

## Supporting information for:

### Evaluation and understanding the performances of various derivatives of carbonyl-stabilized Phosphonium ylides in CO<sub>2</sub> transformation to cyclic carbonates

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Table 1(S): degree of TOF control ( $X_{TOF}$ ) of the reaction for all functional groups

Mechanism A

M062X/6-31G(d,p)						MPW1PW91/6-311++G(d,p)			
Substituent	Step	Intermediate	$X_{TOF,j}$	Transition state	$X_{TOF,Ti}$	Intermediate	$X_{TOF,j}$	Transition state	$X_{TOF,Ti}$
Me	1	In0A	0.00	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	1.00	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
CF <sub>3</sub>	1	In0A	0.70	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.30	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-		In2A	0.00	-	
OMe	1	In0A	0.00	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	1.00	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
Br	1	In0A	0.06	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.94	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
Cl	1	In0A	0.04	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.96	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
CO <sub>2</sub> Me	1	In0A	0.83	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.17	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
CHO	1	In0A	0.97	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.03	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
CN	1	In0A	0.99	TS1	0.00	In0A	0.00	TS1	0.00
	2	In1A	0.01	TS2	1.00	In1A	1.00	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00
NMe <sub>2</sub>	1	In0A	0.00	TS1	0.00	In0A	0.01	TS1	0.00
	2	In1A	1.00	TS2	1.00	In1A	0.99	TS2	1.00
	3	In2A	0.00	-	0.00	In2A	0.00	-	0.00



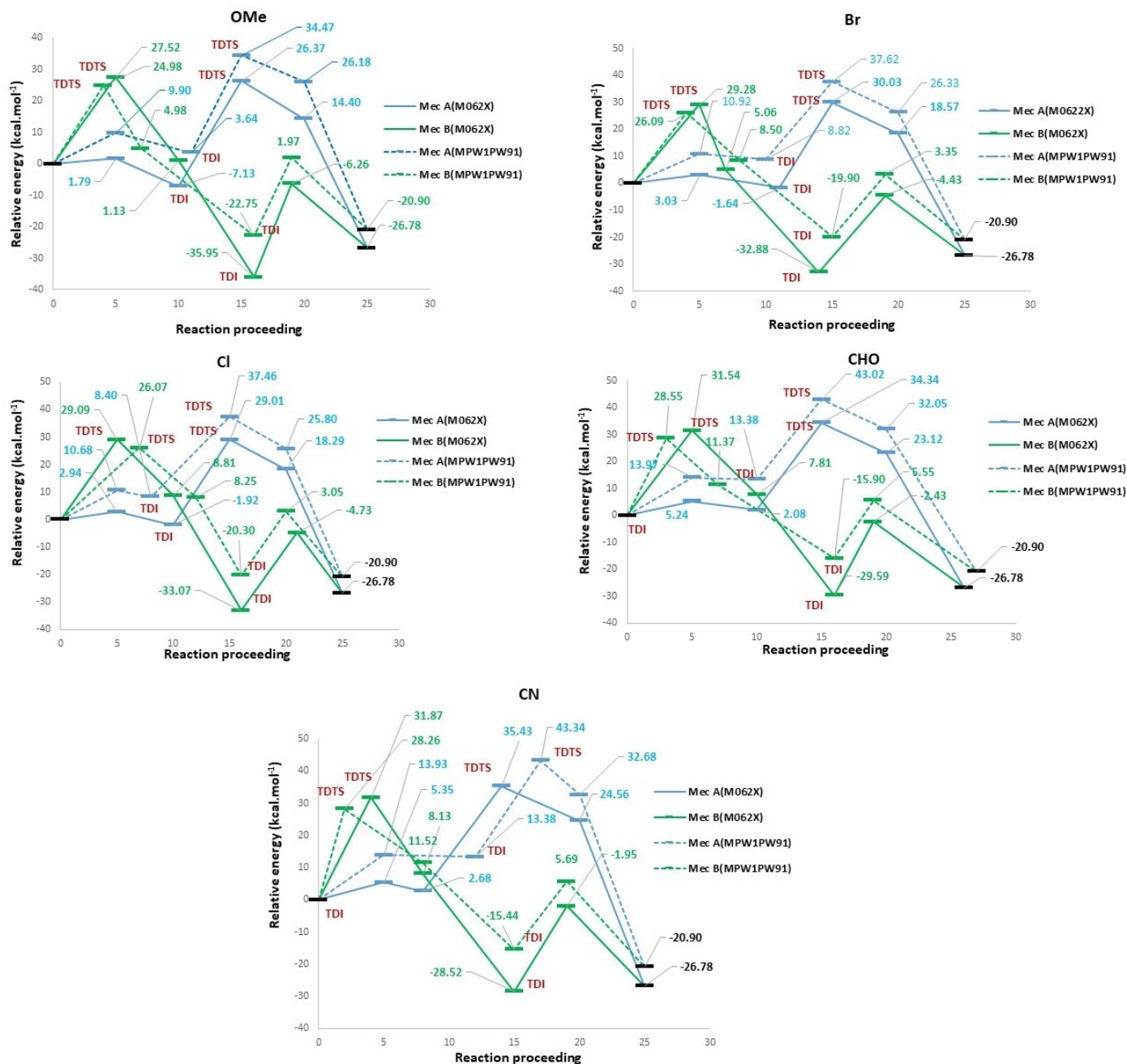


Figure 1(s) PED diagrams for the other substituted organocatalysts

Table 2(S). ESP quantities at nuclear positions (in a.u), electron densities ( $\rho$ ) and their Laplacian ( $\nabla^2\rho$ ) for developing bond at the TSs (in a.u) and the obtained  $\Delta E^\ddagger$  values (in kcal.mol<sup>-1</sup>) in two studied levels in kcal.mol<sup>-1</sup> for the first strategy

G		$V_{n-D}$	$V_{n-A}$	$V_{n-D}$	$V_{n-A}$	$\Delta V_{n-D}$	$\Delta V_{n-A}$	$\rho$	$\nabla^2\rho$	$\Delta\Delta V_n$	$\Delta E^\ddagger$ M062X	$\Delta E^\ddagger$ mpw1pw91
Step 1 Mechanism A	Me	-22.4233	-14.6273	-22.4434		0.0202	-0.0872	0.0632	0.1432	0.1074	1.75	9.47
	CF <sub>3</sub>	-22.3932	-14.6239	-22.4183		0.0251	-0.0839	0.0797	0.1485	0.1089	4.08	12.46
	OMe	-22.4195	-14.6260	-22.4395		0.0200	-0.0860	0.0639	0.1441	0.1060	1.79	9.89
	Br	-22.4036	-14.6235	-22.4259		0.0223	-0.0835	0.0721	0.1475	0.1058	3.03	10.92
	Cl	-22.4046	-14.6240	-22.4268	-14.5400	0.0222	-0.0840	0.0720	0.1472	0.1062	2.94	10.68
	CO <sub>2</sub> Me	-22.3939	-14.6270	-22.4178		0.0238	-0.0870	0.0817	0.1483	0.1108	4.44	12.93
	CHO	-22.3860	-14.6241	-22.4094		0.0236	-0.0841	0.0850	0.1480	0.1076	5.24	13.97
	CN	-22.3778	-14.6203	-22.4047		0.0269	-0.0803	0.0877	0.1470	0.1072	5.34	13.93
NMe <sub>2</sub>	-22.4291	-14.6271	-22.4443		0.0152	-0.0871	0.0597	0.1404	0.1023	1.13	9.01	
Step 1 Mechanism B	Me	-22.3717	-14.7599	-22.4434		0.0718	-0.0769	0.0935	0.1385	0.1487	27.14	24.64
	CF <sub>3</sub>	-22.3553	-14.7510	-22.4183		0.0714	-0.0643	0.0971	0.1351	0.1357	30.48	27.27
	OMe	-22.3681	-14.7581	-22.4395		0.0714	-0.0751	0.0938	0.1384	0.1465	27.52	24.98
	Br	-22.3553	-14.7510	-22.4259		0.0706	-0.0680	0.0959	0.1364	0.1386	29.28	26.09
	Cl	-22.3561	-14.7513	-22.4268	-14.6830	0.0707	-0.0684	0.0957	0.1364	0.1391	29.09	26.07
	CO <sub>2</sub> Me	-22.3469	-14.7487	-22.4178		0.0709	-0.0657	0.0973	0.1354	0.1366	30.62	27.21
	CHO	-22.3419	-14.7454	-22.4094		0.0676	-0.0625	0.0982	0.1338	0.1300	31.54	28.55
	CN	-22.3334	-14.7405	-22.4047		0.0713	-0.0575	0.0989	0.1332	0.1288	31.87	28.26
NMe <sub>2</sub>	-22.3787	-14.7624	-22.4443		0.0657	-0.0795	0.0923	0.1398	0.1451	26.57	23.86	

Table 3(S). Absolute energy values of the species in two studied levels

G	species	M06-2X/6-31G(d,p)	MPW1PW91/6-311++G(d,p)
	CO <sub>2</sub>	-188.51134	-188.5946257
	Ethylene oxide	-153.724899	-153.7986199
	Carbonate	-342.2789132	-342.4265573
Me	Organocatalyst	-1381.427165	-1381.912491
	TS step1 mechanism A	-1569.9357119	-1570.4920309
	In1A	-1569.9464082	-1570.4980415
	TS step2 mechanism A	-1723.6222587	-1724.252097
	In2A	-1723.6419201	-1724.271322
	In1B	-1535.1479978	-1535.7010731
	TS step1 mechanism B	-1535.1088203	-1535.6718385
	In2B	-1723.7215419	-1724.3428491
	TS step 3 mechanism B	-1723.67399	-1724.3034272
CF <sub>3</sub>	Organocatalyst	-1679.074177	-1679.674268
	TS step1 mechanism A	-1867.57901	-1868.249037
	In1A	-1867.584697	-1868.250679
	TS step2 mechanism A	-2021.258453	-2022.002515
	In2A	-2021.276417	-2022.019791
	In1B	-1832.788585	-1833.456764
	TS step1 mechanism B	-1832.750497	-1833.429431
	In2B	-2021.359551	-2022.095282
	TS step 3 mechanism B	-2021.315552	-2022.06024

Table 3(S).continued

OMe	Organocatalyst	-1456.603798	-1457.116741
	TS step1 mechanism A	-1645.112279	-1645.695598
	In1A	-1645.126499	-1645.705559
	TS step2 mechanism A	-1798.798017	-1799.455052
	In2A	-1798.817095	-1799.473994
	In1B	-1610.326891	-1610.90743
	TS step1 mechanism B	-1610.284844	-1610.875555
	In2B	-1798.897333	-1799.546245
	TS step 3 mechanism B	-1798.850014	-1799.506851
Br	Organocatalyst	-3913.312901	-3916.303012
	TS step1 mechanism A	-4101.819406	-4104.880232
	In1A	-4101.826862	-4104.883587
	TS step2 mechanism A	-4255.501281	-4258.63631
	In2A	-4255.519543	-4258.654295
	In1B	-4067.029736	-4070.08809
	TS step1 mechanism B	-4066.991144	-4070.060051
	In2B	-4255.601545	-4258.727964
	TS step 3 mechanism B	-4255.556202	-4258.69092
Cl	Organocatalyst	-1801.699784	-1802.227535
	TS step1 mechanism A	-1990.206446	-1990.80514
	In1A	-1990.214189	-1990.808772
	TS step2 mechanism A	-2143.889793	-2144.561079
	In2A	-2143.906878	-2144.579668
	In1B	-1955.41064	-1956.013012
	TS step1 mechanism B	-1955.378318	-1955.984607
	In2B	-2143.988726	-2144.653131
	TS step 3 mechanism B	-2143.943554	-2144.615926
CO <sub>2</sub> Me	Organocatalyst	-1569.937356	-1570.493994
	TS step1 mechanism A	-1758.441621	-1759.068018
	In1A	-1758.447193	-1759.069917
	TS step2 mechanism A	-1912.121263	-1912.821889
	In2A	-1912.139253	-1912.839716
	In1B	-1723.65123	-1724.276187
	TS step1 mechanism B	-1723.613451	-1724.249253
	In2B	-1912.222601	-1912.915065
	TS step 3 mechanism B	-1912.178725	-1912.880088
CHO	Organocatalyst	-1455.425289	-1455.936635
	TS step1 mechanism A	-1643.928278	-1644.50899
	In1A	-1643.93331	-1644.509943
	TS step2 mechanism A	-1797.60681	-1798.261326
	In2A	-1797.624687	-1798.278806
	In1B	-1609.137738	-1609.71713
	TS step1 mechanism B	-1609.099926	-1609.689762
	In2B	-1797.708678	-1798.355221
	TS step 3 mechanism B	-1797.665393	-1798.321029

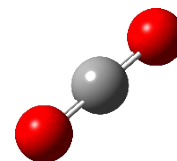
Table 3(S).continued

CN	Organocatalyst	-1434.356718	-1434.847294
	TS step1 mechanism A	-1622.859539	-1623.419727
	In1A	-1622.863789	-1623.420603
	TS step2 mechanism A	-1776.536499	-1777.17147
	In2A	-1776.55381	-1777.188454
	In1B	-1588.068662	-1588.627559
	TS step1 mechanism B	-1588.030831	-1588.600882
	In2B	-1776.638414	-1777.265143
	TS step 3 mechanism B	-1776.59607	-1777.231473
NMe <sub>2</sub>	Organocatalyst	-1476.034865	-1476.559704
	TS step1 mechanism A	-1664.544401	-1665.139972
	In1A	-1664.558506	-1665.150343
	TS step2 mechanism A	-1818.235656	-1818.905709
	In2A	-1818.256396	-1818.926384
	In1B	-1629.758342	-1630.351749
	TS step1 mechanism B	-1629.717427	-1630.320307
	In2B	-1818.333598	-1818.995113
	TS step 3 mechanism B	-1818.281228	-1818.949961

## Cartesian coordinate of the species, imaginary frequency of TSs and optimized structures

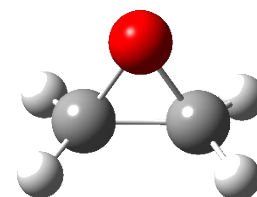
### CO<sub>2</sub>

0 1			
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16272900
O	0.00000000	0.00000000	-1.16272900



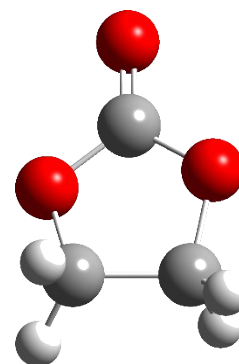
### Ethylene oxide

0 1			
C	0.00000000	0.82112200	0.00000000
C	0.65931200	-0.48972000	0.00000000
O	-0.75787900	-0.38111100	0.00000000
H	-0.04259100	1.39586500	0.92171100
H	-0.04259100	1.39586500	-0.92171100
H	1.09617000	-0.86562500	0.92168700
H	1.09617000	-0.86562500	-0.92168700



### Carbonate

0 1			
C	0.00000000	0.00000000	0.83854700
C	0.00000000	0.76454200	-1.29774700
H	0.97179600	1.18519100	-1.56490400
C	0.00000000	-0.76454200	-1.29774700
H	0.78245500	-1.20081100	-1.91598400
O	0.27009100	-1.07413300	0.07623500
O	-0.27009100	1.07413300	0.07623500
O	0.00000000	0.00000000	2.03546100
H	-0.97179600	-1.18519100	-1.56490400
H	-0.78245500	1.20081100	-1.91598400



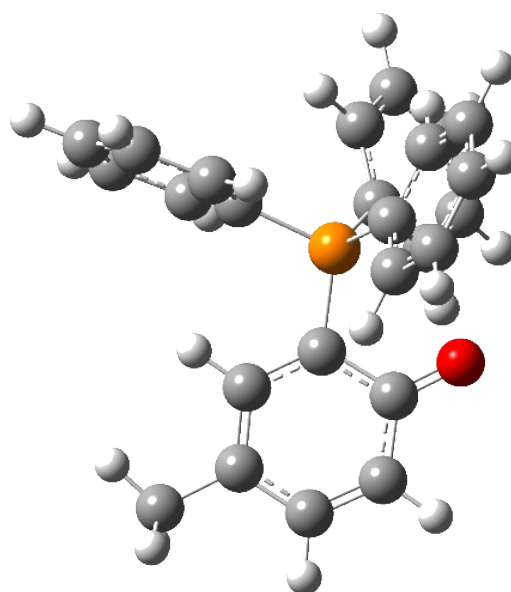
### Me

#### Organocatalyst

0 1			
C	3.98087000	-1.44640700	0.90000200
C	2.92530500	-2.31788900	1.01331800
C	1.56635100	-1.89661600	0.78845900
C	1.43066500	-0.51217500	0.41918100
C	2.53444500	0.35833500	0.29871400
C	3.81895300	-0.08358800	0.54489100
H	4.98896500	-1.81405800	1.08739900
H	3.08425800	-3.35792800	1.28334600
H	2.37457400	1.39384600	0.00516000



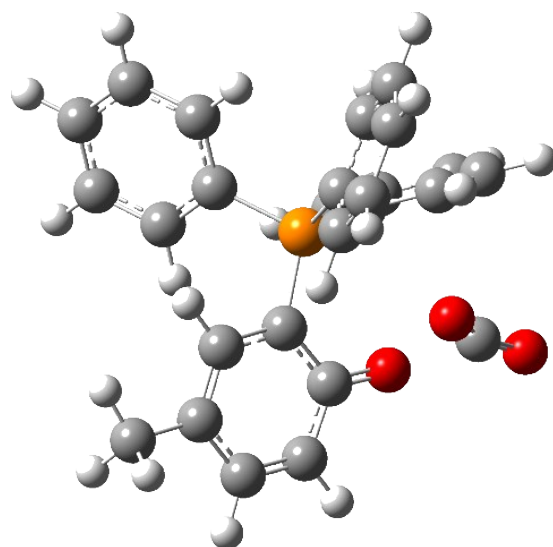
O	0.56201300	-2.65916800	0.90014400
P	-0.22088600	-0.01532900	0.03528600
C	-0.94992000	-1.07418100	-1.24400100
C	-2.33517200	-1.13521000	-1.40907900
C	-0.10458000	-1.76906200	-2.11291200
C	-2.87308100	-1.88818200	-2.44954600
H	-2.99536400	-0.60643800	-0.72790800
C	-0.64912600	-2.51760500	-3.15116200
H	0.97109800	-1.72700400	-1.96810200
C	-2.03158500	-2.57608200	-3.32026600
H	-3.94921000	-1.93825300	-2.57656900
H	0.00584100	-3.06088700	-3.82403700
H	-2.45373700	-3.16283900	-4.12965100
C	-1.34598200	0.06569700	1.45817500
C	-1.12033200	-0.75170000	2.57088200
C	-2.43228500	0.95019600	1.44352200
C	-1.98158700	-0.67824600	3.66155200
H	-0.29727600	-1.45765600	2.55661500
C	-3.29288200	1.00820500	2.53581400
H	-2.60176100	1.60131100	0.59045100
C	-3.06526900	0.19713700	3.64537800
H	-1.80504200	-1.30981400	4.52584800
H	-4.13477100	1.69199000	2.52145200
H	-3.73336200	0.24838900	4.49901700
C	-0.16505400	1.66344700	-0.65109700
C	-0.20958600	1.86318700	-2.03292400
C	0.01077700	2.75439200	0.20968900
C	-0.07927300	3.14969800	-2.55105100
H	-0.34594800	1.02049400	-2.70379300
C	0.14188100	4.03551900	-0.31480000
H	0.04365100	2.60273000	1.28526300
C	0.09677700	4.23269200	-1.69472400
H	-0.11700500	3.30287400	-3.62416500
H	0.27791400	4.87904500	0.35339300
H	0.19805600	5.23337900	-2.10169200
C	5.01480200	0.82814600	0.43903400
H	5.52548800	0.93625600	1.40215300
H	5.75199800	0.44348800	-0.27356900
H	4.71814300	1.82611300	0.10665000



### TS step1 mechanism A (iv = 286.53cm<sup>-1</sup>)

01			
C	-2.06695300	-3.70155300	-0.51923600
C	-0.76457200	-3.55713800	-0.93100300
C	-0.04115300	-2.33006600	-0.77892700
C	-0.78828900	-1.26139400	-0.19776400
C	-2.13088500	-1.43523900	0.21830200
C	-2.78608200	-2.64149600	0.08028200

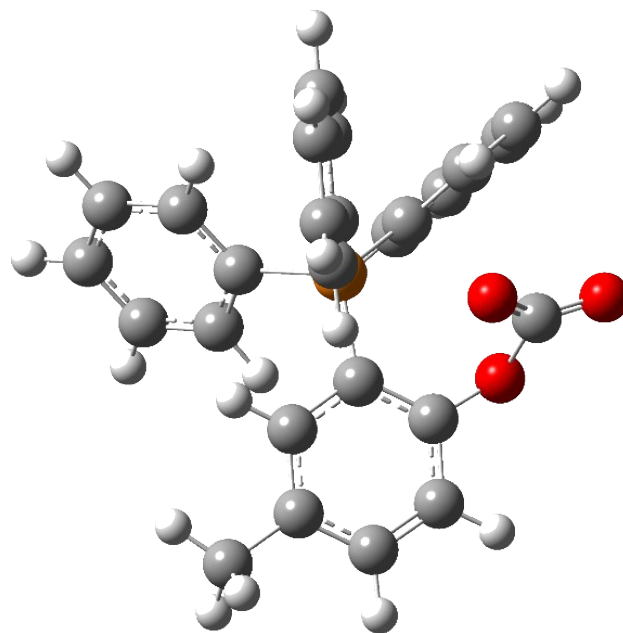
H	-2.56481100	-4.65988100	-0.65424200
H	-0.22639400	-4.38340600	-1.38532700
H	-2.66900400	-0.59395900	0.65300000
O	1.18542200	-2.23845100	-1.15173500
P	-0.09633600	0.36607700	-0.00329000
C	0.30573900	0.75712400	1.71892600
C	1.01433100	1.92304900	2.03696900
C	-0.13599100	-0.09404700	2.73438900
C	1.26661100	2.23696700	3.36851400
H	1.37796100	2.57949800	1.25103900
C	0.11934600	0.22770600	4.06409300
H	-0.65778900	-1.01152200	2.48224200
C	0.81670300	1.39104500	4.38084800
H	1.81760000	3.13839300	3.61314300
H	-0.22058100	-0.43566100	4.85181800
H	1.01677700	1.63676700	5.41847000
C	1.36698000	0.70163600	-1.02222800
C	1.19489100	0.96046300	-2.38528600
C	2.64874000	0.70418800	-0.46480900
C	2.30411400	1.20028400	-3.18898900
H	0.20226000	0.97626900	-2.82390600
C	3.75303500	0.94911100	-1.27529300
H	2.78770400	0.50459700	0.59264400
C	3.58290800	1.19408100	-2.63553500
H	2.16761500	1.39628900	-4.24688400
H	4.74662800	0.94483600	-0.84052200
H	4.44636200	1.38392800	-3.26431700
C	-1.38446500	1.53903500	-0.54437700
C	-1.56752300	2.77168100	0.08801300
C	-2.17642600	1.20048400	-1.65027500
C	-2.52494900	3.66262800	-0.39102000
H	-0.98105600	3.03857000	0.95995500
C	-3.12600800	2.09773500	-2.12668500
H	-2.06127900	0.23116000	-2.12653300
C	-3.29981100	3.32971100	-1.49843800
H	-2.66633900	4.61515900	0.10793300
H	-3.73485400	1.83007000	-2.98334700
H	-4.04537700	4.02590600	-1.86778400
C	-4.21133300	-2.83452000	0.52934600
H	-4.62143700	-1.91114600	0.94472100
H	-4.85192000	-3.14364800	-0.30265600
H	-4.28421300	-3.61048700	1.29808800
C	2.55275500	-2.19348400	0.32632600
O	3.52015200	-2.50720200	-0.26732200
O	1.91153800	-1.85820300	1.26342700



## In1A

0 1

C	-2.86766400	-3.18340700	-0.23791700
C	-1.53248600	-3.41459300	-0.52015800
C	-0.58426400	-2.38917800	-0.42052100
C	-1.02564900	-1.10696900	-0.05955000
C	-2.38502200	-0.89334600	0.23441700
C	-3.31882400	-1.91844600	0.16411500
H	-3.58011400	-3.99993900	-0.32199300
H	-1.18088900	-4.39654900	-0.81749200
H	-2.72142800	0.10225600	0.51441600
O	0.69622900	-2.69319200	-0.72279600
P	0.05196000	0.33618700	0.00808300
C	0.43070300	0.84746900	1.69858000
C	1.35734800	1.87102200	1.92475100
C	-0.23883700	0.25059600	2.76875000
C	1.60104700	2.30322700	3.22523400
H	1.89458800	2.32547300	1.09670600
C	0.00926400	0.69113100	4.06406100
H	-0.92753200	-0.56833800	2.58968100
C	0.92507300	1.71660300	4.29235100
H	2.32259000	3.09349100	3.40096100
H	-0.50603200	0.22497000	4.89679500
H	1.11813500	2.05410200	5.30532600
C	1.57353600	0.23145000	-0.97588400
C	1.48926000	0.37011600	-2.36609800
C	2.81736400	0.05597300	-0.36113700
C	2.64481500	0.31851900	-3.13684600
H	0.53224700	0.52276300	-2.85320300
C	3.96915300	0.02106400	-1.14094100
H	2.87679700	-0.08784800	0.71188200
C	3.88506600	0.15009200	-2.52433300
H	2.57505800	0.41884800	-4.21445800
H	4.93260700	-0.11732800	-0.66270900
H	4.78644500	0.11871500	-3.12747000
C	-0.94070300	1.66565700	-0.75632200
C	-0.90745700	2.97238600	-0.26259800
C	-1.71868400	1.37150300	-1.88565300
C	-1.63262900	3.97610700	-0.90109900
H	-0.33231700	3.21488400	0.62378600
C	-2.43441100	2.37932100	-2.52131600
H	-1.78173600	0.35338200	-2.25893500
C	-2.39046100	3.68327600	-2.03063700
H	-1.60560700	4.98664900	-0.50815700
H	-3.03215600	2.14225700	-3.39465200
H	-2.95331700	4.46807700	-2.52496400

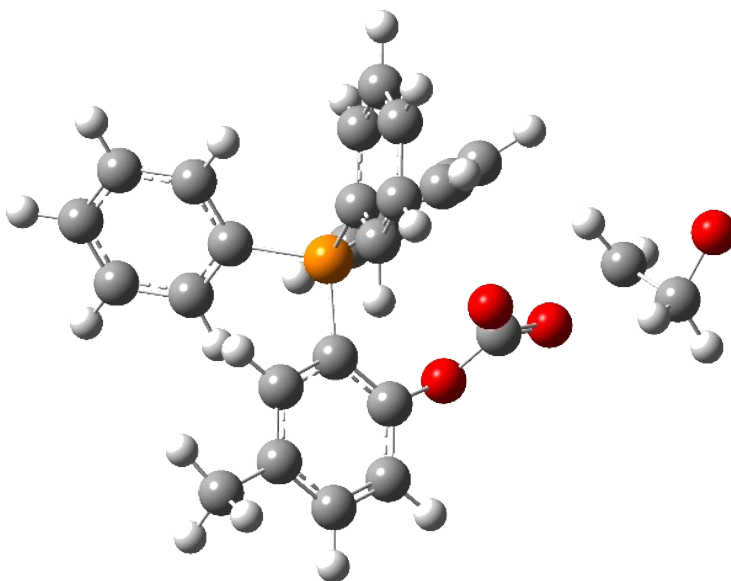


C	-4.77023200	-1.68562100	0.49376700
H	-5.41244100	-1.98584200	-0.33896400
H	-5.07062900	-2.27261400	1.36669500
H	-4.96279500	-0.63316300	0.71088300
C	1.70806000	-2.54861400	0.33971100
O	2.75758500	-3.09467700	0.03652500
O	1.32980500	-1.88951500	1.31830200

### TS step2 mechanism A (iv = 632.18cm<sup>-1</sup>)

0 1

C	1.22249300	4.13091400	-0.59167400
C	0.09875700	3.50452500	-1.10592100
C	-0.09438500	2.13572200	-0.92460500
C	0.86974800	1.39130900	-0.23733600
C	2.00044400	2.04661900	0.28166700
C	2.18962900	3.41441700	0.12463500
H	1.35404000	5.19881500	-0.74274000
H	-0.65637100	4.05644600	-1.65447500
H	2.75441400	1.47230600	0.81491100
O	-1.20861400	1.58451800	-1.49643000
P	0.78859700	-0.39150000	0.03732700
C	0.35871300	-0.76239700	1.74977600
C	0.19000800	-2.09637100	2.14414000
C	0.20838400	0.27376000	2.67400300
C	-0.10891400	-2.38782400	3.47037600
H	0.27633700	-2.90362700	1.42155700
C	-0.08991400	-0.02930900	3.99878000
H	0.29717000	1.30673400	2.35550100
C	-0.24418500	-1.35497600	4.39655100
H	-0.24224800	-3.41944600	3.77649900
H	-0.21205900	0.77288200	4.71804200
H	-0.48060100	-1.58504200	5.43012200
C	-0.32911300	-1.28897400	-1.06995600
C	0.03248800	-1.47370500	-2.40929500
C	-1.53744500	-1.80163700	-0.58758600
C	-0.82348800	-2.15838400	-3.26332500
H	0.97441600	-1.09155900	-2.78870200
C	-2.38301400	-2.49319100	-1.44920800
H	-1.82769700	-1.63604100	0.44430500
C	-2.02885800	-2.66927400	-2.78344000
H	-0.54612500	-2.29726800	-4.30239600
H	-3.32246400	-2.88533900	-1.07455700
H	-2.69220800	-3.20662000	-3.45305400
C	2.47797700	-0.97729700	-0.29771200
C	3.08730700	-1.94187600	0.50873800
C	3.16225000	-0.45931000	-1.40678800
C	4.36613000	-2.39685600	0.19609200

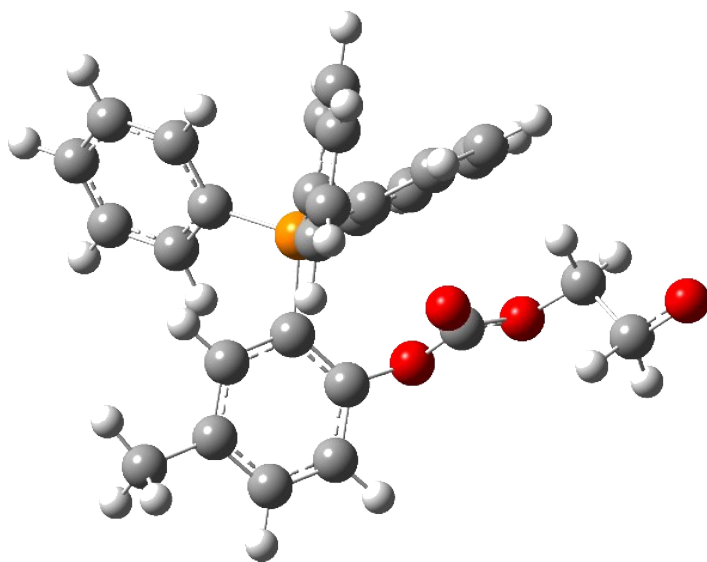


H	2.58430300	-2.32975900	1.38727200
C	4.43530500	-0.92374600	-1.71428000
H	2.71551500	0.32046300	-2.01732300
C	5.03686000	-1.89406600	-0.91439900
H	4.83717500	-3.14088100	0.82907500
H	4.96013900	-0.51912000	-2.57273400
H	6.03374400	-2.24963800	-1.15267800
C	3.39717800	4.11007100	0.69539300
H	3.95571400	4.62584300	-0.09046100
H	3.09773200	4.86127900	1.43180700
H	4.06833400	3.40183000	1.18443100
C	-2.19839100	1.07956600	-0.63336400
O	-3.23073900	0.77647500	-1.29566800
O	-1.95079800	0.97647100	0.56039400
C	-4.57916300	0.10603200	-0.27717200
H	-5.06264000	-0.36806100	-1.12022000
H	-3.96007400	-0.51517200	0.35542500
C	-5.37285400	1.11809600	0.43009500
H	-5.87487600	1.84353800	-0.23997100
H	-4.79253600	1.69467800	1.17665300
O	-6.12631800	0.06931700	0.89404400

## In2A

01

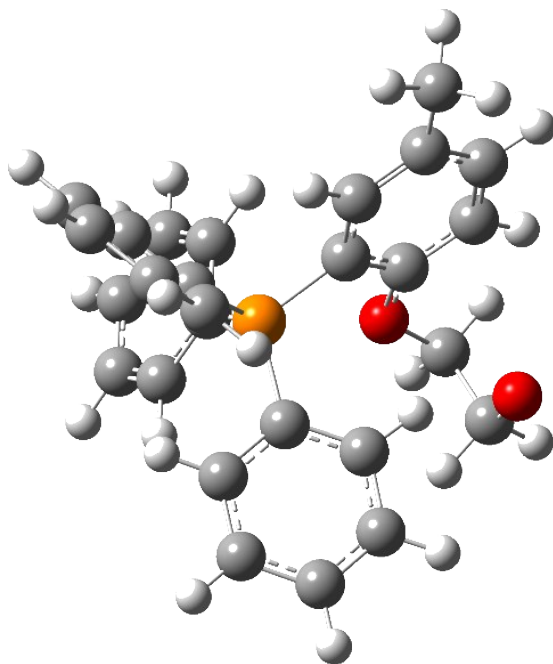
C	0.91121800	4.16218000	-0.60644800
C	-0.19504400	3.45689400	-1.05434800
C	-0.26807500	2.08173600	-0.86391600
C	0.77988000	1.40068900	-0.23992400
C	1.88964600	2.13713000	0.20920700
C	1.96977300	3.51575900	0.04316300
H	0.95546400	5.23651000	-0.76003000
H	-1.02023500	3.95186700	-1.55367700
H	2.71374900	1.61952100	0.69442200
O	-1.38058400	1.44439000	-1.37542600
P	0.83570400	-0.38401000	0.04933400
C	0.52099800	-0.74795300	1.78675300
C	0.45140400	-2.08444200	2.20492300
C	0.36277800	0.29119900	2.70711300
C	0.24313900	-2.37369000	3.54828800
H	0.54435800	-2.89567700	1.48790600
C	0.15393500	-0.01067700	4.04937800
H	0.38115200	1.32465800	2.37835800
C	0.09802900	-1.33709900	4.46907900
H	0.18786800	-3.40682100	3.87256400
H	0.02598800	0.79331100	4.76546500
H	-0.06893400	-1.56539700	5.51639300
C	-0.30343800	-1.34158000	-0.98216200
C	-0.03537500	-1.47423800	-2.35008300



C	-1.43581200	-1.94178700	-0.42181200
C	-0.90953600	-2.19549900	-3.15326100
H	0.84712500	-1.02183200	-2.79081300
C	-2.29816600	-2.67215100	-1.23442400
H	-1.65839800	-1.82127100	0.63316900
C	-2.03799500	-2.79597300	-2.59586400
H	-0.70605500	-2.29340000	-4.21378400
H	-3.17795200	-3.13350300	-0.79906300
H	-2.71458900	-3.36304900	-3.22635600
C	2.52918200	-0.87055800	-0.39311900
C	3.22721100	-1.82077300	0.35683500
C	3.11481800	-0.30997300	-1.53691200
C	4.49823000	-2.22029100	-0.04839300
H	2.79878700	-2.24035800	1.25991100
C	4.38179900	-0.71899200	-1.93542100
H	2.59679100	0.45720200	-2.10519500
C	5.07193700	-1.67622400	-1.19364500
H	5.03965900	-2.95440600	0.53797100
H	4.83147900	-0.28313100	-2.82064400
H	6.06241100	-1.99068900	-1.50481700
C	3.16060000	4.29539300	0.53362500
H	3.65138000	4.81293400	-0.29509700
H	2.85222800	5.05382900	1.25838800
H	3.89262800	3.64215500	1.01137200
C	-2.25780000	0.91615700	-0.47185300
O	-3.29315400	0.47966400	-1.13452100
O	-2.03259400	0.85963400	0.71419300
C	-4.37820600	-0.09971400	-0.34428800
H	-4.86648700	-0.79652200	-1.02819600
H	-3.94342300	-0.64977400	0.49426800
C	-5.38477400	0.94510000	0.17382900
H	-5.69458600	1.52541400	-0.74684000
H	-4.75065100	1.69767300	0.73416000
O	-6.35335000	0.34095700	0.86103300

## In1B

O 1			
C	-2.19750000	3.41002000	0.56148100
C	-2.68838400	2.14096000	0.80644000
C	-1.84358400	1.02832500	0.67335500
C	-0.51759900	1.24624400	0.25673400
C	-0.04211100	2.54670700	0.01456300
C	-0.86879300	3.64723600	0.16936500
H	-2.87119100	4.25679000	0.66865700
H	-3.73008300	2.00278900	1.05712900
H	0.98789800	2.69157600	-0.29881700
O	-2.15177500	-0.23879200	0.99465500
P	0.53452400	-0.17748300	-0.00512500

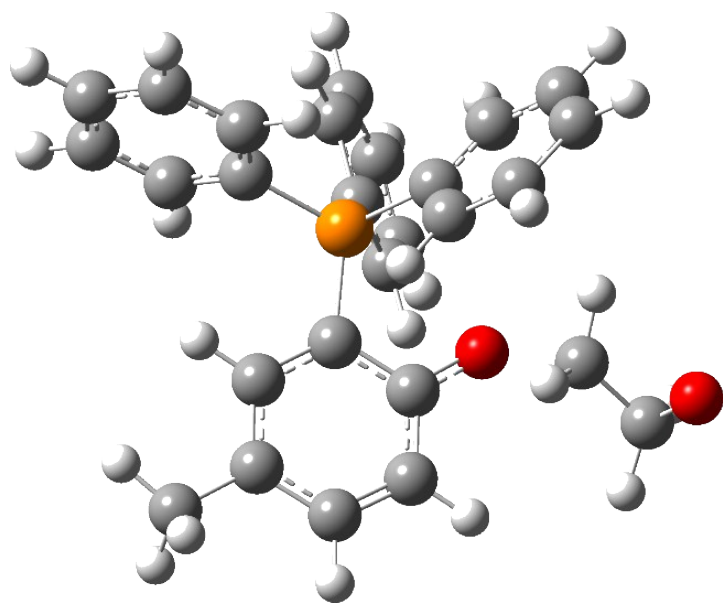


C	0.61277500	-1.18951000	1.49425400
C	0.86173000	-2.56077100	1.40991100
C	0.46676600	-0.57030200	2.73980100
C	0.97606000	-3.31078600	2.57729600
H	0.95494300	-3.04787900	0.44457600
C	0.58723300	-1.32679500	3.90055700
H	0.25058200	0.49292500	2.79849400
C	0.84236700	-2.69500000	3.81898100
H	1.16473300	-4.37689500	2.51366700
H	0.47275100	-0.84964000	4.86781300
H	0.92950800	-3.28286700	4.72676700
C	0.01386500	-1.15353700	-1.43196000
C	-1.27849700	-1.01948900	-1.94775600
C	0.93641700	-2.04045800	-2.01042700
C	-1.63780500	-1.80217600	-3.04619200
H	-2.04750600	-0.33915000	-1.54256100
C	0.55478400	-2.81391300	-3.09901700
H	1.94911900	-2.11756200	-1.62287100
C	-0.73660400	-2.69461800	-3.61668200
H	-2.64307100	-1.69769700	-3.44269400
H	1.26450500	-3.50158600	-3.54599900
H	-1.03158100	-3.29724200	-4.46992100
C	2.21197500	0.40891700	-0.35449200
C	3.16450800	0.48339400	0.66532200
C	2.52825600	0.83980200	-1.64926900
C	4.43213800	0.98772600	0.38751000
H	2.92291400	0.14596600	1.66851400
C	3.79563900	1.34455500	-1.91657400
H	1.78986000	0.77640000	-2.44367400
C	4.74643800	1.41702400	-0.89909600
H	5.17349200	1.04229600	1.17727400
H	4.04168100	1.67683900	-2.91918900
H	5.73611300	1.80789100	-1.11150700
C	-0.37870900	5.04960300	-0.08162100
H	-0.97175300	5.54042700	-0.85900600
H	-0.45573000	5.66162600	0.82213500
H	0.66533200	5.05017400	-0.40182600
C	-3.52705700	-0.65403400	1.07371100
H	-4.10581700	0.10404100	1.61115400
H	-3.50506700	-1.56709600	1.67685700
C	-4.05504800	-0.88303200	-0.35306100
H	-3.54162400	-1.82892700	-0.68686400
H	-5.12396200	-1.19980000	-0.20990900
O	-3.85440800	0.17657800	-1.15217100

## TS step1 mechanism B (iv = 656.23cm<sup>-1</sup>)

0 1

C	-1.48726400	3.61923600	-1.16624900
C	-2.15833300	2.41058500	-1.18798500
C	-1.47838400	1.20410400	-0.89668300
C	-0.10812800	1.31602900	-0.54851400
C	0.55695800	2.55190100	-0.53052100
C	-0.11937500	3.72088300	-0.84824800
H	-2.03415400	4.52854900	-1.40649400
H	-3.21173300	2.35869900	-1.44645700
H	1.60735600	2.59735600	-0.25331600
O	-2.03977000	0.02439600	-0.92446300
P	0.64354700	-0.20199700	0.00646900
C	-0.38053500	-0.91486200	1.31790200
C	-0.60098500	-2.29097000	1.39027100
C	-0.96721200	-0.05206300	2.24993200
C	-1.41258200	-2.80296100	2.39982500
H	-0.16066900	-2.95980300	0.65748400
C	-1.77093700	-0.57309600	3.25816200
H	-0.81262200	1.02133000	2.17579400
C	-1.99604000	-1.94696100	3.33084700
H	-1.59357300	-3.87105100	2.45251300
H	-2.23039500	0.09517100	3.97837700
H	-2.63328000	-2.34969300	4.11105900
C	0.91739600	-1.42150600	-1.30147300
C	0.17491200	-1.37741400	-2.48482500
C	1.88372100	-2.41712400	-1.10660100
C	0.40080600	-2.33516500	-3.46932400
H	-0.58556600	-0.61698000	-2.61941100
C	2.09368400	-3.37500400	-2.09287700
H	2.47282100	-2.44165000	-0.19402400
C	1.35386000	-3.33203400	-3.27345300
H	-0.17241700	-2.30289700	-4.38943700
H	2.83894600	-4.14818300	-1.94192800
H	1.52252000	-4.07754000	-4.04353300
C	2.27841400	0.17587900	0.68819500
C	2.48902300	0.22797900	2.06789100
C	3.32756400	0.45924800	-0.19679300
C	3.74718900	0.56654700	2.56060100
H	1.68164800	0.00074100	2.75651100
C	4.57848900	0.80005800	0.30366800
H	3.16833500	0.40906100	-1.27078000
C	4.78749900	0.85332600	1.68178500
H	3.91182600	0.60226700	3.63192900
H	5.39046700	1.01972800	-0.38092500
H	5.76623700	1.11625200	2.06937000



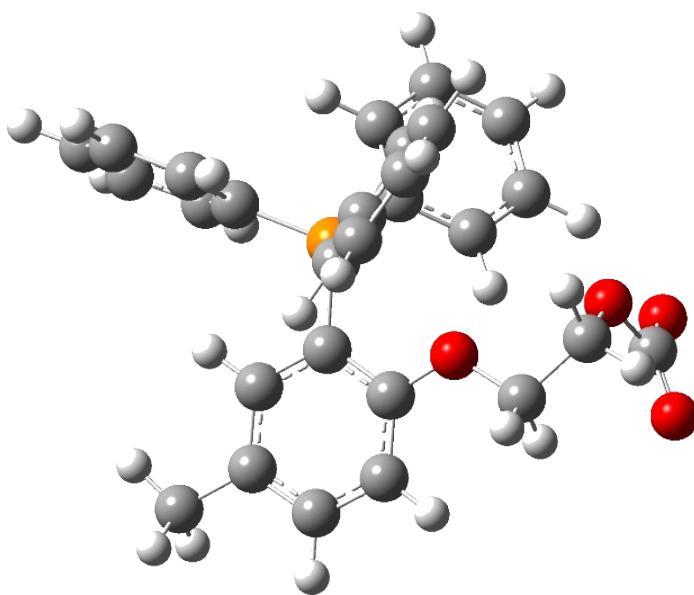


C	0.57004100	5.06122900	-0.84283900
H	0.51805000	5.53674500	-1.82715500
H	0.10261300	5.74485800	-0.12745300
H	1.62368000	4.96026200	-0.57317300
C	-3.58535500	-0.12739800	0.05774200
H	-3.44763500	0.78173300	0.63259300
H	-3.26302600	-1.05328200	0.51802800
C	-4.81457700	-0.19518800	-0.73643400
H	-5.03458400	0.71887400	-1.32364000
H	-4.86133500	-1.05721800	-1.42900500
O	-5.44720400	-0.32626300	0.47471700

## In2B

0 1

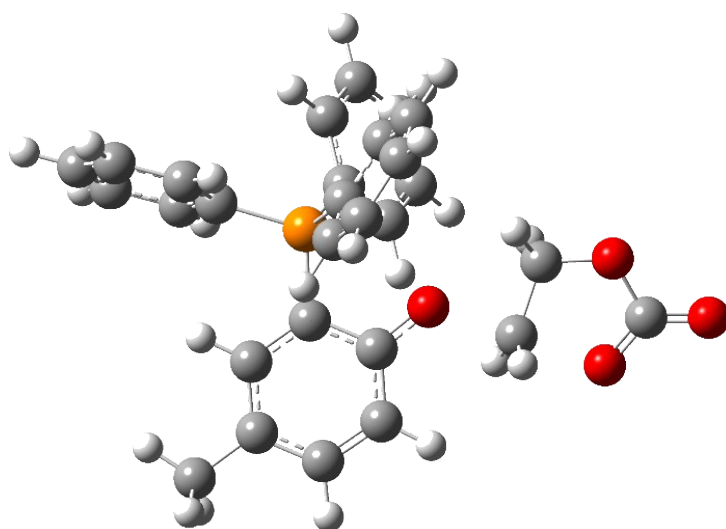
C	0.06765500	4.15366700	-0.50958200
C	-0.91235500	3.31923200	0.01325700
C	-0.66032000	1.95128600	0.13797000
C	0.59386700	1.44416800	-0.25357500
C	1.56675300	2.31245200	-0.76363200
C	1.31786200	3.67414700	-0.91053400
H	-0.14651200	5.21519600	-0.60177600
H	-1.86382400	3.73138000	0.32476800
H	2.54088700	1.92378200	-1.04318600
O	-1.53976000	1.05683000	0.62625400
P	0.96299200	-0.30500600	0.00174500
C	0.53825000	-0.74281200	1.70281000
C	0.04218900	-2.01566200	1.99051800
C	0.72816900	0.19717300	2.72174600
C	-0.26172200	-2.34854500	3.30836200
H	-0.11643500	-2.73802400	1.19556800
C	0.42409700	-0.14631000	4.03378200
H	1.10155500	1.19133100	2.49038600
C	-0.07149100	-1.41692400	4.32571800
H	-0.65278900	-3.33420800	3.53583900
H	0.56678700	0.58004100	4.82626800
H	-0.31392300	-1.67875800	5.35032500
C	0.11597400	-1.42542800	-1.13273900
C	-1.22437300	-1.20820600	-1.46990600
C	0.77790200	-2.58071400	-1.57496100
C	-1.90110300	-2.14223700	-2.24918000
H	-1.76859600	-0.34854100	-1.09858500
C	0.09646700	-3.50035900	-2.36444000
H	1.81238100	-2.76685700	-1.30568300
C	-1.23903900	-3.28139700	-2.70037700
H	-2.95095900	-1.95383500	-2.45776000
H	0.60982100	-4.39130900	-2.70990600
H	-1.76594500	-4.00986800	-3.30859500
C	2.74213000	-0.53294200	-0.22970600



C	3.58052200	-0.70798700	0.87327000
C	3.27476000	-0.50657200	-1.52675800
C	4.95199400	-0.85357300	0.67824100
H	3.17070700	-0.73736000	1.87751200
C	4.64435200	-0.65051300	-1.71034400
H	2.62197100	-0.38245400	-2.38697000
C	5.48173800	-0.82416100	-0.60805500
H	5.60316200	-0.99379900	1.53400400
H	5.05706200	-0.63107100	-2.71292600
H	6.55025200	-0.94033400	-0.75592900
C	2.35977200	4.60733000	-1.47090900
H	2.01590400	5.05904000	-2.40586800
H	2.57241900	5.42118700	-0.77222500
H	3.29365200	4.07955800	-1.67357800
C	-2.84804100	1.49438500	1.01008700
H	-3.31105200	2.05817100	0.19503600
H	-2.77429800	2.12292100	1.90579400
C	-3.66589100	0.24754100	1.27144800
H	-3.14735800	-0.38405300	2.00123100
H	-4.63763400	0.55058200	1.67152400
O	-3.80990100	-0.52123500	0.09950300
C	-4.71485100	-0.01015700	-0.87482000
O	-4.69779700	-0.66781400	-1.92675900
O	-5.37050400	0.99360500	-0.54994900

### TS step 3 mechanism B (iv = 646.78cm<sup>-1</sup>)

01			
C	-0.14309000	4.10086100	-0.11342600
C	-1.08583900	3.11102100	0.10264200
C	-0.70178300	1.74812900	0.13685600
C	0.67720900	1.47534200	-0.06867800
C	1.61857800	2.49623100	-0.26666000
C	1.22344600	3.82548300	-0.29973600
H	-0.47158200	5.13791900	-0.13042500
H	-2.12494000	3.37623800	0.26327300
H	2.66846200	2.24501200	-0.39581800
O	-1.50748300	0.74298700	0.34215300
P	1.12796700	-0.24579600	0.02247400
C	0.59248300	-0.94447600	1.60326200
C	0.09155800	-2.24455000	1.69068800
C	0.71060600	-0.15137100	2.74947700
C	-0.28610500	-2.75182400	2.93135400
H	-0.01956900	-2.85602200	0.80104500
C	0.33782400	-0.66940400	3.98497900
H	1.08114900	0.86757200	2.67441200
C	-0.16069200	-1.96814500	4.07537300
H	-0.68270800	-3.75888100	3.00079600



H	0.42680200	-0.05578800	4.87489600
H	-0.45848500	-2.36694800	5.03942900
C	0.48919900	-1.22860000	-1.35517800
C	-0.53253700	-0.74832200	-2.17795800
C	1.06836400	-2.47977000	-1.60349100
C	-0.98249700	-1.53009100	-3.23874900
H	-0.97262000	0.22466700	-1.98829900
C	0.60546500	-3.25741300	-2.65884400
H	1.88336100	-2.84238900	-0.98235000
C	-0.41940800	-2.78213800	-3.47532800
H	-1.77332200	-1.15770900	-3.88103800
H	1.05116400	-4.22791400	-2.84741300
H	-0.77432500	-3.38712700	-4.30310100
C	2.93148400	-0.38588100	-0.08120000
C	3.70443900	-0.66585000	1.04755700
C	3.54509100	-0.18003000	-1.32440900
C	5.09105600	-0.73636500	0.93145900
H	3.23203200	-0.83519100	2.00976900
C	4.92899000	-0.24583900	-1.42941600
H	2.94379800	0.02781000	-2.20570600
C	5.70106000	-0.52522900	-0.30152500
H	5.69123800	-0.96109700	1.80632500
H	5.40404300	-0.08551300	-2.39106600
H	6.78109600	-0.58251500	-0.38773700
C	2.21271900	4.94232800	-0.51468500
H	1.95273500	5.53772400	-1.39506400
H	2.23514800	5.62223000	0.34252200
H	3.22160100	4.54980600	-0.65923500
C	-3.32719600	0.94069400	-0.03879900
H	-3.08804600	1.51472300	-0.92229100
H	-3.50831000	1.47036800	0.88610700
C	-3.50564800	-0.56650800	-0.08332500
H	-3.24629500	-0.93720800	-1.08222600
H	-2.85318100	-1.03891600	0.65032200
O	-4.83837100	-0.91909100	0.23880300
C	-5.73344100	0.06974000	-0.12529900
O	-5.15734800	1.14467000	-0.50705700
O	-6.92514200	-0.17882000	-0.03588600

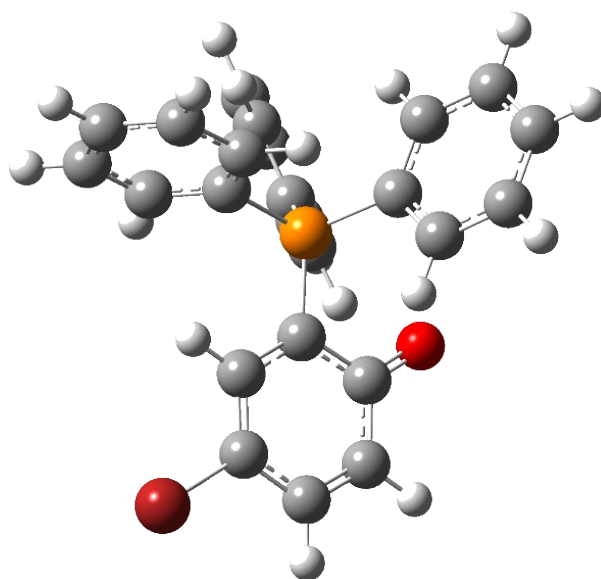
**Br**

## **Organocatalyst**

01

C	3.13857400	-2.00838600	0.86311800
C	1.96949300	-2.69074400	1.09248600
C	0.67648200	-2.08779200	0.88211400
C	0.71897200	-0.72852200	0.40018200
C	1.92069600	-0.04155700	0.15492800

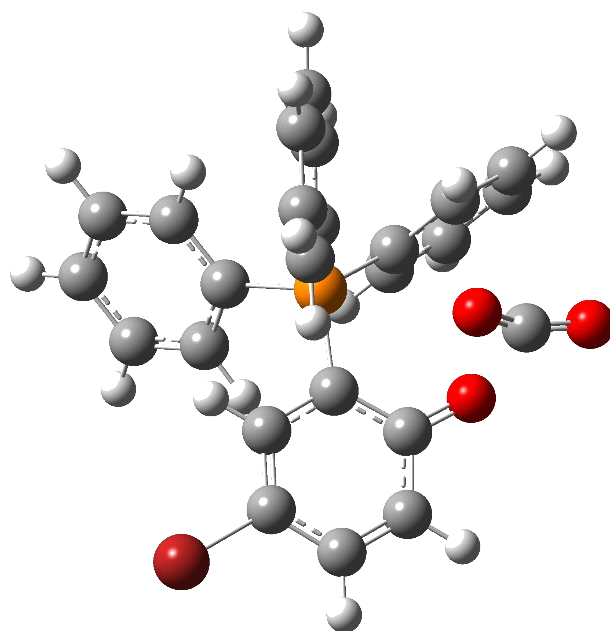
C	3.11596200	-0.67954900	0.39608500
H	4.09544600	-2.49148100	1.03722800
H	1.98879200	-3.71652000	1.44671000
H	1.91440400	0.97645500	-0.22190900
O	-0.41652000	-2.68156000	1.09304000
P	-0.86139600	-0.01647400	0.03456600
C	-1.78314400	-1.04802000	-1.13437600
C	-3.16916600	-0.91721200	-1.24674200
C	-1.08469000	-1.92161000	-1.97171100
C	-3.85493500	-1.66047900	-2.20349100
H	-3.71518800	-0.24722000	-0.58905600
C	-1.77723600	-2.65977000	-2.92582300
H	-0.00834000	-2.02564200	-1.86925900
C	-3.16010400	-2.52894600	-3.04195100
H	-4.93168500	-1.56201400	-2.29028100
H	-1.23684600	-3.34069700	-3.57464500
H	-3.69756900	-3.10709800	-3.78639300
C	-1.89950100	0.33553500	1.48121400
C	-1.78772300	-0.43901400	2.64117200
C	-2.81816300	1.39196700	1.42502900
C	-2.59321300	-0.14766600	3.73848900
H	-1.09963500	-1.27690800	2.66172800
C	-3.62473200	1.66716600	2.52480700
H	-2.89859300	2.00672700	0.53316400
C	-3.50906300	0.90062700	3.68196700
H	-2.50628300	-0.74507500	4.63985500
H	-4.33558600	2.48503200	2.47795800
H	-4.13341100	1.12205400	4.54144100
C	-0.58720800	1.58451800	-0.77273900
C	-0.72664400	1.71649200	-2.15600300
C	-0.17717400	2.67893600	0.00066800
C	-0.45833400	2.94127600	-2.76346000
H	-1.04568100	0.87094800	-2.75738400
C	0.09109800	3.89668500	-0.61334200
H	-0.07358700	2.58014500	1.07810100
C	-0.05119700	4.02761600	-1.99476300
H	-0.57143800	3.04439300	-3.83723800
H	0.40621000	4.74394400	-0.01408700
H	0.15353700	4.98092100	-2.47072800
Br	4.75812100	0.22606600	0.08528100



### TS step1 mechanism A (iv = 271.66 cm<sup>-1</sup>)

01			
C	-2.91190200	-2.25531700	-0.92681100
C	-1.65571000	-2.71843500	-1.23797400
C	-0.46581300	-1.97793100	-0.95172800
C	-0.66887300	-0.69641300	-0.35373900

C	-1.96043600	-0.22393000	-0.03879700
C	-3.06136400	-1.00293700	-0.30969700
H	-3.79012500	-2.85190400	-1.15112400
H	-1.52538400	-3.68761200	-1.70813300
H	-2.09622100	0.75575300	0.41173900
O	0.68996700	-2.46816900	-1.23093400
P	0.68199500	0.41909700	-0.00264300
C	1.03986800	0.53247800	1.76736100
C	2.16429000	1.23989600	2.21244300
C	0.16880300	-0.05408100	2.68819400
C	2.40232100	1.36998500	3.57659700
H	2.85885500	1.67804000	1.50065700
C	0.41451600	0.08144500	4.05112000
H	-0.68254400	-0.63076300	2.34181800
C	1.52591400	0.79372000	4.49459200
H	3.27397200	1.91668300	3.91940600
H	-0.26084700	-0.37600700	4.76581800
H	1.71484900	0.89519500	5.55818500
C	2.22398300	0.04877000	-0.88106000
C	2.33428700	0.39047100	-2.23214200
C	3.29272300	-0.56473500	-0.22134200
C	3.50527300	0.10039900	-2.92341000
H	1.51606500	0.88317800	-2.74722500
C	4.46205300	-0.84739900	-0.92003000
H	3.21024400	-0.83076800	0.82742500
C	4.56851100	-0.51859300	-2.26891400
H	3.58732600	0.36279700	-3.97255000
H	5.28794700	-1.32857900	-0.40753600
H	5.48161400	-0.74193400	-2.81056900
C	0.12970700	2.05996100	-0.57091100
C	0.45813600	3.22404700	0.12899500
C	-0.60393700	2.14638300	-1.76244000
C	0.06781200	4.46514700	-0.36774300
H	1.00275300	3.17179000	1.06507000
C	-0.98358000	3.38976100	-2.25512000
H	-0.89217800	1.24484100	-2.29560500
C	-0.64648300	4.54949600	-1.55946700
H	0.32019400	5.36461100	0.18310200
H	-1.55033500	3.45010600	-3.17782900
H	-0.95007600	5.51809100	-1.94256200
C	1.74989400	-3.08290800	0.29316100
O	2.52879800	-3.79541600	-0.23433600
O	1.26192000	-2.52662500	1.22193100
Br	-4.79661300	-0.38440000	0.14398400

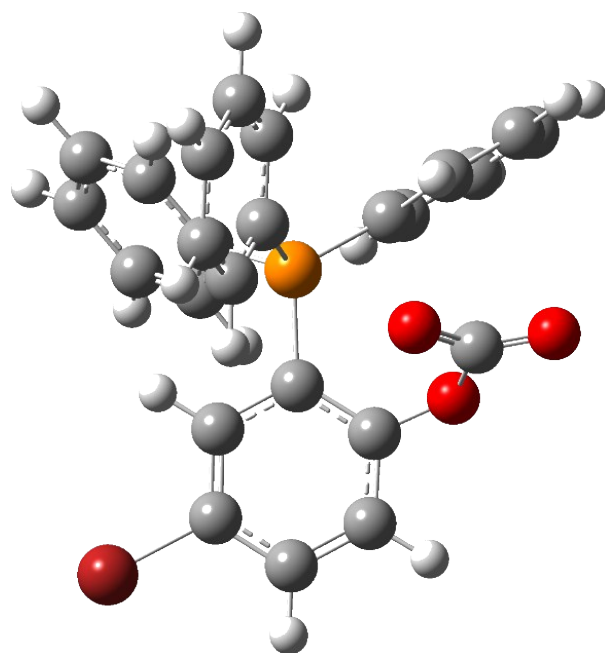


## In1A

01

C	-2.95779600	-2.37745200	-0.48144500
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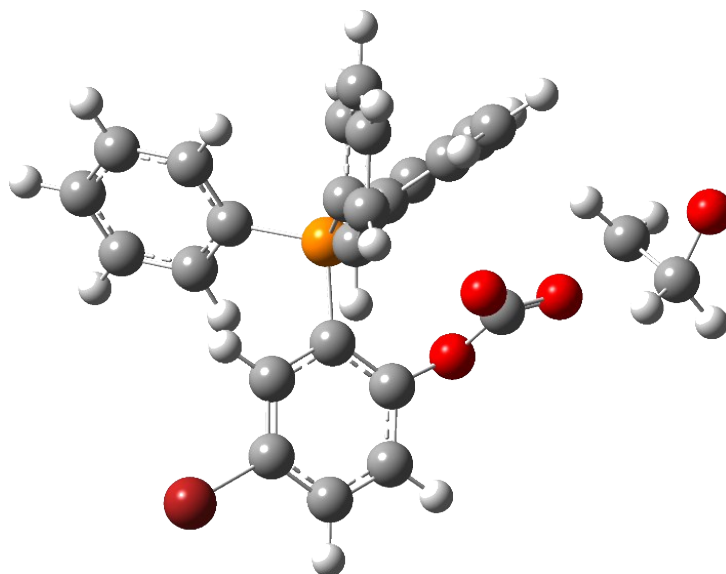
C	-1.69784200	-2.91958100	-0.66911800
C	-0.53851700	-2.15286900	-0.49657400
C	-0.67285200	-0.79538900	-0.15100700
C	-1.95075500	-0.24795100	0.04781800
C	-3.07405900	-1.04028000	-0.10820000
H	-3.84552900	-2.98523400	-0.61574900
H	-1.57628200	-3.96040200	-0.94714400
H	-2.06938400	0.79920300	0.30823000
O	0.64044500	-2.76229300	-0.71701800
P	0.72177900	0.34591800	-0.00677800
C	1.13437300	0.73696300	1.70699600
C	2.28833700	1.47622500	1.98767600
C	0.27215200	0.35088800	2.73496500
C	2.57144000	1.83402900	3.30284600
H	2.96773000	1.76796500	1.19127900
C	0.56176800	0.71667600	4.04470500
H	-0.60255600	-0.25205700	2.51497400
C	1.70802700	1.45708100	4.32841200
H	3.46788100	2.40304400	3.52322200
H	-0.10339800	0.41381000	4.84592800
H	1.93236600	1.73503900	5.35288800
C	2.20899600	-0.13380000	-0.92745000
C	2.23526400	0.05277700	-2.31464300
C	3.33238300	-0.63829000	-0.26424200
C	3.37625700	-0.28160800	-3.03456000
H	1.37836300	0.46226100	-2.83838400
C	4.47375100	-0.95604900	-0.99327400
H	3.29991700	-0.81024500	0.80586300
C	4.49672200	-0.78144300	-2.37415200
H	3.39058900	-0.14238300	-4.10989700
H	5.34256600	-1.35007700	-0.47752400
H	5.38831000	-1.03537200	-2.93780800
C	0.11548800	1.88349700	-0.78068300
C	0.42493200	3.13190600	-0.23435400
C	-0.64157600	1.81067000	-1.95946400
C	-0.00655600	4.29479800	-0.86825100
H	0.98702200	3.20771600	0.68947400
C	-1.06358900	2.97554700	-2.58895300
H	-0.91836300	0.84740800	-2.37865400
C	-0.74465300	4.21873200	-2.04497100
H	0.23187100	5.25960400	-0.43393300
H	-1.64896700	2.91119400	-3.49962800
H	-1.08052700	5.12668000	-2.53479800
C	1.59230900	-2.85681300	0.41521200
O	2.48815300	-3.64923800	0.17880300
O	1.32099700	-2.10752900	1.36214100
Br	-4.78940200	-0.28525800	0.15394800



## TS step 2 mechanism A (iv = 628.50cm<sup>-1</sup>)

0 1

C	-2.19905700	-2.98723200	-1.16138400
C	-0.88468400	-2.80401200	-1.56301200
C	-0.18288700	-1.65141900	-1.21201900
C	-0.82010200	-0.65182000	-0.46373100
C	-2.14936900	-0.83939600	-0.05687500
C	-2.81951100	-2.00276200	-0.39729800
H	-2.73677100	-3.88849400	-1.43208800
H	-0.37086800	-3.55624900	-2.15048000
H	-2.66349200	-0.07716500	0.52019000
O	1.09543600	-1.54201300	-1.67802100
P	-0.05347800	0.91083800	0.03594700
C	0.37508800	0.88292600	1.78813800
C	1.05091200	1.97529600	2.34788700
C	-0.00296200	-0.20010900	2.58508400
C	1.32832800	1.98557300	3.71048500
H	1.36852800	2.80945700	1.72795600
C	0.27852100	-0.17842400	3.94713800
H	-0.48945000	-1.06253200	2.14288100
C	0.93786700	0.91215800	4.50891600
H	1.85181100	2.82977000	4.14517800
H	-0.01061200	-1.02010700	4.56647700
H	1.15710100	0.92270400	5.57130600
C	1.38646100	1.38413100	-0.95133800
C	1.20142800	1.80212200	-2.27423200
C	2.66872600	1.34352800	-0.39558600
C	2.30371800	2.16047100	-3.04055500
H	0.20876800	1.85385700	-2.70975100
C	3.76406100	1.71671300	-1.16822700
H	2.81337800	0.99765000	0.62214800
C	3.58303900	2.12013100	-2.48778600
H	2.16154100	2.47734000	-4.06776500
H	4.75867800	1.68054000	-0.73674400
H	4.44020100	2.40471800	-3.08868000
C	-1.34901000	2.15810400	-0.23491100
C	-1.54890000	3.19102300	0.68478900
C	-2.12906100	2.09655400	-1.39896600
C	-2.51075400	4.16565100	0.43252000
H	-0.97571600	3.23602800	1.60335700
C	-3.08405000	3.07661400	-1.64383800
H	-2.01021400	1.27754300	-2.10266600
C	-3.27270800	4.11279900	-0.73036400
H	-2.66569600	4.96089800	1.15312100
H	-3.68617100	3.02520800	-2.54421300
H	-4.02292200	4.87271600	-0.92137300

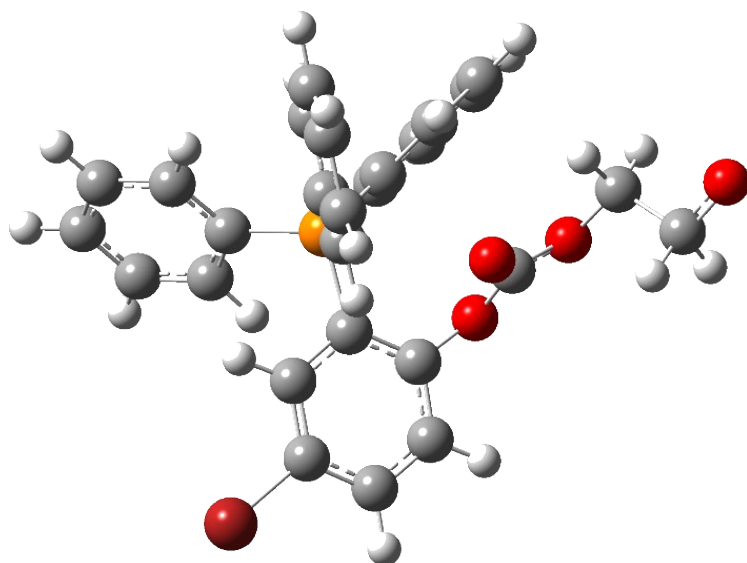


C	2.13308100	-1.55026300	-0.72305200
O	3.25104700	-1.62761800	-1.30451000
O	1.84471000	-1.46071800	0.46174300
C	4.65947200	-1.62836300	-0.16199700
H	5.35334100	-1.26786600	-0.90940300
H	4.26152900	-0.90339400	0.53478000
C	4.96967700	-2.93959200	0.42292700
H	5.22850600	-3.71353300	-0.32693500
H	4.15297600	-3.34385600	1.05341400
O	6.00959900	-2.31840900	1.06437500
Br	-4.60150200	-2.24257500	0.17957500

## In2A

0 1

C	-2.00167100	-3.09781000	-1.00241800
C	-0.67991600	-2.87618900	-1.35844400
C	-0.05808900	-1.67328000	-1.04152400
C	-0.76106100	-0.66323800	-0.37633000
C	-2.09751800	-0.89272000	-0.01668500
C	-2.69907200	-2.10285400	-0.32298000
H	-2.48697100	-4.03549300	-1.24675100
H	-0.10745600	-3.63125000	-1.88460200
H	-2.67092400	-0.12447500	0.49277700
O	1.23926600	-1.52037800	-1.47473000
P	-0.10015500	0.97176900	0.05224600
C	0.22204600	1.06342700	1.82085500
C	0.78061800	2.23445500	2.35309100
C	-0.08972700	-0.01541800	2.65219800
C	1.00682600	2.32484700	3.72135800
H	1.05204700	3.06510800	1.70678700
C	0.14192800	0.08726100	4.02022500
H	-0.48897000	-0.93441300	2.23739700
C	0.68437800	1.25343300	4.55328000
H	1.43959600	3.22886200	4.13469500
H	-0.09578600	-0.75023800	4.66644600
H	0.86536600	1.32633900	5.62037500
C	1.39048200	1.42202900	-0.86771300
C	1.28906700	1.70089200	-2.23612900
C	2.63035100	1.48454300	-0.22241700
C	2.43168700	2.02703000	-2.95544500
H	0.33061600	1.66530400	-2.74374500
C	3.76622500	1.82458300	-0.95157500
H	2.71741300	1.24737700	0.83263400
C	3.66815700	2.09061100	-2.31408500
H	2.35480500	2.23577900	-4.01660100
H	4.72748700	1.86966400	-0.45117800
H	4.55676000	2.34915300	-2.87994500
C	-1.43163300	2.11516800	-0.40925900



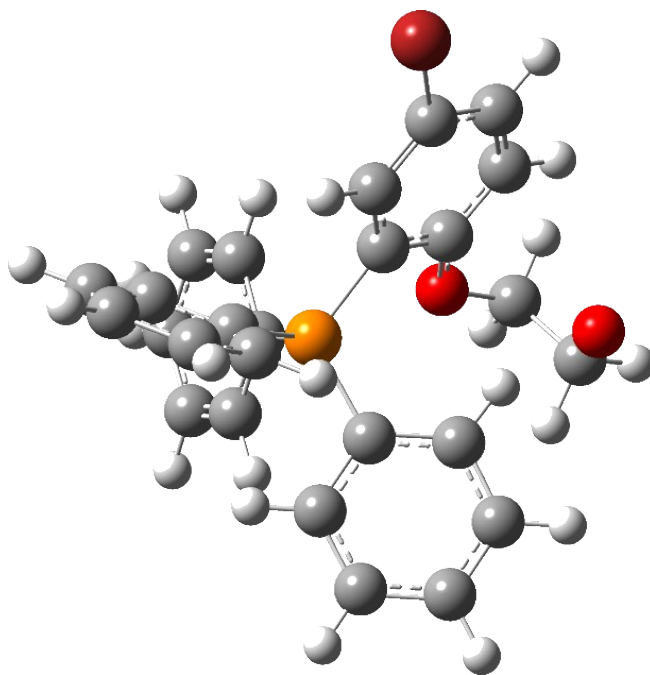


C	-1.77866400	3.19461200	0.40755100
C	-2.09831600	1.91038500	-1.62595000
C	-2.77728700	4.07434100	-0.00307800
H	-1.29302400	3.34596600	1.36489600
C	-3.08894300	2.79681900	-2.02848400
H	-1.86623900	1.05110100	-2.24861000
C	-3.42668700	3.88019000	-1.21860200
H	-3.04955200	4.90818200	0.63431100
H	-3.60231000	2.63470800	-2.96964100
H	-4.20513600	4.56734200	-1.53269300
C	2.20831200	-1.45081000	-0.50986700
O	3.36252800	-1.44077800	-1.11264000
O	1.95775200	-1.37383800	0.66951500
C	4.54933600	-1.43390000	-0.25600100
H	5.31853200	-0.95638900	-0.86583900
H	4.34014800	-0.82059700	0.62413600
C	4.99613700	-2.84496000	0.17234800
H	5.07621600	-3.42577400	-0.79515600
H	4.07783800	-3.29974500	0.65503400
O	6.09488200	-2.76531900	0.92150200
Br	-4.49672500	-2.39689200	0.16996800

## In1B

0 1

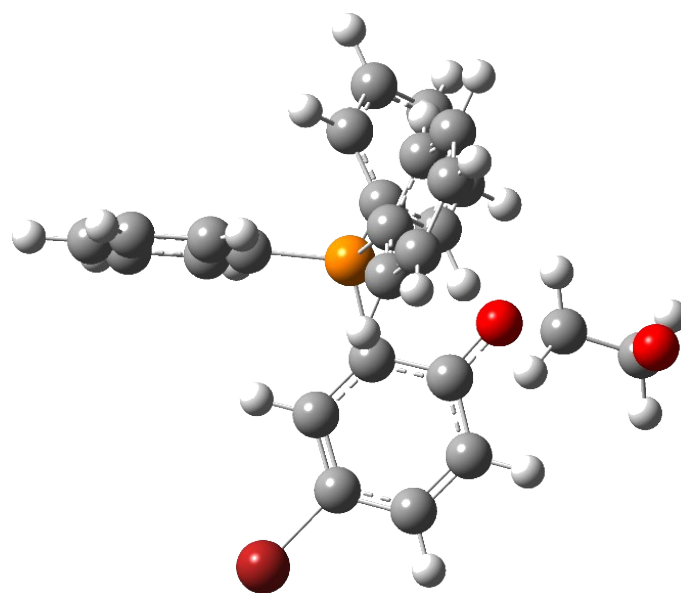
C	-2.94570800	-2.03659400	0.57066600
C	-1.69900700	-2.59509600	0.77814100
C	-0.54317300	-1.80664700	0.64647800
C	-0.68809100	-0.46131500	0.25324800
C	-1.95642300	0.10066500	0.04518700
C	-3.07371000	-0.69005800	0.21673400
H	-3.83390900	-2.64998200	0.67519300
H	-1.61579700	-3.64853600	1.00074800
H	-2.06049100	1.14059000	-0.24416000
O	0.70294900	-2.18264000	0.95793800
P	0.79550900	0.51373700	0.00166700
C	1.79244800	0.51427200	1.51042300
C	3.18368300	0.60938900	1.44264700
C	1.14330500	0.45763400	2.74818200
C	3.92506500	0.65832700	2.62024100
H	3.69081400	0.63274300	0.48345500
C	1.89243000	0.51142500	3.91848500
H	0.06171700	0.36346800	2.79614800
C	3.28151900	0.61264100	3.85400100
H	5.00624100	0.72732500	2.57029100
H	1.39197400	0.46568600	4.87962500
H	3.86348000	0.64861800	4.76890500
C	1.74446000	-0.04543600	-1.42696400
C	1.53483900	-1.31252200	-1.97995000



C	2.68926200	0.83888400	-1.97288800
C	2.30244100	-1.68436600	-3.08544900
H	0.80470200	-2.04739800	-1.59684800
C	3.44766800	0.44279700	-3.06640700
H	2.82326900	1.83385300	-1.55607200
C	3.25318400	-0.82301300	-3.62257600
H	2.14322300	-2.66752600	-3.51754600
H	4.17993800	1.12243400	-3.48836200
H	3.84303000	-1.12946500	-4.48063300
C	0.29754400	2.22057600	-0.33926500
C	0.31866400	3.18641700	0.67002000
C	-0.15063200	2.55008300	-1.62536500
C	-0.10946200	4.48164700	0.39067400
H	0.67235700	2.93547400	1.66501800
C	-0.58032900	3.84445300	-1.89284100
H	-0.15980700	1.80119400	-2.41274600
C	-0.55801700	4.80895400	-0.88581500
H	-0.08716200	5.23393900	1.17160000
H	-0.92699200	4.10112000	-2.88782900
H	-0.88852500	5.82001900	-1.09966800
C	1.04442800	-3.57984200	1.02018900
H	0.26792700	-4.11774900	1.57339200
H	1.97151200	-3.61060700	1.60001500
C	1.20191800	-4.10177800	-0.41935800
H	2.17696800	-3.66095800	-0.76980400
H	1.43080400	-5.19450700	-0.30141300
O	0.14146800	-3.79822200	-1.18464100
Br	-4.79808800	0.05234600	-0.03575200

### TS step1 mechanism B (iv = 651.06 cm<sup>-1</sup>)

01			
C	2.46217600	-2.50444800	0.73237300
C	1.10961200	-2.74707200	0.88609600
C	0.16269300	-1.70677400	0.72418800
C	0.66562300	-0.42818100	0.36257200
C	2.03429200	-0.18193100	0.20433000
C	2.92064700	-1.22465400	0.40051600
H	3.17834000	-3.30733100	0.87210500
H	0.75225900	-3.73614000	1.15426300
H	2.39679400	0.80062300	-0.08029900
O	-1.12166500	-1.86096400	0.88086200
P	-0.58222600	0.79150200	-0.02153800
C	-1.70690900	0.09028900	-1.25206000
C	-3.07859000	0.34174600	-1.19697900
C	-1.17209500	-0.71951200	-2.25994300
C	-3.91606500	-0.21883400	-2.15820700
H	-3.49632000	0.95510500	-0.40491200



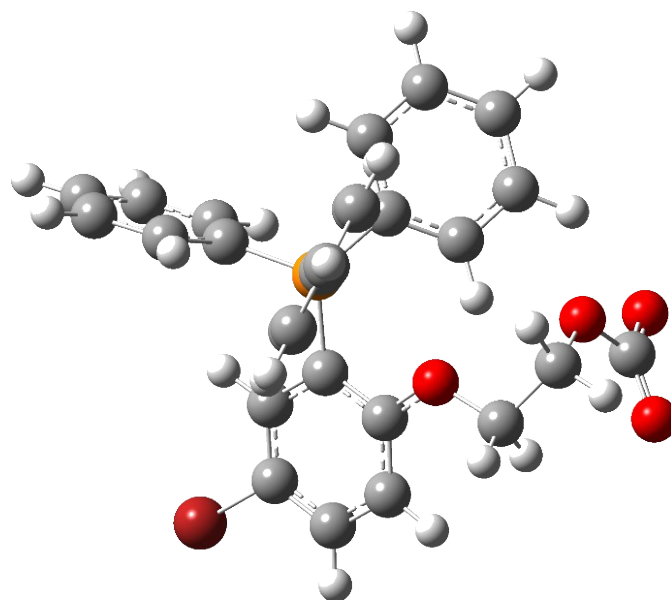
C	-2.01622900	-1.27117100	-3.21752100
H	-0.10658300	-0.93287900	-2.28645700
C	-3.38685800	-1.02209000	-3.16542200
H	-4.98332900	-0.03126800	-2.11424900
H	-1.60472100	-1.90420200	-3.99608000
H	-4.04476200	-1.46028400	-3.90843200
C	-1.49200100	1.37565500	1.42564000
C	-1.49129000	0.64051500	2.61419900
C	-2.18807400	2.58873100	1.34024200
C	-2.19371300	1.12193600	3.71502600
H	-0.96272600	-0.30413000	2.67076500
C	-2.89623400	3.05359000	2.44282900
H	-2.17180400	3.17183400	0.42332800
C	-2.89624700	2.32128800	3.62919100
H	-2.19216000	0.55585200	4.63999100
H	-3.43899000	3.99021000	2.37777900
H	-3.44387100	2.68959000	4.49051700
C	0.23529200	2.24233400	-0.72835400
C	0.23622600	2.46783800	-2.10692500
C	0.91397600	3.11593100	0.13205800
C	0.91891100	3.56636500	-2.62338100
H	-0.29615400	1.79769100	-2.77428100
C	1.59621800	4.20675900	-0.39329200
H	0.90572700	2.94684400	1.20557200
C	1.59756800	4.43136500	-1.76989200
H	0.91614800	3.74524500	-3.69293600
H	2.12298600	4.88291800	0.27116200
H	2.12729700	5.28647300	-2.17664700
C	-1.86207700	-3.25665700	-0.03122400
H	-1.04583000	-3.39914700	-0.73100800
H	-2.69913500	-2.66187500	-0.37606100
C	-2.20049800	-4.42454500	0.78922700
H	-1.32723500	-4.92149200	1.25914000
H	-2.93370400	-4.21395900	1.59188700
O	-2.68028700	-4.97295300	-0.37178900
Br	4.78167600	-0.92290600	0.19610300

## In2B

01

C	1.53781900	3.26701100	0.64327000
C	0.23646100	2.89398200	0.95729300
C	-0.19289400	1.58558800	0.71916600
C	0.71270900	0.64547700	0.18383700
C	2.02212400	1.02778600	-0.11579300
C	2.41991800	2.33798500	0.10445700
H	1.86437200	4.28481300	0.82469200
H	-0.43545300	3.62427700	1.38873000
H	2.73155500	0.31123900	-0.51326000

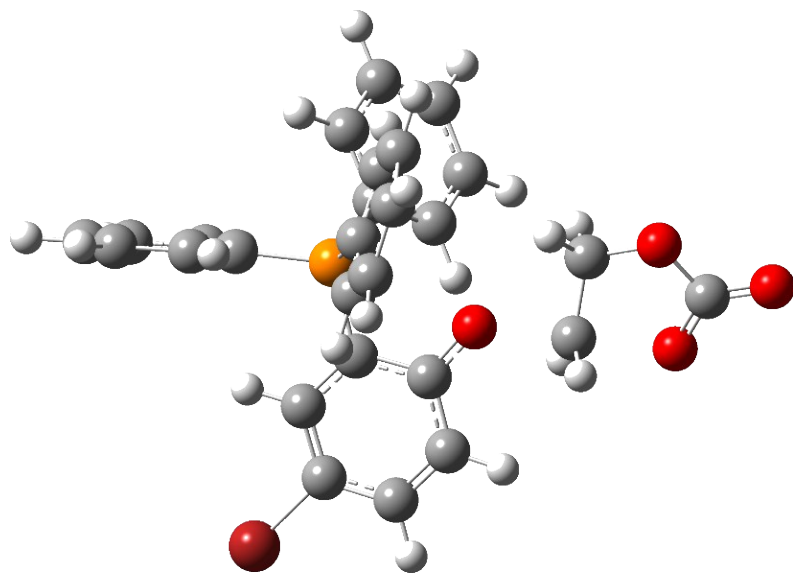
O	-1.43118200	1.13479100	0.97294500
P	0.20530300	-1.07923800	-0.01262300
C	-0.49357100	-1.64449000	1.55370000
C	-1.52777600	-2.58275600	1.55313800
C	0.02300300	-1.15064700	2.75682700
C	-2.04248500	-3.03189900	2.76641500
H	-1.93678900	-2.95263800	0.61792200
C	-0.49661700	-1.60831300	3.96228700
H	0.81837200	-0.40990900	2.75244700
C	-1.52811000	-2.54662000	3.96609800
H	-2.84980200	-3.75601400	2.77141300
H	-0.10136700	-1.22695300	4.89735700
H	-1.93475600	-2.89722600	4.90882500
C	-0.96682900	-1.35403900	-1.35286700
C	-1.91309200	-0.38257400	-1.68896000
C	-0.97704500	-2.60670900	-1.98692800
C	-2.87628200	-0.66371600	-2.65461600
H	-1.94915600	0.57519100	-1.18524500
C	-1.93568200	-2.87233200	-2.95729500
H	-0.24564500	-3.36628700	-1.72738900
C	-2.88274500	-1.90269700	-3.28856000
H	-3.61851500	0.10337800	-2.85797600
H	-1.94425100	-3.83818800	-3.45083900
H	-3.63350300	-2.12126700	-4.04146000
C	1.69345400	-2.03609900	-0.37817000
C	2.33406400	-2.76300500	0.62815900
C	2.22933200	-1.99023900	-1.67268000
C	3.51558300	-3.44077700	0.33821700
H	1.91543700	-2.80594200	1.62857000
C	3.41113900	-2.66669100	-1.94984000
H	1.72554500	-1.43348300	-2.45811500
C	4.05297000	-3.39048300	-0.94474600
H	4.01275500	-4.00796900	1.11725800
H	3.82857600	-2.63097300	-2.94998300
H	4.97388200	-3.91950400	-1.16597400
C	-2.43611700	2.05448600	1.42674800
H	-2.40716100	2.96716000	0.82645700
H	-2.25744400	2.29072900	2.48196200
C	-3.78090100	1.39037800	1.21850600
H	-3.79463000	0.41205700	1.71038300
H	-4.54796200	2.03277300	1.66093600
O	-4.02829700	1.16318100	-0.14961200
C	-4.33663600	2.31646800	-0.92757200
O	-4.40561100	2.06376600	-2.14031900
O	-4.48066200	3.38212100	-0.30551500
Br	4.19033300	2.84834300	-0.32079700



### TS step 3 mechanism B (iv = 643.89cm<sup>-1</sup>)

0 1

C	0.91595600	3.47779100	0.31342600
C	-0.31869800	2.86882400	0.45407000
C	-0.45063100	1.46157900	0.35462500
C	0.74002200	0.72157900	0.10733500
C	1.98869400	1.33898700	-0.01811000
C	2.06399300	2.71627900	0.07789500
H	0.99738600	4.55689100	0.39298600
H	-1.19476600	3.47405000	0.65655300
H	2.88509200	0.75228200	-0.19245300
O	-1.56979300	0.80854600	0.47036500
P	0.55197200	-1.05371200	0.01043700
C	-0.27301500	-1.66700900	1.49715500
C	-1.10505600	-2.78712900	1.44155500
C	-0.03630800	-1.01671300	2.71274800
C	-1.69709600	-3.25925200	2.61002300
H	-1.30469800	-3.28281700	0.49705600
C	-0.62793300	-1.49944000	3.87474300
H	0.59596100	-0.13382800	2.74774800
C	-1.45765700	-2.61860800	3.82299300
H	-2.34816700	-4.12556600	2.56942500
H	-0.44821800	-0.99654900	4.81866100
H	-1.92215300	-2.98866500	4.73094000
C	-0.33166800	-1.57206900	-1.47874200
C	-1.10203000	-0.66302000	-2.20869900
C	-0.21781000	-2.90295500	-1.90193700
C	-1.77321000	-1.09322800	-3.34951400
H	-1.17797600	0.36964000	-1.88792400
C	-0.89878600	-3.32477800	-3.03875600
H	0.40746800	-3.60419600	-1.35552600
C	-1.67732400	-2.42092400	-3.75942800
H	-2.36989000	-0.38791900	-3.91788500
H	-0.81437400	-4.35555000	-3.36471200
H	-2.20457400	-2.75079500	-4.64844300
C	2.19817300	-1.79755400	-0.08107200
C	2.80317900	-2.32891700	1.06080700
C	2.88549600	-1.77554600	-1.30185100
C	4.09756800	-2.83634400	0.97958500
H	2.26923100	-2.35274100	2.00561000
C	4.17869100	-2.28032100	-1.37142900
H	2.41337400	-1.36964300	-2.19234100
C	4.78295200	-2.81045700	-0.23180800
H	4.56637100	-3.25359100	1.86396700
H	4.71273700	-2.26344800	-2.31511400
H	5.79089300	-3.20737700	-0.29151100
C	-3.16740200	1.67162800	0.07829300



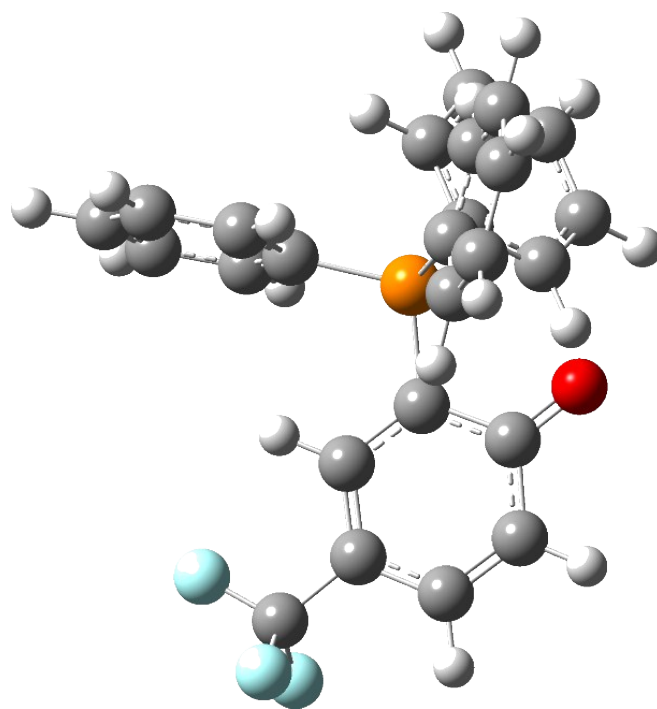
H	-2.70402300	2.18925600	-0.74949800
H	-3.20252400	2.16626400	1.03931100
C	-3.88473900	0.34559800	-0.10210400
H	-3.74395700	-0.01047200	-1.12976300
H	-3.47771700	-0.39275200	0.58799700
O	-5.26335000	0.48326900	0.18519800
C	-5.72744700	1.75103000	-0.12036300
O	-4.78923400	2.56508900	-0.41585800
O	-6.93179100	1.94310900	-0.06491500
Br	3.74230900	3.57654000	-0.11281700

**CF<sub>3</sub>**

### Organocatalyst

O 1

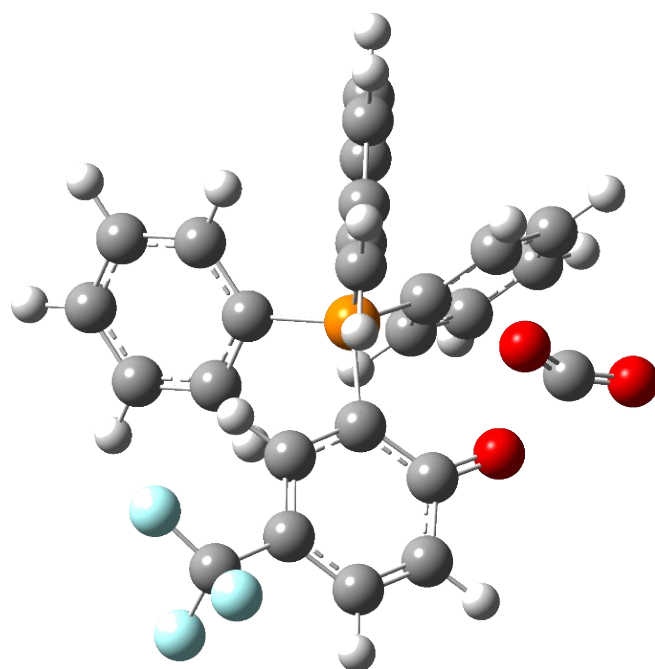
C	3.21421800	-1.93105400	0.89631600
C	2.06519900	-2.63155600	1.14678200
C	0.75893100	-2.05406200	0.92637800
C	0.77160800	-0.70395700	0.40904200
C	1.95820900	-0.00736600	0.14557600
C	3.17587700	-0.60767700	0.39603100
H	4.18032300	-2.39539900	1.08007900
H	2.09917300	-3.64757800	1.52649300
H	1.93140300	1.00112500	-0.25581200
O	-0.31845500	-2.66088900	1.15862800
P	-0.82227400	-0.02547100	0.03672800
C	-1.73815200	-1.09909100	-1.09819000
C	-3.12677000	-0.99024900	-1.20242300
C	-1.03396500	-1.98277100	-1.92019800
C	-3.80937000	-1.76524800	-2.13573600
H	-3.67720500	-0.31219000	-0.55692000
C	-1.72355000	-2.75291000	-2.85088600
H	0.04459100	-2.06921900	-1.82488700
C	-3.10894500	-2.64387500	-2.95889000
H	-4.88799000	-1.68364300	-2.21622200
H	-1.17875300	-3.44163600	-3.48763200
H	-3.64419500	-3.24717200	-3.68474400
C	-1.85406000	0.34706100	1.48233500
C	-1.71324800	-0.38697700	2.66488400
C	-2.79731800	1.38008900	1.40217200
C	-2.51496700	-0.07973800	3.76069600
H	-1.00370000	-1.20573000	2.70746800
C	-3.60002600	1.67128900	2.50058100
H	-2.90007600	1.96393000	0.49191900
C	-3.45568900	0.94460500	3.68016000
H	-2.40451900	-0.64512700	4.67991600
H	-4.33036100	2.47046900	2.43480200
H	-4.07680300	1.17878600	4.53855100



C	-0.57766600	1.55929600	-0.80981800
C	-0.73314100	1.65922500	-2.19404800
C	-0.17682400	2.67612400	-0.06406500
C	-0.48979100	2.87473800	-2.83017700
H	-1.04563100	0.79636300	-2.77399200
C	0.06728500	3.88402200	-0.70669800
H	-0.06164700	2.60241900	1.01418300
C	-0.09100300	3.98318600	-2.08908700
H	-0.61532300	2.95297500	-3.90465000
H	0.37596200	4.74834600	-0.12884400
H	0.09542100	4.92889400	-2.58714200
C	4.45602800	0.09859200	0.12829900
F	5.20522100	-0.52703300	-0.80480200
F	4.27087100	1.35785900	-0.30323200
F	5.23989200	0.17177400	1.22506200

### TS step1 mechanism A (iv = 265.34 cm<sup>-1</sup>)

0 1			
C	-2.97393200	-2.24915400	-0.84746300
C	-1.72999900	-2.73261800	-1.16449000
C	-0.53289700	-1.99619900	-0.89622400
C	-0.71192500	-0.70472800	-0.31207900
C	-1.99415300	-0.22012600	0.00596400
C	-3.11407900	-0.98436200	-0.24279000
H	-3.85945400	-2.84252500	-1.05854700
H	-1.60758000	-3.70780600	-1.62352800
H	-2.11566400	0.76681900	0.44480000
O	0.61476400	-2.50210500	-1.18447400
P	0.65325900	0.40855800	-0.00237600
C	1.03665300	0.55514800	1.75927500
C	2.16963600	1.26812200	2.17285500
C	0.17762600	-0.00990300	2.70453400
C	2.42828300	1.42496100	3.53041100
H	2.85477100	1.69030000	1.44267500
C	0.44380300	0.15282700	4.06060500
H	-0.67965800	-0.59177600	2.38262300
C	1.56389100	0.87052900	4.47281900
H	3.30623700	1.97608700	3.84904200
H	-0.22214400	-0.28813400	4.79421400
H	1.76876500	0.99318000	5.53120400
C	2.17842700	0.01288900	-0.89872900
C	2.26497700	0.32334300	-2.25939500
C	3.25824300	-0.58636600	-0.24408800
C	3.42320600	0.01621400	-2.96432800
H	1.43858300	0.80555300	-2.77131100
C	4.41514800	-0.88542900	-0.95675100
H	3.19328500	-0.83045400	0.81116900

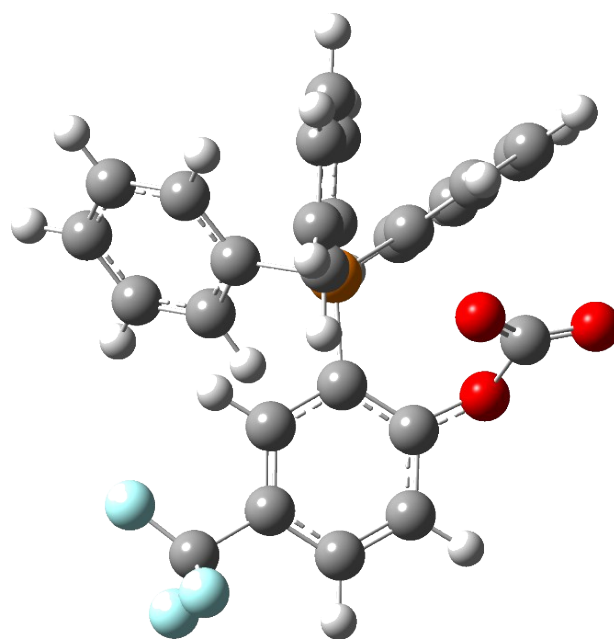


C	4.49779400	-0.58797800	-2.31444600
H	3.48661600	0.25405200	-4.02056900
H	5.24958700	-1.35566200	-0.44800900
H	5.40102500	-0.82446600	-2.86691900
C	0.09765800	2.03881300	-0.59740400
C	0.43941900	3.21625500	0.07300600
C	-0.65305700	2.10238200	-1.77981300
C	0.04491600	4.44769800	-0.44410300
H	0.99780100	3.18236300	1.00177700
C	-1.03628800	3.33610700	-2.29323400
H	-0.95195200	1.19076900	-2.28956300
C	-0.68616400	4.50912300	-1.62701500
H	0.30700100	5.35779200	0.08429100
H	-1.61654500	3.37856100	-3.20846800
H	-0.99295700	5.47037000	-2.02579100
C	-4.48099400	-0.49040800	0.09418900
C	1.69258100	-3.06609600	0.28980900
O	2.47162800	-3.78749500	-0.23032900
O	1.23546600	-2.50368200	1.23406300
F	-4.46032500	0.71060900	0.69246600
F	-5.12909400	-1.33370100	0.91981700
F	-5.25992400	-0.37395100	-0.99830700

## In1A

0 1

C	-3.02929900	-2.31641200	-0.51729600
C	-1.78424300	-2.88103100	-0.71261100
C	-0.61090400	-2.13532700	-0.51842000
C	-0.72065200	-0.77894300	-0.15632600
C	-1.98994600	-0.21617400	0.04836300
C	-3.13098100	-0.98098200	-0.11723600
H	-3.92721900	-2.90785100	-0.66811200
H	-1.67582800	-3.91776900	-1.00961100
H	-2.08939400	0.82955400	0.32323000
O	0.55408100	-2.76355100	-0.73552100
P	0.69218700	0.33715900	-0.00443000
C	1.10074500	0.72139700	1.71180300
C	2.25800600	1.45341400	1.99850200
C	0.23379000	0.33640800	2.73618900
C	2.53855100	1.80664600	3.31536900
H	2.94225000	1.74255700	1.20532100
C	0.52088900	0.69753500	4.04783600
H	-0.64249400	-0.26269900	2.51222300
C	1.66958300	1.43193900	4.33708800
H	3.43718000	2.37047500	3.54001600
H	-0.14833300	0.39568400	4.84605500
H	1.89168600	1.70663100	5.36292800
C	2.17777900	-0.16574400	-0.91544100

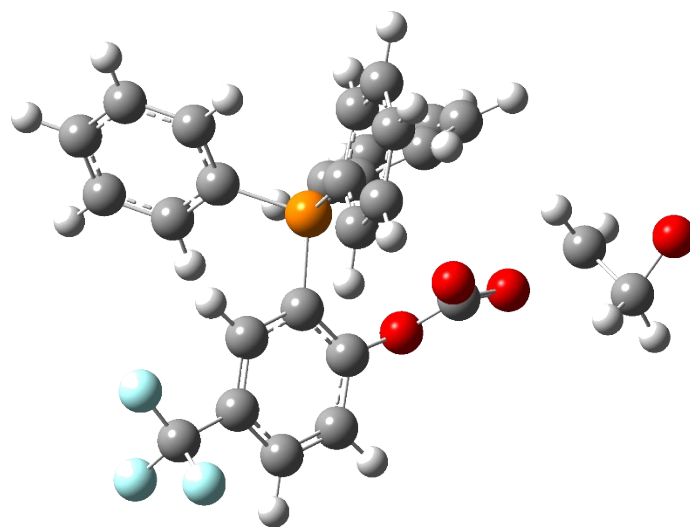




C	2.21220300	0.00944200	-2.30390400
C	3.29262600	-0.67687200	-0.24309700
C	3.35316800	-0.34202600	-3.01565700
H	1.36150300	0.42280600	-2.83483200
C	4.43428800	-1.01171300	-0.96399300
H	3.25335900	-0.84078100	0.82809400
C	4.46556000	-0.84760800	-2.34598600
H	3.37403300	-0.21161500	-4.09199200
H	5.29663700	-1.41049900	-0.44109900
H	5.35733200	-1.11415200	-2.90349400
C	0.11498300	1.88278600	-0.78508000
C	0.44681800	3.12824100	-0.24516900
C	-0.63954400	1.81752400	-1.96591000
C	0.04096900	4.29541000	-0.88796800
H	1.00651200	3.19894200	0.68046000
C	-1.03573400	2.98664900	-2.60441800
H	-0.93374700	0.85733600	-2.38025400
C	-0.69378700	4.22662300	-2.06732700
H	0.29734300	5.25797900	-0.45893300
H	-1.61905600	2.92809900	-3.51679900
H	-1.00918000	5.13784100	-2.56461300
C	-4.48953900	-0.39540300	0.11961000
C	1.50956800	-2.87711900	0.40267800
O	2.39051500	-3.68190100	0.15918500
O	1.24429800	-2.12945700	1.35079000
F	-4.44006800	0.92326200	0.35628300
F	-5.09944100	-0.96628100	1.17207400
F	-5.29781400	-0.58505100	-0.93584100

### TS step 2 mechanism A (iv = 628.82cm<sup>-1</sup>)

01			
C	-2.19154300	-3.04186900	-1.11038600
C	-0.88565300	-2.84842100	-1.52390900
C	-0.20055500	-1.67988600	-1.18406200
C	-0.84498300	-0.68068800	-0.44073200
C	-2.16894300	-0.88701800	-0.02536400
C	-2.82802400	-2.06068100	-0.34855300
H	-2.71716500	-3.95481200	-1.37148400
H	-0.36059900	-3.59467600	-2.10850200
H	-2.69026500	-0.12651200	0.54799500
O	1.07053800	-1.55856700	-1.65982500
P	-0.09731800	0.89938700	0.03216600
C	0.34662900	0.90183700	1.78086000
C	1.00924800	2.01238900	2.32014200
C	-0.00731800	-0.17606600	2.59553000
C	1.29765900	2.04567200	3.68006800
H	1.30878300	2.84297400	1.68662900

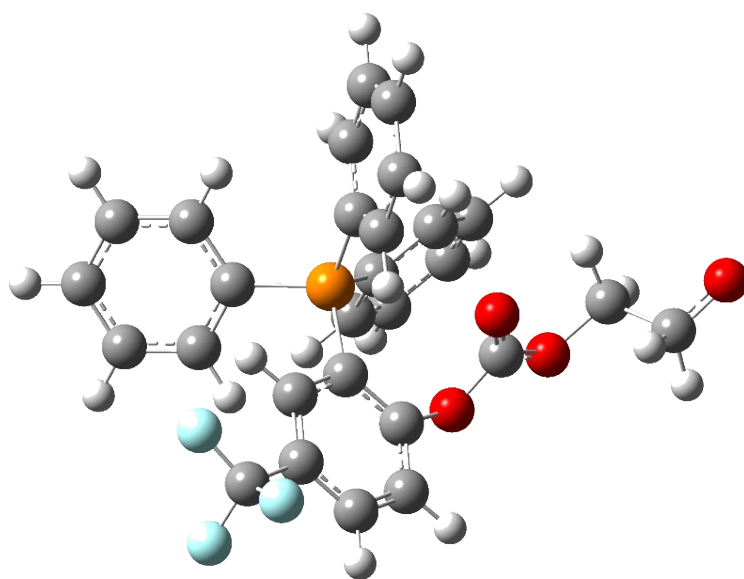


C	0.28486700	-0.13131200	3.95475200
H	-0.48266500	-1.05269700	2.16939700
C	0.93107000	0.97715900	4.49624100
H	1.81114400	2.90406300	4.09861400
H	0.01387700	-0.96893000	4.58765000
H	1.15869100	1.00567400	5.55653600
C	1.32736500	1.38236300	-0.97274300
C	1.12621700	1.78295900	-2.29862200
C	2.61454500	1.36644500	-0.42685500
C	2.21718600	2.14873000	-3.07765800
H	0.12960300	1.81484200	-2.72688500
C	3.69827800	1.74607500	-1.21244700
H	2.77238400	1.03413200	0.59351700
C	3.50128900	2.13234700	-2.53481100
H	2.06223700	2.45171800	-4.10721500
H	4.69673300	1.72886700	-0.78873300
H	4.34972100	2.42196700	-3.14560100
C	-1.41447100	2.12261900	-0.24296100
C	-1.62815700	3.15870900	0.67016500
C	-2.19853100	2.03935500	-1.40299900
C	-2.60676700	4.11558400	0.41456200
H	-1.05267900	3.21981700	1.58639700
C	-3.17030600	3.00191900	-1.65126900
H	-2.06947800	1.21737900	-2.10145100
C	-3.37203500	4.04187600	-0.74491200
H	-2.77181400	4.91354100	1.12993000
H	-3.77493100	2.93405000	-2.54890600
H	-4.13481700	4.78846500	-0.93875400
C	-4.24011700	-2.29814900	0.10148700
C	2.11829100	-1.53352000	-0.71348000
O	3.23085200	-1.60170300	-1.30523400
O	1.83790700	-1.43100300	0.47159200
C	4.64772500	-1.57815700	-0.17789900
H	5.33310400	-1.22092100	-0.93469300
H	4.25250400	-0.84825500	0.51546300
C	4.97429400	-2.88074200	0.41866000
H	5.23117300	-3.66008100	-0.32646700
H	4.16608400	-3.28514000	1.06016600
O	6.01568800	-2.24747500	1.04489400
F	-4.72449300	-1.27101400	0.81053500
F	-4.33005200	-3.39594000	0.86746800
F	-5.06048700	-2.49120900	-0.94293000

## In2A

0 1

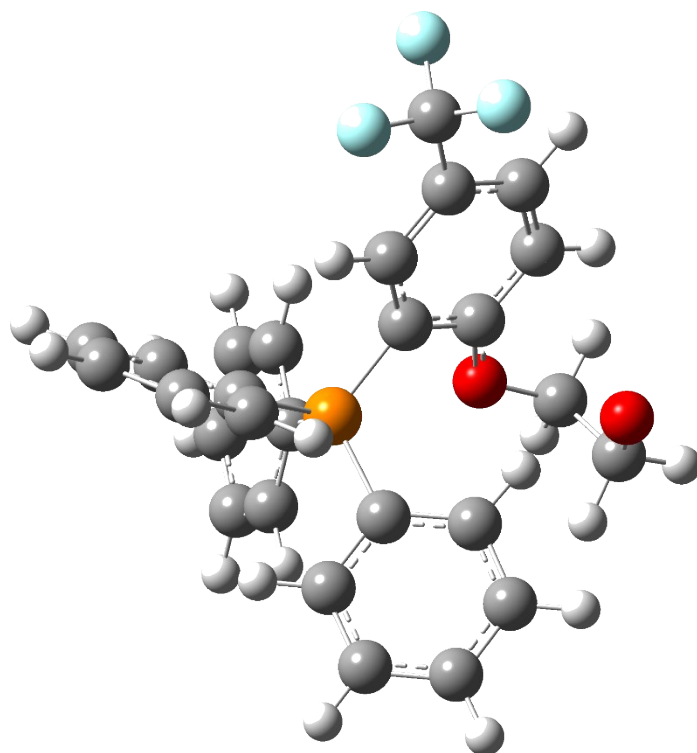
C	-2.00541900	-3.13811300	-0.98525800
C	-0.69094000	-2.90887600	-1.35462300
C	-0.07854100	-1.69877400	-1.03747800
C	-0.78293400	-0.69250800	-0.36788300
C	-2.11334700	-0.93851600	0.00256700
C	-2.71007900	-2.15181100	-0.29482600
H	-2.48255100	-4.08244300	-1.22655700
H	-0.11213800	-3.65520000	-1.88573300
H	-2.68841200	-0.17658200	0.51990700
O	1.21388900	-1.53807900	-1.47648200
P	-0.13878800	0.95172400	0.04947800
C	0.18656000	1.05637600	1.81686000
C	0.72472400	2.23975200	2.34292200
C	-0.10345400	-0.02439100	2.65365900
C	0.95165500	2.34041700	3.71035400
H	0.97984200	3.07236600	1.69246100
C	0.12855700	0.08872300	4.02079600
H	-0.48580500	-0.95295800	2.24423000
C	0.65019200	1.26714800	4.54770700
H	1.36861700	3.25405700	4.11872400
H	-0.09262800	-0.75001600	4.67129800
H	0.83133000	1.34827300	5.61417900
C	1.34272700	1.41699800	-0.87777400
C	1.23528600	1.68249000	-2.24842000
C	2.58158300	1.50724700	-0.23383500
C	2.37151100	2.02310400	-2.97122900
H	0.27715700	1.62483300	-2.75473200
C	3.71062800	1.86194200	-0.96646900
H	2.67333900	1.28011100	0.82302400
C	3.60691900	2.11485400	-2.33103200
H	2.29038700	2.22129700	-4.03407900
H	4.67123800	1.92890100	-0.46730500
H	4.49038900	2.38476900	-2.89961000
C	-1.48714800	2.07456500	-0.41396100
C	-1.84537400	3.15392000	0.39804200
C	-2.15584200	1.85385300	-1.62674800
C	-2.85723900	4.01789400	-0.01350300
H	-1.35851500	3.31692800	1.35274100
C	-3.16006800	2.72457100	-2.03014500
H	-1.91461400	0.99446500	-2.24580100
C	-3.50902200	3.80798100	-1.22508900
H	-3.13796400	4.85161400	0.62033800
H	-3.67528200	2.55008200	-2.96807200
H	-4.29807200	4.48264700	-1.53969100
C	-4.13354300	-2.42270800	0.10340200



C	2.18785300	-1.43810100	-0.51732200
O	3.33752400	-1.41095400	-1.12680600
O	1.94137200	-1.35571200	0.66229900
C	4.52824300	-1.37377100	-0.27499500
H	5.28703200	-0.89298700	-0.89518800
H	4.31232500	-0.75062000	0.59648300
C	4.99845500	-2.77090100	0.17364400
H	5.09027700	-3.36417800	-0.78512000
H	4.08782200	-3.23456500	0.66207300
O	6.09467800	-2.66083400	0.92283100
F	-4.22380400	-3.52593500	0.85935000
F	-4.66192300	-1.40897800	0.79950700
F	-4.91019600	-2.62533200	-0.97070800

## In1B

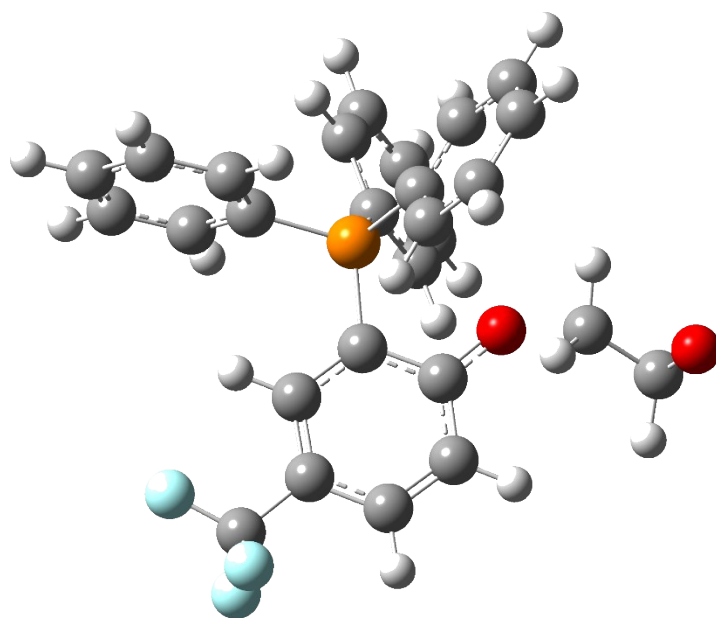
0 1			
C	-3.04192600	-1.94178400	0.56166100
C	-1.82024200	-2.54194000	0.77508200
C	-0.63763400	-1.78935100	0.63561200
C	-0.73691000	-0.43806200	0.24159700
C	-1.98649300	0.15821800	0.02807200
C	-3.13467500	-0.59019700	0.19460600
H	-3.94930100	-2.52840400	0.67173300
H	-1.76814500	-3.59457800	1.00968200
H	-2.05624900	1.20053700	-0.26317400
O	0.59097800	-2.20308900	0.95346200
P	0.77716900	0.49197200	0.00616000
C	1.76673900	0.44825900	1.51913800
C	3.16123600	0.47366700	1.45881900
C	1.10931400	0.42376600	2.75371000
C	3.89785900	0.48599900	2.64043200
H	3.67394700	0.47047100	0.50237500
C	1.85381200	0.44075700	3.92800500
H	0.02412400	0.38249300	2.79632300
C	3.24653400	0.47274100	3.87078600
H	4.98134900	0.50071700	2.59619700
H	1.34652000	0.42048700	4.88642100
H	3.82498800	0.48041300	4.78855500
C	1.71914600	-0.08055500	-1.42120300
C	1.46989200	-1.33107000	-1.99451100
C	2.69835300	0.77830900	-1.94615900
C	2.23314400	-1.71293400	-3.09987500
H	0.71015900	-2.04252400	-1.62460200
C	3.45139100	0.37264500	-3.03968400
H	2.86272900	1.76168300	-1.51291000
C	3.21722800	-0.87702700	-3.61662500
H	2.04504800	-2.68334400	-3.54890700
H	4.20986900	1.03269700	-3.44611800



H	3.80281000	-1.19083000	-4.47494700
C	0.33288900	2.21604400	-0.32412800
C	0.38190100	3.17587300	0.68980600
C	-0.09978700	2.56607800	-1.61017500
C	-0.00351400	4.48559400	0.41542000
H	0.72506200	2.90960600	1.68441100
C	-0.48750900	3.87465700	-1.87248900
H	-0.12974400	1.82186700	-2.40148400
C	-0.43770000	4.83311400	-0.86067900
H	0.04153300	5.23315200	1.19983900
H	-0.82240800	4.14723700	-2.86724700
H	-0.73452800	5.85533700	-1.07084900
C	-4.48618800	0.01547800	-0.00598900
C	0.89311500	-3.61007800	1.00065500
H	0.10623500	-4.13124800	1.55455700
H	1.82426200	-3.67255700	1.57082100
C	1.02011500	-4.11612600	-0.44897600
H	2.00879200	-3.70971600	-0.80110400
H	1.20299000	-5.21864300	-0.35004200
O	-0.03369100	-3.75580800	-1.19877000
F	-5.21766300	-0.01105400	1.12361100
F	-4.41651600	1.29494900	-0.40224800
F	-5.20208800	-0.65119600	-0.92880000

### TS step1 mechanism B (iv = 647.75 cm<sup>-1</sup>)

01			
C	-2.48536200	2.52558100	0.65597400
C	-1.13695700	2.77449600	0.79980700
C	-0.19359500	1.72348700	0.66393900
C	-0.69769600	0.43475300	0.33315900
C	-2.06597200	0.19220200	0.18642700
C	-2.95809600	1.23672500	0.35832900
H	-3.19801000	3.33664000	0.77770800
H	-0.77337700	3.76749400	1.04248700
H	-2.43034500	-0.79707400	-0.07195000
O	1.08752300	1.87618300	0.81987300
P	0.54647400	-0.79843000	-0.01957000
C	1.68695600	-0.12460500	-1.25139100
C	3.05338000	-0.40245400	-1.19279500
C	1.16955100	0.68936600	-2.26495000
C	3.90296500	0.13588900	-2.15627200
H	3.45829000	-1.01909600	-0.39664100
C	2.02561300	1.21942300	-3.22407100
H	0.10827900	0.92242400	-2.29453700
C	3.39114300	0.94388600	-3.16846200
H	4.96625000	-0.07254500	-2.10974100
H	1.62766500	1.85603300	-4.00672700



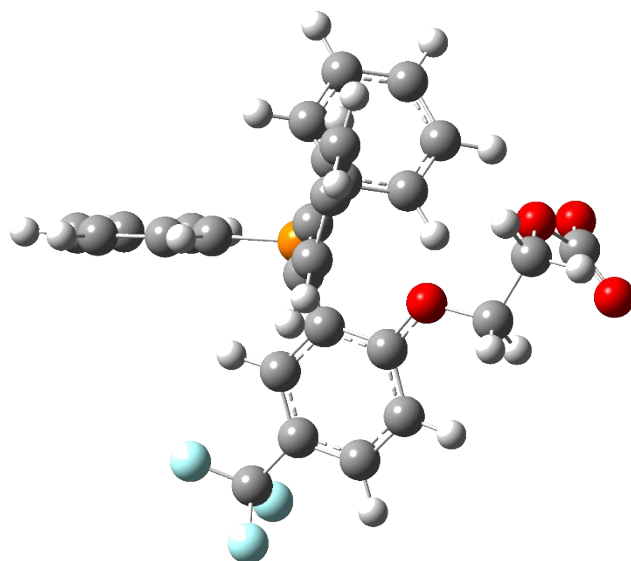
H	4.05863000	1.36508200	-3.91271800
C	1.43817000	-1.35839200	1.44798000
C	1.42518800	-0.59811400	2.62066800
C	2.13092600	-2.57525600	1.39736000
C	2.11221100	-1.05753500	3.74033800
H	0.89735500	0.34812600	2.65188900
C	2.82325000	-3.01863200	2.51878700
H	2.12365600	-3.17799700	0.49308800
C	2.81126700	-2.26082900	3.68909400
H	2.10109100	-0.47175000	4.65285400
H	3.36359600	-3.95809200	2.48083700
H	3.34669900	-2.61233800	4.56494900
C	-0.27206700	-2.25584400	-0.71072200
C	-0.27296500	-2.49188100	-2.08770100
C	-0.95264800	-3.12119600	0.15634700
C	-0.95733200	-3.59303700	-2.59588500
H	0.26059400	-1.82762500	-2.76006300
C	-1.63660700	-4.21487500	-0.36101100
H	-0.94458700	-2.94360600	1.22844700
C	-1.63776900	-4.45016600	-1.73578100
H	-0.95452100	-3.78025700	-3.66401000
H	-2.16498000	-4.88494000	0.30830800
H	-2.16889700	-5.30752800	-2.13592800
C	-4.43062800	1.02407300	0.22711500
C	1.83419400	3.29069900	-0.04307300
H	1.03917100	3.43852600	-0.76587100
H	2.68724800	2.71165600	-0.37472900
C	2.14343200	4.45191300	0.80062200
H	1.25424500	4.93446500	1.25629800
H	2.85534400	4.23202300	1.62034300
O	2.65078100	5.02588900	-0.33477400
F	-4.97287200	1.82951400	-0.70504900
F	-4.73663200	-0.23713800	-0.11290900
F	-5.08163500	1.29453400	1.37412500

## In2B

0 1

C	1.47315100	3.32812600	0.63376500
C	0.18431800	2.92667300	0.94942000
C	-0.20773000	1.60462800	0.70765400
C	0.72236700	0.68677900	0.17236300
C	2.01825000	1.10734200	-0.12876800
C	2.38697000	2.42700200	0.08999400
H	1.77285500	4.35404000	0.82379100
H	-0.50750800	3.63468100	1.38579100
H	2.74683800	0.40774900	-0.52266200
O	-1.42949700	1.12112600	0.96074300
P	0.26220200	-1.05235200	-0.00929700

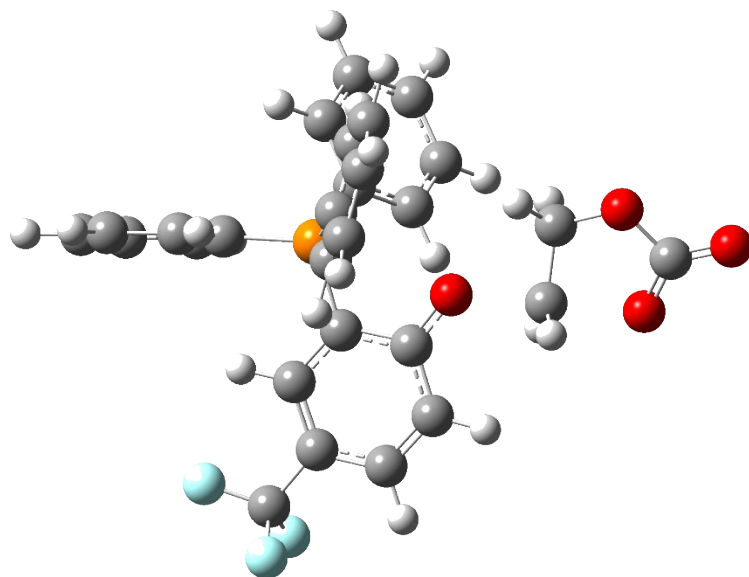
C	-0.41653100	-1.62543200	1.56333000
C	-1.42700700	-2.58920600	1.57232100
C	0.09321400	-1.11334300	2.76179900
C	-1.92424800	-3.04569900	2.79017300
H	-1.83126200	-2.97352400	0.64093100
C	-0.40869100	-1.57855400	3.97192000
H	0.86992700	-0.35309600	2.75066800
C	-1.41614900	-2.54250400	3.98510600
H	-2.71283200	-3.79015500	2.80255200
H	-0.01798600	-1.18370100	4.90328700
H	-1.80896100	-2.89925100	4.93136500
C	-0.90339100	-1.37570800	-1.34431400
C	-1.87740900	-0.43776100	-1.69618100
C	-0.87662400	-2.63789500	-1.95875400
C	-2.82983000	-0.76244200	-2.65892900
H	-1.94328400	0.52704000	-1.20904200
C	-1.82549000	-2.94720500	-2.92529400
H	-0.12352200	-3.37137400	-1.68650800
C	-2.79981000	-2.01086200	-3.27327100
H	-3.59241000	-0.01966000	-2.87550700
H	-1.80452100	-3.92072900	-3.40315200
H	-3.54253700	-2.26325200	-4.02364500
C	1.77541800	-1.96995400	-0.37141800
C	2.43221300	-2.68192100	0.63500100
C	2.30968600	-1.91291400	-1.66629700
C	3.62812000	-3.33392900	0.34480700
H	2.01451500	-2.73404000	1.63531600
C	3.50586900	-2.56332600	-1.94364100
H	1.79312100	-1.36809300	-2.45186400
C	4.16367400	-3.27262800	-0.93840700
H	4.13766300	-3.89008700	1.12377500
H	3.92205200	-2.51895200	-2.94395900
H	5.09566500	-3.78189000	-1.15966400
C	3.76126700	2.90406200	-0.26979400
C	-2.45974400	2.00404600	1.43475000
H	-2.46237000	2.92428200	0.84602200
H	-2.28035100	2.23003700	2.49178100
C	-3.78317400	1.29945100	1.22364900
H	-3.77033300	0.32291200	1.71901200
H	-4.57069500	1.92076800	1.66042300
O	-4.01504500	1.05997100	-0.14465200
C	-4.34341300	2.20176400	-0.93183200
O	-4.38345400	1.94334600	-2.14452600
O	-4.52900400	3.26437500	-0.31574100
F	4.29222900	3.65615400	0.70717300
F	4.60247900	1.88642400	-0.50091900
F	3.75054200	3.66736300	-1.37522800



### TS step 3 mechanism B (iv = 644.08cm<sup>-1</sup>)

0 1

C	0.81602300	3.53255700	0.20774100
C	-0.39890000	2.89165400	0.33514100
C	-0.47500900	1.47550500	0.26711900
C	0.74540800	0.76947200	0.05858400
C	1.97059500	1.42977700	-0.05372000
C	2.00443500	2.81225000	0.01395200
H	0.85575000	4.61674500	0.26812000
H	-1.30172900	3.46623500	0.50445100
H	2.89056600	0.87054300	-0.19268700
O	-1.56794700	0.78561500	0.38004600
P	0.61796600	-1.01254700	0.01456300
C	-0.19185400	-1.60503500	1.51854700
C	-1.00308300	-2.74154800	1.49352200
C	0.03458900	-0.91990100	2.71702000
C	-1.58354500	-3.19520300	2.67501000
H	-1.19635400	-3.26381600	0.56217400
C	-0.54545200	-1.38432700	3.89234100
H	0.65089800	-0.02509300	2.72971200
C	-1.35360800	-2.52019000	3.87097900
H	-2.21839200	-4.07420600	2.65752800
H	-0.37251000	-0.85486100	4.82289200
H	-1.80872200	-2.87634000	4.78918800
C	-0.24043600	-1.61489600	-1.45764300
C	-1.03489800	-0.76267900	-2.22969700
C	-0.08013400	-2.95766100	-1.82434600
C	-1.68125100	-1.26216500	-3.35672500
H	-1.15006900	0.27900100	-1.95278700
C	-0.73743100	-3.44899800	-2.94690700
H	0.56283200	-3.61458000	-1.24449300
C	-1.53842600	-2.60166500	-3.71052300
H	-2.29607600	-0.60165000	-3.95848200
H	-0.61661300	-4.48925800	-3.22822500
H	-2.04600500	-2.98570800	-4.58920300
C	2.28986700	-1.69849000	-0.04980200
C	2.90994900	-2.17615400	1.10750300
C	2.97874200	-1.68790900	-1.26992700
C	4.22074300	-2.64208500	1.04212400
H	2.37514600	-2.19121100	2.05195400
C	4.28818600	-2.15087400	-1.32371900
H	2.49498300	-1.32403500	-2.17231900
C	4.90729200	-2.62800500	-0.16876500
H	4.70146100	-3.01807500	1.93854600
H	4.82322400	-2.14318700	-2.26695500
H	5.92798300	-2.99271600	-0.21575900





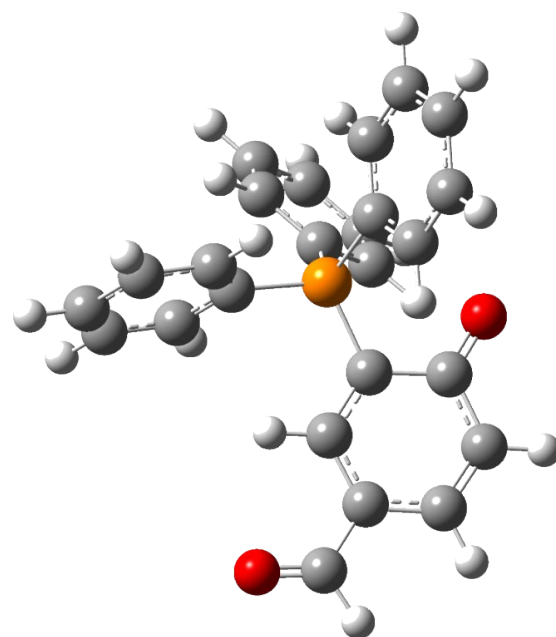
C	3.29028800	3.56150300	-0.11157500
C	-3.19691100	1.58784100	0.02613800
H	-2.77872100	2.11209200	-0.82119500
H	-3.22651400	2.09356300	0.98167200
C	-3.87788700	0.23839200	-0.12361700
H	-3.74758800	-0.12456300	-1.15034600
H	-3.43239600	-0.47939800	0.56480400
O	-5.25296900	0.33447200	0.19409500
C	-5.76695200	1.58428900	-0.11011900
O	-4.86490100	2.42649700	-0.43467600
O	-6.97568000	1.73528900	-0.02571800
F	3.51370200	4.35398000	0.95291600
F	3.29770400	4.37334100	-1.18533700
F	4.34740300	2.74390400	-0.22744800

## CHO

### Organocatalyst

O 1

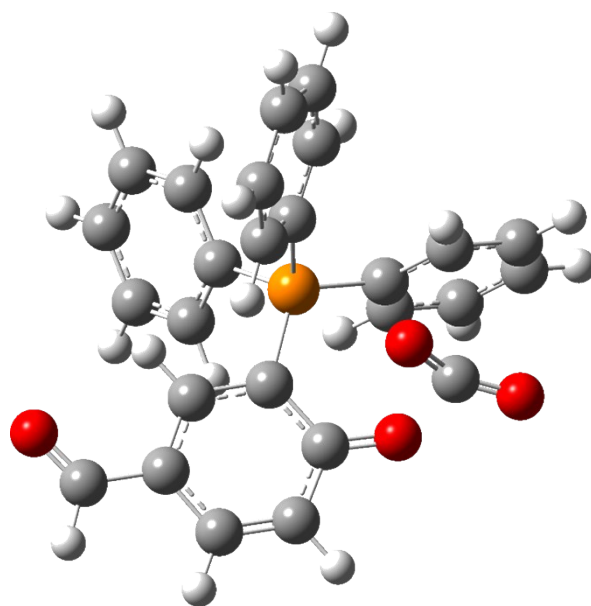
C	3.53218100	-2.12987700	0.99938700
C	2.34866300	-2.80394600	1.13076500
C	1.08098100	-2.15940400	0.87459300
C	1.17152100	-0.76933500	0.45542100
C	2.38635100	-0.10961800	0.31525500
C	3.58166900	-0.77162600	0.59453200
H	4.47019100	-2.64305000	1.20620100
H	2.31991700	-3.84468100	1.43704200
H	2.43736000	0.92471200	-0.01631100
O	-0.02983900	-2.72996200	0.99582000
P	-0.37477000	-0.00318300	0.02971500
C	-1.24126200	-0.97642800	-1.22678000
C	-2.62407200	-0.85665600	-1.38140400
C	-0.50189100	-1.79887800	-2.08152500
C	-3.26564000	-1.55971200	-2.39739300
H	-3.20204100	-0.22757800	-0.71103200
C	-1.15070400	-2.49650100	-3.09509700
H	0.57192200	-1.89588200	-1.94827000
C	-2.53051500	-2.37683800	-3.25298300
H	-4.34004700	-1.47039300	-2.51673600
H	-0.57834800	-3.13714600	-3.75725700
H	-3.03414500	-2.92380100	-4.04316800
C	-1.48493200	0.30833400	1.42889500
C	-1.44970800	-0.50959400	2.56358900
C	-2.39094600	1.37472800	1.35610800
C	-2.32059600	-0.25359200	3.61880300
H	-0.76715300	-1.35104200	2.59948400
C	-3.26288600	1.61483700	2.41305000
H	-2.41199000	2.02213100	0.48428600



C	-3.22555700	0.80288000	3.54457900
H	-2.29311300	-0.88487200	4.50045000
H	-3.96472600	2.43953400	2.35355600
H	-3.90280200	0.99537000	4.37025800
C	-0.01731700	1.61908800	-0.69507900
C	-0.04644800	1.79989700	-2.07973800
C	0.35328500	2.67661800	0.14621300
C	0.29238500	3.03787900	-2.62080900
H	-0.33430500	0.98259600	-2.73342300
C	0.69201400	3.90796800	-0.40207800
H	0.37260900	2.53861700	1.22399000
C	0.66043000	4.08799100	-1.78490300
H	0.26560000	3.17955800	-3.69568900
H	0.97854300	4.72694100	0.24853800
H	0.92270300	5.05135300	-2.20977000
C	4.85526900	-0.08161700	0.45352600
O	4.99386600	1.08079300	0.10524200
H	5.74550800	-0.70086300	0.69207300

### TS step1 mechanism A (iv = 275.57 cm<sup>-1</sup>)

0 1			
C	-2.63095300	-3.18888100	-0.66775800
C	-1.30074500	-3.34266300	-0.97060100
C	-0.35006800	-2.29841300	-0.75582800
C	-0.86799200	-1.06440400	-0.23962300
C	-2.22683900	-0.92548900	0.05925600
C	-3.11440500	-1.97734800	-0.13377600
H	-3.32638900	-4.00861700	-0.83547100
H	-0.91643500	-4.27261600	-1.37562000
H	-2.62798500	0.01180400	0.44093000
O	0.89189000	-2.49029900	-1.03274000
P	0.14382600	0.39861400	-0.01679900
C	0.44781900	0.75626300	1.73001900
C	1.32299600	1.78857300	2.09209700
C	-0.22323400	0.02553700	2.71311000
C	1.50990100	2.09426300	3.43596300
H	1.86516500	2.34606700	1.33295500
C	-0.03075700	0.33913600	4.05497900
H	-0.87182900	-0.79746000	2.43220400
C	0.83073200	1.37203100	4.41565900
H	2.18810700	2.89282800	3.71582800
H	-0.54877000	-0.23041500	4.81873800
H	0.98056400	1.61074300	5.46339100
C	1.72959400	0.38298600	-0.89572400
C	1.74401600	0.59792700	-2.27782600
C	2.92613900	0.17183800	-0.20467800
C	2.95208300	0.58308900	-2.96498500

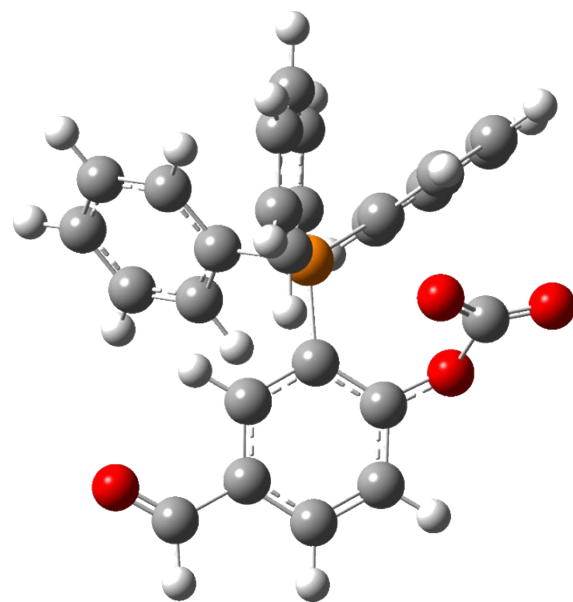


H	0.82207400	0.77927900	-2.82056400
C	4.13111400	0.16419800	-0.90054400
H	2.91792100	-0.00122000	0.86620900
C	4.14508500	0.36672300	-2.27768200
H	2.96074200	0.74594100	-4.03713600
H	5.05783400	-0.00459000	-0.36311600
H	5.08634100	0.35926600	-2.81722400
C	-0.83502000	1.76793100	-0.71585400
C	-0.85445700	3.03124400	-0.11950500
C	-1.55009600	1.54542500	-1.90103400
C	-1.57170100	4.06693300	-0.71348500
H	-0.33048400	3.21261200	0.81222700
C	-2.25688600	2.58666000	-2.49149100
H	-1.57149300	0.55778000	-2.35289500
C	-2.26642400	3.84810900	-1.89947200
H	-1.58982400	5.04357100	-0.24206800
H	-2.80689300	2.40791600	-3.40896800
H	-2.82376400	4.65764000	-2.35895500
C	2.08600100	-2.60539900	0.41766200
O	3.03960800	-3.10861900	-0.07086900
O	1.50523900	-2.13271300	1.34563800
C	-4.53565000	-1.81257400	0.19092200
O	-5.02644400	-0.79712700	0.64725400
H	-5.16613400	-2.70185800	-0.01155000

## In1A

01

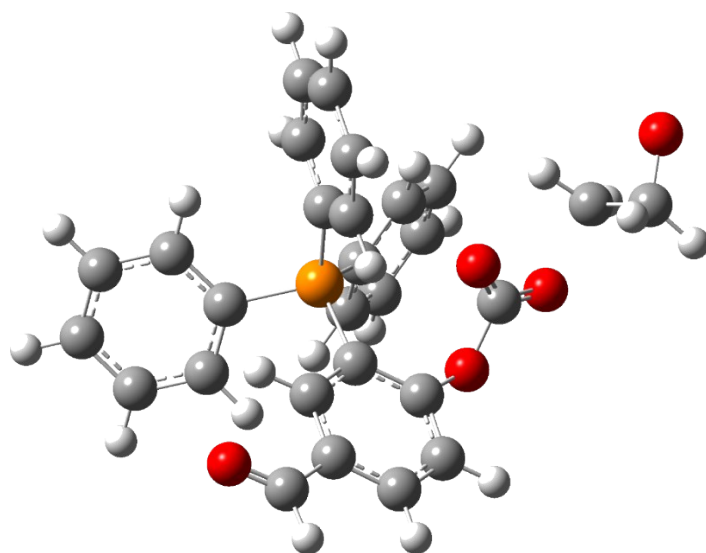
C	-2.85773800	-3.06697300	-0.36861800
C	-1.52344000	-3.36302600	-0.58040500
C	-0.53513400	-2.37983400	-0.42724700
C	-0.92510000	-1.06145500	-0.09856600
C	-2.27486300	-0.77857700	0.12122200
C	-3.24068100	-1.77481800	0.00500700
H	-3.61217700	-3.84111100	-0.48211100
H	-1.19894300	-4.36083200	-0.85224900
H	-2.60653300	0.22555600	0.37499400
O	0.73518300	-2.74635500	-0.64440900
P	0.21569900	0.33843800	-0.01444000
C	0.53445100	0.87942300	1.67769600
C	1.49903500	1.86537300	1.91362100
C	-0.21723800	0.35723300	2.73163100
C	1.69835200	2.33541200	3.20837500
H	2.09781300	2.26155200	1.09791900
C	-0.01234600	0.83536600	4.02126100
H	-0.93723200	-0.43347000	2.54934600
C	0.94086800	1.82390100	4.25916100
H	2.44755800	3.09762400	3.39189600
H	-0.59224600	0.42827800	4.84238000



H	1.09834700	2.19209700	5.26749400
C	1.77910400	0.14443600	-0.91401000
C	1.78874400	0.29904700	-2.30543100
C	2.97097500	-0.10777000	-0.22576200
C	2.98504600	0.18370000	-3.00389000
H	0.87494800	0.51530500	-2.84790300
C	4.16387800	-0.20729300	-0.93375000
H	2.95683900	-0.25804800	0.84826000
C	4.17253000	-0.06456700	-2.31855500
H	2.98839700	0.29734100	-4.08231200
H	5.08609400	-0.40594100	-0.39891800
H	5.10595600	-0.14691700	-2.86564600
C	-0.69266300	1.67804400	-0.85705400
C	-0.65422100	2.98968500	-0.37708800
C	-1.41295200	1.38646500	-2.02485000
C	-1.31883800	4.00133300	-1.06692200
H	-0.12242900	3.22931100	0.53678200
C	-2.06758800	2.40242600	-2.71110800
H	-1.47850500	0.36580100	-2.39112600
C	-2.01989600	3.71108700	-2.23312200
H	-1.29019600	5.01590000	-0.68486100
H	-2.62255900	2.16838400	-3.61291200
H	-2.53741700	4.50184500	-2.76583900
C	1.70114300	-2.61097200	0.48566000
O	2.73453500	-3.21080500	0.25316400
O	1.28357300	-1.91018000	1.41446700
C	-4.66131300	-1.45319500	0.25115200
O	-5.05944400	-0.35489800	0.57717500
H	-5.36466900	-2.29804300	0.11778000

### TS step 2 mechanism A (iv = 629.58 cm<sup>-1</sup>)

01			
C	1.50536400	3.87296600	-0.96128600
C	0.30352600	3.33528300	-1.39430700
C	-0.02238600	2.01167900	-1.09954100
C	0.88185000	1.20351400	-0.38430000
C	2.08907800	1.75937200	0.04553200
C	2.39801200	3.08925200	-0.22827700
H	1.75142600	4.90689800	-1.18716900
H	-0.41250700	3.92133900	-1.95856700
H	2.81617700	1.16920600	0.59850000
O	-1.20639300	1.55164500	-1.59015500
P	0.61820400	-0.54216600	0.01908700
C	0.21115700	-0.74573300	1.76350000
C	-0.07584800	-2.02532400	2.25756400
C	0.21316900	0.35903700	2.61775500
C	-0.34202600	-2.19424800	3.61187900



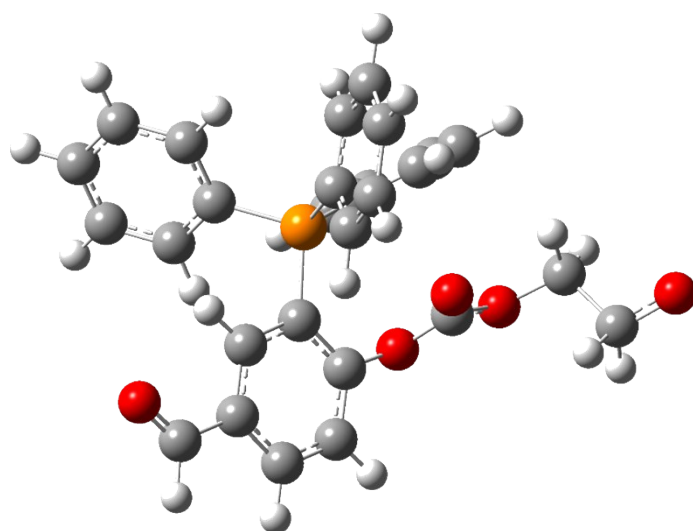
H	-0.10333600	-2.88450900	1.59268000
C	-0.05308800	0.17815200	3.97116000
H	0.39448300	1.35385800	2.22598100
C	-0.32590600	-1.09414800	4.46738600
H	-0.56565800	-3.18357400	3.99519900
H	-0.05534900	1.03542000	4.63490200
H	-0.53526500	-1.22954400	5.52318700
C	-0.62344900	-1.36196700	-1.00984800
C	-0.35146600	-1.57635600	-2.36592600
C	-1.83902400	-1.77782400	-0.45853900
C	-1.30181000	-2.19703300	-3.16672400
H	0.59162200	-1.26258200	-2.80137100
C	-2.77874600	-2.41028100	-1.26679800
H	-2.06094700	-1.58651600	0.58579300
C	-2.51261000	-2.61664200	-2.61715500
H	-1.09440600	-2.35661900	-4.21897100
H	-3.72251900	-2.73066000	-0.83854300
H	-3.25011900	-3.10438800	-3.24580400
C	2.22635000	-1.32615600	-0.31182300
C	2.75152800	-2.28253400	0.56132200
C	2.92888300	-0.98232800	-1.47624300
C	3.95950600	-2.90591000	0.26031600
H	2.23877300	-2.53485400	1.48191500
C	4.13197500	-1.61274800	-1.77003200
H	2.55496800	-0.21023800	-2.14256900
C	4.64555400	-2.57779200	-0.90469400
H	4.36435000	-3.64295600	0.94486800
H	4.67244300	-1.34267900	-2.67044600
H	5.58742300	-3.06457300	-1.13438000
C	-2.19530400	1.17477000	-0.65516000
O	-3.27816400	0.92947600	-1.25458600
O	-1.89402200	1.11672700	0.52785500
C	-4.62340300	0.44856000	-0.14198900
H	-5.17559600	-0.06183200	-0.91955000
H	-4.02960500	-0.16259400	0.52414200
C	-5.31500300	1.57399800	0.50182900
H	-5.78710100	2.27535300	-0.21489800
H	-4.65974300	2.16912100	1.16857900
O	-6.12731000	0.64012300	1.09033300
C	3.68199200	3.65596800	0.24787800
O	4.49901300	3.02316900	0.87944800
H	3.85519000	4.71712100	-0.01381900

## In2A

01

C	1.19146800	3.91528800	-0.94141300
C	0.00685600	3.29517900	-1.31169200
C	-0.19263400	1.95187500	-1.01382600

C	0.79721900	1.19918400	-0.36187800
C	1.98468600	1.83913300	0.00244500
C	2.17842000	3.18988300	-0.27422900
H	1.34920500	4.96602100	-1.16718200
H	-0.78259100	3.82953300	-1.82690300
H	2.78548500	1.30140600	0.50437000
O	-1.37287200	1.39959100	-1.45085800
P	0.68306900	-0.56609000	0.04339200
C	0.41618300	-0.77406700	1.81289800
C	0.24882100	-2.06578900	2.33309500
C	0.38232800	0.33952600	2.65606500
C	0.06505900	-2.23470900	3.70025300
H	0.24527400	-2.93335100	1.67874500
C	0.19643700	0.15742800	4.02280500
H	0.47812400	1.34096000	2.25138400
C	0.04186500	-1.12451800	4.54336700
H	-0.06626500	-3.23190100	4.10490400
H	0.16561200	1.02095500	4.67752300
H	-0.10583700	-1.26087000	5.60940000
C	-0.60169200	-1.45172400	-0.87234000
C	-0.42789700	-1.68010400	-2.24275300
C	-1.75482900	-1.90293300	-0.22088000
C	-1.41429600	-2.34740400	-2.95774300
H	0.46754800	-1.34428200	-2.75545100
C	-2.73046900	-2.58135200	-0.94544200
H	-1.90636000	-1.70520600	0.83499400
C	-2.56307900	-2.79977400	-2.30963900
H	-1.28237900	-2.51797300	-4.02032500
H	-3.62571700	-2.92709600	-0.44000000
H	-3.32960100	-3.32348900	-2.87080600
C	2.29930000	-1.23303000	-0.44058800
C	2.96421100	-2.17111500	0.35337500
C	2.86458200	-0.80986100	-1.65223600
C	4.18217000	-2.69439400	-0.07450100
H	2.55366500	-2.48536600	1.30639500
C	4.07696300	-1.34273000	-2.07213100
H	2.37760200	-0.05166200	-2.25881000
C	4.73432800	-2.28663700	-1.28493900
H	4.69993400	-3.41715100	0.54624400
H	4.51119800	-1.01139200	-3.00889900
H	5.68412000	-2.69570000	-1.61264400
C	-2.26971800	1.01543700	-0.48848800
O	-3.35855700	0.64024800	-1.09481700
O	-2.00721000	1.01710800	0.69066600
C	-4.48645000	0.25744700	-0.24394700
H	-5.06015900	-0.44075200	-0.85613300
H	-4.09977800	-0.25635600	0.64000700
C	-5.36044800	1.45507500	0.17494400
H	-5.61042300	1.97997700	-0.79544200

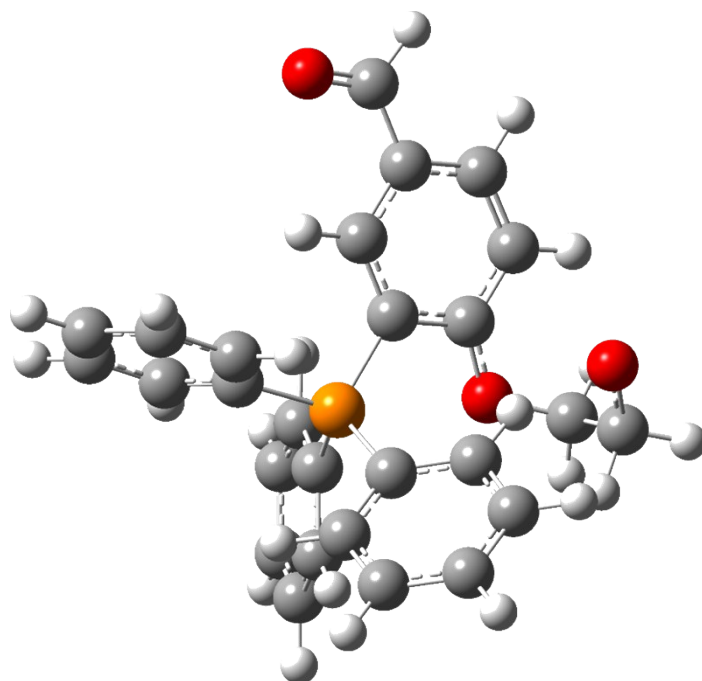


H	-4.63747200	2.17722700	0.66402800
O	-6.38420700	1.03262700	0.91487200
C	3.44866800	3.84350400	0.13188000
O	4.34049500	3.26162800	0.70724500
H	3.53327800	4.91529900	-0.12792600

## In1B

0 1

C	-0.55335000	3.92737600	0.59563300
C	-1.56809400	3.01470100	0.79170400
C	-1.30945500	1.64104400	0.62581300
C	-0.00781200	1.23155200	0.23938200
C	1.00362800	2.16973300	0.04593200
C	0.74010900	3.52361500	0.22512300
H	-0.75980900	4.98689800	0.72632100
H	-2.56461800	3.35168600	1.03527700
H	2.00652900	1.86859600	-0.24164100
O	-2.14985800	0.65005000	0.92130000
P	0.30459700	-0.52094700	0.00933900
C	-0.14034200	-1.41986100	1.51369700
C	-0.67188100	-2.70870400	1.44541400
C	0.08986500	-0.80984900	2.75191900
C	-0.96263400	-3.39241500	2.62332100
H	-0.86981100	-3.17403800	0.48513600
C	-0.19875400	-1.50293700	3.92204100
H	0.48432200	0.20166400	2.80138200
C	-0.72377000	-2.79301800	3.85711900
H	-1.38017100	-4.39208800	2.57298500
H	-0.02218700	-1.03290700	4.88336000
H	-0.95354200	-3.32923800	4.77182500
C	-0.53757100	-1.18795600	-1.43750700
C	-1.59389500	-0.49867400	-2.04050400
C	-0.08260500	-2.41478800	-1.94768100
C	-2.19801400	-1.07073700	-3.16184400
H	-1.98419100	0.47103700	-1.68169500
C	-0.70384400	-2.96727000	-3.05923000
H	0.75775200	-2.92874400	-1.48783700
C	-1.76489200	-2.29250600	-3.66630200
H	-3.01943900	-0.54148100	-3.63502000
H	-0.35626700	-3.91508800	-3.45550400
H	-2.24700500	-2.72306600	-4.53828300
C	2.07838400	-0.74422500	-0.27563600
C	2.92558100	-1.16447700	0.75253200
C	2.59621100	-0.45076100	-1.54435200
C	4.29165400	-1.28666500	0.51047700
H	2.52610900	-1.40271200	1.73311700
C	3.96156800	-0.56966600	-1.77393700
H	1.93594500	-0.13568600	-2.34775400

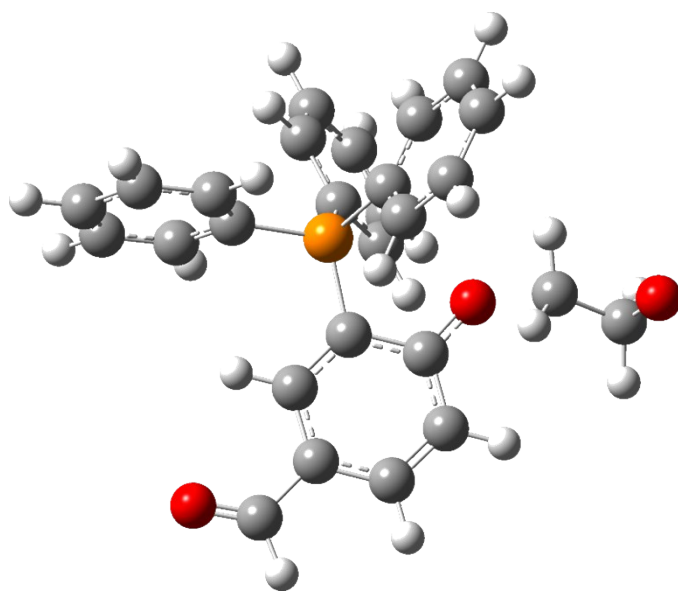


C	4.80776800	-0.98765600	-0.74706500
H	4.94951800	-1.61851700	1.30614700
H	4.36408300	-0.34165500	-2.75482800
H	5.87255400	-1.08452100	-0.93136000
C	-3.57015800	0.88400200	0.92674100
H	-3.78450800	1.80668200	1.47426000
H	-3.98760800	0.03943700	1.48197200
C	-4.03913700	0.95176700	-0.54096800
H	-4.01499800	-0.11746500	-0.89072000
H	-5.13334500	1.18991900	-0.47717300
O	-3.29154100	1.79614700	-1.26868900
C	1.80715400	4.51542500	0.02506300
O	2.94816600	4.23931100	-0.28957700
H	1.50331800	5.56915300	0.18436200

### TS step1 mechanism B (iv = 650.77 cm<sup>-1</sup>)

0 1

C	-0.80809700	3.77667100	-0.93649900
C	-1.71570900	2.73825000	-0.98077200
C	-1.28512200	1.40600300	-0.75970800
C	0.09383500	1.20318200	-0.44041800
C	0.99596600	2.25850000	-0.39529700
C	0.55208400	3.55499500	-0.65679600
H	-1.14637500	4.79301200	-1.12688400
H	-2.76157900	2.91172700	-1.21196200
H	2.04297200	2.10314600	-0.14780500
O	-2.06427400	0.37070400	-0.82639900
P	0.52994000	-0.46876700	0.02795200
C	-0.62989400	-1.02428600	1.29940400
C	-1.11219700	-2.33388000	1.29981200
C	-1.05898200	-0.10824400	2.26662400
C	-2.02660200	-2.72667600	2.27383400
H	-0.79421200	-3.03960400	0.53895000
C	-1.96951900	-0.51139900	3.23708000
H	-0.70086600	0.91800400	2.25045700
C	-2.45460100	-1.81853700	3.23908500
H	-2.40899400	-3.74152800	2.27167300
H	-2.30975900	0.19855700	3.98304300
H	-3.17252600	-2.12763600	3.99147700
C	0.54427400	-1.61872300	-1.36390000
C	-0.13985100	-1.31585600	-2.54413600
C	1.24958200	-2.82325200	-1.24008700
C	-0.12132700	-2.22497900	-3.59749100
H	-0.69268100	-0.38785900	-2.63137500
C	1.25221900	-3.72875500	-2.29520100
H	1.79790300	-3.05130800	-0.33002400
C	0.56830600	-3.42852000	-3.47230000



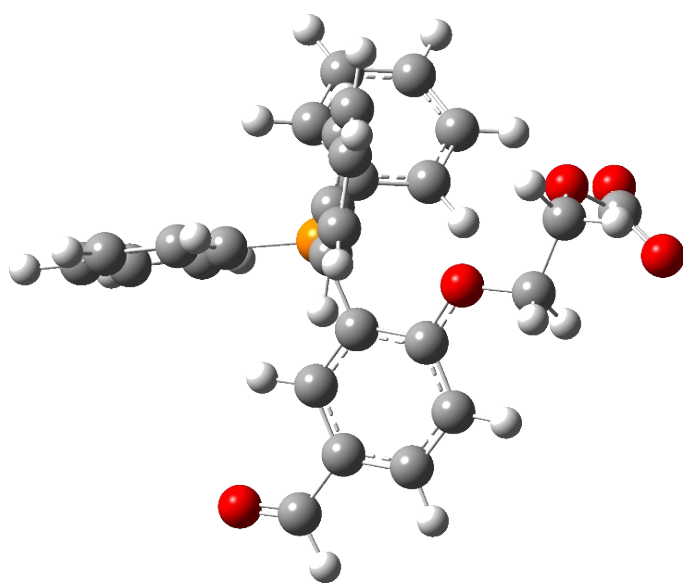


H	-0.64902900	-1.99150000	-4.51564100
H	1.79302500	-4.66394500	-2.20029500
H	0.57659800	-4.13467500	-4.29603400
C	2.20390800	-0.45493200	0.71017800
C	2.41407400	-0.48560500	2.09107700
C	3.29083300	-0.36258800	-0.16965000
C	3.71242200	-0.41956400	2.59024600
H	1.57493200	-0.56653300	2.77440700
C	4.58252600	-0.29292400	0.33871600
H	3.12934800	-0.34905600	-1.24417300
C	4.79218500	-0.32130700	1.71733500
H	3.87724300	-0.44761600	3.66167500
H	5.42459400	-0.22062600	-0.34073300
H	5.80197900	-0.26974000	2.11061800
C	-3.63740400	0.48382800	0.06386500
H	-3.37935400	1.32931000	0.69288600
H	-3.52578800	-0.49776400	0.50884700
C	-4.82400100	0.67262800	-0.78050900
H	-4.83172800	1.63203500	-1.33859400
H	-4.97956100	-0.13821800	-1.51917100
O	-5.55484700	0.61861900	0.37598000
C	1.49743700	4.67825600	-0.62074800
O	2.68616800	4.56913000	-0.38946600
H	1.05031400	5.67196000	-0.82398600

## In2B

01

C	0.33567700	4.05053500	0.19501000
C	-0.72252500	3.24061700	0.58276500
C	-0.59394600	1.85128300	0.48443800
C	0.61899100	1.28377900	0.01898500
C	1.66877500	2.11529900	-0.35139000
C	1.52825300	3.50194200	-0.27731200
H	0.23304700	5.13023800	0.26608500
H	-1.63648000	3.68092300	0.95884800
H	2.61642900	1.71329000	-0.69648800
O	-1.55179100	0.97955500	0.81116500
P	0.82355100	-0.51362100	0.00864400
C	0.34081900	-1.15765100	1.62523200
C	-0.23926200	-2.42484800	1.71550200
C	0.57071000	-0.39324400	2.77429100
C	-0.58637400	-2.92922800	2.96596900
H	-0.43152700	-3.00884600	0.82065300
C	0.22206800	-0.90761400	4.01769000
H	1.01054500	0.59776100	2.69812300
C	-0.35679000	-2.17308100	4.11216400
H	-1.04188400	-3.91044100	3.04164300
H	0.39675400	-0.31873300	4.91145100



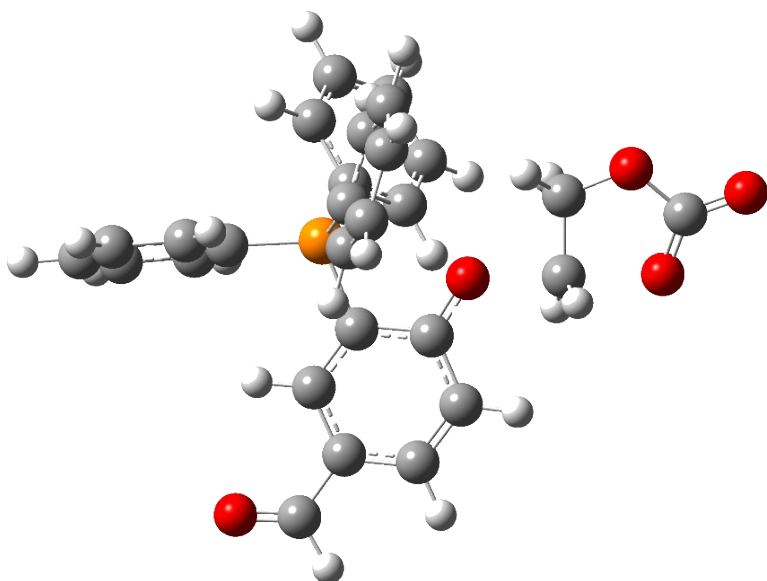
H	-0.63353000	-2.56802400	5.08402900
C	-0.10436400	-1.35703800	-1.28700800
C	-1.37129700	-0.90617100	-1.66970800
C	0.42008200	-2.54335500	-1.82320300
C	-2.11494600	-1.64134500	-2.58899600
H	-1.81312200	-0.01795700	-1.23527500
C	-0.32643800	-3.26303200	-2.74852500
H	1.39866600	-2.90371500	-1.52188300
C	-1.59018700	-2.81216700	-3.12993200
H	-3.11063000	-1.28087700	-2.83127300
H	0.07829300	-4.17858300	-3.16597800
H	-2.17034100	-3.38513800	-3.84635900
C	2.57777000	-0.85248200	-0.25811600
C	3.39641600	-1.20910500	0.81618700
C	3.11563500	-0.71639400	-1.54614500
C	4.75500300	-1.42699300	0.60164500
H	2.97982000	-1.32305700	1.81161300
C	4.47318500	-0.93318800	-1.74815200
H	2.47887100	-0.44858300	-2.38505700
C	5.29112100	-1.28832100	-0.67522500
H	5.39023300	-1.70844400	1.43406900
H	4.89181100	-0.82815900	-2.74284100
H	6.34965000	-1.46036300	-0.83898900
C	-2.83062700	1.45420400	1.26216800
H	-3.20640600	2.21947800	0.57833200
H	-2.72409500	1.86564200	2.27213700
C	-3.77039800	0.26785100	1.22979600
H	-3.35328800	-0.55094300	1.82580300
H	-4.72882400	0.58009900	1.65456600
O	-3.92060300	-0.21977400	-0.08275400
C	-4.70275100	0.58461600	-0.96187200
O	-4.67572000	0.17072000	-2.13080000
O	-5.27813900	1.56088900	-0.45294600
C	2.64954300	4.37492900	-0.68051900
O	3.71232200	3.95970400	-1.09145200
H	2.45932200	5.46120600	-0.58301600

### TS step 3 mechanism B (iv = 645.35cm<sup>-1</sup>)

0 1

C	0.14053600	3.98821000	0.12470000
C	-0.88932900	3.08217200	0.28020500
C	-0.62346700	1.68909400	0.24509700
C	0.73531600	1.28372900	0.04046200
C	1.76003100	2.20962400	-0.10059800
C	1.46892400	3.57389500	-0.06548700
H	-0.07821800	5.05340400	0.15613800
H	-1.90346300	3.42694600	0.44341100

H	2.79214300	1.89908700	-0.24219600
O	-1.51498700	0.75938300	0.37574000
P	1.02265300	-0.48253600	0.02566000
C	0.37703500	-1.20608900	1.55105100
C	-0.27665200	-2.43949700	1.54645800
C	0.55309300	-0.49907300	2.74559400
C	-0.74701300	-2.96937300	2.74537100
H	-0.43596000	-2.97765900	0.61761000
C	0.08557000	-1.04011400	3.93811000
H	1.04325900	0.47108800	2.74453900
C	-0.56379000	-2.27356600	3.93757100
H	-1.26216500	-3.92373200	2.74382500
H	0.22048800	-0.49447300	4.86559700
H	-0.93454700	-2.68898400	4.86866500
C	0.30271700	-1.28010000	-1.42704500
C	-0.62737400	-0.61077000	-2.22611500
C	0.71274500	-2.57928200	-1.75528000
C	-1.16295200	-1.25088500	-3.33991200
H	-0.93128700	0.40096300	-1.98294500
C	0.16534500	-3.21326300	-2.86539500
H	1.45986900	-3.09229400	-1.15503600
C	-0.77342600	-2.55045800	-3.65426500
H	-1.88416500	-0.73056300	-3.96082100
H	0.47737700	-4.22077000	-3.11733500
H	-1.19654400	-3.04621000	-4.52159800
C	2.80479300	-0.77436800	-0.05760800
C	3.53231700	-1.12713100	1.08180300
C	3.45424300	-0.59435200	-1.28626500
C	4.91134900	-1.29744100	0.98947700
H	3.03072200	-1.27584800	2.03247000
C	4.83142200	-0.76206400	-1.36665900
H	2.88681500	-0.32832100	-2.17407700
C	5.55833900	-1.11382700	-0.22937000
H	5.47745500	-1.57596800	1.87143400
H	5.33552900	-0.62179400	-2.31642000
H	6.63288300	-1.24786700	-0.29627800
C	-3.28955600	1.13125300	0.02645800
H	-3.01984900	1.75940800	-0.81014600
H	-3.44779800	1.59618000	0.98967900
C	-3.61141000	-0.34219400	-0.15378300
H	-3.39478100	-0.63787200	-1.18750200
H	-2.99852500	-0.94032400	0.52040500
O	-4.96572300	-0.60147600	0.15973600
C	-5.77942400	0.48304400	-0.12448700
O	-5.12070100	1.53240700	-0.42826700
O	-6.98683400	0.31913400	-0.04427300
C	2.54359900	4.56201900	-0.22021600
O	3.71549300	4.28289500	-0.38494100
H	2.21509700	5.61972600	-0.17750100

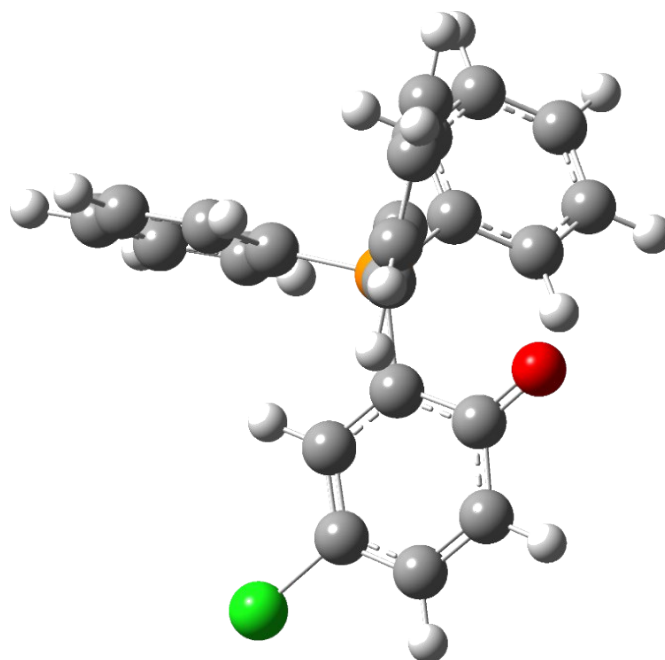


Cl

## Organocatalyst

0 1

C	3.67650900	-1.78738700	0.85665000
C	2.54857900	-2.54492600	1.05394300
C	1.22352500	-2.01548900	0.84610100
C	1.18809300	-0.64523900	0.39716000
C	2.34844200	0.12015500	0.18479600
C	3.57744000	-0.44990800	0.42541000
H	4.65973400	-2.21539200	1.02876900
H	2.62609300	-3.57634200	1.38276300
H	2.28572500	1.14566200	-0.16637600
O	0.16612600	-2.67856100	1.03344800
P	-0.42866000	-0.01903900	0.03461200
C	-1.28699700	-1.07441600	-1.16117100
C	-2.67593500	-1.00032900	-1.28866900
C	-0.54268700	-1.90400500	-2.00399100
C	-3.31881900	-1.75456900	-2.26607200
H	-3.25763800	-0.36458000	-0.62769900
C	-1.19264700	-2.65383800	-2.97878100
H	0.53580800	-1.96417300	-1.89034200
C	-2.57835600	-2.57869600	-3.11047500
H	-4.39756400	-1.69908200	-2.36494600
H	-0.61623600	-3.30005000	-3.63205100
H	-3.08209400	-3.16525000	-3.87174500
C	-1.49224000	0.24149000	1.48212000
C	-1.33916800	-0.54929800	2.62621700
C	-2.47051400	1.24383800	1.44415000
C	-2.16363200	-0.32843500	3.72575400
H	-0.60275500	-1.34563700	2.63268300
C	-3.29551800	1.44812900	2.54559200
H	-2.58319900	1.87259000	0.56548400
C	-3.13911000	0.66534600	3.68695300
H	-2.04418900	-0.93834400	4.61500300
H	-4.05296800	2.22389500	2.51228400
H	-3.77873000	0.83149700	4.54775600
C	-0.23999500	1.61129800	-0.73841600
C	-0.35722400	1.75713600	-2.12234600
C	0.09132400	2.71474700	0.05948400
C	-0.14517700	3.00412400	-2.70639800
H	-0.61610800	0.90480100	-2.74258200
C	0.30412200	3.95501200	-0.53124100
H	0.17839000	2.60504200	1.13726900
C	0.18456200	4.09932300	-1.91338800
H	-0.24099900	3.11727800	-3.78083700
H	0.56051600	4.80875200	0.08650800
H	0.34687100	5.06966200	-2.37089400

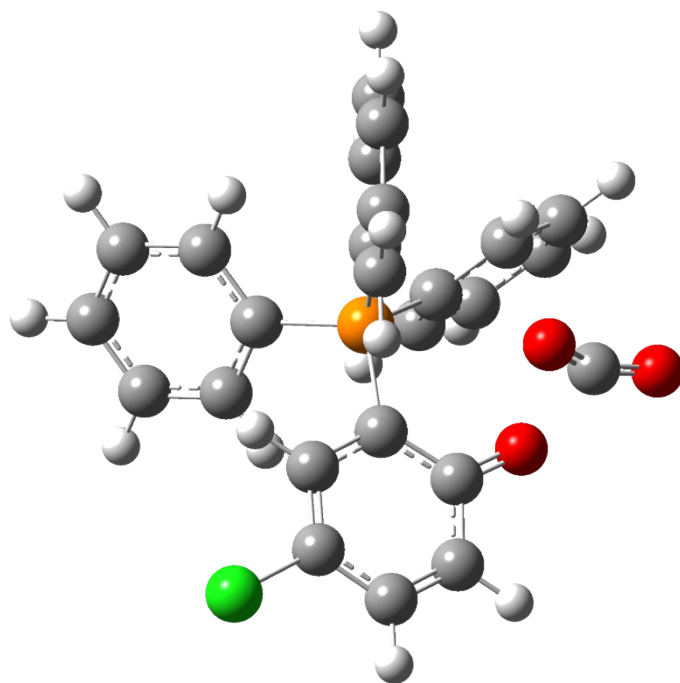


Cl 5.04428000 0.48584500 0.18069900

### TS step1 mechanism A (iv = 272.58 cm<sup>-1</sup>)

0 1

C	-3.00578600	-2.72353200	-0.69466700
C	-1.71152900	-3.02387100	-1.04692800
C	-0.62422200	-2.11855100	-0.83834100
C	-0.97451900	-0.86017200	-0.26223000
C	-2.30450400	-0.55384000	0.09612900
C	-3.29985600	-1.48191500	-0.10851800
H	-3.80385500	-3.43967500	-0.86235800
H	-1.47000800	-3.98147800	-1.49629400
H	-2.55465800	0.41346500	0.52444700
O	0.57502200	-2.45214400	-1.16324800
P	0.23216500	0.43428900	-0.01082100
C	0.66416700	0.64689800	1.73276400
C	1.70758400	1.50877800	2.09500700
C	-0.07047300	-0.02058100	2.71514100
C	2.00126800	1.70913900	3.43949600
H	2.29629900	2.01258100	1.33285300
C	0.23014300	0.18601600	4.05813400
H	-0.85565700	-0.71339200	2.43030600
C	1.26037700	1.05041000	4.41948500
H	2.81114400	2.37371100	3.71960100
H	-0.33659200	-0.33543500	4.82167400
H	1.49286000	1.20674300	5.46769400
C	1.76532700	0.23871000	-0.95734800
C	1.77400100	0.55461300	-2.31910100
C	2.92657600	-0.22931800	-0.33617700
C	2.93825900	0.38045100	-3.05904600
H	0.88214500	0.93624700	-2.80569900
C	4.08751200	-0.39691300	-1.08347700
H	2.92148700	-0.47374600	0.72117800
C	4.09353500	-0.09665000	-2.44329900
H	2.94237200	0.62186900	-4.11639900
H	4.98571200	-0.76679400	-0.60101400
H	5.00076200	-0.23043000	-3.02324200
C	-0.56334000	1.97017000	-0.58472400
C	-0.38176600	3.18344900	0.08425400
C	-1.34657800	1.92426000	-1.74654800
C	-0.96846000	4.34371000	-0.41484100
H	0.19939500	3.23053900	0.99835800
C	-1.92325800	3.08827100	-2.24185100
H	-1.51882100	0.97824500	-2.25191200
C	-1.73305800	4.29846000	-1.57700200
H	-0.82982600	5.28222600	0.11071500
H	-2.52791200	3.04781200	-3.14123400
H	-2.18844600	5.20507700	-1.96144600

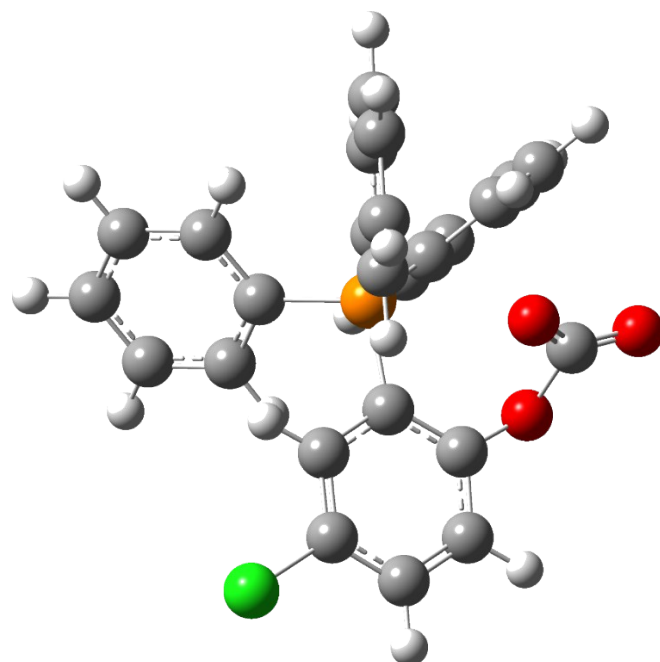


C	1.76335100	-2.90751800	0.32314300
O	2.60725800	-3.52053000	-0.22923400
O	1.24268100	-2.40738600	1.26588500
Cl	-4.95041600	-1.10966200	0.34183100

## In1A

0 1

C	-3.21338700	-2.59315800	-0.39828100
C	-1.92904700	-3.05897100	-0.62351500
C	-0.81256000	-2.22658100	-0.47562400
C	-1.01690300	-0.88084500	-0.12175700
C	-2.31788000	-0.40989900	0.11604100
C	-3.39668700	-1.26710000	-0.01147100
H	-4.06799000	-3.25115900	-0.51038600
H	-1.75366000	-4.08984200	-0.90982400
H	-2.49276400	0.62663800	0.38752800
O	0.39637300	-2.76419600	-0.72253400
P	0.30939000	0.34182200	-0.00364900
C	0.70949200	0.77147000	1.70394200
C	1.81362200	1.58895900	1.96833300
C	-0.11531500	0.33657000	2.74311600
C	2.08315200	1.97654700	3.27774300
H	2.46583900	1.91758100	1.16369100
C	0.16008500	0.73279800	4.04713500
H	-0.94818300	-0.32746700	2.53715200
C	1.25552600	1.55190900	4.31422200
H	2.94142700	2.60603500	3.48550400
H	-0.47644900	0.39281000	4.85669900
H	1.46901300	1.85384800	5.33421900
C	1.81858200	-0.04256600	-0.93279500
C	1.83008600	0.15052000	-2.31931400
C	2.97474000	-0.47345500	-0.27344700
C	2.98912600	-0.10629100	-3.04231600
H	0.94754700	0.50571500	-2.84016800
C	4.13277800	-0.71345400	-1.00528800
H	2.95566900	-0.64973300	0.79608200
C	4.14129100	-0.53391000	-2.38568900
H	2.99222200	0.03725900	-4.11716200
H	5.02677700	-1.05018300	-0.49192400
H	5.04658900	-0.72791500	-2.95144100
C	-0.40313700	1.82879200	-0.78538600
C	-0.16635300	3.10230800	-0.26097300
C	-1.17142300	1.68988300	-1.95062300
C	-0.68243300	4.22549200	-0.90329300
H	0.40405000	3.22741100	0.65256800
C	-1.67816000	2.81568200	-2.58865800
H	-1.38921600	0.70454600	-2.35325400
C	-1.43276500	4.08461200	-2.06618000

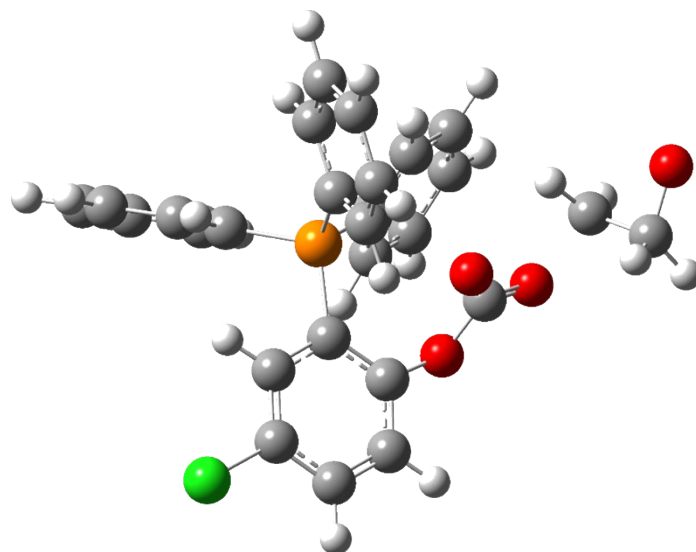


H	-0.50101000	5.20983000	-0.48560800
H	-2.27112600	2.70025500	-3.48943500
H	-1.83519700	4.96170900	-2.56195600
C	1.37467100	-2.79837900	0.39015800
O	2.31640500	-3.52854400	0.13224100
O	1.07402200	-2.07255000	1.34674000
Cl	-5.00772800	-0.66811400	0.29437700

### TS step 2 mechanism A (iv = 627.07 cm<sup>-1</sup>)

0 1

C	1.79479500	3.82592400	-0.65850900
C	0.50207600	3.45604900	-0.99352600
C	0.06110900	2.14248200	-0.83580000
C	0.94549300	1.16773500	-0.33890800
C	2.25277600	1.54750700	-0.00150500
C	2.66257800	2.86137600	-0.15566900
H	2.12797000	4.84971900	-0.78454700
H	-0.20018100	4.18041800	-1.38960000
H	2.96166000	0.81854100	0.37533600
O	-1.20099300	1.88460300	-1.28273400
P	0.53556300	-0.58068000	-0.06267400
C	0.27568200	-0.90859700	1.69181800
C	0.26809200	-2.24427100	2.11596300
C	0.14842300	0.13225500	2.61351800
C	0.10837100	-2.53388700	3.46571200
H	0.39461000	-3.05246600	1.40047700
C	0.00571000	-0.16972400	3.96457200
H	0.13716900	1.16078000	2.27168800
C	-0.01942300	-1.49620000	4.38814300
H	0.09371100	-3.56646700	3.79620500
H	-0.09175400	0.63416800	4.68572400
H	-0.13598600	-1.72360500	5.44260800
C	-0.85238600	-1.11603700	-1.08135800
C	-0.88577200	-0.77067900	-2.43807600
C	-1.88439700	-1.86731300	-0.51436200
C	-1.94297900	-1.20362300	-3.22867500
H	-0.10804200	-0.14619900	-2.86992000
C	-2.94085600	-2.29117800	-1.31497700
H	-1.87911900	-2.10303600	0.54481400
C	-2.96762800	-1.96424500	-2.66784500
H	-1.97266100	-0.93408500	-4.27852900
H	-3.74797800	-2.86613100	-0.87415100
H	-3.79640700	-2.29200700	-3.28646700
C	1.99390900	-1.56810100	-0.52004700
C	3.01223000	-1.76086800	0.42433800
C	2.11534900	-2.11968300	-1.79931700
C	4.14902200	-2.48358700	0.07992500

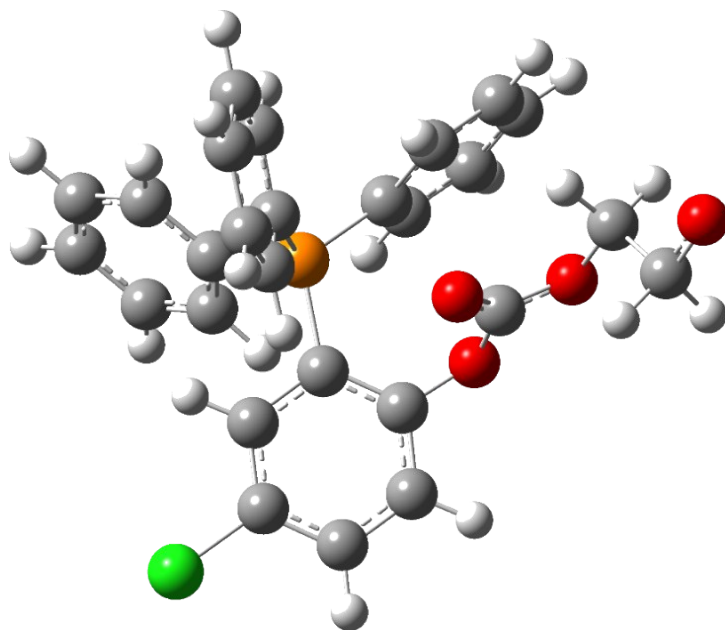


H	2.91540100	-1.36120400	1.42957500
C	3.25480000	-2.84624700	-2.13294200
H	1.32525400	-2.00326100	-2.53223200
C	4.27087300	-3.02520700	-1.19819300
H	4.93315800	-2.62960800	0.81441400
H	3.34268800	-3.27756400	-3.12397800
H	5.15526100	-3.59500800	-1.46262200
C	-2.15349400	1.36170000	-0.38859400
O	-3.24831900	1.17950500	-0.98881800
O	-1.82125500	1.14514100	0.76801400
C	-4.55569000	0.50118900	0.06888400
H	-5.07139700	0.03179300	-0.75797800
H	-3.91610300	-0.12778300	0.67319800
C	-5.32140300	1.51062100	0.81157600
H	-5.84143500	2.24421200	0.16390200
H	-4.71040000	2.08217500	1.53889000
O	-6.06620700	0.46826000	1.30021700
Cl	4.29186900	3.30249400	0.27370600

## In2A

0 1

C	1.33379800	3.83067800	-0.84105800
C	0.13465200	3.25543700	-1.23413800
C	-0.12119500	1.91369500	-0.97339100
C	0.83296900	1.11935200	-0.32975400
C	2.04493800	1.70403600	0.06606400
C	2.27784000	3.04808000	-0.18220000
H	1.53502000	4.87701200	-1.03939400
H	-0.62489500	3.83564400	-1.74516600
H	2.80936100	1.11409700	0.56276000
O	-1.31841800	1.41429600	-1.43391100
P	0.64816500	-0.64631800	0.04374000
C	0.34458400	-0.87405600	1.80451800
C	0.12659400	-2.16868100	2.29793600
C	0.33398400	0.22501200	2.66678200
C	-0.08250600	-2.35605700	3.65899900
H	0.10437400	-3.02337400	1.62709000
C	0.12193000	0.02453700	4.02727000
H	0.46643700	1.22955000	2.28050500
C	-0.08134900	-1.26087200	4.52184600
H	-0.25215300	-3.35556700	4.04330700
H	0.10849200	0.87671300	4.69724000
H	-0.24871600	-1.41151100	5.58301500
C	-0.65521100	-1.46659000	-0.90501100
C	-0.47076000	-1.68530300	-2.27549400
C	-1.83550200	-1.87661400	-0.27520700
C	-1.47401000	-2.30149200	-3.01253300
H	0.44528500	-1.38104200	-2.77104400

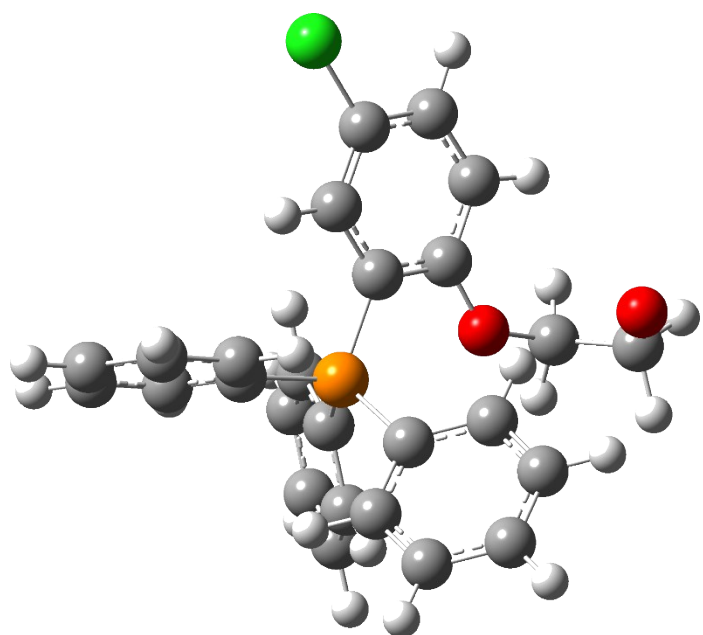




C	-2.82816700	-2.50440900	-1.02189600
H	-1.99299200	-1.68549100	0.78103800
C	-2.65023400	-2.71258400	-2.38638600
H	-1.33416500	-2.46452100	-4.07528600
H	-3.74436600	-2.81839000	-0.53355900
H	-3.42969900	-3.19673400	-2.96505900
C	2.24681400	-1.36693200	-0.42119000
C	2.87018300	-2.32454100	0.38314500
C	2.84294300	-0.96347200	-1.62501400
C	4.07557700	-2.88874400	-0.02719500
H	2.43699200	-2.62308000	1.33109500
C	4.04247000	-1.53724200	-2.02747600
H	2.39014700	-0.18920600	-2.23806700
C	4.65709400	-2.50187600	-1.23058100
H	4.56014000	-3.62722900	0.60181100
H	4.50080700	-1.22210900	-2.95834400
H	5.59689200	-2.94324800	-1.54508700
C	-2.24161500	1.06168800	-0.48592700
O	-3.34100200	0.74449600	-1.10744700
O	-1.99263400	1.03473400	0.69600700
C	-4.49112700	0.39341000	-0.27372400
H	-5.08639400	-0.27127900	-0.90227700
H	-4.13484900	-0.14924900	0.60580900
C	-5.32313100	1.61680200	0.15608600
H	-5.54206800	2.16664100	-0.80801400
H	-4.57893800	2.30280600	0.66483900
O	-6.37069100	1.22189200	0.87791800
Cl	3.78149400	3.75949500	0.32701900

## In1B

01			
C	2.65015700	2.80224100	0.27171000
C	2.95286800	1.44784200	0.25110600
C	1.90265000	0.52617400	0.21415300
C	0.56867300	0.96621000	0.18582800
C	0.27186200	2.33434600	0.21271700
C	1.32235300	3.23519700	0.25812400
H	3.44679000	3.53821500	0.31156400
H	3.96963800	1.01484900	0.33386800
H	-0.75289000	2.68835100	0.17958400
O	2.08949200	-0.80786700	0.22036900
P	-0.71395100	-0.27606700	-0.01136000
C	-0.27187700	-1.33640000	-1.40648100
C	-0.57078600	-2.69965700	-1.37824700
C	0.37504200	-0.77072900	-2.51106400
C	-0.22502400	-3.49818600	-2.46565600
H	-1.05526900	-3.14225900	-0.51363600
C	0.71326700	-1.57697300	-3.59222300



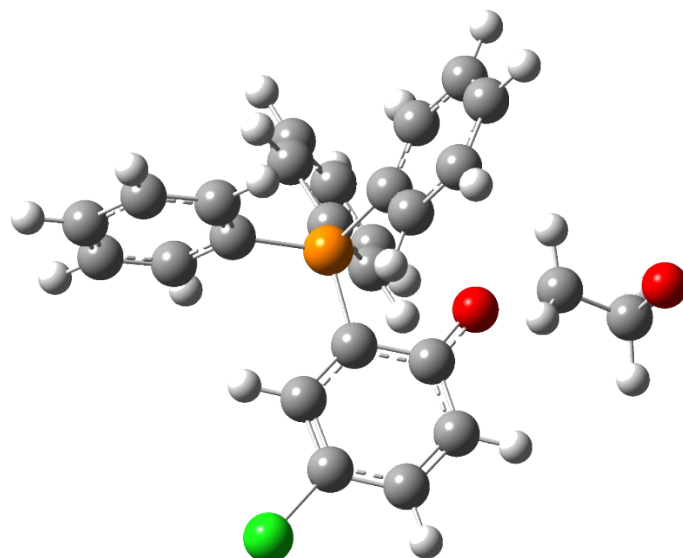
H	0.62538700	0.28678300	-2.52214700
C	0.41402400	-2.93869000	-3.56889800
H	-0.45070600	-4.55869600	-2.44477300
H	1.21702300	-1.14224800	-4.44856800
H	0.68579100	-3.56501500	-4.41191200
C	-0.97256100	-1.25312800	1.48400600
C	0.02392200	-1.35681400	2.45926600
C	-2.19774000	-1.91444400	1.64491900
C	-0.21066200	-2.12805900	3.59380000
H	0.97474000	-0.85147000	2.33238000
C	-2.41664800	-2.68824700	2.77844100
H	-2.97914500	-1.81779500	0.89626600
C	-1.42425800	-2.79296000	3.75189800
H	0.55815100	-2.20869800	4.35430900
H	-3.36405100	-3.20043100	2.90464500
H	-1.60093200	-3.39171700	4.63932600
C	-2.27529500	0.56099000	-0.36502800
C	-2.77624100	0.61305700	-1.66802200
C	-2.96041500	1.18780200	0.68531100
C	-3.96400500	1.29528600	-1.91943600
H	-2.25105100	0.12029700	-2.47991100
C	-4.14156800	1.87098200	0.42222600
H	-2.57705400	1.13784000	1.70097200
C	-4.64274800	1.92266300	-0.87851000
H	-4.35801100	1.33228100	-2.92899500
H	-4.67242100	2.35841700	1.23243300
H	-5.56822000	2.45210700	-1.07893000
C	3.23988700	-1.35448000	-0.47875000
H	3.45628300	-0.70207400	-1.33514300
H	2.88341800	-2.32446500	-0.84464800
C	4.48483900	-1.50197100	0.41168500
H	4.12905200	-2.15562400	1.25869700
H	5.11673900	-2.21045600	-0.20043100
O	5.09122300	-0.36317100	0.77374000
Cl	0.97717600	4.94934200	0.28972400

### TS step1 mechanism B (iv = 651.14 cm<sup>-1</sup>)

01

C	0.87545300	3.71744900	0.87945400
C	1.74392200	2.64556300	0.97368700
C	1.28754200	1.32109700	0.76850900
C	-0.08044100	1.15812200	0.42077100
C	-0.96079800	2.24189500	0.32357700
C	-0.47304800	3.51299000	0.56528700
H	1.23449000	4.72672100	1.05293200
H	2.78742800	2.80081600	1.22849000
H	-2.00178200	2.09656100	0.05241200

O	2.04484400	0.26563700	0.87416700
P	-0.55089700	-0.50826500	-0.02336600
C	0.60916900	-1.11322500	-1.27254700
C	1.06430900	-2.43212600	-1.24301700
C	1.06364700	-0.22598900	-2.25461200
C	1.97765200	-2.86308100	-2.20180600
H	0.72656700	-3.11557700	-0.47048000
C	1.97213100	-0.66734600	-3.21047200
H	0.72754900	0.80781100	-2.26042700
C	2.43065700	-1.98365200	-3.18237100
H	2.33973700	-3.88504900	-2.17591300
H	2.33165400	0.02053700	-3.96793700
H	3.14744600	-2.32272300	-3.92276100
C	-0.61360800	-1.63780000	1.38431500
C	0.05531000	-1.33164800	2.57233300
C	-1.34162800	-2.82908100	1.26451800
C	-0.00146900	-2.22503300	3.63783700
H	0.62784600	-0.41509100	2.65359200
C	-1.38155400	-3.71956200	2.33170000
H	-1.87809900	-3.05837600	0.34767100
C	-0.71284600	-3.41631400	3.51670800
H	0.51440200	-1.98958300	4.56223600
H	-1.93963200	-4.64491100	2.24011200
H	-0.75020000	-4.11052500	4.34975500
C	-2.21589600	-0.46701900	-0.72867500
C	-2.40862900	-0.50734000	-2.11179100
C	-3.31234200	-0.33906400	0.13478300
C	-3.69809100	-0.41459900	-2.62962700
H	-1.56278800	-0.61603300	-2.78291700
C	-4.59515200	-0.24321700	-0.39199400
H	-3.16507300	-0.31818000	1.21125400
C	-4.78690500	-0.28052300	-1.77294600
H	-3.84891400	-0.44988500	-3.70292300
H	-5.44421800	-0.14385200	0.27530500
H	-5.78965600	-0.20795900	-2.18068400
C	3.61014300	0.32042100	-0.06288000
H	3.35108700	1.16182000	-0.69667100
H	3.46228900	-0.66703100	-0.48340800
C	4.81286300	0.49820300	0.75718400
H	4.85772900	1.46696500	1.29574200
H	4.97276300	-0.30390900	1.50339900
O	5.50616900	0.40771200	-0.42226700
Cl	-1.55103700	4.88764200	0.45876300

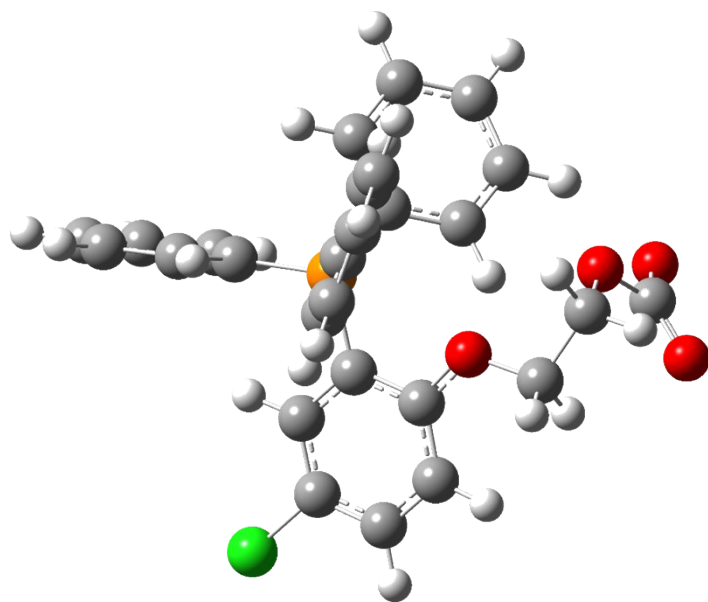


## In2B

01

C	0.41341100	3.97891100	0.18273900
C	-0.65148700	3.18159800	0.58360300

C	-0.55677700	1.79065100	0.48872200
C	0.63356400	1.20821000	0.00595000
C	1.70286200	2.01762200	-0.38406300
C	1.57869300	3.39701600	-0.30316900
H	0.33697100	5.05810400	0.25496200
H	-1.54770900	3.64708600	0.97230600
H	2.62963800	1.58201800	-0.74040400
O	-1.53114000	0.93619600	0.83729300
P	0.80928900	-0.59119800	0.01048000
C	0.39004800	-1.19075600	1.66155500
C	-0.24177100	-2.42731800	1.81091000
C	0.71436800	-0.41382300	2.77942500
C	-0.54491800	-2.88896000	3.08899000
H	-0.50647700	-3.01994500	0.94080400
C	0.41047300	-0.88653800	4.05082500
H	1.19023200	0.55555900	2.65788100
C	-0.21940400	-2.12133100	4.20432600
H	-1.03973000	-3.84623500	3.21034000
H	0.65871000	-0.28811700	4.92040900
H	-0.46111300	-2.48339400	5.19807700
C	-0.18359600	-1.44185900	-1.22928600
C	-1.43060100	-0.95049100	-1.62468400
C	0.28244900	-2.67424600	-1.71512200
C	-2.21436400	-1.69183300	-2.50572300
H	-1.82610400	-0.02356700	-1.22853800
C	-0.50334800	-3.40045300	-2.60106600
H	1.24736600	-3.06378800	-1.40513600
C	-1.74857300	-2.90933200	-2.99467700
H	-3.19453700	-1.29706400	-2.75829300
H	-0.14368900	-4.35110000	-2.97951400
H	-2.36011500	-3.48725000	-3.68034800
C	2.54227100	-0.96634400	-0.34035100
C	3.41835100	-1.31878100	0.68883700
C	3.00222900	-0.86270700	-1.66083700
C	4.75739900	-1.56585500	0.39491400
H	3.06116200	-1.40680400	1.70980500
C	4.34080300	-1.10694300	-1.94190800
H	2.31936600	-0.59958700	-2.46419500
C	5.21633300	-1.45917500	-0.91458500
H	5.43789600	-1.84519900	1.19159000
H	4.69913300	-1.02768300	-2.96223100
H	6.25958500	-1.65483200	-1.13890600
C	-2.79803800	1.45174500	1.27194700
H	-3.14356700	2.22591400	0.58168500
H	-2.69137900	1.86608800	2.28109400
C	-3.77963100	0.29974800	1.23737400
H	-3.39309400	-0.53442600	1.83248100
H	-4.72609900	0.64603100	1.66254800
O	-3.94989200	-0.18156300	-0.07524600

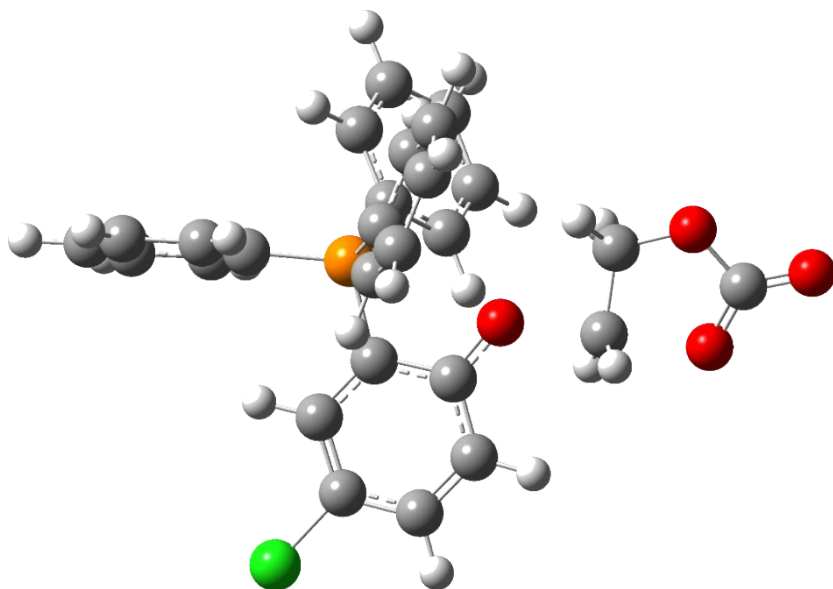


C	-4.70578600	0.64995000	-0.95114400
O	-4.69665600	0.23654100	-2.12079900
O	-5.24598500	1.64546900	-0.44080000
Cl	2.91140300	4.40769200	-0.79518700

### TS step 3 mechanism B (iv = 645.61cm<sup>-1</sup>)

0 1

C	0.17537300	3.93017100	0.15711300
C	-0.85347800	3.02105300	0.32796600
C	-0.60530500	1.62705000	0.27964900
C	0.73928000	1.22234300	0.04549900
C	1.78021100	2.14367300	-0.11092300
C	1.48540100	3.49405100	-0.06043300
H	-0.03100300	4.99457600	0.19916800
H	-1.85921100	3.37930000	0.51431600
H	2.80122900	1.81146800	-0.27179800
O	-1.50890500	0.70283400	0.42812000
P	1.01665600	-0.54299400	0.01729600
C	0.39298000	-1.27520200	1.54803100
C	-0.24140800	-2.51849800	1.54834400
C	0.57176400	-0.56797100	2.74186700
C	-0.68994900	-3.05779400	2.75141900
H	-0.40293900	-3.05779600	0.62051800
C	0.12640200	-1.11832400	3.93852800
H	1.04572700	0.41015100	2.73616300
C	-0.50399600	-2.36156600	3.94291900
H	-1.19029800	-4.02004400	2.75378100
H	0.26319700	-0.57223500	4.86550200
H	-0.85804000	-2.78435500	4.87722400
C	0.27350800	-1.32963800	-1.43009400
C	-0.67303700	-0.65338600	-2.20339100
C	0.67986900	-2.62404200	-1.78043600
C	-1.22774300	-1.28177500	-3.31451100
H	-0.97497400	0.35386000	-1.93974000
C	0.11390400	-3.24619600	-2.88808400
H	1.43875700	-3.14221900	-1.19980400
C	-0.84055700	-2.57638400	-3.65181700
H	-1.96242900	-0.75640900	-3.91509900
H	0.42374800	-4.24981900	-3.15759600
H	-1.27820900	-3.06291700	-4.51714400
C	2.79655200	-0.84609800	-0.09104100
C	3.53726100	-1.19308600	1.04182200
C	3.43201600	-0.67743600	-1.32869100
C	4.91434700	-1.36931100	0.93418600
H	3.04679200	-1.33268700	1.99970600
C	4.80761500	-0.85123000	-1.42461700
H	2.85497800	-0.41539800	-2.21147100



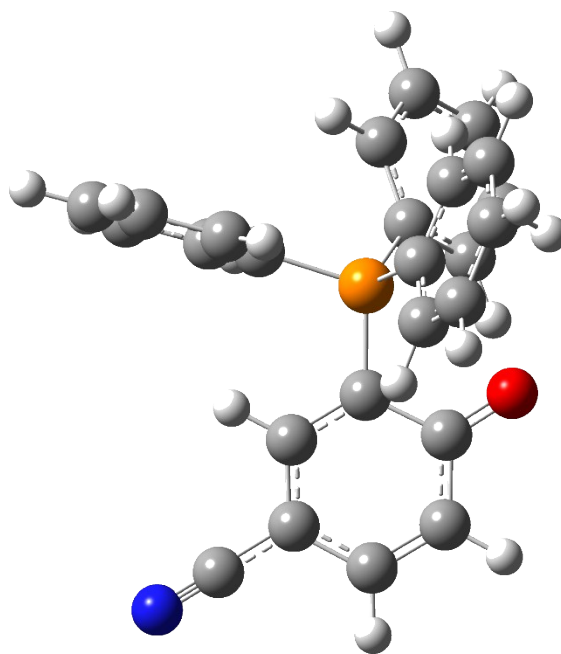
C	5.54721600	-1.19741000	-0.29384900
H	5.48993300	-1.64367000	1.81130900
H	5.30053200	-0.72022100	-2.38158600
H	6.62031700	-1.33638800	-0.37300100
C	-3.28411100	1.10282500	0.05515900
H	-2.98878700	1.72097200	-0.78049900
H	-3.43545800	1.57383600	1.01633900
C	-3.61801300	-0.36870000	-0.11608500
H	-3.38946900	-0.67792800	-1.14305200
H	-3.02291300	-0.96638400	0.57402200
O	-4.98166400	-0.60856400	0.17621100
C	-5.77229400	0.48858000	-0.11668200
O	-5.09111700	1.52725400	-0.41210400
O	-6.98340800	0.34839300	-0.05253400
Cl	2.76450500	4.66974600	-0.26266700

## CN

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0 1

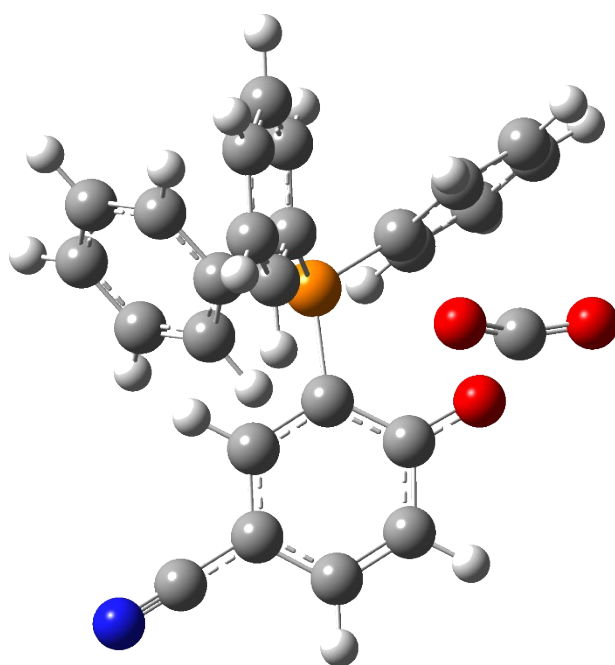
C	3.70521600	-1.85035400	0.98371600
C	2.56711200	-2.58867000	1.15281400
C	1.25416500	-2.03677600	0.90533700
C	1.24642400	-0.65945400	0.45072400
C	2.41439900	0.07860500	0.26916000
C	3.65092500	-0.50011500	0.54257000
H	4.67597000	-2.29488300	1.18334500
H	2.61485900	-3.62034700	1.48531500
H	2.37363200	1.10340500	-0.08846200
O	0.18800500	-2.67944400	1.06316700
P	-0.35151900	-0.00690900	0.03264500
C	-1.17040100	-1.06300200	-1.18751400
C	-2.55930100	-1.02345300	-1.33002800
C	-0.39376200	-1.85947600	-2.03407500
C	-3.16982200	-1.77983200	-2.32631600
H	-3.16506700	-0.41358600	-0.66654000
C	-1.01204700	-2.61087000	-3.02792500
H	0.68491300	-1.89366600	-1.91025400
C	-2.39775000	-2.57040700	-3.17444900
H	-4.24843600	-1.75242300	-2.43683900
H	-0.41138800	-3.23157100	-3.68394000
H	-2.87703000	-3.15876500	-3.94996100
C	-1.45631800	0.26771600	1.44326300
C	-1.34812900	-0.51159000	2.60009800
C	-2.43038400	1.27143300	1.35734000
C	-2.21458800	-0.27918200	3.66452700
H	-0.61186500	-1.30602700	2.64807700
C	-3.29723300	1.48723000	2.42356300



H	-2.50727700	1.89091200	0.46847500
C	-3.18675200	0.71479800	3.57747600
H	-2.13079700	-0.88013300	4.56372600
H	-4.05167300	2.26320700	2.35299400
H	-3.85974200	0.88918400	4.41062400
C	-0.11084300	1.61803600	-0.73446700
C	-0.17458600	1.76419800	-2.12197700
C	0.20454600	2.71683200	0.07632900
C	0.07540600	3.00823000	-2.69675000
H	-0.42142400	0.91537400	-2.75179200
C	0.45557200	3.95383500	-0.50570900
H	0.24919100	2.60628900	1.15653900
C	0.38976200	4.09897200	-1.89141800
H	0.02091300	3.12272800	-3.77384100
H	0.69997800	4.80432300	0.12124600
H	0.58135800	5.06695900	-2.34252900
C	4.85082700	0.25246900	0.36382100
N	5.82828700	0.86188400	0.21973300

### TS step1 mechanism A (iv = 266.33 cm<sup>-1</sup>)

01			
C	-2.87949400	-3.00477200	-0.56293900
C	-1.56684000	-3.24390000	-0.87850800
C	-0.54392000	-2.26360300	-0.69470300
C	-0.96792700	-0.99255000	-0.19295600
C	-2.31194400	-0.75486000	0.12501500
C	-3.26718000	-1.75008900	-0.04134200
H	-3.62898600	-3.77607800	-0.70706700
H	-1.25319200	-4.20408900	-1.27312700
H	-2.62639200	0.21754600	0.49526100
O	0.67650800	-2.55009200	-0.98787000
P	0.14638000	0.40183400	-0.01246000
C	0.53320700	0.75104400	1.71909000
C	1.50530300	1.70748400	2.03905200
C	-0.17345200	0.09916600	2.73224600
C	1.75590000	2.01595600	3.37218200
H	2.07189200	2.20465200	1.25623700
C	0.08341600	0.41512800	4.06261900
H	-0.90147500	-0.66660900	2.48524500
C	1.04317100	1.37232200	4.38211100
H	2.51047200	2.75481700	3.61888900
H	-0.46140300	-0.09462500	4.84958300
H	1.24285000	1.61266500	5.42110800
C	1.68930100	0.26380100	-0.95310400
C	1.65751700	0.46428000	-2.33703400
C	2.89598000	-0.03102100	-0.31207100
C	2.82897000	0.35119500	-3.07648300

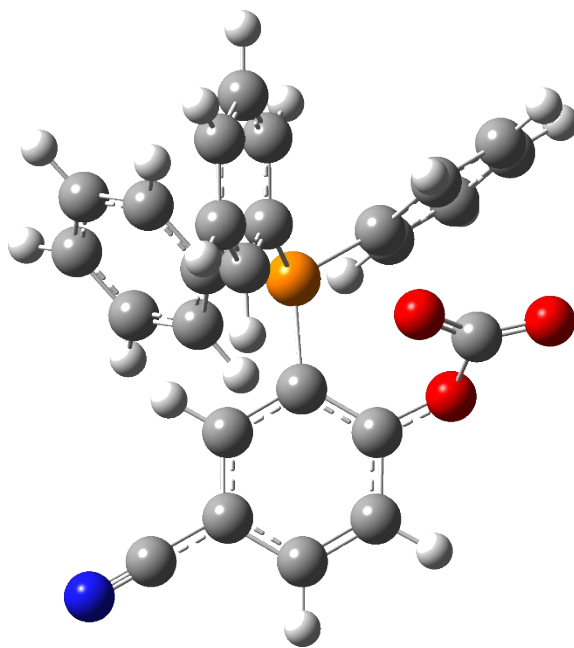


H	0.72846300	0.70895800	-2.84149300
C	4.06423100	-0.13647200	-1.06042700
H	2.92270700	-0.19423700	0.76012100
C	4.03168400	0.05152600	-2.43940500
H	2.80175900	0.50248300	-4.14999300
H	4.99859900	-0.36929000	-0.56156900
H	4.94498000	-0.03201300	-3.01914700
C	-0.76054900	1.83222900	-0.68475600
C	-0.66525900	3.09397100	-0.09166700
C	-1.53289600	1.66256700	-1.84244500
C	-1.32484500	4.17983200	-0.66192400
H	-0.09427200	3.23625900	0.81905800
C	-2.18391900	2.75289200	-2.40799400
H	-1.64062000	0.67991500	-2.29270800
C	-2.07851700	4.01205800	-1.81961100
H	-1.25068400	5.15547000	-0.19410600
H	-2.77952100	2.61562300	-3.30397300
H	-2.59169000	4.86004200	-2.26077100
C	1.87952200	-2.71131900	0.43285200
O	2.78790000	-3.29609700	-0.05246600
O	1.35643900	-2.17125400	1.35979500
C	-4.63608300	-1.49094600	0.29236500
N	-5.74403200	-1.28213900	0.56124600

## In1A

0 1

C	-3.10824600	-2.83360100	-0.32024600
C	-1.80198800	-3.21752000	-0.54631600
C	-0.74001500	-2.31001200	-0.40732400
C	-1.02776800	-0.96964100	-0.07390800
C	-2.35210600	-0.58421900	0.16035200
C	-3.38701000	-1.51084600	0.05510500
H	-3.91666300	-3.54923400	-0.42075400
H	-1.55648600	-4.23707500	-0.82003600
H	-2.58993200	0.44464500	0.41399800
O	0.49285200	-2.77295800	-0.64053000
P	0.21653300	0.34197700	-0.00542300
C	0.59517500	0.85598500	1.68255800
C	1.63556900	1.76447400	1.90681100
C	-0.18362000	0.39401900	2.74525000
C	1.88450900	2.21811900	3.19875000
H	2.25503900	2.11295200	1.08497400
C	0.07072800	0.85651900	4.03163000
H	-0.96254900	-0.34126600	2.57332100
C	1.10039600	1.76799400	4.25804400
H	2.69188000	2.92049300	3.37394800
H	-0.53069900	0.49717100	4.85944200
H	1.29640500	2.12334800	5.26423900

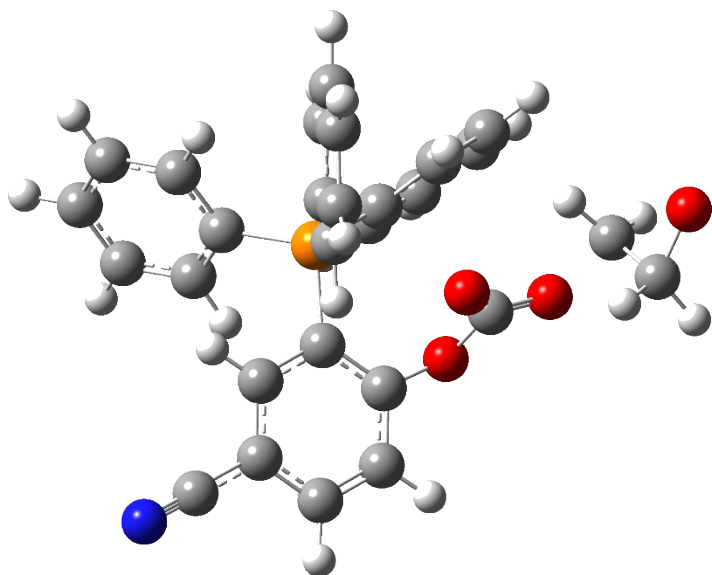




C	1.74235100	0.02269400	-0.93128600
C	1.73222300	0.15396500	-2.32497100
C	2.92829000	-0.30149000	-0.26339400
C	2.90164800	-0.05732700	-3.04587900
H	0.82460600	0.42463800	-2.85311700
C	4.09550100	-0.49593100	-0.99406900
H	2.92757000	-0.43330000	0.81301300
C	4.08364000	-0.37749400	-2.38106900
H	2.88889800	0.03750000	-4.12602700
H	5.01277500	-0.74981500	-0.47438200
H	4.99660300	-0.53578800	-2.94564500
C	-0.60015300	1.74530500	-0.83735000
C	-0.45324800	3.05023600	-0.35942300
C	-1.35399800	1.51084200	-1.99692500
C	-1.04360800	4.11093500	-1.04283900
H	0.10540800	3.24787600	0.54850700
C	-1.93462400	2.57519400	-2.67617000
H	-1.50179700	0.49911600	-2.36437400
C	-1.77860700	3.87626300	-2.20053000
H	-0.93087600	5.11992100	-0.66165600
H	-2.51534200	2.38501500	-3.57213100
H	-2.23925600	4.70454800	-2.72844100
C	1.48869100	-2.70580200	0.47679900
O	2.46771200	-3.38343000	0.22807400
O	1.13781800	-1.97242100	1.40676100
C	-4.73974500	-1.09998900	0.31038900
N	-5.83065000	-0.77171100	0.51686800

### TS step 2 mechanism A (iv = 629.45 cm<sup>-1</sup>)

0 1			
C	1.55580000	3.89099200	-0.85447200
C	0.36316000	3.35844000	-1.30959800
C	0.02665700	2.03029400	-1.04211700
C	0.91661100	1.20924600	-0.32961200
C	2.12141800	1.75144700	0.13066600
C	2.43438100	3.08628600	-0.11839800
H	1.80874200	4.92508000	-1.05892100
H	-0.34082400	3.95795100	-1.87459800
H	2.82664700	1.13613600	0.68153900
O	-1.15196500	1.58737400	-1.55537300
P	0.64684600	-0.54831300	0.02702700
C	0.20970000	-0.79338600	1.75783900
C	-0.09122100	-2.08470800	2.21154000
C	0.20280200	0.28797200	2.64148800
C	-0.38106700	-2.28877300	3.55607800
H	-0.11147300	-2.92527500	1.52298300
C	-0.08640600	0.07149400	3.98487200
H	0.39371300	1.29273600	2.28066500



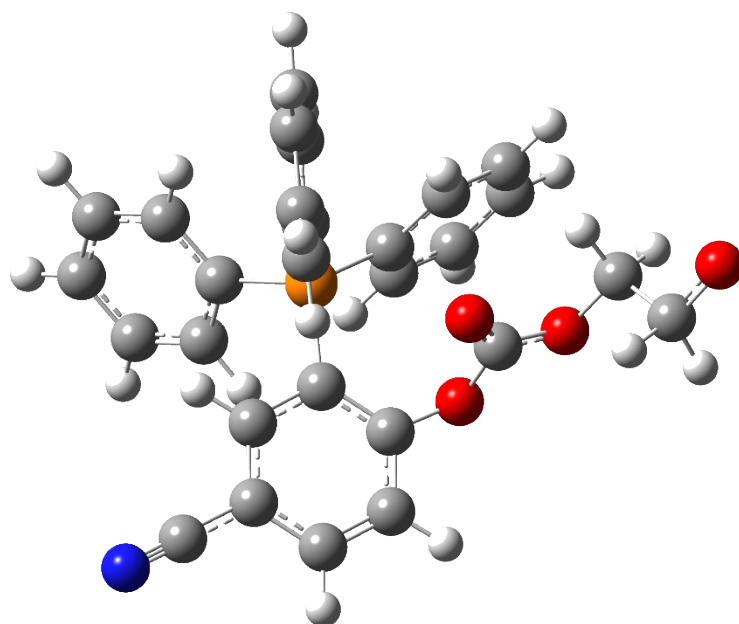
C	-0.37373300	-1.21249700	4.44134400
H	-0.61662900	-3.28683700	3.90813800
H	-0.09568600	0.91027300	4.67179200
H	-0.60153400	-1.37558000	5.48936800
C	-0.57711200	-1.33753600	-1.04519400
C	-0.27642900	-1.53354500	-2.39806100
C	-1.80772900	-1.75185300	-0.52657300
C	-1.21503300	-2.13217500	-3.22893200
H	0.67896600	-1.22292700	-2.80784100
C	-2.73555300	-2.36160100	-1.36534600
H	-2.04949800	-1.57660300	0.51622600
C	-2.44176400	-2.54798100	-2.71284400
H	-0.98620400	-2.27754100	-4.27877500
H	-3.69093500	-2.68072200	-0.96282900
H	-3.16980700	-3.01767900	-3.36575600
C	2.26231200	-1.31969500	-0.29481500
C	2.77587700	-2.29050600	0.56938500
C	2.98278700	-0.95180600	-1.44105800
C	3.99078800	-2.90434600	0.27699900
H	2.24814000	-2.56179300	1.47604900
C	4.19240800	-1.57345900	-1.72643100
H	2.61799800	-0.16861500	-2.09951700
C	4.69465200	-2.55272900	-0.87042000
H	4.38690000	-3.65254300	0.95447200
H	4.74664000	-1.28563100	-2.61284700
H	5.64180200	-3.03233000	-1.09333700
C	-2.15486700	1.19542100	-0.63808800
O	-3.23135200	0.97017900	-1.25525000
O	-1.86519200	1.10984100	0.54552400
C	-4.59172400	0.47820500	-0.17087600
H	-5.13888700	-0.01509400	-0.96298000
H	-4.01252100	-0.14982000	0.49264200
C	-5.28403400	1.59662400	0.48544300
H	-5.74128400	2.31422700	-0.22490000
H	-4.63117300	2.17544500	1.16916400
O	-6.11108600	0.66137700	1.04940400
C	3.67354500	3.62710000	0.37195000
N	4.67051500	4.06144300	0.76725700

## In2A

0 1

C	1.24837600	3.93528800	-0.83618700
C	0.07122400	3.32245200	-1.23043100
C	-0.14131200	1.97372700	-0.96000800
C	0.83351400	1.20637600	-0.30933900
C	2.02182800	1.83070200	0.08595900
C	2.22225700	3.18669600	-0.16563500
H	1.41561900	4.98651300	-1.04005600

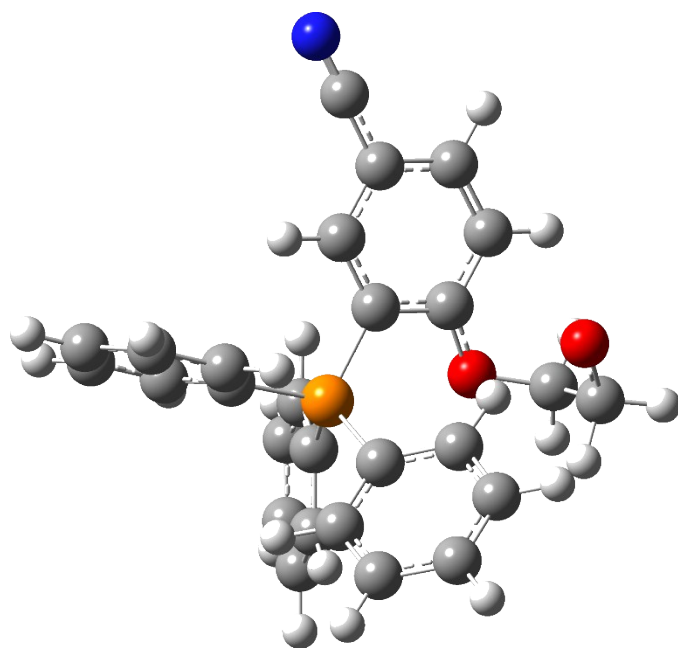
H	-0.70667800	3.87188900	-1.74709900
H	2.80219900	1.26539000	0.58657300
O	-1.31745500	1.43909600	-1.42244800
P	0.71045600	-0.57040200	0.05148700
C	0.42533100	-0.81780900	1.81214700
C	0.25977000	-2.12260700	2.29942400
C	0.37167800	0.27589200	2.68000300
C	0.05997000	-2.32453400	3.65978000
H	0.26903800	-2.97435800	1.62467100
C	0.17018600	0.06043000	4.03964700
H	0.46170400	1.28753900	2.30019200
C	0.01872400	-1.23447300	4.52803000
H	-0.07007400	-3.33169700	4.03930300
H	0.12378400	0.90810300	4.71388900
H	-0.14153900	-1.39671900	5.58855800
C	-0.56765100	-1.42750000	-0.89826300
C	-0.38143200	-1.62787600	-2.27151300
C	-1.72721100	-1.88981400	-0.26592100
C	-1.36297300	-2.27778100	-3.00867600
H	0.51931200	-1.28374500	-2.76911200
C	-2.69756300	-2.55082000	-1.01307500
H	-1.88718400	-1.71401200	0.79263400
C	-2.51829500	-2.74090400	-2.38005300
H	-1.22208100	-2.42680500	-4.07333000
H	-3.59775600	-2.90581800	-0.52315900
H	-3.28063100	-3.25150600	-2.95875400
C	2.33101900	-1.22266200	-0.43562600
C	2.99379400	-2.17509900	0.34302900
C	2.90217700	-0.77166600	-1.63459700
C	4.21613900	-2.68508200	-0.08849900
H	2.57822600	-2.51069700	1.28654700
C	4.11904900	-1.29121500	-2.05785300
H	2.41603500	-0.00294900	-2.22853700
C	4.77446300	-2.24948900	-1.28643400
H	4.73245100	-3.41954000	0.51953200
H	4.55778400	-0.93882600	-2.98472500
H	5.72757700	-2.64850500	-1.61674400
C	-2.22764900	1.03557000	-0.47786400
O	-3.30920000	0.67772300	-1.10512000
O	-1.97655900	1.01096300	0.70320800
C	-4.45050900	0.28359100	-0.27620200
H	-5.01875500	-0.40002800	-0.90945100
H	-4.07741500	-0.24859200	0.60260700
C	-5.32391300	1.47747300	0.15447400
H	-5.56172400	2.02050600	-0.80881100
H	-4.60311600	2.18774600	0.66391900
O	-6.35662700	1.04559900	0.87607000
C	3.44884600	3.80956200	0.25668400
N	4.43515500	4.30921900	0.59676800



## In1B

0 1

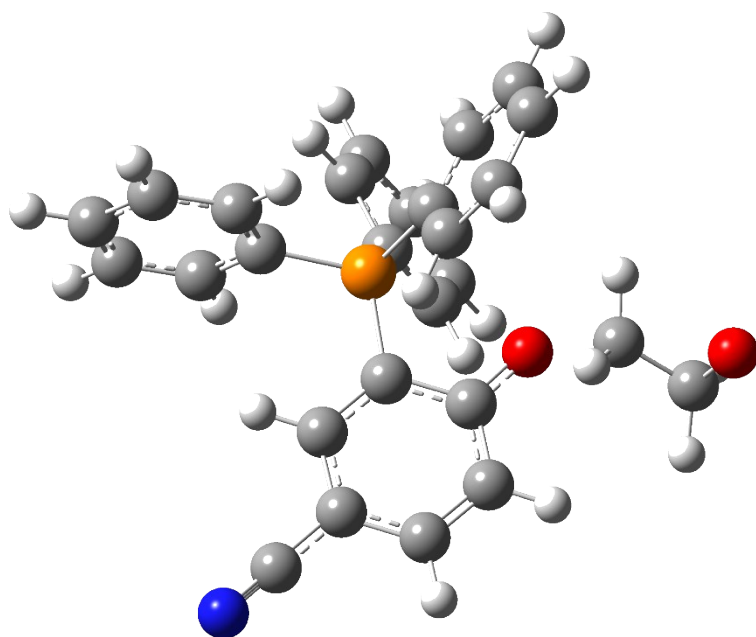
C	-2.13304300	3.34922400	0.57290800
C	-2.65620000	2.09511200	0.78989200
C	-1.84155000	0.95519500	0.63905500
C	-0.49670900	1.12891000	0.23604200
C	0.02492800	2.40519700	0.01603800
C	-0.78756500	3.51967500	0.18872300
H	-2.76619600	4.22202800	0.69094700
H	-3.70109300	1.98341300	1.03711200
H	1.05915700	2.53369600	-0.28527800
O	-2.18249600	-0.29143200	0.96102700
P	0.52551700	-0.32791300	-0.00172600
C	0.54281500	-1.31313300	1.51439300
C	0.69118600	-2.70028300	1.45577200
C	0.44728400	-0.65975200	2.74774800
C	0.75484200	-3.43284800	2.63804700
H	0.74480300	-3.21163300	0.50008900
C	0.51588200	-1.40016800	3.92274900
H	0.31280900	0.41779400	2.78931900
C	0.67074800	-2.78471200	3.86738400
H	0.86549100	-4.51082300	2.59516700
H	0.44032200	-0.89684300	4.88045000
H	0.71853800	-3.35977200	4.78610200
C	0.00098400	-1.29710300	-1.42896100
C	-1.26477000	-1.11135100	-1.99293200
C	0.90670100	-2.22767600	-1.96432400
C	-1.61488300	-1.88839000	-3.09872500
H	-2.01089800	-0.38951200	-1.61663300
C	0.53220800	-2.99596500	-3.05855800
H	1.90093200	-2.34229700	-1.54015700
C	-0.73240000	-2.82556200	-3.62543000
H	-2.59648400	-1.74768000	-3.54066300
H	1.22771400	-3.71736700	-3.47322300
H	-1.02152300	-3.42293700	-4.48420300
C	2.21707300	0.22369400	-0.33112400
C	3.16202700	0.27623300	0.69726600
C	2.55290700	0.64623400	-1.62420300
C	4.44254100	0.75226900	0.42932800
H	2.90579100	-0.05614600	1.69831100
C	3.83293100	1.12379400	-1.88022200
H	1.82049200	0.59802500	-2.42530300
C	4.77616600	1.17534200	-0.85448400
H	5.17854000	0.78974200	1.22497400
H	4.09461900	1.45085600	-2.88047300
H	5.77564000	1.54495500	-1.05852900
C	-3.57087600	-0.67199400	1.00630800



H	-4.13276300	0.07737000	1.57204300
H	-3.58040400	-1.61315400	1.56240400
C	-4.06784600	-0.80338000	-0.44754600
H	-3.61745400	-1.76735900	-0.81211200
H	-5.16099500	-1.03377800	-0.35386700
O	-3.75136400	0.27597400	-1.18100000
C	-0.25535000	4.83325300	-0.02803700
N	0.17584300	5.89469900	-0.20049100

### TS step1 mechanism B (iv = 648.01 cm<sup>-1</sup>)

0 1			
C	-1.17091800	3.69618900	-0.85920900
C	-1.96731600	2.57289800	-0.90313900
C	-1.40880200	1.28326600	-0.70848200
C	-0.01450300	1.20962100	-0.41760400
C	0.78656400	2.34734800	-0.36991400
C	0.21201300	3.59633700	-0.60359000
H	-1.60729200	4.67544500	-1.02730100
H	-3.02818500	2.65179500	-1.11497400
H	1.84534300	2.27460900	-0.14093200
O	-2.08896200	0.18153100	-0.77567600
P	0.59814800	-0.41353000	0.02386700
C	-0.46213700	-1.08876700	1.32366400
C	-0.74771500	-2.45433900	1.36674100
C	-0.99556200	-0.21962000	2.28217600
C	-1.57057300	-2.95028300	2.37478300
H	-0.34820600	-3.12715600	0.61460800
C	-1.81384800	-0.72546600	3.28605300
H	-0.78732200	0.84616600	2.23676600
C	-2.10247500	-2.08885200	3.33100400
H	-1.80086500	-4.00957300	2.40596300
H	-2.23331300	-0.05270500	4.02602800
H	-2.74931000	-2.47851700	4.10986100
C	0.69842200	-1.54389800	-1.38052200
C	-0.05323500	-1.31239300	-2.53595200
C	1.54871200	-2.65486700	-1.29651000
C	0.04610400	-2.19842900	-3.60443300
H	-0.71992700	-0.45970500	-2.59195700
C	1.63067100	-3.53940400	-2.36621300
H	2.15003800	-2.82559100	-0.40765200
C	0.88196400	-3.30918500	-3.51911900
H	-0.53180400	-2.01837700	-4.50427200
H	2.28517500	-4.40167500	-2.30216900
H	0.95371700	-3.99733700	-4.35489900
C	2.27809900	-0.22404600	0.66405600
C	2.51997500	-0.20699400	2.04016400
C	3.32886800	-0.02940100	-0.24274700

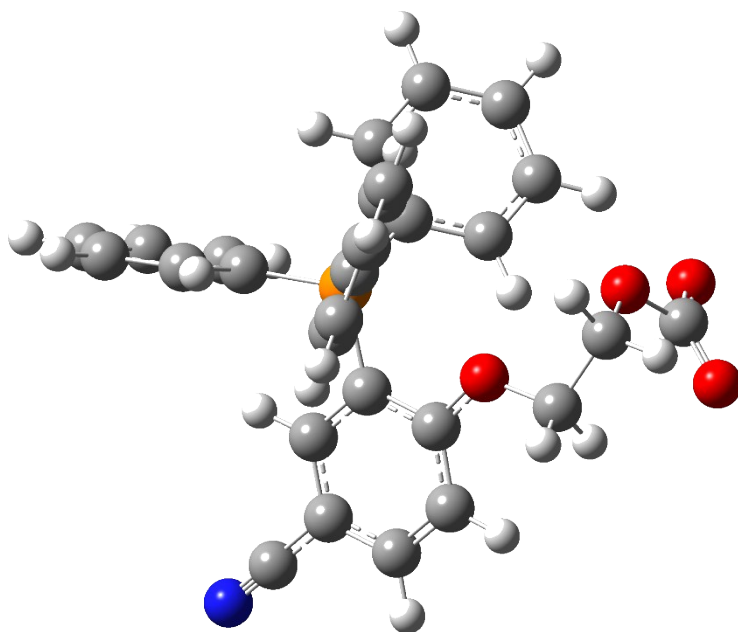


C	3.81426900	0.00767200	2.50686000
H	1.70924600	-0.36448300	2.74445800
C	4.61631900	0.18834000	0.23353700
H	3.14265900	-0.05037000	-1.31320900
C	4.85773100	0.20644400	1.60709900
H	4.00475800	0.01696200	3.57434900
H	5.42982400	0.34020000	-0.46717000
H	5.86425500	0.37328100	1.97608100
C	-3.69240400	0.16412200	0.05971800
H	-3.50519200	0.99461300	0.73224900
H	-3.53742000	-0.82736800	0.46692500
C	-4.86702700	0.31376100	-0.81054400
H	-4.92167100	1.29033700	-1.33562700
H	-4.95237400	-0.47745000	-1.58151400
O	-5.62374500	0.17299400	0.32117600
C	1.02629200	4.77529200	-0.56877300
N	1.68434200	5.72879600	-0.54318000

## In2B

0 1

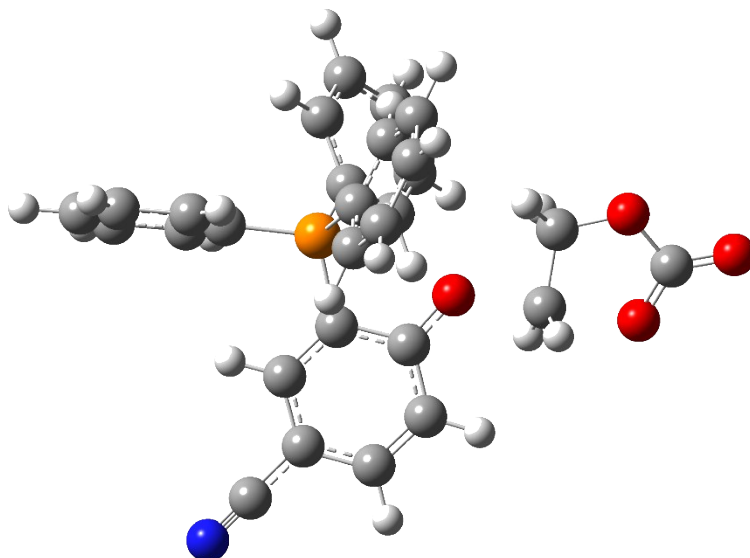
C	0.31889000	4.06199500	0.12887200
C	-0.71873000	3.23996900	0.53658500
C	-0.57635700	1.84962400	0.45543700
C	0.63551700	1.29283700	-0.01573900
C	1.67460600	2.12946100	-0.41087200
C	1.51444600	3.51546700	-0.35140500
H	0.20553500	5.13881000	0.18720400
H	-1.63240000	3.67658400	0.91749000
H	2.61487800	1.71647300	-0.75905000
O	-1.51962300	0.97320300	0.80412400
P	0.86271900	-0.50357000	-0.00115300
C	0.40563200	-1.11912400	1.63315600
C	-0.18292100	-2.38001200	1.75332700
C	0.65760800	-0.33616400	2.76506800
C	-0.51545500	-2.85977300	3.01740600
H	-0.39311400	-2.97756500	0.87169900
C	0.32333500	-0.82628400	4.02204300
H	1.10242300	0.65044900	2.66551500
C	-0.26341500	-2.08561500	4.14674800
H	-0.97716700	-3.83594300	3.11658300
H	0.51540000	-0.22324800	4.90264700
H	-0.52880000	-2.46153500	5.12922100
C	-0.07300700	-1.37232000	-1.27240600
C	-1.34022200	-0.92795700	-1.66120600
C	0.44800600	-2.57218100	-1.78188100
C	-2.08820300	-1.68357200	-2.56018300
H	-1.77915100	-0.02855600	-1.24758300
C	-0.30285600	-3.31200600	-2.68732600



H	1.42720800	-2.92667000	-1.47536600
C	-1.56727600	-2.86774300	-3.07479100
H	-3.08460900	-1.32814100	-2.80658900
H	0.09871300	-4.23775000	-3.08480200
H	-2.15117600	-3.45656200	-3.77508700
C	2.61720500	-0.82278100	-0.28722600
C	3.46082500	-1.13200400	0.78274400
C	3.12970300	-0.71516000	-1.58825300
C	4.81909600	-1.33190100	0.54977700
H	3.06399000	-1.22390800	1.78847700
C	4.48737800	-0.91333100	-1.80827600
H	2.47334000	-0.48399700	-2.42297000
C	5.33002000	-1.22181600	-0.74020200
H	5.47411500	-1.57745800	1.37822900
H	4.88655300	-0.83061000	-2.81299300
H	6.38849000	-1.38004100	-0.91762000
C	-2.80044900	1.43576600	1.26500700
H	-3.19167300	2.19267600	0.58078100
H	-2.68878600	1.85221800	2.27212200
C	-3.72452000	0.23676500	1.24460100
H	-3.29071300	-0.57416800	1.83947200
H	-4.68342800	0.53738400	1.67658500
O	-3.87818100	-0.25659900	-0.06521300
C	-4.67609400	0.53601400	-0.94132900
O	-4.65133900	0.11957700	-2.10932500
O	-5.25970800	1.50650500	-0.43086400
C	2.58867600	4.37369300	-0.76676200
N	3.45596800	5.06322200	-1.10199000

### TS step 3 mechanism B (iv = 642.15cm<sup>-1</sup>)

0 1			
C	0.12695000	4.00655500	0.11458500
C	-0.88429300	3.08380200	0.27540100
C	-0.60281200	1.69290100	0.24508300
C	0.75677700	1.30531800	0.03754200
C	1.77424200	2.24196800	-0.10996100
C	1.46211100	3.60138200	-0.07794900
H	-0.10374000	5.06654100	0.14248100
H	-1.90129600	3.41914800	0.43974300
H	2.80331800	1.92614100	-0.25278700
O	-1.48410200	0.75537500	0.38296600
P	1.06392900	-0.45835200	0.02167100
C	0.42987800	-1.18406800	1.55028800
C	-0.21972400	-2.41964300	1.54785500
C	0.60979400	-0.47692400	2.74419300
C	-0.68186700	-2.95179500	2.74888100
H	-0.38261100	-2.95748900	0.61946900



C	0.15030700	-1.02039800	3.93868200
H	1.09630500	0.49507700	2.74167300
C	-0.49475100	-2.25609500	3.94054800
H	-1.19388400	-3.90782400	2.74939900
H	0.28807400	-0.47484300	4.86577200
H	-0.85939800	-2.67335000	4.87321700
C	0.34421300	-1.25791000	-1.42931500
C	-0.58795000	-0.59235500	-2.22907200
C	0.75774800	-2.55666400	-1.75504100
C	-1.12252800	-1.23618800	-3.34115100
H	-0.89372900	0.41960300	-1.98921600
C	0.21108700	-3.19429700	-2.86335600
H	1.50680700	-3.06641000	-1.15442900
C	-0.73003700	-2.53551400	-3.65279500
H	-1.84536400	-0.71897900	-3.96272000
H	0.52552800	-4.20148700	-3.11345400
H	-1.15264600	-3.03418300	-4.51868400
C	2.84836000	-0.73211600	-0.06977600
C	3.58462900	-1.07421500	1.06747100
C	3.48984900	-0.55119000	-1.30270700
C	4.96452900	-1.23264600	0.96866100
H	3.08914600	-1.22444900	2.02106700
C	4.86811700	-0.70675000	-1.38918000
H	2.91575300	-0.29457000	-2.18901800
C	5.60371600	-1.04775900	-0.25418900
H	5.53735700	-1.50346400	1.84863400
H	5.36616500	-0.56618700	-2.34207300
H	6.67901300	-1.17283900	-0.32610300
C	-3.26006500	1.09803600	0.02833300
H	-3.00171300	1.72282800	-0.81442400
H	-3.43011700	1.56958800	0.98640900
C	-3.56364500	-0.38070100	-0.13956700
H	-3.34745000	-0.68072800	-1.17214900
H	-2.94032800	-0.96612100	0.53629900
O	-4.91251600	-0.65515000	0.18259700
C	-5.74345200	0.41315600	-0.11590000
O	-5.10117900	1.46765400	-0.43549300
O	-6.94798700	0.23126100	-0.03093400
C	2.49728300	4.57958700	-0.23621200
N	3.33162300	5.37332700	-0.36505200

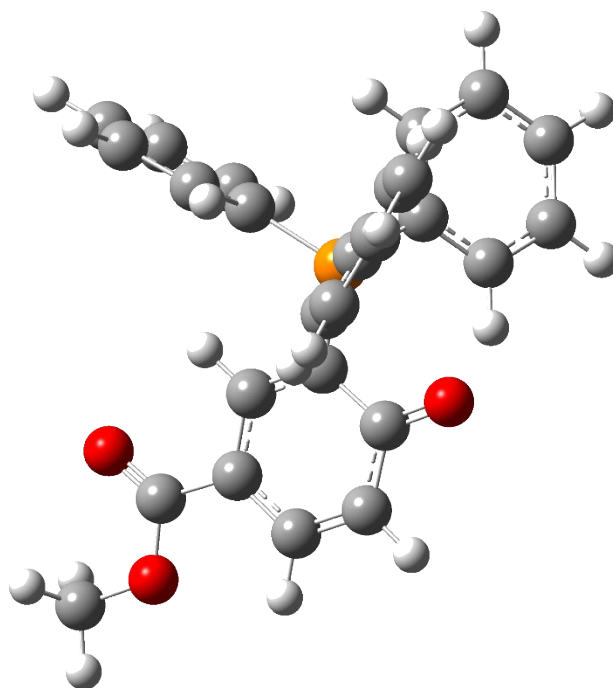


# CO<sub>2</sub>Me

## Organocatalyst

0 1

C	3.14936000	-2.00944100	0.78398200
C	1.99345700	-2.71581300	0.98169200
C	0.69210800	-2.11572400	0.80027200
C	0.71630700	-0.72767600	0.38041300
C	1.90429500	-0.02877600	0.17304200
C	3.13028100	-0.64931000	0.38005000
H	4.11001700	-2.49231500	0.93445400
H	2.01728100	-3.75714500	1.28712100
H	1.90014700	1.00663700	-0.15650800
O	-0.39123300	-2.72541500	0.98354000
P	-0.87023900	-0.01256700	0.03513400
C	-1.76840400	-1.00773700	-1.18186800
C	-3.15882800	-0.91777400	-1.27876800
C	-1.04832400	-1.81505900	-2.06671500
C	-3.82731000	-1.63539600	-2.26678600
H	-3.72144700	-0.30013500	-0.58502300
C	-1.72388700	-2.52769400	-3.05197400
H	0.03183600	-1.88834600	-1.97789600
C	-3.11129300	-2.43763500	-3.15215000
H	-4.90738300	-1.56884400	-2.34137100
H	-1.16636300	-3.15677700	-3.73751100
H	-3.63542600	-2.99578000	-3.92091300
C	-1.91932600	0.26459400	1.48842800
C	-1.79193800	-0.54391400	2.62304900
C	-2.86197800	1.30111400	1.46353900
C	-2.60634800	-0.30712900	3.72684100
H	-1.08234000	-1.36383200	2.62222300
C	-3.67693900	1.52183400	2.56903600
H	-2.95384500	1.94321000	0.59210500
C	-3.54607300	0.72086100	3.70110800
H	-2.50697500	-0.93085800	4.60885700
H	-4.40609800	2.32455000	2.54680300
H	-4.17741600	0.90009200	4.56535700
C	-0.60171400	1.62240700	-0.70171000
C	-0.69487600	1.80108700	-2.08370600
C	-0.22802200	2.69179300	0.12300300
C	-0.41601400	3.04782900	-2.63884600
H	-0.98497800	0.97447100	-2.72461100
C	0.05051200	3.93211800	-0.43913400
H	-0.15802100	2.55554300	1.19890800
C	-0.04454000	4.10958100	-1.81930800
H	-0.49238100	3.18723300	-3.71171300
H	0.33943800	4.76007200	0.19896500

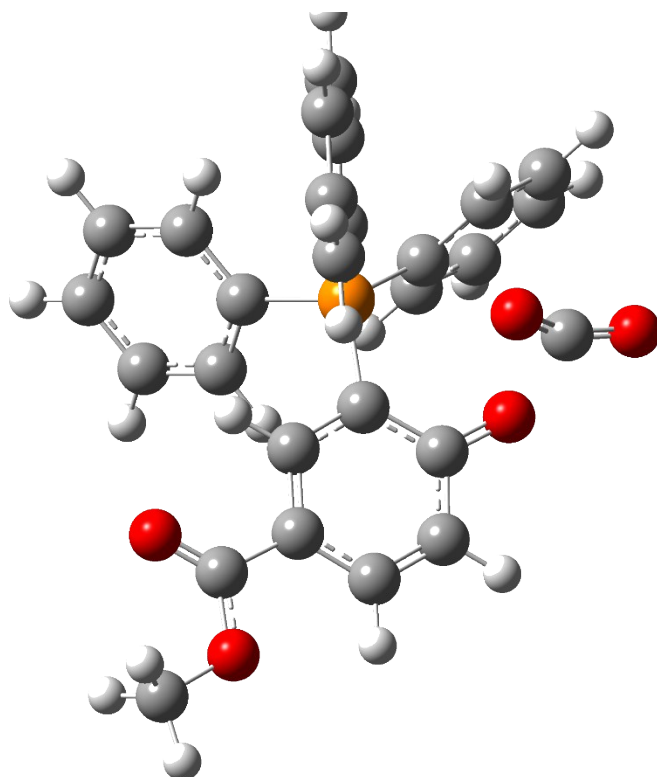


H	0.16970000	5.07993300	-2.25502500
C	4.35155900	0.13395100	0.14938200
O	4.38085700	1.30134800	-0.19496700
O	5.47582500	-0.57920100	0.35819900
C	6.69486300	0.13192900	0.14739100
H	6.76357400	0.98421600	0.82647500
H	7.49369900	-0.57951000	0.34812300
H	6.75539800	0.49211700	-0.88158100

### TS step1 mechanism A (iv = 275.35 cm<sup>-1</sup>)

O 1

C	-2.99772400	-2.22012900	-0.72739700
C	-1.76432100	-2.75311800	-1.00759600
C	-0.54958400	-2.03901000	-0.76878300
C	-0.69455500	-0.71034500	-0.25506900
C	-1.96139500	-0.17962500	0.02438100
C	-3.11269500	-0.92085600	-0.18948000
H	-3.89709600	-2.79711300	-0.91549000
H	-1.66521600	-3.75348300	-1.41545200
H	-2.07316900	0.83247100	0.40752700
O	0.58500900	-2.58977900	-1.02304400
P	0.69680800	0.38904700	-0.01477700
C	1.08099500	0.64984200	1.73370000
C	2.22961500	1.36400800	2.09906800
C	0.20695600	0.17488800	2.71395000
C	2.49015900	1.61069800	3.44288300
H	2.92453300	1.71937200	1.34306500
C	0.47484600	0.42760600	4.05595700
H	-0.66415900	-0.40653700	2.43078200
C	1.61162600	1.14558700	4.41968500
H	3.37992200	2.16291500	3.72451000
H	-0.20262000	0.05543000	4.81660100
H	1.81793300	1.33837000	5.46727200
C	2.21285800	-0.09978000	-0.88197600
C	2.29422100	0.09753900	-2.26420200
C	3.29036600	-0.65589300	-0.18709400
C	3.44520300	-0.27676900	-2.94775100
H	1.46876700	0.54321700	-2.80991500
C	4.44066900	-1.02259600	-0.87917900
H	3.22866900	-0.81568800	0.88414700
C	4.51840900	-0.83575000	-2.25644700
H	3.50468500	-0.12632100	-4.02014300
H	5.27365700	-1.45847100	-0.33836400
H	5.41666900	-1.12298500	-2.79283100
C	0.18144400	1.98882900	-0.72141000
C	0.55010800	3.20027100	-0.13079900
C	-0.56242700	1.99073300	-1.90969700

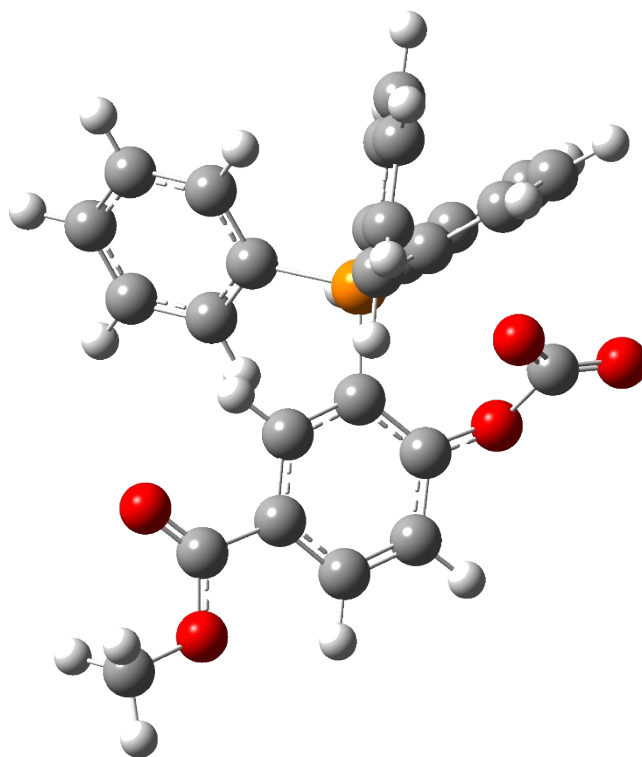


C	0.18953500	4.40308800	-0.73288700
H	1.10298100	3.21651700	0.80163800
C	-0.91152400	3.19578000	-2.50848000
H	-0.88273800	1.05423100	-2.35750000
C	-0.53411200	4.40226600	-1.92184900
H	0.47269100	5.34031200	-0.26618700
H	-1.48699500	3.19079900	-3.42766200
H	-0.81339400	5.34154700	-2.38761600
C	1.66633400	-3.05700700	0.46825700
O	2.42769400	-3.83036400	-0.00236300
O	1.23396600	-2.41976300	1.37694300
C	-4.41306200	-0.29759300	0.13717800
O	-4.54773300	0.81602200	0.60304900
O	-5.45243200	-1.10087600	-0.13624000
C	-6.73927400	-0.55789400	0.16538700
H	-7.45774900	-1.33013300	-0.10157800
H	-6.81105600	-0.31837400	1.22795300
H	-6.91651300	0.34768600	-0.41796900

## In1A

01

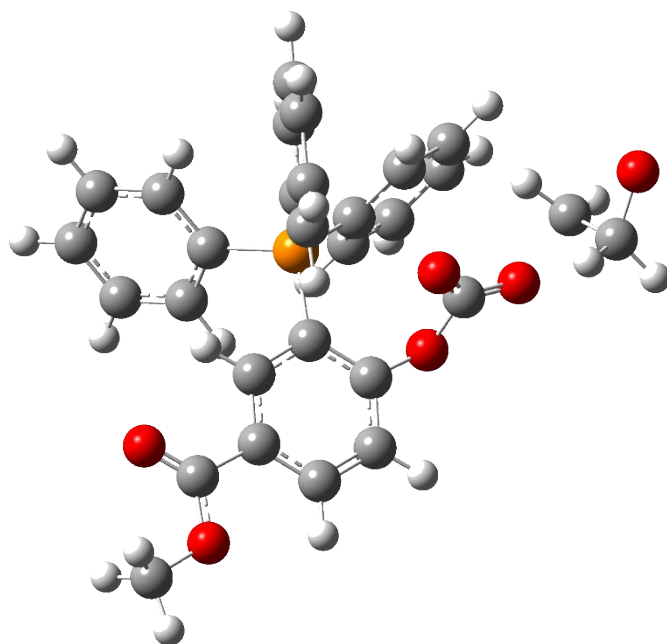
C	-3.03997600	-2.26259000	-0.50431500
C	-1.80343900	-2.85314700	-0.68834600
C	-0.61674400	-2.13045500	-0.49844100
C	-0.70040600	-0.76386500	-0.15704900
C	-1.95687500	-0.17767800	0.03140000
C	-3.12221400	-0.91854900	-0.12331800
H	-3.94816100	-2.83802000	-0.64431700
H	-1.71375600	-3.89664900	-0.96794000
H	-2.05195000	0.87290000	0.29286000
O	0.53723900	-2.78467900	-0.69656800
P	0.73238600	0.32533300	-0.00484300
C	1.12672500	0.72812500	1.71093000
C	2.29503100	1.44028800	2.00274100
C	0.23857000	0.37698900	2.72927700
C	2.56520900	1.80825200	3.31769400
H	2.99631800	1.70168900	1.21488700
C	0.51597300	0.75162900	4.03922700
H	-0.64803100	-0.20563900	2.50268000
C	1.67552400	1.46674400	4.33315400
H	3.47212200	2.35727500	3.54571200
H	-0.17003100	0.47598900	4.83269200
H	1.88962000	1.75247500	5.35769200
C	2.22085600	-0.21639700	-0.88923900
C	2.27597300	-0.06060000	-2.27935100
C	3.31810500	-0.73748100	-0.19592300
C	3.42006300	-0.44008300	-2.97145200
H	1.43864000	0.35936200	-2.82632200



C	4.46348600	-1.10010000	-0.89723300
H	3.26189200	-0.88716900	0.87664300
C	4.51542400	-0.95431000	-2.28066300
H	3.45710200	-0.32441200	-4.04906900
H	5.31240100	-1.50597300	-0.35801600
H	5.41010200	-1.24169900	-2.82305200
C	0.19962200	1.87034800	-0.81821400
C	0.56679000	3.11690400	-0.30417100
C	-0.55134800	1.80175400	-2.00090200
C	0.19905900	4.28138000	-0.97417400
H	1.12465500	3.19094900	0.62236500
C	-0.90970300	2.96809400	-2.66657600
H	-0.87202500	0.84162700	-2.39498800
C	-0.53277100	4.20877000	-2.15521600
H	0.48339300	5.24492500	-0.56542600
H	-1.49081400	2.90708600	-3.58022700
H	-0.81836700	5.11770000	-2.67412100
C	1.48148900	-2.89751800	0.45003000
O	2.35000800	-3.72157400	0.22631600
O	1.22228100	-2.13177200	1.38555500
C	-4.41758500	-0.22574200	0.10991000
O	-4.51725400	0.94115000	0.42207300
O	-5.46838000	-1.03444000	-0.05975400
C	-6.74647700	-0.42812100	0.15763700
H	-7.47963000	-1.21491900	-0.00415700
H	-6.81312300	-0.04352300	1.17671600
H	-6.89945700	0.39070500	-0.54746100

### TS step 2 mechanism A (iv = 628.92 cm<sup>-1</sup>)

01			
C	-2.40842900	-2.85833200	-1.06416700
C	-1.08599900	-2.77933600	-1.46907900
C	-0.30813300	-1.66823500	-1.14368600
C	-0.87362900	-0.60223000	-0.42336200
C	-2.21040100	-0.69343800	-0.01989900
C	-2.97193500	-1.81554300	-0.32458700
H	-3.00597800	-3.72721900	-1.31427700
H	-0.61930500	-3.57619700	-2.03647400
H	-2.68497100	0.11150200	0.53527100
O	0.97125800	-1.66239900	-1.61230300
P	-0.00348200	0.92010900	0.02356100
C	0.42377700	0.92976500	1.77638400
C	1.15740800	2.00111900	2.30281800
C	-0.00747000	-0.10813500	2.60536800
C	1.44163100	2.03555200	3.66362900
H	1.51547700	2.79913100	1.65797600
C	0.27973700	-0.06187500	3.96558000



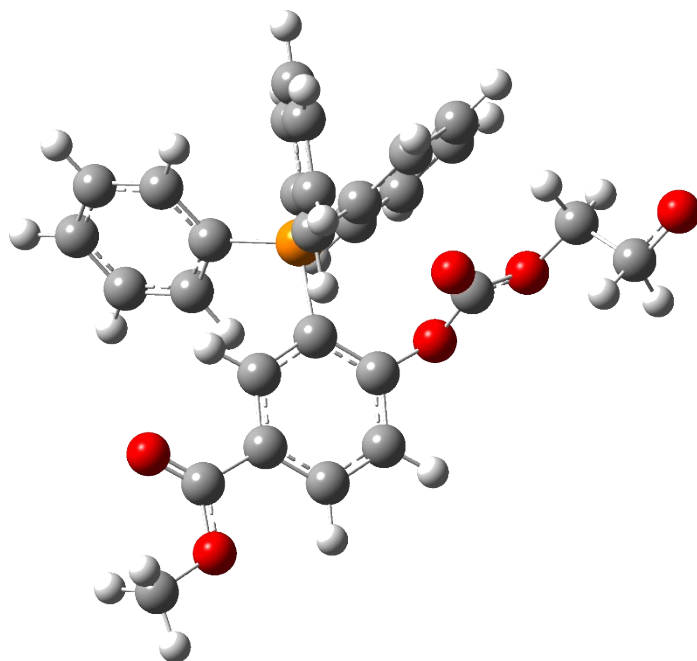
H	-0.53828900	-0.95696300	2.18836500
C	0.99880900	1.00742800	4.49365700
H	2.01165300	2.86276600	4.07174900
H	-0.05102900	-0.86855000	4.61021000
H	1.22350600	1.03639400	5.55457400
C	1.46377000	1.25309700	-0.98186900
C	1.30385000	1.56470200	-2.33697000
C	2.74074300	1.19607500	-0.41624900
C	2.42384700	1.80795800	-3.12192000
H	0.31639400	1.61707400	-2.78421000
C	3.85509100	1.45474800	-1.20852500
H	2.86780200	0.92680800	0.62661500
C	3.69793600	1.75695000	-2.55771800
H	2.30027200	2.04118900	-4.17362800
H	4.84535300	1.40624900	-0.76843300
H	4.56930700	1.95288500	-3.17361900
C	-1.21115200	2.24187600	-0.29937700
C	-1.35480000	3.31388000	0.58528100
C	-1.98211000	2.19330800	-1.47000600
C	-2.24996400	4.33900600	0.29120400
H	-0.78963800	3.35141300	1.50906700
C	-2.86993700	3.22340200	-1.75702900
H	-1.91092700	1.34576600	-2.14572300
C	-3.00169100	4.29795100	-0.87866800
H	-2.36125900	5.16496700	0.98486700
H	-3.46542100	3.18120800	-2.66226400
H	-3.69976900	5.09753700	-1.10271900
C	2.01380300	-1.68417300	-0.66131200
O	3.12182700	-1.83931500	-1.24504400
O	1.73613300	-1.53765200	0.51993400
C	4.53619200	-1.87554100	-0.11263600
H	5.23691500	-1.54722300	-0.86853300
H	4.16752000	-1.12980300	0.57835600
C	4.80568300	-3.19049000	0.48463300
H	5.02952100	-3.98146600	-0.25872200
H	3.98039900	-3.55897500	1.12608900
O	5.87238800	-2.60068800	1.11122400
C	-4.38640700	-1.84072800	0.14724600
O	-4.90630600	-0.94148200	0.76982500
O	-5.01541600	-2.96629700	-0.19514100
C	-6.38264700	-3.05616800	0.22239100
H	-6.73621600	-4.02245400	-0.12919500
H	-6.44902600	-2.99287900	1.30966300
H	-6.96459200	-2.24769400	-0.22317500

## In2A

O 1

C	-2.23539700	-2.95310100	-0.96410500
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C	-0.90181500	-2.83349600	-1.32501900
C	-0.19675300	-1.67499100	-1.01699900
C	-0.82179300	-0.60629200	-0.36011300
C	-2.16737500	-0.74114300	-0.00123000
C	-2.86773600	-1.90637600	-0.29033600
H	-2.78791500	-3.85491200	-1.20036000
H	-0.38076600	-3.62912600	-1.84442400
H	-2.69622800	0.06285800	0.50389300
O	1.10699100	-1.62006100	-1.44967100
P	-0.04337800	0.97914700	0.04903200
C	0.27577900	1.07194400	1.81876200
C	0.90558500	2.20950900	2.34367700
C	-0.10625300	0.02213900	2.65773100
C	1.13030000	2.29766600	3.71234700
H	1.23392700	3.01432700	1.69127200
C	0.12518200	0.12162000	4.02602100
H	-0.55727500	-0.87443400	2.24712500
C	0.73659300	1.25639400	4.55178900
H	1.61758100	3.17592600	4.12059300
H	-0.16644500	-0.69412400	4.67790500
H	0.91663100	1.32758100	5.61917400
C	1.48233200	1.31077300	-0.86434400
C	1.40971100	1.57652200	-2.23718700
C	2.71868400	1.30399500	-0.20969300
C	2.57572600	1.82161400	-2.95105000
H	0.45502900	1.59754400	-2.75258300
C	3.87898600	1.56460100	-0.93327100
H	2.78252700	1.07585900	0.84908100
C	3.80852900	1.81862600	-2.29980300
H	2.52001200	2.02097800	-4.01532700
H	4.83710200	1.55659300	-0.42496700
H	4.71602400	2.01621800	-2.86036500
C	-1.27913600	2.21456900	-0.44241100
C	-1.53717900	3.33931700	0.34558600
C	-1.95422300	2.03799200	-1.65884100
C	-2.45294600	4.29197100	-0.09445400
H	-1.04817200	3.47154800	1.30405300
C	-2.86058400	2.99767100	-2.09149500
H	-1.79376600	1.14688400	-2.25910600
C	-3.10744700	4.12606800	-1.31152900
H	-2.65793600	5.16050500	0.52157000
H	-3.37950400	2.85755500	-3.03318200
H	-3.82000800	4.87093000	-1.64955500
C	2.07924100	-1.60311400	-0.48424100
O	3.23065100	-1.67071700	-1.08749900
O	1.83257800	-1.50405600	0.69413800
C	4.42022900	-1.72949700	-0.23676200
H	5.20987700	-1.29181400	-0.85011700
H	4.25001000	-1.10781000	0.64614800

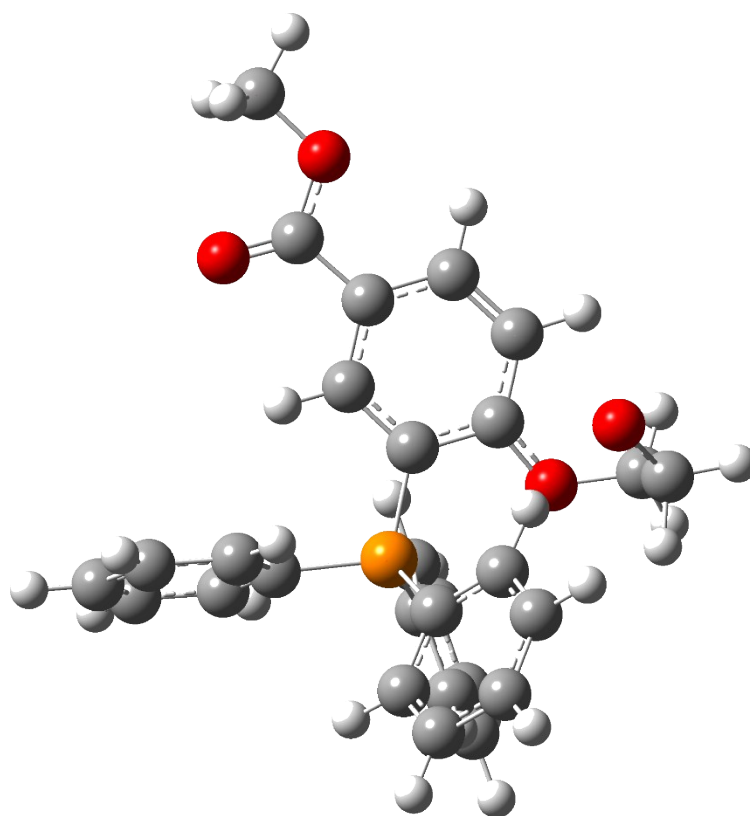


C	4.79651200	-3.16258800	0.18426200
H	4.82886300	-3.74656600	-0.78398200
H	3.86340000	-3.56765200	0.68267000
O	5.91052100	-3.14046100	0.91436600
C	-4.30038700	-1.97106600	0.12590800
O	-4.87243000	-1.07413300	0.70346400
O	-4.87423500	-3.12487800	-0.21330900
C	-6.25387400	-3.25405000	0.15235300
H	-6.84351100	-2.47359000	-0.33106300
H	-6.56036400	-4.23809900	-0.19401400
H	-6.36398800	-3.17359800	1.23485900

## In1B

0 1

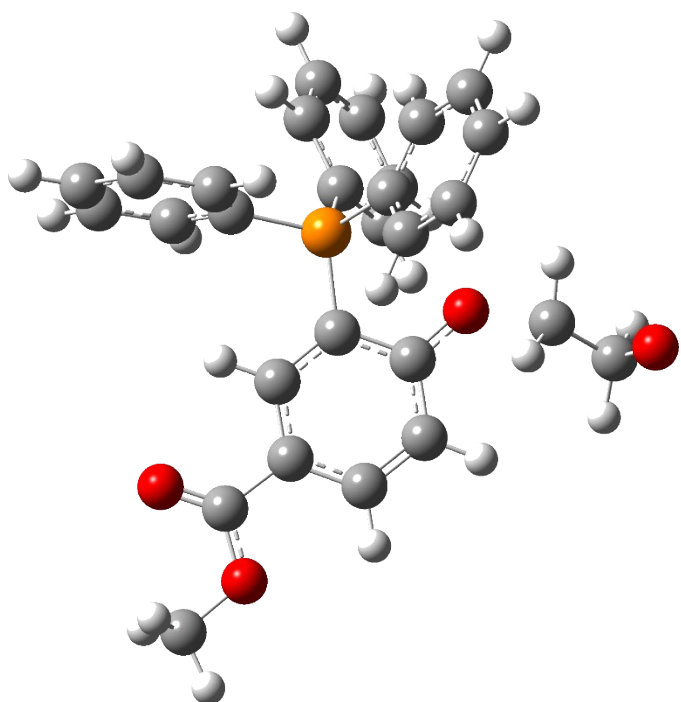
C	-3.03655600	-1.90107000	0.55344600
C	-1.82143700	-2.52198500	0.75346400
C	-0.62786800	-1.78926300	0.61421900
C	-0.70770700	-0.42799400	0.23737100
C	-1.94602000	0.18525700	0.04058300
C	-3.11629000	-0.54231700	0.20249800
H	-3.95183500	-2.47222300	0.66355700
H	-1.78477800	-3.57745300	0.97887200
H	-2.01591700	1.23216200	-0.23672000
O	0.59584200	-2.22274600	0.91985400
P	0.81818700	0.48579400	0.01274200
C	1.80810400	0.40810300	1.52419500
C	3.20279500	0.40049300	1.46368000
C	1.15063000	0.39043700	2.75896400
C	3.93977700	0.38751800	2.64508100
H	3.71496200	0.39148600	0.50699000
C	1.89558300	0.38193900	3.93308500
H	0.06475400	0.37534700	2.80211100
C	3.28864300	0.38159000	3.87558000
H	5.02330700	0.37677900	2.60052900
H	1.38814700	0.36757700	4.89153600
H	3.86731300	0.37012200	4.79318100
C	1.75480400	-0.07589000	-1.42258900
C	1.48960700	-1.31229300	-2.01841800
C	2.74645800	0.77876300	-1.93060700
C	2.24919600	-1.68462100	-3.12963800
H	0.72013200	-2.01975100	-1.66131500
C	3.49561200	0.38268900	-3.03026600
H	2.92343400	1.75169600	-1.47907300
C	3.24518200	-0.85297200	-3.63010800
H	2.04890100	-2.64430900	-3.59612300
H	4.26372700	1.03942800	-3.42376800
H	3.82770100	-1.15931400	-4.49319800
C	0.39565000	2.21938900	-0.29473200



C	0.46620300	3.16895200	0.72736400
C	-0.04154500	2.58727800	-1.57423900
C	0.09708700	4.48650600	0.46787900
H	0.81343500	2.88879500	1.71669700
C	-0.41323900	3.90329800	-1.82155400
H	-0.08784800	1.85076400	-2.37190400
C	-0.34245000	4.85160600	-0.80141500
H	0.15872100	5.22620700	1.25854200
H	-0.75251900	4.18965500	-2.81093000
H	-0.62720300	5.87956900	-0.99998400
C	0.88097800	-3.63344200	0.94419500
H	0.08659800	-4.15490500	1.48661600
H	1.81052800	-3.71740900	1.51427400
C	1.00528000	-4.11458100	-0.51484100
H	1.99930000	-3.71258900	-0.85702300
H	1.17636300	-5.22059600	-0.43437300
O	-0.04231000	-3.73035800	-1.26073000
C	-4.40354000	0.15974200	-0.01185700
O	-4.50265900	1.33379600	-0.30242300
O	-5.46291500	-0.64374400	0.15177700
C	-6.73551800	-0.01974500	-0.03809500
H	-6.81224400	0.38529400	-1.04863900
H	-7.47612900	-0.80089000	0.11818500
H	-6.87182100	0.78774100	0.68353400

### TS step1 mechanism B (iv = 654.68 cm<sup>-1</sup>)

01			
C	-2.78904500	2.16969100	0.57573900
C	-1.48861000	2.61542900	0.69258300
C	-0.40208300	1.71010200	0.58740500
C	-0.71516400	0.34447500	0.31769100
C	-2.03211900	-0.09240500	0.19547800
C	-3.07801400	0.81400100	0.33476200
H	-3.60972500	2.87235600	0.67442000
H	-1.27291200	3.65956500	0.89313500
H	-2.26694600	-1.13058600	-0.02054300
O	0.84352100	2.05182800	0.71630600
P	0.68145900	-0.72662700	0.00336400
C	1.73375400	0.03333500	-1.25613100
C	3.11689100	-0.15230900	-1.22718000
C	1.13980500	0.79658300	-2.26723500
C	3.90705200	0.42700000	-2.21669000
H	3.58010200	-0.73028400	-0.43364000
C	1.93724000	1.36919900	-3.25183700
H	0.06440000	0.95420400	-2.27680300
C	3.31925300	1.18532600	-3.22583800
H	4.98256300	0.28965900	-2.19285500
H	1.47991700	1.96535800	-4.03402500





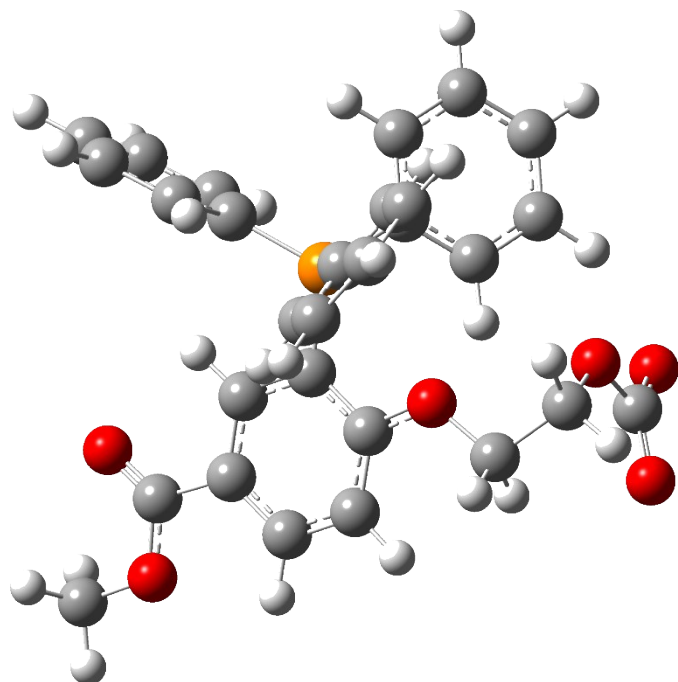
H	3.93905300	1.63922400	-3.99193300
C	1.65152100	-1.11982900	1.47743400
C	1.64885700	-0.26454600	2.58330100
C	2.41866000	-2.29243100	1.48823800
C	2.41815300	-0.58689700	3.69767800
H	1.06804100	0.65038500	2.56243100
C	3.19050800	-2.59897400	2.60370900
H	2.40917200	-2.96541900	0.63545200
C	3.18803300	-1.74782400	3.70725600
H	2.41580000	0.07195200	4.55903300
H	3.78726200	-3.50432800	2.61215400
H	3.78632500	-1.99290600	4.57853900
C	0.05379500	-2.29843200	-0.63648400
C	0.09398600	-2.57616700	-2.00487200
C	-0.52323300	-3.21315700	0.25494600
C	-0.44502900	-3.76907400	-2.48038400
H	0.54561600	-1.87184100	-2.69627900
C	-1.06285300	-4.39861700	-0.22994600
H	-0.54653800	-3.00199900	1.32066900
C	-1.02279200	-4.67587100	-1.59638900
H	-0.40997500	-3.98805600	-3.54189900
H	-1.50934800	-5.10725200	0.45886600
H	-1.44032000	-5.60453000	-1.97099100
C	1.35894200	3.58475100	-0.11014700
H	0.54856900	3.62565300	-0.83014600
H	2.28964400	3.15114000	-0.45328300
C	1.48966500	4.76046300	0.75963100
H	0.53801400	5.09543200	1.22163300
H	2.22563200	4.63124300	1.57716600
O	1.90608900	5.42848600	-0.36122200
C	-4.46036800	0.30168300	0.20230900
O	-4.74481900	-0.85899000	-0.01247400
O	-5.38374000	1.26315200	0.34417700
C	-6.74045700	0.82794400	0.22615600
H	-7.35058700	1.71938300	0.35520900
H	-6.91192100	0.38375300	-0.75597300
H	-6.97021300	0.09079000	0.99779300

## In2B

0 1

C	1.89654200	3.08775200	0.58215200
C	0.56323500	2.86570500	0.89559400
C	0.00194700	1.60281500	0.67877100
C	0.80509500	0.55748500	0.16568800
C	2.14390300	0.79785600	-0.12912700
C	2.69179800	2.06377700	0.06507100
H	2.32864900	4.06855300	0.74552800
H	-0.03470300	3.66716700	1.30894500

H	2.78857100	0.01091200	-0.50649200
O	-1.27349000	1.28787200	0.93070200
P	0.11234900	-1.10393800	-0.00241600
C	-0.66907100	-1.55166100	1.56270700
C	-1.82477900	-2.33546500	1.56446700
C	-0.10234900	-1.11065800	2.76383200
C	-2.41292300	-2.68152200	2.77815900
H	-2.26953700	-2.66374100	0.63007400
C	-0.69589000	-1.46502000	3.96965700
H	0.78839600	-0.48806800	2.75721800
C	-1.85061000	-2.24741800	3.97574100
H	-3.31374900	-3.28507300	2.78464900
H	-0.26304200	-1.12287100	4.90331300
H	-2.31557200	-2.51495500	4.91879500
C	-1.06681600	-1.27636200	-1.35448900
C	-1.90881500	-0.21917600	-1.70995800
C	-1.19739000	-2.52888500	-1.97521500
C	-2.88683100	-0.41324700	-2.68218800
H	-1.85264800	0.74304300	-1.21679500
C	-2.16836800	-2.70790500	-2.95325400
H	-0.55000100	-3.35541600	-1.69875400
C	-3.01070500	-1.65233600	-3.30431300
H	-3.54792300	0.42079200	-2.90124300
H	-2.26941800	-3.67389100	-3.43606100
H	-3.77223700	-1.80376000	-4.06266100
C	1.48686600	-2.23090900	-0.32551700
C	2.01814600	-3.01659500	0.70013400
C	2.04265300	-2.27067700	-1.61176900
C	3.10887600	-3.84154100	0.43686500
H	1.58474100	-2.99219300	1.69484900
C	3.13295300	-3.09456900	-1.86241600
H	1.62258800	-1.66658800	-2.41138100
C	3.66464400	-3.87861500	-0.83855900
H	3.52052800	-4.45563300	1.23015300
H	3.56463400	-3.12781300	-2.85658600
H	4.51415400	-4.52279200	-1.03965900
C	-2.18676100	2.30475200	1.37282800
H	-2.07943200	3.19925600	0.75423100
H	-1.97808600	2.54210600	2.42197800
C	-3.58401800	1.75221200	1.18605100
H	-3.66657800	0.78124700	1.68609100
H	-4.29226300	2.45673200	1.63112900
O	-3.86496600	1.53314000	-0.17698000
C	-4.08686400	2.70097500	-0.96269200
O	-4.19526700	2.44420900	-2.17152800
O	-4.13186300	3.77999400	-0.34849400
C	4.12669200	2.25734800	-0.27545200
O	4.84320600	1.38309600	-0.71220900
O	4.54228800	3.50607700	-0.04567500

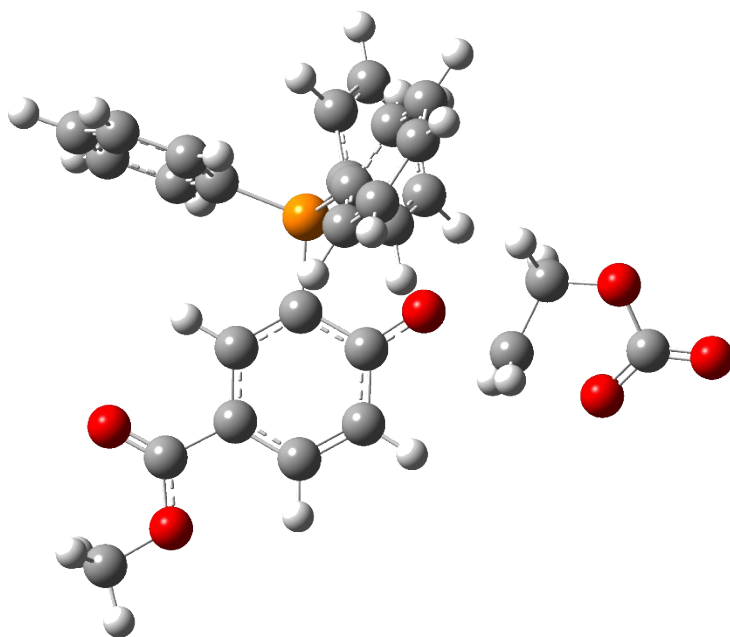


C	5.91747100	3.76006800	-0.35217800
H	6.11186400	3.55904300	-1.40688700
H	6.08239600	4.81072100	-0.12493500
H	6.56236100	3.12808900	0.26065900

### TS step 3 mechanism B (iv = 645.64cm<sup>-1</sup>)

0 1

C	1.10864200	3.43253400	0.09952600
C	-0.16211900	2.90023100	0.18602700
C	-0.35845400	1.49547100	0.15252700
C	0.80657000	0.67842000	0.02191600
C	2.08237200	1.22989200	-0.04530300
C	2.24366200	2.61137700	-0.01486800
H	1.24075900	4.50900400	0.12857500
H	-1.01824800	3.55591600	0.29111700
H	2.96551500	0.60219000	-0.12117500
O	-1.50669900	0.90055000	0.23033700
P	0.52868400	-1.08732000	0.00939900
C	-0.41671200	-1.57209800	1.47336200
C	-1.29803400	-2.65407700	1.42551900
C	-0.22563100	-0.86279900	2.66355800
C	-1.98563200	-3.02878300	2.57693400
H	-1.46144900	-3.19514800	0.49907500
C	-0.91302000	-1.24838800	3.80915600
H	0.44721400	-0.01008100	2.69188400
C	-1.79244900	-2.32934100	3.76526800
H	-2.67498800	-3.86522200	2.54115500
H	-0.76807600	-0.69991900	4.73349400
H	-2.33270700	-2.62279000	4.65913500
C	-0.29723900	-1.65928900	-1.49435200
C	-1.02452200	-0.77895300	-2.30077300
C	-0.19576300	-3.01375600	-1.83879100
C	-1.66167300	-1.26133300	-3.44025200
H	-1.09853400	0.27003500	-2.03834100
C	-0.84309400	-3.48692100	-2.97496100
H	0.39330600	-3.69458500	-1.23014400
C	-1.57634000	-2.61113400	-3.77331600
H	-2.22538400	-0.57936700	-4.06759600
H	-0.76801500	-4.53603500	-3.23891300
H	-2.07697500	-2.98119000	-4.66194900
C	2.13345100	-1.91957600	0.06282200
C	2.62028500	-2.44813400	1.26083200
C	2.90439500	-1.98411000	-1.10572000
C	3.87969700	-3.04121600	1.28818600
H	2.02121500	-2.40476500	2.16478700
C	4.16172600	-2.57468800	-1.06715000
H	2.52240500	-1.57949300	-2.03914100
C	4.64760800	-3.10358000	0.12865100

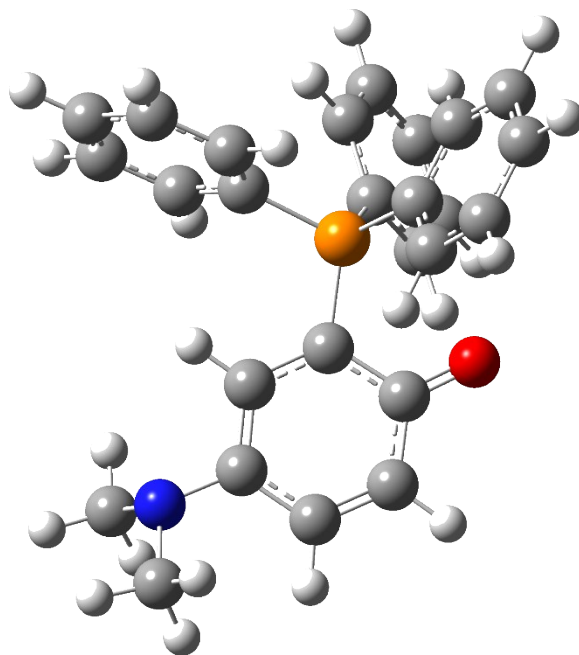


H	4.25738100	-3.45603900	2.21623800
H	4.76023000	-2.62445800	-1.97005200
H	5.62795200	-3.56777200	0.15434700
C	-3.07132500	1.84357700	-0.05850700
H	-2.64710500	2.32494200	-0.92757100
H	-3.01089100	2.35202300	0.89405300
C	-3.87064100	0.55634400	-0.16957900
H	-3.81033900	0.17795800	-1.19729400
H	-3.46079300	-0.19250200	0.50791500
O	-5.21902200	0.77053800	0.19885400
C	-5.63571000	2.06050800	-0.08376100
O	-4.67908300	2.82378200	-0.44503400
O	-6.82259500	2.31308800	0.05093800
C	3.61956200	3.15085100	-0.09104900
O	4.62127300	2.46807600	-0.15801000
O	3.65082400	4.49084300	-0.07706700
C	4.95584100	5.07173100	-0.13598300
H	4.80200900	6.14857700	-0.12622600
H	5.54840600	4.76160800	0.72662400
H	5.46656400	4.76534700	-1.05063500

**NMe<sub>2</sub>**

**Organocatalyst**

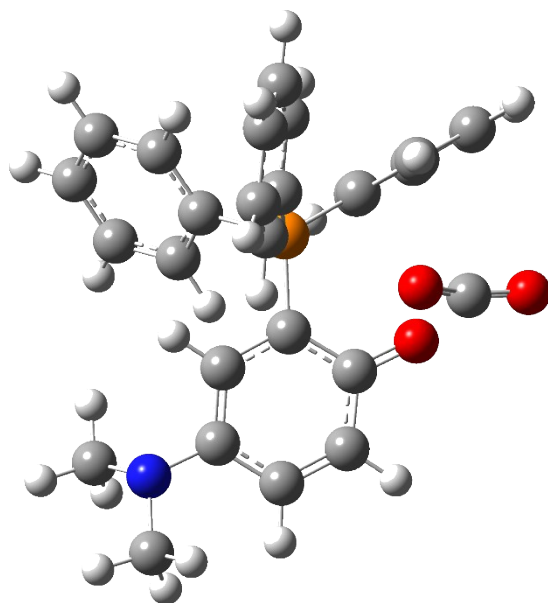
O 1			
C	3.45389600	-1.67398700	1.00383400
C	2.32352300	-2.33965400	1.42287000
C	1.00168300	-1.83091100	1.18009400
C	0.97339100	-0.59449500	0.44061100
C	2.13730500	0.05011400	-0.01431000
C	3.38921000	-0.46420800	0.27319600
H	4.42614500	-2.10303300	1.23290600
H	2.40162000	-3.27687300	1.96621200
H	2.07551600	0.96195900	-0.60331300
O	-0.06214300	-2.40159500	1.56569700
P	-0.64888600	-0.01518100	0.03400200
C	-1.59920400	-1.28033800	-0.84909300
C	-2.99276200	-1.20602800	-0.90319300
C	-0.91751400	-2.28599900	-1.53940800
C	-3.70332400	-2.13700700	-1.65600500
H	-3.52450600	-0.43149600	-0.35822200
C	-1.63438100	-3.21114300	-2.29110100
H	0.16540700	-2.34387200	-1.47846500
C	-3.02518700	-3.13626500	-2.35026700
H	-4.78586000	-2.08180600	-1.69705600
H	-1.10755200	-3.99484100	-2.82486900
H	-3.58167400	-3.86116400	-2.93531100
C	-1.62562400	0.59148300	1.44034300



C	-1.43246400	0.04919500	2.71606200
C	-2.57479600	1.60271800	1.24173000
C	-2.18911500	0.52372800	3.78335000
H	-0.72002200	-0.75759600	2.84921000
C	-3.33249900	2.06215500	2.31480800
H	-2.71700800	2.03940100	0.25745900
C	-3.13734900	1.52525400	3.58537200
H	-2.03924700	0.10521000	4.77299400
H	-4.06895200	2.84283500	2.15796900
H	-3.72522700	1.88812500	4.42231900
C	-0.48491300	1.39776400	-1.09213600
C	-0.72595700	1.25374300	-2.46006500
C	-0.05050800	2.62823400	-0.58125200
C	-0.53454400	2.33820300	-3.31377500
H	-1.06367200	0.30230100	-2.85896600
C	0.14069100	3.70470200	-1.43931800
H	0.13437800	2.74357700	0.48366300
C	-0.10231200	3.55937100	-2.80535500
H	-0.72548800	2.22569000	-4.37553100
H	0.47778800	4.65643900	-1.04309300
H	0.04521200	4.40170600	-3.47322600
N	4.54797200	0.25268300	-0.17355400
C	4.87286100	1.38498100	0.68852700
H	5.67501500	1.97214100	0.23069900
H	3.99748500	2.02756900	0.80500500
H	5.20658900	1.06549300	1.69123100
C	5.72385200	-0.57124300	-0.39984200
H	6.47568800	0.01999800	-0.93096800
H	6.18930900	-0.93860800	0.53119600
H	5.45993800	-1.43367700	-1.01663500

### TS step1 mechanism A (iv = 285.93 cm<sup>-1</sup>)

0 1			
C	-3.05712800	-2.39800700	-0.61282900
C	-1.80612100	-2.82364100	-1.00349100
C	-0.62617300	-2.03512600	-0.83804600
C	-0.84728200	-0.76267300	-0.22377300
C	-2.12870000	-0.35202200	0.19856800
C	-3.24854900	-1.14391600	0.00894400
H	-3.90796200	-3.04932400	-0.78793200
H	-1.67716500	-3.79544000	-1.47052500
H	-2.25940700	0.61600600	0.67887400
O	0.52328400	-2.46408800	-1.22123100
P	0.47105500	0.41271200	0.00563100
C	1.00944200	0.54039700	1.73082200
C	2.15986700	1.26642000	2.06495300
C	0.23704300	-0.05141100	2.73278700



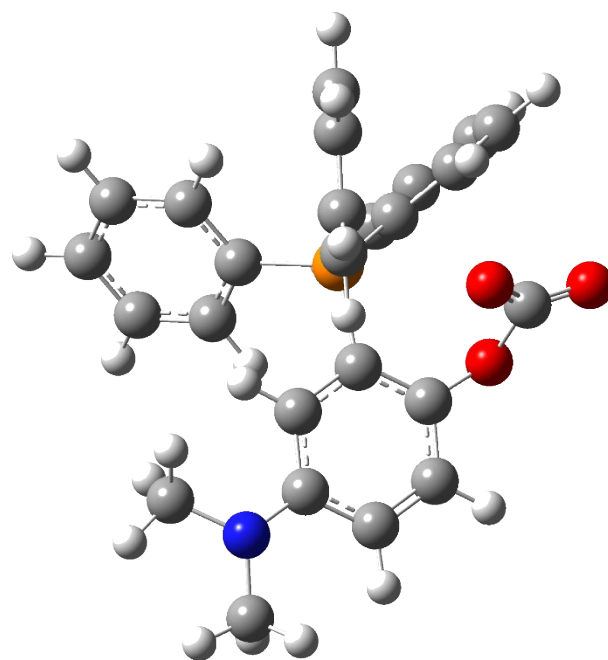
C	2.52505000	1.40541700	3.40001500
H	2.77480600	1.71529200	1.28953200
C	0.60858600	0.09357200	4.06590200
H	-0.63698400	-0.63725500	2.46735600
C	1.74861800	0.82134800	4.39905000
H	3.41677200	1.96625400	3.65768100
H	0.01103000	-0.36979500	4.84344700
H	2.03702800	0.92913200	5.43949000
C	1.93157200	0.13129200	-1.03214900
C	1.88194500	0.50225000	-2.37862100
C	3.08718400	-0.45321200	-0.50652900
C	2.98065300	0.27103800	-3.19945100
H	0.99342600	0.97011500	-2.79089400
C	4.18343900	-0.67633500	-1.33334300
H	3.12966600	-0.74209700	0.53887100
C	4.13033000	-0.31819100	-2.67821800
H	2.93873200	0.55601500	-4.24514900
H	5.07805600	-1.13312700	-0.92411900
H	4.98689000	-0.49559400	-3.32022500
C	-0.21094600	2.03651700	-0.47352000
C	0.16419600	3.20914200	0.18691900
C	-1.10628800	2.10045600	-1.55019600
C	-0.34350000	4.43618800	-0.23353000
H	0.83596200	3.17422400	1.03753700
C	-1.60661400	3.32958000	-1.96618200
H	-1.42443600	1.18975600	-2.04958900
C	-1.22495400	4.49795300	-1.30888500
H	-0.05346900	5.34190800	0.28798200
H	-2.29938800	3.37224800	-2.79970800
H	-1.62085500	5.45506700	-1.63199700
C	1.78359800	-3.06725500	0.26512900
O	2.52566900	-3.73786600	-0.35422400
O	1.33089200	-2.52161600	1.21150800
N	-4.51973300	-0.65586500	0.43159300
C	-5.56801100	-1.65604800	0.52824500
H	-6.43352800	-1.21090600	1.02611000
H	-5.90297500	-2.03368000	-0.45315800
H	-5.22369700	-2.50318400	1.12630100
C	-4.97779000	0.50274000	-0.33164100
H	-5.25315800	0.23426700	-1.36553700
H	-5.85506600	0.93490800	0.15806700
H	-4.19752700	1.26531900	-0.37202500

## In1A

01

C	-3.11184300	-2.45615100	-0.34331100
C	-1.84793900	-2.97277700	-0.56839300
C	-0.69589100	-2.19196700	-0.44766200

C	-0.86073100	-0.84225100	-0.11281700
C	-2.13893300	-0.31593200	0.13169400
C	-3.29138800	-1.11069400	0.04343800
H	-3.96681900	-3.10941300	-0.46637200
H	-1.72363300	-4.01304500	-0.85009200
H	-2.23055200	0.73504000	0.37785000
O	0.49992500	-2.77840700	-0.70615700
P	0.51041100	0.32515500	-0.00688500
C	0.94812100	0.73567800	1.69804400
C	2.10300700	1.47908000	1.96271800
C	0.09715900	0.35666700	2.73840600
C	2.39848300	1.84800400	3.27232600
H	2.77527000	1.76407600	1.15793500
C	0.39916400	0.73266200	4.04252800
H	-0.78106800	-0.24554700	2.53055900
C	1.54644400	1.47746600	4.30964100
H	3.29620500	2.42014700	3.47941500
H	-0.25769700	0.43502100	4.85263500
H	1.78026300	1.76388700	5.32969900
C	1.99590100	-0.11121300	-0.95356100
C	1.99819000	0.09978300	-2.33746100
C	3.13924400	-0.60394500	-0.31621400
C	3.13410700	-0.20044400	-3.08047000
H	1.12495500	0.50236600	-2.83975600
C	4.27516900	-0.88727900	-1.06762800
H	3.12453400	-0.79527200	0.75085400
C	4.27379900	-0.68986300	-2.44561400
H	3.12954700	-0.04284800	-4.15340700
H	5.15922600	-1.27305800	-0.57179700
H	5.16137900	-0.91824700	-3.02641500
C	-0.13444500	1.85140000	-0.77636000
C	0.21167200	3.11011200	-0.27828400
C	-0.95658400	1.75672900	-1.90878100
C	-0.25102200	4.26136000	-0.91177500
H	0.82784500	3.20259400	0.60907100
C	-1.41142600	2.90975200	-2.53800700
H	-1.25812100	0.78468700	-2.28807900
C	-1.05831200	4.16315400	-2.04054000
H	0.01783100	5.23431200	-0.51488900
H	-2.04779500	2.82842500	-3.41258500
H	-1.41931100	5.06191200	-2.52954400
C	1.46439400	-2.86064100	0.39071600
O	2.37703200	-3.63561000	0.13918800
O	1.21443400	-2.11906700	1.35402800
N	-4.54668500	-0.59119400	0.31640500
C	-5.70862800	-1.36247700	-0.08773300
H	-5.73987600	-2.31952000	0.44085700
H	-6.60825600	-0.80952000	0.18065400
H	-5.72978900	-1.56421000	-1.16869800

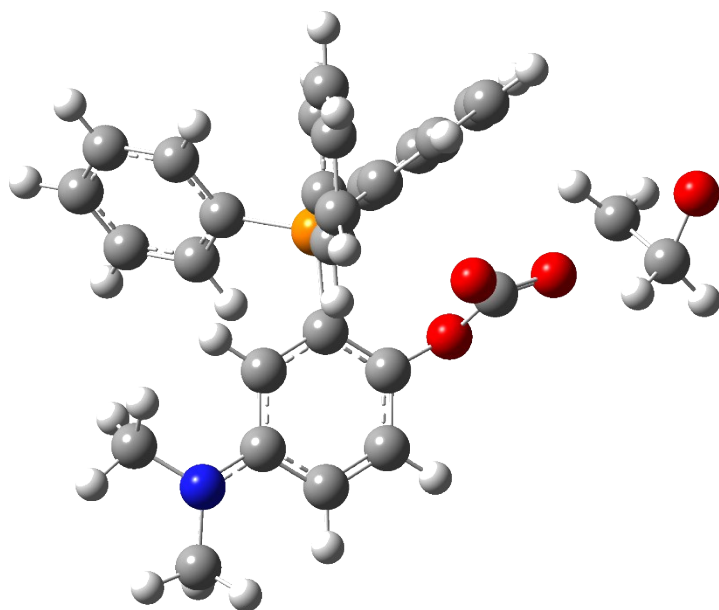


C	-4.68501400	0.85250000	0.37519800
H	-4.11925400	1.26289600	1.21768100
H	-4.33754600	1.34668900	-0.54477500
H	-5.73403400	1.10205300	0.53056100

### TS step 2 mechanism A (iv = 636.64 cm<sup>-1</sup>)

0 1

C	2.02334700	3.37483000	-0.88245700
C	0.74313300	3.07365100	-1.31186100
C	0.15918200	1.83540300	-1.05377200
C	0.90455600	0.88144100	-0.35873900
C	2.20012700	1.18285700	0.08555700
C	2.78495100	2.43928200	-0.14737100
H	2.43467800	4.34710900	-1.12253100
H	0.16568700	3.80202800	-1.87093300
H	2.76240500	0.41868400	0.60920100
O	-1.09318700	1.60433400	-1.56372300
P	0.32601500	-0.78568900	0.02829300
C	-0.07339300	-0.93094700	1.78147000
C	-0.58758000	-2.13745700	2.27585800
C	0.13802600	0.15137900	2.63883000
C	-0.86810500	-2.26090200	3.63204200
H	-0.78613800	-2.97105500	1.60729800
C	-0.14651300	0.01686100	3.99416300
H	0.50140100	1.09545000	2.24795000
C	-0.64405500	-1.18561000	4.49009800
H	-1.26771800	-3.19336500	4.01481300
H	0.01309200	0.85707100	4.66090600
H	-0.86727300	-1.28346500	5.54727500
C	-1.07732800	-1.36390500	-0.95977900
C	-0.88232400	-1.67485300	-2.31022900
C	-2.34079600	-1.50639100	-0.37787500
C	-1.95499700	-2.11573900	-3.07561700
H	0.09676700	-1.57494700	-2.76750600
C	-3.40584000	-1.95844400	-1.15077500
H	-2.49818900	-1.23980700	0.66155500
C	-3.21509100	-2.26001500	-2.49580100
H	-1.80476700	-2.35010400	-4.12364000
H	-4.38624600	-2.06482600	-0.69884300
H	-4.04954700	-2.60679000	-3.09620100
C	1.74636700	-1.85294500	-0.36647100
C	2.09663700	-2.93897200	0.43924900
C	2.48232500	-1.57680200	-1.52771800
C	3.16783700	-3.75213300	0.07525100
H	1.55582200	-3.14694100	1.35552700
C	3.54559600	-2.39640600	-1.88592800
H	2.24305000	-0.71122000	-2.13880900



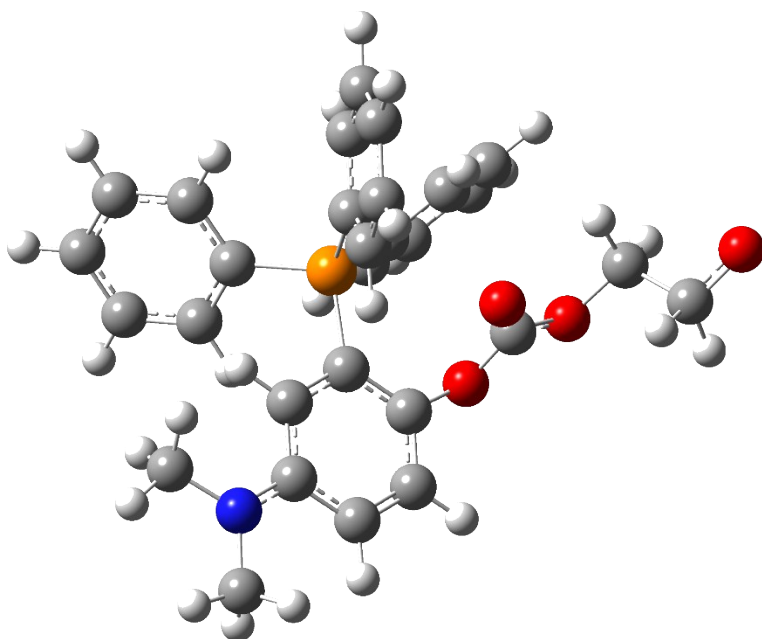


C	3.88774400	-3.48536200	-1.08540500
H	3.44079300	-4.59061700	0.70645000
H	4.11212400	-2.17725200	-2.78422400
H	4.72328400	-4.11918500	-1.36283600
C	-2.14642600	1.45206600	-0.64884800
O	-3.24982500	1.41878500	-1.26571300
O	-1.89211200	1.34495500	0.54425000
C	-4.69923800	1.20159400	-0.17992000
H	-5.30127200	0.78031200	-0.97338500
H	-4.23006400	0.51473500	0.51082100
C	-5.20049500	2.44462000	0.41525300
H	-5.52664200	3.20043500	-0.32565900
H	-4.48119800	2.93278500	1.10139300
O	-6.17544500	1.66054700	0.98072900
N	4.04805900	2.73775900	0.31450000
C	4.70065700	3.94215700	-0.16699100
H	5.68628300	4.01590600	0.29067800
H	4.82064800	3.94692300	-1.25942600
H	4.13405200	4.83250600	0.12143700
C	4.87351400	1.65814200	0.82355100
H	5.01871300	0.85853600	0.08269700
H	5.84855800	2.05735400	1.09939000
H	4.42871400	1.21739500	1.72176800

## In2A

01

C	1.76469900	3.47588300	-0.85582200
C	0.48556400	3.10130600	-1.22639500
C	0.01038100	1.81929300	-0.97816900
C	0.84609900	0.89022800	-0.35765000
C	2.14018800	1.26684600	0.02549300
C	2.62718400	2.56866000	-0.19924300
H	2.09526800	4.48165000	-1.08121700
H	-0.17225400	3.80449400	-1.72547700
H	2.78006200	0.53082800	0.49700200
O	-1.26329800	1.52159900	-1.43172600
P	0.38352500	-0.81693100	0.02823800
C	0.02034300	-0.98574300	1.78655700
C	-0.45681100	-2.20873400	2.27909800
C	0.22929800	0.09173700	2.65100400
C	-0.70549600	-2.35123500	3.63932300
H	-0.64957500	-3.04109000	1.60753100
C	-0.02416600	-0.06236100	4.01048200
H	0.56945300	1.04668700	2.26537600
C	-0.48647800	-1.27977500	4.50357400
H	-1.07698600	-3.29583100	4.02047600
H	0.13295400	0.77388200	4.68259000
H	-0.68548800	-1.39311500	5.56397500



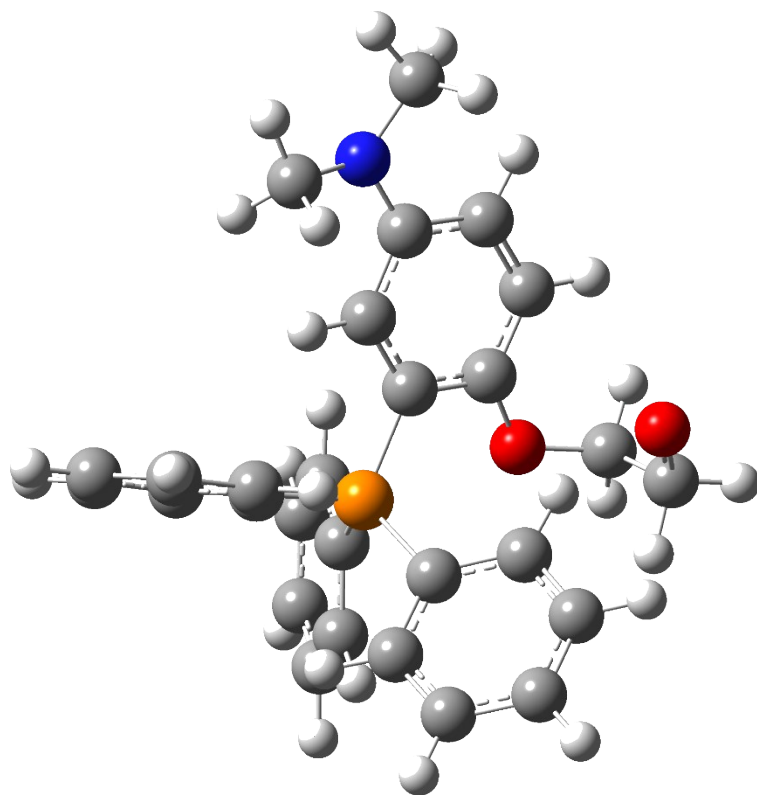
C	-1.01381500	-1.43893600	-0.94064400
C	-0.82805600	-1.70897200	-2.30186700
C	-2.26187600	-1.64438600	-0.34316500
C	-1.89565400	-2.16942100	-3.06219100
H	0.14039500	-1.56388100	-2.76993400
C	-3.32090100	-2.11838100	-1.11202300
H	-2.41806200	-1.41193000	0.70494800
C	-3.14027300	-2.37582400	-2.46750100
H	-1.75374300	-2.37132700	-4.11803000
H	-4.28924800	-2.27259300	-0.64838300
H	-3.97063700	-2.73771200	-3.06452500
C	1.84422800	-1.81021400	-0.39852100
C	2.22595600	-2.89760700	0.39136500
C	2.56599000	-1.49679700	-1.55907400
C	3.31683700	-3.67621800	0.01330600
H	1.69285900	-3.13429600	1.30505100
C	3.65144400	-2.28212800	-1.92952400
H	2.29916800	-0.63195700	-2.15966200
C	4.02547600	-3.37251800	-1.14527700
H	3.61322000	-4.51648400	0.63125300
H	4.20943000	-2.03592600	-2.82607100
H	4.87681100	-3.97948500	-1.43431200
C	-2.22129400	1.32117100	-0.48413500
O	-3.36627100	1.19385800	-1.09976900
O	-1.98189400	1.24001500	0.69820600
C	-4.54432900	0.98381700	-0.26314400
H	-5.23685200	0.43661300	-0.90567800
H	-4.26376700	0.36088600	0.59017300
C	-5.19238800	2.29101600	0.23056700
H	-5.33782700	2.91055700	-0.70520800
H	-4.35730900	2.84137600	0.76158000
O	-6.28237500	2.01332700	0.94579700
N	3.88817200	2.93200200	0.19566300
C	4.79920300	1.91405200	0.68418600
H	4.42480000	1.46071500	1.60869100
H	4.95615500	1.11491200	-0.05327200
H	5.76106500	2.37489300	0.90279100
C	4.40458000	4.23516900	-0.18003900
H	3.77308900	5.03504800	0.21972800
H	5.40067300	4.35467800	0.24311300
H	4.47135600	4.35839400	-1.26921400

## In1B

01

C	3.18132900	-1.88366800	-0.78269300
C	1.94768400	-2.48924300	-0.94360200
C	0.76451600	-1.76692800	-0.74725600
C	0.88555600	-0.42836900	-0.34748900

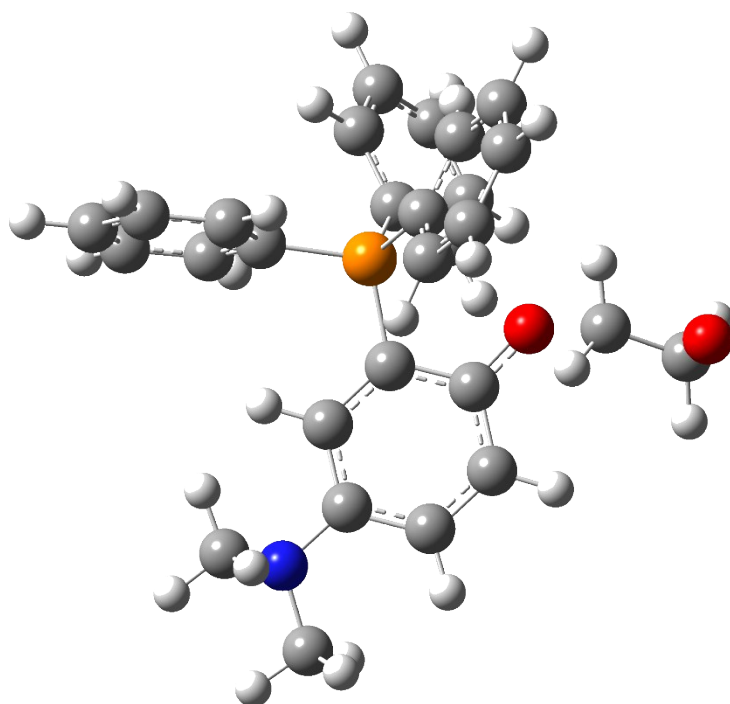
C	2.13730100	0.18564300	-0.18729900
C	3.31763200	-0.52441400	-0.42238800
H	4.06330700	-2.49384900	-0.93599300
H	1.90894400	-3.54225000	-1.18452800
H	2.17364300	1.22197300	0.12032400
O	-0.48909200	-2.20644300	-0.98165300
P	-0.61357900	0.48907800	0.00466200
C	-1.71451000	0.46252400	-1.43074900
C	-3.09250700	0.62177500	-1.27108000
C	-1.15796400	0.33847000	-2.70779200
C	-3.91317300	0.66475000	-2.39510500
H	-3.52872900	0.70120500	-0.28027700
C	-1.98520700	0.38559400	-3.82461700
H	-0.08726200	0.19629200	-2.82543600
C	-3.36064100	0.54961300	-3.66833700
H	-4.98432000	0.78344700	-2.27292700
H	-1.55598300	0.28634800	-4.81568400
H	-4.00342700	0.58063500	-4.54176200
C	-1.44099100	-0.10637800	1.49329700
C	-1.16106500	-1.38022900	1.99604700
C	-2.35934500	0.74038700	2.13536500
C	-1.83211200	-1.80069100	3.14513200
H	-0.44515600	-2.09147800	1.54797600
C	-3.01747300	0.29933800	3.27600600
H	-2.54761000	1.74215900	1.75732600
C	-2.75426200	-0.97609200	3.77997200
H	-1.61508900	-2.79321900	3.52803800
H	-3.72718200	0.95097900	3.77419100
H	-3.26838500	-1.31784000	4.67295600
C	-0.16370400	2.21744200	0.30822400
C	-0.27170700	3.16861600	-0.70934500
C	0.35743000	2.57542000	1.55850600
C	0.14348100	4.47707400	-0.47517600
H	-0.68060100	2.89395000	-1.67681300
C	0.77446500	3.88263000	1.78114300
H	0.43605600	1.83679200	2.35146900
C	0.66656600	4.83203100	0.76510200
H	0.05397100	5.21760200	-1.26240200
H	1.17884600	4.16139900	2.74813000
H	0.98880500	5.85257900	0.94388300
C	-0.76659500	-3.61731700	-1.01631300
H	0.02274900	-4.13176300	-1.57431300
H	-1.70092100	-3.70073600	-1.58141700
C	-0.88714000	-4.14507500	0.42247800
H	-1.85668400	-3.70583100	0.79450900
H	-1.12513200	-5.23774300	0.30080200
O	0.18610600	-3.85506200	1.17404700
N	4.56818400	0.08296500	-0.31135700
C	4.62415200	1.35195600	0.39147900



H	4.06255500	2.11896600	-0.15092700
H	4.21972900	1.29073100	1.41386600
H	5.66153000	1.68191000	0.44462400
C	5.72452200	-0.78571200	-0.17210300
H	5.86869700	-1.38576400	-1.07477000
H	6.61426400	-0.16846600	-0.04662600
H	5.64622600	-1.46779900	0.68776900

### TS step1 mechanism B (iv = 653.94 cm<sup>-1</sup>)

0 1			
C	2.34139800	2.76265200	-0.95530800
C	0.96047700	2.85867900	-1.05660200
C	0.13111600	1.74213500	-0.82751200
C	0.79270700	0.53737600	-0.47410200
C	2.18428900	0.43732500	-0.39598600
C	2.98712200	1.55375900	-0.63475200
H	2.92992500	3.65574200	-1.13529900
H	0.49353200	3.80283000	-1.32106300
H	2.64916200	-0.51348600	-0.15196100
O	-1.17569200	1.75587000	-0.91267900
P	-0.29509800	-0.79626500	-0.00392400
C	-1.41332500	-0.20013500	1.28681300
C	-2.75034300	-0.59907500	1.32177300
C	-0.91090300	0.68446600	2.24712800
C	-3.58588100	-0.10789700	2.32193400
H	-3.14512800	-1.27285100	0.56793900
C	-1.75133200	1.16463900	3.24574400
H	0.12427100	1.01276700	2.20115200
C	-3.08814800	0.77092100	3.28120800
H	-4.62777500	-0.40848500	2.34571100
H	-1.36526000	1.85622000	3.98660900
H	-3.74504100	1.15528400	4.05429900
C	-1.23225600	-1.51381600	-1.37327600
C	-1.42275100	-0.80395100	-2.56174500
C	-1.75969800	-2.80331800	-1.22383600
C	-2.14520900	-1.38912700	-3.59793000
H	-1.02804200	0.20067100	-2.66180800
C	-2.48942400	-3.37317700	-2.26115800
H	-1.59561600	-3.36240800	-0.30653000
C	-2.67903400	-2.66701700	-3.44765600
H	-2.29224200	-0.84364100	-4.52378100
H	-2.90206200	-4.36934300	-2.14520100
H	-3.24222800	-3.11677400	-4.25881000
C	0.70965200	-2.14421300	0.67036000
C	0.82391500	-2.34017100	2.04851100
C	1.41612000	-2.96425300	-0.21961500
C	1.64530000	-3.35495100	2.53442300

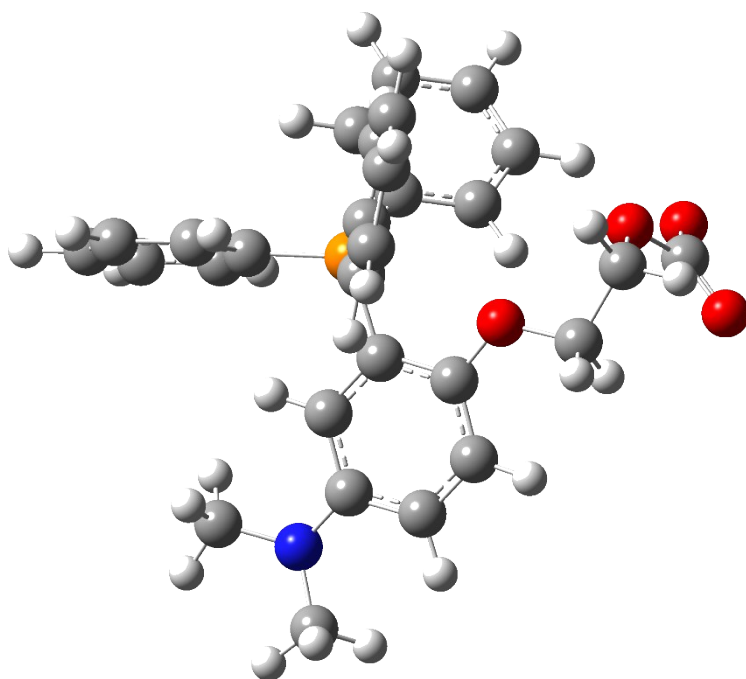


H	0.27204000	-1.71220300	2.74061300
C	2.23659500	-3.97156600	0.27409900
H	1.32208500	-2.81871600	-1.29248200
C	2.34978900	-4.16693000	1.65046500
H	1.72974500	-3.51060200	3.60441500
H	2.78428900	-4.60584500	-0.41435400
H	2.98818500	-4.95659400	2.03259000
C	-2.00365100	3.06336200	0.09115400
H	-1.13900100	3.29504000	0.70301500
H	-2.72536800	2.36624700	0.49821500
C	-2.54569600	4.17442600	-0.69229000
H	-1.78514300	4.77563800	-1.22898000
H	-3.32251300	3.88248600	-1.42423100
O	-2.97373800	4.64926200	0.52373700
N	4.39904600	1.42068000	-0.56588300
C	5.16298900	2.55923600	-1.04298200
H	6.21830000	2.27883600	-1.08194800
H	4.84283300	2.83155000	-2.05139200
H	5.07210200	3.44669900	-0.39362800
C	4.90119800	0.95697800	0.72521300
H	5.96118800	0.70865200	0.62745500
H	4.79336200	1.72345400	1.50980400
H	4.37288800	0.05883500	1.04679000

## In2B

01

C	1.02433400	3.69325300	0.37075500
C	-0.17728800	3.09706900	0.73019500
C	-0.36018600	1.72154000	0.59213800
C	0.71170900	0.95345500	0.10942400
C	1.92548800	1.55562000	-0.23282900
C	2.10174600	2.94642400	-0.14222600
H	1.11710700	4.76407000	0.50231200
H	-0.97128400	3.71694200	1.12758400
H	2.74400200	0.93195400	-0.56293000
O	-1.49584900	1.05622300	0.90900700
P	0.54993800	-0.84297900	0.00449500
C	-0.05690700	-1.48013300	1.58231000
C	-0.81354500	-2.65372800	1.60576200
C	0.27119100	-0.81733600	2.76943200
C	-1.24104000	-3.16687900	2.82737400
H	-1.07549200	-3.15849700	0.68065500
C	-0.15915500	-1.33938300	3.98395200
H	0.85050500	0.10153200	2.74326800
C	-0.91452800	-2.51159900	4.01192300
H	-1.83410300	-4.07441400	2.85024600
H	0.08888000	-0.82754600	4.90731400
H	-1.25416100	-2.91167800	4.96151300



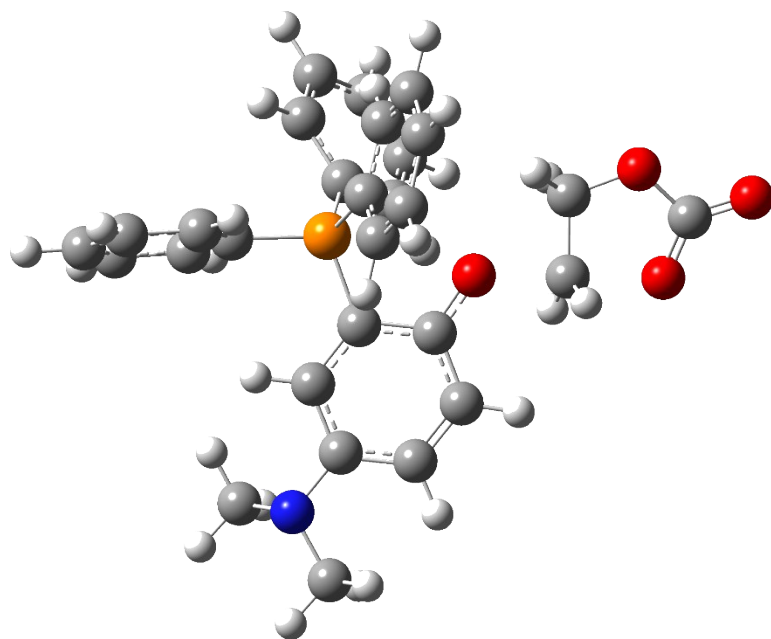
C	-0.52017000	-1.40384300	-1.33728300
C	-1.68841300	-0.69990200	-1.64623700
C	-0.21975900	-2.60394100	-1.99890600
C	-2.55558500	-1.19297700	-2.61739200
H	-1.96127800	0.20131100	-1.11143000
C	-1.08639400	-3.08133700	-2.97582100
H	0.67867700	-3.16226400	-1.75575800
C	-2.25003200	-2.37672500	-3.28405400
H	-3.47141800	-0.63739600	-2.80278500
H	-0.85336400	-4.00667200	-3.49150700
H	-2.92522300	-2.76148300	-4.04184000
C	2.19740900	-1.53099500	-0.28903300
C	2.89702100	-2.15269700	0.74759700
C	2.78086300	-1.39929800	-1.55792100
C	4.18146300	-2.63903100	0.51557700
H	2.44514100	-2.26283800	1.72805500
C	4.06458700	-1.88324900	-1.77761400
H	2.23471800	-0.92358600	-2.36835600
C	4.76365500	-2.50301300	-0.74103700
H	4.72282000	-3.12632500	1.31891800
H	4.51707900	-1.78051300	-2.75773500
H	5.76412300	-2.88398300	-0.91706400
C	-2.64470200	1.80939300	1.30649600
H	-2.81827000	2.63139200	0.60588100
H	-2.48987900	2.20911800	2.31644000
C	-3.83418700	0.87405200	1.25724900
H	-3.62003200	-0.02404500	1.84670200
H	-4.69848400	1.39365900	1.68074200
O	-4.09237500	0.44389200	-0.05996400
C	-4.70500200	1.39949800	-0.91984900
O	-4.80652200	0.98855700	-2.08649100
O	-5.03783500	2.47933600	-0.40332900
N	3.28523300	3.54804000	-0.53894200
C	4.43770700	2.69868600	-0.77682100
H	5.28187500	3.32235300	-1.06888200
H	4.72424600	2.11282200	0.10930000
H	4.24215700	2.00180500	-1.59834600
C	3.53100400	4.91515300	-0.11645700
H	3.51193100	5.03048800	0.97703100
H	4.50906100	5.22652400	-0.48187800
H	2.78790900	5.59315100	-0.54630000

### TS step 3 mechanism B (iv = 648.73cm<sup>-1</sup>)

01

C	0.58669200	3.70471400	0.13495400
C	-0.56053300	2.94335200	0.27481000
C	-0.49631900	1.52860300	0.23245300

C	0.79019700	0.95475500	0.03443800
C	1.94396600	1.74020500	-0.08565300
C	1.85398600	3.12270400	-0.04480100
H	0.50408400	4.78866200	0.17603100
H	-1.51772200	3.42720500	0.43423100
H	2.92219200	1.28596100	-0.21289500
O	-1.51772400	0.72925800	0.36542200
P	0.84057600	-0.82707800	0.01676500
C	0.08359800	-1.48480200	1.52218800
C	-0.64760600	-2.67403100	1.49871300
C	0.26143000	-0.78410800	2.71980600
C	-1.19513000	-3.16568200	2.68120700
H	-0.80517200	-3.20777900	0.56694600
C	-0.28399700	-1.28640900	3.89620900
H	0.81262300	0.15248200	2.73022300
C	-1.01133400	-2.47564100	3.87670600
H	-1.76989400	-4.08518800	2.66451800
H	-0.14818700	-0.74511300	4.82616700
H	-1.44075800	-2.86103600	4.79547100
C	0.05881300	-1.54229900	-1.44946400
C	-0.82268700	-0.79115100	-2.23052500
C	0.36617600	-2.86293200	-1.80258300
C	-1.40684600	-1.36821600	-3.35458000
H	-1.05211100	0.23338600	-1.95966500
C	-0.22900200	-3.43338400	-2.92259700
H	1.07188700	-3.44213300	-1.21278400
C	-1.11580200	-2.68677100	-3.69649600
H	-2.08851700	-0.78353600	-3.96306300
H	0.00626600	-4.45689500	-3.19313000
H	-1.57522200	-3.13262600	-4.57242700
C	2.57183600	-1.35667900	-0.03349600
C	3.21743800	-1.81985500	1.11494400
C	3.27073400	-1.25157300	-1.24339300
C	4.56283800	-2.17574800	1.05153400
H	2.67676700	-1.90910100	2.05185700
C	4.61408000	-1.60405000	-1.29596100
H	2.76708700	-0.89924500	-2.13966200
C	5.25862800	-2.06668500	-0.14887600
H	5.06362600	-2.54061900	1.94169000
H	5.15543400	-1.52225700	-2.23213000
H	6.30614700	-2.34578000	-0.19345400
C	-3.23726400	1.35915900	-0.01146300
H	-2.87573600	1.93748900	-0.85027300
H	-3.29975800	1.83812700	0.95515300
C	-3.74987400	-0.06293900	-0.17863600
H	-3.59543500	-0.38762200	-1.21461600
H	-3.20929500	-0.73533600	0.48675200
O	-5.12225900	-0.14184100	0.15734200
C	-5.78078900	1.04878900	-0.08412800



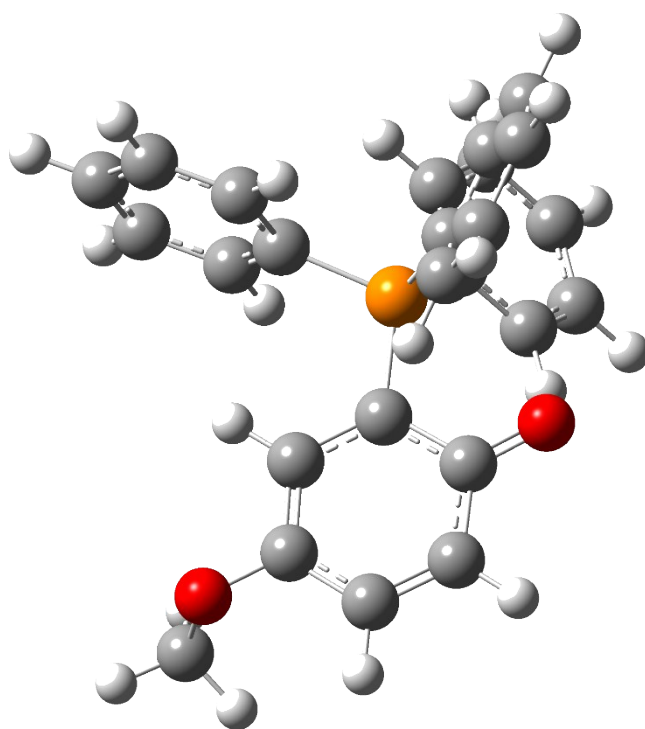
O	-4.98732400	2.00024000	-0.39503900
O	-6.99582700	1.06257400	0.03393900
N	3.05273200	3.90377300	-0.17598400
C	3.34717400	4.67391800	1.02828000
H	4.32373900	5.15433200	0.91647800
H	2.60172100	5.46162000	1.23056500
H	3.38535400	4.00453300	1.89075700
C	3.02989600	4.76427100	-1.35484100
H	2.27397700	5.56514300	-1.29154000
H	4.01021400	5.23520000	-1.47378600
H	2.82219200	4.16296300	-2.24279900

## OMe

### Organocatalyst

0 1

C	3.69246600	-1.78856600	0.69104000
C	2.57889700	-2.44878300	1.15191300
C	1.25381500	-1.90001400	1.00853200
C	1.20312800	-0.62400900	0.34194200
C	2.35380300	0.03899900	-0.13117800
C	3.59132200	-0.53773800	0.04523000
H	4.67997000	-2.23023300	0.80500100
H	2.66529300	-3.41685200	1.63594200
H	2.28674300	0.99308100	-0.64642700
O	0.20502300	-2.47845200	1.41896700
P	-0.42862700	-0.01203500	0.04030900
C	-1.42134700	-1.21434100	-0.88428400
C	-2.81543600	-1.12634300	-0.88747800
C	-0.77316800	-2.18152700	-1.65634400
C	-3.55931700	-2.00556300	-1.66978200
H	-3.32194800	-0.38191000	-0.28012800
C	-1.52330700	-3.05578500	-2.43632800
H	0.31060800	-2.25003700	-1.63880600
C	-2.91434300	-2.96733800	-2.44380900
H	-4.64199400	-1.93942600	-1.67113000
H	-1.02142500	-3.80997600	-3.03294800
H	-3.49739700	-3.65159300	-3.05147600
C	-1.35062900	0.51677700	1.51311900
C	-1.11135800	-0.09001500	2.75119700
C	-2.30391600	1.53758100	1.40154300
C	-1.82657700	0.33041000	3.86892800
H	-0.39594200	-0.90244300	2.81649200
C	-3.01983100	1.94254000	2.52407500
H	-2.48172500	2.02398500	0.44678900
C	-2.77866400	1.34145200	3.75747800
H	-1.64104600	-0.13705800	4.83020500
H	-3.75899300	2.73113900	2.43363500

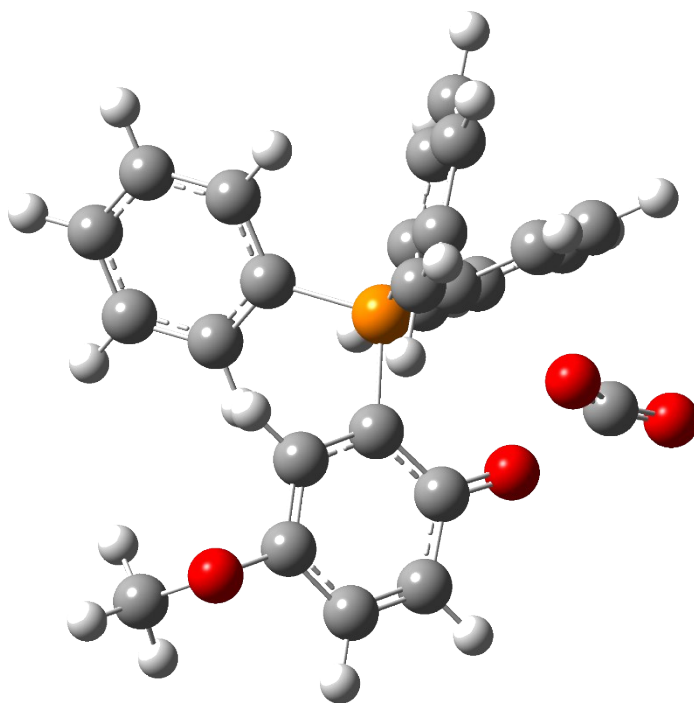




H	-3.33379800	1.66180100	4.63319200
C	-0.29036800	1.46692000	-1.00265800
C	-0.56242700	1.40527100	-2.37085900
C	0.16268600	2.66259700	-0.42944600
C	-0.38322100	2.53762800	-3.16276200
H	-0.91454500	0.48086400	-2.81815800
C	0.34201200	3.78707000	-1.22626500
H	0.37146700	2.71315900	0.63598700
C	0.06837200	3.72410800	-2.59263600
H	-0.59863700	2.48988700	-4.22468900
H	0.69344300	4.71217100	-0.78217000
H	0.20686500	4.60424600	-3.21206800
O	4.72507400	0.08499100	-0.44544400
C	5.45663900	0.77530300	0.55582600
H	5.80282900	0.08967500	1.33901000
H	6.32073300	1.23017600	0.06857500
H	4.84273900	1.55776000	1.01837500

### TS step1 mechanism A (iv = 283.10 cm<sup>-1</sup>)

01			
C	-2.90253300	-2.92431500	-0.08219600
C	-1.64121200	-3.20527100	-0.55096700
C	-0.57990000	-2.24191000	-0.54186900
C	-0.92997100	-0.95577800	-0.02502400
C	-2.23030600	-0.67989900	0.45686100
C	-3.20349700	-1.65297300	0.44080300
H	-3.68407300	-3.67975100	-0.09807200
H	-1.40012400	-4.18687800	-0.94664200
H	-2.49089600	0.30403700	0.84099200
O	0.58737100	-2.55234900	-0.98048200
P	0.21753300	0.40640300	-0.01247400
C	0.83329900	0.79003800	1.64713200
C	1.86651300	1.71921900	1.82342800
C	0.23678100	0.18503700	2.75566800
C	2.28997700	2.04605100	3.10749500
H	2.34668800	2.18114400	0.96495300
C	0.66528300	0.51862800	4.03691200
H	-0.54252200	-0.55672200	2.61420700
C	1.68774900	1.44787200	4.21292700
H	3.09057100	2.76497200	3.24243000
H	0.20395600	0.04572600	4.89702500
H	2.02093600	1.70307600	5.21347300
C	1.63720900	0.22293800	-1.12710700
C	1.44400000	0.40494400	-2.49967900
C	2.90470500	-0.09641700	-0.63310500
C	2.51324100	0.24800600	-3.37427000
H	0.46611500	0.66870100	-2.89012900

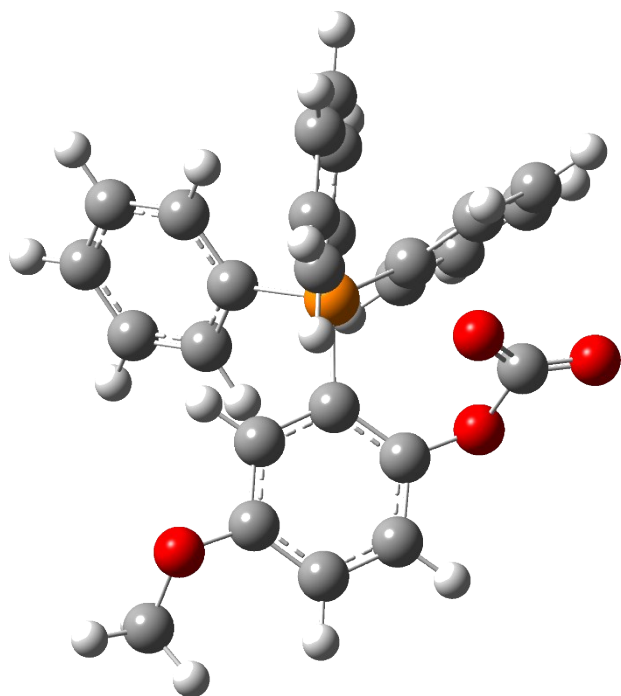


C	3.97007100	-0.24848700	-1.51512300
H	3.05876300	-0.23909700	0.43155300
C	3.77563000	-0.07934700	-2.88341500
H	2.35970700	0.38568700	-4.43911300
H	4.95139700	-0.50254000	-1.12922600
H	4.60814000	-0.19925300	-3.56872300
C	-0.72229800	1.85834000	-0.59536800
C	-0.50227200	3.13220100	-0.06504500
C	-1.66072800	1.68491900	-1.62227100
C	-1.20556700	4.22434900	-0.56700800
H	0.20169800	3.27958300	0.74633300
C	-2.35546200	2.78094500	-2.12159700
H	-1.85956000	0.69298200	-2.01807200
C	-2.12726900	4.05137800	-1.59550200
H	-1.03546900	5.20942100	-0.14608100
H	-3.08137700	2.64009700	-2.91500800
H	-2.67500400	4.90461000	-1.98192200
C	2.03705800	-2.76787900	0.39305600
O	2.82914300	-3.38213900	-0.22501400
O	1.59548000	-2.19605200	1.33122800
O	-4.46506000	-1.38245200	0.92935500
C	-5.36213300	-0.94737900	-0.08413100
H	-6.32348100	-0.76042200	0.39605200
H	-4.99972600	-0.02428700	-0.55329200
H	-5.48441600	-1.71444700	-0.85797500

## In1A

01

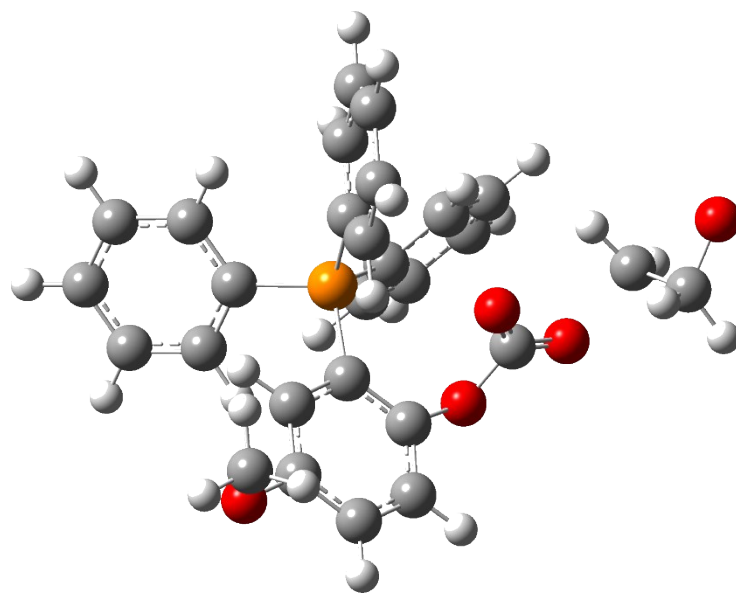
C	-3.54431700	-2.02438700	-0.45765900
C	-2.33806500	-2.66311000	-0.71822000
C	-1.11208800	-2.01770800	-0.55854700
C	-1.11833500	-0.67213500	-0.15135100
C	-2.32971400	-0.02772700	0.12252700
C	-3.54317900	-0.69923000	-0.01377900
H	-4.47124400	-2.56783600	-0.59490600
H	-2.32346200	-3.69667700	-1.04643700
H	-2.35829400	1.01214000	0.43514900
O	0.01230800	-2.71664800	-0.84239300
P	0.37589200	0.32798300	0.01395500
C	0.82138800	0.62608600	1.73830500
C	2.02437600	1.27334000	2.04059700
C	-0.05802100	0.25638200	2.75778700
C	2.33673000	1.56111300	3.36629200
H	2.72123500	1.54474100	1.25221600
C	0.26197800	0.55009800	4.07880100
H	-0.97119200	-0.27920500	2.52151100
C	1.45473700	1.20335900	4.38291700
H	3.27020100	2.06077600	3.60076700



H	-0.41769200	0.25954300	4.87245600
H	1.70062600	1.42766500	5.41560700
C	1.82413600	-0.23820500	-0.92115600
C	1.87592400	-0.00315400	-2.30008300
C	2.89885800	-0.85476500	-0.27185100
C	2.99300900	-0.39916900	-3.02630100
H	1.05688400	0.49069300	-2.81162800
C	4.01824500	-1.23285000	-1.00622400
H	2.84009800	-1.06840500	0.78965000
C	4.06638900	-1.00831000	-2.37924600
H	3.02696500	-0.22205500	-4.09563700
H	4.84902000	-1.71344800	-0.50139700
H	4.94074500	-1.30813200	-2.94749200
C	-0.08942700	1.93474000	-0.71872900
C	0.34696700	3.13932800	-0.16122200
C	-0.86288200	1.95156000	-1.88875100
C	0.02500700	4.34707100	-0.77629100
H	0.92477100	3.14718800	0.75604600
C	-1.17428000	3.16000000	-2.50044500
H	-1.23591900	1.02415500	-2.31398700
C	-0.72870600	4.35882900	-1.94581000
H	0.36290900	5.27833600	-0.33472700
H	-1.77239200	3.16435200	-3.40506800
H	-0.97749400	5.30146700	-2.42190400
C	0.95670500	-2.95330100	0.25694600
O	1.78403600	-3.80530500	-0.03150900
O	0.77130600	-2.23836800	1.25384900
O	-4.65547200	0.01834300	0.28876700
C	-5.90467000	-0.64271700	0.18259600
H	-5.94829000	-1.51546100	0.84311400
H	-6.65710400	0.08221700	0.48945500
H	-6.10076800	-0.95679200	-0.84845500

### TS step 2 mechanism A (iv = 636.44 cm<sup>-1</sup>)

0 1			
C	1.54767600	3.55455200	-1.62907300
C	0.33816600	2.95853400	-1.95436100
C	0.00262300	1.70559700	-1.44461100
C	0.90873600	1.02540500	-0.62128300
C	2.13325800	1.62953400	-0.30077000
C	2.44385900	2.89141200	-0.79158900
H	1.81356500	4.53244400	-2.01627000
H	-0.37784300	3.45305300	-2.60111000
H	2.86412100	1.12067700	0.32248800
O	-1.19744000	1.17519600	-1.83277900
P	0.62619000	-0.61813500	0.07978800
C	0.28576800	-0.49778800	1.84682800
C	-0.03279300	-1.65633900	2.56842200

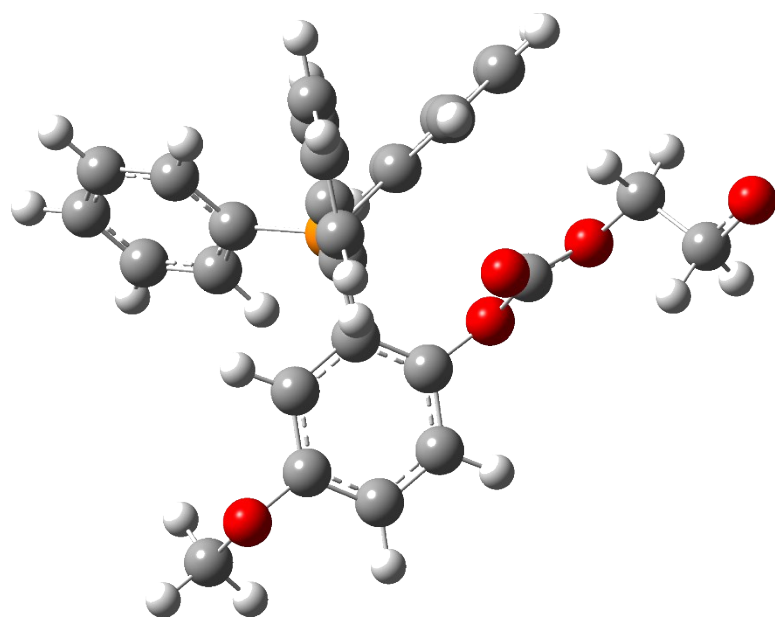


C	0.35241900	0.74024000	2.49037700
C	-0.26502100	-1.57108300	3.93668200
H	-0.11771500	-2.61690100	2.06721600
C	0.11906100	0.81364400	3.85988800
H	0.56181500	1.64153000	1.92469300
C	-0.18532200	-0.33801000	4.58132800
H	-0.51521700	-2.46607400	4.49520100
H	0.16657200	1.77459200	4.36013900
H	-0.37069500	-0.27438400	5.64833700
C	-0.67531800	-1.58459600	-0.72609600
C	-0.44048300	-2.12561800	-1.99563100
C	-1.89811800	-1.79880400	-0.08207900
C	-1.43709000	-2.86407600	-2.62182600
H	0.51106700	-1.97819800	-2.49620400
C	-2.88512800	-2.54841800	-0.71428300
H	-2.08860100	-1.36156100	0.89216700
C	-2.65719600	-3.07688900	-1.98129900
H	-1.25852400	-3.27819900	-3.60797900
H	-3.83533300	-2.70848400	-0.21614900
H	-3.43143000	-3.65618900	-2.47318300
C	2.19940800	-1.49071100	-0.18259700
C	2.72596900	-2.34946600	0.78592600
C	2.86767500	-1.31641200	-1.40265500
C	3.90757600	-3.03977200	0.52697900
H	2.23528600	-2.47350000	1.74472400
C	4.04379500	-2.01303300	-1.65362000
H	2.48522000	-0.62469300	-2.14777800
C	4.56281600	-2.87612300	-0.68986700
H	4.31631200	-3.70141500	1.28269500
H	4.55733700	-1.87364000	-2.59843900
H	5.48416700	-3.41418100	-0.88602200
C	-2.19096700	1.04743300	-0.84351300
O	-3.29224000	0.73750700	-1.37937700
O	-1.88400000	1.20914900	0.32963800
C	-4.64969500	0.52039500	-0.18909100
H	-5.21944800	-0.10703500	-0.86077900
H	-4.06776700	0.02778500	0.57809000
C	-5.29733700	1.77016300	0.22610200
H	-5.75275300	2.33843100	-0.60873000
H	-4.62309600	2.45811300	0.77327300
O	-6.13320700	0.98138500	0.97519600
O	3.64582400	3.47192600	-0.48674400
C	3.68290700	4.03918600	0.82170500
H	3.50747500	3.27448200	1.58655800
H	4.67837100	4.46256000	0.95156400
H	2.92929300	4.82776800	0.92125400

In2A

01

C	1.46305500	3.85463500	-0.23211400
C	0.26632500	3.37721200	-0.74474800
C	-0.04285300	2.02319100	-0.66379800
C	0.85457800	1.12473400	-0.08010700
C	2.06409600	1.61541600	0.43427700
C	2.36083100	2.97056300	0.36969300
H	1.70147600	4.91203800	-0.28058600
H	-0.45392900	4.04219600	-1.20747400
H	2.79433200	0.95046400	0.88633500
O	-1.23188500	1.62561200	-1.23862000
P	0.60975400	-0.66555500	0.04695000
C	0.23506300	-1.11981600	1.74985800
C	-0.03893600	-2.46017500	2.05834500
C	0.21873400	-0.14468700	2.75015200
C	-0.30860600	-2.81946600	3.37351700
H	-0.06260600	-3.21695600	1.27845200
C	-0.05482100	-0.51663100	4.06279400
H	0.39651400	0.89719700	2.50730800
C	-0.31333200	-1.84871400	4.37411500
H	-0.52338500	-3.85482600	3.61324700
H	-0.07438900	0.23945000	4.83987000
H	-0.52999300	-2.13139700	5.39884600
C	-0.67062300	-1.32361400	-1.04885200
C	-0.43268200	-1.37216500	-2.42778600
C	-1.88412100	-1.78065700	-0.52350000
C	-1.41578900	-1.86627700	-3.27580000
H	0.50931200	-1.02848100	-2.84294700
C	-2.85644800	-2.28583700	-1.38191200
H	-2.08133200	-1.72200700	0.54165200
C	-2.62489000	-2.32482000	-2.75357400
H	-1.23485700	-1.89773900	-4.34435600
H	-3.79776100	-2.63794500	-0.97409800
H	-3.38704000	-2.71381700	-3.42032500
C	2.20381000	-1.36508000	-0.46837100
C	2.76029000	-2.47302700	0.17555000
C	2.85641200	-0.78857500	-1.56740800
C	3.95740200	-3.01037200	-0.29231400
H	2.28105500	-2.90983600	1.04462400
C	4.04669600	-1.33574700	-2.02965600
H	2.45153100	0.09645300	-2.05002000
C	4.59549300	-2.44834500	-1.39423500
H	4.39192800	-3.86631600	0.21209600
H	4.54835700	-0.88642000	-2.87947900
H	5.52809100	-2.87032900	-1.75346200
C	-2.20786300	1.18079200	-0.39082600
O	-3.28146600	0.97613100	-1.10155400
O	-2.02385000	0.99388500	0.78889500
C	-4.48062300	0.55858700	-0.37738600

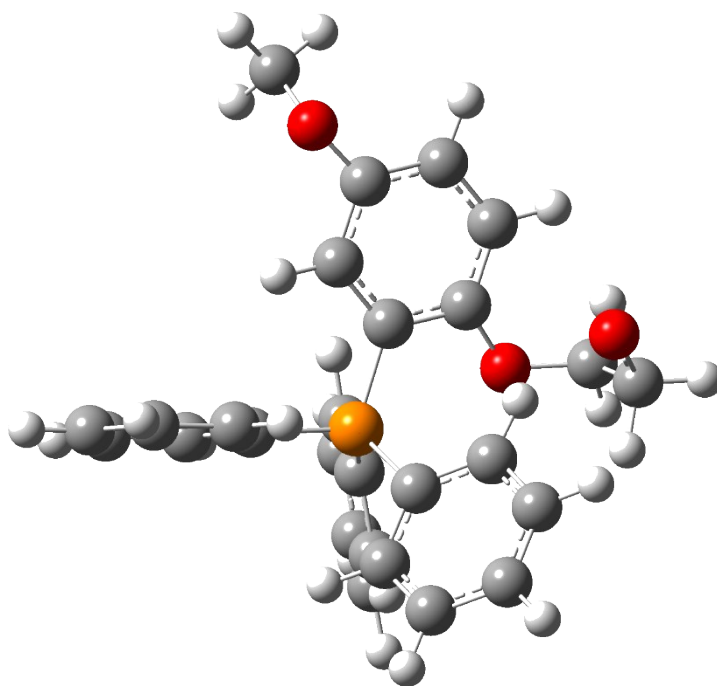


H	-5.05708100	-0.00611000	-1.11252400
H	-4.18385600	-0.09881200	0.44397700
C	-5.30397200	1.74407800	0.16187200
H	-5.46743200	2.41074700	-0.73764900
H	-4.56607600	2.34354300	0.77833000
O	-6.39169900	1.29848200	0.78836100
O	3.52936800	3.41318500	0.92140100
C	4.51156100	3.79823200	-0.04007800
H	4.14769200	4.61323400	-0.67421500
H	5.38094900	4.13589800	0.52261600
H	4.78572900	2.94413800	-0.66858400

## In1B

0 1

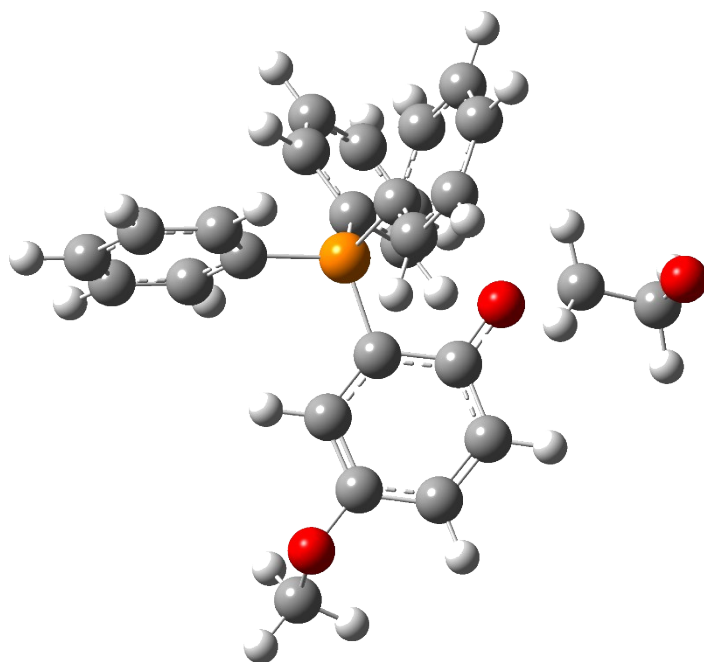
C	-3.85936700	0.00375200	0.56070500
C	-3.06101900	-1.10206000	0.82094800
C	-1.67146600	-1.02540300	0.69060300
C	-1.11426100	0.19338700	0.25649000
C	-1.91926700	1.30813800	-0.00013800
C	-3.29692500	1.22054700	0.15702400
H	-4.93248300	-0.09941500	0.66997500
H	-3.53072300	-2.03760000	1.08862200
H	-1.49256900	2.25073700	-0.32635100
O	-0.78806400	-1.98844100	1.01722000
P	0.65848900	0.27326400	-0.01053500
C	1.53236400	-0.21372900	1.49539200
C	2.79206300	-0.81116300	1.42629100
C	0.94308400	0.06160700	2.73370500
C	3.46705200	-1.12426800	2.60333200
H	3.24104500	-1.04320300	0.46553700
C	1.62681100	-0.25082200	3.90338700
H	-0.04695900	0.50700400	2.78236800
C	2.88756200	-0.84233400	3.83775200
H	4.44373900	-1.59309400	2.55226700
H	1.17117600	-0.04140000	4.86511900
H	3.41637800	-1.09027900	4.75204000
C	1.16054800	-0.71697800	-1.43251600
C	0.31225400	-1.71019400	-1.92829500
C	2.40661200	-0.46366600	-2.02937000
C	0.73916200	-2.46293000	-3.02259200
H	-0.67856200	-1.96091000	-1.51253400
C	2.81194500	-1.22716300	-3.11679000
H	3.04882100	0.33102600	-1.65797600
C	1.97650100	-2.23059700	-3.61257300
H	0.07619600	-3.23752200	-3.39531900
H	3.77367700	-1.03600100	-3.58046700
H	2.29532000	-2.82419800	-4.46361500
C	1.10171600	1.99090500	-0.37360400



C	1.58693300	2.83053500	0.63254400
C	0.89707900	2.48353100	-1.66900200
C	1.86526600	4.16339600	0.34056200
H	1.75181200	2.44865500	1.63513000
C	1.17429000	3.81653700	-1.94970200
H	0.52589200	1.82864600	-2.45237100
C	1.65872800	4.65435300	-0.94575900
H	2.24618900	4.81535500	1.11898000
H	1.01667800	4.20003700	-2.95175500
H	1.87828300	5.69317000	-1.16917100
C	-1.20812500	-3.36258700	1.09538600
H	-2.16793900	-3.42229900	1.61933000
H	-0.44514300	-3.84792800	1.71282200
C	-1.29133300	-3.94474000	-0.32517600
H	-0.21518900	-4.02543000	-0.65030600
H	-1.59924100	-5.01538600	-0.17121200
O	-2.07094700	-3.21735200	-1.14009900
O	-4.00692500	2.35216400	-0.11078800
C	-5.41522900	2.27807500	0.01380600
H	-5.79477300	3.26582300	-0.24420800
H	-5.83685700	1.53600100	-0.67331700
H	-5.71248200	2.03150700	1.03930800

### TS step1 mechanism B (iv = 657.46 cm<sup>-1</sup>)

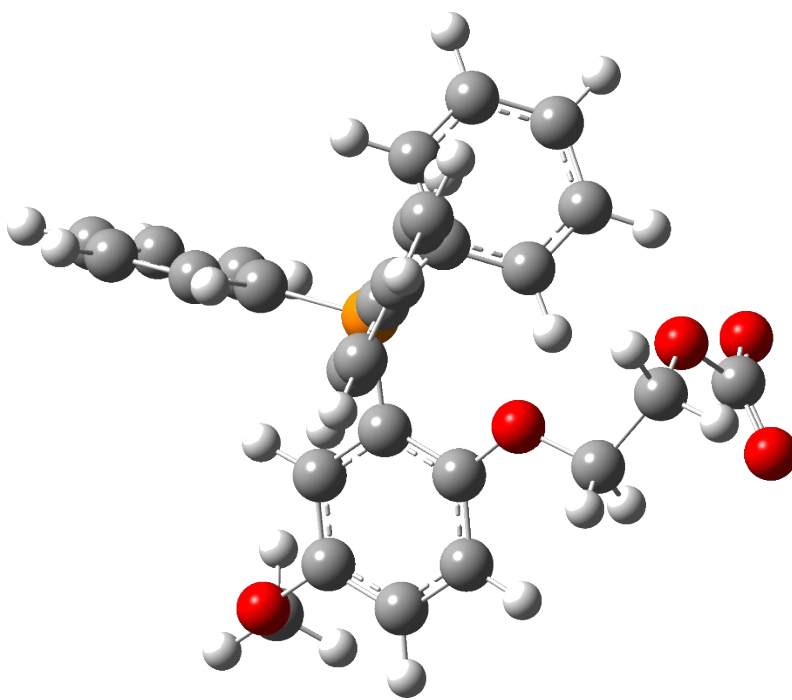
0 1			
C	0.90967900	3.78525100	0.37936400
C	1.75565900	2.72759100	0.66055800
C	1.28382800	1.39345000	0.61679300
C	-0.07084300	1.20282700	0.23794800
C	-0.92687000	2.27781500	-0.04014400
C	-0.43258900	3.56889900	0.03543800
H	1.27816900	4.80695200	0.41316700
H	2.79318300	2.89944400	0.93007700
H	-1.96012400	2.12132600	-0.33574600
O	2.02272800	0.35039900	0.88952900
P	-0.53949200	-0.50091800	-0.01222400
C	0.64322100	-1.25895200	-1.15252300
C	1.08282700	-2.57056800	-0.96890000
C	1.11970300	-0.49180700	-2.22077600
C	2.00435900	-3.11468400	-1.86101500
H	0.72621800	-3.15898800	-0.12915500
C	2.03432000	-1.04598500	-3.10969800
H	0.79199900	0.53699700	-2.34645700
C	2.47787200	-2.35506200	-2.92797200
H	2.35607200	-4.13042100	-1.71641900
H	2.40810000	-0.45176400	-3.93646800
H	3.19905500	-2.78095200	-3.61747500
C	-0.66707600	-1.46506400	1.51200900



C	-0.00074600	-1.05913200	2.67194200
C	-1.45134300	-2.62619600	1.51301300
C	-0.12137400	-1.82075700	3.83035700
H	0.62196100	-0.17206100	2.65772700
C	-1.55483600	-3.38552100	2.67348300
H	-1.98463100	-2.93183700	0.61703200
C	-0.89215800	-2.98114100	3.83098900
H	0.39154600	-1.50726800	4.73315100
H	-2.15879500	-4.28618500	2.67467000
H	-0.97889200	-3.57139800	4.73735900
C	-2.18207400	-0.54105000	-0.77281000
C	-2.33750700	-0.81388400	-2.13363800
C	-3.30027600	-0.25444300	0.02209600
C	-3.61052200	-0.79670600	-2.69873200
H	-1.47512400	-1.04581400	-2.74994700
C	-4.56602800	-0.23443700	-0.55146700
H	-3.18169700	-0.05388200	1.08375200
C	-4.72032600	-0.50602200	-1.91100500
H	-3.73186100	-1.01325900	-3.75444000
H	-5.43166000	-0.01007600	0.06210200
H	-5.71044400	-0.49319000	-2.35456400
C	3.61615100	0.26005100	-0.01705300
H	3.37151400	1.00881900	-0.76255100
H	3.46157900	-0.77567100	-0.29357200
C	4.80020100	0.54011500	0.79897800
H	4.84794800	1.57202400	1.20139400
H	4.94172500	-0.15677700	1.64726900
O	5.50688300	0.28409700	-0.34942700
O	-1.25203700	4.63239800	-0.27159100
C	-1.74057200	5.31263900	0.87806600
H	-0.91646300	5.70604100	1.48446100
H	-2.35440300	6.14046300	0.52172200
H	-2.34927000	4.64275000	1.49636800

## In2B

01			
C	0.28169400	3.91776800	0.80459200
C	-0.76369000	3.03801200	1.06183100
C	-0.61675300	1.67919200	0.77169800
C	0.60258000	1.21246700	0.23886700
C	1.64833600	2.10734700	-0.00381800
C	1.48430800	3.45947900	0.27328700
H	0.17534600	4.97383000	1.03171200
H	-1.68352900	3.41134200	1.49293500
H	2.60370100	1.76861700	-0.39024100
O	-1.56715800	0.74776400	0.97801900
P	0.84519200	-0.55960600	-0.00812600
C	0.44186300	-1.41150800	1.53250700



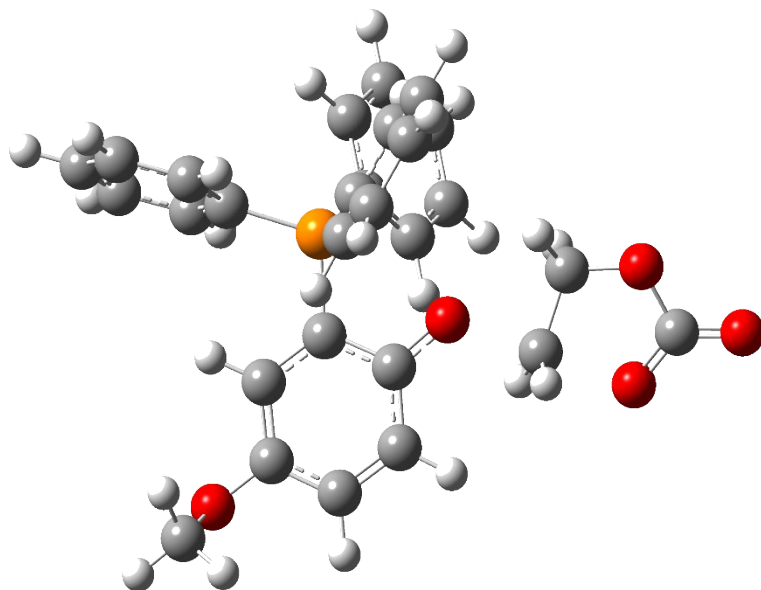


C	-0.13131800	-2.68428600	1.49880300
C	0.73206300	-0.79150400	2.75285700
C	-0.41081500	-3.33965900	2.69514000
H	-0.36823700	-3.15721200	0.55076000
C	0.45294300	-1.45679100	3.94129200
H	1.16455200	0.20529700	2.77511600
C	-0.11893400	-2.72811400	3.91160600
H	-0.86147700	-4.32584900	2.67317600
H	0.67394600	-0.97930100	4.88958500
H	-0.34181500	-3.24122800	4.84115300
C	-0.10019100	-1.26895600	-1.36969600
C	-1.36389300	-0.77969100	-1.71020100
C	0.42196400	-2.40003600	-2.01729200
C	-2.11100800	-1.42519700	-2.69304900
H	-1.80104000	0.06723100	-1.19663200
C	-0.32683100	-3.02959700	-3.00375300
H	1.40215600	-2.78665000	-1.75497600
C	-1.59086400	-2.54299900	-3.33909400
H	-3.10531600	-1.03824700	-2.89927500
H	0.07655200	-3.90220700	-3.50613600
H	-2.17247300	-3.04639300	-4.10497400
C	2.59308600	-0.82293000	-0.38522800
C	3.46889200	-1.31883400	0.58286600
C	3.06114000	-0.49280600	-1.66470300
C	4.81622600	-1.48203200	0.26848800
H	3.10574000	-1.58297300	1.57088800
C	4.40742700	-0.65494400	-1.96645300
H	2.37581800	-0.11733700	-2.41992400
C	5.28323500	-1.14996900	-0.99964300
H	5.49795400	-1.87236600	1.01593300
H	4.77168200	-0.39980200	-2.95546400
H	6.33325300	-1.28039500	-1.23941800
C	-2.86109300	1.16068000	1.43565800
H	-3.21290300	2.01275400	0.84781900
H	-2.80015000	1.43668000	2.49511900
C	-3.80700400	-0.00026400	1.21365500
H	-3.40719800	-0.90020200	1.69299600
H	-4.77217200	0.25537300	1.66036800
O	-3.93816100	-0.29534100	-0.15763900
C	-4.70831500	0.62487800	-0.92377800
O	-4.66522500	0.37935800	-2.13953600
O	-5.29278400	1.52099900	-0.29226500
O	2.52576500	4.32707800	0.06284900
C	2.49435900	4.93869100	-1.22455900
H	3.35109200	5.61038300	-1.27472500
H	2.57112000	4.18342300	-2.01476700
H	1.56958700	5.51006100	-1.36184500

**TS step 3 mechanism B (iv = 651.02cm<sup>-1</sup>)**

0 1

C	0.18542400	3.91942300	-0.31572800
C	-0.83899900	3.04207400	-0.00443700
C	-0.59078000	1.65166000	0.10645300
C	0.74436200	1.21985600	-0.12456100
C	1.78077100	2.11734600	-0.41362000
C	1.49536600	3.46789200	-0.52099300
H	-0.01694900	4.98305500	-0.40812100
H	-1.84193400	3.41865600	0.16203100
H	2.80019300	1.77568100	-0.56784400
O	-1.49255500	0.75318600	0.39292600
P	1.00912700	-0.53879700	0.01295000
C	0.42649100	-1.13129700	1.61911200
C	-0.16270000	-2.38980800	1.75338200
C	0.59723200	-0.30447500	2.73413300
C	-0.57640900	-2.82178900	3.01104200
H	-0.31563800	-3.02589800	0.88742200
C	0.18623700	-0.74730000	3.98663000
H	1.03834500	0.68230600	2.62114300
C	-0.40095800	-2.00445100	4.12426100
H	-1.04041500	-3.79630100	3.11745000
H	0.31561200	-0.10690800	4.85241900
H	-0.72802500	-2.34430800	5.10122900
C	0.22524900	-1.45752100	-1.33392100
C	-0.75558500	-0.86018200	-2.12948100
C	0.63466700	-2.77353300	-1.58469100
C	-1.34033300	-1.58871800	-3.16141200
H	-1.05971600	0.16385200	-1.94290900
C	0.03750900	-3.49667200	-2.61199400
H	1.42212100	-3.22908100	-0.98972600
C	-0.95041900	-2.90493800	-3.39703800
H	-2.10107300	-1.12508700	-3.78024400
H	0.34977700	-4.51744500	-2.80333900
H	-1.41222700	-3.46908600	-4.20055700
C	2.78265100	-0.87539400	-0.11182100
C	3.54125700	-1.16057500	1.02600500
C	3.39359100	-0.80758200	-1.37104900
C	4.91154400	-1.37636700	0.90215300
H	3.06855200	-1.22285300	2.00102400
C	4.76243900	-1.01971000	-1.48393300
H	2.80243100	-0.59285800	-2.25742400
C	5.51979300	-1.30520300	-0.34787900
H	5.50026800	-1.60488900	1.78375900
H	5.23669000	-0.96598300	-2.45777400
H	6.58731100	-1.47556600	-0.44028400
C	-3.27569900	1.09931200	-0.04949600
H	-2.96522600	1.56765100	-0.97294600
H	-3.41699900	1.72396700	0.82163300



C	-3.61901600	-0.37697000	0.02866100
H	-3.41559700	-0.85278600	-0.93818300
H	-3.01765600	-0.86112100	0.79729000
O	-4.98057900	-0.54593600	0.38036200
C	-5.76089000	0.49141500	-0.09616100
O	-5.06862700	1.45014900	-0.58073000
O	-6.97289100	0.38652200	0.00432700
O	2.49481200	4.35521800	-0.85284800
C	3.01022700	5.06218100	0.26889400
H	3.46286400	4.37053800	0.98882900
H	3.76955900	5.74782800	-0.10821500
H	2.22144600	5.63341900	0.77170300