680906	4.92202568	0.22241500				
1	1.64280903	-1.46687412	5.02391529	1	3.40550923	5.15062571	1.63511503				
6	-4.73509073	0.40662593	0.13511500	6	2.37270927	3.15282583	0.19351499				
6	-5.46679068	-0.74597406	0.56891501	1	1.86960900	2.18862581	0.10831501				
6	-6.76079082	-0.56727409	1.06831503	1	1.65050900	3.86932588	0.60451502				
1	-7.32799101	-1.42377412	1.41631496	1	2.64900923	3.49112582	-0.81178498				
6	-7.36349106	0.68362594	1.13151503	6	3.22890925	2.63902593	2.51961493				
6	-6.67079067	1.78942585	0.65211499	1	4.10580921	2.66062593	3.17581511				
1	-7.16769075	2.75322580	0.68001497	1	2.48120928	3.32552576	2.93661499				
6	-5.37409067	1.68892586	0.13941500	1	2.82700920	1.62422585	2.53321505				
6	-4.88309097	-2.16827416	0.46641499	1	-8.36929131	0.79232591	1.53001499				
6	-4.68309069	2.94142580	-0.43178502	1	7.91550922	2.07182598	-0.52848500				
6	-5.88029099	-3.24607420	0.92991501	1	0.62140900	-2.84207416	4.52491522				
1	-6.15229082	-3.13807416	1.98551500	1	-1.00659096	1.61212587	3.97121501				
1	-6.79929066	-3.24187422	0.33481500	1	-1.33769095	2.34502578	2.38921499				
1	-5.42139101	-4.23437452	0.81201500	1	0.33730900	2.04672575	2.88491488				
6	-4.53669071	-2.49187422	-1.00118494	8	1.13110900	-0.44267407	-1.65878499				
1	-4.11959076	-3.50387406	-1.08168495	8	-0.75819099	1.62712586	-1.71488500				
1	-5.43989086	-2.45247412	-1.61978495	8	0.51380897	2.71832585	-3.18688512				
1	-3.81329083	-1.78947413	-1.41578496	6	1.13250899	0.46712592	-2.74368501				
6	-3.63759089	-2.32267404	1.35991502	6	2.56680918	0.85042590	-3.08658504				
1	-3.88299084	-2.10367417	2.40511489	1	0.66660899	-0.01177408	-3.61568499				

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1	-3.25209093	-3.34887409	1.31101501	6	0.21020900	1.65352583	-2.46878505
1	-2.83799076	-1.64707410	1.05241501	6	-0.35999101	3.86262584	-3.04778504
6	-5.58609104	4.18702555	-0.38168502	1	-1.37629092	3.59352589	-3.33708501
1	-6.50849104	4.05362558	-0.95638502	1	-0.34879100	4.21182585	-2.01518512
1	-5.85509062	4.46502542	0.64291501	1	0.05080899	4.61542559	-3.71738505
1	-5.05009079	5.03772545	-0.81798500	1	2.59470916	1.55062592	-3.92348504
6	-4.33369064	2.71292591	-1.91638505	1	3.11180925	-0.05417408	-3.36238503
1	-3.68269086	1.84782588	-2.04878497	1	3.06810927	1.29872584	-2.22698498
1	-5.24479103	2.53992581	-2.49918509	8	-1.01439095	-1.34057415	-1.79978502
1	-3.83339071	3.59802580	-2.33068490	6	0.23290899	-1.67987418	-1.75708497
6	-3.41849089	3.28832579	0.37621498	6	0.73070902	-2.58327413	-2.88588500
1	-2.69839072	2.47002578	0.36701500	8	0.65450901	-2.18097425	-0.42908502
1	-2.92889094	4.17992544	-0.03558500	6	-0.22909100	-3.73497415	-3.19498491
1	-3.67839074	3.49932575	1.41951501	1	1.74140906	-2.93777418	-2.65888500
6	4.39080906	0.67282593	0.43941501	1	0.81070900	-1.96697414	-3.78658509
6	4.66170931	2.07792592	0.53331500	6	0.67010897	-3.58747411	-0.12038500
6	5.92800903	2.54242587	0.16451499	1	-1.23629093	-3.31757402	-3.29028511
1	6.14450932	3.60482597	0.20111500	1	0.03650899	-4.15487432	-4.17198467
6	6.94190931	1.68202591	-0.24148500	1	1.64270902	-4.00077438	-0.41658500
6	6.70320940	0.31242591	-0.23408501	1	0.61950898	-3.61037421	0.97061497
1	7.51910925	-0.34967408	-0.50398499	6	-0.22549102	-4.86127424	-2.16218495
6	5.46020937	-0.22527409	0.11371500	1	0.73320901	-5.39637423	-2.20868492
6	3.62140918	3.06822586	1.09131503	1	-0.99419099	-5.59227419	-2.43828511
6	5.28130913	-1.75497413	0.15461500	6	-0.46199101	-4.41387415	-0.71818501
6	6.60620928	-2.50877404	-0.06028500	1	-1.40559089	-3.86757421	-0.62448502
1	7.35940933	-2.23867416	0.68721497	1	-0.55099100	-5.30847454	-0.08928500

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### TS-23\_LC



Zero-point vibrational energy	2700224.7 (Joules/Mol)
	645.36920 (Kcal/Mol)
Zero-point correction=	1.028461 (Hartree/Particle)
Thermal correction to Energy=	1.091343
Thermal correction to Enthalpy=	1.092287
Thermal correction to Gibbs Free Energy=	0.929516
Sum of electronic and zero-point Energies=	-2791.110764
Sum of electronic and thermal Energies=	-2791.047882
Sum of electronic and thermal Enthalpies=	-2791.046938
Sum of electronic and thermal Free Energies=	-2791.209709

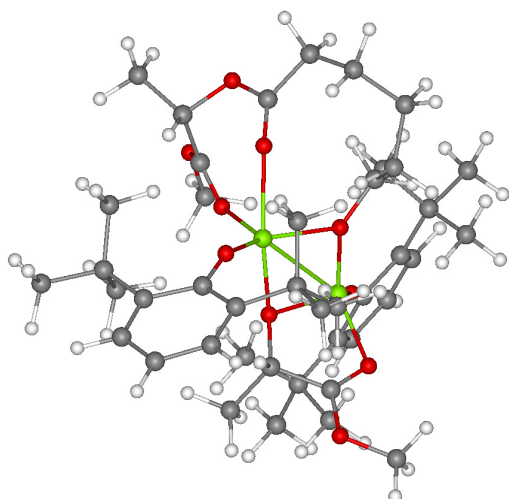
cartesian							
12	1.08600318	0.24337737	0.04757904	1	-5.62019682	3.39997721	-1.46772099
12	-1.92779672	0.36827737	2.00847888	1	-5.35489655	2.23697710	-2.76722097
8	2.81670332	-0.22502263	-0.51302099	6	-5.15259695	1.87597740	0.66537905
8	-3.09209681	-0.36762264	0.72177905	1	-6.15329695	1.45887744	0.82217902
8	0.08590332	-0.11182262	1.67387903	1	-4.48649693	1.45337749	1.41737902
8	-1.55179679	-0.85022265	3.66227913	1	-5.20799685	2.95787716	0.83567905
8	0.14360332	-1.23502254	5.07457924	6	-3.27749681	2.18887711	-1.00642097
6	0.71430337	-0.48972264	2.87567902	1	-2.52429676	1.70957744	-0.37822098
6	1.70510328	-1.64362252	2.69587898	1	-2.98079681	2.07177711	-2.05642104
1	1.24400318	0.36607736	3.32327914	1	-3.28469682	3.26117730	-0.77822095
6	-0.34619668	-0.87532270	3.89887905	6	-3.74049687	-4.71992254	0.18927902
6	-0.82639664	-1.55652261	6.09527922	1	-4.81889677	-4.90792274	0.22097903
1	-0.24049668	-1.79282260	6.98137951	1	-3.36929679	-5.00642252	-0.80102098
1	-1.42489672	-2.41472268	5.78657913	1	-3.27159667	-5.39202261	0.91677904
6	4.00960302	-0.80262268	-0.32462096	6	-1.85559678	-3.15992284	0.51267904
6	5.05800343	-0.09002262	0.34117904	1	-1.50869679	-2.15832281	0.76527905
6	6.26690340	-0.75242269	0.58027905	1	-1.40759683	-3.87142277	1.21807909
1	7.07020330	-0.24032263	1.09827900	1	-1.47979677	-3.40632272	-0.48712099
6	6.48640347	-2.06082273	0.16827902	6	-3.91559672	-3.03082275	1.98207903
6	5.48790312	-2.72252274	-0.53582096	1	-4.99879694	-3.19002271	2.02107906
1	5.68890333	-3.73172283	-0.87802094	1	-3.44579673	-3.73412275	2.68117905
6	4.25290346	-2.12712288	-0.81182098	1	-3.71179676	-2.01782274	2.32837915
6	4.91090345	1.38547742	0.76587903	1	7.43380308	-2.55242276	0.37527904
6	3.21490312	-2.89932275	-1.65082097	1	-6.10559654	-2.21432281	-3.14092088
6	6.21070337	1.95627749	1.36377907	1	-1.47669673	-0.69942266	6.27447939
1	6.50250340	1.44817746	2.28877902	1	2.18010330	-1.90452254	3.64497900
1	7.04780340	1.90157747	0.66047901	1	2.49430323	-1.35862255	1.99477899
1	6.05930328	3.01327729	1.60967898	1	1.19460320	-2.52552271	2.29987907
6	4.57630301	2.25337720	-0.46362096	8	0.56600332	2.70737720	-2.63292098

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1	4.44360304	3.30227733	-0.16972098	8	-0.16379668	-0.13352263	-1.54732096
1	5.39210320	2.20787716	-1.19312096	8	-0.91129667	0.02747737	-3.64652085
1	3.66420317	1.90657747	-0.95002091	6	0.97310340	1.37867749	-3.06212091
6	3.83490324	1.55317748	1.85497904	6	1.25790322	1.46687746	-4.54572058
1	4.07650328	0.94737732	2.73457909	1	1.87300324	1.09887743	-2.50342107
1	3.76380324	2.59967732	2.17347908	6	-0.10089668	0.35487735	-2.67782092
1	2.84480333	1.25597739	1.50567901	6	-1.92029679	-0.98822272	-3.35852098
6	3.75170326	-4.25142241	-2.15472102	1	-2.44359684	-1.13182259	-4.29992056
1	4.64630318	-4.13562250	-2.77532101	1	-1.42279673	-1.90262258	-3.03682089
1	3.98610306	-4.93992233	-1.33632100	1	-2.59789681	-0.63372266	-2.58182096
1	2.98590326	-4.73392248	-2.77222085	1	1.58190322	0.49287736	-4.91852093
6	2.84730315	-2.08362269	-2.90572095	1	2.06110334	2.18717718	-4.71542072
1	2.47010326	-1.09992254	-2.62602091	1	0.37140331	1.77887750	-5.09982061
1	3.72830319	-1.94122255	-3.54092097	8	0.98420334	2.26727724	-0.45842099
1	2.08430314	-2.60672283	-3.49602103	6	0.74420333	3.06887722	-1.35572100
6	1.95410323	-3.21532273	-0.82622099	6	0.68490332	4.56127739	-1.18952096
1	1.45900321	-2.31342268	-0.46492094	8	-2.02479672	2.00597715	2.88157892
1	1.22730327	-3.77252269	-1.42892098	6	0.62490332	5.07077742	0.24927902
1	2.20600319	-3.82792282	0.04537904	1	-0.15419668	4.93007755	-1.78902102
6	-3.90489674	-0.83322269	-0.20702097	1	1.58650327	4.93087769	-1.69812095
6	-4.04229689	-2.24922276	-0.40742096	6	-1.97659671	3.37567711	2.71537900
6	-4.82359695	-2.70322275	-1.47402096	1	1.45000327	4.62867737	0.81737906
1	-4.92409658	-3.76892281	-1.65152097	1	0.82910335	6.14597750	0.20857903
6	-5.50209665	-1.83112252	-2.32142091	1	-2.77009678	3.72977710	2.02717900
6	-5.43369675	-0.46422264	-2.07252097	1	-2.17599678	3.88587713	3.67557907
1	-6.00619698	0.20007737	-2.71152091	6	-0.71869665	4.79997730	0.96027905
6	-4.66359663	0.06607737	-1.03122091	1	-1.42879677	4.36547756	0.24507904
6	-3.39159679	-3.26502275	0.55007905	1	-1.17079675	5.74887753	1.27257907
6	-4.67489672	1.58397746	-0.77182096	6	-0.61119664	3.86097717	2.16257906
6	-5.63689661	2.33207726	-1.71252096	1	-0.06039668	2.96287727	1.86397898
1	-6.67069674	1.98897743	-1.60052097	1	-0.01089668	4.33877754	2.94867897

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# I-3\_LC



Zero-point vibrational energy	2705348.6 (Joules/Mol)
	646.59384 (Kcal/Mol)
Zero-point correction=	1.030413 (Hartree/Particle)
Thermal correction to Energy=	1.093067
Thermal correction to Enthalpy=	1.094011
Thermal correction to Gibbs Free Energy=	0.932463
Sum of electronic and zero-point Energies=	-2791.143767
Sum of electronic and thermal Energies=	-2791.081113
Sum of electronic and thermal Enthalpies=	-2791.080169
Sum of electronic and thermal Free Energies=	-2791.241717

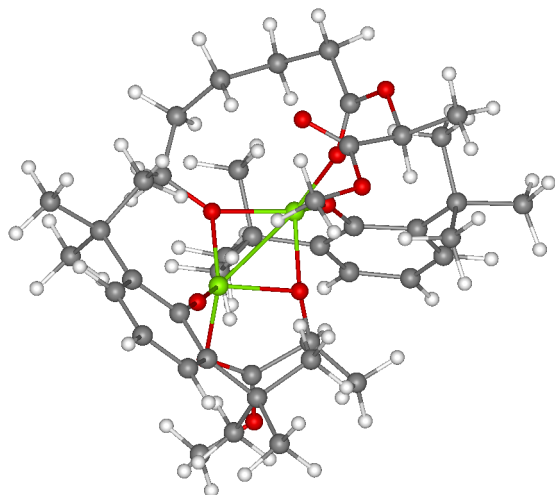
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12	1.44325101	-0.68472838	-0.76404667	1	2.97565079	1.78487158	-0.35844666				
8	-3.01134920	0.00067163	0.15125336	6	5.96015072	2.51137161	-1.91524673				
8	3.24725080	-0.59282833	-0.27964664	1	6.42765093	3.04017162	-1.07814670				
8	-0.15884900	-1.29292846	0.26915336	1	6.74635077	2.00717163	-2.48684669				
8	0.94865096	-2.39032841	-1.87644672	1	5.51615095	3.26927161	-2.57104659				
8	-0.46814901	-4.12502861	-1.87624669	6	4.26225090	0.92267162	-2.73194671				
6	-0.66224903	-2.54612827	-0.07014666	1	5.03515100	0.38497165	-3.29154658				
6	-0.44624901	-3.58912826	1.03415334	1	3.46725082	0.20977162	-2.50714660				
1	-1.74104893	-2.50292826	-0.28594664	1	3.85745072	1.70507157	-3.38604665				
6	0.01075100	-3.01022840	-1.35724664	6	5.06435061	-3.67292833	2.35585332				
6	0.15635100	-4.59752846	-3.08844662	1	5.87185097	-4.16922855	1.80775332				
1	-0.37344900	-5.51282835	-3.34464669	1	5.49865103	-3.15982819	3.22055340				
1	1.21425104	-4.79782867	-2.91264677	1	4.40345097	-4.45752859	2.74145341				
6	-4.04824924	-0.82142836	0.23915336	6	3.12715077	-2.15082836	2.35195327				
6	-4.68224907	-1.32152843	-0.94674665	1	2.45785069	-1.48932838	1.80095327				



6	-5.68714905	-2.28462839	-0.81214666	1	2.52685070	-2.95982838	2.78575325
1	-6.15774918	-2.69992828	-1.69714665	1	3.56465077	-1.58282840	3.18165326
6	-6.12624931	-2.72892833	0.43055335	6	3.66765070	-3.58522820	0.32435337
6	-5.59114933	-2.15172839	1.57715333	1	4.47765064	-4.06572866	-0.23574665
1	-5.98694944	-2.46222830	2.53855324	1	3.02535081	-4.37772846	0.72945333
6	-4.57984924	-1.18832839	1.52045333	1	3.08845091	-2.99062824	-0.38274664
6	-4.32594919	-0.78212833	-2.34594679	1	-6.90334940	-3.48582840	0.50375336
6	-4.09564924	-0.51372838	2.81815338	1	8.35735035	-0.52302837	0.90605330
6	-5.25484943	-1.33922839	-3.44044662	1	0.04815099	-3.85392833	-3.87944674
1	-5.15564919	-2.42322826	-3.56294656	1	-0.86854905	-4.55882835	0.75645334
1	-6.30714941	-1.11022842	-3.24284673	1	-0.94464904	-3.23492837	1.93775332
1	-4.99424934	-0.88032836	-4.40094662	1	0.61835098	-3.70542836	1.25125337
6	-4.49404907	0.75127167	-2.36704659	8	0.30655101	0.83517164	-1.26484668
1	-4.22504902	1.15107155	-3.35334659	6	-1.32824898	3.75177169	0.02375335
1	-5.53824902	1.01887155	-2.17014670	6	-1.29814899	4.84867144	-1.00834668
1	-3.87434912	1.23237157	-1.60904670	6	-0.62944901	2.25587177	-3.02234674
6	-2.89354920	-1.16902840	-2.75824666	6	0.50255096	2.00767159	-2.01724672
1	-2.78454924	-2.25932837	-2.78324676	8	-1.76694894	2.62437177	-0.13374664
1	-2.66284919	-0.78412837	-3.75924659	1	0.60475099	2.87477160	-1.34394670
1	-2.14544916	-0.76772839	-2.07274675	1	-0.27654901	5.24487162	-1.03864670
6	-4.94014931	-0.91562837	4.04095316	8	-0.83574903	4.18607140	1.20235336
1	-5.99934912	-0.67222834	3.90735340	8	-0.02214901	1.23337162	1.69885337
1	-4.85854912	-1.98252845	4.27315331	8	1.10425103	2.53837180	3.12395334
1	-4.58404922	-0.36732838	4.92105341	6	-1.01684892	3.33897161	2.36655331
6	-4.22914934	1.01747155	2.68465328	6	-1.01294899	4.24177122	3.58125329
1	-3.68974924	1.38617158	1.81005335	1	-1.96834898	2.81187177	2.26385331
1	-5.28174925	1.29787159	2.56785321	6	0.06925099	2.26187181	2.35875344
1	-3.85134912	1.51427162	3.58915329	6	2.17105079	1.55337155	3.15695333
6	-2.64344931	-0.90952837	3.14355326	1	1.77745104	0.59917164	3.50665331
1	-1.95734894	-0.70322835	2.32165337	1	2.60275078	1.43517160	2.16365337
1	-2.28604913	-0.37582836	4.03445339	1	2.90305090	1.95547163	3.85345340
1	-2.58384919	-1.98222840	3.35765338	1	-1.14484894	3.64747167	4.48855352
6	4.54455090	-0.58302838	0.01305335	1	-1.84294891	4.94807148	3.50755334
6	5.10325098	-1.58482838	0.87275332	1	-0.07684901	4.79617167	3.66045332
6	6.46825075	-1.52842844	1.17085338	1	1.45745099	1.95697153	-2.55724669
1	6.90795088	-2.27682829	1.82125330	1	-1.90244901	5.66107130	-0.58474666
6	7.29905081	-0.53952837	0.65755332	6	-1.81324899	4.49037123	-2.40514660
6	6.75525093	0.42447165	-0.18294664	1	-0.41214901	1.70017159	-3.94164658
1	7.41645098	1.18677163	-0.58084667	6	-0.86874902	3.73487163	-3.35364676
6	5.39915085	0.43497163	-0.52314669	1	-1.55304897	1.82627153	-2.62344670
6	4.24835062	-2.72222829	1.46175337	1	-2.75124931	3.93307161	-2.30804658

6	4.86065102	1.53857160	-1.45174670	1	-2.07344913	5.44117165	-2.88454676
6	3.81585073	2.38977170	-0.70374668	1	0.08935099	4.26917124	-3.42604661
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#### I-4\_LC



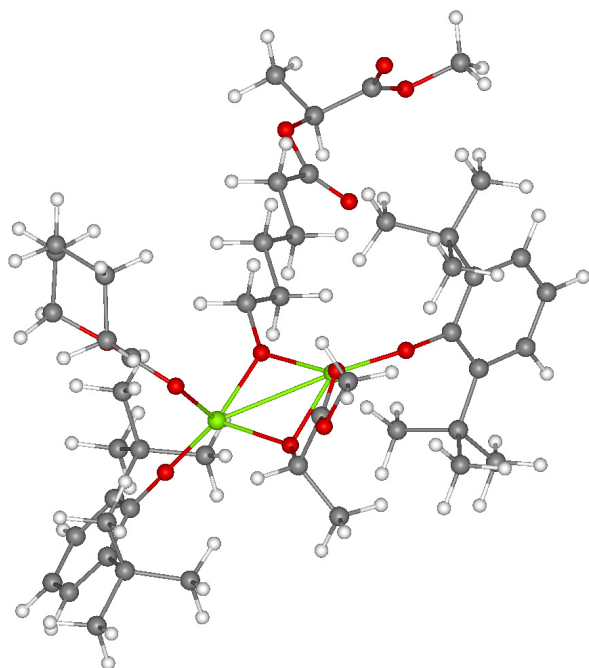
Zero-point vibrational energy	2705362.1 (Joules/Mol)
	646.59707 (Kcal/Mol)
Zero-point correction=	1.030418 (Hartree/Particle)
Thermal correction to Energy=	1.093424
Thermal correction to Enthalpy=	1.094368
Thermal correction to Gibbs Free Energy=	0.931135
Sum of electronic and zero-point Energies=	-2791.147590
Sum of electronic and thermal Energies=	-2791.084584
Sum of electronic and thermal Enthalpies=	-2791.083640
Sum of electronic and thermal Free Energies=	-2791.246873

cartesian							
12	1.34161520	0.34419581	0.42331010	1	-3.21248484	1.01079571	3.49460983
12	-1.18218482	-1.16100430	0.36841011	1	-2.81448483	0.71969587	1.78861010
8	3.21521521	0.17199580	0.35571012	6	-5.63348532	-0.12190420	3.58470988
8	-3.02098489	-1.01010430	0.10571011	1	-6.20078516	0.79059589	3.37310982
8	0.30591515	-0.69970411	-0.92188984	1	-6.34048510	-0.95140415	3.69160986
8	-0.49798486	-3.08500409	-0.08728988	1	-5.14578485	0.01769580	4.55600977
8	0.90381515	-4.17940378	-1.44938982	6	-3.80778480	-1.66410422	2.98940992
6	0.87881517	-1.78120422	-1.59758985	1	-4.50248528	-2.50490403	3.09080982
6	0.58081514	-1.75960422	-3.10029006	1	-3.03378487	-1.96930420	2.28260994
1	1.97301507	-1.80170429	-1.46778989	1	-3.33988476	-1.49470425	3.96680999
6	0.36491516	-3.07440424	-0.97358984	6	-5.02748489	-1.71590424	-3.78948998
6	0.43391514	-5.42530394	-0.88958985	1	-5.75548506	-2.52410412	-3.66329002

1	0.99241519	-6.20020390	-1.41058981	1	-5.56928492	-0.80430412	-4.06399012
1	-0.63708484	-5.53340387	-1.06508982	1	-4.39048529	-1.98250425	-4.64049006
6	4.34301472	-0.33470419	-0.14768989	6	-3.14948487	-0.39720419	-2.89229012
6	4.95131493	-1.48370421	0.45561013	1	-2.44728494	-0.19870420	-2.08169007
6	6.07861471	-2.04170418	-0.15548989	1	-2.57458496	-0.65840411	-3.78939009
1	6.54261494	-2.92530417	0.26981011	1	-3.68748474	0.53229582	-3.10889006
6	6.64621496	-1.49540424	-1.30068982	6	-3.41258478	-2.85570407	-2.31318998
6	6.10291481	-0.33120421	-1.83058989	1	-4.13688517	-3.66370416	-2.16219020
1	6.58561468	0.10639581	-2.69799018	1	-2.80018497	-3.11450410	-3.18689013
6	4.97421503	0.28199580	-1.27728987	1	-2.77168489	-2.81910419	-1.43198991
6	4.43211508	-2.08290410	1.77681017	1	7.51921511	-1.95500422	-1.75748980
6	4.46331501	1.60519576	-1.87968981	1	-8.22908592	-0.64250416	-0.39998990
6	5.30591488	-3.24710417	2.27760983	1	0.63861513	-5.45430374	0.18141012
1	5.29851484	-4.10040379	1.59061015	1	1.07311511	-2.58870411	-3.61539006
1	6.34521484	-2.94420409	2.44010997	1	0.95321512	-0.81830412	-3.50879002
1	4.91651487	-3.60130405	3.23880982	1	-0.49518484	-1.80940425	-3.27969003
6	4.46601486	-1.00360429	2.87700987	8	-0.00658486	-0.30800420	1.71731019
1	4.03871489	-1.38900423	3.81130981	6	0.89531517	3.47769594	0.52011013
1	5.49941492	-0.70160413	3.07950997	6	1.60341513	3.91269588	1.77391016
1	3.91091514	-0.11430420	2.57621002	6	0.84481514	0.66879588	3.80690980
6	3.01021504	-2.65380406	1.62001014	6	-0.10308486	-0.32020420	3.13320994
1	2.99501514	-3.42420411	0.84051013	8	0.80431515	2.31609583	0.12221012
1	2.67591524	-3.11650419	2.55671000	1	-1.13298488	-0.08450420	3.42900991
1	2.28141522	-1.88560426	1.35911012	1	0.98671520	4.68419600	2.24550986
6	5.39781475	2.15439582	-2.97319007	8	0.38481516	4.49549627	-0.15948988
1	6.41311502	2.32379580	-2.60009003	8	-2.08688474	3.72709584	0.48281011
1	5.45631504	1.49479580	-3.84529018	8	-2.71188474	3.55959582	-1.68668985
1	5.01271486	3.11859584	-3.32459021	6	-0.48188484	4.20419598	-1.27398992
6	4.39211512	2.69089580	-0.78698987	6	-0.54028487	5.45089626	-2.14069009
1	3.77551508	2.36689591	0.05171011	1	-0.08278485	3.35499597	-1.83428991
1	5.39461470	2.90799594	-0.40218988	6	-1.84528482	3.80409575	-0.70098984
1	3.98221517	3.62239575	-1.19918990	6	-4.03398514	3.14869595	-1.26698983
6	3.08941507	1.40779579	-2.54649019	1	-3.98518491	2.18859577	-0.75278986
1	2.33831525	1.03289580	-1.85108984	1	-4.46708488	3.90259576	-0.60758984
1	2.72081518	2.35399580	-2.96309018	1	-4.61158514	3.06039596	-2.18469000
1	3.16661525	0.68859583	-3.36889005	1	-1.19268489	5.27059603	-2.99629021
6	-4.34318495	-0.93260413	-0.01708989	1	0.45981514	5.69649601	-2.50539017
6	-4.96328497	-1.14880431	-1.29148984	1	-0.92618483	6.30189610	-1.57428992
6	-6.35338497	-1.03240430	-1.38988984	1	0.11641515	-1.33050430	3.50940990
1	-6.84078503	-1.18980432	-2.34599018	1	2.52691507	4.41169596	1.45411015
6	-7.15008497	-0.72370416	-0.29358989	6	1.90201521	2.75549579	2.72110987

6	-6.54588509	-0.53270411	0.94341016	1	0.69931513	0.58649588	4.89081001
1	-7.18128490	-0.30160421	1.79161012	6	0.64061517	2.12139583	3.32980990
6	-5.16208506	-0.62970412	1.11921012	1	1.87651515	0.34759581	3.62110996
6	-4.14588499	-1.51920426	-2.54269004	1	2.49911523	2.00699592	2.18570995
6	-4.55978489	-0.40340421	2.51770997	1	2.56141520	3.11859584	3.51721001
6	-3.63508487	0.82869583	2.49880981	1	-0.16688487	2.13219595	2.59070992
1	-4.19788504	1.72339571	2.21270990	1	0.29131514	2.75189590	4.15491009

## I-5\_LC



Zero-point vibrational energy	3116563.3 (Joules/Mol)
	744.87651 (Kcal/Mol)
Zero-point correction=	1.187036 (Hartree/Particle)
Thermal correction to Energy=	1.260692
Thermal correction to Enthalpy=	1.261636
Thermal correction to Gibbs Free Energy=	1.064951
Sum of electronic and zero-point Energies=	-3176.019960
Sum of electronic and thermal Energies=	-3175.946304
Sum of electronic and thermal Enthalpies=	-3175.945360
Sum of electronic and thermal Free Energies=	-3176.142045

cartesian							
12	-2.52937508	-0.24490061	-0.04085302	1	1.82562494	3.15809917	3.27634716
12	-0.80797499	2.15919924	0.00774698	6	1.73722494	3.28939915	-4.74675322
8	-3.37567520	-1.65160060	-0.92995298	1	1.95642495	4.32989931	-5.00905323
8	0.62042499	3.24799919	-0.45665303	1	2.64762497	2.69799924	-4.88975334

8	-2.63727498	1.64199936	-0.68085301	1	0.99492496	2.92039919	-5.46345329
8	-2.06747508	3.45979929	1.12854695	6	0.89302498	1.65689933	-3.10735297
8	-4.15217495	4.28569937	1.15714693	1	0.50392497	1.44209933	-2.11055303
6	-3.66387510	2.55039930	-0.44015303	1	0.16772497	1.28729939	-3.84185290
6	-4.02267504	3.37209916	-1.68415308	1	1.81552494	1.07769942	-3.22085285
1	-4.57757521	2.04719925	-0.08645302	6	-0.13797504	3.97049928	-3.29725289
6	-3.22117519	3.47159934	0.69034702	1	0.06032497	5.01629925	-3.55735302
6	-3.74297500	5.20639944	2.19174719	1	-0.85327500	3.56939936	-4.02575302
1	-4.63347530	5.78549957	2.42844701	1	-0.60087502	3.95869923	-2.30945301
1	-2.94547510	5.85359955	1.82454693	1	-5.45527506	-5.74300051	-3.46665287
6	-3.89487505	-2.67650080	-1.59855306	1	5.28592491	5.02989960	-2.03175282
6	-5.29097509	-2.69260073	-1.92325306	1	-3.39367509	4.65699959	3.06734705
6	-5.81307507	-3.80700064	-2.58675289	1	-4.84107494	4.06879950	-1.48295307
1	-6.86827517	-3.84020066	-2.83605289	1	-4.32917500	2.68169928	-2.47225285
6	-5.02097511	-4.88940048	-2.95185304	1	-3.15327501	3.93139935	-2.04035282
6	-3.66137505	-4.85380030	-2.66545296	8	-0.70757502	0.26269940	0.52024704
1	-3.05247498	-5.69630051	-2.97565293	6	0.32682496	-0.44980061	1.17764699
6	-3.06797504	-3.77370071	-2.00515294	6	1.59482491	-0.56760055	0.33914694
6	-6.21997499	-1.51380062	-1.57815301	1	0.56812495	0.04849939	2.13004708
6	-1.54967511	-3.77950072	-1.75295305	6	2.69942498	-1.34370065	1.05814695
6	-7.66407490	-1.73560059	-2.06165290	1	1.95272493	0.43689939	0.08314697
1	-7.72327518	-1.85900068	-3.14805293	1	1.34412491	-1.06060064	-0.60735297
1	-8.13277531	-2.60590076	-1.58985305	8	-3.51767516	-0.04710060	1.81164694
1	-8.26857471	-0.85930055	-1.80025303	6	-3.61217499	-0.85270059	2.73864698
6	-6.29477501	-1.31880069	-0.05165302	6	-4.44497490	-0.55500060	3.95574713
1	-6.93797493	-0.46490061	0.19904697	8	-2.93457508	-1.98580062	2.63594699
1	-6.71827507	-2.21100068	0.42434695	6	-3.63307500	-0.47680059	5.26164675
1	-5.30537510	-1.14580059	0.36994699	1	-5.23107529	-1.31500065	4.04534674
6	-5.72087526	-0.22750062	-2.26605296	1	-4.93747520	0.39639941	3.75184703
1	-5.75837517	-0.34030059	-3.35505295	6	-3.03537512	-3.05600071	3.61124706
1	-6.35867500	0.62439942	-1.99575305	1	-2.73557520	0.13099940	5.09694672
1	-4.69017506	0.00449940	-1.99475300	1	-4.24097490	0.06849940	5.99074697
6	-0.86087501	-5.03780031	-2.31105304	1	-4.08617496	-3.34760070	3.70934701
1	-1.23247504	-5.95730066	-1.84615302	1	-2.50537515	-3.87270069	3.12184715
1	-0.97907501	-5.12770033	-3.39585304	6	-3.25707507	-1.83370066	5.85574675
1	0.21402496	-4.98040056	-2.10515285	1	-4.17687511	-2.37510085	6.11384678
6	-1.25637507	-3.76150084	-0.23985302	1	-2.72487497	-1.67080069	6.79914665
1	-1.74737513	-2.92390084	0.25794700	6	-2.40047503	-2.71690083	4.94904661
1	-1.62347507	-4.68440056	0.22464697	1	-1.42177510	-2.25930071	4.76354694
1	-0.17677501	-3.69750071	-0.05535302	1	-2.20437503	-3.66700077	5.45934677
6	-0.89087504	-2.57860065	-2.46045303	1	-0.02797503	-1.45840061	1.43574691

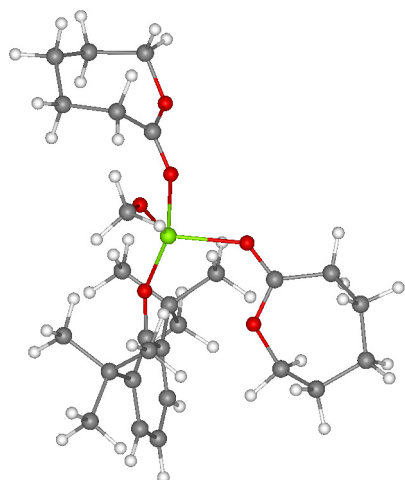
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1	-1.30307508	-1.62500060	-2.12795281	6	3.96772480	-1.50540066	0.21864697
1	0.19062497	-2.56890082	-2.28055286	1	2.32212496	-2.33710074	1.34064698
1	-1.05017507	-2.64340067	-3.54205298	1	2.94992495	-0.83450055	1.99914706
6	1.79432487	3.72119927	-0.86455297	6	5.04772472	-2.29240084	0.95404702
6	2.14622498	3.68769932	-2.25125289	1	4.36132479	-0.52290058	-0.06015302
6	3.40502501	4.16329956	-2.63105297	1	3.72712493	-2.01190066	-0.72285300
1	3.69842482	4.13829947	-3.67515302	6	6.31742477	-2.46410084	0.15974697
6	4.31032515	4.67519951	-1.70835304	1	4.69302511	-3.28720069	1.24764693
6	3.94582486	4.73939943	-0.36805305	1	5.33022499	-1.79310060	1.88954699
1	4.65742493	5.15909958	0.33504698	8	7.16562510	-3.32420087	0.78634703
6	2.70322490	4.28649950	0.08554698	8	6.58372498	-1.92500067	-0.89245301
6	1.17272496	3.15749931	-3.32075286	6	8.44272518	-3.49160075	0.16804697
6	2.33252501	4.42939949	1.57424700	6	9.27692509	-2.22500086	0.35104695
6	3.44442487	5.10809946	2.39404702	1	8.31452465	-3.66070080	-0.90425301
1	3.66642499	6.11769962	2.03284717	6	9.11262512	-4.68710041	0.83134699
1	3.11812496	5.19959927	3.43644714	8	10.29522514	-2.21340084	-0.52805299
1	4.37492514	4.53029966	2.39444709	8	9.08222485	-1.37430060	1.18894696
6	1.07432485	5.30949926	1.72124696	6	11.17032528	-1.07680058	-0.43575302
1	1.26952493	6.31499958	1.33194697	1	11.92112446	-1.22330058	-1.21095300
1	0.22762498	4.89299965	1.17514694	1	11.63882446	-1.03370059	0.54984701
1	0.79592496	5.40589952	2.77894711	1	10.61172485	-0.15560061	-0.61115301
6	2.10012484	3.04919934	2.21924710	1	10.09252453	-4.86450052	0.38254699
1	1.30472493	2.49859929	1.71444690	1	8.49662495	-5.57880068	0.69094700
1	3.01042485	2.44219923	2.16674709	1	9.23722458	-4.51350069	1.90314698

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### S1.3. CC sequence, mononuclear mechanism

#### I-1\_CC

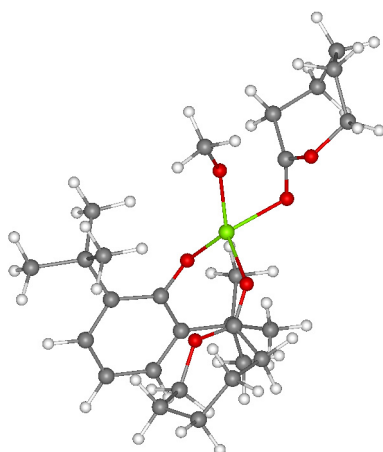


Zero-point vibrational energy	1784683.0 (Joules/Mol)
	426.54948 (Kcal/Mol)
Zero-point correction=	0.679750 (Hartree/Particle)
Thermal correction to Energy=	0.719103
Thermal correction to Enthalpy=	0.720047
Thermal correction to Gibbs Free Energy=	0.604580
Sum of electronic and zero-point Energies=	-1705.797246
Sum of electronic and thermal Energies=	-1705.757893
Sum of electronic and thermal Enthalpies=	-1705.756949
Sum of electronic and thermal Free Energies=	-1705.872416

cartesian											
8	-1.63320374	0.75279218	-2.54900122	1	-0.22190370	0.54409218	1.85919869				
6	-1.40160370	0.82269216	-3.91410136	8	0.18789630	2.31889224	-0.29470125				
1	-1.03700376	-0.13080782	-4.33640146	6	1.31929624	2.47839212	0.17269874				
1	-0.65780371	1.59449220	-4.18610144	8	2.16109633	1.46659219	0.10809873				
12	-0.80780369	0.56899220	-0.88910127	6	1.73529625	3.79649210	0.77209872				
8	0.13459630	-0.89550781	-0.14480126	6	3.46119618	1.46709216	0.74919873				
6	1.22249627	-1.51050782	0.28239873	6	2.92789626	4.46169233	0.06189874				
6	2.20499635	-1.99840784	-0.64440125	6	4.46029615	2.38929224	0.07159874				
6	3.39919639	-2.52220774	-0.13730127	1	3.76279640	0.42199215	0.67419875				
1	4.16589642	-2.87290788	-0.82050127	1	2.92339635	5.52069235	0.34079874				
6	3.64339638	-2.62950778	1.22909880	1	2.76799631	4.43219233	-1.02230132				
6	2.64119625	-2.25680780	2.12049866	1	1.96859622	3.64189219	1.83319879				
1	2.82149625	-2.40140772	3.18099880	1	0.85299629	4.43609238	0.72429872				
6	1.42389631	-1.72120786	1.68899870	6	4.29299641	3.86909223	0.41459873				

6	1.96959639	-1.98390794	-2.16870117	1	3.33159637	1.70519221	1.81019878
6	0.32569629	-1.39340782	2.71959877	1	4.40389633	2.22809219	-1.01120126
6	2.00169635	-0.54830784	-2.72600126	1	5.45969629	2.06109214	0.38019875
1	1.22779632	0.08459218	-2.29080129	1	4.47169638	4.00689220	1.48959875
1	1.84669626	-0.55240786	-3.81130123	1	5.07019615	4.44599199	-0.09900127
1	2.97029638	-0.07790782	-2.52240133	8	-2.44980359	0.88429219	0.33769873
6	0.62799633	-2.66250777	-2.51400137	6	-3.67240381	0.92199218	0.20779873
1	-0.21590370	-2.15730786	-2.04460120	6	-4.36730385	0.67469215	-1.10120130
1	0.63289630	-3.70440793	-2.17460132	8	-4.36890364	1.18019211	1.31499875
1	0.47189629	-2.66190791	-3.59970117	6	-5.16870356	-0.64060783	-1.11420131
6	3.05809641	-2.76440787	-2.93000126	1	-5.03230381	1.51969218	-1.32210124
1	3.12749624	-3.80500793	-2.59570122	1	-3.56980371	0.66189218	-1.85710120
1	4.04889631	-2.30600786	-2.83710122	6	-5.81350374	1.21099222	1.31009877
1	2.80979633	-2.77670789	-3.99730134	1	-4.55880356	-1.44370782	-0.68430126
6	0.69249630	-1.87250781	4.13579845	1	-5.32900381	-0.91320783	-2.16200137
1	1.56999624	-1.35650778	4.54119873	1	-6.16040373	1.96529222	0.59519875
1	0.88229632	-2.95060778	4.16879845	1	-6.05050373	1.56709218	2.31359863
1	-0.14370370	-1.66490781	4.81319857	6	-6.52230358	-0.56210786	-0.40940127
6	-0.98840368	-2.10860777	2.34219885	1	-7.16130352	0.15109217	-0.94790125
1	-1.32730365	-1.81810784	1.34779871	1	-7.02310371	-1.53420782	-0.48150125
1	-1.77440369	-1.86410785	3.06779885	6	-6.45480347	-0.14640781	1.06049871
1	-0.84570372	-3.19510794	2.35229874	1	-5.91880369	-0.89490783	1.65619874
6	0.09229630	0.12619218	2.81439877	1	-7.47280359	-0.10070782	1.46559870
1	1.01079631	0.63259214	3.13669872	1	-2.32560372	1.07689226	-4.46610165
1	-0.69010371	0.35279217	3.54929876	1	4.58229637	-3.04120779	1.59229875

## TS-12\_CC



Zero-point vibrational energy

1783379.8 (Joules/Mol)

426.23801 (Kcal/Mol)

Zero-point correction=

0.679254 (Hartree/Particle)

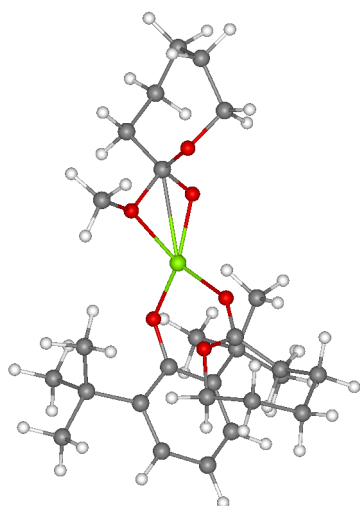


Thermal correction to Energy=	0.717627
Thermal correction to Enthalpy=	0.718571
Thermal correction to Gibbs Free Energy=	0.606288
Sum of electronic and zero-point Energies=	-1705.775815
Sum of electronic and thermal Energies=	-1705.737442
Sum of electronic and thermal Enthalpies=	-1705.736497
Sum of electronic and thermal Free Energies=	-1705.848780

cartesian							
8	0.41141027	-1.15696788	-0.07369613	1	-2.06328964	1.48363209	-2.98629618
6	1.69001031	-1.49026787	-0.03679613	8	-2.59148979	-0.21696796	1.08880389
6	2.30881023	-1.84046793	1.20880389	12	-0.98018974	0.10603204	-0.06809613
6	3.68981028	-2.06046796	1.22960389	1	5.53981018	-2.16926789	0.12200387
1	4.18301010	-2.30446792	2.16520381	6	-3.57408977	-0.00136795	0.32490388
6	4.46741009	-1.99406791	0.07620387	6	-4.36918974	-1.17096794	-0.22409612
6	3.84031034	-1.76226795	-1.14559615	8	-4.13858986	1.23363209	0.39440387
1	4.44991016	-1.77586794	-2.04339623	6	-5.60708952	-1.49636793	0.62680387
6	2.46371031	-1.53326786	-1.24389613	1	-4.65528965	-0.97646797	-1.25979614
6	1.48361027	-2.01206779	2.50000381	1	-3.67498970	-2.01206779	-0.23259613
6	1.80941033	-1.37266791	-2.63079619	6	-5.53198957	1.45693207	0.67950386
6	0.91351026	-0.66596794	2.98640370	1	-5.38068962	-1.31876791	1.68450391
1	0.25141028	-0.21386795	2.24790382	1	-5.82098961	-2.56746793	0.55030388
1	0.33271030	-0.80276799	3.90650368	1	-5.63078976	2.53813219	0.56390387
1	1.72361028	0.04093205	3.20330381	1	-5.70948982	1.22123206	1.73700392
6	0.33601028	-3.01746798	2.26750374	6	-6.84738970	-0.70086795	0.19940388
1	-0.32858971	-2.69306779	1.46680391	1	-7.33648968	-1.20586789	-0.64189613
1	0.74171031	-3.99906802	1.99850392	1	-7.57548952	-0.70156795	1.01930380
1	-0.25518972	-3.13586783	3.18390369	6	-6.53958988	0.74493206	-0.21359614
6	2.32831025	-2.57186794	3.65860367	1	-7.46748972	1.32913208	-0.19399613
1	2.78131032	-3.53636789	3.40650368	1	-6.17908955	0.79373205	-1.24669611
1	3.12621021	-1.88756788	3.96840382	8	-0.20808974	1.96393204	0.47260389
1	1.68311024	-2.72986794	4.53010368	6	0.94761026	2.36193204	0.65290385
6	2.79891038	-1.65776789	-3.77539635	8	1.93371034	1.60823214	0.21490386
1	3.62341022	-0.93686795	-3.81029630	6	1.21631026	3.68193221	1.32550383
1	3.22491026	-2.66426802	-3.70729613	6	1.97771025	4.68893194	0.44520387
1	2.27051020	-1.58856785	-4.73289633	1	1.77321029	3.49763203	2.25290370
6	0.65211028	-2.38096786	-2.79249620	1	0.23911029	4.07623196	1.60690391
1	-0.11508973	-2.24266791	-2.03059626	6	3.33221030	1.87703204	0.49130389
1	0.18671027	-2.26826787	-3.77949619	1	1.52491033	4.71423197	-0.55309612
1	1.02981031	-3.40636802	-2.71309614	1	1.81881022	5.68303204	0.87590390
6	1.29531026	0.06283205	-2.84889627	1	3.46591020	1.96803212	1.57440388

1	2.12041020	0.78233200	-2.80179620	1	3.81631017	0.95493203	0.16850388
1	0.81961030	0.15553205	-3.83279634	6	3.48191023	4.43523169	0.34190387
1	0.55941027	0.35193205	-2.09759617	1	3.92411017	4.51903200	1.34390390
8	-2.42238975	0.30173206	-1.32939613	1	3.93341017	5.23423195	-0.25669613
6	-2.89018965	1.03173208	-2.41749620	6	3.86871028	3.08373213	-0.25889611
1	-3.55088973	1.85293210	-2.09219623	1	3.54871035	3.01313210	-1.30499613
1	-3.45608974	0.39653206	-3.11979628	1	4.96131039	2.99503207	-0.26549613

## I-2\_CC

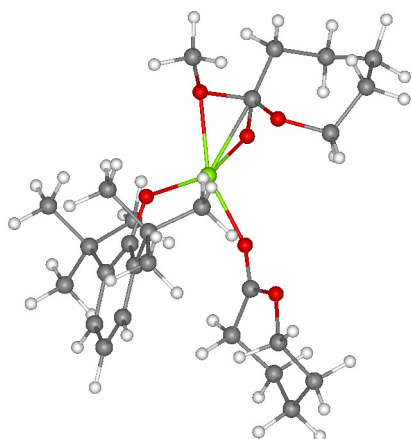


Zero-point vibrational energy	1790760.0 (Joules/Mol)
	428.00192 (Kcal/Mol)
Zero-point correction=	0.682064 (Hartree/Particle)
Thermal correction to Energy=	0.719931
Thermal correction to Enthalpy=	0.720875
Thermal correction to Gibbs Free Energy=	0.610171
Sum of electronic and zero-point Energies=	-1705.786682
Sum of electronic and thermal Energies=	-1705.748816
Sum of electronic and thermal Enthalpies=	-1705.747872
Sum of electronic and thermal Free Energies=	-1705.858576

cartesian							
8	0.25038970	-1.54128444	-0.52589613	1	-3.08721042	2.34221578	-2.03589606
6	1.55038965	-1.49038446	-0.25979611	8	-3.96351027	1.47891557	0.02840389
6	2.04138970	-1.90178442	1.02160394	6	-3.55441022	0.16831554	-0.34559610
6	3.38618970	-1.66128445	1.32230389	8	-2.88151026	-0.48128444	0.59690386
1	3.77998972	-1.92938447	2.29760385	6	-4.69181013	-0.64958447	-0.97319609
6	4.25868988	-1.09088445	0.39690387	12	-1.07961035	-0.25568444	-0.06869611
6	3.80318975	-0.83638448	-0.89599609	1	-5.21001053	-0.06388445	-1.74139607
1	4.51898956	-0.47988445	-1.63059604	1	5.29918957	-0.91248447	0.65930390
6	2.47238970	-1.05808449	-1.26819611	6	-4.86801052	1.53341556	1.13160396

6	1.14478970	-2.68048429	2.00710392	1	-4.53901052	0.83841556	1.91380394
6	2.04238963	-0.95208442	-2.74569607	6	-6.31771040	1.29591560	0.71040386
6	-0.09141032	-1.88158441	2.47390389	1	-4.76451015	2.54961562	1.52370393
1	-0.89181030	-1.89168441	1.73110390	1	-6.97701025	1.77911556	1.44270396
1	-0.52021033	-2.33808422	3.37380385	6	-6.75461054	-0.17248444	0.54540390
1	0.15808968	-0.84528446	2.72550392	1	-6.46301031	1.84231555	-0.22909610
6	0.66888970	-3.97908449	1.32170391	1	-4.21801043	-1.50208449	-1.46999609
1	0.11828968	-3.75778437	0.40500388	6	-5.67481041	-1.16488445	0.08390389
1	1.52198970	-4.61748409	1.06830394	1	-5.08111048	-1.50418448	0.93860388
1	0.00998968	-4.54408455	1.99260390	1	-6.17911053	-2.05678439	-0.30569613
6	1.91628969	-3.08808422	3.27440405	1	-7.59651041	-0.19698445	-0.15749609
1	2.79738975	-3.69548440	3.04440403	1	-7.15621042	-0.53948444	1.49780393
1	2.23938966	-2.22208428	3.86430383	8	0.05928968	1.24481559	0.70280391
1	1.26478970	-3.69228435	3.91470385	6	1.14918971	1.81891561	0.66840386
6	3.21938968	-0.56968445	-3.65929604	8	1.43688965	2.51341558	-0.42329612
1	3.61468959	0.42821556	-3.43489599	6	2.09968972	1.78121555	1.83130395
1	4.04348946	-1.28758442	-3.59569597	6	2.75248981	3.08281565	-0.64669609
1	2.87978959	-0.55708444	-4.70069599	6	2.42978978	3.15791559	2.43530393
6	1.53138971	-2.33438444	-3.20529604	6	3.04598975	4.29811573	0.21720390
1	0.68218970	-2.65698433	-2.59939599	1	2.71668959	3.36051559	-1.70069611
1	1.21378970	-2.29388428	-4.25479603	1	2.81878972	2.98181558	3.44340396
1	2.32318974	-3.08648443	-3.12059617	1	1.50578964	3.73481560	2.56270385
6	0.93418968	0.09231555	-2.98299599	1	3.01308966	1.26161551	1.51130390
1	1.19908965	1.06801558	-2.56409597	1	1.62688971	1.14341557	2.57770395
1	0.76808971	0.22291555	-4.05949593	6	3.45868969	3.96971560	1.65070391
1	-0.01091032	-0.23308444	-2.54619598	1	3.50038958	2.29251575	-0.52989614
8	-2.51511025	0.44661555	-1.40109611	1	2.16978979	4.95741558	0.20140390
6	-2.79721022	1.37281561	-2.44719601	1	3.85688972	4.85051584	-0.27229610
1	-3.59261036	0.99051553	-3.09539604	1	4.40668964	3.41641569	1.63060391
1	-1.88301027	1.47491550	-3.03479600	1	3.66058969	4.90341568	2.18740392

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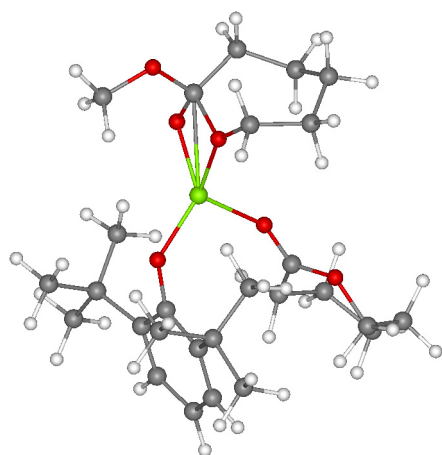


Zero-point vibrational energy	1788747.1 (Joules/Mol)
	427.52081 (Kcal/Mol)
Zero-point correction=	0.681298 (Hartree/Particle)
Thermal correction to Energy=	0.718427
Thermal correction to Enthalpy=	0.719371
Thermal correction to Gibbs Free Energy=	0.611018
Sum of electronic and zero-point Energies=	-1705.780691
Sum of electronic and thermal Energies=	-1705.743562
Sum of electronic and thermal Enthalpies=	-1705.742618
Sum of electronic and thermal Free Energies=	-1705.850971

cartesian							
8	0.24478835	-1.67412949	-0.32297692	1	-3.45271158	-1.51352954	-2.20877695
6	1.54718840	-1.43452954	-0.26237693	8	-3.17851162	0.34757045	-0.68777692
6	2.27778840	-1.73972952	0.93122309	6	-3.53521156	-0.62462956	0.37402308
6	3.61268830	-1.33162951	1.01452315	8	-2.83101153	-0.37542954	1.45772302
1	4.18368816	-1.52022958	1.91822302	6	-5.04001188	-0.79232955	0.56262308
6	4.25228834	-0.68542951	-0.04217692	12	-1.18441164	-0.62062955	0.38092306
6	3.56978846	-0.51442951	-1.24617696	1	-5.53341198	-0.97352952	-0.39847693
1	4.11058807	-0.08632953	-2.08467698	1	5.29098797	-0.37612954	0.05032308
6	2.23468852	-0.90412956	-1.40257692	6	-3.56971169	1.70197046	-0.43477693
6	1.64438844	-2.59272933	2.04992318	1	-3.29821157	1.97757041	0.59212309
6	1.56468844	-0.87412953	-2.79167700	6	-5.04951191	1.94217050	-0.72647691
6	0.33978835	-1.99292958	2.62472296	1	-2.95571160	2.29797053	-1.11557698
1	-0.52971166	-2.25762939	2.01732302	1	-5.18411160	2.99567056	-1.00187695
1	0.13608834	-2.40432930	3.61992311	6	-6.03201199	1.60237050	0.40952307
1	0.39358833	-0.90442955	2.73692298	1	-5.29131174	1.36547041	-1.62707698
6	1.33308840	-3.99182940	1.47692311	1	-5.15571165	-1.69632959	1.16902304
1	0.65868837	-3.91782951	0.62072307	6	-5.66531181	0.39937046	1.29302311
1	2.25298834	-4.48992920	1.15282309	1	-4.96581173	0.70217049	2.07842302
1	0.85648835	-4.62072945	2.23932314	1	-6.57301188	0.06577048	1.80862308
6	2.60698843	-2.78162932	3.23542309	1	-7.02021170	1.43997049	-0.03827692
1	3.54128838	-3.26732945	2.93682313	1	-6.14401197	2.47607064	1.06302309
1	2.85348845	-1.83252954	3.72592306	8	-0.11161165	1.08457041	0.78702307
1	2.13558841	-3.42522931	3.98582315	6	0.87358832	1.80287051	0.62592310
6	2.52298832	-0.35772952	-3.87887692	8	0.89628834	2.57047057	-0.45817691
1	2.82088852	0.68407047	-3.71087694	6	1.98798847	1.86657047	1.63232303
1	3.42988849	-0.96622956	-3.95687699	6	2.08128834	3.30927062	-0.84657693
1	2.02058840	-0.39762953	-4.85157681	6	2.22078848	3.25917053	2.24472308
6	1.17138839	-2.31702948	-3.17457700	6	2.34998846	4.53097057	0.01702308

1	0.48208833	-2.74002934	-2.44107699	1	1.85418844	3.60627055	-1.87127697
1	0.68588835	-2.33132935	-4.15847683	1	2.77268839	3.11157060	3.17872310
1	2.05758834	-2.95882940	-3.22597694	1	1.25848842	3.70307064	2.52732301
6	0.31018835	0.01947048	-2.84337687	1	2.90358829	1.48577046	1.16032302
1	0.51898837	1.03187048	-2.48517704	1	1.72428846	1.15067041	2.41042304
1	-0.05021165	0.09747048	-3.87647700	6	3.00998831	4.22187042	1.35942304
1	-0.50371164	-0.39632952	-2.24847698	1	2.93148851	2.62047052	-0.87437695
8	-2.91061163	-1.82912958	-0.21447693	1	1.40648842	5.07177067	0.15862308
6	-3.37271166	-2.31852937	-1.47297692	1	3.00338840	5.19577074	-0.56037694
1	-4.34011173	-2.81902933	-1.35757697	1	4.00668812	3.79937053	1.17652309
1	-2.63431168	-3.04852939	-1.80907691	1	3.16958833	5.15917063	1.90412307

### I-3\_CC



Zero-point vibrational energy	1789228.3 (Joules/Mol)
	427.63583 (Kcal/Mol)
Zero-point correction=	0.681481 (Hartree/Particle)
Thermal correction to Energy=	0.719233
Thermal correction to Enthalpy=	0.720177
Thermal correction to Gibbs Free Energy=	0.610751
Sum of electronic and zero-point Energies=	-1705.795191
Sum of electronic and thermal Energies=	-1705.757440
Sum of electronic and thermal Enthalpies=	-1705.756495
Sum of electronic and thermal Free Energies=	-1705.865921

### cartesian

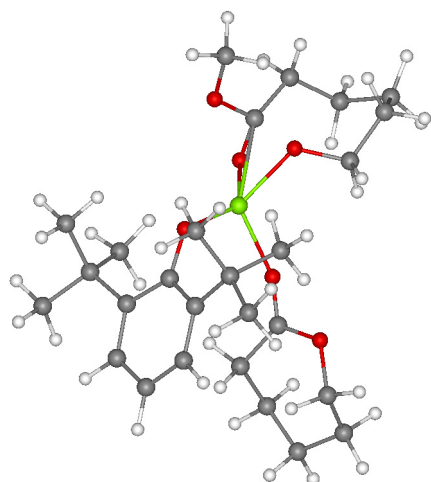
12	-1.32603967	-0.55938852	0.35671797	1	0.27376026	-3.02628875	3.33641791
8	-4.71623993	-1.63358855	0.46611795	1	-0.46963978	-2.26688862	1.95091796
6	-4.11123991	-2.89658856	0.21591796	8	-2.79233980	-0.95398855	1.56241798
1	-3.42143965	-2.85068870	-0.63568205	6	-3.83493972	-0.60638857	0.82461792
1	-4.92984009	-3.57638860	-0.02838204	6	-4.70974016	0.52411151	1.37811792

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1	-3.57683969	-3.26008868	1.09751797	8	-3.13833976	-0.13808854	-0.49248204
8	-0.00773977	-1.66278851	-0.46178207	6	-4.15483999	1.94351149	1.23261797
6	1.30666029	-1.47548854	-0.49968204	1	-5.70673990	0.46231148	0.92911792
6	1.90356016	-0.80138850	-1.61558211	1	-4.82863998	0.27191147	2.43601799
6	3.25946021	-0.46368855	-1.53578210	6	-3.89053965	0.54091144	-1.49598205
1	3.73326039	0.07141146	-2.35298204	1	-3.07163978	1.94511151	1.40541792
6	4.04646015	-0.82498848	-0.44348204	1	-4.58614016	2.55911136	2.03121805
6	3.48826027	-1.61348855	0.56121790	1	-4.92884016	0.19221146	-1.44818211
1	4.13585997	-1.95308852	1.36291790	1	-3.48633981	0.22941145	-2.46498203
6	2.13806033	-1.97798848	0.55391794	6	-4.49064016	2.61881137	-0.10438204
6	1.11556029	-0.56578851	-2.92128205	1	-5.57764006	2.56281137	-0.25488204
6	1.59136033	-2.96728873	1.60391796	1	-4.25224018	3.68751144	-0.03338205
6	-0.10053977	0.36361146	-2.74048209	6	-3.78433967	2.05161142	-1.33808208
1	-0.88833976	-0.12358854	-2.16378212	1	-2.71853971	2.31041145	-1.31108212
1	-0.52963978	0.61281145	-3.71888208	1	-4.19553995	2.52441144	-2.23998213
1	0.17136024	1.30241144	-2.24838209	8	-0.24823976	1.09011149	0.85171795
6	0.62716019	-1.93038857	-3.45228195	6	0.79226023	1.74681151	0.77931792
1	-0.01243977	-2.42758870	-2.72028208	8	0.82596022	2.71761131	-0.12328205
1	1.47666025	-2.58598852	-3.67118216	6	1.95486021	1.51011145	1.69951797
1	0.05546023	-1.79538846	-4.37898207	6	2.03556037	3.47061133	-0.39678204
6	1.99446034	0.06441145	-4.01548195	6	2.31036019	2.70961142	2.59651804
1	2.86916018	-0.55048859	-4.25058174	6	2.40736032	4.44751120	0.70651793
1	2.34226036	1.06831145	-3.74498200	1	1.78336024	4.00291157	-1.31458211
1	1.40946031	0.16221146	-4.93638182	1	2.90166020	2.32081127	3.43161798
6	2.69586039	-3.44798875	2.56231785	1	1.39566028	3.12281132	3.03861785
1	3.10186028	-2.63328862	3.17311788	1	2.81986022	1.19611144	1.10011792
1	3.52486038	-3.92758870	2.03181791	1	1.67886031	0.65101147	2.30941796
1	2.27756023	-4.19068861	3.25031781	6	3.11096025	3.81011128	1.90301788
6	1.04066026	-4.21328878	0.87841791	1	2.84346032	2.76741147	-0.62218207
1	0.24966024	-3.94058871	0.17741796	1	1.50166023	4.98011160	1.02041793
1	0.63056022	-4.92578840	1.60491788	1	3.06866026	5.19961119	0.26011795
1	1.83736026	-4.71878862	0.32201797	1	4.07066011	3.39391136	1.57021797
6	0.47646022	-2.36618853	2.48481798	1	3.35196018	4.59041119	2.63341784
1	0.76066023	-1.39088857	2.89521790	1	5.09935999	-0.55408859	-0.40948203

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# TS-34\_CC

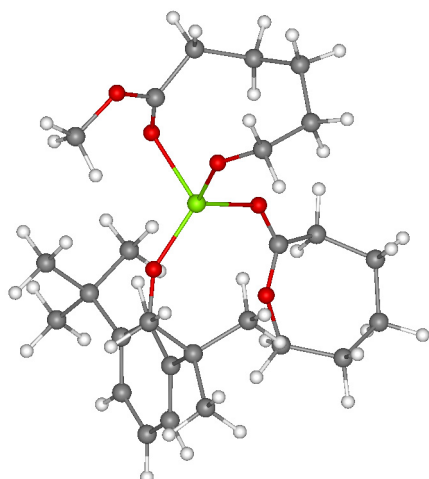


Zero-point vibrational energy	1786096.1 (Joules/Mol)
	426.88722 (Kcal/Mol)
Zero-point correction=	0.680288 (Hartree/Particle)
Thermal correction to Energy=	0.717896
Thermal correction to Enthalpy=	0.718841
Thermal correction to Gibbs Free Energy=	0.609286
Sum of electronic and zero-point Energies=	-1705.777674
Sum of electronic and thermal Energies=	-1705.740065
Sum of electronic and thermal Enthalpies=	-1705.739121
Sum of electronic and thermal Free Energies=	-1705.848676

cartesian													
8	0.05624477	-1.57122314	-0.39618218	1	-4.37425518	-1.57902312	-1.53418219						
6	1.37754476	-1.45982313	-0.42278218	8	-2.96445537	0.19687694	-0.64928216						
6	2.17114472	-1.98902309	0.64811784	6	-3.60495520	-0.69972306	0.84801787						
6	3.53784466	-1.69412315	0.66631782	8	-2.68215537	-0.44902307	1.69331777						
1	4.15784454	-2.05532289	1.48061776	6	-5.01335526	-0.20202306	1.10591781						
6	4.14734459	-0.94912302	-0.34208214	12	-1.25645530	-0.36332306	0.27131784						
6	3.39364481	-0.57122302	-1.45228219	1	-5.68015528	-0.45692307	0.27911782						
1	3.90454483	-0.07602306	-2.27248216	1	5.21164465	-0.72922307	-0.29788220						
6	2.02414465	-0.84532303	-1.54648221	6	-3.21575522	1.56867695	-0.91658217						
6	1.56134474	-2.92422295	1.71291780	1	-2.77495527	2.21737695	-0.14088216						
6	1.27204478	-0.61362302	-2.87488222	6	-4.70205545	1.88307691	-1.07418227						
6	0.53204477	-2.21162295	2.61091781	1	-2.69615531	1.80627692	-1.85488224						
1	-0.37365526	-1.93732309	2.06961775	1	-4.81645536	2.74487710	-1.74368227						
1	0.21684477	-2.87582302	3.42471790	6	-5.44525528	2.18587708	0.23511782						
1	0.95464474	-1.31182313	3.07161784	1	-5.16145515	1.03587687	-1.59728217						
6	0.88294476	-4.12022305	1.01161778	1	-5.34085512	-0.79462302	1.96971774						
1	0.09744477	-3.78632307	0.33181781	6	-5.08565521	1.29307687	1.43031776						

1	1.61744475	-4.69512320	0.43711782	1	-4.12705517	1.59347689	1.86421776
1	0.43584475	-4.79092312	1.75561774	1	-5.83135509	1.45707691	2.21591783
6	2.63744473	-3.50162292	2.64991784	1	-6.52445507	2.12237692	0.04461783
1	3.41394472	-4.04512310	2.10171771	1	-5.25455523	3.22717690	0.52411783
1	3.12154484	-2.72942305	3.25911784	8	-0.09695524	1.24047685	0.77591783
1	2.16844463	-4.20982313	3.34151769	6	0.98724478	1.82047689	0.70571786
6	2.20404482	-0.06312306	-3.96858239	8	1.11084473	2.75087690	-0.23328216
1	2.58974481	0.93377697	-3.72438216	6	2.10854483	1.54397690	1.66541779
1	3.05534482	-0.72442305	-4.15958214	6	2.37964463	3.39537692	-0.51068217
1	1.64584470	0.02707694	-4.90678215	6	2.53144479	2.75407696	2.51761770
6	0.73364478	-1.97232306	-3.37228227	6	2.80394483	4.39097691	0.55671787
1	0.05994476	-2.41722298	-2.63718224	1	2.18824482	3.90377712	-1.45628226
1	0.18374476	-1.84152305	-4.31278181	1	3.07084465	2.36207700	3.38581777
1	1.55724478	-2.67072296	-3.55558228	1	1.64034474	3.25537705	2.91441774
6	0.09504475	0.37497693	-2.75848222	1	2.96204472	1.14247692	1.10251784
1	0.39314476	1.31187689	-2.27808213	1	1.75554478	0.73607695	2.30501771
1	-0.28235525	0.62177694	-3.75858212	6	3.43004465	3.75827694	1.79781783
1	-0.74295521	-0.05692307	-2.20898223	1	3.13574481	2.62367702	-0.68698215
8	-3.47085524	-1.95982313	0.29901785	1	1.93604469	5.00587654	0.82391787
6	-4.32905531	-2.35782290	-0.76918215	1	3.53104472	5.06857681	0.09331783
1	-5.33185530	-2.60052299	-0.40168220	1	4.36224461	3.25577712	1.50871778
1	-3.87985539	-3.25822306	-1.19058216	1	3.71384478	4.55097675	2.49901772

#### I-4\_CC



Zero-point vibrational energy	1785379.5 (Joules/Mol)
	426.71594 (Kcal/Mol)
Zero-point correction=	0.680015 (Hartree/Particle)
Thermal correction to Energy=	0.718940
Thermal correction to Enthalpy=	0.719884
Thermal correction to Gibbs Free Energy=	0.606721

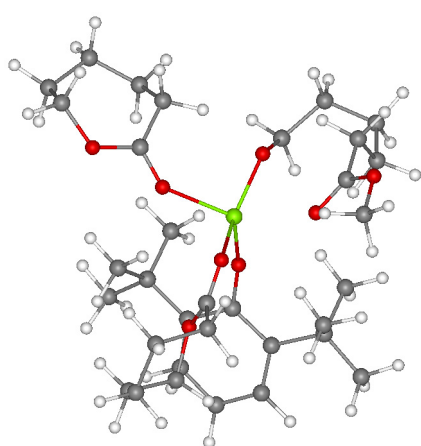


Sum of electronic and zero-point Energies=	-1705.795516
Sum of electronic and thermal Energies=	-1705.756591
Sum of electronic and thermal Enthalpies=	-1705.755647
Sum of electronic and thermal Free Energies=	-1705.868810

cartesian											
12	-1.31694233	-0.37061539	0.06525776	1	0.59645766	-1.11561537	3.93375778				
8	-4.11644220	-2.53401542	0.44225776	1	0.16045766	-0.56181538	2.31735778				
6	-3.08504224	-3.52941537	0.32925773	8	-2.63994241	-1.15431535	1.43725777				
1	-2.35734224	-3.21721530	-0.42234224	6	-3.75714231	-1.34901536	0.92015779				
1	-3.59404230	-4.43581533	0.00475775	6	-4.93104267	-0.41631538	1.03005779				
1	-2.59114242	-3.68531537	1.28935766	8	-2.81434226	-0.38061538	-1.08194232				
8	0.29085767	-1.35411537	-0.04504225	6	-4.64674234	1.09118462	0.94165778				
6	1.60835767	-1.38961542	-0.16484225	1	-5.68024254	-0.72811538	0.29905778				
6	2.23075771	-1.23641539	-1.44854224	1	-5.35644245	-0.65131539	2.01625776				
6	3.62595773	-1.14701545	-1.50544226	6	-3.49894238	0.36258462	-2.03124213				
1	4.11855745	-1.00551534	-2.46184206	1	-3.60854220	1.29068458	1.22495770				
6	4.42395735	-1.25001538	-0.36894226	1	-5.26184273	1.57818460	1.70725775				
6	3.81735778	-1.51241541	0.85625780	1	-4.39934254	-0.18531539	-2.36784220				
1	4.45565748	-1.65471542	1.72255766	1	-2.88744235	0.51458460	-2.93974209				
6	2.42895770	-1.61201537	0.99135774	6	-4.98244238	1.75928462	-0.40544224				
6	1.41225767	-1.20921540	-2.75604224	1	-5.91834259	1.33058465	-0.79064220				
6	1.81855774	-1.99531543	2.35415792	1	-5.21224260	2.81228471	-0.19624224				
6	0.56825763	0.07378461	-2.87534213	6	-3.92484236	1.73968458	-1.51574230				
1	-0.19644235	0.14078462	-2.10044217	1	-3.02454233	2.26438451	-1.16584229				
1	0.04755765	0.09988461	-3.84004211	1	-4.31594276	2.32548451	-2.36054206				
1	1.20115769	0.96528459	-2.80724216	8	-0.88794237	1.52528465	0.82615775				
6	0.50065762	-2.45101547	-2.83864212	6	0.17585765	2.15278459	0.88395774				
1	-0.18944235	-2.49651551	-1.99614227	8	1.19855773	1.69108462	0.19675776				
1	1.10365772	-3.36561537	-2.83794212	6	0.28685766	3.42208457	1.68575776				
1	-0.08524235	-2.43131542	-3.76554227	6	2.54085779	2.23448467	0.29915774				
6	2.31595778	-1.24731541	-4.00314236	6	0.65885764	4.65878439	0.84745777				
1	2.97025776	-2.12531543	-4.01004219	6	2.68005776	3.59928465	-0.35244226				
1	2.94025779	-0.35171539	-4.09834194	1	3.13985777	1.47878456	-0.20944224				
1	1.68835771	-1.29841542	-4.89964199	1	0.38035762	5.54238462	1.43105769				
6	2.89535761	-2.35411549	3.39385772	1	0.03975765	4.68448448	-0.05704224				
1	3.53945780	-1.50351536	3.64385772	1	1.02575767	3.27288461	2.48315787				
1	3.53195763	-3.18001533	3.05975795	1	-0.68324238	3.55868459	2.16525793				
1	2.40715766	-2.67161536	4.32215786	6	2.14005780	4.76078463	0.48205775				
6	0.92315763	-3.24171543	2.19795775	1	2.83755779	2.24498463	1.35305774				
1	0.11915766	-3.06381536	1.48345768	1	2.19925761	3.56588459	-1.33704233				

1	0.48095763	-3.51541543	3.16415787	1	3.74875760	3.75808454	-0.53714222
1	1.51495767	-4.09321547	1.84435773	1	2.72835779	4.83808470	1.40625775
6	1.00145769	-0.83561540	2.95365787	1	2.30405760	5.69788456	-0.06144224
1	1.63455772	0.04908461	3.09485793	1	5.50635767	-1.17701542	-0.44584227

### TS-45\_CC



Zero-point vibrational energy	2202689.7 (Joules/Mol)
	526.45548 (Kcal/Mol)
Zero-point correction	0.838960 (Hartree/Particle)
Thermal correction to Energy	0.886166
Thermal correction to Enthalpy	0.887110
Thermal correction to Gibbs Free Energy	0.754432
Sum of electronic and zero-point Energies	-2090.658608
Sum of electronic and Thermal Energies	-2090.611402
Sum of electronic and Thermal Enthalpies	-2090.610457
Sum of electronic and Thermal Free Energies	-2090.743136

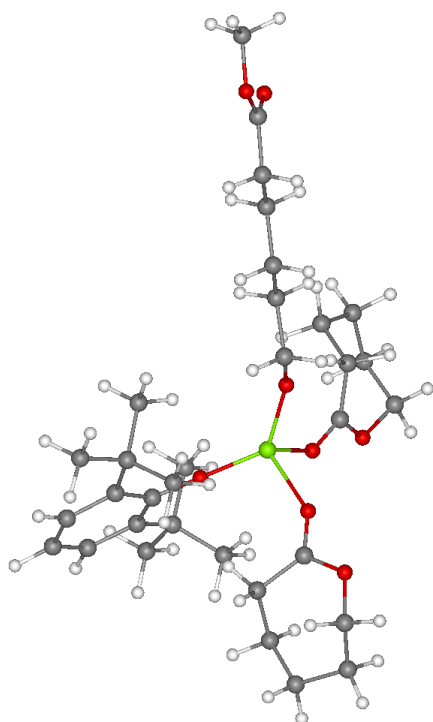
cartesian							
8	0.70412910	-0.07527923	1.06377423	1	-0.63107091	5.26272058	1.27927423
6	1.82382905	-0.64457923	1.47887421	1	-0.53757089	3.50122070	1.12777424
6	1.86502910	-2.04957914	1.81007421	6	-3.06387091	2.92782068	2.33197427
6	3.10332918	-2.64157915	2.09337425	6	-2.17767096	4.18692064	2.34927416
1	3.14902902	-3.70697927	2.31467414	1	-3.87237096	3.03302073	1.58847427
6	4.28932905	-1.91067922	2.11867428	12	-0.63257092	0.50382078	-0.19302575
6	4.22962904	-0.53097922	1.92987418	1	-2.65407085	3.54242086	-0.24062575
1	5.15012932	0.04312077	2.02547431	1	-2.50997090	5.33692074	-0.34792575
6	3.03002906	0.13342077	1.64537418	1	5.23942900	-2.40107918	2.33437419
6	0.58752912	-2.91887927	1.86227417	1	-3.55997086	2.84952068	3.31527424
6	3.02282906	1.67692077	1.56157422	1	-2.82017088	5.07982063	2.44397426
6	0.07322913	-3.19937921	0.43377426	1	-1.55317092	4.16482067	3.25807428

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1	-0.10647088	-2.27867913	-0.12752575	8	-1.85177088	-0.95287919	-1.20672584
1	-0.86717087	-3.77427912	0.46567425	6	-3.02797079	-1.32247925	-1.18362582
1	0.81082910	-3.79497910	-0.12552576	6	-4.08907080	-0.66807920	-0.33992577
6	-0.50967085	-2.23287916	2.70977426	8	-3.32077098	-2.38067913	-1.96602583
1	-0.76127088	-1.24047923	2.32277417	6	-4.60017109	-1.57107925	0.80517423
1	-0.16937086	-2.11447930	3.74907422	1	-4.93307066	-0.36867923	-0.98432577
1	-1.41697085	-2.85827923	2.72387433	1	-3.60387087	0.24302077	0.06207424
6	0.84032911	-4.29237938	2.51957417	6	-4.67177105	-2.93207932	-2.00302577
1	1.24762905	-4.19117928	3.53547430	1	-3.74057078	-2.03897929	1.31037426
1	1.52582908	-4.92027950	1.93257427	1	-5.07017088	-0.91677922	1.55337417
1	-0.11497088	-4.83377934	2.59227419	1	-5.37817097	-2.14397931	-2.30752587
6	4.37752914	2.29232073	1.96867418	1	-4.60617113	-3.66657925	-2.81452584
1	5.18782902	2.01672077	1.27767420	6	-5.61217070	-2.63637924	0.37157425
1	4.67472887	1.99732077	2.98487425	1	-6.51627111	-2.13227916	-0.01202575
1	4.28952932	3.38882089	1.95077419	1	-5.93277073	-3.21337914	1.25277424
6	1.96852911	2.24642086	2.53947425	6	-5.09987068	-3.60237932	-0.70222580
1	0.97392911	1.83862078	2.33017421	1	-4.25407076	-4.20017958	-0.32542574
1	1.92862916	3.34422088	2.45977426	1	-5.89807081	-4.31957960	-0.95412576
1	2.23482919	1.99102080	3.57557416	8	0.36852914	0.46722075	-2.06332564
6	2.73502922	2.16752076	0.12637424	6	1.40732908	-0.09357923	-2.42722583
1	3.50082922	1.78912079	-0.56902575	6	2.02432919	0.19772077	-3.77482581
1	2.75852919	3.26782084	0.08527425	8	1.95822906	-0.98467922	-1.60702574
1	1.75262916	1.84552085	-0.22862574	6	2.10482907	-1.02877915	-4.70922565
8	-0.96197093	5.22452068	-2.21242571	1	3.03352904	0.61522079	-3.61872578
6	-0.05207087	5.05812073	-3.32452583	1	1.40872908	0.98732078	-4.22042561
1	-0.32717088	4.17622042	-3.91722584	6	3.26302910	-1.59367919	-1.86402583
1	-0.15127087	5.97182035	-3.91912580	1	1.14712906	-1.57277918	-4.67942572
1	0.97762913	4.93942070	-2.96402574	1	2.21472907	-0.65447921	-5.73792553
8	-0.30797088	3.17542076	-1.49242580	1	4.00082922	-0.79387921	-2.03062582
6	-0.99697089	4.17492056	-1.34032583	1	3.49092913	-2.07357931	-0.90472579
8	-2.08487082	1.41472077	0.66647422	6	3.26742911	-1.98087931	-4.40552568
6	-1.96017087	4.39722061	-0.20732576	1	4.21632910	-1.43117917	-4.53172541
6	-2.33467078	1.60282075	2.03517413	1	3.27612901	-2.78487921	-5.15762568
6	-1.23427093	4.34882069	1.14997423	6	3.23952913	-2.60157919	-3.00452590
1	-1.40297091	1.56862080	2.64277411	1	2.35722899	-3.24957919	-2.87792587
1	-2.97247100	0.78012079	2.43727422	1	4.12092924	-3.25057912	-2.87892580

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## I-5\_CC



Zero-point vibrational energy	2200979.7 (Joules/Mol)
	526.04676 (Kcal/Mol)
Zero-point correction=	0.838309 (Hartree/Particle)
Thermal correction to Energy=	0.887169
Thermal correction to Enthalpy=	0.888113
Thermal correction to Gibbs Free Energy=	0.747361
Sum of electronic and zero-point Energies=	-2090.672967
Sum of electronic and thermal Energies=	-2090.624107
Sum of electronic and thermal Enthalpies=	-2090.623163
Sum of electronic and thermal Free Energies=	-2090.763914

cartesian											
8	-1.25303173	0.46260831	-0.91945100	6	3.85036826	-1.57279170	3.39174891				
6	-2.31623173	-0.32219172	-1.34725094	1	4.65946817	-1.17689168	3.99624896				
6	-3.63003159	0.06570829	-0.66225100	6	3.15536833	-0.72649169	2.52264905				
6	-4.82033205	-0.79089171	-1.09295106	6	0.49376822	-3.25419188	1.19834900				
6	-6.13663197	-0.37349170	-0.43515098	6	3.50556827	0.77320832	2.47344899				
6	-7.30663204	-1.25789165	-0.85415095	6	0.68556821	-3.28739166	-0.33005098				
6	-8.63063145	-0.83559173	-0.26265097	1	0.85546821	-2.28999186	-0.73745096				
8	-9.58473110	-1.76839173	-0.49635097	1	-0.20013174	-3.70659161	-0.82265097				
1	-2.14063168	-1.39809167	-1.15685105	1	1.54656827	-3.91279173	-0.59415096				
1	-2.45823169	-0.23199171	-2.44215107	6	-0.77013177	-2.44969177	1.56464911				
1	-3.48663163	-0.00929171	0.42344904	1	-0.69683176	-1.40429175	1.26234913				

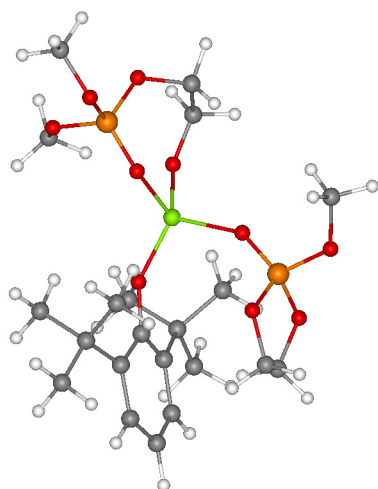
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1	-3.83713174	1.12320828	-0.87745100	1	-0.93383175	-2.47749186	2.64744902
1	-4.61243200	-1.84419167	-0.85795099	1	-1.65303171	-2.88319159	1.07914901
1	-4.92963171	-0.74169171	-2.18585110	6	0.22676824	-4.70809174	1.62934899
6	-10.88983154	-1.44729173	0.00434902	1	0.04166825	-4.79279137	2.70524907
12	0.57596827	0.37700829	-0.56125098	1	1.05096829	-5.38069153	1.36754894
8	1.06506824	2.38550806	-0.53875101	1	-0.66793174	-5.07649136	1.11474895
6	0.46066827	3.45830822	-0.55155098	6	4.59316826	1.15640831	3.49334908
6	-1.03763175	3.55460835	-0.57595098	1	5.54676819	0.65420830	3.29634905
8	1.21646833	4.55430841	-0.52225101	1	4.29316807	0.93280828	4.52264929
6	-1.62233174	4.11240864	0.73474902	1	4.77766800	2.23520851	3.43304896
1	-1.34573174	4.18380833	-1.42095089	6	2.26036835	1.61260831	2.82554889
1	-1.39723170	2.53350830	-0.75925100	1	1.42876828	1.39430833	2.15494895
6	0.63196826	5.87720823	-0.49725097	1	2.49066830	2.68340826	2.75934887
1	-1.13893175	3.62210846	1.58774900	1	1.93516827	1.39760828	3.84944892
1	-2.67433167	3.81350851	0.77374899	6	4.04736805	1.16900826	1.08664894
1	-0.00253175	6.01190853	-1.38015103	1	4.97326803	0.62250829	0.87244904
1	1.50166833	6.52620840	-0.60745096	1	4.27406788	2.24180841	1.05214906
6	-1.53173172	5.63130856	0.86954904	1	3.32676840	0.95480829	0.29784903
1	-2.13903165	6.09420824	0.07974902	8	1.67166829	-0.03809170	-2.27645111
1	-1.98383164	5.93690825	1.81974912	6	2.59546828	-0.70059168	-2.74295115
6	-0.11243175	6.19640827	0.79124904	8	2.68436837	-0.72869170	-4.07065105
1	0.49536824	5.85000849	1.63574910	6	3.59966826	-1.42799175	-1.89015102
1	-0.15833175	7.28900862	0.87234902	6	3.68036819	-1.52029169	-4.75895071
1	-6.36563206	0.66840827	-0.68395096	6	5.03696823	-0.89369172	-2.03445101
1	-6.03283215	-0.40499172	0.65564901	6	5.09836817	-0.99479175	-4.60405064
1	-7.13383198	-2.30629158	-0.58665097	1	3.35866833	-1.45909166	-5.79925060
1	-7.42783213	-1.25289166	-1.94535089	1	5.58996820	-1.22489166	-1.15055108
8	-8.85013103	0.19820829	0.33494902	1	5.02446795	0.20120829	-1.99075103
1	-11.52273178	-2.29269171	-0.26415098	1	3.57056832	-2.49759150	-2.13305116
1	-10.86513138	-1.31809175	1.08874893	1	3.25776839	-1.32359171	-0.85955095
1	-11.26413155	-0.52939171	-0.45475098	6	5.77266788	-1.37129176	-3.28545094
8	1.49596834	-0.52699172	0.81274903	1	3.59416819	-2.56529188	-4.44165087
6	2.10396838	-1.27949166	1.71854901	1	5.08116817	0.09320830	-4.74055099
6	1.72176826	-2.64909172	1.90644908	1	5.68516827	-1.40139174	-5.43645096
6	2.46516824	-3.43399191	2.79384899	1	5.87846804	-2.46359158	-3.24065113
1	2.20576835	-4.47759151	2.93744898	1	6.79066801	-0.96629167	-3.27635098
6	3.53486824	-2.92119169	3.51984906	1	4.09686804	-3.55799150	4.19894934

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## S1.4. PP sequence, mononuclear mechanism

### I-1\_PP

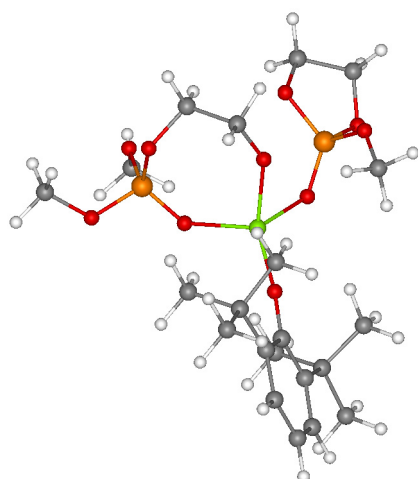


Zero-point vibrational energy	1565337.6 (Joules/Mol)
	374.12466 (Kcal/Mol)
Zero-point correction=	0.596206 (Hartree/Particle)
Thermal correction to Energy=	0.637320
Thermal correction to Enthalpy=	0.638265
Thermal correction to Gibbs Free Energy=	0.519129
Sum of electronic and zero-point Energies=	-2457.219233
Sum of electronic and thermal Energies=	-2457.178118
Sum of electronic and thermal Enthalpies=	-2457.177174
Sum of electronic and thermal Free Energies=	-2457.296310

cartesian											
12	1.04106259	0.46429029	-0.51320416	6	-0.06723739	-2.78090978	2.05299592				
8	4.91156292	0.12579030	1.73039579	1	-0.61943740	-3.70210981	1.83579588				
8	-0.31403738	-0.82090962	-0.21170413	1	0.64906263	-2.99660969	2.85539603				
6	6.29556274	-0.26580968	1.72299588	1	0.48886263	-2.49670959	1.15899587				
1	6.69126272	0.01549029	2.69829607	1	6.38236284	-1.34560966	1.58329582				
1	6.83856249	0.26389030	0.93609583	8	2.61926270	0.40089029	0.77769583				
6	-1.59023738	-1.07430971	0.01999586	15	3.99266267	-0.09800971	0.45569587				
6	-2.53813720	-1.09500968	-1.05890417	8	4.71986294	0.61379027	-0.76440418				
6	-3.89733744	-1.21540964	-0.74570417	8	2.13116264	0.34819031	-2.06280398				
1	-4.63643742	-1.20110965	-1.53980422	6	4.10096264	1.66549027	-1.56730413				
6	-4.34753752	-1.36200964	0.56409585	6	3.16106272	1.07349026	-2.61140394				
6	-3.41013718	-1.47650969	1.58849585	1	4.94266272	2.19369030	-2.02360415				
1	-3.77173710	-1.67380965	2.59279585	1	3.56926274	2.34689021	-0.89510417				
6	-2.03503728	-1.37450969	1.35289586	1	2.81276274	1.93389034	-3.21850395				

6	-2.09403729	-1.04770970	-2.53580403	1	3.77196264	0.45199031	-3.29300404
6	-1.03533745	-1.66200972	2.49179602	8	4.15866280	-1.65220964	0.19549584
6	-1.08473742	-2.18080974	-2.81260395	1	-5.41103745	-1.44600964	0.77579582
1	-0.20483740	-2.09350967	-2.17450404	6	3.75476265	-2.29200959	-1.04470420
1	-0.75613737	-2.14680958	-3.85840416	1	3.04986262	-1.66840971	-1.60130417
1	-1.54763734	-3.15780973	-2.63390398	1	3.29206276	-3.23720980	-0.76170415
6	-1.47173738	0.30949029	-2.92030406	1	4.65366268	-2.47220969	-1.63720417
1	-0.48333740	0.45689029	-2.48410416	8	0.26696262	2.31459022	-0.12050415
1	-2.11753726	1.14269030	-2.62430406	15	-0.92173743	3.08829021	0.33689585
1	-1.33363736	0.36309028	-4.00710392	8	-2.28433728	2.97299027	-0.47570416
6	-3.28023720	-1.26570964	-3.49430394	8	-1.45113742	2.65049028	1.78199589
1	-4.01353741	-0.45250973	-3.44590402	6	-3.29463720	2.30009031	0.32909587
1	-3.79953718	-2.21080971	-3.30380416	6	-2.89643717	2.56189036	1.78299582
1	-2.90643740	-1.29980969	-4.52360392	8	-0.63553739	4.64799023	0.32499588
6	-1.73983741	-2.16340971	3.76529598	6	0.69686264	5.16429043	0.53309584
1	-2.33063722	-3.06740975	3.58289599	1	1.41316259	4.62679052	-0.08940414
1	-2.39683723	-1.40670967	4.20929575	1	0.96996260	5.07759047	1.58709586
1	-0.98373735	-2.41200972	4.51829576	1	0.65566260	6.21339035	0.24409586
6	-0.23563738	-0.40990970	2.89459586	1	-3.17413735	1.73489034	2.43549585
1	0.35836262	-0.02070969	2.06919599	1	-3.29583716	3.50559044	2.16549587
1	0.45746261	-0.65010965	3.71009588	1	-4.25633717	2.74199033	0.06929585
1	-0.89983737	0.38719028	3.24399590	1	-3.28363729	1.23719025	0.08139586

### TS-12\_PP



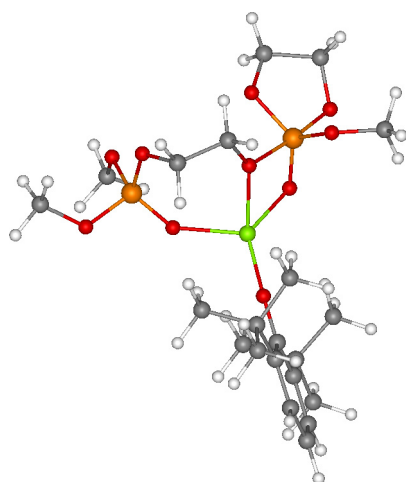
Zero-point vibrational energy	1565406.4 (Joules/Mol)
	374.14112 (Kcal/Mol)
Zero-point correction=	0.596232 (Hartree/Particle)
Thermal correction to Energy=	0.636346
Thermal correction to Enthalpy=	0.637290
Thermal correction to Gibbs Free Energy=	0.521406
Sum of electronic and zero-point Energies=	-2457.215883

Sum of electronic and thermal Energies=	-2457.175769
Sum of electronic and thermal Enthalpies=	-2457.174824
Sum of electronic and thermal Free Energies=	-2457.290708

cartesian											
12	-0.52497226	-0.17979024	-0.12329715	6	1.74002779	2.58320999	0.97760284				
8	-1.52607226	3.78060985	-1.48109710	1	2.36912775	3.24040985	0.36730283				
8	1.32692766	-0.28209025	-0.04479715	1	1.15312767	3.21320987	1.65830290				
6	-2.17277217	5.04501009	-1.23559713	1	1.05622768	2.07070994	0.29970282				
1	-1.55597234	5.79461002	-1.72909713	1	-3.17937207	5.05160999	-1.66159713				
1	-2.21477222	5.24060965	-0.16279715	8	-1.54717231	-1.89929020	-0.48859715				
6	2.65212774	-0.23429024	-0.07189716	15	-2.66597223	-2.24179006	0.45280284				
6	3.38422775	-1.07299030	-0.97249711	8	-3.40027213	-3.54679012	-0.20009714				
6	4.78042746	-1.00739026	-0.96089715	8	-4.02247238	-1.35909021	0.58510286				
1	5.35512781	-1.63579023	-1.63339710	6	-4.78337240	-3.55689001	0.14750285				
6	5.47362757	-0.15549025	-0.10729715	6	-5.18627262	-2.08489013	0.13610286				
6	4.75622749	0.66180974	0.75950289	1	-4.91617250	-4.00729036	1.13770282				
1	5.31192780	1.32280970	1.41640282	1	-5.31997252	-4.14729023	-0.59679711				
6	3.35882783	0.65200973	0.80300289	1	-5.43677235	-1.73999023	-0.87139714				
6	2.66772771	-2.03529024	-1.93849719	1	-6.00477219	-1.85739028	0.82110286				
6	2.61422777	1.59060979	1.77120292	8	-2.29977226	-2.77099013	1.90330291				
6	1.76542771	-1.24719024	-2.91059732	6	-0.97427225	-2.69909024	2.47160268				
1	1.05002773	-0.61489022	-2.38289714	1	-0.22947228	-3.05059004	1.75500286				
1	1.20802772	-1.93279028	-3.56089735	1	-0.76527226	-1.67189026	2.76710272				
1	2.37132788	-0.59329027	-3.54749727	1	-0.99397230	-3.36129022	3.33700275				
6	1.84472764	-3.07219005	-1.14809716	8	-1.23447227	1.29740977	-1.30989718				
1	1.10632765	-2.59329009	-0.50549716	15	-2.17387223	2.41730976	-1.00219715				
1	2.50552773	-3.67749023	-0.51719713	8	-2.56817222	2.69550991	0.49400285				
1	1.31592774	-3.74739003	-1.83199716	8	-1.81887233	-0.08349024	1.30320287				
6	3.65212798	-2.83289003	-2.81189728	6	-3.36147213	1.78760970	1.33310282				
1	4.31552744	-3.46729016	-2.21429729	6	-2.47447228	0.82770973	2.10920286				
1	4.27032757	-2.18389010	-3.44129729	1	-4.06287241	1.24480975	0.69690287				
1	3.08582783	-3.49229002	-3.47989726	1	-3.91117215	2.45500994	2.00170279				
6	3.57382774	2.43960977	2.62310266	1	-1.76767230	1.42110980	2.71360278				
1	4.20922756	3.08850980	2.01130271	1	-3.14887214	0.32020974	2.82270265				
1	4.22012758	1.82330978	3.25710273	8	-3.58397222	2.25010991	-1.73679709				
1	2.98872781	3.08820987	3.28560281	6	-3.63007212	1.68810976	-3.06689715				
6	1.75452769	0.77990973	2.76230264	1	-3.20187211	2.38930988	-3.78739715				
1	1.01782775	0.16180976	2.24810266	1	-3.08767223	0.74170977	-3.09869719				
1	1.22522771	1.45250976	3.44960284	1	6.56072760	-0.12759024	-0.11899716				
1	2.38882780	0.11770976	3.36220264	1	-4.68467236	1.52890980	-3.28849721				



## I-2\_PP

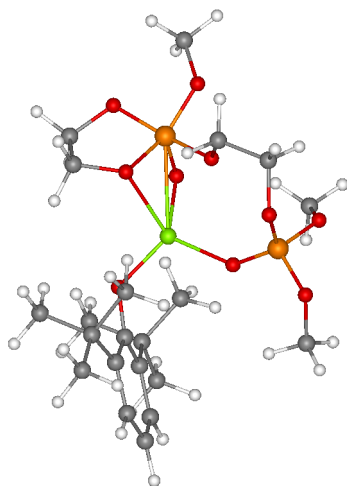


Zero-point vibrational energy	1568556.2 (Joules/Mol)
	374.89393 (Kcal/Mol)
Zero-point correction=	0.597432 (Hartree/Particle)
Thermal correction to Energy=	0.637567
Thermal correction to Enthalpy=	0.638511
Thermal correction to Gibbs Free Energy=	0.521551
Sum of electronic and zero-point Energies=	-2457.215133
Sum of electronic and thermal Energies=	-2457.174997
Sum of electronic and thermal Enthalpies=	-2457.174053
Sum of electronic and thermal Free Energies=	-2457.291014

cartesian											
12	-0.47606266	-0.23479718	-0.38737077	6	1.81143737	-2.51239705	-2.02967072				
8	-1.57166266	3.96430278	-0.85387081	1	2.43263745	-3.32379723	-1.63487077				
8	1.34773731	-0.14809719	-0.10777077	1	1.27093732	-2.89569712	-2.90347075				
6	-2.33476257	5.14460278	-0.53717077	1	1.07743740	-2.26639724	-1.26197076				
1	-1.65846264	5.98560238	-0.68187076	1	-3.19396257	5.23730278	-1.20627069				
1	-2.67326260	5.11390257	0.50102919	8	-1.57836270	-1.81929719	-0.78307080				
6	2.67413735	-0.19149718	-0.07857077	15	-2.66296268	-1.92169714	0.29882926				
6	3.37373734	0.32940280	1.05532932	8	-3.39906263	-3.32069707	-0.31647074				
6	4.76963758	0.25970283	1.07052922	8	-4.10376263	-1.11669719	0.27312922				
1	5.32083750	0.64420283	1.92242932	6	-4.78666258	-3.33379722	-0.06447077				
6	5.49023724	-0.29149717	0.01622923	6	-5.20756245	-1.87939715	-0.22137077				
6	4.80353737	-0.78299713	-1.08907068	1	-5.00706244	-3.69749713	0.95092922				
1	5.38213730	-1.20449710	-1.90447068	1	-5.27376270	-3.99249721	-0.78797078				
6	3.40833735	-0.74899715	-1.17277074	1	-5.36786270	-1.61799717	-1.27257073				
6	2.61933732	0.97030282	2.23452926	1	-6.09146261	-1.61339712	0.36322922				
6	2.69663739	-1.31049716	-2.41767073	8	-2.28846264	-2.54669714	1.75832927				
6	1.67213726	-0.05039717	2.89742923	6	-2.06786251	-3.95279717	1.94012928				

1	0.94883740	-0.45749718	2.19002938	1	-3.00696254	-4.51109743	1.92112923
1	1.12673736	0.41680282	3.72822928	1	-1.39666259	-4.34999752	1.17602932
1	2.24403739	-0.89069718	3.30572939	1	-1.60306263	-4.04949760	2.92282939
6	1.83453727	2.20370293	1.74262929	8	-1.17306256	1.52170289	-1.10807073
1	1.15783739	1.94630289	0.92522919	15	-2.22626257	2.51640296	-0.74887079
1	2.52183723	2.97060275	1.36902928	8	-2.91696262	2.39860296	0.66722924
1	1.25713730	2.64590287	2.56632924	8	-1.99426270	-0.32629719	0.96792918
6	3.56783724	1.46570289	3.34052920	6	-2.22866249	1.88070285	1.84442925
1	4.26293755	2.23160291	2.98052931	6	-2.53346276	0.41120282	2.04002929
1	4.15163755	0.65010285	3.78002930	1	-2.61276269	2.46820283	2.68122935
1	2.97723746	1.91480279	4.14752913	1	-1.15336263	2.05930281	1.75622928
6	3.68533754	-1.82619715	-3.47867084	1	-2.09126282	0.09190283	2.99382925
1	4.29543734	-2.65649724	-3.10767078	1	-3.61646271	0.26670283	2.08802938
1	4.35583735	-1.03839719	-3.83827066	8	-3.51036263	2.50840282	-1.68177068
1	3.12283731	-2.19779706	-4.34277105	6	-3.34076262	2.32500291	-3.10577083
6	1.86713743	-0.20729718	-3.10837078	1	-2.85966253	1.36620283	-3.30537081
1	1.17833734	0.28830281	-2.42187071	1	-2.74936271	3.13920283	-3.53197074
1	1.29153740	-0.62359715	-3.94447064	1	6.57613754	-0.33439717	0.05392923
1	2.52743745	0.57020283	-3.50827074	1	-4.34516239	2.33640289	-3.52577066

## TS-24\_PP



Zero-point vibrational energy	1569309.1 (Joules/Mol)
	375.07388 (Kcal/Mol)
Zero-point correction=	0.597718 (Hartree/Particle)
Thermal correction to Energy=	0.636766
Thermal correction to Enthalpy=	0.637710
Thermal correction to Gibbs Free Energy=	0.524904
Sum of electronic and zero-point Energies=	-2457.202690
Sum of electronic and thermal Energies=	-2457.163642
Sum of electronic and thermal Enthalpies=	-2457.162698

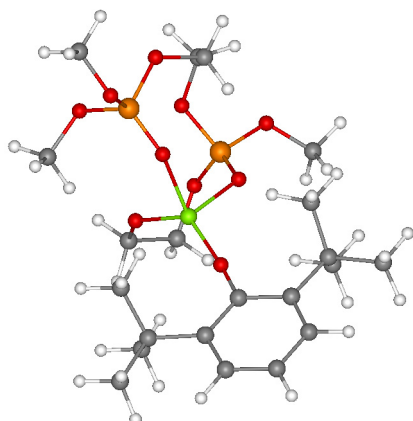
Sum of electronic and thermal Free Energies=

-2457.275504

cartesian

12	-0.69835955	-0.22166945	0.20521393	1	3.10524035	-2.19056964	-2.88118625
8	-2.25265956	3.34293056	1.38901401	1	1.66334033	-1.88716948	-3.86748624
8	0.97394043	-1.03766942	-0.14218606	1	1.50864053	-2.18006945	-2.11758614
6	-2.47685957	2.42083049	2.48761392	1	-2.80295968	1.45003057	2.11401391
1	-1.56295943	2.31483054	3.07451391	8	-2.23395944	-1.00926936	1.27501392
6	2.19234037	-0.49366945	-0.04688606	15	-3.21295953	-1.07616937	0.08971395
6	2.86104035	-0.45216948	1.21611392	8	-3.58445954	-2.69436955	-0.12918606
6	4.07714081	0.23343053	1.30341399	8	-2.05855966	-1.24076939	-1.25578606
1	4.59104061	0.30513054	2.25591397	6	-2.47995949	-3.45106959	-0.59728611
6	4.66724062	0.82983053	0.19351393	6	-1.85265946	-2.58706951	-1.68678606
6	4.05984068	0.69293052	-1.05078602	1	-2.85575962	-4.40176916	-0.98098606
1	4.56074047	1.11843061	-1.91408598	1	-1.77975965	-3.63766956	0.22461393
6	2.84274030	0.02283055	-1.21168602	1	-0.78165954	-2.76376963	-1.79908597
6	2.29874039	-1.18836939	2.44871378	1	-2.35455942	-2.72276950	-2.65058613
6	2.26334047	-0.19376947	-2.62368608	8	-4.78305960	-0.74036950	0.38671395
6	2.18814039	-2.69546962	2.13821387	6	-5.75085926	-1.69966936	0.83411390
1	1.55914044	-2.86656952	1.26231396	1	-6.01995945	-2.38836956	0.03151394
1	1.75314045	-3.23166943	2.99121380	1	-5.37945938	-2.26636958	1.69041395
1	3.17824030	-3.12036943	1.94111395	1	-6.62275934	-1.11276937	1.13041401
6	0.91294044	-0.65226948	2.87511396	8	-0.48225954	1.74703062	0.41721395
1	0.10264045	-1.10756946	2.30101395	15	-1.26775956	3.00493050	0.18891394
1	0.86014050	0.43893054	2.78961396	8	-2.11575961	3.12113047	-1.13998604
1	0.70684046	-0.91006953	3.92081380	8	-3.03755951	0.60613054	-0.30018604
6	3.22134042	-1.04326940	3.67271376	6	-3.49725962	2.70243049	-1.26288605
1	3.30294037	-0.00436945	4.01211405	6	-3.61085963	1.20613062	-1.44578600
1	4.22964048	-1.42216945	3.47741389	1	-3.87425971	3.23293042	-2.13908625
1	2.81104040	-1.62716937	4.50411367	1	-4.04555941	3.02843046	-0.37558606
6	3.18444037	0.36993054	-3.72038603	1	-4.67555952	0.95213050	-1.53008604
1	4.18404055	-0.07546945	-3.68998623	1	-3.08855963	0.88033050	-2.35358620
1	3.28994036	1.45873058	-3.65688610	8	-0.32305953	4.25733089	-0.00768606
1	2.75634050	0.14193054	-4.70288610	6	0.92944044	4.33853054	0.71091390
6	0.89734048	0.49683052	-2.80488610	1	1.48804045	3.40653038	0.61351395
1	0.11614048	0.00313054	-2.22478604	1	0.74034041	4.56723070	1.76261401
1	0.58714044	0.45553052	-3.85648608	1	5.60934067	1.36433053	0.29101396
1	0.94434041	1.55023062	-2.51048613	1	-3.25675964	2.88123035	3.09311390
6	2.12214041	-1.70716941	-2.88658619	1	1.47884035	5.15773058	0.24991393

# I-4\_PP

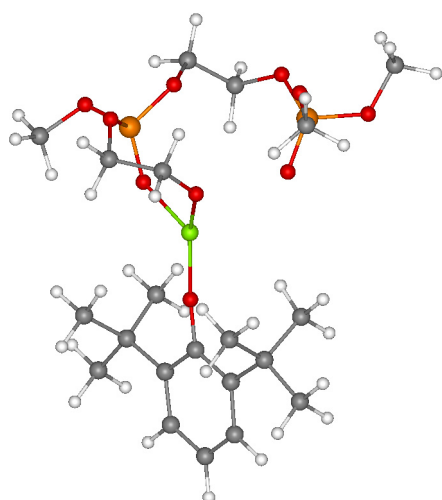


Zero-point vibrational energy	1566502.0 (Joules/Mol)
	374.40297 (Kcal/Mol)
Zero-point correction=	0.596649 (Hartree/Particle)
Thermal correction to Energy=	0.637223
Thermal correction to Enthalpy=	0.638167
Thermal correction to Gibbs Free Energy=	0.521953
Sum of electronic and zero-point Energies=	-2457.222104
Sum of electronic and thermal Energies=	-2457.181530
Sum of electronic and thermal Enthalpies=	-2457.180586
Sum of electronic and thermal Free Energies=	-2457.296800

cartesian				
12	0.49715561	-0.04940699	-0.48172364	1 -1.86334443 -2.08550715 -3.29362369
8	2.33065557	-3.19190717	2.15207624	1 -1.48534441 -0.61670697 -2.37682366
8	-1.31954432	0.15189300	-0.13852362	1 3.90665579 -4.53280687 1.83787644
6	3.34785557	-4.07690668	2.65877628	8 1.56215572 1.69349301 -0.17762363
1	2.82125568	-4.84600687	3.22187638	15 2.91635561 1.90569305 -0.78972358
1	4.02645540	-3.53060699	3.31777620	8 2.98425579 1.93989301 -2.35932374
6	-2.61174440	0.10679300	0.15277638	8 1.48415565 -0.54320699 -2.03182364
6	-3.17904425	1.07909298	1.03837645	6 1.90285563 1.49599302 -3.24522376
6	-4.54674435	1.01259303	1.31867635	6 1.77715564 -0.01810699 -3.26842380
1	-4.99704409	1.73969305	1.98657644	1 2.17965555 1.90519309 -4.21962357
6	-5.36714411	0.03479301	0.76577640	1 0.97335565 1.96399307 -2.90572381
6	-4.80984449	-0.90830696	-0.09132362	1 1.00155568 -0.23490700 -4.02962351
1	-5.46354437	-1.66440701	-0.51352358	1 2.72375560 -0.42880699 -3.66572380
6	-3.45024443	-0.90490699	-0.41692364	8 1.45885563 -1.22220695 0.87467641
6	-2.31664443	2.18409300	1.67637634	15 2.69345570 -1.99880695 1.16987646
6	-2.88564444	-1.97700691	-1.36742365	8 3.83555579 -1.18040693 1.92127645
6	-1.69944429	3.07889295	0.58247638	8 4.04915571 0.87509304 -0.35482362
1	-1.08474445	2.50289297	-0.10892362	6 3.83035564 0.25799301 2.03117633

1	-1.07444429	3.85909295	1.03687644	6	4.66045570	0.91689301	0.95017642
1	-2.49014425	3.57369280	0.00707638	1	4.28945541	0.47209302	2.99967623
6	-1.21474433	1.56219304	2.55887628	1	2.80305576	0.63029301	2.03917623
1	-0.58704442	0.87069303	1.99617636	1	4.85945559	1.95489299	1.23227644
1	-1.66284442	1.00479305	3.38907623	1	5.61035585	0.39279300	0.83387637
1	-0.57514435	2.34619284	2.98477626	8	3.48845577	-2.61780715	-0.04692363
6	-3.13414431	3.11229300	2.59197617	6	2.77915573	-3.27150702	-1.13942361
1	-3.59164429	2.57299280	3.42827630	1	2.20415568	-2.51620698	-1.68382359
1	-3.92494440	3.64039302	2.04837632	1	2.13885570	-4.06760693	-0.75002360
1	-2.46934438	3.87209296	3.01917624	1	-6.42854452	0.00759301	1.00087643
6	-3.96874428	-2.95020700	-1.86692357	8	3.55725574	3.28839302	-0.31132364
1	-4.75004435	-2.44090700	-2.44122362	6	2.77075577	4.49509335	-0.39562362
1	-4.44514418	-3.49820709	-1.04722357	1	3.34325576	5.26469326	0.12067638
1	-3.50764441	-3.69170713	-2.52972364	1	2.63475561	4.77789307	-1.44232357
6	-1.83624434	-2.83900714	-0.63572359	1	1.80365562	4.35429335	0.09107638
1	-1.04534435	-2.23540711	-0.18822363	1	3.55915570	-3.70060706	-1.76732361
1	-1.37754440	-3.55750704	-1.32702363	6	-2.27954435	-1.32120693	-2.62522364
1	-2.30844426	-3.40410709	0.17557637	1	-3.05314422	-0.77450699	-3.17592382

#### TS-45\_PP



Zero-point vibrational energy	1563528.3 (Joules/Mol)
	373.69222 (Kcal/Mol)
Zero-point correction=	0.595516 (Hartree/Particle)
Thermal correction to Energy=	0.635976
Thermal correction to Enthalpy=	0.636920
Thermal correction to Gibbs Free Energy=	0.518929
Sum of electronic and zero-point Energies=	-2457.197842
Sum of electronic and thermal Energies=	-2457.157383
Sum of electronic and thermal Enthalpies=	-2457.156439

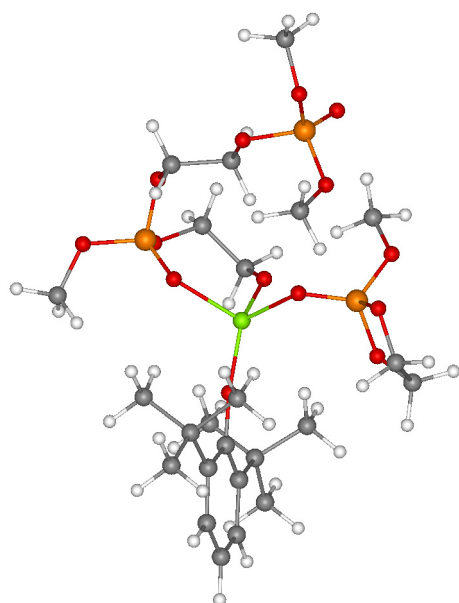
Sum of electronic and thermal Free Energies=

-2457.274430

cartesian

12	0.15823469	0.15365970	-0.73387504	6	-2.25516534	-1.95184028	-2.38117504
8	3.91033459	-3.14894032	1.89312506	1	-3.14666533	-1.67634022	-2.95517492
8	-1.56066525	0.01215971	-0.10997502	1	-1.68906534	-2.68834043	-2.96387506
6	5.27503490	-3.58674049	2.00042486	1	-1.63856518	-1.05684030	-2.28687501
1	5.24343491	-4.55734015	2.49472499	1	5.72813463	-3.68854046	1.01092505
1	5.85233498	-2.88194036	2.60402513	8	1.16733468	1.81065977	-0.17477500
6	-2.82076550	-0.26074028	0.22072499	15	2.50983453	2.28455973	-0.65977502
6	-3.56826520	0.68765974	0.98602498	8	2.69293451	2.32705951	-2.22047496
6	-4.89256525	0.38255972	1.31432509	8	1.23543465	-0.29904029	-2.19867492
1	-5.48186541	1.08615971	1.89282501	6	1.72933471	1.84995973	-3.21497488
6	-5.49306536	-0.80884027	0.92222500	6	1.70313466	0.33405972	-3.32807493
6	-4.75656509	-1.72644031	0.18142499	1	2.06413460	2.31895971	-4.14307499
1	-5.24046516	-2.65094042	-0.11467502	1	0.74083471	2.24335957	-2.95337486
6	-3.42846537	-1.48914027	-0.18627501	1	1.08063471	0.12425971	-4.22007513
6	-2.94686532	2.01795959	1.45222509	1	2.72543454	0.00095971	-3.58277488
6	-2.66296530	-2.53834033	-1.01397491	8	2.08143473	-1.53884029	1.16042507
6	-2.51926541	2.86815953	0.23842499	15	3.53173470	-1.81384027	1.10422504
1	-1.78706539	2.34635973	-0.37877503	8	4.47453451	-0.69824028	1.77962506
1	-2.07886553	3.81635952	0.57332498	8	3.77593470	1.47835970	-0.16527501
1	-3.38636541	3.10305953	-0.38887504	6	3.95183468	0.59445965	2.11972499
6	-1.74346530	1.75085974	2.37882495	6	4.39443493	1.64825976	1.13102508
1	-0.97526526	1.15695977	1.88322508	1	4.37153482	0.84545970	3.09862494
1	-2.06586552	1.20605969	3.27282500	1	2.86273456	0.55295968	2.20452499
1	-1.29316533	2.69735956	2.70512509	1	4.17293453	2.64375973	1.52492499
6	-3.93816543	2.87665963	2.25782514	1	5.46683502	1.56925976	0.94582498
1	-4.27556515	2.37305951	3.16982508	8	4.20883465	-1.95244026	-0.33287501
1	-4.82006502	3.15575957	1.67132509	6	3.48443460	-2.62624049	-1.39397502
1	-3.44346547	3.80555964	2.56412506	1	2.63533449	-2.01284027	-1.70707500
6	-3.51846528	-3.78144050	-1.32157493	1	3.15333462	-3.61584044	-1.06657493
1	-4.40466499	-3.53994036	-1.91807497	1	-6.52476501	-1.02054024	1.19262505
1	-3.84416556	-4.29614019	-0.41167504	8	2.82123470	3.75255966	-0.12177501
1	-2.92046547	-4.49344015	-1.90177500	6	1.80583465	4.77515984	-0.20447502
6	-1.43276525	-3.05024028	-0.23687501	1	2.18753457	5.62366009	0.36162499
1	-0.77086532	-2.24684048	0.09012499	1	1.65563476	5.06655979	-1.24697495
1	-0.84986532	-3.74604034	-0.85227501	1	0.87133467	4.41905975	0.23272499
1	-1.74916518	-3.58264041	0.66642499	1	4.19973469	-2.73384047	-2.20947504

# I-5\_PP



Zero-point vibrational energy	1870434.4 (Joules/Mol)
	447.04454 (Kcal/Mol)
Zero-point correction=	0.712411 (Hartree/Particle)
Thermal correction to Energy=	0.764194
Thermal correction to Enthalpy=	0.765139
Thermal correction to Gibbs Free Energy=	0.618509
Sum of electronic and zero-point Energies=	-3217.786351
Sum of electronic and thermal Energies=	-3217.734568
Sum of electronic and thermal Enthalpies=	-3217.733624
Sum of electronic and thermal Free Energies=	-3217.880253

				cartesian				
12	0.23214152	-0.61861616	0.58668512	6	-3.54245830	-2.53571630	-0.89501488	
8	-4.43975830	1.95198393	-0.44291493	6	-3.91905832	-1.34491611	-0.03301492	
8	1.88374150	-0.10371612	-0.14261490	1	-3.01985836	-2.21761632	-1.79991484	
6	-4.06435871	2.26268387	-1.79871488	1	-4.42685843	-3.11001611	-1.17591488	
1	-3.67575836	1.37468398	-2.30261493	1	-3.03305840	-0.75201613	0.21008509	
1	-4.92495823	2.65948391	-2.34171510	1	-4.39445829	-1.67881608	0.89298511	
6	3.08934164	0.32098389	-0.48951492	8	-6.68625832	1.09328389	-1.06241488	
6	4.18484163	0.25448388	0.43378508	6	-7.88265848	0.29948390	-0.95531487	
6	5.42814159	0.75468385	0.03578509	1	-8.24885845	0.30098388	0.07368509	
1	6.26714182	0.72048384	0.72278512	1	-7.68875837	-0.72331613	-1.28841484	
6	5.63984156	1.29678392	-1.22741485	1	6.61864138	1.67878389	-1.50761485	
6	4.58484173	1.32368386	-2.13301492	8	-0.58805847	-2.04861617	-0.61641490	
1	4.77184153	1.72838390	-3.12221503	15	-1.13415849	-3.39291620	-0.23101491	
6	3.31274152	0.84418386	-1.80641484	8	-0.61905849	-4.05371618	1.09788513	

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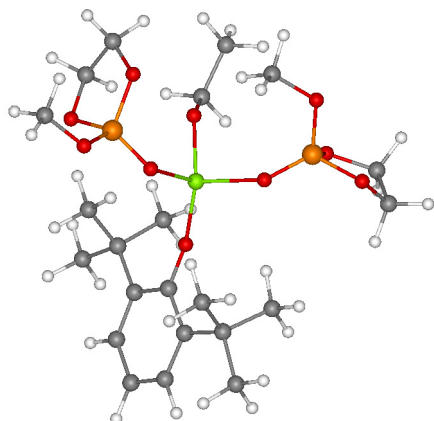
6	4.02704144	-0.36971611	1.83288515	8	-0.38985848	-1.32831609	2.23558497
6	2.19304156	0.87258387	-2.86361504	6	-1.00395846	-3.64931631	2.45698500
6	3.02764153	0.43918389	2.68248510	6	-0.17425850	-2.47881627	2.95978498
1	2.05364156	0.53328383	2.20328498	1	-2.06935835	-3.40431619	2.44498491
1	2.87864161	-0.03441612	3.66038489	1	-0.84465849	-4.55181599	3.05238509
1	3.41024160	1.45188391	2.85218501	1	0.88414145	-2.79591632	2.97458506
6	3.58044147	-1.84071612	1.70718515	1	-0.46675849	-2.35951614	4.02278519
1	2.65134168	-1.93661606	1.14328516	8	-0.82315850	-4.48401642	-1.34041488
1	4.34604168	-2.42571616	1.18528509	6	0.50904143	-4.59411621	-1.88991487
1	3.43304157	-2.28451610	2.69938493	1	1.18784153	-5.00581598	-1.13971484
6	5.34834146	-0.38891611	2.62318492	1	0.86194146	-3.61971617	-2.23191500
1	6.12784147	-0.96681613	2.11528492	1	0.42674151	-5.28051615	-2.73141503
1	5.73434162	0.61848384	2.81308508	8	-1.04545844	0.98138386	0.55628508
1	5.17564154	-0.85851616	3.59818506	15	-1.16165853	2.26738381	1.30458510
6	2.67324162	1.42388391	-4.21761465	8	0.25034150	2.76828384	1.88808513
1	3.02184153	2.46008372	-4.14681482	8	-1.52665854	3.57138371	0.44338506
1	3.47854161	0.81968385	-4.64851475	6	0.44004151	4.17068386	1.61938512
1	1.83854139	1.40968394	-4.92801476	6	-0.38095850	4.45028400	0.35938507
6	1.67364156	-0.55511612	-3.12871504	1	0.08244148	4.74488401	2.47908497
1	1.29124153	-1.01651609	-2.21811509	1	1.50694144	4.33848381	1.47298515
1	0.86904144	-0.53831613	-3.87531495	1	0.17454150	4.21068382	-0.55011487
1	2.48274159	-1.18261611	-3.51971507	1	-0.75505853	5.47348356	0.31478509
6	1.03934145	1.78408396	-2.40141511	8	-2.23275852	2.26208377	2.44798493
1	1.39744151	2.81648374	-2.30311513	6	-2.70465851	1.03978395	3.09898496
1	0.22434148	1.78018391	-3.13681507	1	-2.05835843	0.19148389	2.85468507
1	0.63774145	1.46308386	-1.44021487	1	-3.73075843	0.87748384	2.76868510
8	-5.70735836	0.62798387	1.34078515	1	-2.67085838	1.24558389	4.16898537
15	-5.44915819	0.77268386	-0.10381491	1	-3.28215837	3.01628375	-1.72421491
8	-2.71975851	-3.42551613	-0.10841491	1	-8.61545849	0.76738387	-1.61191487
8	-4.85075855	-0.55911613	-0.80291492				

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## S1.5. CP sequence, mononuclear mechanism

### I-1\_CP

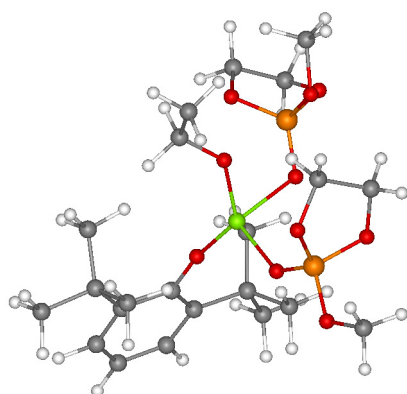


Zero-point vibrational energy	1638160.6 (Joules/Mol)
	391.52977 (Kcal/Mol)
Zero-point correction=	0.623942 (Hartree/Particle)
Thermal correction to Energy=	0.666703
Thermal correction to Enthalpy=	0.667647
Thermal correction to Gibbs Free Energy=	0.543208
Sum of electronic and zero-point Energies=	-2496.480479
Sum of electronic and thermal Energies=	-2496.437719
Sum of electronic and thermal Enthalpies=	-2496.436775
Sum of electronic and thermal Free Energies=	-2496.561213

				cartesian			
12	0.61740255	0.17141742	0.16157193	1	-1.30479741	1.32141745	3.73557210
8	1.97870255	0.01081741	-1.17392814	1	-0.86489737	0.18811741	2.44897199
8	-1.24289739	-0.05588260	0.07257193	6	3.28400254	0.73591739	-3.09402800
6	1.97560263	0.14851740	-2.56452799	8	1.49490261	-0.99968261	1.59577191
1	1.14980257	0.79141742	-2.91522789	15	2.53400254	-2.05778265	1.54237187
1	1.81180263	-0.82768261	-3.06222796	8	4.00910282	-1.57008255	1.12457192
6	-2.49749756	-0.47388262	0.17457193	8	2.36990237	-3.22068262	0.45137194
6	-3.02579761	-1.42018259	-0.76382810	6	4.43480253	-2.19108272	-0.11222808
6	-4.34529734	-1.85518253	-0.60912806	6	3.20340252	-2.90098262	-0.69282806
1	-4.75969744	-2.57748270	-1.30472803	1	5.24590254	-2.88268256	0.13177192
6	-5.16269732	-1.39028251	0.41517192	1	4.79240227	-1.40458250	-0.77622807
6	-4.65569735	-0.44968259	1.30527186	1	2.64110255	-2.23288274	-1.34672809
1	-5.30979776	-0.08498260	2.09047198	1	3.44850254	-3.84148264	-1.18622804
6	-3.34659743	0.03191741	1.21347189	8	2.61410236	-2.75338268	2.95797205
6	-2.18149757	-1.95198262	-1.93662798	6	3.54550242	-3.82268262	3.21027207

6	-2.85389757	1.09531748	2.21207190	1	3.34680247	-4.66408253	2.54297209
6	-0.96769738	-2.74448276	-1.41382813	1	4.57180262	-3.46718264	3.08917212
1	-0.33879742	-2.13978267	-0.76012808	1	3.37930250	-4.12248278	4.24377203
1	-0.35119745	-3.10078263	-2.24932790	8	1.04790258	2.03171730	0.89767194
1	-1.29819739	-3.61648273	-0.83902812	15	1.60740256	3.27651739	0.30687195
6	-1.72569740	-0.78298259	-2.83272791	8	1.17740262	4.65801716	1.00037193
1	-1.16219735	-0.04118259	-2.26632786	8	1.06320262	3.59051728	-1.17422807
1	-2.59599757	-0.28248259	-3.27202797	6	0.23190257	5.35401726	0.15877193
1	-1.09559739	-1.14838254	-3.65332794	6	0.60440254	4.95481730	-1.26962805
6	-2.96929741	-2.91578269	-2.84172797	1	0.34820256	6.42151737	0.34637195
1	-3.84809732	-2.43918276	-3.28882790	1	-0.77799737	5.03231716	0.42517191
1	-3.29869747	-3.81328273	-2.30702806	1	-0.24739745	4.97201729	-1.94962800
1	-2.32319760	-3.24528265	-3.66382790	1	1.41660261	5.56841755	-1.66952813
6	-3.94919729	1.52651751	3.20407200	8	3.18310237	3.33451724	0.31357193
1	-4.29589748	0.69521743	3.82727194	6	3.97180247	2.13351727	0.55597192
1	-4.81779766	1.96471751	2.70027208	1	3.93100238	1.88961744	1.61837196
1	-3.54259753	2.28911734	3.87847209	1	3.59490252	1.30451751	-0.04792808
6	-2.42649746	2.36861730	1.45257187	1	4.98750257	2.40101743	0.26737192
1	-1.65039742	2.14671731	0.71997190	1	3.27290249	0.80491740	-4.18892813
1	-2.04479742	3.12081742	2.15557194	1	3.44890237	1.74171746	-2.69252801
1	-3.28709745	2.79721737	0.92557192	1	4.13880253	0.11251741	-2.80412793
6	-1.69089746	0.54651743	3.06167197	1	-6.18459749	-1.74908257	0.51297194
1	-2.03389764	-0.29438260	3.67447209				

## TS-12\_CP



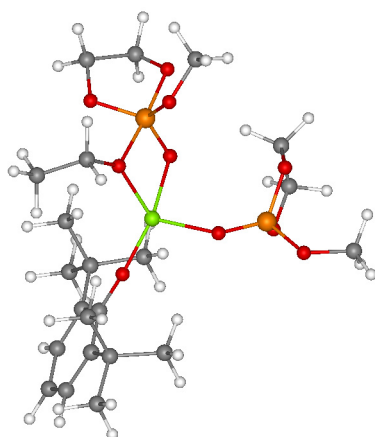
Zero-point vibrational energy	1639406.3 (Joules/Mol)
	391.82751 (Kcal/Mol)
Zero-point correction=	0.624417 (Hartree/Particle)
Thermal correction to Energy=	0.665903
Thermal correction to Enthalpy=	0.666847
Thermal correction to Gibbs Free Energy=	0.547305
Sum of electronic and zero-point Energies=	-2496.473564

Sum of electronic and thermal Energies=	-2496.432077
Sum of electronic and thermal Enthalpies=	-2496.431133
Sum of electronic and thermal Free Energies=	-2496.550676

cartesian							
12	0.41053650	-0.26081076	0.00927469	1	-0.99606347	0.42068923	3.92087483
8	1.70083654	0.20168923	-1.33782530	1	-0.92176342	-0.48121077	2.39757466
8	-1.44706345	-0.08801077	0.07387469	1	1.42073655	1.32478929	-3.04362535
6	1.65293658	0.29098922	-2.73432517	8	1.01333654	-2.01641083	0.84527469
1	0.84523654	-0.33471078	-3.14752531	15	2.32193661	-2.67321086	1.09177470
6	2.96323657	-0.13601077	-3.39512539	8	3.31803656	-1.86601079	2.06067467
6	-2.75746346	-0.23241076	0.21807469	8	3.31543660	-2.83241081	-0.15822530
6	-3.53666353	-0.83991075	-0.81902528	6	4.49573660	-1.42741072	1.34067476
6	-4.91456366	-0.97861075	-0.62862527	6	4.20833635	-1.68381071	-0.14432532
1	-5.52156353	-1.43981075	-1.40082526	1	5.34263659	-2.01081085	1.71227467
6	-5.54876328	-0.53931075	0.52877468	1	4.64263630	-0.36821079	1.55047476
6	-4.78966331	0.06338924	1.52637470	1	3.69033647	-0.84441078	-0.61892533
1	-5.30016327	0.40738922	2.42017484	1	5.09973669	-1.96281075	-0.70622528
6	-3.40726352	0.23388924	1.40677476	8	2.07273650	-4.11221075	1.68447471
6	-2.88956356	-1.32431078	-2.12922525	6	3.17173648	-4.96501112	2.06267476
6	-2.61666346	0.91208923	2.54017472	1	3.79483652	-5.18691111	1.19377470
6	-1.86916351	-2.44581079	-1.84572530	1	3.76103663	-4.49251080	2.85187483
1	-1.11956346	-2.14651084	-1.11232531	1	2.71853662	-5.88081121	2.43847466
1	-1.35426342	-2.74311066	-2.76802516	8	1.47173655	1.11868930	1.12057471
1	-2.37706351	-3.32891083	-1.44272530	15	2.18853641	2.15588927	0.32037470
6	-2.22156358	-0.13981077	-2.85652518	8	2.39523649	3.51798916	1.19717467
1	-1.47936344	0.35518926	-2.22922540	8	1.42913651	2.86898923	-0.91042531
1	-2.97606349	0.60538924	-3.13312531	6	1.36103654	4.45328903	0.85837471
1	-1.73136353	-0.47991079	-3.77752519	6	1.14133656	4.25988913	-0.64302528
6	-3.91676331	-1.91561079	-3.11122537	1	1.71523654	5.45428896	1.10787475
1	-4.67496347	-1.18321073	-3.40802526	1	0.46003652	4.22528887	1.43537474
1	-4.42716360	-2.79301071	-2.69992518	1	0.11253650	4.44938898	-0.95112526
1	-3.39906335	-2.23751068	-4.02232552	1	1.82723653	4.86548901	-1.24212527
6	-3.52086353	1.37238920	3.69767475	8	3.69383645	1.76108921	-0.00962530
1	-4.03886366	0.53598922	4.17897463	6	4.52263641	2.66868925	-0.75712526
1	-4.27116346	2.10148931	3.37317467	1	4.10643625	2.82318926	-1.75512528
1	-2.90396357	1.85578930	4.46417427	1	4.62253666	3.61878920	-0.22612530
6	-1.91006351	2.17748928	2.01087475	1	5.49823666	2.19028926	-0.83912528
1	-1.26306343	1.94288921	1.16517472	1	2.90783644	-0.02351077	-4.48502541
1	-1.30366349	2.63438916	2.80407476	1	3.80183649	0.47188926	-3.03512526
1	-2.65376353	2.91258931	1.68147469	1	3.18493652	-1.18611073	-3.17512536

6	-1.59826350	-0.07291076	3.14817476	1	-6.62266350	-0.66091073	0.64997470
1	-2.12096357	-0.91671073	3.61177468				

## I-2\_CP

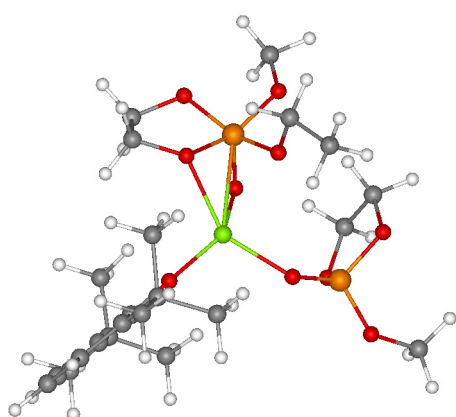


Zero-point vibrational energy	1643868.5 (Joules/Mol)
	392.89400 (Kcal/Mol)
Zero-point correction=	0.626116 (Hartree/Particle)
Thermal correction to Energy=	0.667507
Thermal correction to Enthalpy=	0.668451
Thermal correction to Gibbs Free Energy=	0.549132
Sum of electronic and zero-point Energies=	-2496.488615
Sum of electronic and thermal Energies=	-2496.447225
Sum of electronic and thermal Enthalpies=	-2496.446280
Sum of electronic and thermal Free Energies=	-2496.565600

cartesian							
12	0.40965077	0.16324402	0.40965867	1	-0.26054922	-0.64395601	-3.51344132
8	1.38165081	-1.14505601	1.59255862	1	-0.62824929	0.37664402	-2.10824132
8	-1.41184926	0.10424402	0.11315867	1	2.22695065	-2.21815610	3.13935876
6	1.26205075	-1.77715588	2.87625861	8	1.00705075	2.09214401	0.63155866
6	0.16595076	-2.82685614	2.87855864	15	1.86575079	2.98484397	-0.18914133
1	1.05445075	-0.98825592	3.60785866	8	1.57025075	2.92744398	-1.76704133
6	-2.68734932	-0.06195597	-0.21684134	8	3.44295073	2.70274401	-0.24764132
6	-3.71524906	0.47494403	0.62185866	6	2.75785089	2.58334398	-2.51904130
6	-5.04834938	0.27384403	0.25275868	6	3.77115083	2.04324412	-1.50104129
1	-5.84524918	0.66924405	0.87385869	1	3.10675073	3.48874402	-3.02304125
6	-5.39964914	-0.42285597	-0.89884132	1	2.47655082	1.83074403	-3.25544143
6	-4.39484930	-0.93205601	-1.71394134	1	3.66755080	0.96604401	-1.35974133
1	-4.68664932	-1.46955609	-2.61034131	1	4.79785061	2.31524396	-1.74664128
6	-3.03974915	-0.77125597	-1.40884137	8	1.68635082	4.46114397	0.34075868

6	-3.38214922	1.26914406	1.89865863	6	2.35285068	5.56894398	-0.29484132
6	-1.96684933	-1.35285592	-2.34784126	1	3.43525076	5.42224407	-0.27984133
6	-2.57604933	2.53564405	1.54535866	1	1.99105084	5.68804407	-1.31894135
1	-1.64724922	2.29684401	1.02725863	1	2.09055066	6.44804430	0.29125869
1	-2.32734919	3.09714389	2.45485878	8	2.08045077	-0.42135596	-0.50814134
1	-3.16654921	3.19164395	0.89585871	15	2.79535079	-1.35045600	0.50555867
6	-2.59784913	0.39234403	2.89525867	8	4.18625069	-1.65595603	-0.44914132
1	-1.67254925	0.01654403	2.45655870	8	2.45885086	-2.96635604	0.55045867
1	-3.19764924	-0.47205597	3.20095873	6	4.00825071	-2.83215594	-1.20814133
1	-2.34644914	0.96554404	3.79645872	6	3.31445074	-3.78915596	-0.24654132
6	-4.64474916	1.74384403	2.64025879	1	4.98425102	-3.20155597	-1.53484130
1	-5.27504921	0.90924400	2.96625876	1	3.38335085	-2.63475609	-2.09034133
1	-5.25504923	2.41934395	2.03115869	1	2.69275069	-4.53425598	-0.74814135
1	-4.34694910	2.29644394	3.53865862	1	4.03095055	-4.29235601	0.41205868
6	-2.57644916	-2.05665612	-3.57384133	8	3.68005085	-0.71055597	1.71355867
1	-3.17654920	-1.37605596	-4.18724155	6	5.10645056	-0.60865599	1.74125862
1	-3.20284915	-2.90985608	-3.29314137	1	5.57895088	-1.59195590	1.69365871
1	-1.76834917	-2.43995595	-4.20754147	1	5.48005056	0.00764403	0.92145866
6	-1.12894917	-2.41915607	-1.61344135	1	5.34075069	-0.13295597	2.69595861
1	-0.66624916	-2.03695607	-0.70294130	1	0.06895077	-3.25945592	3.88075876
1	-0.33344921	-2.80135608	-2.26514125	1	-0.79834926	-2.39145613	2.60295868
1	-1.76394916	-3.26345611	-1.32354128	1	0.39985076	-3.62695599	2.17275858
6	-1.07044923	-0.22625598	-2.90234137	1	-6.44584942	-0.56425595	-1.15974128
1	-1.65874910	0.44984403	-3.53254128				

### TS-23\_CP



Zero-point vibrational energy

1643386.5 (Joules/Mol)

392.77879 (Kcal/Mol)

Zero-point correction=

0.625933 (Hartree/Particle)

Thermal correction to Energy=

0.666641

Thermal correction to Enthalpy=

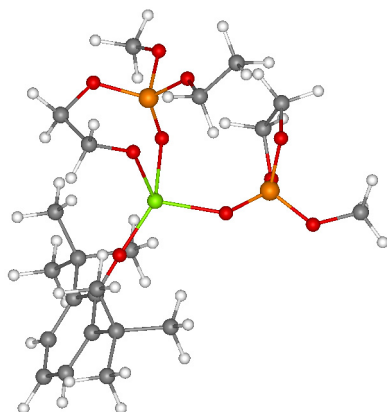
0.667585

Thermal correction to Gibbs Free Energy=	0.550969
Sum of electronic and zero-point Energies=	-2496.472669
Sum of electronic and thermal Energies=	-2496.431961
Sum of electronic and thermal Enthalpies=	-2496.431016
Sum of electronic and thermal Free Energies=	-2496.547633

				cartesian			
12	-0.46078813	-0.07986808	-0.08209602	1	0.91301191	1.99273193	3.36870384
8	-2.48428822	-1.05306804	-1.10749602	1	0.91201186	1.78903198	1.60400391
8	1.38161194	0.08873192	0.01360398	6	-2.78728819	-0.75856811	-3.46929598
6	-2.75938821	-1.75566804	-2.32859612	8	-1.19088817	1.73093200	-0.60479605
1	-3.72698808	-2.26016808	-2.22699594	15	-2.36728811	2.54853177	-0.20409602
1	-1.98288810	-2.51246810	-2.49289608	8	-2.74498820	2.51143193	1.34900391
6	2.69871187	0.22153193	0.09280398	8	-3.79758811	2.13223195	-0.79209602
6	3.50461197	0.11553192	-1.08599603	6	-3.96658802	1.76873195	1.58040392
6	4.89331198	0.21093193	-0.95479608	6	-4.52028799	1.35403192	0.19620398
1	5.52511168	0.12433192	-1.83249605	1	-4.64158821	2.43453193	2.12210393
6	5.50731182	0.41823190	0.27570397	1	-3.71168804	0.89563191	2.18000388
6	4.71571207	0.55553192	1.41080391	1	-4.35138798	0.29703194	-0.01009602
1	5.21011209	0.73443192	2.35990405	1	-5.57568789	1.60313201	0.07920398
6	3.32121181	0.47253191	1.35770392	8	-2.10258818	4.04253197	-0.63319600
6	2.87721181	-0.08456808	-2.47829604	6	-3.06578803	5.07783222	-0.35169601
6	2.49121189	0.66803193	2.64060402	1	-4.01688814	4.85243225	-0.83899605
6	1.93631196	1.09133196	-2.81299615	1	-3.19948816	5.18393230	0.72700393
1	1.16201186	1.23183191	-2.05769610	1	-2.64418817	5.99283218	-0.76419604
1	1.45181191	0.93043190	-3.78469610	8	-1.93638813	-0.66336811	1.22650397
1	2.50411177	2.02623200	-2.87339616	15	-2.33268809	-1.88506806	0.37540397
6	2.11921191	-1.42506802	-2.54819608	8	-2.15548801	-3.28226805	1.26180398
1	1.32821190	-1.49046803	-1.80049610	8	-0.69828808	-2.23676825	-0.30899602
1	2.80731177	-2.26076818	-2.37699604	6	-0.80588812	-3.57026815	1.60860395
1	1.66931200	-1.55966806	-3.54029608	6	0.00811189	-3.27786803	0.34980398
6	3.93321180	-0.12516807	-3.59779596	1	-0.75458813	-4.61816788	1.90980399
1	4.62861204	-0.96406811	-3.48509598	1	-0.50138813	-2.93066812	2.44340396
1	4.51591206	0.80043191	-3.65199614	1	1.02341187	-2.94686818	0.57900393
1	3.42891192	-0.24916808	-4.56309605	1	0.04901189	-4.14746809	-0.31559601
6	3.36911178	0.95323193	3.87230396	8	-3.96598816	-2.11186814	0.33580399
1	3.96691179	1.86293197	3.75290394	6	-4.69828796	-2.84896827	1.31940401
1	4.04631186	0.12363192	4.10240412	1	-4.53238821	-3.92236805	1.20970392
1	2.72491193	1.09993196	4.74690390	1	-4.42638826	-2.54566813	2.33400393
6	1.68521190	-0.60426807	2.96880388	1	-5.75148821	-2.62006807	1.13760400
1	0.99731183	-0.86216807	2.16320395	1	-3.01908803	-1.27436805	-4.40659618

1	1.09901190	-0.46506810	3.88550401	1	-3.54798818	0.00793192	-3.29829597
1	2.36111188	-1.45306802	3.12310386	1	-1.81888807	-0.26376808	-3.58309603
6	1.55111194	1.88073194	2.48340392	1	6.59051180	0.48293191	0.34750399
1	2.13561177	2.80023193	2.36880398				

### I-3\_CP

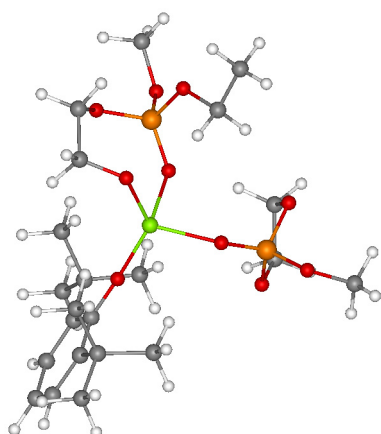


Zero-point vibrational energy	1643197.0 (Joules/Mol)
	392.73350 (Kcal/Mol)
Zero-point correction=	0.625861 (Hartree/Particle)
Thermal correction to Energy=	0.667501
Thermal correction to Enthalpy=	0.668446
Thermal correction to Gibbs Free Energy=	0.549508
Sum of electronic and zero-point Energies=	-2496.490683
Sum of electronic and thermal Energies=	-2496.449042
Sum of electronic and thermal Enthalpies=	-2496.448098
Sum of electronic and thermal Free Energies=	-2496.567035

cartesian							
12	0.26832652	0.02891735	0.22843331	1	-0.89907342	-0.87418264	-3.62356663
8	3.69682670	-1.03028262	1.22113335	1	-0.97147352	0.19851735	-2.21186662
8	-1.57337356	0.05761734	0.09073333	1	2.99442649	0.64781737	2.22873354
6	3.61282659	-0.23198265	2.41413355	8	1.13502645	1.83421731	-0.07396667
6	5.02822638	0.15801734	2.79023337	15	2.30052662	2.34731722	-0.84406668
1	3.14902663	-0.81368262	3.21433353	8	2.44092655	1.90691733	-2.37596655
6	-2.88367343	0.09791735	-0.12576666	8	3.73302650	1.85031736	-0.32856667
6	-3.73677349	0.80691737	0.77853334	6	3.44752669	0.86461735	-2.49686646
6	-5.11367321	0.80421734	0.53603333	6	4.44272661	1.09821737	-1.34706664
1	-5.78077364	1.33021736	1.21073329	1	3.90732670	0.97901738	-3.47866654
6	-5.67097330	0.14531735	-0.55456668	1	2.94822669	-0.09948265	-2.40276647
6	-4.83347321	-0.52508265	-1.43906665	1	4.76852655	0.15991735	-0.89776665
1	-5.28387356	-1.02558267	-2.28966665	1	5.30332661	1.69971740	-1.65056670

6	-3.44737339	-0.56758261	-1.26056671	8	2.24772644	3.92411733	-0.80686671
6	-3.17327332	1.57501733	1.98953331	6	3.25982666	4.72041702	-1.45456672
6	-2.56567335	-1.31468260	-2.27936649	1	4.23022652	4.55481720	-0.98056668
6	-2.22547340	2.69541717	1.51593328	1	3.30352664	4.48571730	-2.52036667
1	-1.40347338	2.31101727	0.91163331	1	2.95402670	5.75601721	-1.31646669
1	-1.80107331	3.22901726	2.37593341	8	1.72392654	-1.00528264	-0.66266668
1	-2.77217340	3.42291737	0.90583330	15	2.52572656	-1.78088260	0.40713331
6	-2.43817329	0.61571735	2.94693351	8	2.02012658	-3.21408272	0.99613333
1	-1.62617350	0.09311734	2.44013333	8	1.16712654	-1.01538265	1.69013333
1	-3.12947345	-0.13818264	3.34023333	6	0.81632650	-3.30688286	1.76293337
1	-2.01907349	1.16701734	3.79813337	6	0.69402653	-2.01478267	2.55683351
6	-4.27647352	2.25521731	2.81883335	1	0.90812653	-4.19448280	2.39253354
1	-4.98867321	1.53441739	3.23453355	1	-0.02687347	-3.43258286	1.07593334
1	-4.83557320	2.99581718	2.23723340	1	-0.34417349	-1.82828259	2.84913349
1	-3.81747341	2.78351736	3.66223335	1	1.30932653	-2.05748272	3.46803355
6	-3.38597345	-1.94148266	-3.42106652	8	3.68002653	-2.48408270	-0.53786665
1	-3.93707323	-1.19048262	-3.99656653	6	3.25802660	-3.35738277	-1.58016670
1	-4.09937334	-2.68878269	-3.05796647	1	2.80382657	-4.26558256	-1.17096663
1	-2.70677352	-2.45028281	-4.11506701	1	2.54432654	-2.86478281	-2.25016665
6	-1.81787348	-2.47738266	-1.59666669	1	4.15442657	-3.62948275	-2.14206648
1	-1.20657349	-2.13058281	-0.76266670	1	5.01112652	0.75081736	3.71033335
1	-1.16347337	-2.99008274	-2.31206656	1	5.64592648	-0.72808266	2.95933342
1	-2.53227329	-3.20958281	-1.20436668	1	5.49062681	0.76041734	2.00393343
6	-1.57477355	-0.33848265	-2.94556665	1	-6.74617338	0.15901735	-0.71646667
1	-2.11707330	0.41211733	-3.53066659				

#### I-4\_CP



Zero-point vibrational energy

1640580.5 (Joules/Mol)

392.10815 (Kcal/Mol)

Zero-point correction=

0.624864 (Hartree/Particle)

Thermal correction to Energy=

0.667099

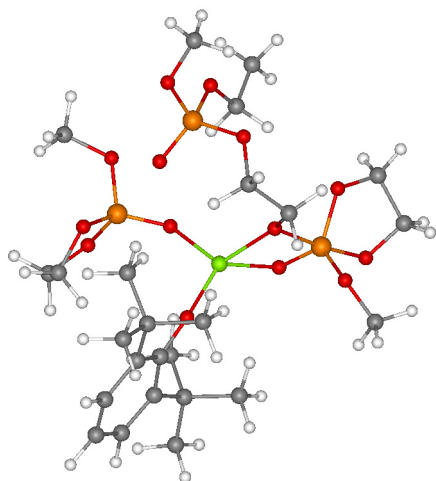


Thermal correction to Enthalpy=	0.668043
Thermal correction to Gibbs Free Energy=	0.546623
Sum of electronic and zero-point Energies=	-2496.494176
Sum of electronic and thermal Energies=	-2496.451941
Sum of electronic and thermal Enthalpies=	-2496.450997
Sum of electronic and thermal Free Energies=	-2496.572417

				cartesian			
12	0.39618522	-0.00831600	0.80612534	1	-0.33831477	-0.68631601	-3.48837471
8	3.54258537	-2.15861607	-1.44747472	1	-0.63811475	0.18698400	-1.96587467
8	-1.36531472	-0.18701601	0.21162534	1	5.41748524	-2.85931611	-0.85347468
6	4.53808498	-3.19411612	-1.40997469	8	0.95178527	1.96198404	0.72722536
1	4.81038523	-3.38791609	-2.44717479	15	1.35068536	2.95688391	-0.29767466
1	4.12698507	-4.10021591	-0.95947468	8	0.39468524	3.05168390	-1.58157468
6	-2.64871478	-0.36481601	-0.06987467	8	2.73628521	2.69568396	-1.07477462
6	-3.66251469	0.07508401	0.84232533	6	1.11698532	2.76018405	-2.80207467
6	-5.00301504	-0.12451599	0.49862534	6	2.43178535	2.10508394	-2.36687469
1	-5.78631496	0.20168400	1.17482531	1	1.27628517	3.70498395	-3.32907486
6	-5.38011503	-0.73411602	-0.69337469	1	0.49808526	2.09408402	-3.40257478
6	-4.39211512	-1.16281605	-1.57307470	1	2.33418536	1.02518404	-2.23507476
1	-4.70201492	-1.64001596	-2.49717474	1	3.26118541	2.33858395	-3.03437471
6	-3.03171468	-0.99821603	-1.29727471	8	1.46518517	4.37308407	0.38792533
6	-3.30861473	0.75348401	2.17912531	6	1.75338531	5.55788422	-0.38107467
6	-1.98071480	-1.50101602	-2.30407476	1	2.72298527	5.46388435	-0.87557465
6	-2.52911472	2.05998397	1.92722535	1	0.95998526	5.73498440	-1.11077464
1	-1.63121486	1.89248395	1.33272529	1	1.78208518	6.37598419	0.33662534
1	-2.23391461	2.52318406	2.87722516	8	1.87628531	-0.57601601	-0.52157468
1	-3.15691471	2.77548409	1.38372529	15	2.88228536	-1.61151600	-0.10287467
6	-2.49721479	-0.20691600	3.07182527	8	2.38328528	-2.94841599	0.58532536
1	-1.58361483	-0.55391598	2.58772516	8	1.26348519	-0.94961596	2.21922517
1	-3.09581470	-1.09091604	3.31862521	6	2.24408531	-3.11081600	2.02972531
1	-2.21691465	0.28428400	4.01192522	6	1.08688521	-2.27861595	2.55992532
6	-4.55741501	1.14458394	2.99002528	1	3.18908525	-2.80691600	2.48962522
1	-5.16711473	0.27548400	3.25942516	1	2.09378529	-4.18401575	2.17062521
1	-5.19241476	1.86008406	2.45662522	1	0.14578524	-2.70831609	2.17102528
1	-4.24181509	1.62268400	3.92452526	1	1.06778526	-2.43271589	3.65522528
6	-2.61491466	-2.13541603	-3.55437469	8	4.10738516	-1.08261597	0.76332533
1	-3.24151468	-1.42761600	-4.10787487	6	4.10708523	0.20038401	1.46172535
1	-3.22171474	-3.01371598	-3.31037474	1	3.97438526	0.98998398	0.71772534
1	-1.81931472	-2.46761608	-4.23167467	1	3.25978541	0.20028400	2.15102530
6	-1.10101485	-2.58901596	-1.65707469	6	5.43298483	0.32948402	2.17612529

1	-0.61651474	-2.22701597	-0.75047469	1	5.46268511	1.28628397	2.70632529
1	-0.32201475	-2.92431593	-2.35317469	1	5.56278515	-0.47031599	2.91002512
1	-1.71221471	-3.45731592	-1.38757467	1	6.26998520	0.29908401	1.47282529
6	-1.11541486	-0.32541600	-2.80157471	1	-6.43161488	-0.87481600	-0.93257469
1	-1.73981476	0.40008399	-3.33647490				

## TS-45\_CP



Zero-point vibrational energy	1949671.9 (Joules/Mol)
	465.98276 (Kcal/Mol)
Zero-point correction=	0.742591 (Hartree/Particle)
Thermal correction to Energy=	0.793301
Thermal correction to Enthalpy=	0.794245
Thermal correction to Gibbs Free Energy=	0.655007
Sum of electronic and zero-point Energies=	-3257.059837
Sum of electronic and thermal Energies=	-3257.009126
Sum of electronic and thermal Enthalpies=	-3257.008182
Sum of electronic and thermal Free Energies=	-3257.147421

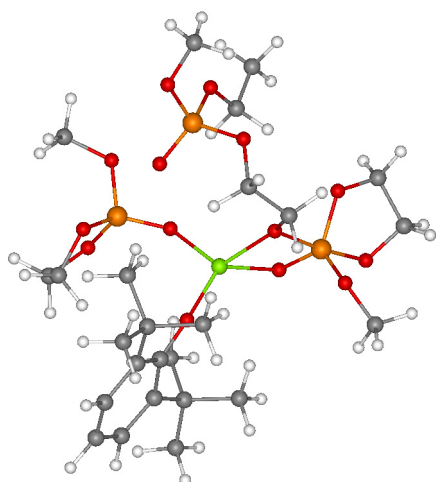
cartesian							
12	-0.10523887	0.60592556	0.45948553	6	-2.38783884	-0.08727442	-2.44541430
8	-3.87353897	-3.23817420	-1.69531453	1	-1.50293887	1.83552551	-2.67241430
8	1.60886109	0.37242556	-0.27001446	1	-3.14113879	1.85762560	-1.98391449
6	-5.22003889	-3.18237424	-2.19191432	1	-2.66273880	-0.08047442	-3.50501442
1	-5.36953878	-2.28767443	-2.80231452	1	-1.48033893	-0.68247443	-2.31961441
1	-5.93093872	-3.19097424	-1.36221457	8	-4.34663868	-1.86157441	0.30078554
6	2.89426112	0.16092558	-0.51581448	6	-4.16563892	-0.82287443	1.30668545
6	3.28926110	-0.53407443	-1.70731449	1	-3.25853896	-1.05067444	1.87138546
6	4.63826132	-0.86317444	-1.87411451	1	-4.03683901	0.13832557	0.80188555
1	4.95426130	-1.40937448	-2.75681448	6	-5.38843870	-0.82667446	2.19628549

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6	5.60786152	-0.50327444	-0.94411451	1	6.64876127	-0.77927446	-1.09591448
6	5.23256111	0.25902557	0.15728553	8	-0.76333886	2.24552560	1.33788550
1	6.00896120	0.58222556	0.84278554	15	-1.78053892	2.88952565	0.39088553
6	3.90356088	0.62822556	0.39188552	8	-2.06553888	4.26472569	1.34818542
6	2.27416110	-0.89087445	-2.81031442	8	-3.40323901	2.56412578	0.33818552
6	3.57036114	1.56222558	1.57158554	6	-3.37853885	4.75012589	1.18758547
6	1.53546107	0.38072556	-3.27601433	6	-4.22463894	3.49252558	1.05098546
1	1.02306116	0.87532556	-2.45001435	1	-3.46813893	5.38092566	0.28948551
1	0.79946113	0.12892558	-4.05061483	1	-3.64923882	5.34512568	2.06388545
1	2.24286103	1.09712553	-3.70821428	1	-4.46603870	3.06542563	2.03018546
6	1.27086115	-1.94707441	-2.31591439	1	-5.14243889	3.64172578	0.47708553
1	0.72126114	-1.62297440	-1.43271446	8	-1.24203885	3.70572567	-0.91811448
1	1.78846121	-2.87887430	-2.06081438	6	-0.60113883	4.98252583	-0.79711443
1	0.54206109	-2.18627429	-3.10071445	1	-1.32543886	5.77552557	-0.59441447
6	2.95436120	-1.47947443	-4.05981445	1	0.15396112	4.97362566	-0.00881447
1	3.44966102	-2.43497443	-3.85531449	1	-0.12213886	5.16152573	-1.76161456
1	3.69146109	-0.79427445	-4.49171448	8	-0.42933887	-0.88297445	1.76598549
1	2.19386101	-1.67007446	-4.82571459	15	-0.07483886	-2.30377436	2.02568555
6	4.83186150	2.05332565	2.30558562	8	1.04176116	-2.46877432	3.17738557
1	5.51156139	2.59672570	1.64078546	8	0.66666114	-3.14627433	0.88738555
1	5.39026117	1.23642552	2.77618551	6	2.21396112	-3.15127420	2.68018556
1	4.53486156	2.74232578	3.10428572	6	2.09196115	-3.14687443	1.15248549
6	2.70966101	0.84742558	2.62968564	1	2.21456122	-4.16377449	3.09418559
1	1.79806113	0.42092556	2.21268559	1	3.09436107	-2.60897422	3.02528548
1	2.41666102	1.54032552	3.42668557	1	2.53526115	-2.25737429	0.69858551
1	3.27586102	0.02952558	3.09108567	1	2.50616121	-4.04317427	0.69168556
6	2.85676122	2.82672572	1.04988551	8	-1.37093890	-3.07987428	2.47548556
1	3.51626110	3.37452579	0.36748552	6	-1.36163890	-4.50837421	2.65898561
1	2.59816122	3.49112558	1.88238549	1	-1.10353887	-5.00257444	1.72108543
1	1.93866110	2.59082580	0.51228553	1	-0.66403890	-4.78597450	3.45378566
8	-1.85423887	-2.27447438	-0.47051448	1	-2.37553883	-4.77537441	2.95278549
15	-3.25963879	-2.02737427	-0.85421449	1	-5.27103853	-0.07037442	2.97818565
8	-1.64153886	1.36812556	-0.66011447	1	-6.29173851	-0.59547442	1.62488544
8	-3.48503900	-0.70207441	-1.73141456	1	-5.51973867	-1.79967439	2.67798567
6	-2.18143892	1.33172560	-1.97311461	1	-5.35413885	-4.07317448	-2.80591440

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# I-5\_CP



Zero-point vibrational energy	1944471.0 (Joules/Mol)
	464.73972 (Kcal/Mol)
Zero-point correction=	0.740610 (Hartree/Particle)
Thermal correction to Energy=	0.793970
Thermal correction to Enthalpy=	0.794915
Thermal correction to Gibbs Free Energy=	0.643328
Sum of electronic and zero-point Energies=	-3257.061075
Sum of electronic and thermal Energies=	-3257.007714
Sum of electronic and thermal Enthalpies=	-3257.006770
Sum of electronic and thermal Free Energies=	-3257.158357

cartesian											
12	-0.78191978	0.80300331	0.25762117	6	3.13168025	0.86020327	3.39682126				
8	0.83498025	1.41350329	-0.52077883	6	2.86308026	-0.56529677	2.91732121				
8	-1.97581971	-0.58359671	-0.17047884	1	3.42058015	0.90120327	4.45042086				
6	1.98348033	0.91010332	-1.10357881	1	3.86988020	1.35500324	2.76872134				
1	1.86898029	0.72880328	-2.18597865	1	2.99818015	-0.65699673	1.83972120				
1	2.30588007	-0.05429673	-0.66697884	1	3.47338009	-1.30459678	3.43492126				
6	-2.67501974	-1.69249678	-0.35637885	8	0.04948026	0.65800327	4.76662111				
6	-2.06531978	-2.85199666	-0.93887889	6	-1.32901967	0.31890327	5.04992104				
6	-2.83681989	-4.00569677	-1.10437882	1	-1.98221982	0.68850327	4.25912094				
1	-2.39181972	-4.89329672	-1.54187882	1	-1.42581975	-0.76419675	5.14692116				
6	-4.17431974	-4.06279659	-0.72737885	1	-1.56361973	0.80240327	5.99712086				
6	-4.76741982	-2.93019676	-0.17997883	8	-1.77261972	2.58810329	0.15462117				
1	-5.81441975	-2.98629665	0.09952117	15	-1.81491971	3.70770335	-0.82487887				
6	-4.06011963	-1.74009681	0.01262116	8	-3.18701982	4.53910303	-0.89547884				
6	-0.59221977	-2.84669685	-1.38607883	8	-1.75891972	3.23600316	-2.35997868				
6	-4.78031969	-0.50989676	0.59402114	6	-3.89301991	4.21950340	-2.11417866				
6	0.33268026	-2.62909675	-0.17207883	6	-2.80141973	3.87070322	-3.12727880				

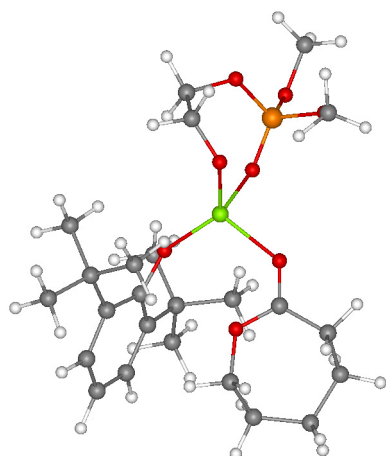
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1	0.08858025	-1.71499681	0.37112117	1	-4.47271967	5.09790325	-2.39887881
1	1.38138032	-2.57369685	-0.48997885	1	-4.55891943	3.37460327	-1.92227876
1	0.23568025	-3.46039677	0.53512114	1	-3.13741994	3.15920329	-3.88177896
6	-0.35921979	-1.76519680	-2.46047878	1	-2.38731980	4.76090336	-3.60927868
1	-0.62621975	-0.76899672	-2.10657883	8	-0.72921973	4.82210302	-0.57177883
1	-0.96761972	-1.97889686	-3.34657884	6	0.40698025	4.58150339	0.30762118
1	0.69298023	-1.75059676	-2.76957870	1	0.08268026	4.70280313	1.34242117
6	-0.16281976	-4.18299675	-2.01817870	1	0.81228024	3.58060336	0.13912116
1	-0.74441975	-4.42299652	-2.91477871	1	1.13378024	5.35040331	0.04802117
1	-0.24641974	-5.02189684	-1.31877887	8	4.39028025	1.47060323	-1.43347883
1	0.88838023	-4.11509657	-2.32167864	1	2.89718008	2.84540319	-1.43727887
6	-6.26611948	-0.77999675	0.89072114	1	3.22478008	2.14110327	0.16622117
1	-6.40481949	-1.56969678	1.63712120	1	-4.74891949	-4.97559690	-0.86547887
1	-6.82571936	-1.05659676	-0.00927883	15	5.32568026	0.49280328	-0.60427886
1	-6.72401953	0.13130328	1.29262114	8	5.15968037	-0.90089679	-1.35967886
6	-4.73731947	0.65070331	-0.42107886	8	6.80798054	0.91180325	-1.05567884
1	-3.70921993	0.90680325	-0.67797887	8	5.10408020	0.48060328	0.86602116
1	-5.22951937	1.53960323	-0.00387883	6	7.39258051	2.09380341	-0.48817885
1	-5.26451969	0.36560327	-1.33907890	6	5.92628050	-2.04749680	-0.91587889
6	-4.13671970	-0.08379671	1.92862117	6	5.49418020	-3.24299669	-1.73557889
1	-4.24311972	-0.88479674	2.66942120	1	6.98948050	-1.83019686	-1.05937886
1	-4.62931967	0.81360328	2.32482123	1	5.74068022	-2.20559669	0.15122117
1	-3.07411981	0.12820329	1.81142116	1	6.85728025	2.98380327	-0.83137888
6	3.11018014	1.91980326	-0.89847887	1	7.37968063	2.04400325	0.60362118
8	-0.40501976	0.71120328	2.26802135	1	8.42168045	2.12820339	-0.84587884
15	0.64738023	0.53580326	3.30532122	1	6.06318045	-4.12519693	-1.42677879
8	1.86738026	1.56330323	3.25702119	1	4.43068027	-3.44959664	-1.59247887
8	1.47488034	-0.83399677	3.24612117	1	5.67478037	-3.06909680	-2.79937863

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## S1.6. PC sequence, mononuclear mechanism

### I-1\_PC

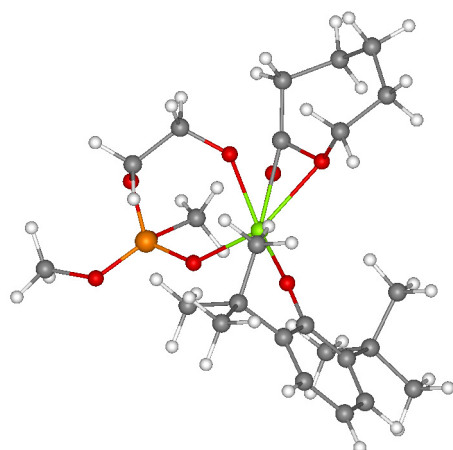


Zero-point vibrational energy	1675286.6 (Joules/Mol)
	400.40310 (Kcal/Mol)
Zero-point correction=	0.638083 (Hartree/Particle)
Thermal correction to Energy=	0.678025
Thermal correction to Enthalpy=	0.678969
Thermal correction to Gibbs Free Energy=	0.563290
Sum of electronic and zero-point Energies=	-2081.514540
Sum of electronic and thermal Energies=	-2081.474598
Sum of electronic and thermal Enthalpies=	-2081.473654
Sum of electronic and thermal Free Energies=	-2081.589333

cartesian							
12	1.31035209	-0.13747860	0.45031193	1	0.20125212	1.82692134	-3.20378828
8	5.10425234	0.56482142	-1.80868804	1	0.24685213	1.17592132	-1.56848812
8	-0.08244789	-1.05097866	-0.44058806	1	6.93575239	1.32642138	-1.16308808
6	6.54165220	0.54452139	-1.81648803	8	0.70545208	1.71762133	1.17021191
1	6.83845234	0.73742139	-2.84688830	6	-0.42414787	2.13762140	1.44321191
1	6.91135216	-0.43477857	-1.50208807	8	-1.43434787	1.30272138	1.31841195
6	-1.37864792	-1.17727864	-0.67538810	6	-2.81774783	1.66482139	1.56751192
6	-2.20344782	-1.96447861	0.19571191	6	-3.35934782	2.70992136	0.60861194
6	-3.58804798	-1.94957864	-0.00608808	1	-2.91794777	1.96812141	2.61641192
1	-4.23614788	-2.51487851	0.65601194	1	-3.33244777	0.71472144	1.42511189
6	-4.17794800	-1.24257863	-1.05088806	1	-3.07964778	2.41602159	-0.40878808
6	-3.35814786	-0.58647859	-1.96518803	1	-4.45214796	2.63682151	0.65471190
1	-3.82764769	-0.10137860	-2.81528831	6	-0.63514793	3.55922151	1.89011192
6	-1.96674788	-0.55547857	-1.82728803	6	-1.43794787	4.40502167	0.88481194
6	-1.60224783	-2.85027862	1.30661190	1	-1.04054797	4.24382162	-0.12358808

6	-1.10204792	0.09852140	-2.92398810	6	-2.94444776	4.14912128	0.91291195
6	-0.98424792	-2.01227856	2.44281173	1	-1.25304794	5.45782137	1.12271190
1	-0.09634790	-1.46337867	2.12751174	8	2.83435225	0.37312141	-0.79398805
1	-0.67274785	-2.66417861	3.26851177	15	4.29295206	0.30532143	-0.46878806
1	-1.71294796	-1.29687870	2.84021187	8	4.82425213	-1.06827867	0.12361192
6	-0.53614783	-3.79107857	0.70811194	8	2.46865225	-0.83777857	1.79341197
1	0.25585210	-3.22737861	0.21381192	6	3.95875216	-2.19907856	0.46031192
1	-0.98974788	-4.46207857	-0.02968808	6	3.25525212	-1.96957862	1.79301190
1	-0.08974788	-4.40857840	1.49751198	1	4.63275242	-3.05897856	0.49081191
6	-2.66484785	-3.75257850	1.96221197	1	3.24005222	-2.33827853	-0.35408807
1	-3.17604780	-4.38757849	1.23091197	1	2.68335223	-2.89707851	1.99161196
1	-3.42194772	-3.18057847	2.51041174	1	4.03275204	-1.91687870	2.57831192
1	-2.17564774	-4.41387844	2.68611193	8	4.87185240	1.43252134	0.48921192
6	-1.93654788	0.51522142	-4.14878798	1	-5.25764799	-1.24947870	-1.18208802
1	-2.66814780	1.29652131	-3.91348815	1	-3.42824769	4.81812143	0.19261192
1	-2.46954775	-0.33277857	-4.59158802	1	-3.33364773	4.43252134	1.90051198
1	-1.26904786	0.92112142	-4.91718817	1	-1.14044785	3.55922151	2.86411190
6	-0.04574788	-0.90547860	-3.43148828	1	0.36145213	3.97842145	2.03331184
1	0.60545212	-1.24167860	-2.62468815	6	4.79045200	1.34972131	1.93491197
1	0.57355213	-0.44267857	-4.20958805	1	3.88965225	0.81352139	2.24501181
1	-0.53624785	-1.78327870	-3.86658812	1	4.77635241	2.38022137	2.29031181
6	-0.41104791	1.37652135	-2.41318822	1	5.68275213	0.83842140	2.30301189
1	-1.15664792	2.11892152	-2.10378814				

## TS-12\_PC



Zero-point vibrational energy	1676085.2 (Joules/Mol)
	400.59398 (Kcal/Mol)
Zero-point correction=	0.638387 (Hartree/Particle)
Thermal correction to Energy=	0.677014
Thermal correction to Enthalpy=	0.677958
Thermal correction to Gibbs Free Energy=	0.566048

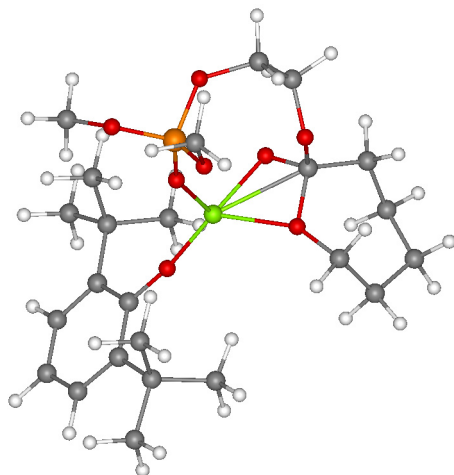
Sum of electronic and zero-point Energies=	-2081.492462
Sum of electronic and thermal Energies=	-2081.453835
Sum of electronic and thermal Enthalpies=	-2081.452891
Sum of electronic and thermal Free Energies=	-2081.564802

cartesian							
12	0.57755464	-0.08190262	-0.27801067	1	-1.59994531	1.98449743	-3.26191068
8	2.50175476	-4.09530258	-0.28111067	1	-1.32684529	1.60719740	-1.55051064
8	-1.25474524	-0.28190264	-0.10251068	1	4.02775478	-5.10330296	-1.28001070
6	3.64075470	-4.97860289	-0.26701069	8	2.17805457	0.95949745	-1.12331069
1	3.27445459	-5.93050289	0.11468932	6	2.12025476	1.70069742	-0.07751068
1	4.42205477	-4.58990288	0.39098933	8	0.81875461	2.22139716	0.03658932
6	-2.55504537	-0.53690267	-0.10161068	6	0.49185467	3.12589717	1.10698938
6	-3.18054533	-1.05020261	1.07948935	6	0.73275465	4.56669712	0.68308938
6	-4.55804539	-1.28680265	1.05728936	1	1.04665470	2.84579730	2.00868917
1	-5.05384541	-1.67320263	1.94188941	1	-0.56904536	2.95649719	1.30168939
6	-5.33034515	-1.04310262	-0.07391068	1	0.21805465	4.72199726	-0.27211070
6	-4.71354532	-0.55640262	-1.22181070	1	0.24155465	5.22229719	1.41298938
1	-5.32954550	-0.37730265	-2.09701085	6	3.26295471	2.64349723	0.26228932
6	-3.34064531	-0.29710263	-1.27411067	6	3.06725478	4.05399752	-0.31811067
6	-2.36714530	-1.34930265	2.35278916	1	2.65355468	3.98479748	-1.33051062
6	-2.70534539	0.23069736	-2.57411075	6	2.20435452	4.96749735	0.55968928
6	-1.69914532	-0.06530263	2.88518929	1	4.05675459	4.51389742	-0.41931069
1	-1.02834535	0.37779739	2.14868927	8	1.30345476	-1.92600262	-0.68101072
1	-1.12234533	-0.28140262	3.79388928	15	2.65205479	-2.56170273	-0.64241064
1	-2.46054530	0.68029737	3.14118934	8	3.64385462	-1.89550257	0.41308931
6	-1.30774534	-2.43280268	2.06278920	8	1.93635476	0.56909740	1.21878934
1	-0.66124535	-2.15890265	1.22788930	6	3.16825461	-1.49430263	1.72918940
1	-1.79274535	-3.37970281	1.80138934	6	3.06815481	0.01509738	1.84258938
1	-0.68594533	-2.60890269	2.95098925	1	3.91585469	-1.86940265	2.43338919
6	-3.24324536	-1.88980258	3.49668932	1	2.20775461	-1.96840262	1.95198929
1	-3.73804522	-2.83030272	3.23238921	1	3.04335475	0.25189736	2.91808915
1	-4.01024532	-1.17160261	3.80568933	1	3.99555469	0.44159737	1.43908930
1	-2.61204529	-2.08850265	4.37068939	8	3.49285460	-2.57520270	-1.97701061
6	-3.73604536	0.40349737	-3.70391083	1	-6.40074539	-1.23460269	-0.06221068
1	-4.51204538	1.13269734	-3.44811082	1	2.25455475	5.98859739	0.16338933
1	-4.22354507	-0.54060262	-3.96931076	1	2.65305471	5.01059723	1.56198931
1	-3.22724533	0.77129745	-4.60241032	1	3.39915466	2.71569729	1.34578931
6	-1.65264535	-0.76760268	-3.09981084	1	4.16495466	2.18829727	-0.15421069
1	-0.89614540	-1.00400257	-2.34991074	6	3.63635468	-1.39220262	-2.81171083
1	-1.15054536	-0.36520264	-3.98861074	1	2.84255481	-1.40610266	-3.55961084



1	-2.13024521	-1.71280265	-3.38051081	1	4.61065483	-1.48320258	-3.29031086
6	-2.07574534	1.61949742	-2.34281087	1	3.57415462	-0.47800264	-2.22021079
1	-2.84884524	2.34099722	-2.05541062				

## I-2\_PC

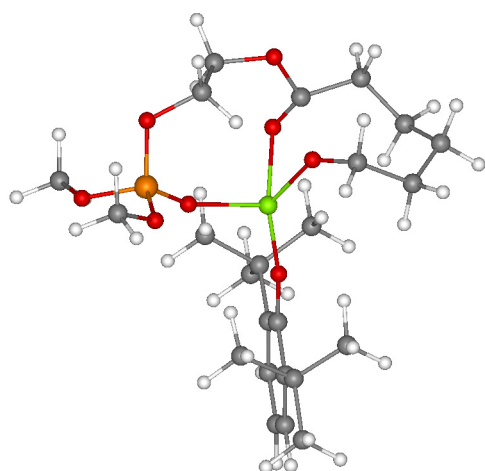


Zero-point vibrational energy	1678490.5 (Joules/Mol)
	401.16885 (Kcal/Mol)
Zero-point correction=	0.639303 (Hartree/Particle)
Thermal correction to Energy=	0.678320
Thermal correction to Enthalpy=	0.679264
Thermal correction to Gibbs Free Energy=	0.565282
Sum of electronic and zero-point Energies=	-2081.501711
Sum of electronic and thermal Energies=	-2081.462694
Sum of electronic and thermal Enthalpies=	-2081.461749
Sum of electronic and thermal Free Energies=	-2081.575732

cartesian							
12	-0.42749742	0.09922667	0.37556538	1	1.72230256	0.69012666	3.91556525
8	-3.29609728	-2.16277337	-1.72723460	1	1.46440256	1.06872678	2.20546532
8	1.39050257	-0.03817332	0.09696537	1	-3.76929736	-4.00827312	-2.56813478
6	-4.26499748	-3.08267331	-2.27173471	8	-1.60419738	0.90922672	1.71946537
1	-4.68979740	-2.58597350	-3.14283466	6	-2.42499733	1.51502669	0.88166535
1	-5.05329752	-3.29797339	-1.54573464	8	-1.66289747	1.61202669	-0.38103464
6	2.69020271	-0.28937334	0.00016536	6	-2.12739730	2.42792654	-1.46593463
6	3.32950258	-0.25037333	-1.27913463	6	-1.52459741	3.82312655	-1.38873458
6	4.69920254	-0.52097332	-1.34793460	1	-3.22229743	2.44062662	-1.45963454
1	5.20760250	-0.49797332	-2.30643463	1	-1.80779743	1.92302668	-2.38163471
6	5.44920254	-0.82237333	-0.21583465	1	-0.43629742	3.71092653	-1.32333457
6	4.82040262	-0.85497332	1.02446544	1	-1.72689748	4.33532667	-2.33863473
1	5.42270231	-1.08807325	1.89646542	6	-2.95279741	2.87922668	1.34116542

6	3.45410275	-0.59627330	1.17026544	6	-1.97419739	4.04442692	1.15966535
6	2.54200268	0.08192669	-2.55993462	1	-0.95639741	3.71132660	1.39316535
6	2.80410266	-0.64347333	2.56526518	6	-2.03289747	4.68722677	-0.23203464
6	1.92320263	1.49112678	-2.45733476	1	-2.21849728	4.81862688	1.89626539
1	1.27900255	1.58502674	-1.58213460	8	-1.37069750	-1.58727324	-0.17203465
1	1.33410251	1.71772671	-3.35543466	15	-2.58259726	-2.43467331	-0.34083462
1	2.71120262	2.24752665	-2.37293482	8	-3.67189741	-2.35527349	0.80966532
6	1.44760251	-0.97627336	-2.80733466	8	-3.55359721	0.67342669	0.47216538
1	0.76430261	-1.06327331	-1.96193457	6	-4.70159769	-1.34217334	0.98076534
1	1.90140259	-1.96047330	-2.96953464	6	-4.18479729	-0.02877332	1.51996541
1	0.86320257	-0.72457331	-3.70183468	1	-5.39999771	-1.79577327	1.68686545
6	3.43520260	0.08882667	-3.81323481	1	-5.20719767	-1.18737328	0.02316536
1	3.89300275	-0.88797337	-4.00313425	1	-5.05269766	0.53142667	1.90506542
1	4.23270226	0.83652669	-3.74863482	1	-3.48669744	-0.20557332	2.34526539
1	2.82500267	0.33752668	-4.68913460	8	-2.24069738	-3.98467350	-0.37473464
6	3.81640267	-0.98137331	3.67436528	1	6.51390266	-1.02747333	-0.29903463
1	4.61110258	-0.23177332	3.75096536	1	-1.45169747	5.61712694	-0.22003464
1	4.28100252	-1.96257329	3.52986526	1	-3.07189727	4.98432684	-0.43293464
1	3.29800272	-1.00507331	4.63976574	1	-3.89669728	3.10302663	0.83106536
6	1.72790253	-1.74817324	2.61736536	1	-3.18619728	2.74692655	2.40216517
1	0.98830259	-1.63997328	1.82136536	6	-1.23199737	-4.54067326	0.49976537
1	1.20380259	-1.73527324	3.58086538	1	-0.30769742	-3.96677351	0.42106536
1	2.19200277	-2.73357344	2.49626517	1	-1.07159746	-5.56107330	0.15536535
6	2.20410275	0.72982669	2.93116522	1	-1.59449744	-4.54737329	1.52986538
1	2.99520278	1.48652673	2.97236538				

### TS-24\_PC



Zero-point vibrational energy

1675248.8 (Joules/Mol)

400.39407 (Kcal/Mol)

Zero-point correction=

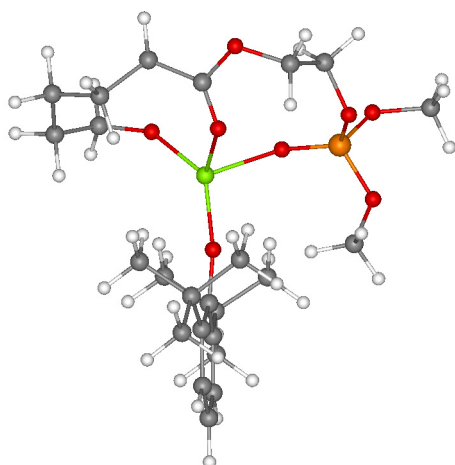
0.638069 (Hartree/Particle)

Thermal correction to Energy=	0.677002
Thermal correction to Enthalpy=	0.677946
Thermal correction to Gibbs Free Energy=	0.564773
Sum of electronic and zero-point Energies=	-2081.499104
Sum of electronic and thermal Energies=	-2081.460171
Sum of electronic and thermal Enthalpies=	-2081.459227
Sum of electronic and thermal Free Energies=	-2081.572400

cartesian											
12	0.61558270	0.32051325	-0.11976940	1	-1.62871718	2.48651338	-2.94996929				
8	2.89808273	-2.95788670	1.01483059	1	-1.42471719	1.94921327	-1.27486944				
8	-1.19951725	-0.05128676	-0.02806940	1	3.76618290	-4.83858681	0.77983063				
6	3.92308283	-3.91898680	1.34623063	8	1.50598264	1.61641335	-1.40606940				
1	3.81438279	-4.11128664	2.41223073	6	2.33538270	2.27121329	-0.71386939				
1	4.91398239	-3.50798678	1.13973057	8	1.87588263	1.33391333	0.98663056				
6	-2.46261716	-0.44718677	-0.14106940	6	2.06528282	1.87341332	2.26953053				
6	-3.09381723	-1.14538670	0.93803060	6	0.96608275	2.85101342	2.67533064				
6	-4.43031740	-1.52958679	0.79513061	1	3.04838276	2.37311339	2.31533051				
1	-4.92991734	-2.05448675	1.60253060	1	2.10248280	1.05521321	3.00623059				
6	-5.15711737	-1.26118684	-0.35966939	1	0.00128272	2.34081340	2.56643057				
6	-4.53471756	-0.59348679	-1.40856934	1	1.07608271	3.07411337	3.74553061				
1	-5.11491728	-0.39508677	-2.30376935	6	2.13478279	3.71971321	-0.34016940				
6	-3.20221710	-0.17638676	-1.33716941	6	0.83108270	4.08741283	0.37613058				
6	-2.33401728	-1.48688674	2.23303056	1	0.03088272	3.40161324	0.07793060				
6	-2.56541729	0.55711323	-2.53146935	6	0.93448275	4.17301321	1.90553057				
6	-1.83011723	-0.20328675	2.92073059	1	0.52308273	5.07401323	0.01193060				
1	-1.17451715	0.36811322	2.26353073	8	1.61178279	-1.41388679	-0.51806939				
1	-1.28001738	-0.44788677	3.83833051	15	2.79398274	-2.31188679	-0.42176938				
1	-2.67261720	0.44131327	3.19453073	8	4.17928267	-1.59058666	-0.75106937				
6	-1.15631723	-2.43198681	1.92133069	8	3.67608285	2.02021337	-0.82706940				
1	-0.48191726	-2.00968671	1.17533064	6	4.37558270	-0.22418675	-0.27576941				
1	-1.52811718	-3.38518667	1.52883065	6	4.05628252	0.76751322	-1.39416933				
1	-0.57941729	-2.64368677	2.83053064	1	5.41928244	-0.17668675	0.03783061				
6	-3.21891713	-2.21328664	3.26213050	1	3.72808290	-0.01028675	0.57793063				
1	-3.59351730	-3.17208672	2.88783073	1	4.93048239	0.96761328	-2.01746941				
1	-4.07591724	-1.60668683	3.57433057	1	3.25098276	0.38251323	-2.02266955				
1	-2.62581730	-2.42488670	4.15933037	8	2.79068279	-3.55468678	-1.40026939				
6	-3.54551721	0.74111325	-3.70396948	1	-6.19651747	-1.57008672	-0.44166940				
1	-4.41461754	1.34661317	-3.42556930	1	0.07688272	4.75161314	2.27033067				
1	-3.90461707	-0.21428676	-4.10116959	1	1.82338262	4.76611328	2.16303062				
1	-3.03401732	1.26231313	-4.52136946	1	3.00488281	4.05751324	0.22923060				

6	-1.38051724	-0.25928676	-3.08876944	1	2.18378282	4.23661327	-1.30786943
1	-0.65221727	-0.50748676	-2.31526947	6	2.51688290	-3.37928677	-2.81006932
1	-0.86511725	0.29511324	-3.88256931	1	1.55888271	-2.87498665	-2.94526935
1	-1.74101710	-1.20418668	-3.51106930	1	2.47368288	-4.38278675	-3.22976947
6	-2.11911726	1.97261333	-2.11446929	1	3.32398272	-2.81268668	-3.27926946
1	-2.98881721	2.56641340	-1.81226933				

#### I-4\_PC

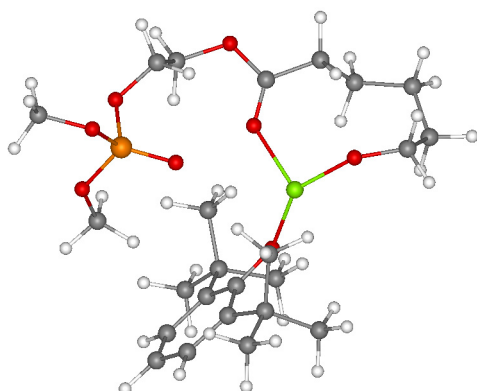


Zero-point vibrational energy	1677306.1 (Joules/Mol)
	400.88577 (Kcal/Mol)
Zero-point correction=	0.638852 (Hartree/Particle)
Thermal correction to Energy=	0.678429
Thermal correction to Enthalpy=	0.679373
Thermal correction to Gibbs Free Energy=	0.566976
Sum of electronic and zero-point Energies=	-2081.499513
Sum of electronic and thermal Energies=	-2081.459937
Sum of electronic and thermal Enthalpies=	-2081.458993
Sum of electronic and thermal Free Energies=	-2081.571389

				cartesian			
12	0.69860518	0.29152530	0.82502133	1	-1.23529482	-2.70487452	3.03842115
8	3.16020513	-3.54417467	1.05952132	1	-0.66229486	-2.07047462	1.49072134
8	-0.94459474	-0.15427467	0.02382131	1	2.85140514	-5.50627470	0.42962131
6	3.67540503	-4.81377506	0.60882133	8	2.09390521	0.84802526	-0.68377870
1	4.30720520	-5.18157482	1.41592133	6	3.10620499	1.53802538	-0.55757868
1	4.26830530	-4.69097471	-0.30117869	8	1.26910520	1.49112535	2.11752129
6	-2.22559500	-0.33477467	-0.28277868	6	0.99940515	2.54722548	2.97312117
6	-2.72709489	0.11842531	-1.54727864	6	0.62310517	3.85462546	2.26392126
6	-4.04739475	-0.18707469	-1.89197862	1	1.87580526	2.74832535	3.62092113
1	-4.44259501	0.12942532	-2.85157871	1	0.17260519	2.30392528	3.66502118

6	-4.89129496	-0.88577467	-1.03607869	1	-0.27009478	3.67012548	1.65062141
6	-4.41989470	-1.26067472	0.21702132	1	0.32100520	4.57712507	3.03592134
1	-5.10359478	-1.77267480	0.88552129	6	3.21660519	2.74042535	0.31662130
6	-3.11099482	-0.99437469	0.63192129	6	2.09280515	3.77212548	0.10952131
6	-1.86659467	0.96402532	-2.50617886	1	1.20740521	3.27542543	-0.29677871
6	-2.67239499	-1.38777471	2.05642128	6	1.69730520	4.52412510	1.39212132
6	-0.63229477	0.18032533	-2.99217868	1	2.42190504	4.48802519	-0.65297872
1	0.01450518	-0.09877469	-2.16097879	8	1.76260519	-1.46887469	0.88052130
1	-0.04609481	0.78812534	-3.69367886	15	2.30410504	-2.61517453	0.10522132
1	-0.94239473	-0.73077470	-3.51737881	8	3.24450517	-2.18207479	-1.12117863
6	-1.42919481	2.26272535	-1.80007863	8	4.24460506	1.19022536	-1.17247868
1	-0.88769484	2.05132532	-0.87687868	6	4.34290504	-1.26247478	-0.92677867
1	-2.30279493	2.87142539	-1.54327869	6	4.23010540	-0.06757468	-1.88097858
1	-0.78099477	2.85892534	-2.45467877	1	5.25310516	-1.83287477	-1.12497866
6	-2.63849497	1.38942528	-3.76767874	1	4.37980509	-0.91067469	0.10742132
1	-3.52729487	1.98292542	-3.52997875	1	5.09670496	-0.00397468	-2.53857875
1	-2.94949484	0.53192532	-4.37457848	1	3.32170510	-0.15367469	-2.47877884
1	-1.98919475	2.01202536	-4.39377832	8	1.28290522	-3.60197473	-0.57257867
6	-3.81739473	-2.01877475	2.86992121	1	-5.91199493	-1.11477470	-1.33287859
1	-4.17539501	-2.95557451	2.42932129	1	1.31550527	5.50902510	1.09602141
1	-4.67029476	-1.34117460	2.98172116	1	2.59420514	4.72452497	1.99512136
1	-3.45389485	-2.25297451	3.87682128	6	0.20890519	-3.13547468	-1.43917859
6	-2.23069501	-0.13507468	2.84082127	1	-0.29179481	-2.27257466	-0.99687868
1	-1.42239475	0.40912533	2.34962130	1	-0.48249480	-3.97197461	-1.51947868
1	-1.88819468	-0.41067469	3.84552121	1	0.62400520	-2.88957453	-2.41777873
1	-3.07089496	0.55932534	2.94872117	1	4.21030521	3.18322539	0.21762133
6	-1.54219472	-2.43437457	2.02062130	1	3.09900498	2.31212544	1.32302141
1	-1.88449466	-3.34737468	1.51972139				

### TS-45\_PC



Zero-point vibrational energy

1675725.9 (Joules/Mol)

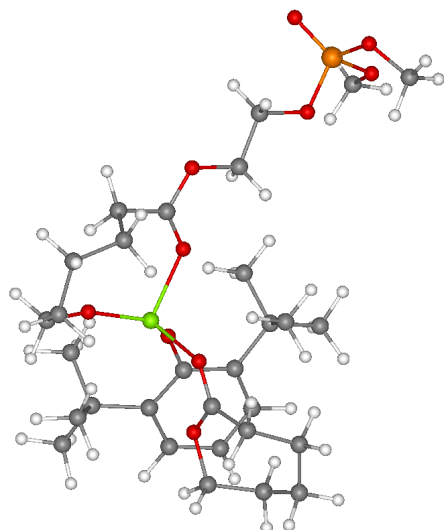
400.50810 (Kcal/Mol)

Zero-point correction=	0.638250 (Hartree/Particle)
Thermal correction to Energy=	0.677414
Thermal correction to Enthalpy=	0.678358
Thermal correction to Gibbs Free Energy=	0.564735
Sum of electronic and zero-point Energies=	-2081.478881
Sum of electronic and thermal Energies=	-2081.439717
Sum of electronic and thermal Enthalpies=	-2081.438773
Sum of electronic and thermal Free Energies=	-2081.552396

cartesian							
12	1.30094266	-0.24956931	0.86555600	1	0.77594268	0.52253067	2.87405610
8	-4.13595724	-3.14476943	1.41965604	1	-0.80465734	0.12683070	2.05235600
8	0.74014258	1.35163069	0.08955602	1	-6.01725769	-2.86286926	0.56745601
6	-5.34535742	-3.67586923	0.84965605	8	0.86504269	-1.81116939	-0.40254396
1	-5.80265760	-4.28476954	1.62905598	6	1.45164263	-2.87006927	-0.65394396
1	-5.12075758	-4.29726934	-0.02154398	8	2.71184254	-0.97906935	1.78455603
6	-0.31835741	2.14493060	-0.04924398	6	4.02994251	-1.01886928	2.21215606
6	-0.70805740	2.59443069	-1.34964395	6	5.05804253	-0.89226937	1.08115602
6	-1.87475741	3.35753059	-1.46284401	1	4.22734261	-1.96226931	2.75715613
1	-2.20035744	3.70293069	-2.43884397	1	4.23864269	-0.21126932	2.93625593
6	-2.64145756	3.70473075	-0.35334396	1	4.86704254	0.05023068	0.54835600
6	-2.21095753	3.32633066	0.91515601	1	6.05124235	-0.78866935	1.54045606
1	-2.79825759	3.64013076	1.77195597	6	2.84214258	-3.18476939	-0.21034399
6	-1.04935741	2.57063055	1.10245597	6	3.89394236	-2.23746920	-0.82804400
6	0.14684260	2.28763056	-2.59344387	1	3.44404244	-1.26036930	-1.03254402
6	-0.51855743	2.28453064	2.51975608	6	5.13504267	-2.03646922	0.05845602
6	0.17394260	0.77383065	-2.88054395	1	4.19154263	-2.64626932	-1.80044401
1	0.56354260	0.21543068	-2.02924395	8	-1.98185742	-1.77106929	1.35105598
1	0.80454266	0.56103063	-3.75334406	15	-3.12205744	-2.27136922	0.55855602
1	-0.83515739	0.40593067	-3.10194397	8	-2.67425752	-3.20896935	-0.69104397
6	1.58424258	2.80863070	-2.38514400	8	0.84774268	-3.83136940	-1.34904397
1	2.05174255	2.35093069	-1.51244402	6	-1.45905733	-3.96706939	-0.57384396
1	1.57914269	3.89433050	-2.23934388	6	-0.52955741	-3.58546925	-1.72564399
1	2.19814253	2.59113073	-3.26824403	1	-1.72235739	-5.02736950	-0.60214400
6	-0.39775741	2.97243071	-3.85874391	1	-0.96735740	-3.74846935	0.37665603
1	-0.43355739	4.06213045	-3.75584388	1	-0.68715739	-4.19916916	-2.61214399
1	-1.39955735	2.61933064	-4.12754440	1	-0.66105735	-2.53276944	-1.97384405
1	0.26224259	2.74583054	-4.70364428	8	-4.08885717	-1.22696936	-0.14674398
6	-1.48745739	2.78453064	3.60625601	1	-3.54885745	4.29183054	-0.47364396
1	-2.45855737	2.28013062	3.55495596	1	5.98744249	-1.83256936	-0.60104400
1	-1.65375733	3.86453056	3.54595613	1	5.37704229	-2.97796941	0.57045603

1	-1.05995739	2.57943058	4.59375572	6	-3.53825760	-0.11536932	-0.89584398
6	0.80934262	3.04953074	2.71095610	1	-2.86305737	0.47253069	-0.27294397
1	1.54934263	2.75353074	1.96325600	1	-4.39055729	0.49333069	-1.19204402
1	1.22604263	2.85573077	3.70715594	1	-3.01975751	-0.48606932	-1.78254402
1	0.64594257	4.12803078	2.61605597	1	3.07244253	-4.22986937	-0.42824399
6	-0.29365739	0.76633060	2.78265595	1	2.82704258	-3.02116942	0.87265605
1	-0.71105742	0.46173069	3.74795604				

## I-5\_PC



Zero-point vibrational energy	2091309.6 (Joules/Mol)
	499.83499 (Kcal/Mol)
Zero-point correction=	0.796538 (Hartree/Particle)
Thermal correction to Energy=	0.846224
Thermal correction to Enthalpy=	0.847169
Thermal correction to Gibbs Free Energy=	0.704841
Sum of electronic and zero-point Energies=	-2466.366023
Sum of electronic and thermal Energies=	-2466.316337
Sum of electronic and thermal Enthalpies=	-2466.315392
Sum of electronic and thermal Free Energies=	-2466.457719

## cartesian

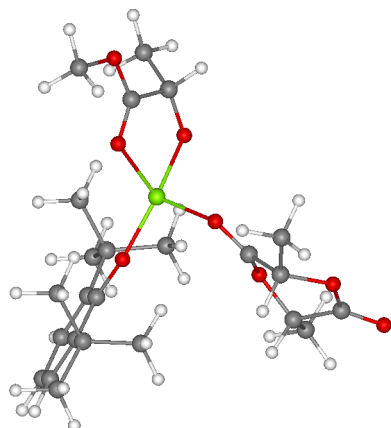
8	8.20359135	-0.16865267	-0.95956987	6	-1.30060852	-2.62235260	0.76143008
6	7.89339161	-0.79575270	-2.21596980	6	-3.76970816	-0.23085265	2.60673022
1	8.53209114	-0.31695265	-2.95786977	6	0.19319150	-2.72135258	0.39363009
1	6.84279156	-0.64115268	-2.47646976	6	-4.09580851	0.97574735	1.70623004
1	8.11269093	-1.86435258	-2.16776991	1	-3.20800829	1.43124735	1.26633000
8	1.23279142	1.57554734	0.27893010	1	-4.58810854	1.76024735	2.29403019
6	1.98279154	2.53424740	0.48623008	1	-4.77850819	0.68764734	0.89893013

8	-1.29560852	3.10914731	0.94553012	6	-2.77720833	0.19174734	3.71053028
6	-1.89000857	4.35414743	0.97843009	1	-1.81020844	0.47624731	3.29553008
6	-1.50310862	5.26074743	-0.19816990	1	-2.61760855	-0.63165265	4.41573000
1	-1.63490856	4.88604736	1.91703010	1	-3.17750835	1.04524732	4.27083015
1	-2.99360847	4.27514744	0.97993010	6	-5.08320856	-0.60235268	3.32173014
1	-1.77510846	4.74664736	-1.13106990	1	-4.96370840	-1.46795261	3.98163009
1	-2.12730837	6.16474724	-0.14826991	1	-5.89920855	-0.81285268	2.62113023
6	1.52409148	3.93294740	0.74143010	1	-5.40410852	0.24224734	3.94143009
6	0.99099147	4.59434748	-0.55026990	6	0.62779152	-4.17085266	0.10993010
1	0.53079152	3.83494735	-1.19057000	1	0.13469151	-4.59365273	-0.77256989
6	-0.03670853	5.70814753	-0.28666991	1	0.43409151	-4.83275270	0.96043009
1	1.84569144	4.99804735	-1.10596991	1	1.70639145	-4.19165277	-0.08446990
8	7.86989164	0.19724734	1.55993009	6	1.05669141	-2.22455263	1.57173002
15	7.36879158	-0.48895270	0.35853010	1	0.82399154	-1.18995261	1.82553005
8	5.82269144	-0.15505266	-0.00276990	1	2.12219143	-2.29795265	1.31633008
8	3.30449152	2.37944746	0.47913009	1	0.88139153	-2.84255266	2.45923018
6	5.31519175	1.15864742	0.28593010	6	0.51629150	-1.90845263	-0.87336987
6	3.80409145	1.04774737	0.23003009	1	-0.06500852	-2.28125262	-1.72536993
1	5.67639160	1.87074733	-0.46316987	1	1.57929146	-2.00285268	-1.13056993
1	5.65119171	1.48384738	1.27373004	1	0.29639149	-0.84975266	-0.74146986
1	3.46179152	0.70524734	-0.74896991	8	-1.18410850	1.22854733	-1.67386997
1	3.42379141	0.36344731	0.99103010	6	-2.11140871	0.64044732	-2.23866987
8	7.34019184	-2.08705258	0.35233009	8	-3.01320839	0.05054734	-1.47816992
1	0.04089150	6.43604755	-1.10416996	6	-4.11640835	-0.73175269	-2.00486994
1	0.23959148	6.25714731	0.62413013	6	-3.68110847	-1.97675252	-2.75746989
6	6.77039146	-2.77985263	1.48003006	1	-4.75380850	-0.07715267	-2.61086988
1	7.23789167	-2.44315267	2.40753007	1	-4.65680838	-1.00685263	-1.09986997
1	6.97719145	-3.83765268	1.32063007	1	-2.91560841	-2.48665261	-2.16246986
1	5.69039154	-2.61655259	1.51723003	1	-4.54720831	-2.64835262	-2.77466989
1	2.34039164	4.51794720	1.17133009	6	-2.20850849	0.59554732	-3.74026990
1	0.69599152	3.84544730	1.45063007	6	-2.00300837	-0.81185269	-4.32916975
12	-0.85670853	1.40324736	0.39643008	1	-1.11920846	-1.26975262	-3.87136984
8	-1.17310846	-0.27815264	1.20213008	6	-3.21430874	-1.73365259	-4.19266987
6	-1.87510860	-1.39885259	1.24533010	1	-1.76940858	-0.68985265	-5.39216995
6	-3.19500828	-1.42185259	1.80983007	1	-4.06220818	-4.63325262	0.98493010
6	-3.95270824	-2.59045267	1.67423010	1	-2.97700834	-2.69695258	-4.65736961
1	-4.96520853	-2.62275267	2.06313014	1	-4.04700851	-1.31255257	-4.77276993
6	-3.44650841	-3.74135256	1.07583010	1	-3.18460846	0.98974735	-4.04906988
6	-2.11670828	-3.75425267	0.66573012	1	-1.44310856	1.27944744	-4.10926962
1	-1.71130860	-4.68195248	0.27433008				



## S1.7. LL sequence, mononuclear mechanism

### I-1\_LL

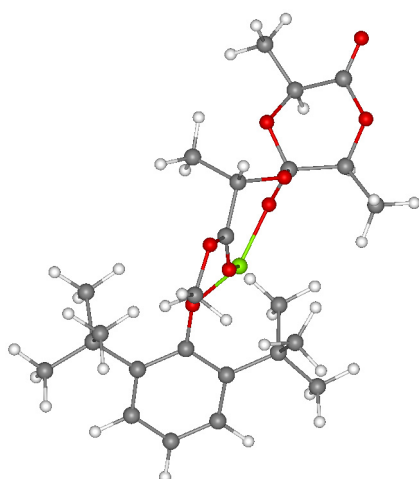


Zero-point vibrational energy	1512976.3 (Joules/Mol)
	361.61000 (Kcal/Mol)
Zero-point correction=	0.576262 (Hartree/Particle)
Thermal correction to Energy=	0.614223
Thermal correction to Enthalpy=	0.615167
Thermal correction to Gibbs Free Energy=	0.501162
Sum of electronic and zero-point Energies=	-1737.213316
Sum of electronic and thermal Energies=	-1737.175356
Sum of electronic and thermal Enthalpies=	-1737.174412
Sum of electronic and thermal Free Energies=	-1737.288417

cartesian							
8	-1.82028842	-1.42980576	-0.37500733	6	2.51421142	3.28749442	0.97629267
6	-4.08538818	-0.72760570	-0.80200732	1	3.08151150	3.63079429	1.83519268
6	-2.77188849	-0.73690581	-0.04470732	6	1.97221160	1.99879420	0.97329271
8	-2.68808842	0.06179425	1.00569272	6	0.31601161	2.02799439	-2.55650735
6	-3.75938845	1.02419424	1.22529268	6	2.20821142	1.06499422	2.17359281
6	-5.11728811	0.34599426	1.08219266	6	-1.15778840	1.73399425	-2.21140718
8	-5.19058800	-0.59640574	0.11149268	1	-1.21068835	0.96799421	-1.43750727
8	-6.07348824	0.60819423	1.76349270	1	-1.70028830	1.38729417	-3.10110736
1	-4.06098843	0.15589425	-1.45670736	1	-1.65028834	2.64259434	-1.84450734
6	-4.30638838	-1.97620583	-1.62900734	6	0.97441155	0.78309429	-3.18550730
6	-3.54348850	1.64609420	2.58539271	1	1.00001168	-0.05480576	-2.48850727
1	-3.67138839	1.78609419	0.44019267	1	2.00471163	1.00819421	-3.48150730
1	-4.31448841	2.39659429	2.76449275	1	0.42651159	0.47379425	-4.08480740
1	-2.56168842	2.12099433	2.61929274	6	0.30811161	3.12069440	-3.63940740
1	-3.60718846	0.88919425	3.36919260	1	1.31841159	3.37749434	-3.97480726

1	-5.26028824	-1.89660573	-2.15340734	1	-0.18618840	4.03859425	-3.30320740
1	-4.32318830	-2.86170578	-0.99090731	1	-0.24198841	2.75639439	-4.51480722
1	-3.50318837	-2.08330584	-2.35910726	6	3.00371146	-0.17810576	1.71959269
12	0.20461160	-1.38890576	0.23319268	1	4.01781178	0.11619425	1.42799270
8	0.31901157	-2.77470565	1.53379273	1	2.56121159	-0.67010576	0.85109270
6	0.78061157	-3.98930573	1.10319269	1	3.07691145	-0.91330576	2.52829266
6	1.10891151	-3.92460561	-0.39080733	6	0.86821157	0.67949426	2.83549261
8	1.53521156	-5.04500580	-0.95240736	1	0.43321157	1.55649424	3.32829261
6	1.83911157	-4.98810577	-2.36100721	1	1.01021171	-0.10120575	3.59039259
6	2.00851154	-4.48020601	1.89059269	1	0.12741160	0.32659426	2.11599278
8	0.96821159	-2.87980556	-1.04350734	6	3.05221152	1.72069418	3.28139281
1	0.94731158	-4.71810579	-2.92910719	1	2.56741142	2.60769439	3.70259261
1	2.17421150	-5.98990583	-2.62380719	1	4.04821157	2.00709438	2.92849278
1	2.62631154	-4.25610590	-2.54820728	1	3.18911147	1.00429416	4.09939289
8	0.65741158	0.36919424	-0.20930734	1	2.78901148	5.15489388	-0.06650732
6	1.22191167	1.57289422	-0.16980731	1	0.00891158	-4.78360605	1.17799270
6	1.07661152	2.45619440	-1.28770733	1	2.34371161	-5.47050571	1.56739271
6	1.64811158	3.72979426	-1.21440732	1	1.73031163	-4.52560568	2.94609261
1	1.54701161	4.41549397	-2.04890728	1	2.83421159	-3.76940560	1.79029274
6	2.35671163	4.15769386	-0.09670732				

## I-2\_LL

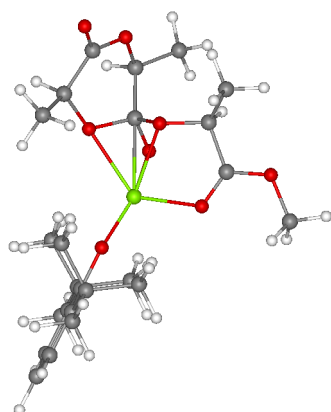


Zero-point vibrational energy	1519322.5 (Joules/Mol)
	363.12680 (Kcal/Mol)
Zero-point correction=	0.578679 (Hartree/Particle)
Thermal correction to Energy=	0.615067
Thermal correction to Enthalpy=	0.616012
Thermal correction to Gibbs Free Energy=	0.509377
Sum of electronic and zero-point Energies=	-1737.186784
Sum of electronic and thermal Energies=	-1737.150396

Sum of electronic and thermal Enthalpies= -1737.149452  
Sum of electronic and thermal Free Energies= -1737.256087

cartesian							
8	1.68072319	-0.92900151	0.78145951	1	-1.16517687	-1.06760144	-1.80194044
8	3.71452332	-0.45760149	1.74355936	1	-1.47927678	-2.70270157	-2.28234053
6	3.00292301	-1.06420159	0.64155942	1	-0.28067678	-2.47430158	-1.02984047
6	3.39162302	-2.57170153	0.54245943	6	-3.13907671	-3.51940179	-0.63954055
8	4.78822327	-2.81200147	0.87885946	1	-3.60397673	-3.49170136	-1.63504052
6	5.20462322	-2.31710148	2.08185935	1	-3.92207670	-3.72410178	0.10275948
6	4.19232321	-1.37650156	2.74175930	1	-2.43477678	-4.36450148	-0.61974055
8	6.29982328	-2.59860158	2.51685929	6	-2.00287676	3.26999831	-0.94664049
12	0.23452324	-0.27520150	-0.21554053	1	-2.46717691	3.27319837	-1.94414043
8	3.55882311	-0.46140152	-0.57244051	1	-1.16867685	2.55939841	-0.95164055
6	3.43082333	0.92609847	-0.86044049	1	-1.60817683	4.27979851	-0.75234056
6	2.28232336	1.15609848	-1.84844065	6	-2.39887667	2.95949841	1.53815937
8	2.62232304	1.96529841	-2.84554052	1	-3.15027666	2.75529838	2.31465936
6	1.56442320	2.30869842	-3.79224062	1	-1.99137676	3.96659851	1.71875930
6	3.28392315	1.92779851	0.29855949	1	-1.59067678	2.22679853	1.63855934
8	1.13822317	0.68159848	-1.76524043	6	-4.14617682	3.96819854	0.08995944
1	1.21722317	1.40299845	-4.30164051	1	-4.91777658	3.79959846	0.85455948
1	2.03402328	3.00039840	-4.49574041	1	-4.63737679	4.01919842	-0.89254057
1	0.72982323	2.78309846	-3.26384068	1	-3.69507694	4.95179844	0.28705949
8	-1.43447673	0.49279848	0.10385948	1	-6.57137680	-0.10180151	-0.79714054
6	-2.74117661	0.33089849	-0.12514052	1	4.34862328	1.18509853	-1.41044044
6	-3.29097700	-0.97170156	-0.36134052	1	3.21202326	2.94339848	-0.11694053
6	-4.66507673	-1.09570146	-0.60054052	1	4.16542339	1.86959839	0.94385952
1	-5.09657669	-2.07930160	-0.78174055	1	2.40032339	1.72349846	0.91385943
6	-5.50367689	0.01569849	-0.60974056	1	2.76392317	-3.07350159	1.29625940
6	-4.96567678	1.28069854	-0.37354052	6	3.16312313	-3.20170140	-0.81914055
1	-5.63657665	2.13809848	-0.38074052	6	4.80512333	-0.57290155	3.87335920
6	-3.60107660	1.47659850	-0.12934053	1	3.35042334	-1.98140168	3.13435936
6	-2.38217688	-2.21470165	-0.32294053	1	5.18762350	-1.24970150	4.64665937
6	-3.04467678	2.89189839	0.13395947	1	4.04612350	0.08639848	4.31285954
6	-1.79437673	-2.39170146	1.10115957	1	5.64272356	0.03179848	3.50405931
1	-1.30827677	-1.48350167	1.48225951	1	3.34422302	-4.28260136	-0.76334053
1	-1.07127678	-3.22140145	1.12965941	1	3.83812332	-2.76230168	-1.56164050
1	-2.60547686	-2.62610149	1.80395937	1	2.12652302	-3.03990149	-1.14234054
6	-1.25307679	-2.09040165	-1.39864051				

## TS-13\_LL

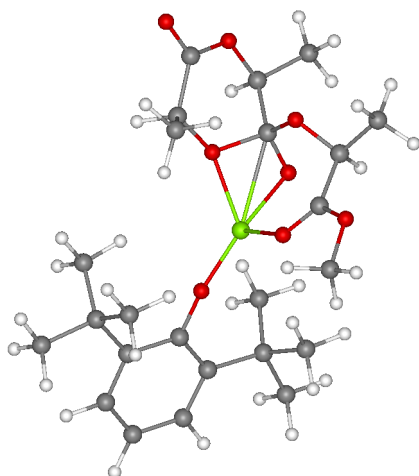


Zero-point vibrational energy	1516662.9 (Joules/Mol)
	362.49112 (Kcal/Mol)
Zero-point correction=	0.577666 (Hartree/Particle)
Thermal correction to Energy=	0.613556
Thermal correction to Enthalpy=	0.614501
Thermal correction to Gibbs Free Energy=	0.509629
Sum of electronic and zero-point Energies=	-1737.195133
Sum of electronic and thermal Energies=	-1737.159243
Sum of electronic and thermal Enthalpies=	-1737.158299
Sum of electronic and thermal Free Energies=	-1737.263170

cartesian							
12	0.55945081	-0.22443183	-0.48413911	1	-1.20244908	2.31796837	-0.02063915
8	-1.18204927	-0.04123183	0.08546085	8	2.04645085	-1.38383186	-1.26863921
6	-2.50364923	-0.20773183	0.12726085	6	2.72085094	-1.14363182	-0.19213915
6	-3.12154913	-1.31283188	-0.53753918	8	1.92725086	-1.48793185	0.95546085
6	-4.51064920	-1.44993186	-0.45463914	8	0.94885081	1.47736812	-1.61273921
1	-5.00154924	-2.28253174	-0.94753915	8	2.73565078	0.39586818	0.05676085
6	-5.29794931	-0.54503185	0.24816084	6	2.11335087	1.86696815	-1.71133912
6	-4.68884897	0.53176814	0.88446081	6	3.27125096	1.21646821	-0.96553916
1	-5.31914902	1.22986817	1.42526078	1	3.76575089	0.60426813	-1.72953916
6	-3.30624914	0.73296815	0.84416085	1	-6.37604904	-0.67623186	0.29866087
6	-2.29164910	-2.33863163	-1.32983911	8	2.46535087	2.86076832	-2.50003910
6	-2.68134904	1.94776821	1.55476081	6	1.40905070	3.47706819	-3.27603912
6	-1.56914926	-1.64733183	-2.50813913	1	1.89795089	4.26616812	-3.84293914
1	-1.06634927	-0.72093183	-2.21653914	1	0.64965081	3.88706827	-2.60983896
1	-0.83404917	-2.31543183	-2.97103906	1	0.95925081	2.73976827	-3.94203901
1	-2.29554915	-1.35733187	-3.27473903	6	4.11945057	-1.73833179	-0.00333915
6	-1.30094910	-3.06533170	-0.39523914	6	2.56245089	-1.47563183	2.25166106
1	-0.68334919	-2.38263178	0.19036084	6	3.99655080	-0.93793184	2.25066090

1	-1.85324907	-3.67873168	0.32496086	1	2.65325093	-2.52903175	2.55466104
1	-0.63734919	-3.72613168	-0.96483916	1	3.93595099	-2.80313182	0.19276084
6	-3.15744901	-3.44303179	-1.96303916	8	4.75095081	-1.15613186	1.14926088
1	-3.69124889	-4.03053188	-1.20923913	8	4.48645067	-0.41073185	3.21986103
1	-3.89054918	-3.04243183	-2.67063904	6	4.25495052	2.22126818	-0.37543914
1	-2.51134920	-4.13363171	-2.51723909	1	3.75795078	2.85326838	0.36466086
6	-3.73324919	2.81686831	2.26536083	1	4.68485069	2.85586834	-1.15313911
1	-4.46974897	3.23186827	1.56886089	1	5.05575085	1.67586815	0.12766086
1	-4.26934910	2.26616836	3.04566097	6	1.68325090	-0.74143183	3.24426103
1	-3.23254919	3.66246819	2.75026107	1	1.62975073	0.32086819	2.99716091
6	-1.68394923	1.48676813	2.63586092	1	2.09275079	-0.84043187	4.25086117
1	-0.88424915	0.88366818	2.20556092	1	0.67685080	-1.16493189	3.22376084
1	-1.23714924	2.35286832	3.14036083	6	5.07745075	-1.62523186	-1.17143917
1	-2.19294906	0.88216817	3.39466095	1	5.93655109	-2.27963161	-1.00403917
6	-1.97404909	2.85816836	0.52956080	1	5.45905066	-0.60883182	-1.28653920
1	-2.69604921	3.24886823	-0.19653915	1	4.57245111	-1.93433189	-2.08903909
1	-1.50974917	3.71406817	1.03626084				

### I-3\_LL

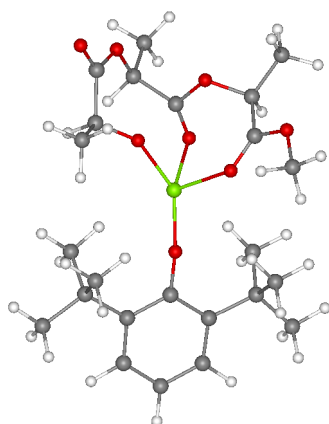


Zero-point vibrational energy	1516772.9 (Joules/Mol)
	362.51742 (Kcal/Mol)
Zero-point correction=	0.577708 (Hartree/Particle)
Thermal correction to Energy=	0.613538
Thermal correction to Enthalpy=	0.614483
Thermal correction to Gibbs Free Energy=	0.510079
Sum of electronic and zero-point Energies=	-1737.206633
Sum of electronic and thermal Energies=	-1737.170803
Sum of electronic and thermal Enthalpies=	-1737.169858
Sum of electronic and thermal Free Energies=	-1737.274262

cartesian

8	-1.33347368	0.07431158	0.19583914	8	3.69382644	-0.51208842	-0.04446086
6	-2.66207361	0.14941159	0.25663912	6	3.44652629	-1.59208834	-0.92736083
6	-3.43087363	-0.98608845	0.65563911	1	3.03482628	-2.43718839	-0.35866088
6	-4.82317400	-0.86098844	0.69903910	6	2.34162641	-1.24128830	-1.93046093
1	-5.43317366	-1.70678830	0.99783915	12	0.44522631	-0.32718843	0.24103914
6	-5.46627378	0.32691157	0.36993915	1	-6.55037403	0.39561158	0.41393912
6	-4.70667410	1.42661166	-0.01496086	8	2.61642647	-1.56128836	-3.17886090
1	-5.22637367	2.34501171	-0.26596087	8	1.25602627	-0.73918843	-1.62196076
6	-3.31157351	1.37481165	-0.08416086	6	1.58122635	-1.31308842	-4.16006088
6	-2.76367354	-2.31968832	1.04103911	1	2.00112629	-1.65028834	-5.10506105
6	-2.51157355	2.61621165	-0.52126086	1	1.34892631	-0.24828842	-4.19376087
6	-1.97097373	-2.89628839	-0.15126087	1	0.68402636	-1.87898839	-3.90686083
1	-1.25557375	-2.17998838	-0.56286085	6	4.76792622	-1.97788835	-1.57246077
1	-1.42807364	-3.80178833	0.14593914	8	1.88202643	-1.27858841	1.20323920
1	-2.65217352	-3.16278839	-0.96666092	6	3.61932635	-0.04278841	2.31713915
6	-1.85627365	-2.13428831	2.27463913	6	2.79542637	-0.34618843	1.06843913
1	-1.09337378	-1.36688840	2.12993908	8	2.03042626	0.91241157	0.78933913
1	-2.45327353	-1.82828832	3.14003921	6	2.75132632	2.14741158	0.65783912
1	-1.34887362	-3.07268834	2.52823925	6	4.10972643	2.14861155	1.36363924
6	-3.79097342	-3.39958835	1.42773914	8	4.48382616	1.10051167	2.11663914
1	-4.38557386	-3.11108828	2.30063915	8	4.83982611	3.10751176	1.25713921
1	-4.47597408	-3.63328838	0.60613912	1	2.89842629	0.21001159	3.10143924
1	-3.26337361	-4.32488823	1.68563914	6	4.49602604	-1.19428837	2.75583911
6	-3.42037368	3.81881166	-0.83186090	6	2.89102626	2.57441163	-0.79786086
1	-4.11377382	3.61281157	-1.65396082	1	2.15222621	2.89251161	1.19273913
1	-4.00297403	4.13431168	0.03993914	1	4.64552593	-2.83698845	-2.23486090
1	-2.80087352	4.67061186	-1.13486087	1	5.47472620	-2.24138832	-0.78326088
6	-1.55787373	3.06781173	0.60423911	1	5.18532610	-1.14848840	-2.14736080
1	-0.86737365	2.27361155	0.89273912	1	3.34542632	3.56561160	-0.84586090
1	-0.97467369	3.94091153	0.28483915	1	1.90232635	2.61471152	-1.26206076
1	-2.12667370	3.35321164	1.49573922	1	3.52082634	1.87321162	-1.34866083
6	-1.72307372	2.31721163	-1.81316078	1	5.02012634	-0.93288845	3.67823911
1	-2.41047359	2.07421160	-2.63096070	1	5.23772621	-1.42438841	1.98773921
1	-1.13777375	3.19451165	-2.11646080	1	3.87602639	-2.07458830	2.93883920
1	-1.04567361	1.47101164	-1.68736076				

# TS-34\_LL

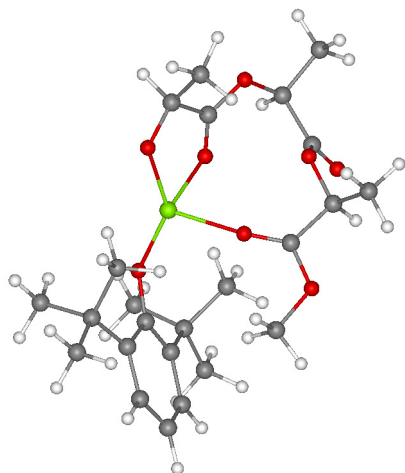


Zero-point vibrational energy	1514951.2 (Joules/Mol)
	362.08202 (Kcal/Mol)
Zero-point correction=	0.577014 (Hartree/Particle)
Thermal correction to Energy=	0.613392
Thermal correction to Enthalpy=	0.614336
Thermal correction to Gibbs Free Energy=	0.508324
Sum of electronic and zero-point Energies=	-1737.199817
Sum of electronic and thermal Energies=	-1737.163439
Sum of electronic and thermal Enthalpies=	-1737.162495
Sum of electronic and thermal Free Energies=	-1737.268507

cartesian											
8	1.26826394	-0.05315214	-0.05739420	8	-3.68013620	0.88504785	0.55160576				
6	2.58456373	-0.18795215	0.09410580	6	-3.24133635	2.21564794	0.23200580				
6	3.38156366	0.95354784	0.41810581	1	-2.58113623	2.56694794	1.03400576				
6	4.76086378	0.78064781	0.56680578	6	-2.36623621	2.19434786	-1.02399421				
1	5.38826370	1.63024783	0.81420577	12	-0.56503612	-0.07875215	-0.03229420				
6	5.37016392	-0.45895216	0.40680581	1	6.44556379	-0.56375217	0.52790576				
6	4.58706379	-1.56245220	0.08760580	8	-2.73893595	3.05654788	-1.94759429				
1	5.08016396	-2.52055216	-0.03659420	8	-1.37443614	1.48174787	-1.15599418				
6	3.20176411	-1.46565211	-0.07589421	6	-1.91713607	3.12424779	-3.13869405				
6	2.75876379	2.35044789	0.59910578	1	-2.36933613	3.90234780	-3.74949408				
6	2.38176394	-2.71875215	-0.43529421	1	-1.93693614	2.16324782	-3.65359402				
6	2.07536411	2.80294776	-0.70749420	1	-0.89243615	3.38134789	-2.86949420				
1	1.31106389	2.09444785	-1.02929425	6	-4.48283625	3.08064795	0.13110580				
1	1.60986388	3.78834796	-0.57239425	8	-1.71163607	0.49254787	1.60730577				
1	2.81346369	2.88834786	-1.51279426	6	-3.52913618	-1.09925210	1.87480581				
6	1.75256383	2.34754777	1.76790571	6	-2.83013630	0.08004786	1.22260582				
1	0.95436382	1.61854780	1.62440574	8	-2.13533616	-1.14905214	-0.31199419				
1	2.25916386	2.09914780	2.70670581	6	-2.72793627	-2.39915204	-0.48979419				

1	1.29756391	3.33944774	1.88530576	6	-4.21293592	-2.33085227	-0.10789420
6	3.81026363	3.42254782	0.93610579	8	-4.53863621	-1.65155220	1.03330576
1	4.33076382	3.21294785	1.87650573	8	-5.10633612	-2.84435225	-0.73709422
1	4.55896378	3.53324795	0.14470580	1	-2.74843597	-1.83475220	2.08870578
1	3.31176376	4.39204788	1.05000579	6	-4.20963621	-0.67635214	3.17010593
6	3.26116371	-3.97295213	-0.58919424	6	-2.57193613	-2.90725207	-1.91759419
1	4.00026369	-3.86485219	-1.38979423	1	-2.28123617	-3.14975214	0.19100580
1	3.78976393	-4.22515202	0.33600581	1	-4.21083593	4.11734772	-0.07459420
1	2.62716389	-4.82945204	-0.84469426	1	-5.01783609	3.04174781	1.08220577
6	1.37026393	-3.04125214	0.68340576	1	-5.14753628	2.72754788	-0.65919423
1	0.70656383	-2.20055223	0.89770579	1	-3.02843618	-3.89255214	-2.03819418
1	0.75366390	-3.90665221	0.41130581	1	-1.50823617	-2.97545218	-2.15869403
1	1.89486396	-3.27975225	1.61470580	1	-3.05063629	-2.21785212	-2.61749411
6	1.66756380	-2.52475214	-1.78849423	1	-4.64893627	-1.55435216	3.64900589
1	2.40226364	-2.37665224	-2.58709407	1	-5.00663614	0.04264786	2.96710587
1	1.07216382	-3.41095209	-2.03979421	1	-3.48183632	-0.23005214	3.85220599
1	1.01056385	-1.65295219	-1.78659427				

#### I-4\_LL



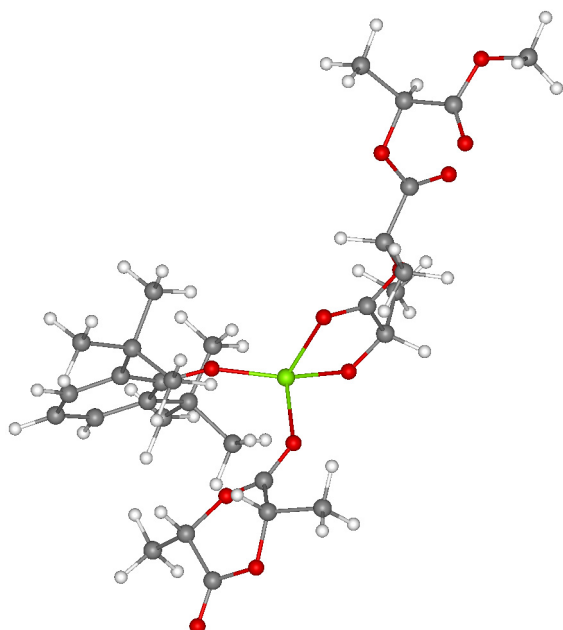
Zero-point vibrational energy	1516356.2 (Joules/Mol)
	362.41784 (Kcal/Mol)
Zero-point correction=	0.577550 (Hartree/Particle)
Thermal correction to Energy=	0.614647
Thermal correction to Enthalpy=	0.615591
Thermal correction to Gibbs Free Energy=	0.507992
Sum of electronic and zero-point Energies=	-1737.217347
Sum of electronic and thermal Energies=	-1737.180250
Sum of electronic and thermal Enthalpies=	-1737.179305
Sum of electronic and thermal Free Energies=	-1737.286905



cartesian

12	0.34762606	1.18167973	0.69020432	1	-1.43967390	-0.89832032	3.06810427
8	-1.29397392	0.41607967	1.19210422	8	1.32472610	2.80427980	0.90390432
6	-2.31117392	-0.13982034	0.53870434	6	3.87452602	-1.26782024	0.00830429
6	-3.21587396	0.68047965	-0.20719571	6	4.57512617	-0.55282032	1.16300428
6	-4.19177389	0.05497966	-0.98989564	8	4.29882574	0.86177963	1.20300424
1	-4.87017393	0.65217966	-1.59019578	6	3.01612592	1.20307970	1.30170429
6	-4.33607388	-1.32982028	-1.01749575	6	2.66392589	2.68667960	1.17350423
6	-3.52347398	-2.11152029	-0.20099571	8	3.77492595	-2.47182035	-0.02579571
1	-3.68807411	-3.18402028	-0.19059572	6	3.54962587	3.38527966	0.13240428
6	-2.51967406	-1.55512023	0.59980434	1	2.92752600	3.11237979	2.16610432
6	-3.17497396	2.21737981	-0.09319571	1	4.19112587	-1.02052033	2.07260442
6	-1.69687390	-2.45182037	1.54480422	6	6.08412600	-0.71182036	1.06730425
6	-3.47907400	2.61727977	1.36620426	8	3.45252609	-0.42562035	-0.96269566
1	-2.76737404	2.15607977	2.05440426	6	2.72112608	-0.99402040	-2.05379558
1	-3.42067409	3.70637965	1.48500431	6	1.26052606	-0.55932033	-1.95399570
1	-4.48767424	2.29907966	1.65030420	8	0.53262603	-1.16182029	-2.87269568
6	-1.80837381	2.81817961	-0.50929570	6	-0.88617384	-0.84482032	-2.91179562
1	-1.13527393	2.94947982	0.34290430	6	3.35742593	-0.53522032	-3.36159563
1	-1.31717396	2.22557974	-1.29019570	1	2.74652600	-2.08442020	-1.97629583
1	-1.93487394	3.82707977	-0.91779566	8	0.81462610	0.25057966	-1.15379572
6	-4.24187422	2.88417983	-0.98039573	1	-1.01737392	0.21357965	-3.13869572
1	-4.07527399	2.69347978	-2.04699564	1	-1.28747392	-1.46372032	-3.71089554
1	-5.25507402	2.55737972	-0.72649568	1	-1.35547388	-1.08652031	-1.95759571
1	-4.20667410	3.96887970	-0.83199567	1	-5.10117388	-1.79152024	-1.63709569
6	-2.21047401	-3.90242028	1.55900431	8	2.13982606	0.34287965	1.44790423
1	-3.26217413	-3.96442032	1.85770428	1	4.61292601	3.33277965	0.38410428
1	-2.09827399	-4.39752007	0.58790433	1	3.24582601	4.43347979	0.08830429
1	-1.62937391	-4.48212051	2.28470445	1	3.39502597	2.94537973	-0.85719568
6	-0.21927392	-2.51062036	1.11420429	1	6.55802584	-0.25082034	1.93660426
1	0.25642607	-1.53142023	1.17040431	1	6.47012615	-0.23352034	0.16380429
1	0.34492606	-3.18712020	1.76720428	1	6.33942604	-1.77302027	1.04810429
1	-0.12697393	-2.88942027	0.08930429	1	2.81092596	-0.94762033	-4.21159554
6	-1.80027401	-1.92482030	2.99110436	1	4.38922596	-0.89092034	-3.40309572
1	-2.84097409	-1.94912028	3.33260441	1	3.36022592	0.55517966	-3.43269563
1	-1.20987391	-2.55602026	3.66670442				

I-5\_LL



Zero-point vibrational energy	1887836.8 (Joules/Mol)
	451.20383 (Kcal/Mol)
Zero-point correction=	0.719039 (Hartree/Particle)
Thermal correction to Energy=	0.768340
Thermal correction to Enthalpy=	0.769284
Thermal correction to Gibbs Free Energy=	0.629422
Sum of electronic and zero-point Energies=	-2271.313314
Sum of electronic and thermal Energies=	-2271.264013
Sum of electronic and thermal Enthalpies=	-2271.263069
Sum of electronic and thermal Free Energies=	-2271.402931

cartesian							
8	1.41838157	2.05061722	0.95030344	6	0.54788154	-1.51258278	-2.69589663
6	2.62498140	3.85281730	-0.09969656	1	0.18978155	-1.49498272	-1.66579652
6	2.48478174	2.47541714	0.51950347	1	0.69938153	-2.55738282	-2.98749661
8	3.57378149	1.73691726	0.57090342	1	-0.23011847	-1.09118295	-3.34499645
6	4.74558163	2.18001723	-0.17609654	6	2.25498152	-0.78478283	-4.33449697
6	5.01178122	3.65511727	0.09780344	1	2.42198133	-1.81288266	-4.67139673
8	3.90288162	4.42621708	0.22850345	1	3.15448141	-0.20018283	-4.55789661
8	6.11028147	4.13551712	0.19630346	1	1.44108152	-0.37138283	-4.94089699
1	2.57098150	3.70971727	-1.18899655	6	2.07988167	-3.20888281	1.93810344
6	1.54988158	4.82151699	0.34660345	1	2.10528135	-4.16968298	1.41260350
6	5.89748144	1.27751708	0.19700345	1	1.24108148	-2.63878274	1.53840351
1	4.50508165	2.06111717	-1.23999655	1	1.88448155	-3.40518284	2.99840355
1	6.77528143	1.56161714	-0.38569653	6	3.47398138	-1.18818283	2.60940337

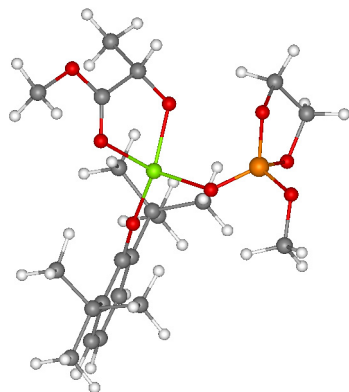
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1	5.63548136	0.24111716	-0.02459656	1	4.49678135	-0.79838282	2.65380335
1	6.13898134	1.37971711	1.25680351	1	3.13178158	-1.37208295	3.63310337
1	1.70638156	5.78391743	-0.14399655	1	2.86278152	-0.38648283	2.19170356
1	1.58498156	4.96351719	1.42830348	6	4.49568129	-3.41318274	2.36440349
1	0.56648153	4.43601704	0.07470345	1	5.49748135	-2.97078276	2.35140347
12	0.69328153	0.09491716	1.29220343	1	4.53688145	-4.37548256	1.84360349
8	-0.04081847	-0.01908283	3.03870344	1	4.24758148	-3.61698270	3.41200352
6	-1.40401852	0.05381717	3.14560342	1	6.01268148	-2.81648278	-2.14829659
6	-2.02471852	0.28861716	1.76670349	1	-1.73241842	0.92591715	3.74720335
8	-3.34141827	0.42941716	1.73840344	1	-3.11101866	-1.11888289	3.89460349
6	-3.97221851	0.63731718	0.45770347	1	-1.57561851	-1.32448292	4.77520323
6	-2.02551842	-1.19938278	3.78760338	1	-1.78441846	-2.08718276	3.19430351
8	-1.32681847	0.34751716	0.74270344	8	-5.80751848	-0.26108283	-0.68669653
6	-4.06291866	2.12601709	0.14290345	8	-5.98681879	-0.16008282	1.57290351
6	-5.36061859	0.02371716	0.55760342	6	-7.17111874	-0.69168282	-0.77939653
1	-3.40011835	0.11711717	-0.31289655	6	-8.09281826	0.50361717	-0.54279655
8	1.65878153	-0.89978284	0.03500345	1	-7.37171841	-1.43578291	-0.00429656
6	2.73638153	-1.44278288	-0.51479656	6	-7.36531878	-1.28468275	-2.16709661
6	2.94288158	-1.31958294	-1.92799664	8	-9.35301781	0.08151717	-0.35509652
6	4.13328123	-1.80908275	-2.47529650	8	-7.74551868	1.66311717	-0.55199653
1	4.31958151	-1.71118283	-3.53979659	6	-10.32661819	1.11991715	-0.14329655
6	5.09588146	-2.44508266	-1.69689655	1	-11.27691841	0.60481715	-0.01299655
6	4.84618139	-2.64178276	-0.34209657	1	-10.36511803	1.78711724	-1.00659657
1	5.58308125	-3.18608284	0.23920345	1	-10.07511806	1.69511724	0.74950343
6	3.68268156	-2.17298269	0.27690345	1	-4.61221838	2.27551723	-0.78889656
6	1.86228156	-0.71868283	-2.84819651	1	-3.05791855	2.53911734	0.03230345
6	3.42848158	-2.47808266	1.76610351	1	-4.58681870	2.65191722	0.94410348
6	1.61168158	0.76651716	-2.52439642	1	-8.39231777	-1.63778281	-2.27989650
1	1.27848148	0.88891715	-1.49379659	1	-6.68671846	-2.12978268	-2.30419660
1	0.84178156	1.18221712	-3.18649650	1	-7.15751839	-0.54018283	-2.93969655
1	2.52978134	1.34891725	-2.67929649				

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## S1.8. LP sequence, mononuclear mechanism

### I-1\_LP

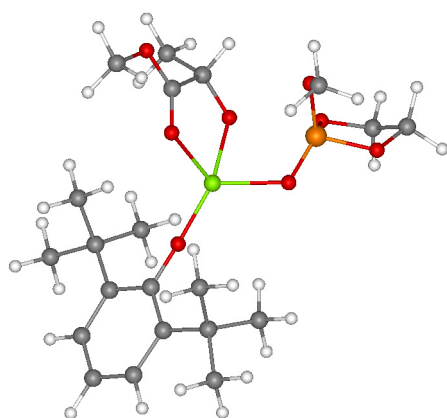


Zero-point vibrational energy	1445611.2 (Joules/Mol)
	345.50936 (Kcal/Mol)
Zero-point correction=	0.550604 (Hartree/Particle)
Thermal correction to Energy=	0.587427
Thermal correction to Enthalpy=	0.588371
Thermal correction to Gibbs Free Energy=	0.477829
Sum of electronic and zero-point Energies=	-1963.699849
Sum of electronic and thermal Energies=	-1963.663026
Sum of electronic and thermal Enthalpies=	-1963.662082
Sum of electronic and thermal Free Energies=	-1963.772624

				cartesian			
12	0.92811191	0.39101970	-0.07618640	1	-1.11408806	-2.71438026	2.30341363
8	-0.90228808	0.10001969	-0.06178640	1	-0.01908806	-1.70538032	3.26951361
6	-2.18398809	-0.21938032	0.06521360	1	-0.10218808	-1.51418030	1.50911355
6	-3.04738808	-0.16918030	-1.07568634	1	-5.96438789	-1.14838028	0.42151362
6	-4.39358807	-0.50718033	-0.90988642	8	1.86371195	-1.04768026	-1.18008637
1	-5.06718779	-0.47438031	-1.75978637	15	3.02651191	-1.92128038	-0.84098643
6	-4.91268778	-0.89028031	0.32241359	8	4.42691231	-1.25468028	-0.47028640
6	-4.06788778	-0.93758035	1.42601359	8	2.79431176	-2.76888037	0.50151360
1	-4.48928785	-1.23758030	2.37971377	6	4.63931227	-1.36788034	0.96591353
6	-2.71108818	-0.61188030	1.33711362	6	3.95851183	-2.67878032	1.35671353
6	-2.52278805	0.24381970	-2.46318626	1	5.71651220	-1.37908030	1.13161361
6	-1.82358801	-0.67438030	2.59371376	1	4.15381193	-0.51048028	1.43991363
6	-1.43898797	-0.74548030	-2.93888640	8	3.39691186	-2.88508034	-2.03738642
1	-0.61678803	-0.82058030	-2.22668624	6	2.39511180	-3.30998039	-2.99438620
1	-1.03348804	-0.43208033	-3.90988636	1	2.94941187	-3.66868043	-3.85998631
1	-1.86898792	-1.74648035	-3.06028628	1	1.75261199	-2.47328043	-3.26918626

6	-1.96728814	1.68211973	-2.42318630	1	1.80231202	-4.11998034	-2.56528640
1	-1.16818798	1.79021966	-1.68988645	8	2.33631182	0.79961967	1.19131362
1	-2.76278806	2.38791966	-2.15868640	6	2.87881184	2.05871964	1.10821354
1	-1.57658803	1.96911979	-3.40798640	1	3.97911191	2.03371978	0.96721363
6	-3.62488818	0.23121969	-3.53718638	6	2.35121202	2.77191973	-0.13758640
1	-4.43258810	0.93591964	-3.31228638	8	2.88281178	3.95451975	-0.40198642
1	-4.06398773	-0.76328033	-3.67198634	8	1.48101199	2.26711965	-0.85828638
1	-3.19228816	0.52861965	-4.49948645	6	2.38501191	4.63951969	-1.57078636
6	-2.60338807	-1.11628032	3.84511375	1	2.93421197	5.57841969	-1.60898638
1	-3.03188825	-2.11838031	3.73621368	1	1.31381190	4.82141972	-1.47298646
1	-1.92118800	-1.14478028	4.70251369	1	2.57461190	4.04401970	-2.46528625
1	-3.41178823	-0.42118031	4.09561348	1	3.60811186	-2.67588043	2.38861370
6	-1.24828804	0.72061968	2.91301370	1	4.58951187	-3.55278039	1.17251360
1	-0.68558800	1.13281965	2.07471371	6	2.59981179	2.91971970	2.35341382
1	-0.58108807	0.67341965	3.78221369	1	3.07161188	3.90521955	2.29241371
1	-2.05988812	1.41961968	3.14371371	1	2.99321175	2.39081979	3.22491360
6	-0.69398808	-1.70768034	2.40471363	1	1.52221203	3.04351974	2.49661374

## TS-12\_LP

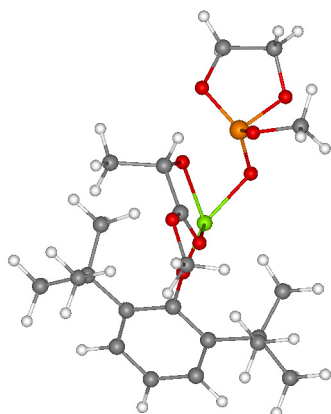


Zero-point vibrational energy	1446277.9 (Joules/Mol)
	345.66872 (Kcal/Mol)
Zero-point correction=	0.550858 (Hartree/Particle)
Thermal correction to Energy=	0.586395
Thermal correction to Enthalpy=	0.587339
Thermal correction to Gibbs Free Energy=	0.481887
Sum of electronic and zero-point Energies=	-1963.687541
Sum of electronic and thermal Energies=	-1963.652004
Sum of electronic and thermal Enthalpies=	-1963.651060
Sum of electronic and thermal Free Energies=	-1963.756513

cartesian

12	-0.70673352	0.03032728	0.13930909	1	2.65036654	3.06662726	0.20700909
8	1.09776652	-0.24557272	-0.09839091	1	1.44556653	3.53472733	-1.00699091
6	2.41486645	-0.41127270	-0.15279092	1	1.15846658	2.13982725	0.05820908
6	3.02256656	-1.54417276	0.47480911	8	-2.00903344	-1.50707269	0.06000908
6	4.41236639	-1.67817271	0.40400910	15	-3.36153340	-1.15287268	-0.50269091
1	4.89726639	-2.52767277	0.87340909	8	-4.10563374	-2.60807276	-0.65609092
6	5.21096659	-0.75187272	-0.25829092	8	-3.64223337	-0.65767276	-2.00409079
6	4.61056662	0.34052730	-0.87489092	6	-5.00673342	-2.57727265	-1.76489091
1	5.24746656	1.04992723	-1.39269102	6	-4.32603359	-1.66697276	-2.78129101
6	3.22726655	0.54142725	-0.84429091	1	-5.97683334	-2.17637277	-1.44919097
6	2.18276644	-2.61157274	1.20120907	1	-5.13433361	-3.59757280	-2.12979102
6	2.61286640	1.76782727	-1.54419100	1	-3.57973337	-2.20097280	-3.37529087
6	1.42326653	-1.99027276	2.39150906	1	-5.02633333	-1.15057278	-3.43869090
1	0.80046654	-1.14767277	2.08680916	8	-4.36733341	-0.35057271	0.45490912
1	0.78086650	-2.73887277	2.87140894	6	-4.56673336	-0.85707271	1.79040909
1	2.12836647	-1.61697268	3.14250898	1	-4.95673370	-1.87747276	1.75860906
6	1.20456648	-3.28147268	0.21490909	1	-3.63093352	-0.83457273	2.35420895
1	0.53636646	-2.56137276	-0.25709090	1	-5.29633331	-0.19387272	2.25450897
1	1.76076651	-3.79097271	-0.57969087	8	-1.11883354	1.37502730	1.72440898
1	0.58966649	-4.02927256	0.73090911	8	-2.24113345	0.97502732	-0.63049090
6	3.04896641	-3.74037266	1.78830910	6	-1.98013353	2.19532728	1.38000906
1	3.60356641	-4.28147268	1.01440907	6	-2.67923355	2.10712719	0.02410909
1	3.76456642	-3.37327266	2.53190899	1	-3.75693345	2.04622722	0.25460911
1	2.40026641	-4.46707249	2.29090905	1	6.28976631	-0.88247275	-0.29719090
6	3.67216635	2.63742733	-2.24439096	8	-2.35273361	3.19342732	2.16290903
1	4.40786648	3.04362726	-1.54199100	6	-1.67713344	3.30632734	3.43420911
1	4.20866632	2.08862734	-3.02569103	1	-2.10683346	4.18572760	3.91010904
1	3.17766643	3.48892736	-2.72559094	1	-0.60493350	3.43422723	3.27940893
6	1.61926651	1.32732725	-2.63869095	1	-1.85573351	2.41442728	4.03690910
1	0.81276655	0.71302724	-2.23689103	6	-2.43833351	3.38762736	-0.78919089
1	1.17416656	2.20152736	-3.13019085	1	-2.81463337	4.27692747	-0.27489090
1	2.13546658	0.73742729	-3.40389085	1	-2.95753360	3.28062725	-1.74419093
6	1.91896653	2.67812729	-0.51029092	1	-1.37223351	3.51552725	-0.99599087

## I-2\_LP

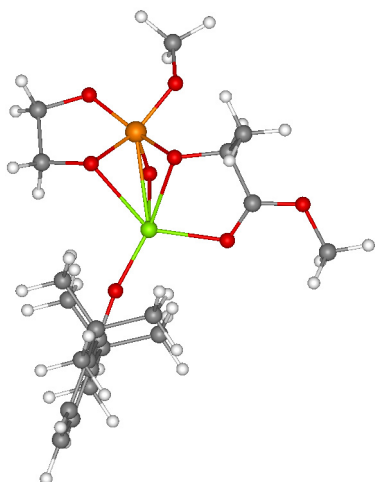


Zero-point vibrational energy	1448529.0 (Joules/Mol)
	346.20674 (Kcal/Mol)
Zero-point correction=	0.551716 (Hartree/Particle)
Thermal correction to Energy=	0.586692
Thermal correction to Enthalpy=	0.587636
Thermal correction to Gibbs Free Energy=	0.484447
Sum of electronic and zero-point Energies=	-1963.689561
Sum of electronic and thermal Energies=	-1963.654584
Sum of electronic and thermal Enthalpies=	-1963.653640
Sum of electronic and thermal Free Energies=	-1963.756829

cartesian							
12	-0.62488794	0.24474543	-0.06886065	1	0.69031197	-1.27885461	1.93073928
8	1.19961214	0.12354544	0.07353935	1	0.88371199	-2.97345448	2.41683936
6	2.50961208	0.20324543	0.28933936	1	1.89111209	-1.70995462	3.14623952
6	3.21601200	1.41044545	-0.00616065	6	1.84991217	-2.82255435	-0.16306065
6	4.59261227	1.44964540	0.23583935	1	2.62521219	-3.05915451	-0.90026069
1	5.15251207	2.35414553	0.02293935	1	1.30371213	-3.74835443	0.05893935
6	5.28341198	0.35714546	0.74873936	1	1.16461205	-2.10845447	-0.62326068
6	4.58821201	-0.81495458	1.02643931	8	-1.89988804	1.36014545	0.93613935
1	5.14371204	-1.65795457	1.42373931	15	-3.25818801	0.64844543	0.92863935
6	3.21211219	-0.92845458	0.80813932	8	-4.12828827	1.85424542	1.71903932
6	2.49761200	2.65034556	-0.57186067	8	-3.77008796	-0.49355456	1.98953938
6	2.48751211	-2.25095439	1.12013936	6	-5.13668776	1.32604539	2.55813956
6	1.83781219	2.32144547	-1.92736065	6	-4.54458809	0.02544544	3.07833934
1	1.15801191	1.47054541	-1.86156070	1	-6.06248808	1.14004540	1.99333930
1	1.27931213	3.18814564	-2.30306053	1	-5.34488773	2.04434538	3.35453939
1	2.60211205	2.06704545	-2.67006063	1	-3.87888789	0.19494544	3.93023944
6	1.45411205	3.17514563	0.43553936	1	-5.29408789	-0.72455460	3.33813953
1	0.72011203	2.41944551	0.71753931	8	-4.10058784	0.68474543	-0.47026068

1	1.94661212	3.50124550	1.35783935	6	-4.83178806	1.85274541	-0.87556064
1	0.91451198	4.03504562	0.02033935	1	-5.72738791	1.99054539	-0.26666063
6	3.46391201	3.81864548	-0.83786064	1	-4.21048784	2.74834561	-0.81376064
1	3.95611191	4.16664553	0.07623935	1	-5.11908770	1.67194545	-1.91316068
1	4.23691225	3.55864549	-1.56876063	8	-1.15708804	-0.24995457	-2.06636047
1	2.90061212	4.66584539	-1.24556065	8	-2.33598804	-0.85575455	0.17253935
6	3.44411206	-3.33405447	1.64993930	6	-2.07678795	-1.07045460	-2.14966059
1	4.22831202	-3.58285451	0.92713934	6	-2.77258801	-1.62755454	-0.91396070
1	3.92241192	-3.04085445	2.59033942	1	-3.85058784	-1.52415454	-1.06846070
1	2.87731218	-4.25145483	1.84553933	1	6.35401201	0.41814545	0.92903936
6	1.42041206	-2.03855443	2.21353936	8	-2.50938797	-1.54415452	-3.30116057
6	-2.42688799	-3.10415435	-0.70846069	6	-1.83898807	-1.06645453	-4.49016094
1	-2.76218796	-3.70705438	-1.55686069	1	-2.32838798	-1.57575452	-5.31766081
1	-2.93088794	-3.44915438	0.19653934	1	-0.77898800	-1.31985462	-4.44906092
1	-1.35088801	-3.24245453	-0.57576066	1	-1.95628786	0.01464544	-4.57516098

### TS-24\_LP



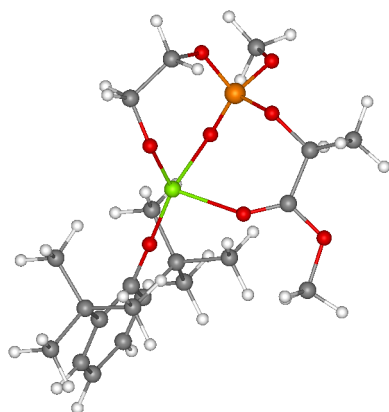
Zero-point vibrational energy	1449157.9 (Joules/Mol)
	346.35705 (Kcal/Mol)
Zero-point correction=	0.551955 (Hartree/Particle)
Thermal correction to Energy=	0.587005
Thermal correction to Enthalpy=	0.587949
Thermal correction to Gibbs Free Energy=	0.484436
Sum of electronic and zero-point Energies=	-1963.676642
Sum of electronic and thermal Energies=	-1963.641592
Sum of electronic and thermal Enthalpies=	-1963.640648
Sum of electronic and thermal Free Energies=	-1963.744162



cartesian

12	0.83857894	-0.06782274	-0.23654543	1	-2.04072094	3.29787731	0.61435461
8	-0.97402108	-0.17032273	0.04475456	1	-0.80892098	3.25557733	1.89015460
6	-2.30332088	-0.15072274	0.05855456	1	-0.70342100	2.15537739	0.49795458
6	-3.04412079	-0.97302276	-0.84744543	8	2.28797913	-1.37452281	-0.83894539
6	-4.44062090	-0.93432271	-0.79024541	15	3.13317919	-1.09572279	0.41665456
1	-5.02562094	-1.55042279	-1.46494544	8	3.65417910	-2.54152274	1.06595457
6	-5.12032080	-0.12392274	0.11255457	8	1.90497899	-1.01972282	1.63525462
6	-4.39132071	0.67667729	0.98535460	6	2.82157898	-3.14262271	2.04405451
1	-4.93772078	1.30397725	1.68155456	6	1.53177893	-2.32552266	2.06755447
6	-2.99322081	0.69037730	0.98675460	1	3.34387875	-3.10742259	3.00615454
6	-2.34172106	-1.88612282	-1.87054539	1	2.63817883	-4.18452311	1.77035463
6	-2.23342085	1.60087717	1.97025454	1	0.78407896	-2.74302268	1.38525462
6	-1.50302100	-1.04532278	-2.85514545	1	1.10227895	-2.24072266	3.06695437
1	-0.78912103	-0.39912274	-2.34174562	8	4.67447901	-0.66512275	0.08895457
1	-0.94702101	-1.69412279	-3.54254556	6	5.69647932	-1.61572278	-0.24534543
1	-2.15372086	-0.39642274	-3.45144558	1	6.04097891	-2.13902259	0.64745456
6	-1.45992100	-2.92612267	-1.15034544	1	5.33757925	-2.33942270	-0.98064542
1	-0.70782101	-2.45162272	-0.51904541	1	6.51207924	-1.02982271	-0.67464542
1	-2.07592106	-3.56782269	-0.51084542	8	1.24857903	1.56777716	-1.45814538
1	-0.94302106	-3.56472278	-1.87674546	8	2.77507877	0.67527729	0.51145458
6	-3.33962107	-2.68432260	-2.72844553	6	2.36247897	2.08487725	-1.34884536
1	-3.96522093	-3.34922266	-2.12374544	6	3.38447905	1.64847720	-0.31154543
1	-3.99572086	-2.03372264	-3.31594563	1	4.22427893	1.22077715	-0.86804539
1	-2.78492117	-3.31212258	-3.43514562	1	-6.20742083	-0.11562274	0.13525458
6	-3.18152094	2.40477729	2.87755442	8	2.77277899	3.05917740	-2.13664556
1	-3.83892107	3.06997728	2.30745435	6	1.84687901	3.49517727	-3.15974545
1	-3.80502081	1.75677717	3.50235438	1	2.36527896	4.29017687	-3.69134545
1	-2.58792114	3.03357744	3.55095458	1	0.93087900	3.86677742	-2.69944549
6	-1.33912098	0.76317728	2.90725446	1	1.61447895	2.66607738	-3.82904553
1	-0.61232102	0.16707727	2.35485458	6	3.88157892	2.81337738	0.54115456
1	-0.79402101	1.41537726	3.60115457	1	4.33857918	3.58867741	-0.07804543
1	-1.95262110	0.07767726	3.50245452	1	4.62647915	2.43177724	1.24185455
6	-1.39062107	2.63527727	1.19635463	1	3.05897903	3.24857736	1.11435461

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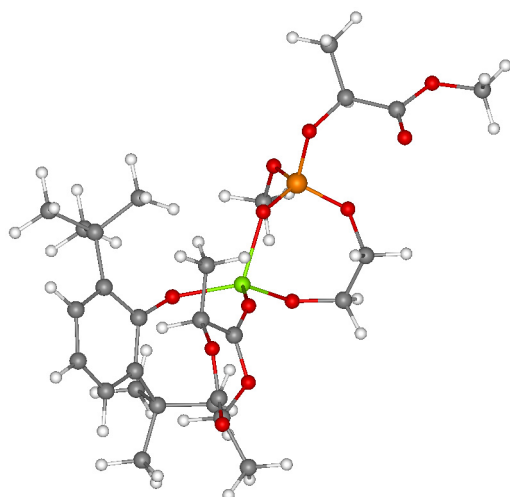


Zero-point vibrational energy	1446312.2 (Joules/Mol)
	345.67691 (Kcal/Mol)
Zero-point correction=	0.550871 (Hartree/Particle)
Thermal correction to Energy=	0.587327
Thermal correction to Enthalpy=	0.588272
Thermal correction to Gibbs Free Energy=	0.480780
Sum of electronic and zero-point Energies=	-1963.692808
Sum of electronic and thermal Energies=	-1963.656352
Sum of electronic and thermal Enthalpies=	-1963.655408
Sum of electronic and thermal Free Energies=	-1963.762900

				cartesian			
12	0.71300149	0.75139695	0.51992869	1	-2.51169872	2.50359702	-2.00287127
8	-1.02909851	0.12829691	0.40542874	1	-1.63069868	3.69579697	-1.02777123
6	-2.31559873	-0.17360309	0.28792873	1	-1.09799862	2.00509691	-1.07597125
6	-2.72869849	-1.54450309	0.30412874	8	2.14990139	-0.65170306	0.97862870
6	-4.08999872	-1.83450317	0.17292874	15	3.57850146	-0.19860309	0.89762872
1	-4.42659855	-2.86590290	0.18382874	8	4.13530159	0.79189694	1.97312880
6	-5.04669857	-0.83530307	0.02982873	8	4.56360149	-1.44590306	0.98402870
6	-4.63859844	0.49419692	0.01902873	6	4.29660130	-2.51380301	1.91982877
1	-5.39909840	1.26039684	-0.08867127	1	4.56390142	-2.19370294	2.92922878
6	-3.29509854	0.86099696	0.14432873	1	3.24510145	-2.80330300	1.87712872
6	-1.71259856	-2.68950295	0.47142875	1	4.93130159	-3.34480309	1.61482882
6	-2.90299869	2.35039711	0.13422874	8	1.39070153	0.67899692	-1.49437118
6	-0.69879860	-2.68310308	-0.69107127	8	3.97350144	0.46999690	-0.50337130
1	-0.17159855	-1.73020315	-0.75097132	6	2.26180148	0.20739692	-2.20787120
1	0.04160145	-3.48290300	-0.56107128	6	3.67590141	-0.15970308	-1.75317121
1	-1.21429849	-2.85210299	-1.64387119	1	3.68570137	-1.25120306	-1.63597119
6	-0.98469859	-2.56480289	1.82532883	1	-6.09939861	-1.08970308	-0.06757127
1	-0.46159858	-1.61290312	1.91682875	8	2.06790137	-0.08440308	-3.48277116

1	-1.70309854	-2.63630295	2.64932871	6	0.72980142	0.14359692	-3.99397135
1	-0.25279856	-3.37410307	1.94382882	1	0.76250148	-0.19240308	-5.02797127
6	-2.38119864	-4.07560301	0.45732874	1	0.48930144	1.20539689	-3.93597126
1	-3.09329867	-4.20130301	1.27972877	1	0.00720146	-0.43220308	-3.41567135
1	-2.90449858	-4.27470303	-0.48427126	6	4.75500154	0.25439692	-2.74297118
1	-1.61209869	-4.84810305	0.57242870	1	4.58790159	-0.21800309	-3.71157122
6	-4.12189865	3.27759695	-0.02617126	1	5.72670126	-0.05710308	-2.35547113
1	-4.65949869	3.10169697	-0.96417135	1	4.76090145	1.33929694	-2.87097120
1	-4.83189869	3.17699695	0.80162871	6	3.87580132	2.23819709	2.07672882
1	-3.78119850	4.31919670	-0.03677126	1	4.50670147	2.54639697	2.91342878
6	-2.23599863	2.74429703	1.46762872	6	2.40840149	2.55409694	2.30502868
1	-1.33679843	2.16339707	1.67452872	1	4.23210144	2.69359708	1.14962876
1	-1.95499849	3.80419707	1.45802879	1	2.37730145	3.64189696	2.51302886
1	-2.93229866	2.58549690	2.29832888	1	2.09560156	2.05719709	3.24362874
6	-1.97429872	2.65479708	-1.05947125	8	1.64220142	2.21579695	1.21892881

# I-5\_LPL



Zero-point vibrational energy	1819608.6 (Joules/Mol)
	434.89689 (Kcal/Mol)
Zero-point correction=	0.693052 (Hartree/Particle)
Thermal correction to Energy=	0.740863
Thermal correction to Enthalpy=	0.741807
Thermal correction to Gibbs Free Energy=	0.606007
Sum of electronic and zero-point Energies=	-2497.786012
Sum of electronic and thermal Energies=	-2497.738201
Sum of electronic and thermal Enthalpies=	-2497.737257
Sum of electronic and thermal Free Energies=	-2497.873057

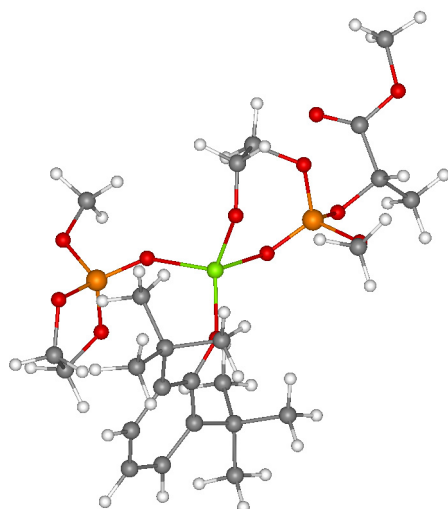
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12	-0.38059509	-0.04624899	-0.77887499	15	-3.47739506	0.31735098	-0.19807494

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8	-4.46909523	0.20575102	1.03842509	8	-3.94239497	-0.71954900	-1.29817498
8	0.92520493	1.34535110	-0.63227499	8	-1.27389514	-0.49164897	-2.38177490
6	-5.89009523	0.13515101	0.86922503	6	-3.14139509	-1.87634897	-1.70187497
6	-6.31179523	-1.32874894	0.73762500	6	-2.15109515	-1.47244895	-2.78747487
1	-6.19279480	0.66385102	-0.04057495	1	-3.87109494	-2.60894895	-2.05487490
6	2.13340497	1.35105109	-0.08937495	1	-2.63619494	-2.27604914	-0.81777495
6	3.25820494	0.83225101	-0.81777495	1	-1.64289510	-2.40914917	-3.09167480
6	4.45530510	0.62455100	-0.11987495	1	-2.73509502	-1.14544892	-3.66757488
1	5.31770515	0.21065103	-0.63437498	8	-3.86919498	1.72975111	-0.80567497
6	4.60240507	0.98455101	1.21952498	1	5.54120493	0.80755097	1.73902500
6	3.56880498	1.68275106	1.84372509	6	-3.34389496	2.16655087	-2.08847475
1	3.74100494	2.06315088	2.84582520	1	-2.91479492	3.15625095	-1.93057501
6	2.34640503	1.92605102	1.20842505	1	-4.18169498	2.22285104	-2.78497481
6	3.21000504	0.65965098	-2.35247493	1	-2.58389497	1.47665107	-2.46657491
6	1.31230485	2.87605095	1.84752500	8	4.58250475	-4.49004889	1.80872500
6	2.81040502	2.01305103	-2.97867489	8	3.00560498	-3.03674912	2.40532517
1	1.82890475	2.33445096	-2.62477493	6	3.82330513	-3.60694909	1.49732506
1	2.77100492	1.92675102	-4.07147503	6	3.70070505	-3.05624914	0.08422505
1	3.54180503	2.78825092	-2.72587490	8	2.30980492	-2.74064898	-0.21677494
6	2.22650504	-0.42344898	-2.83607483	6	1.64060485	-2.01134896	0.66232502
1	1.18190479	-0.12424899	-2.73897481	6	2.25790501	-1.85714889	2.03652501
1	2.37140489	-1.37154889	-2.30947495	1	2.94780493	-1.00024903	1.97522497
1	2.38480496	-0.61674899	-3.90427494	8	0.56250489	-1.51774895	0.35522506
6	4.59200478	0.29155099	-2.92167497	1	4.25340509	-2.10884905	0.03522505
1	4.93580484	-0.69534898	-2.58867478	6	1.22760487	-1.62824893	3.12262511
1	5.35870504	1.02785110	-2.65997481	1	1.73910487	-1.48114896	4.07552481
1	4.53260517	0.25705099	-4.01467514	1	0.55940491	-2.48834896	3.20612526
6	1.88500488	3.59015083	3.08502507	1	0.63770491	-0.74264902	2.89282513
1	2.80270505	4.14205122	2.85602522	6	4.18860483	-4.02114916	-0.97147501
1	2.09480500	2.89875102	3.90892506	1	3.62520504	-4.95574903	-0.93237495
1	1.14940488	4.31285095	3.45502520	1	5.24100494	-4.24664879	-0.79387498
6	0.03560488	2.14925098	2.30322504	1	4.07890511	-3.57434916	-1.96137488
1	-0.47299510	1.64625108	1.48182499	8	-7.60819483	-1.39174891	0.38142505
1	-0.67189509	2.86685085	2.73702526	8	-5.60619497	-2.28874898	0.94082505
1	0.26340491	1.41145110	3.08002520	6	-8.15029526	-2.71894908	0.26262504
6	0.94250494	3.97425103	0.82772505	1	-7.61779499	0.75935102	2.00202513
1	1.83000481	4.54935122	0.54152507	1	-6.20909500	1.83655107	2.14082503
1	0.21910490	4.66985130	1.27042508	1	-6.22119522	0.28305101	2.99922514
1	0.50520492	3.54605103	-0.07537495	1	-9.19579506	-2.58324909	-0.00947495
6	-6.52969503	0.79415101	2.08402514	1	-8.06529522	-3.25114918	1.21212506
8	-2.07839513	0.17345102	0.31272504	1	-7.62109518	-3.27634907	-0.51267499

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## I-5\_LPP



Zero-point vibrational energy	1752800.6 (Joules/Mol)
	418.92940 (Kcal/Mol)
Zero-point correction=	0.667607 (Hartree/Particle)
Thermal correction to Energy=	0.714352
Thermal correction to Enthalpy=	0.715296
Thermal correction to Gibbs Free Energy=	0.582249
Sum of electronic and zero-point Energies=	-2724.269713
Sum of electronic and thermal Energies=	-2724.222968
Sum of electronic and thermal Enthalpies=	-2724.222024
Sum of electronic and thermal Free Energies=	-2724.355071

				cartesian			
12	-0.10930753	0.29227048	0.66469258	8	-1.78880751	0.02857049	-0.46290740
8	-4.15530729	-0.36512953	-1.16370738	15	-3.09450769	-0.52312952	0.01269260
8	1.32659256	-0.86812955	0.25119260	8	-3.71900749	0.14057049	1.30849266
6	-5.53690767	-0.69302952	-0.97950739	8	-1.02300751	0.14437050	2.32219243
6	-6.29440784	0.53647053	-0.47760740	6	-3.12460756	1.29287052	1.98389268
1	-5.64350748	-1.49282956	-0.23990740	6	-2.03580761	0.83327049	2.94659257
6	2.59979248	-1.00332952	-0.07610740	1	-3.96050763	1.77567053	2.49639249
6	3.62199235	-0.95482951	0.93169260	1	-2.72950768	1.97357059	1.22399271
6	4.96019220	-0.94682950	0.52029258	1	-1.68640745	1.75077057	3.46239257
1	5.75129223	-0.88052946	1.26009262	1	-2.51970768	0.21507049	3.72609258
6	5.32409239	-1.02952957	-0.82150739	8	-3.15990758	-2.08272958	0.29409260
6	4.32829237	-1.21422958	-1.77860737	1	6.37239218	-1.01332951	-1.11110735
1	4.63259220	-1.36312962	-2.81000757	6	-2.52140760	-2.67762947	1.45709264
6	2.97059250	-1.24342942	-1.44330740	1	-1.88410747	-1.95552945	1.97529268
6	3.28319240	-0.96302956	2.43689251	1	-1.92910755	-3.51642966	1.09129262
6	1.91989243	-1.60972953	-2.51200747	1	-3.31220770	-3.03162956	2.12059259

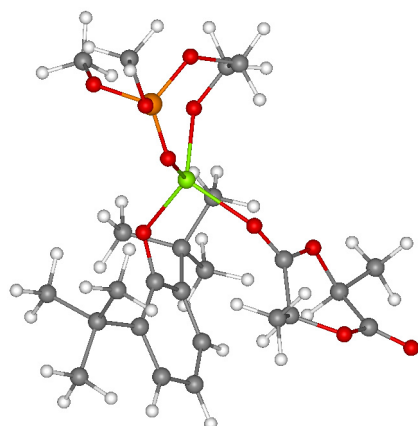
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6	2.37469244	-2.16692948	2.76249242	8	0.44119245	2.19967055	0.17499259
1	1.44589245	-2.13062954	2.19259262	15	1.52119255	3.08787036	-0.34050742
1	2.12419248	-2.17292953	3.83019257	8	2.90399241	3.16097045	0.44449261
1	2.88789248	-3.10652947	2.52889252	8	2.07209229	2.65547037	-1.77950740
6	2.60039234	0.34377050	2.88719249	6	3.96169233	2.55307055	-0.35040739
1	1.58529246	0.44257051	2.50129247	6	3.51849246	2.71247053	-1.80580735
1	3.18079233	1.22107053	2.58259249	8	1.05399251	4.60177040	-0.38190740
1	2.51289248	0.36457050	3.98029256	6	-0.33560753	4.94667053	-0.57910740
6	4.54529238	-1.11542940	3.30589247	1	-0.97020757	4.35827065	0.08449259
1	5.21609259	-0.25192952	3.23009253	1	-0.61740756	4.77727032	-1.62050736
1	5.11419249	-2.01722956	3.05589247	1	-0.41340753	6.00577021	-0.33880740
1	4.24669218	-1.19752955	4.35669279	1	3.86819220	1.89007044	-2.42870736
6	2.57359242	-2.02392960	-3.84260750	1	3.81469250	3.67487049	-2.23290753
1	3.25929236	-2.86922956	-3.72130752	1	4.88129234	3.09327054	-0.12620740
1	3.12119246	-1.20102954	-4.31620741	1	4.05329227	1.50457048	-0.06110740
1	1.79159248	-2.33352947	-4.54500723	8	-7.50040770	0.15897049	-0.01200740
6	0.97529250	-0.43722951	-2.83200741	8	-5.89970779	1.67817044	-0.51780742
1	0.39379245	-0.13012952	-1.96400738	6	-8.34770679	1.22787046	0.44239259
1	0.26339245	-0.72962952	-3.61360741	1	-8.54700756	1.92897058	-0.37070739
1	1.53239250	0.43227050	-3.19470739	1	-7.13870764	-1.41612959	-2.23370743
6	1.09939253	-2.82282948	-2.02480745	1	-5.52690744	-2.04132962	-2.65130734
1	1.75169253	-3.68982959	-1.87210739	1	-5.96350765	-0.37292951	-3.07310748
1	0.34499246	-3.09392953	-2.77350736	1	-9.26930714	0.74997050	0.77099258
1	0.59239244	-2.60562968	-1.08390737	1	-7.87540770	1.76007056	1.27039266
6	-6.08100748	-1.15922952	-2.32360744				

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## S1.9. PL sequence, mononuclear mechanism

### I-1\_PL

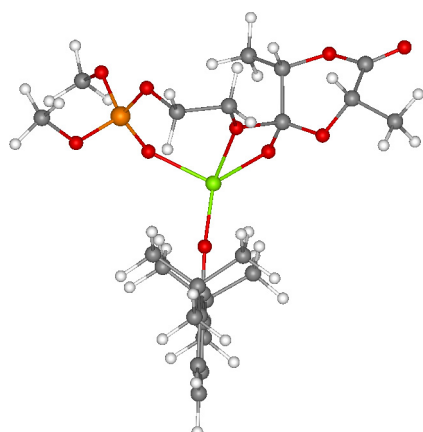


Zero-point vibrational energy	1632022.7 (Joules/Mol)
	390.06278 (Kcal/Mol)
Zero-point correction=	0.621605 (Hartree/Particle)
Thermal correction to Energy=	0.663734
Thermal correction to Enthalpy=	0.664678
Thermal correction to Gibbs Free Energy=	0.542884
Sum of electronic and zero-point Energies=	-2230.735845
Sum of electronic and thermal Energies=	-2230.693716
Sum of electronic and thermal Enthalpies=	-2230.692772
Sum of electronic and thermal Free Energies=	-2230.814566

cartesian											
12	-1.26337743	-0.54803741	-0.29808521	1	-1.43327737	4.52216244	0.60421479				
8	-5.12847710	-0.56613743	1.95051479	1	-1.10137737	3.19166255	-0.52328521				
8	-0.28057736	1.04016256	-0.71098518	1	-7.04097700	-0.04573746	1.30131471				
6	-6.55107737	-0.78373748	1.94021475	8	-2.84437752	-0.40503746	0.96341479				
1	-6.87957716	-0.65943742	2.97131491	15	-4.27257729	-0.70243746	0.62271482				
1	-6.77987719	-1.79603744	1.59791470	8	-4.55957699	-2.14813757	0.03341480				
6	0.95962268	1.38916254	-0.40208519	8	-2.20627737	-1.58643746	-1.56998527				
6	2.06232262	0.92876250	-1.20018530	6	-3.51177740	-3.13013744	-0.24018522				
6	3.35832262	1.11106253	-0.70028520	6	-2.81097746	-2.82373738	-1.55808520				
1	4.21302271	0.75226253	-1.26638520	1	-4.03457737	-4.08973742	-0.26458520				
6	3.60192251	1.79286265	0.49191481	1	-2.80737734	-3.12593746	0.59801477				
6	2.53442264	2.41506267	1.13911474	1	-2.09727740	-3.65583730	-1.71898520				
1	2.75212264	3.04196262	1.99811471	1	-3.56237745	-2.90903735	-2.36468506				
6	1.21412253	2.27596259	0.69771481	8	-5.00347710	0.30826253	-0.35568517				
6	1.84662247	0.40136254	-2.63648510	1	4.61802292	1.91736269	0.85891479				

6	0.09262264	3.13926268	1.31331480	6	-4.86827707	0.25286257	-1.80018520
6	1.09442258	1.48466253	-3.43948507	1	-4.94227743	1.28356266	-2.14618516
1	0.12612262	1.70496249	-2.98578525	1	-5.69447708	-0.33933747	-2.19878507
1	0.92392260	1.14236259	-4.46748495	1	-3.91007733	-0.18673745	-2.08918524
1	1.67642260	2.41166258	-3.48298502	8	4.80602264	-3.39023733	2.10171485
6	1.04932261	-0.91463745	-2.71448517	8	3.10912251	-2.09193754	2.72631478
1	-0.00777738	-0.78483742	-2.47928524	6	3.85492253	-2.71733737	1.79271472
1	1.46322274	-1.68383741	-2.05538511	6	3.39722252	-2.50783730	0.35661477
1	1.08542252	-1.30933738	-3.73758507	8	1.94102263	-2.47923732	0.28991479
6	3.18502259	0.15276253	-3.35478520	6	1.30042267	-1.69393754	1.14101481
1	3.76592255	-0.65493745	-2.89298511	6	2.10262251	-1.14613748	2.30271482
1	3.81252265	1.04906249	-3.39128518	1	2.59902263	-0.23313746	1.93621469
1	2.98632264	-0.14743745	-4.38908529	8	0.10802263	-1.45973754	0.98321480
6	0.65692264	4.21156263	2.26291490	1	3.74542260	-1.52093744	0.02451479
1	1.39102268	4.85566282	1.76751471	6	1.25062251	-0.83183748	3.51391482
1	1.12352252	3.78056240	3.15591478	1	1.88172245	-0.40303746	4.29441500
1	-0.16247737	4.85116243	2.60901475	1	0.77692264	-1.73843741	3.89721489
6	-0.92047739	2.31376266	2.12391472	1	0.47732264	-0.11443746	3.24461484
1	-1.41877747	1.55676246	1.52021480	6	3.87652278	-3.59213734	-0.58058518
1	-1.69907737	2.96966267	2.53261495	1	3.51042247	-4.57013750	-0.26148522
1	-0.43487737	1.82186270	2.97351480	1	4.96712303	-3.61523747	-0.57528520
6	-0.64477736	3.88756275	0.18211479	1	3.52662253	-3.38823748	-1.59408522
1	0.04822263	4.53286266	-0.36858517				

### TS-12\_PL



Zero-point vibrational energy	1632019.7 (Joules/Mol)
	390.06208 (Kcal/Mol)
Zero-point correction=	0.621603 (Hartree/Particle)
Thermal correction to Energy=	0.662683
Thermal correction to Enthalpy=	0.663628
Thermal correction to Gibbs Free Energy=	0.544119

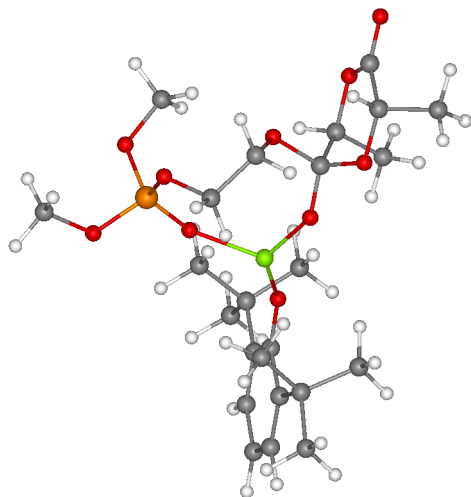


Sum of electronic and zero-point Energies=	-2230.720704
Sum of electronic and thermal Energies=	-2230.679624
Sum of electronic and thermal Enthalpies=	-2230.678680
Sum of electronic and thermal Free Energies=	-2230.798188

				cartesian			
12	-0.40561718	-0.00560797	-0.63097334	1	1.02428281	-2.10510802	-3.70697355
8	-0.09081718	4.11239243	0.26242664	1	0.76898289	-1.97390795	-1.95967329
8	1.35308290	-0.36250797	-0.20157336	1	-0.99801719	5.99639225	0.34502664
6	-0.39531720	5.33229208	0.96902668	8	-1.80571711	-1.21480799	-1.32327330
1	0.56468284	5.79599237	1.18922663	6	-2.70621705	-1.20050800	-0.40907335
1	-0.92481720	5.11379242	1.89902663	8	-2.72811723	-2.32170796	0.39182663
6	2.61538291	-0.76590800	-0.10667336	6	-3.98171711	-2.67600799	0.99012661
6	3.25468278	-0.78610796	1.17252672	6	-5.04161739	-2.79500794	-0.10327336
6	4.57938242	-1.22510803	1.25092661	1	-4.30371714	-1.88550794	1.68602669
1	5.08388281	-1.25590801	2.21102643	8	-5.87331724	-3.66770792	-0.16307336
6	5.28838253	-1.62930799	0.12492663	6	-4.12221718	-0.69810796	-0.75767332
6	4.66458273	-1.59130800	-1.11737335	8	-4.97681761	-1.82810795	-1.04587340
1	5.23578262	-1.90410793	-1.98507333	8	-0.60831720	1.99429202	-0.94967335
6	3.34088278	-1.16810799	-1.27187335	15	-1.24611723	3.15199208	-0.25747335
6	2.52048278	-0.31830797	2.44222665	8	-2.22121716	2.85379195	0.95652664
6	2.69628286	-1.15110803	-2.67007351	8	-2.06901717	0.04799203	0.56462663
6	1.27508283	-1.18880796	2.70782661	6	-1.87241721	1.91709197	2.01582646
1	0.57928276	-1.17390800	1.86802661	6	-2.54201722	0.57689202	1.77292669
1	0.75038278	-0.84030795	3.60772657	1	-2.23671722	2.37129211	2.94032645
1	1.56608284	-2.23130798	2.87532663	1	-0.78631723	1.80639207	2.08272648
6	2.12498283	1.16529202	2.29692650	1	-2.31221724	-0.07600798	2.62862659
1	1.51998281	1.32929206	1.40292668	1	-3.62971711	0.73159200	1.74152672
1	3.01858282	1.79269207	2.20702648	8	-2.22781730	4.00499201	-1.16527331
1	1.56808281	1.50349200	3.18202662	1	6.31798267	-1.96730804	0.21412665
6	3.39878273	-0.41840798	3.70152664	1	-4.55221748	-0.17590797	0.10402664
1	4.29838276	0.20219202	3.63122654	6	-1.84871721	4.29589224	-2.53187346
1	3.70678306	-1.44830799	3.90992665	1	-0.98501718	4.96449232	-2.55247355
1	2.82828283	-0.06720798	4.56932640	1	-2.71151710	4.78739214	-2.97797346
6	3.67828298	-1.57900798	-3.77617335	1	-1.62181711	3.37179208	-3.06567335
1	4.03128242	-2.60680795	-3.64277339	6	-4.14611721	0.20329203	-1.96947336
1	4.55068254	-0.91940796	-3.83567357	1	-5.17521763	0.49749202	-2.19007349
1	3.16888285	-1.53540802	-4.74577332	1	-3.72111726	-0.31390798	-2.83097339
6	2.23778296	0.27589202	-3.03777337	1	-3.55731726	1.10129201	-1.77197337
1	1.58608282	0.71499205	-2.28017354	6	-3.78511715	-3.96980786	1.75112665
1	1.71078277	0.27579203	-4.00017357	1	-3.46431708	-4.76270771	1.07302666

1	3.10468292	0.93959200	-3.13017344	1	-4.72301722	-4.27310753	2.21922660
6	1.52128279	-2.14860797	-2.73017335	1	-3.02311707	-3.83120799	2.52142644
1	1.88738275	-3.17070794	-2.58597350				

## I-2\_PL

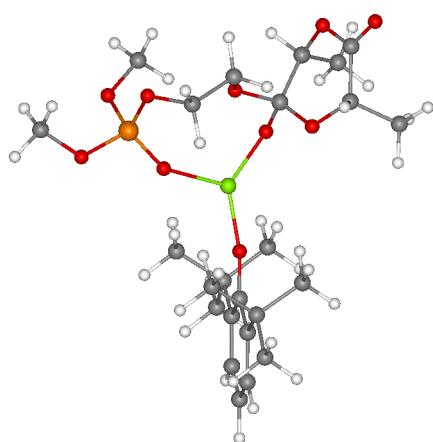


Zero-point vibrational energy	1638080.9 (Joules/Mol)
	391.51073 (Kcal/Mol)
Zero-point correction=	0.623912 (Hartree/Particle)
Thermal correction to Energy=	0.664837
Thermal correction to Enthalpy=	0.665781
Thermal correction to Gibbs Free Energy=	0.547768
Sum of electronic and zero-point Energies=	-2230.720964
Sum of electronic and thermal Energies=	-2230.680039
Sum of electronic and thermal Enthalpies=	-2230.679095
Sum of electronic and thermal Free Energies=	-2230.797108

cartesian							
12	0.03015167	0.08813065	0.30872402	1	0.31965166	-0.37136933	2.52082396
8	-0.53154832	4.41483021	0.79322404	1	1.52375162	0.85953069	1.91722405
8	1.67525172	-0.50216937	-0.29387599	1	-1.34684825	6.14133024	-0.04567598
6	-1.13104832	5.72053051	0.93772405	8	-0.43354833	2.00703073	0.11432403
1	-0.39014834	6.32993031	1.45252407	15	-1.32904840	3.20213079	0.17362402
1	-2.04284835	5.65653038	1.53582406	8	-2.65054822	2.98503065	1.02262402
6	2.98025155	-0.50676930	-0.01267598	8	-3.51894832	0.39583066	0.10442402
6	3.93055177	-0.26626936	-1.04937601	6	-2.83464837	1.87273073	1.94182408
6	5.28635120	-0.25946936	-0.70957595	6	-3.85694838	0.90273070	1.38282406
1	6.03265190	-0.07526934	-1.47497594	1	-3.19824839	2.31093073	2.87512398
6	5.72545147	-0.48356935	0.59242404	1	-1.88114834	1.37763071	2.12492394
6	4.79245186	-0.74026930	1.59102404	1	-3.97954822	0.09283065	2.11242390

1	5.15265179	-0.92676938	2.59772396	1	-4.81754875	1.41693068	1.27062404
6	3.42145157	-0.76586938	1.31932402	8	-1.83554828	3.77253079	-1.20757592
6	3.48625159	-0.02966934	-2.50387597	1	6.78765202	-0.46706936	0.82392406
6	2.40775156	-1.11846936	2.42112398	6	-2.64794827	2.98203063	-2.11437607
6	2.63345170	1.25093067	-2.60547614	1	-3.34274840	2.34563065	-1.56457591
1	1.73815179	1.18673062	-1.98527598	1	-1.98794830	2.37903070	-2.73967600
1	2.32335162	1.42013073	-3.64427614	1	-3.19144821	3.69853067	-2.72817612
1	3.20805168	2.12503052	-2.27947617	8	-6.24664879	-1.88366938	-1.60197592
6	2.68925166	-1.24426937	-3.02187610	8	-4.10284805	-1.43916929	-1.92197597
1	1.80745173	-1.43356931	-2.40847611	6	-5.13544846	-1.77676928	-1.13047600
1	3.31235170	-2.14516926	-3.00757599	6	-4.90524864	-1.99956942	0.36352402
1	2.36765170	-1.07486928	-4.05717564	8	-3.56744838	-1.83126926	0.82562405
6	4.68225193	0.15723065	-3.45397615	6	-2.80334830	-0.87516928	0.10622402
1	5.33915138	-0.71906936	-3.47077608	6	-2.77324843	-1.29756927	-1.37337601
1	5.28555202	1.03523064	-3.19807601	1	-2.33734846	-0.47796932	-1.95377600
1	4.31195164	0.30513066	-4.47467566	8	-1.59694839	-0.79346931	0.65202403
6	3.07845163	-1.31236935	3.79232383	1	-5.55514812	-1.25586927	0.84642404
1	3.60145164	-0.41056934	4.12862396	6	-5.36734867	-3.39146924	0.77692401
1	3.79305148	-2.14066935	3.78182387	1	-6.41274834	-3.53566933	0.49942401
1	2.31475163	-1.55316937	4.54062414	1	-5.26174831	-3.50016928	1.85922408
6	1.71765161	-2.45666933	2.07502389	1	-4.76004791	-4.16096973	0.29312402
1	1.22045171	-2.42356920	1.10332406	6	-1.99244833	-2.57936931	-1.60717595
1	0.97345161	-2.72066927	2.83602381	1	-2.38924837	-3.39326930	-0.99547595
1	2.46195173	-3.25816941	2.03672385	1	-0.93864834	-2.44786930	-1.35227597
6	1.34955168	0.01643066	2.59812403	1	-2.06264830	-2.86096931	-2.66087604
1	1.39515162	0.45683065	3.59942389				

### TS-23\_PL



Zero-point vibrational energy

1635302.2 (Joules/Mol)

390.84660 (Kcal/Mol)

Zero-point correction=

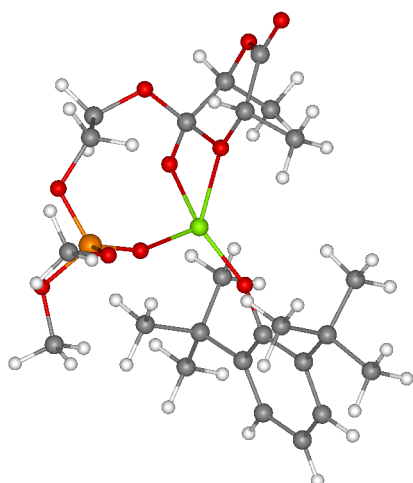
0.622854 (Hartree/Particle)

Thermal correction to Energy=	0.663460
Thermal correction to Enthalpy=	0.664404
Thermal correction to Gibbs Free Energy=	0.547386
Sum of electronic and zero-point Energies=	-2230.713051
Sum of electronic and thermal Energies=	-2230.672444
Sum of electronic and thermal Enthalpies=	-2230.671500
Sum of electronic and thermal Free Energies=	-2230.788518

				cartesian			
12	-0.15403602	0.30497861	-0.49860129	1	1.25136399	0.90477860	2.04599881
8	-0.92023599	4.48237848	0.92329872	1	2.60346389	1.42187858	3.05299878
8	1.54946399	-0.18152142	-0.03280130	1	-1.97023606	6.16457844	0.27729869
6	-1.64513600	5.69677830	1.20839870	8	-0.60823601	2.15157843	0.08619870
1	-0.94193602	6.34517860	1.72809863	15	-1.62033606	3.23737860	0.25349870
1	-2.50313616	5.48617840	1.85089862	8	-2.88543606	2.86427879	1.14459872
6	2.86996388	-0.31912142	0.04369871	8	-2.97833610	0.42727858	-0.07650129
6	3.67596412	-0.21222141	-1.13140130	6	-2.97843599	1.65297854	1.93999863
6	5.06026411	-0.36272138	-1.00350130	6	-3.66723609	0.55597860	1.14869869
1	5.69566441	-0.28682142	-1.87960136	1	-3.55603600	1.92607856	2.82579875
6	5.66236401	-0.61232144	0.22489870	1	-1.97663605	1.34267855	2.24709868
6	4.86746407	-0.71932143	1.36179864	1	-3.62413597	-0.35362142	1.75619864
1	5.35526419	-0.91702139	2.31049871	1	-4.72093582	0.80647856	0.97179872
6	3.47766399	-0.58052140	1.30969870	8	-2.23143601	3.84777880	-1.07150137
6	3.04976392	0.05677859	-2.51180124	1	6.74156427	-0.72452140	0.29579869
6	2.63466406	-0.71072143	2.59189868	6	-3.07773614	3.07927847	-1.95990133
6	2.34836388	1.43207860	-2.52600121	1	-4.00013590	2.80497837	-1.44670129
1	1.66866398	1.57047856	-1.68070138	1	-2.55763602	2.18257856	-2.29870129
1	1.78866386	1.57727861	-3.45850110	1	-3.28963614	3.73827839	-2.80050111
1	3.08726406	2.23677874	-2.44960117	8	-5.56173563	-3.15702152	0.92699873
6	2.07186389	-1.07522142	-2.89290118	8	-4.89823580	-1.81002140	-0.70580125
1	1.29156399	-1.23642147	-2.14710116	6	-4.65213585	-2.59902143	0.35509869
1	2.61446404	-2.02152157	-2.99010110	6	-3.22213602	-2.72092152	0.87129873
1	1.59186399	-0.86342144	-3.85630131	8	-2.27963591	-1.77292144	0.35819870
6	4.10016441	0.10657859	-3.63620114	6	-2.61603594	-0.86902142	-0.69120127
1	4.63726425	-0.84182143	-3.73920131	6	-3.79533601	-1.36892140	-1.53460133
1	4.83506441	0.90407860	-3.48470116	1	-4.19653606	-0.49632144	-2.05260110
1	3.59886384	0.30267859	-4.59110165	8	-1.55143607	-0.61162144	-1.43220139
6	3.49796391	-1.00652146	3.83109879	1	-3.31523609	-2.52632141	1.94669867
1	4.21816397	-0.20752141	4.03709841	6	-2.68083596	-4.14082146	0.71629870
1	4.04716396	-1.94922149	3.73669887	1	-3.35113597	-4.84682131	1.21179867
1	2.84926391	-1.09482145	4.71009874	1	-1.69463611	-4.19522142	1.18279862

6	1.63556397	-1.87892139	2.46209884	1	-2.57853603	-4.42552137	-0.33260131
1	0.97256398	-1.75292146	1.60519862	6	-3.42183614	-2.42952156	-2.55460119
1	1.02446389	-1.96062148	3.37019873	1	-2.96713614	-3.30722141	-2.09150124
1	2.17146397	-2.82572126	2.33309889	1	-2.69883609	-2.01272154	-3.25730133
6	1.88966393	0.60907859	2.87999868	1	-4.31663609	-2.74422121	-3.09830117
1	1.26986396	0.50917858	3.78069878				

### I-3\_PL



Zero-point vibrational energy	1636850.4 (Joules/Mol)
	391.21664 (Kcal/Mol)
Zero-point correction	XXX (Hartree/Particle)
Zero-point correction=	0.623443 (Hartree/Particle)
Thermal correction to Energy=	0.664748
Thermal correction to Enthalpy=	0.665692
Thermal correction to Gibbs Free Energy=	0.547195
Sum of electronic and zero-point Energies=	-2230.728551
Sum of electronic and thermal Energies=	-2230.687246
Sum of electronic and thermal Enthalpies=	-2230.686302
Sum of electronic and thermal Free Energies=	-2230.804799

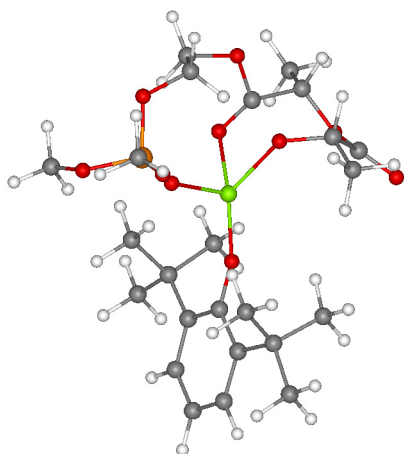
cartesian							
8	-1.18535161	-0.49704006	0.11351198	8	2.33434844	-1.17964005	-0.12448803
6	-2.50895166	-0.40464005	0.00391197	6	2.75974846	-1.20234013	1.32971191
6	-3.31475163	-0.13094005	1.15391195	6	3.01224852	-2.67714000	1.66081190
6	-4.70045185	-0.03814004	0.98951197	8	3.97694826	-3.27234006	0.75761199
1	-5.33305168	0.16795996	1.84651196	6	4.08684826	-2.89684010	-0.52398801
6	-5.30935192	-0.20744005	-0.24888802	6	3.24484825	-1.74234009	-1.07278800
6	-4.51915169	-0.48474005	-1.35938811	8	4.88204813	-3.44774008	-1.25318801
1	-5.01165152	-0.62284005	-2.31598806	1	3.98264837	-0.97913998	-1.35128808
6	-3.12835169	-0.59254003	-1.27118802	1	3.50864840	-2.70654011	2.63301206

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6	-2.69485140	0.05405996	2.55151200	8	2.11224842	3.26365995	-1.71598804
6	-2.29915142	-0.91633999	-2.52738810	6	2.91334820	4.37836027	-2.16268802
6	-1.78305161	1.29865992	2.56971192	1	2.88784838	4.34656000	-3.25058794
1	-1.05265152	1.28845990	1.75761199	1	3.94184828	4.27506018	-1.80978811
1	-1.24185157	1.37805986	3.51991200	1	2.49024820	5.32046032	-1.80668807
1	-2.38445139	2.20625997	2.44401193	8	1.06444836	1.75325990	-0.03718802
6	-1.91835153	-1.21084011	2.97131205	15	1.91564846	2.97016001	-0.16428803
1	-1.14185154	-1.47764003	2.25411201	8	3.34454823	2.90256000	0.51131201
1	-2.60375166	-2.06194019	3.04671192	8	4.02614832	-0.55494004	1.42421198
1	-1.44735157	-1.06694007	3.95101190	6	4.10774851	1.65935993	0.39871198
6	-3.75575161	0.28935996	3.64211202	6	4.00054836	0.83855999	1.68971193
1	-4.44345188	-0.55744004	3.73511195	1	5.12934828	1.97615993	0.18581197
1	-4.34565163	1.19445992	3.46281195	1	3.74304867	1.07205987	-0.44608805
1	-3.25615168	0.41215995	4.60971212	1	4.85354853	1.03915989	2.34221196
6	-3.17615175	-1.11234009	-3.77678800	1	3.08624840	1.10405993	2.22651196
1	-3.74565172	-0.21194005	-4.03058815	8	1.34294844	4.27416039	0.52141201
1	-3.87905169	-1.94444013	-3.66408801	6	-0.05775160	4.61276007	0.35601199
1	-2.53425169	-1.34274006	-4.63468790	1	-0.68635154	3.79235983	0.70361197
6	-1.52105153	-2.23254013	-2.32638812	1	-0.27275157	4.83736038	-0.69118798
1	-0.85895157	-2.17944002	-1.46118808	1	-0.21775156	5.49756002	0.96891201
1	-0.92185152	-2.46304011	-3.21628809	6	2.47374821	-2.17063999	-2.31178808
1	-2.21585178	-3.06394005	-2.16538811	1	1.94294846	-1.31394005	-2.73478794
6	-1.33505154	0.24325997	-2.84948802	1	1.74314845	-2.94573998	-2.06888795
1	-1.89815152	1.15355992	-3.08448815	1	3.16894865	-2.56194019	-3.05638814
1	-0.71585155	-0.00174005	-3.72178817	6	1.74954844	-3.51613998	1.69201195
1	-0.67665160	0.47225994	-2.01018810	1	1.21734846	-3.47943997	0.73711193
12	0.58104843	-0.12514004	0.48641199	1	1.08294845	-3.15514016	2.47731185
1	-6.38965178	-0.13204005	-0.34638801	1	2.00984859	-4.55694008	1.90081191
8	1.76454842	-0.63444000	1.96641195				

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### TS-34\_PL

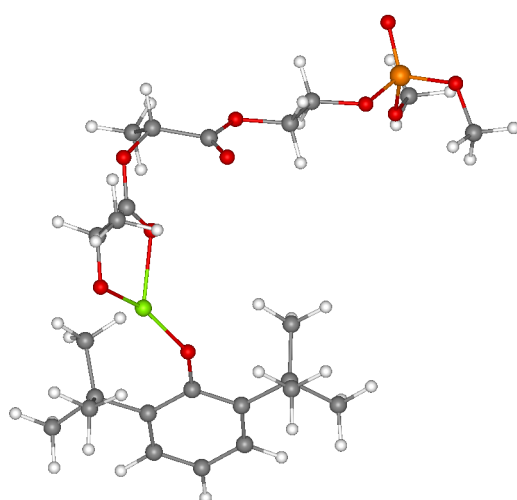


Zero-point vibrational energy	1634251.2 (Joules/Mol)
	390.59540 (Kcal/Mol)
Zero-point correction=	0.622453 (Hartree/Particle)
Thermal correction to Energy=	0.663365
Thermal correction to Enthalpy=	0.664310
Thermal correction to Gibbs Free Energy=	0.547005
Sum of electronic and zero-point Energies=	-2230.725698
Sum of electronic and thermal Energies=	-2230.684786
Sum of electronic and thermal Enthalpies=	-2230.683842
Sum of electronic and thermal Free Energies=	-2230.801147

cartesian									
12	-0.56152666	0.32094792	0.04691336	1	1.31957340	2.01294804	3.40881324		
8	-2.51862669	-3.10005212	-1.54468668	1	1.27187347	1.86434782	1.64261341		
8	1.27987337	0.23234792	-0.04408664	1	-3.07052660	-5.10855246	-1.45698667		
6	-3.39902663	-4.17985201	-1.92608666	8	-1.66152668	1.24844790	1.47081339		
1	-3.31922674	-4.25685215	-3.00908685	6	-2.53332663	1.88524783	0.81191337		
1	-4.42902660	-3.95215201	-1.64218664	8	-2.00382662	1.32854784	-0.93668664		
6	2.54677320	-0.14925209	0.10201336	6	-2.09972668	2.33624792	-1.91468668		
6	3.31467319	-0.52295208	-1.04578662	6	-2.47422671	3.40144801	0.60531336		
6	4.63727331	-0.93505204	-0.85918665	8	-1.32172656	3.82034802	-0.13318664		
1	5.23747349	-1.22555208	-1.71478665	6	-1.25112665	3.52914810	-1.46638668		
6	5.22517347	-0.98255205	0.40011337	8	-1.38472676	-1.53175211	0.07421336		
6	4.47957325	-0.59725207	1.50821340	15	-2.43662667	-2.57455206	-0.05968664		
1	4.95897341	-0.62705207	2.48111320	8	-3.88882661	-2.07565212	0.38071337		
6	3.15107322	-0.17415208	1.39921331	8	-3.85292673	1.52694786	0.87971336		
6	2.72467327	-0.45925209	-2.46638680	6	-4.28612661	-0.71105206	0.05741337		
6	2.38057327	0.25784791	2.66031313	6	-4.13012648	0.18564792	1.28831339		
6	2.29747319	0.98514795	-2.79398680	1	-5.32302666	-0.78285205	-0.27378663		
1	1.57697344	1.36914790	-2.07118678	1	-3.67552662	-0.30955210	-0.75458664		
1	1.85557318	1.03754783	-3.79698682	1	-5.05092669	0.23524792	1.87231338		
1	3.16547322	1.65284789	-2.77798676	1	-3.32282662	-0.18185209	1.92451334		
6	1.53347325	-1.42865217	-2.60408664	8	-2.22532654	-3.88305211	0.80001336		
1	0.75457340	-1.22905207	-1.86698663	1	6.25687313	-1.30645216	0.51531339		
1	1.86407328	-2.46325207	-2.45898676	6	-1.93012667	-3.79985189	2.21511316		
1	1.08977342	-1.35385215	-3.60498667	1	-1.06582665	-3.15505195	2.38071322		
6	3.74217319	-0.87005204	-3.54578686	1	-1.70292664	-4.81695223	2.52921319		
1	4.08397341	-1.90385211	-3.42518663	1	-2.80352664	-3.42775202	2.75491333		
1	4.62017345	-0.21575208	-3.55868673	8	-0.51002663	4.16434765	-2.17458677		
1	3.26817322	-0.79725206	-4.53138685	6	-2.41342664	4.10604763	1.95101333		

6	3.25017333	0.21144792	3.92971325	6	-1.69022655	1.83954787	-3.29188681
1	4.11317348	0.88174796	3.86111331	1	-3.14732671	2.67964792	-1.97238660
1	3.61407328	-0.79755205	4.15171337	1	-3.38032675	3.70084810	0.06881337
1	2.65147328	0.53784794	4.78791332	1	-1.79462671	2.63574791	-4.03278685
6	1.19987345	-0.70195204	2.91641331	1	-2.32892680	0.99954796	-3.57838678
1	0.55737334	-0.80545205	2.04031324	1	-0.64892662	1.51184785	-3.29328680
1	0.58477336	-0.35215211	3.75451326	1	-2.38812661	5.18664789	1.79421341
1	1.57577324	-1.70255208	3.15981317	1	-1.51512671	3.80214810	2.49161315
6	1.89517331	1.71534789	2.52381325	1	-3.29262662	3.85604811	2.55021334
1	2.75437331	2.38904810	2.43681335				

#### I-4\_PL



Zero-point vibrational energy	1633166.1 (Joules/Mol)
	390.33606 (Kcal/Mol)
Zero-point correction=	0.622040 (Hartree/Particle)
Thermal correction to Energy=	0.664669
Thermal correction to Enthalpy=	0.665614
Thermal correction to Gibbs Free Energy=	0.538677
Sum of electronic and zero-point Energies=	-2230.717129
Sum of electronic and thermal Energies=	-2230.674499
Sum of electronic and thermal Enthalpies=	-2230.673555
Sum of electronic and thermal Free Energies=	-2230.800491

cartesian							
12	-3.49188519	2.15444803	-0.57736975	6	0.29411629	4.82924891	0.58003026
8	-3.45548511	0.30874813	-0.67226970	8	-0.94948345	5.25834894	-0.01686999
6	-3.96098518	-0.81945193	-0.16777006	6	-1.88008475	4.35964870	-0.29216987
6	-5.07467985	-0.77965200	0.72543031	6	-3.13578510	4.88324881	-0.98876971
6	-5.56427956	-1.98135138	1.24532902	1	-5.38717985	-4.12725115	1.32462895

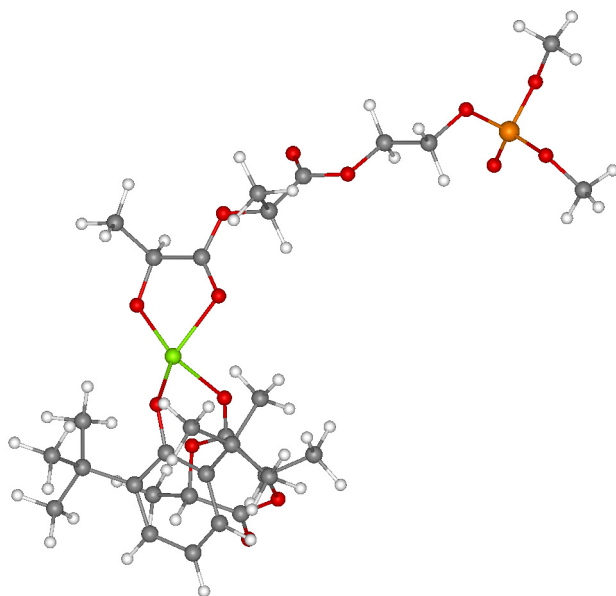


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1	-6.41037989	-1.97475147	1.92522895	8	-1.76178479	3.16094851	0.00903002
6	-4.99307966	-3.20335126	0.90883023	1	0.89031535	5.74714899	0.56633031
6	-3.91498518	-3.23285127	0.02762999	1	-3.50648522	5.69694901	-0.33506984
1	-3.48968506	-4.19795132	-0.22697009	8	0.75101584	3.73654866	-1.54137099
6	-3.37708521	-2.06965137	-0.52996987	8	6.69432020	-0.38645169	-1.07597101
6	-5.73687983	0.56004810	1.08292902	6	5.95202017	-1.31365216	-1.88887107
6	-2.19538450	-2.14245129	-1.51347101	1	6.66852045	-1.73885167	-2.59106898
6	-6.33277988	1.20734811	-0.19147007	1	5.16362047	-0.78875196	-2.43246889
1	-5.64547968	1.22474813	-1.04357076	1	5.51882029	-2.10655141	-1.27387106
1	-6.68187952	2.22834802	-0.00146998	8	6.93902016	1.26064813	0.87783027
1	-7.18827963	0.61644804	-0.53276986	15	6.03692055	0.32504815	0.18722996
6	-4.71688080	1.49404788	1.79372895	8	4.68862057	0.93144822	-0.44646978
1	-3.67668509	1.29794812	1.50262892	8	2.01771498	3.24404860	0.26703021
1	-4.72068071	1.31194806	2.87293100	6	3.86301947	1.77384794	0.37373021
1	-4.96337986	2.55644870	1.65692902	6	2.82661486	2.37604833	-0.55396980
6	-6.91607952	0.40714809	2.05953097	1	4.47132015	2.55534863	0.83753031
1	-6.60997963	-0.05015180	3.00573111	1	3.38431621	1.17504823	1.15442896
1	-7.72527981	-0.19335181	1.63282895	1	3.29831600	2.95694876	-1.34997106
1	-7.32917976	1.39594805	2.29043102	1	2.19661498	1.60684788	-1.00546980
6	-1.74318480	-3.58995104	-1.77127099	8	5.42882013	-0.84775198	1.11042893
1	-2.53988457	-4.20085096	-2.20926905	6	6.25552034	-1.40945232	2.14873099
1	-1.39068437	-4.08485126	-0.85966969	1	6.69662046	-0.61655188	2.75603104
1	-0.90958357	-3.58555126	-2.48236895	1	7.04662037	-2.02675128	1.71412897
6	-0.97668350	-1.38495219	-0.94736969	1	5.59782028	-2.03045130	2.75673103
1	-1.20788395	-0.33305168	-0.77456969	6	-2.75378489	5.51264906	-2.33896899
1	-0.13488387	-1.44485223	-1.64877105	1	-2.06258488	6.35224867	-2.22416902
1	-0.65558386	-1.82745171	0.00253001	1	-3.67298508	5.86624908	-2.81116891
6	-2.60108495	-1.54905200	-2.87846899	1	-2.29778457	4.76424885	-2.99336910
1	-3.43458509	-2.11385131	-3.31046891	6	0.13821614	4.36374855	2.02063107
1	-1.75988483	-1.60175192	-3.58066893	1	-0.37228391	3.40344858	2.08553100
1	-2.90798521	-0.50665176	-2.78516889	1	-0.42668396	5.11244869	2.58193111
8	-4.05528450	3.86974859	-1.11367106	1	1.12541509	4.26804829	2.47643089
6	1.00991511	3.86414862	-0.36816978				

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## I-5\_PLL



Zero-point vibrational energy	2007393.5 (Joules/Mol)
	479.77857 (Kcal/Mol)
Zero-point correction=	0.764576 (Hartree/Particle)
Thermal correction to Energy=	0.818377
Thermal correction to Enthalpy=	0.819321
Thermal correction to Gibbs Free Energy=	0.667725
Sum of electronic and zero-point Energies=	-2764.827696
Sum of electronic and thermal Energies=	-2764.773896
Sum of electronic and thermal Enthalpies=	-2764.772951
Sum of electronic and thermal Free Energies=	-2764.924547

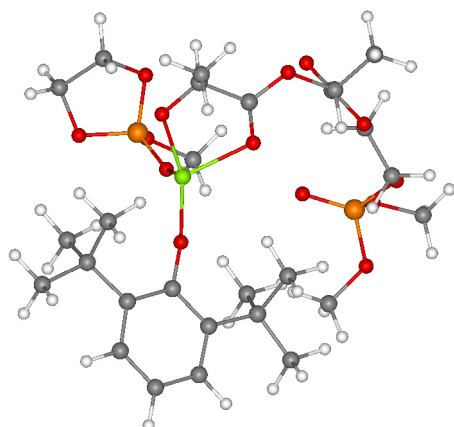
cartesian							
12	1.67067671	-1.24639022	0.80215716	6	1.12657666	3.34460974	-0.19014284
8	2.85827684	-1.32649028	-0.69464284	1	1.24117661	4.26980972	-0.75774288
6	3.66077685	-0.35919032	-1.11964285	1	0.31907672	3.46920967	0.53465712
6	4.90087652	-0.10589030	-0.44484282	1	0.87117666	2.53670979	-0.87414289
6	5.61117649	1.05300975	-0.78384280	6	4.98557663	2.42580962	3.75675726
1	6.54347658	1.28730977	-0.27794284	1	4.29397631	2.61400962	4.58035707
6	5.18347645	1.91010976	-1.79764295	1	5.82087660	3.12200975	3.84245706
6	4.07427645	1.54960978	-2.56354284	1	5.36057663	1.40330970	3.82765722
1	3.81617665	2.17400980	-3.41324282	8	1.34677672	-2.36619020	2.30045724
6	3.31587672	0.40920970	-2.27954292	6	-4.28292322	-1.83269024	1.12015724
6	5.51627636	-1.15659022	0.50425714	6	-2.99932313	-2.22319031	0.39475715
6	2.21887684	-0.06729031	-3.25284290	8	-2.09352326	-2.71079016	1.40155721
6	5.77707672	-2.43879032	-0.31604284	6	-0.82072330	-2.34949017	1.33485711
1	4.84757662	-2.82279038	-0.74234283	6	0.08597672	-2.88039017	2.44495726

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1	6.21017647	-3.21799016	0.32325715	8	-0.38172328	-1.61469030	0.43745714
1	6.47787666	-2.24219036	-1.13434279	1	-2.57622313	-1.32539022	-0.06264284
6	4.62557650	-1.52079022	1.71155715	1	-0.40042329	-2.54619026	3.38295722
1	3.83507657	-2.22409034	1.44395721	8	-4.49992323	-1.96359038	2.29955721
1	4.18377638	-0.63869035	2.18635702	8	-10.30252266	1.37360978	1.09515715
1	5.22057676	-2.02699018	2.48075724	6	-11.39162254	0.67560971	0.46495718
6	6.86987638	-0.68899035	1.06715715	1	-12.26862335	0.86560965	1.08295715
1	6.77557659	0.20550969	1.69485712	1	-11.18272305	-0.39579031	0.43295717
1	7.59977674	-0.47799030	0.27945715	1	-11.56072330	1.05450964	-0.54634285
1	7.29287672	-1.48049033	1.69435716	8	-7.86922359	2.18420982	1.22465718
6	2.14497685	0.81600964	-4.50994301	15	-8.86772251	1.46920967	0.41175717
1	3.09697676	0.84900975	-5.04984283	8	-8.56712341	-0.06989031	0.06025717
1	1.84307671	1.84450972	-4.28114271	8	-5.15252352	-1.30319023	0.23395717
1	1.39567661	0.40550971	-5.19554281	6	-7.25512362	-0.43659028	-0.40384281
6	0.81407672	-0.06829031	-2.62344289	6	-6.41272354	-0.86759031	0.78405714
1	0.74747676	-0.75759029	-1.78304291	1	-6.78212357	0.39170969	-0.93904281
1	0.07147670	-0.38009033	-3.36834288	1	-7.39782333	-1.26379025	-1.10214281
1	0.52927667	0.93160975	-2.27964282	1	-6.25052357	-0.03729030	1.47475719
6	2.56307673	-1.49879026	-3.71784282	1	-6.88672352	-1.69079030	1.32355714
1	3.53287673	-1.51679027	-4.22654295	8	-9.10092258	2.07350969	-1.06394279
1	1.80497670	-1.85999036	-4.42364264	6	-9.07162285	3.50480962	-1.23214281
1	2.60507679	-2.18769026	-2.87204289	1	-8.18372345	3.92750978	-0.75764287
1	5.75407648	2.80320978	-2.04124284	1	-9.97082329	3.95640969	-0.80424285
8	4.15387630	4.99610996	2.85985708	1	-9.04702282	3.68340969	-2.30694294
8	2.74557686	4.15410995	1.35545719	6	0.06387675	-4.41949034	2.44295716
6	3.74777675	4.03840971	2.25215721	1	-0.94012332	-4.82329035	2.60365725
6	4.30097675	2.63090968	2.42495728	1	0.71827668	-4.76089048	3.24815726
8	3.22927690	1.64790976	2.32555723	1	0.46387672	-4.80449009	1.49925721
6	2.39027667	1.74440968	1.30735719	6	-3.21722317	-3.29789019	-0.66314286
6	2.43197680	3.02880979	0.50805718	1	-3.60712314	-4.21259022	-0.20954284
1	3.23697686	2.89990973	-0.23344284	1	-2.26912332	-3.52429032	-1.15614283
8	1.62137675	0.82360971	1.05385709	1	-3.92422318	-2.94389033	-1.41574287
1	4.98957634	2.42680979	1.59465718				

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# I-5\_PLP



Zero-point vibrational energy	1939469.4 (Joules/Mol)
	463.54431 (Kcal/Mol)
Zero-point correction=	0.738705 (Hartree/Particle)
Thermal correction to Energy=	0.791599
Thermal correction to Enthalpy=	0.792544
Thermal correction to Gibbs Free Energy=	0.642759
Sum of electronic and zero-point Energies=	-2991.317977
Sum of electronic and thermal Energies=	-2991.265082
Sum of electronic and thermal Enthalpies=	-2991.264138
Sum of electronic and thermal Free Energies=	-2991.413923

				cartesian			
8	2.20130348	-0.79025316	0.15639110	6	-2.08059669	1.18014681	-3.32890892
6	2.80280352	-1.97205317	0.15799110	1	-2.55339646	0.84734678	-4.25000906
6	2.07160354	-3.14145303	0.54179108	1	-2.76139665	1.81614673	-2.76520896
6	2.73060346	-4.37415314	0.54139107	1	-1.76839674	0.32704681	-2.72930884
1	2.19560337	-5.27295351	0.82999104	1	3.13010335	3.76394701	-3.68920898
6	4.06850338	-4.49465322	0.18049107	1	1.66360331	4.28584671	-4.57530880
6	4.77260303	-3.35475302	-0.19290891	12	1.52190328	0.92304683	-0.05890891
1	5.81530333	-3.46755314	-0.47130889	8	2.21060348	2.69804692	0.27819109
6	4.17950296	-2.08895302	-0.21780892	6	-2.50459647	2.50444698	2.04409099
6	0.58920336	-3.06155300	0.95039111	6	-1.50119674	2.55104685	3.19539094
6	5.00630331	-0.86105323	-0.64170891	8	-0.31409666	3.24184680	2.75909114
6	-0.26049668	-2.52895308	-0.22150892	6	0.42020336	2.62704682	1.83679104
1	0.08870333	-1.55645323	-0.56950891	6	1.64270329	3.38434696	1.32189107
1	-1.31189668	-2.43335319	0.08059110	8	0.12260333	1.50354683	1.41619098
1	-0.21339667	-3.22175312	-1.06940889	1	-1.24009669	1.52874672	3.47629094
6	0.42300335	-2.16455317	2.19379115	1	1.24080324	4.36954689	1.01059103
1	0.79990327	-1.15725327	2.01629114	8	-2.57449651	3.32184696	1.15689099
1	0.97270334	-2.58695316	3.04239106	8	-7.00179672	-0.84895325	-1.83090901

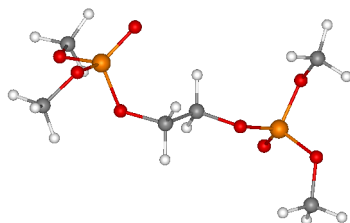
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1	-0.63519669	-2.09505320	2.47829103	6	-8.17509651	-1.41845322	-1.22120893
6	0.00700334	-4.43705320	1.32089102	1	-8.96269703	-1.36015320	-1.97180891
1	0.51780331	-4.88725328	2.17879105	1	-8.45649719	-0.84085321	-0.33820891
1	0.04860333	-5.14495325	0.48599112	1	-7.99979687	-2.46165299	-0.94650888
1	-1.04769671	-4.31875324	1.59639108	8	-4.51309681	-0.24995318	-1.88690901
6	6.45980310	-1.22375321	-0.99600887	15	-5.58319664	-0.90545321	-1.11170888
1	6.52160311	-1.92935312	-1.83140898	8	-5.92829704	-0.30065319	0.33499110
1	6.99340296	-0.31475320	-1.29720891	8	-3.32719660	1.44834673	2.18299103
1	6.99950314	-1.64985323	-0.14350891	6	-4.87399673	-0.10835320	1.29789102
6	5.08590317	0.16094682	0.51059109	6	-4.32059669	1.29814672	1.14999104
1	4.10230303	0.50324678	0.83219105	1	-4.08419657	-0.85325325	1.16799104
1	5.66540337	1.04084682	0.20519109	1	-5.32929659	-0.25435320	2.27919102
1	5.58310318	-0.28815320	1.37749100	1	-3.86309648	1.43824673	0.16979109
6	4.40180302	-0.22105318	-1.90820897	1	-5.10619688	2.04684687	1.28409100
1	4.48250341	-0.90785325	-2.75780892	8	-5.30819702	-2.44485307	-0.73970890
1	4.93440342	0.70244682	-2.16690898	6	-4.59289694	-3.27815318	-1.67630899
1	3.34240341	0.01234680	-1.78870893	1	-3.66729665	-2.79245305	-1.98880899
1	4.55720329	-5.46605349	0.19029109	1	-5.21729660	-3.49075317	-2.54810905
8	0.44680330	1.13164675	-1.76140893	1	-4.37039661	-4.20385313	-1.14680898
15	0.30070332	2.21004677	-2.78610897	6	2.62270331	3.63414693	2.48299098
8	0.18050334	3.71004701	-2.23420906	1	2.17060351	4.21374655	3.29399109
8	1.58260334	2.40634680	-3.72370887	1	3.47890353	4.18514681	2.08689094
6	1.46680331	4.36474657	-2.39070892	1	2.99140334	2.68304682	2.87899113
6	2.04020333	3.77914691	-3.68280888	6	-2.05809665	3.32574701	4.37859106
1	1.27920330	5.43634653	-2.46010900	1	-2.30809665	4.34814644	4.08629084
1	2.07680345	4.11834669	-1.51520896	1	-1.31719673	3.35814691	5.18079090
8	-0.92159665	1.96214676	-3.74190903	1	-2.95709658	2.83234692	4.75549126

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## S1.10. Transesterification of PP

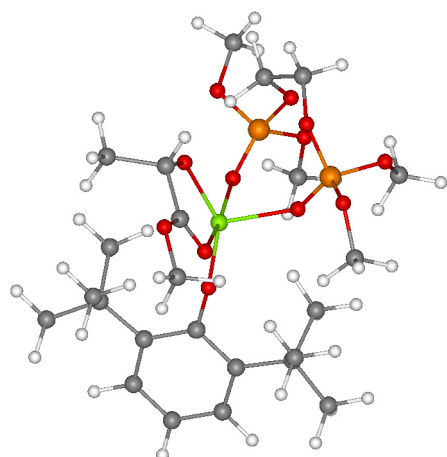
PP



Zero-point vibrational energy	662155.7 (Joules/Mol)
	158.25901 (Kcal/Mol)
Zero-point correction=	0.252202 (Hartree/Particle)
Thermal correction to Energy=	0.273321
Thermal correction to Enthalpy=	0.274265
Thermal correction to Gibbs Free Energy=	0.197927
Sum of electronic and zero-point Energies=	-1522.311875
Sum of electronic and thermal Energies=	-1522.290756
Sum of electronic and thermal Enthalpies=	-1522.289812
Sum of electronic and thermal Free Energies=	-1522.366150

cartesian											
8	-2.23931909	-1.30730009	1.28460002	15	3.11028099	-0.37279999	-0.36570004				
15	-2.87011909	-0.34270000	0.36739996	8	4.19738150	0.62959999	0.24689996				
8	-3.79121900	0.72490001	1.10769999	8	3.13768101	-0.61720002	-1.81729996				
6	-4.51551867	1.72620010	0.37159997	8	3.33588099	-1.68499994	0.50709999				
1	-3.84041905	2.29600000	-0.27230003	1	-4.96001863	2.38569999	1.11660004				
1	-5.29891872	1.25830007	-0.22840002	1	-0.30411887	1.85730004	-0.35800004				
8	-3.85401893	-0.90130001	-0.76230001	1	-0.61371887	0.93699998	1.13250005				
6	-3.41521907	-1.98600006	-1.60169995	1	0.23648113	-1.13279998	0.03799997				
1	-3.06591892	-2.82200003	-0.99180001	6	3.34458113	-1.63849998	1.94540000				
1	-2.62231898	-1.64650011	-2.27300000	6	4.41398144	1.89820004	-0.39650002				
1	-4.28501892	-2.28920007	-2.18359995	1	5.26738119	2.35189986	0.10699997				
8	-1.82561886	0.51059997	-0.52860004	1	3.53478098	2.53740001	-0.27940005				
6	-0.55301887	0.87229997	0.04279997	1	4.63858128	1.75410008	-1.45560002				
6	0.48948115	-0.15080000	-0.37120003	1	3.41308093	-2.67340016	2.27940011				
8	1.74268115	0.30109999	0.17809996	1	2.42268109	-1.18889999	2.32279992				
1	0.55938113	-0.21260001	-1.46070004	1	4.21018124	-1.07360005	2.29820013				

# I-1\_L\_PP

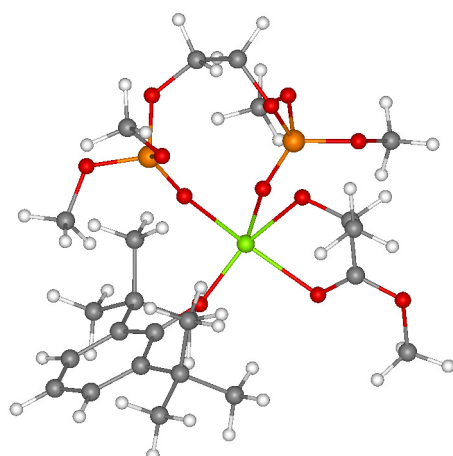


Zero-point vibrational energy	1805576.4 (Joules/Mol)
	431.54311 (Kcal/Mol)
Zero-point correction=	0.687708 (Hartree/Particle)
Thermal correction to Energy=	0.736443
Thermal correction to Enthalpy=	0.737388
Thermal correction to Gibbs Free Energy=	0.603169
Sum of electronic and zero-point Energies=	-2725.458342
Sum of electronic and thermal Energies=	-2725.409606
Sum of electronic and thermal Enthalpies=	-2725.408662
Sum of electronic and thermal Free Energies=	-2725.542881

				cartesian			
12	0.36787078	0.46353373	0.43730843	8	3.91067076	-0.15746626	-2.42979169
8	-1.40112925	0.02943373	-0.10029157	6	3.40087080	-1.47216618	-2.75199175
6	-2.64592934	-0.34476626	-0.32619157	1	2.31117082	-1.48406625	-2.71749163
6	-3.05842924	-0.71616632	-1.65109158	1	3.80237079	-2.19366646	-2.03949165
6	-4.37832928	-1.12416625	-1.86209154	1	3.75257063	-1.69486618	-3.75959158
1	-4.70242929	-1.41056621	-2.85749173	8	0.17597078	2.65273356	0.11660843
6	-5.30982924	-1.17556620	-0.83059156	8	1.46197081	1.17433381	1.89710844
6	-4.91432905	-0.79936630	0.44910842	6	0.75437081	3.25823355	1.01910841
1	-5.65392923	-0.83466631	1.24250841	6	1.53587079	2.52633357	2.10910845
6	-3.61202908	-0.38136625	0.73630846	6	1.03937078	2.94623375	3.50310826
6	-2.07682920	-0.66596627	-2.83529162	1	2.57207084	2.91343355	2.00310850
6	-3.24582934	0.03823373	2.17120838	1	-6.33082914	-1.49736619	-1.02219152
6	-1.54742932	0.76943368	-3.02619171	8	0.75157082	4.58753347	1.10170841
1	-1.06842923	1.13963377	-2.11929154	6	0.00927079	5.28683376	0.08640844
1	-0.82522923	0.80193371	-3.85349154	1	0.06837079	6.34003353	0.35720843
1	-2.37252927	1.44653380	-3.27399158	1	-1.02812910	4.94883347	0.07190844
6	-0.91082925	-1.64636624	-2.60019159	1	0.45917079	5.11953354	-0.89439154

1	-0.38342923	-1.41936624	-1.67319155	8	4.10017061	1.30263376	-0.36409158
1	-1.29142928	-2.67316628	-2.54149175	6	4.86747074	0.39083374	0.44450843
1	-0.19692922	-1.60066628	-3.43419170	6	4.03817081	-0.43936628	1.39620841
6	-2.73052931	-1.07506621	-4.16679144	8	3.58087063	-1.62836623	0.68370843
1	-3.10322928	-2.10496640	-4.14839172	1	3.18257070	0.14343372	1.77780843
1	-3.56002927	-0.41496626	-4.44189167	15	2.19337082	-2.31126642	1.07810843
1	-1.98512936	-1.01346624	-4.96889162	8	2.27567077	-3.57776642	0.11420844
6	-4.44152927	-0.04816628	3.13670826	8	0.96567076	-1.49846625	0.93860847
1	-5.26752949	0.60493368	2.83460832	8	2.32897067	-2.84126639	2.57600832
1	-4.82682943	-1.06916618	3.23210835	1	2.24937081	3.52283359	-3.64809155
1	-4.12012911	0.27203372	4.13460827	1	1.13777077	4.02293348	3.67350841
6	-2.15702939	-0.89086628	2.74450827	1	1.63337088	2.41223359	4.24950838
1	-1.26852918	-0.93136632	2.11560845	1	-0.00602922	2.65463376	3.63570833
1	-1.85422921	-0.56006628	3.74580836	1	5.47937059	-0.24256626	-0.20519157
1	-2.54422927	-1.91296625	2.82990837	1	5.52517080	1.04153371	1.02340841
6	-2.78212929	1.50883377	2.18720841	1	4.67487049	-0.77576631	2.22100830
1	-3.60312939	2.16653371	1.87920845	6	3.37137079	-3.76176643	2.94340825
1	-2.47382927	1.80383372	3.19830823	6	1.05567074	-4.31236649	-0.15729158
1	-1.95072937	1.67793381	1.50250840	1	0.73617077	-4.85476637	0.73600847
8	1.75977087	0.37903374	-1.14519155	1	1.30547071	-5.01646614	-0.94959152
15	3.10967064	0.88293368	-1.52629149	1	0.26857078	-3.63286638	-0.48499158
8	3.11237073	2.25493360	-2.31939173	1	3.26627064	-3.92256641	4.01560831
6	2.09687090	2.49663353	-3.31669164	1	4.35777092	-3.34226632	2.72800827
1	2.22787070	1.81663382	-4.16239166	1	3.25227070	-4.70846653	2.41110826
1	1.10247076	2.38103366	-2.88419175				

### TS-12\_L\_PP



Zero-point vibrational energy

1804775.0 (Joules/Mol)

431.35159 (Kcal/Mol)

Zero-point correction=

0.687403 (Hartree/Particle)

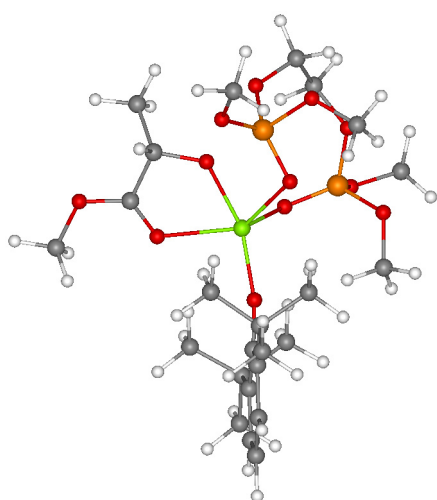


Thermal correction to Energy=	0.735223
Thermal correction to Enthalpy=	0.736168
Thermal correction to Gibbs Free Energy=	0.602895
Sum of electronic and zero-point Energies=	-2725.440521
Sum of electronic and thermal Energies=	-2725.392700
Sum of electronic and thermal Enthalpies=	-2725.391756
Sum of electronic and thermal Free Energies=	-2725.525029

cartesian							
12	0.62231660	0.57682663	-0.00058195	8	4.23031664	-0.79087335	-2.03178215
8	-1.22688329	0.73242664	-0.42718196	6	3.63361669	-0.99977338	-3.31778216
6	-2.48148322	0.34672663	-0.55478191	1	3.36951661	-0.05037338	-3.79058194
6	-2.95438337	-0.20377338	-1.79568195	1	2.73191667	-1.61217332	-3.24398208
6	-4.26728344	-0.68097335	-1.86168194	1	4.38621664	-1.51377344	-3.91908216
1	-4.63638353	-1.11477339	-2.78548217	8	0.82891667	2.75272655	0.18431805
6	-5.13828373	-0.61227334	-0.77858192	8	2.34171653	0.77862662	1.03791809
6	-4.70238352	-0.00527338	0.39561805	6	1.75461662	3.06232667	0.93321806
1	-5.40718365	0.08302662	1.21621811	6	2.64671659	2.00992656	1.58101809
6	-3.40558338	0.49722660	0.53681803	6	2.46111655	2.02762651	3.10681796
6	-2.05678344	-0.26597339	-3.04658198	1	3.68371677	2.30722666	1.36071801
6	-3.00618339	1.22762656	1.83341801	1	-6.15288353	-0.99517339	-0.85968190
6	-1.49108338	1.13152671	-3.37488198	8	2.04041672	4.32622671	1.23181808
1	-0.92408335	1.54482651	-2.54088211	6	1.18021667	5.32562637	0.64821810
1	-0.83548331	1.07732654	-4.25328159	1	1.55241668	6.27922678	1.01901805
1	-2.30718327	1.82542658	-3.60618210	1	0.14741664	5.16482639	0.96081805
6	-0.91138339	-1.27627349	-2.84108210	1	1.23891664	5.28562641	-0.44098195
1	-0.30458334	-1.04087329	-1.96748197	8	3.60231662	-1.21097326	0.31551805
1	-1.31428337	-2.28807354	-2.71278214	6	3.94781661	-2.57207346	0.04541805
1	-0.24888334	-1.28937340	-3.71608210	6	3.20511675	-3.44857335	1.02921808
6	-2.82658339	-0.72647339	-4.29788160	8	1.83431661	-3.67577338	0.63721806
1	-3.20078325	-1.75237346	-4.20918179	1	3.25131655	-3.01527333	2.03231812
1	-3.67318320	-0.06977338	-4.52538204	15	0.60821664	-2.79227352	1.14951801
1	-2.15218329	-0.70407337	-5.16168165	8	-0.56738341	-3.78557348	0.77211809
6	-4.19128370	1.40282655	2.80061793	8	0.47641665	-1.42607331	0.60451806
1	-5.01188374	1.97072649	2.34961796	8	0.72001660	-2.73997355	2.74291801
1	-4.58938360	0.44542664	3.15461802	1	5.60171652	2.63332653	-1.07848191
1	-3.85428357	1.95832658	3.68371797	1	2.71571660	3.00052667	3.53861785
6	-1.93318343	0.43572664	2.60431790	1	3.11511660	1.26482654	3.53621793
1	-1.06328332	0.21172664	1.98731804	1	1.42961669	1.77672672	3.37151790
1	-1.59728336	0.99352664	3.48761797	1	3.71101665	-2.86617351	-0.97828197
1	-2.34028339	-0.52107334	2.95151806	1	5.02541637	-2.69487333	0.20041806

6	-2.49928331	2.64632654	1.50081801	1	3.66291666	-4.44087362	1.04471803
1	-3.30218339	3.23372650	1.04091799	6	0.63631666	-3.94397354	3.52591801
1	-2.18908334	3.16352654	2.41881800	6	-1.91568327	-3.27657342	0.57421809
1	-1.65948343	2.62172651	0.80641806	1	-2.37258339	-3.05557346	1.54061806
8	2.03211665	0.17412663	-1.42518198	1	-2.45868325	-4.07847309	0.07721805
15	3.38831663	-0.08517338	-0.80728191	1	-1.90618324	-2.38167334	-0.04778195
8	4.41131639	1.10862660	-0.48228195	1	0.77101660	-3.63837337	4.56291819
6	5.02941656	1.83672667	-1.55538189	1	1.42151666	-4.65137339	3.24451804
1	5.69471645	1.18762660	-2.12798214	1	-0.34108338	-4.41487360	3.39971805
1	4.27601671	2.27902651	-2.21378207				

## I-2\_L\_PP



Zero-point vibrational energy	1808418.4 (Joules/Mol)
	432.22237 (Kcal/Mol)
Zero-point correction=	0.688790 (Hartree/Particle)
Thermal correction to Energy=	0.736646
Thermal correction to Enthalpy=	0.737590
Thermal correction to Gibbs Free Energy=	0.605468
Sum of electronic and zero-point Energies=	-2725.444065
Sum of electronic and thermal Energies=	-2725.396209
Sum of electronic and thermal Enthalpies=	-2725.395265
Sum of electronic and thermal Free Energies=	-2725.527388

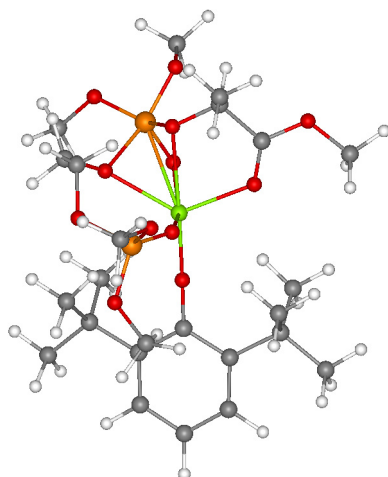
cartesian							
12	0.34140223	0.15011327	0.48016381	8	3.99010229	0.73071325	-1.86023617
8	-1.44929779	-0.10288674	-0.09183620	6	3.49400234	0.18591326	-3.08083630
6	-2.71569777	0.04901326	-0.46133620	1	2.68550229	0.79351330	-3.49953628
6	-3.06579757	0.94911331	-1.52443624	1	3.12040234	-0.83118671	-2.93643618
6	-4.40279770	1.03461325	-1.92433619	1	4.33750200	0.17741327	-3.77713633

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1	-4.68119812	1.70191324	-2.73293614	8	-0.20199779	1.31361318	2.32796383
6	-5.40589809	0.28671324	-1.32003617	8	1.92750216	1.31231320	0.97726381
6	-5.06979799	-0.55868673	-0.26933622	6	0.62450224	2.15781331	2.66356373
1	-5.86699772	-1.12268674	0.20246381	6	1.97620225	2.28361320	1.97796381
6	-3.75639749	-0.69748670	0.19066380	6	3.12760234	2.11081314	2.97006369
6	-2.01339769	1.82251322	-2.23423624	1	2.02890229	3.28971314	1.53806376
6	-3.48299766	-1.61798680	1.39786375	1	-6.43689775	0.36891323	-1.65613627
6	-1.33159781	2.76551318	-1.22193623	8	0.41370225	3.03161311	3.63756371
1	-0.93169785	2.22471333	-0.36293620	6	-0.87029779	2.95181322	4.29386425
1	-0.51129782	3.31981325	-1.69363618	1	-0.85949779	3.74291325	5.04126406
1	-2.05579758	3.49121332	-0.83503622	1	-0.99199784	1.97501326	4.76406384
6	-0.97759783	0.93971330	-2.95693612	1	-1.67149770	3.11051321	3.57076383
1	-0.43049774	0.29641324	-2.27033615	8	4.05610228	0.37361324	0.52346379
1	-1.47949779	0.30791324	-3.69883633	6	4.89310217	-0.74898672	0.28826380
1	-0.24429777	1.56241322	-3.48473620	6	4.22980213	-2.03328681	0.74276376
6	-2.62879777	2.73311329	-3.31293631	8	3.27770233	-2.46608686	-0.25753617
1	-3.09069777	2.16031313	-4.12423611	1	3.73800230	-1.88448679	1.70766377
1	-3.37839770	3.41871333	-2.90363622	15	1.75490224	-2.77148676	0.08296380
1	-1.83549774	3.34461331	-3.75813627	8	1.25020218	-3.07228684	-1.38283622
6	-4.75289774	-2.33278680	1.89516377	8	1.01220226	-1.76468682	0.89446378
1	-5.52169800	-1.63208675	2.23776388	8	1.73140216	-4.14338636	0.90346378
1	-5.19329786	-2.98008680	1.12866378	1	3.81750226	4.38581324	-1.24303627
1	-4.49199772	-2.96908689	2.74866390	1	3.08230233	2.87691331	3.74886370
6	-2.47339773	-2.72508669	1.04366386	1	4.07390213	2.20151329	2.43496370
1	-1.50509775	-2.30488682	0.77746379	1	3.09060240	1.12181318	3.43486381
1	-2.33049774	-3.39778686	1.89866376	1	5.18850231	-0.81568670	-0.76153624
1	-2.84419775	-3.32368684	0.20276380	1	5.79010201	-0.59288675	0.89756376
6	-2.95329762	-0.78358674	2.57976389	1	4.97610188	-2.82858682	0.83516377
1	-3.70839763	-0.05528674	2.89796376	6	2.30860233	-5.33378649	0.33846378
1	-2.72659779	-1.43148673	3.43666387	6	-0.15099776	-3.00168681	-1.75353622
1	-2.05069757	-0.23588674	2.31376386	1	-0.68769777	-3.85318685	-1.33103621
8	1.74660218	0.22021325	-1.04163623	1	-0.16259778	-3.05048680	-2.84093618
15	2.97830224	0.99301332	-0.55293620	1	-0.59749782	-2.06588674	-1.41333616
8	3.12290239	2.61561322	-0.57363623	1	2.21220231	-6.10688639	1.09986377
6	3.92340231	3.33441329	-1.51903617	1	3.36410236	-5.17928648	0.09856380
1	4.97260189	3.03871322	-1.46013618	1	1.76720226	-5.63068676	-0.56283623
1	3.56330228	3.19011331	-2.53973627				

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# TS-23\_L\_PP

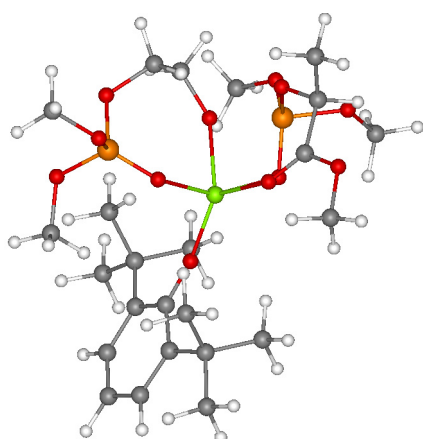


Zero-point vibrational energy	1809287.4 (Joules/Mol)
	432.43006 (Kcal/Mol)
Zero-point correction=	0.689121 (Hartree/Particle)
Thermal correction to Energy=	0.735856
Thermal correction to Enthalpy=	0.736800
Thermal correction to Gibbs Free Energy=	0.606774
Sum of electronic and zero-point Energies=	-2725.431937
Sum of electronic and thermal Energies=	-2725.385202
Sum of electronic and thermal Enthalpies=	-2725.384258
Sum of electronic and thermal Free Energies=	-2725.514284

cartesian											
12	-0.35848781	0.22092885	-0.20759629	8	-3.80738783	1.87062883	2.01450372				
8	1.50071216	0.33802885	-0.07209629	6	-3.49618769	1.44172883	3.33520365				
6	2.80041218	0.45152885	0.17140371	1	-2.43288779	1.20502889	3.43650365				
6	3.26791215	1.17512882	1.31720376	1	-4.08798790	0.56692886	3.62010360				
6	4.64361191	1.21752882	1.56510377	1	-3.74438787	2.27812886	3.99530363				
1	5.01791191	1.75112891	2.43230367	8	-0.97278780	0.94692886	-2.04419637				
6	5.56671190	0.59912884	0.72910368	8	-3.36048770	0.19202885	-0.80699629				
6	5.11011219	-0.06327115	-0.40509629	6	-2.05518794	1.25522888	-2.54229641				
1	5.84511185	-0.51977116	-1.05949628	6	-3.40718770	0.70442885	-2.11279631				
6	3.75031209	-0.14837116	-0.71939629	6	-3.78408766	-0.43777114	-3.06359625				
6	2.30231214	1.92022896	2.25910354	1	-4.13388777	1.51372886	-2.20949626				
6	3.31101227	-0.85677117	-2.01509643	1	6.63031197	0.64642888	0.95010370				
6	1.51021218	2.98502874	1.47290373	8	-2.13888788	2.07562876	-3.57609630				
1	0.95691222	2.55342889	0.63900369	6	-0.89318782	2.60212874	-4.08589649				
1	0.79131216	3.49152875	2.12750363	1	-1.17378783	3.23492885	-4.92549658				
1	2.19451213	3.73902893	1.06800377	1	-0.24478783	1.78782880	-4.41109657				
6	1.34921217	0.93362892	2.96120358	1	-0.39058784	3.18412876	-3.31239629				

1	0.75581223	0.35882887	2.25010371	8	-3.43948770	-0.39307114	1.41860378
1	1.91951227	0.22872886	3.57720375	6	-4.38458824	-1.37587118	1.08300376
1	0.65191215	1.46912885	3.61600375	6	-3.75638771	-2.52947116	0.32510370
6	3.04001212	2.67292881	3.38140368	8	-2.67928767	-3.11447120	1.11630380
1	3.59811234	1.99842882	4.03990364	1	-3.36888766	-2.18317103	-0.63179630
1	3.73321223	3.42512894	2.99040365	15	-1.17548776	-2.95887113	0.66040373
1	2.30531216	3.19792891	4.00210381	8	-0.43298781	-3.15117121	2.04540372
6	4.50611210	-1.37167120	-2.83769631	8	-0.81808782	-1.73767114	-0.11429629
1	5.18101215	-0.56457114	-3.14209628	8	-0.81948781	-4.21717119	-0.25629631
1	5.09081221	-2.12337112	-2.29639626	1	-3.73378778	4.38492870	-0.62359631
1	4.13361216	-1.84787118	-3.75199628	1	-3.85798788	-0.07917115	-4.09389639
6	2.43611217	-2.08517122	-1.70049620	1	-4.75788784	-0.83387113	-2.76459646
1	1.54051208	-1.81497109	-1.14199626	1	-3.04698777	-1.24427116	-3.01989627
1	2.12371230	-2.58317113	-2.62699628	1	-4.80928802	-1.74907112	2.02360368
1	3.00421214	-2.81177115	-1.10749626	1	-5.20828819	-0.98847115	0.47080371
6	2.54881215	0.13092884	-2.92199636	1	-4.48398781	-3.33137107	0.17040370
1	3.20451212	0.95912886	-3.21389627	6	-1.11788785	-5.55057144	0.19710371
1	2.21251225	-0.37267113	-3.83789635	6	1.01141214	-3.01097107	2.09240365
1	1.67951226	0.55132884	-2.41609645	1	1.48541212	-3.83107114	1.54810381
8	-1.62848783	1.24192882	0.82900369	1	1.27471209	-3.05767107	3.14730358
15	-3.15218782	1.11432886	0.68200368	1	1.32011223	-2.05307126	1.67140377
8	-3.70328784	2.40172887	-0.22409630	1	-0.73818779	-6.22217131	-0.57169628
6	-3.66338778	3.74402881	0.26090372	1	-2.19668794	-5.68317127	0.30850372
1	-4.50348806	3.94352889	0.92920369	1	-0.62078786	-5.75777149	1.14840376
1	-2.72608781	3.94972873	0.78470373				

### I-3\_L\_PP



Zero-point vibrational energy

1805168.3 (Joules/Mol)

431.44557 (Kcal/Mol)

Zero-point correction=

0.687552 (Hartree/Particle)

Thermal correction to Energy=

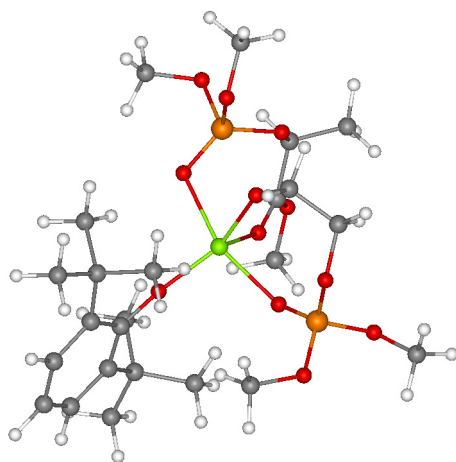
0.735150

Thermal correction to Enthalpy=	0.736094
Thermal correction to Gibbs Free Energy=	0.604724
Sum of electronic and zero-point Energies=	-2725.440129
Sum of electronic and thermal Energies=	-2725.392532
Sum of electronic and thermal Enthalpies=	-2725.391588
Sum of electronic and thermal Free Energies=	-2725.522958

cartesian											
12	-0.57742542	0.12980369	-0.12309286	8	-3.41372538	2.28010368	1.83130717				
8	1.24757457	0.56770366	-0.31139287	6	-2.53082538	2.55930376	2.92530727				
6	2.55947447	0.71650368	-0.31089285	1	-1.48792553	2.37780356	2.66660714				
6	3.23017454	1.25210369	0.83990717	1	-2.81012559	1.94940376	3.78850722				
6	4.62697458	1.31330371	0.83450711	1	-2.67122555	3.61430359	3.17340708				
1	5.15267467	1.70180368	1.70070720	8	-1.87582541	-0.51099634	-1.76739287				
6	5.38247442	0.90130365	-0.25849286	8	-3.82422543	0.18370366	0.03850714				
6	4.72507429	0.44750369	-1.39759278	6	-3.03102541	-0.41719633	-2.15769291				
1	5.32687473	0.16600367	-2.25559282	6	-4.23822546	-0.04369632	-1.29659283				
6	3.33177447	0.35490367	-1.46579278	6	-5.28352547	-1.15499628	-1.28419280				
6	2.44627452	1.79510367	2.05040717	1	-4.66702557	0.86580366	-1.72709286				
6	2.65797448	-0.10659632	-2.77209282	1	6.46817446	0.95800364	-0.23279285				
6	1.48957467	2.91640377	1.59530711	8	-3.37892556	-0.63149631	-3.42159271				
1	0.76867455	2.57320356	0.85240710	6	-2.30532551	-0.95219630	-4.33249331				
1	0.94017464	3.31930375	2.45640707	1	-2.78232551	-1.08219635	-5.30209303				
1	2.06047463	3.74040365	1.15310717	1	-1.80752540	-1.87049627	-4.01779318				
6	1.66507459	0.66980368	2.75540709	1	-1.58342552	-0.13529631	-4.36099291				
1	0.96677452	0.17560366	2.07920718	8	-1.96702552	0.29710367	1.47230721				
1	2.35067463	-0.09029632	3.14660716	6	-2.57282543	-0.48689634	2.47970724				
1	1.09177446	1.06780362	3.60230708	6	-2.58882546	-1.97919631	2.21370721				
6	3.36847448	2.41380358	3.11600709	8	-1.28952539	-2.58709621	2.49020720				
1	4.06087446	1.68320370	3.54860711	1	-2.90322542	-2.19269633	1.18980718				
1	3.95337439	3.24950361	2.71790719	15	-0.30302542	-2.87969637	1.28490722				
1	2.75667453	2.80520368	3.93700719	8	1.06767464	-3.02969623	2.05950713				
6	3.67167449	-0.32449633	-3.90939283	8	-0.34482542	-1.89189637	0.17530714				
1	4.23257446	0.58630365	-4.14419317	8	-0.67622542	-4.31299639	0.68840718				
1	4.38807440	-1.12149632	-3.68229294	1	-4.45772552	4.27400351	-1.26159286				
1	3.13527441	-0.62209630	-4.81789303	1	-5.64662552	-1.35089636	-2.29489279				
6	1.93567443	-1.45169628	-2.56289291	1	-6.12272549	-0.83789635	-0.66139281				
1	1.19357467	-1.40129638	-1.76639283	1	-4.87092543	-2.07929635	-0.87059283				
1	1.43097448	-1.76639628	-3.48599291	1	-2.04922533	-0.32179633	3.43090725				
1	2.65957451	-2.23259640	-2.30089283	1	-3.61692548	-0.17969632	2.61890721				
6	1.66887450	0.96840370	-3.26829290	1	-3.27352548	-2.46929622	2.91010714				

1	2.19917440	1.90200365	-3.48609281	6	-0.69022542	-5.47269630	1.54250717
1	1.18167448	0.63710368	-4.19499302	6	2.32067442	-2.87769628	1.33630717
1	0.90107459	1.18830371	-2.52619290	1	2.43387461	-3.68499637	0.60900712
8	-1.62772536	1.85010362	-0.24229285	1	3.10037446	-2.94269633	2.09270716
15	-2.94932556	1.53750372	0.46130714	1	2.35667443	-1.90749633	0.84010708
8	-4.00302553	2.47680378	-0.43429288	1	-0.96532542	-6.31249619	0.90590715
6	-3.70642543	3.85910368	-0.58469284	1	-1.42842531	-5.35289621	2.33960724
1	-3.77262545	4.37980366	0.37770715	1	0.29857457	-5.64229631	1.97530723
1	-2.70922542	4.00260353	-1.01279283				

### TS-34\_L\_PP



Zero-point vibrational energy	1808585.4 (Joules/Mol)
	432.26228 (Kcal/Mol)
Zero-point correction=	0.688854 (Hartree/Particle)
Thermal correction to Energy=	0.736437
Thermal correction to Enthalpy=	0.737381
Thermal correction to Gibbs Free Energy=	0.607186
Sum of electronic and zero-point Energies=	-2725.439618
Sum of electronic and thermal Energies=	-2725.392034
Sum of electronic and thermal Enthalpies=	-2725.391090
Sum of electronic and thermal Free Energies=	-2725.521285

cartesian							
12	0.47402164	0.07619025	0.00941206	8	3.29002166	-1.74690974	2.01311207
8	-1.30277836	-0.54150975	-0.20968795	6	4.58232164	-2.22970963	2.42051196
6	-2.59367824	-0.81750977	-0.18918794	1	5.37522173	-1.58140981	2.03911209
6	-3.20347834	-1.38490975	0.98171210	1	4.74852180	-3.25290966	2.07901192
6	-4.58997822	-1.56490982	0.99471211	1	4.57232141	-2.19600964	3.51021194
1	-5.07137823	-1.97240984	1.87771213	8	1.74202168	0.51119024	-1.72988796
6	-5.39067841	-1.25010979	-0.09848794	8	3.84102154	-0.31190974	-0.07748793

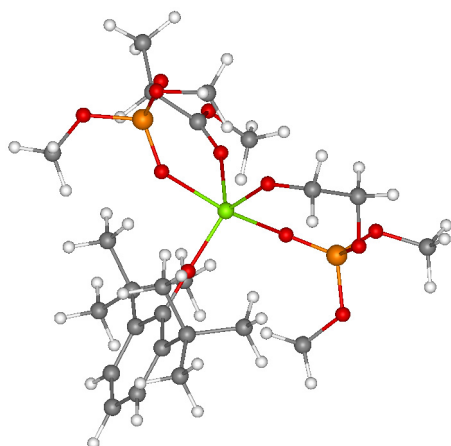
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6	-4.78577852	-0.78040975	-1.25968790	6	2.84892154	0.34359026	-2.20928812
1	-5.41747856	-0.57960975	-2.11898804	6	4.09212160	-0.15790977	-1.47028792
6	-3.40647840	-0.57040977	-1.34758794	6	5.26842165	0.80039024	-1.61598790
6	-2.36577845	-1.84230971	2.19181204	1	4.34872150	-1.12800980	-1.91298795
6	-2.79007840	-0.10380976	-2.68028808	1	-6.46747828	-1.39650977	-0.05578794
6	-1.32717836	-2.89080954	1.74351203	8	3.11882162	0.56239027	-3.49328804
1	-0.65597838	-2.50510955	0.97661209	6	2.00532150	0.99909025	-4.30578756
1	-0.72047836	-3.21440959	2.59911203	1	2.41352177	1.11969030	-5.30738783
1	-1.83637834	-3.77280974	1.33841205	1	1.61422169	1.94399023	-3.92658806
6	-1.66717839	-0.65200979	2.87551188	1	1.21662164	0.24629024	-4.29348803
1	-1.01687837	-0.10970975	2.18871188	8	1.77232170	0.22499025	1.44401205
1	-2.41157842	0.04899025	3.27051187	6	2.11892176	0.91979021	2.58161187
1	-1.05117834	-0.99730980	3.71491194	6	2.10892153	2.43069029	2.41441202
6	-3.22477841	-2.51570964	3.27811193	8	0.75102162	2.97189045	2.31091189
1	-3.96557856	-1.83410978	3.71111202	1	2.68582153	2.72399044	1.53171206
1	-3.74977827	-3.39950967	2.90041208	15	0.08842164	3.26229024	0.89581209
1	-2.57397842	-2.84770966	4.09541225	8	-1.34837830	3.81209040	1.27231205
6	-3.82687855	-0.04190975	-3.81658792	8	0.12012164	2.13219023	-0.06808794
1	-4.30157852	-1.01220977	-3.99788785	8	0.81512165	4.53249025	0.27001208
1	-4.61387825	0.69569021	-3.62558794	1	3.94652176	-4.60081005	-1.00788796
1	-3.32537842	0.25689024	-4.74478769	1	5.52542162	0.93429023	-2.66778803
6	-2.20197845	1.31279027	-2.54118800	1	6.13002157	0.38509023	-1.08918786
1	-1.44327831	1.36849022	-1.76188791	1	5.02762175	1.77279019	-1.17938793
1	-1.75047827	1.63729024	-3.48858809	1	1.46462166	0.67069024	3.43571186
1	-2.99377847	2.02879024	-2.29108810	1	3.14712167	0.66829026	2.90121198
6	-1.70507836	-1.10020971	-3.13858795	1	2.52732158	2.92199039	3.29761195
1	-2.14507842	-2.08880973	-3.31108809	6	0.80462164	5.79749012	0.95781207
1	-1.25827837	-0.76510978	-4.08458757	6	-2.41547847	2.89459038	1.62671208
1	-0.91647840	-1.21110976	-2.39378810	1	-3.33447838	3.47609043	1.57271206
8	1.54832160	-1.73920977	-0.07208794	1	-2.25787830	2.53049040	2.64281201
15	2.93332171	-1.53810978	0.47121206	1	-2.45607829	2.06219029	0.92241210
8	3.83122158	-2.73170972	-0.21558794	1	1.44572163	6.46079016	0.37791207
6	3.22722173	-4.01490974	-0.43328795	1	1.20132160	5.69149017	1.97101212
1	3.02622175	-4.52020979	0.51761210	1	-0.21127835	6.19588995	0.99351209
1	2.29222155	-3.91160941	-0.98758793				

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# I-4\_L\_PP



Zero-point vibrational energy	1804531.9 (Joules/Mol)
	431.29349 (Kcal/Mol)
Zero-point correction=	0.687310 (Hartree/Particle)
Thermal correction to Energy=	0.736113
Thermal correction to Enthalpy=	0.737057
Thermal correction to Gibbs Free Energy=	0.601785
Sum of electronic and zero-point Energies=	-2725.452142
Sum of electronic and thermal Energies=	-2725.403339
Sum of electronic and thermal Enthalpies=	-2725.402395
Sum of electronic and thermal Free Energies=	-2725.537668

cartesian											
12	-0.38796747	-0.72640973	0.54118788	8	-4.01126766	-0.06290971	2.70028782				
8	0.65093255	0.79829031	0.02078790	6	-3.39076734	-1.18350971	3.39798784				
6	1.40003252	1.85789025	-0.20511210	1	-2.35816741	-1.33740962	3.06038785				
6	2.23993254	2.40469027	0.82638788	1	-3.99876738	-2.07030964	3.20798779				
6	3.07333255	3.48229027	0.51288790	1	-3.42436743	-0.92510974	4.45608807				
1	3.72493267	3.89609027	1.27548790	8	-1.87836754	-1.46190965	-0.93021208				
6	3.10073256	4.06059027	-0.75241208	8	-4.24816751	-0.62060970	0.28228790				
6	2.24873257	3.56549025	-1.73391211	6	-2.89836740	-1.34080970	-1.58281219				
1	2.26033258	4.04269028	-2.70851207	6	-4.10356760	-0.50570971	-1.14301217				
6	1.39043248	2.48789024	-1.49781215	6	-5.42566776	-0.90010971	-1.77581215				
6	2.21833253	1.85359037	2.26518774	1	-3.85996747	0.53089029	-1.40981221				
6	0.44243255	2.00979018	-2.61311221	1	3.76353264	4.89619064	-0.96451205				
6	0.80223250	1.99449027	2.85988784	8	-3.06526732	-1.89360964	-2.77691221				
1	0.04893254	1.50049031	2.24638796	6	-1.93456745	-2.64400983	-3.28341222				
1	0.76393259	1.56149030	3.86728787	1	-2.24276733	-2.98920989	-4.26831198				
1	0.53263259	3.05439019	2.93768787	1	-1.72206748	-3.48400974	-2.62131214				
6	2.67453265	0.38279027	2.30448794	1	-1.05716741	-2.00090981	-3.34591222				

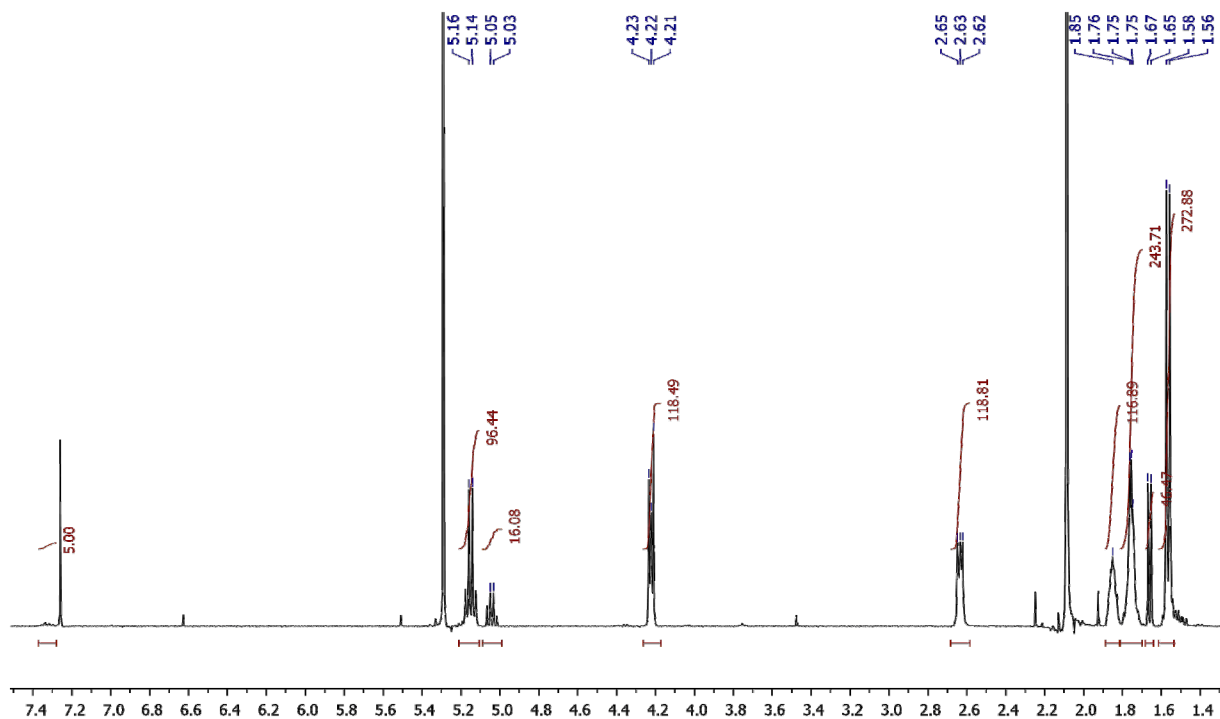
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1	2.02433252	-0.26020971	1.71198785	8	-0.55206746	-1.83610964	2.08548784
1	3.69533253	0.28689027	1.91738784	6	0.09333253	-2.75250983	2.87188792
1	2.66963267	0.00529030	3.33418775	6	0.74723256	-3.90190983	2.11448789
6	3.16533256	2.62369013	3.20368791	8	1.95353258	-3.46450973	1.40668786
1	4.21393251	2.54339027	2.89658785	1	0.04343253	-4.34320974	1.40078783
1	2.90723252	3.68579030	3.27358794	15	1.89873254	-3.03970981	-0.11501210
1	3.08913255	2.20309019	4.21308804	8	3.39353251	-2.55710983	-0.33981210
6	0.55203259	2.86239028	-3.88961220	8	0.83893251	-2.08250976	-0.52821207
1	0.31283250	3.91569018	-3.70821214	8	1.72843254	-4.38480949	-0.97051209
1	1.54893255	2.80939031	-4.34031200	1	-4.24776745	3.79259038	0.98168790
1	-0.16076747	2.48919034	-4.63471174	1	-5.37286758	-0.80860972	-2.86171222
6	0.77123249	0.56139028	-3.02401209	1	-6.20836782	-0.23820971	-1.40001214
1	0.70463252	-0.12720971	-2.18131208	1	-5.68486738	-1.93020964	-1.52121210
1	0.08603254	0.22599031	-3.81541204	1	0.87803245	-2.29950976	3.50768781
1	1.78863251	0.50719029	-3.42901206	1	-0.60706747	-3.25490975	3.57468796
6	-1.02146745	2.11659026	-2.13811207	1	1.10273254	-4.67660952	2.80018783
1	-1.28306746	3.16509032	-1.95491219	6	2.68163252	-5.45170975	-0.82371211
1	-1.70306754	1.73349035	-2.91111207	6	3.67973256	-1.34310961	-1.08001220
1	-1.17756748	1.56379032	-1.21041214	1	3.59763265	-1.53980970	-2.15111208
8	-2.03396749	0.48629028	1.09228790	1	4.70493221	-1.07930970	-0.82451212
15	-3.50476742	0.39079028	1.27998781	1	2.99973273	-0.54220968	-0.78981209
8	-4.26746750	1.75809038	1.01208782	1	2.35123253	-6.24880934	-1.48931217
6	-3.68266749	3.00029016	1.47058785	1	2.69943261	-5.81480932	0.20728791
1	-3.79136729	3.07969022	2.55438781	1	3.67973256	-5.11460972	-1.11431217
1	-2.63076735	3.05269027	1.18588781				

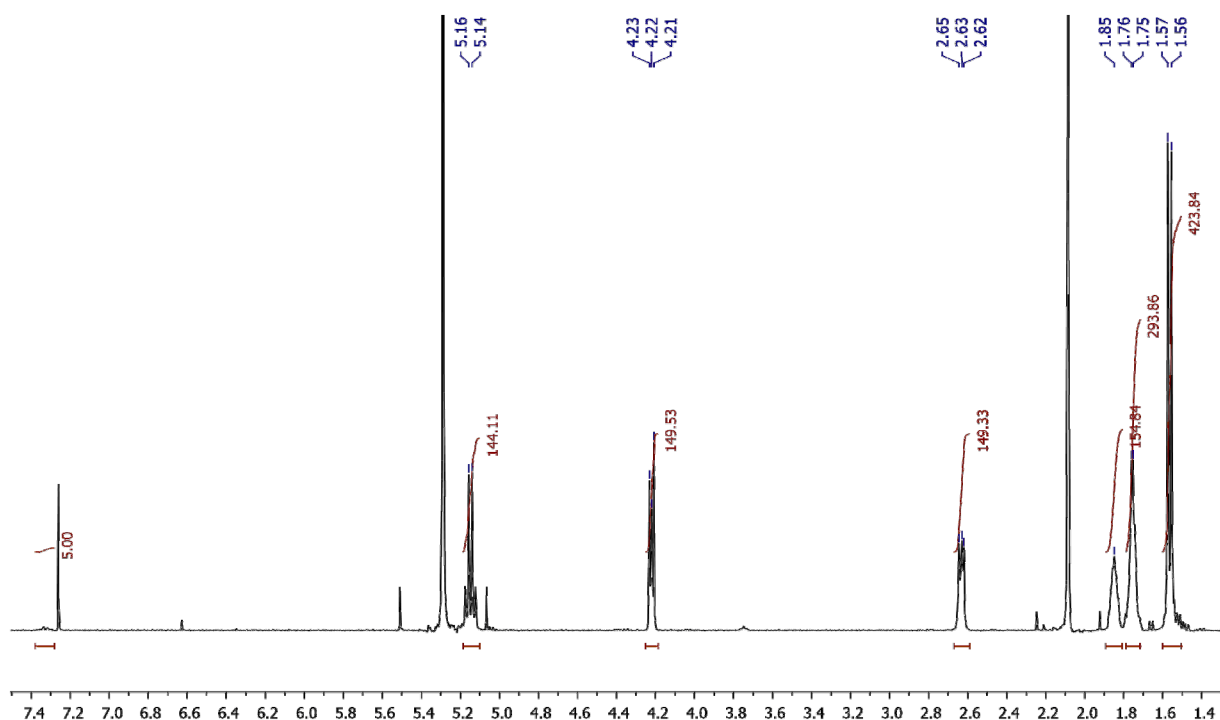
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## S2. Polymerization experiments

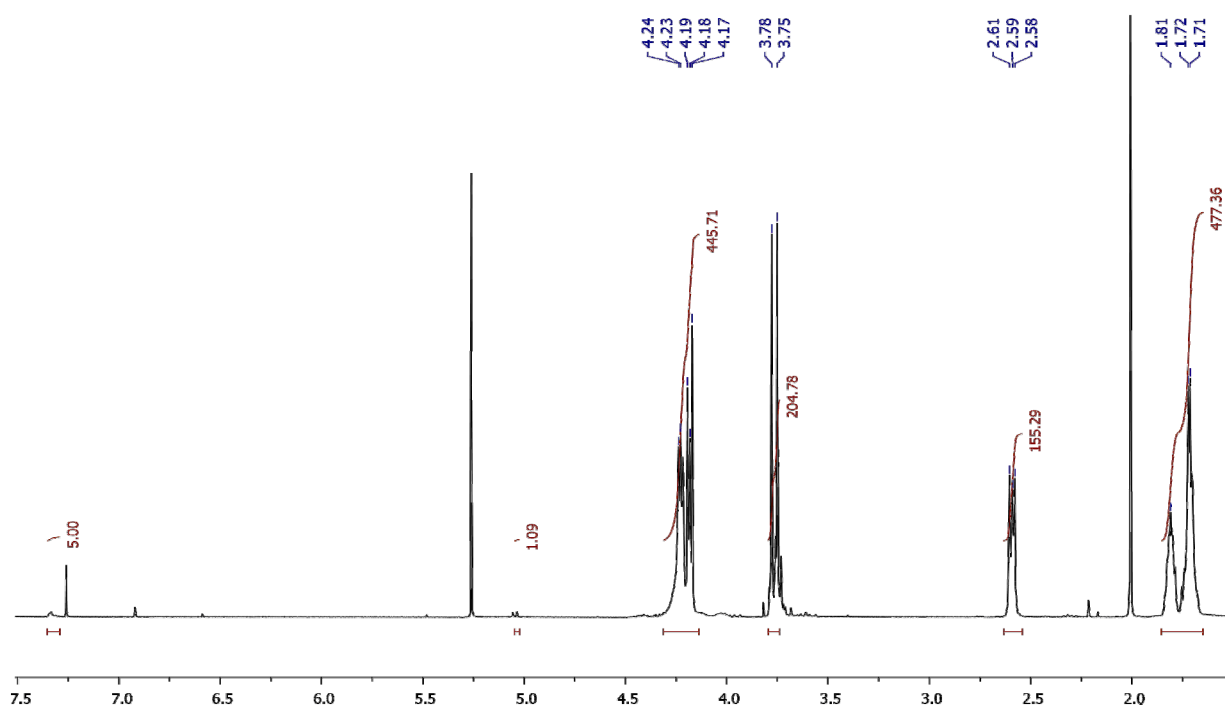
The common reaction protocol of the polymerization experiments was presented in the section 4.3 of the manuscript. NMR spectra of the reaction mixtures and separated polymer samples are given below.



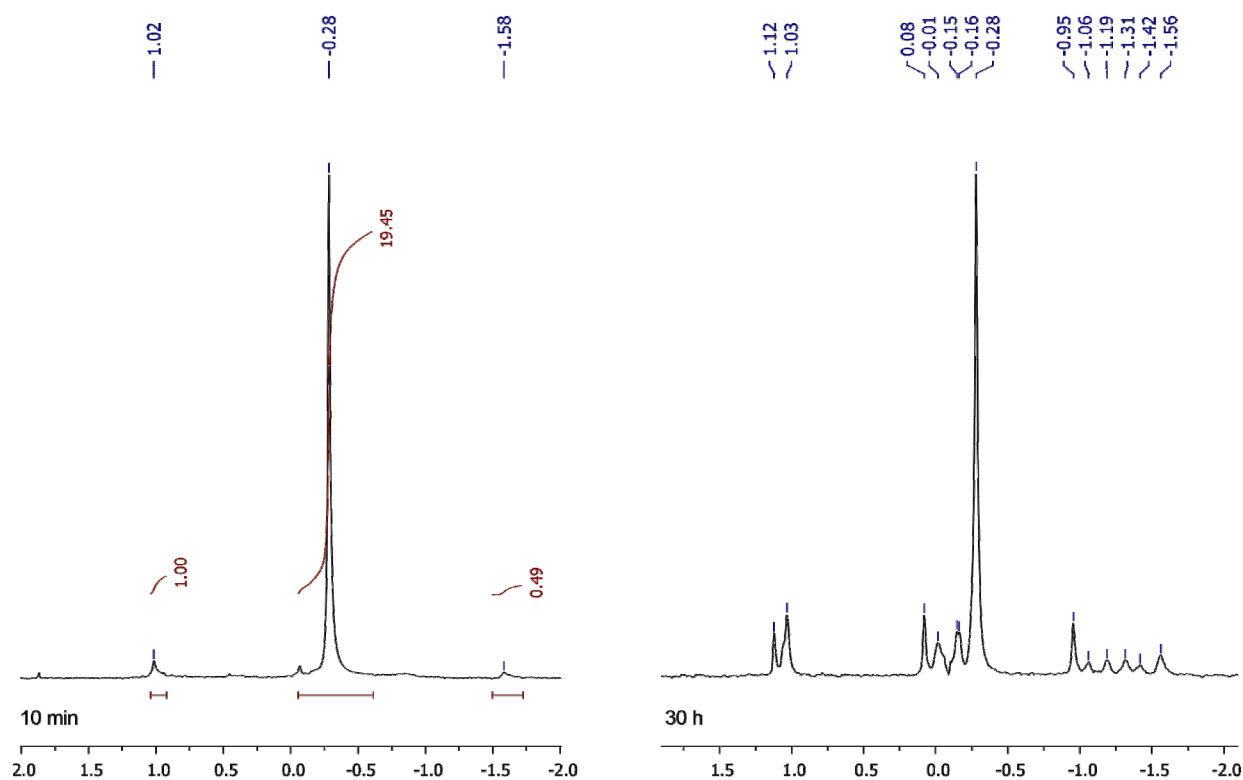
**Figure S1.** <sup>1</sup>H NMR spectrum of the probe taken from  $\epsilon$ -CL/*L*-LA reaction mixture after 10 min (Table 3, rin 1a).



**Figure S2.** <sup>1</sup>H NMR spectrum of the probe taken from  $\epsilon$ -CL/*L*-LA reaction mixture after 30 h (Table 3, rin 1b).



**Figure S3.**  $^1\text{H}$  NMR spectrum of the probe taken from  $\epsilon\text{-CL/MeOEP}$  reaction mixture after 10 min (Table 3, rin 2a).



**Figure S4.**  $^{31}\text{P}$   $\{^1\text{H}\}$  NMR spectra of the probes taken from  $\epsilon\text{-CL/L-LA}$  reaction mixture after 10 min and 30 h (Table 3, rins 1a and 1b, respectively).