

Supporting Information

Mapping the Catalytic Landscape of Triphenylborane (BPh₃)-Catalyzed CO₂-Epoxide Coupling to Carbonates: An In-Silico Approach to Solve Substrate-Dependent Selectivity

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Table of Contents

S1.	BPh ₃ catalyzed coupling reaction of CO ₂ and propylene oxide (PO)	S3-S4
S2.	BPh ₃ catalyzed coupling reaction of CO ₂ and cyclohexene oxide (CHO)	S4-S4
S3.	Distortion-Interaction Analysis (DIA)	S5-S6
S4.	BEt ₃ catalyzed coupling reaction of CO ₂ and propylene oxide (PO)	S7-S7
S5.	BEt ₃ catalyzed coupling reaction of CO ₂ and cyclohexene oxide (CHO)	S7-S11
S6.	Electronic energies and Gibbs free energies	S11-S14
S7.	Cartesian coordinates of the optimized structures	S14-S161

S1. BPh₃ catalyzed coupling reaction of CO₂ and propylene oxide (PO):

The three-dimensional structures of optimized transition states involved in the BPh₃-catalyzed coupling reaction between CO₂ and propylene oxide (PO) are illustrated in **Fig. S1**. In addition to the most favorable transition states reported in the manuscript, we also explored alternative transition states leading to cyclic-carbonate (CC) and poly-carbonate (PC) products.

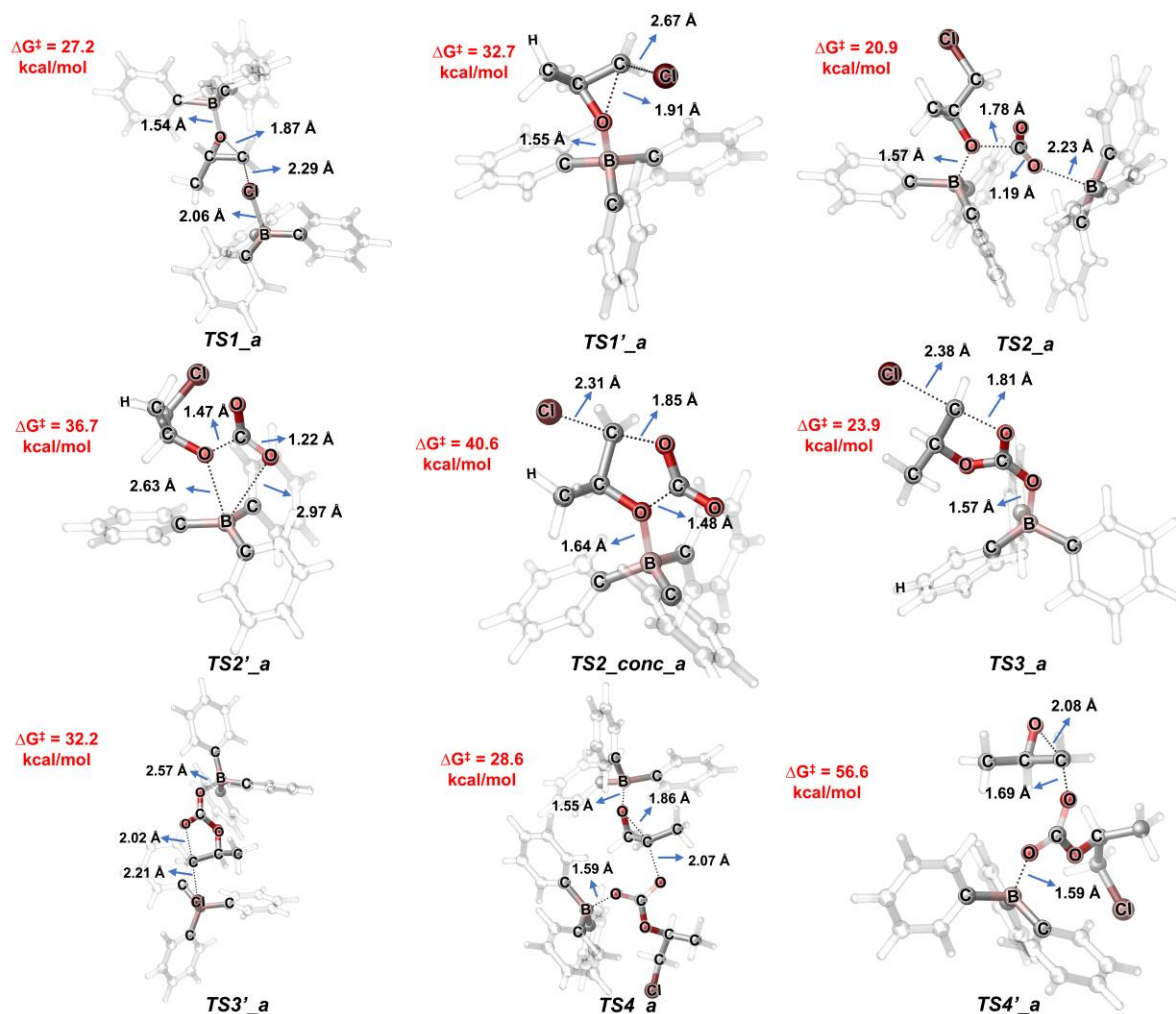


Fig. S1. Optimized geometries of the transition state structures involved in the BPh₃ catalyzed coupling reaction of CO₂ and propylene oxide (PO).

TS1'_a, where no additional BPh₃ molecule is involved in the ring opening step, which exhibited a high energy activation barrier ($\Delta G^\ddagger = 32.7$ kcal/mol) that is not feasible to account for the catalytic activity at 100 °C. **TS2'_a**, a four-membered where CO₂ insertion transition state, wherein the negatively charged oxygen of the alkoxide species attacks the carbon center of CO₂. However, this transition state requires a high activation barrier of 36.7 kcal/mol, which is not feasible to account for the catalytic activity at 100 °C. **TS2_conc_a**, where CO₂ insertion and ring-closing occur concertedly to form the CC product, exhibited a higher activation barrier

($\Delta G^\ddagger = 40.6$ kcal/mol), which is 19.7 kcal/mol above that of **TS2_a** ($\Delta G^\ddagger = 20.9$ kcal/mol). **TS3'a**, where an additional BPh₃ molecule is introduced to carry out the ring-closing step to provide the CC product. The activation barrier required for **TS3'a** ($\Delta G^\ddagger = 32.2$ kcal/mol) is 8.3 kcal/mol higher than the **TS3_a** ($\Delta G^\ddagger = 23.9$ kcal/mol) where only 1 BPh₃ molecule is involved. Similarly, **TS4'_a**, representing epoxide addition with a single BPh₃ molecule in the PC formation pathway, required a significantly higher activation barrier ($\Delta G^\ddagger = 56.6$ kcal/mol), 28.0 kcal/mol more than **TS4_a** ($\Delta G^\ddagger = 28.6$ kcal/mol), where two BPh₃ molecules were involved. These findings reinforce that the transition states reported in the manuscript correspond to the most favorable reaction pathways.

S2. BPh₃ catalyzed coupling reaction of CO₂ and cyclohexene oxide (CHO):

The three-dimensional structures of optimized transition states involved in the BPh₃-catalyzed coupling reaction between CO₂ and cyclohexene oxide (CHO) are illustrated in **Fig. S2**.

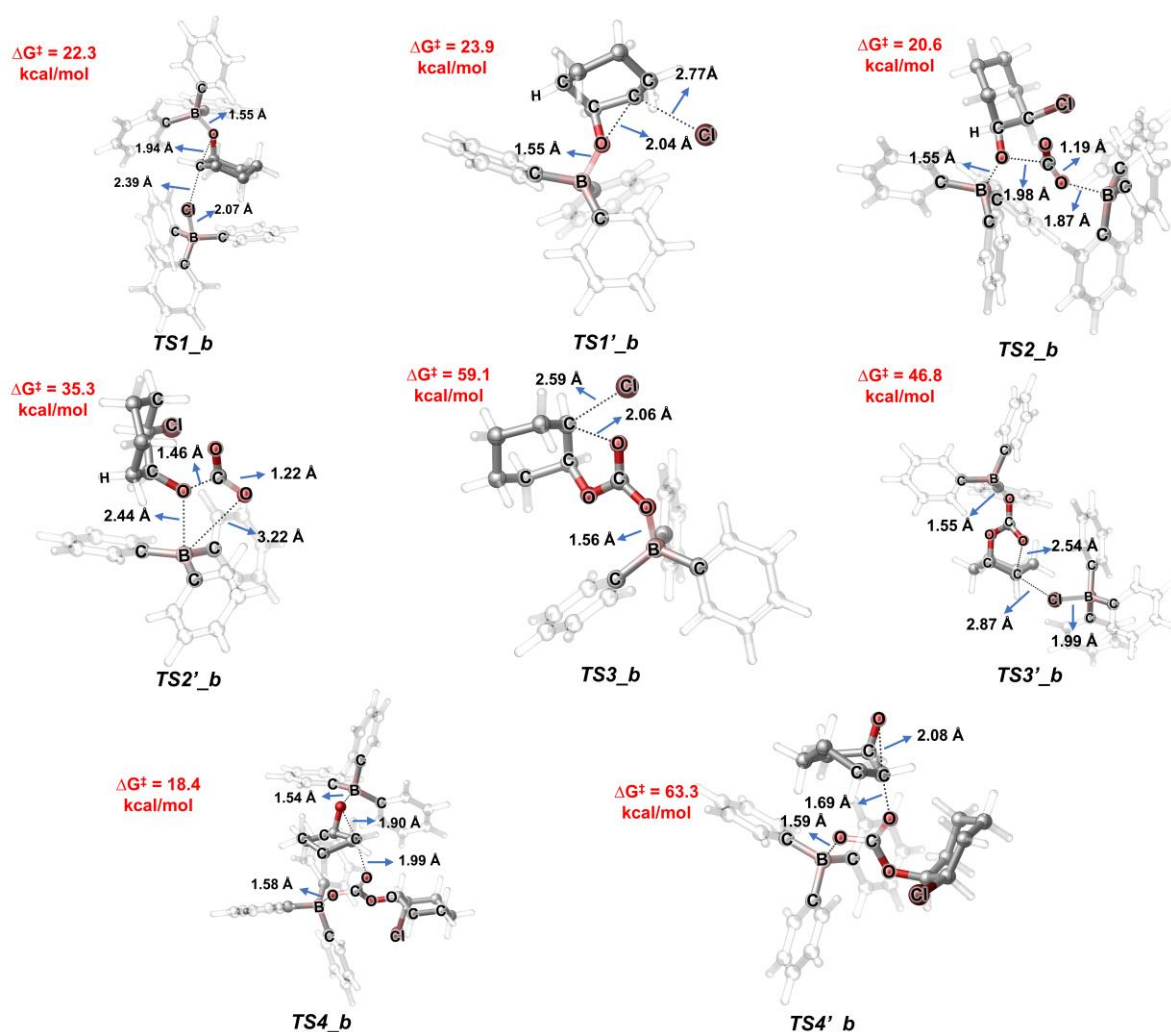


Fig. S2. Optimized geometries of the transition state structures involved in the BPh₃ catalyzed coupling reaction of CO₂ and cyclohexene oxide (CHO).

S3. Distortion-Interaction Analysis (DIA)

A distortion-interaction energy analysis (DIA) was conducted to elucidate the distinct catalytic behavior of BPh₃-catalyzed coupling reactions of CO₂ and epoxides. In the distortion/interaction model, the activation energy ($\Delta E^\ddagger$) is decomposed into two contributions along the reaction coordinate: the reaction strain or distortion energy (ΔE_{dist}), which reflects the structural deformation the reactants undergo during the reaction, and the interaction energy (ΔE_{int}) which represents the change in interactions between these increasingly distorted reactants.

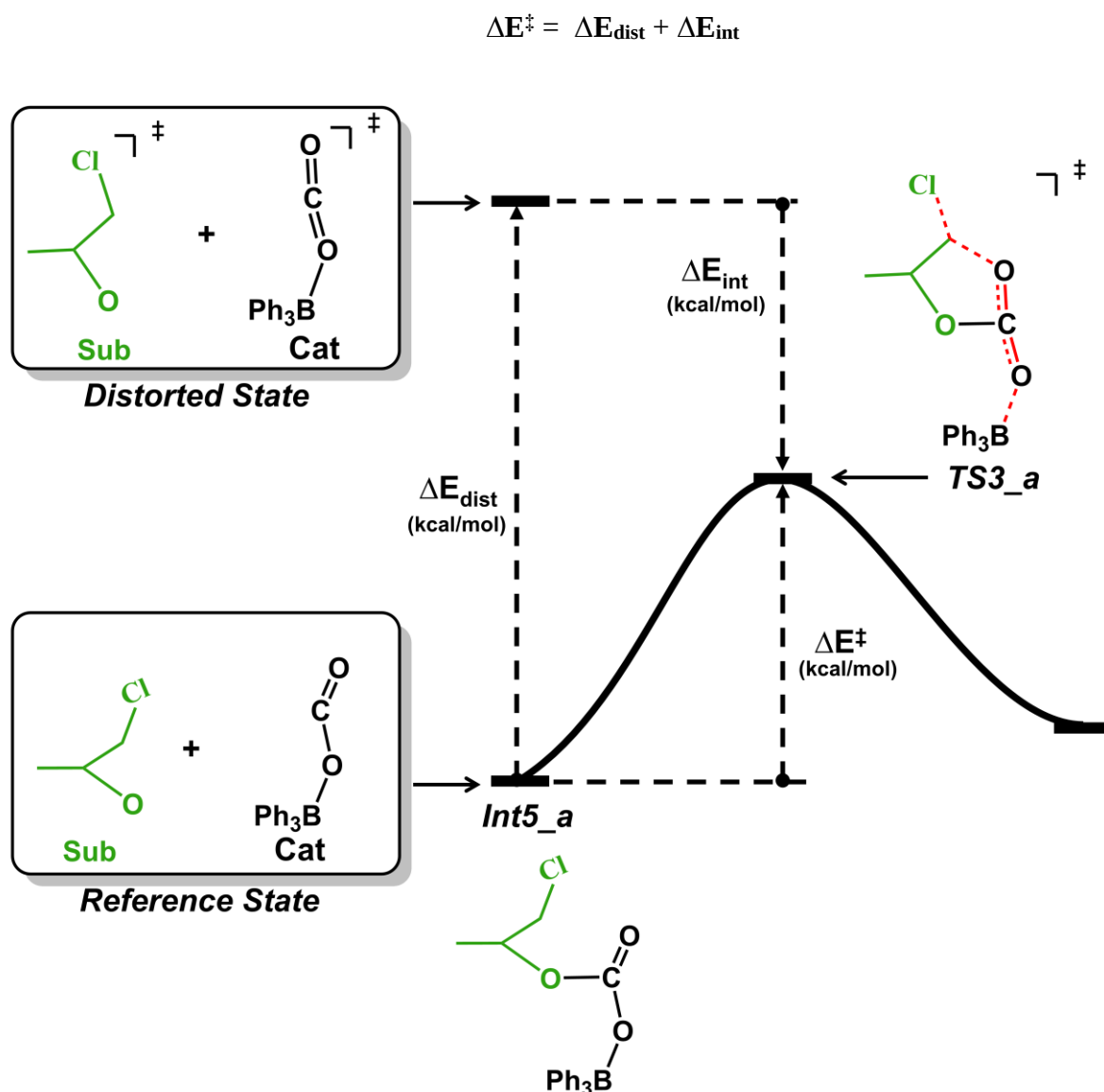


Fig. S3. Distortion-interaction analysis of the ring-closing step of BPh₃ catalyzed coupling reaction of CO₂ and PO.

It is important to note that in the DIA, electronic energies are used without accounting for zero-point energy and thermal corrections. We performed (DIA) on the selectivity determining transition states: ring-closing and epoxide addition steps of both BPh₃ and BEt₃-catalyzed CO₂ with PO and CO₂ with CHO coupling reactions. In the DIA framework, the frozen geometries of the reactive fragments are extracted from the optimized transition state and reference intermediate structures. As illustrated in **Fig. S3**, for the ring-closing step of the BPh₃-catalyzed CO₂ and PO coupling reaction, the transition state and reference intermediate were decomposed into two fragments: the catalyst (**Cat**), which includes the BPh₃-activated CO₂ molecule, and the substrate (**Sub**), which comprises the remaining part of the system. Single-point energy calculations were performed on these isolated fragments for both the reference intermediate and the transition state. The changes in the energies of the respective fragments allowed us to compute the distortion energies for the **Cat** (referred to as $\Delta E^{\text{Cat}}_{\text{dist}}$) and **Sub** (referred to as $\Delta E^{\text{Sub}}_{\text{dist}}$). The cumulative distortion energy ΔE_{dist} was obtained by summing both distortion energies together. To quantify the interaction between the fragments, the sum of the electronic energies of the individual fragments from the electronic energy of the optimized transition state and the reference intermediate. To quantify the interaction between the fragments, we subtracted the sum of the electronic energies of the individual fragments from the electronic energy of the optimized transition state and the reference intermediate. The difference between the interaction energies of the distorted fragments and those of the reference intermediate fragments provided the change in interaction energy (ΔE_{int}). This DIA methodology was similarly applied to the critical steps of the all coupling reaction pathways to provide a comprehensive understanding of the reaction energetics.

S4. BEt_3 catalyzed coupling reaction of CO_2 and propylene oxide (PO):

The three-dimensional structures of optimized transition states involved in the BEt_3 -catalyzed coupling reaction between CO_2 and PO are illustrated in **Fig. S4**.

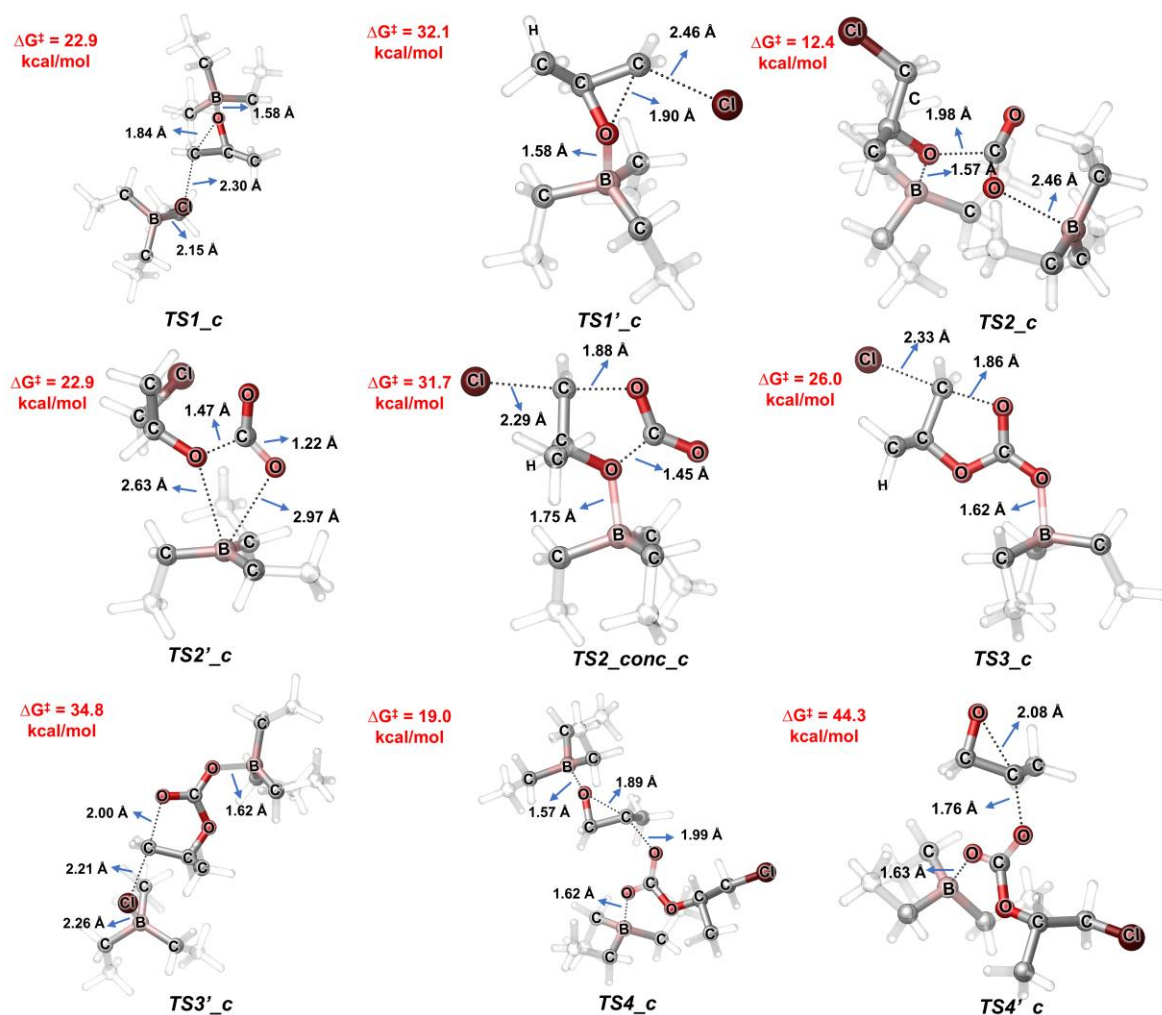


Fig. S4. Optimized geometries of the transition state structures involved in the BEt_3 catalyzed coupling reaction of CO_2 and propylene oxide (PO).

S5. BEt_3 catalyzed coupling reaction of CO_2 and cyclohexene oxide (CHO):

The BEt_3 -catalyzed coupling of CO_2 and CHO follows a similar mechanism as BEt_4 -catalyzed coupling of CO_2 and PO. The Gibbs energy profile for BEt_3 -catalyzed coupling of CO_2 and CHO is presented in **Fig. S5**.

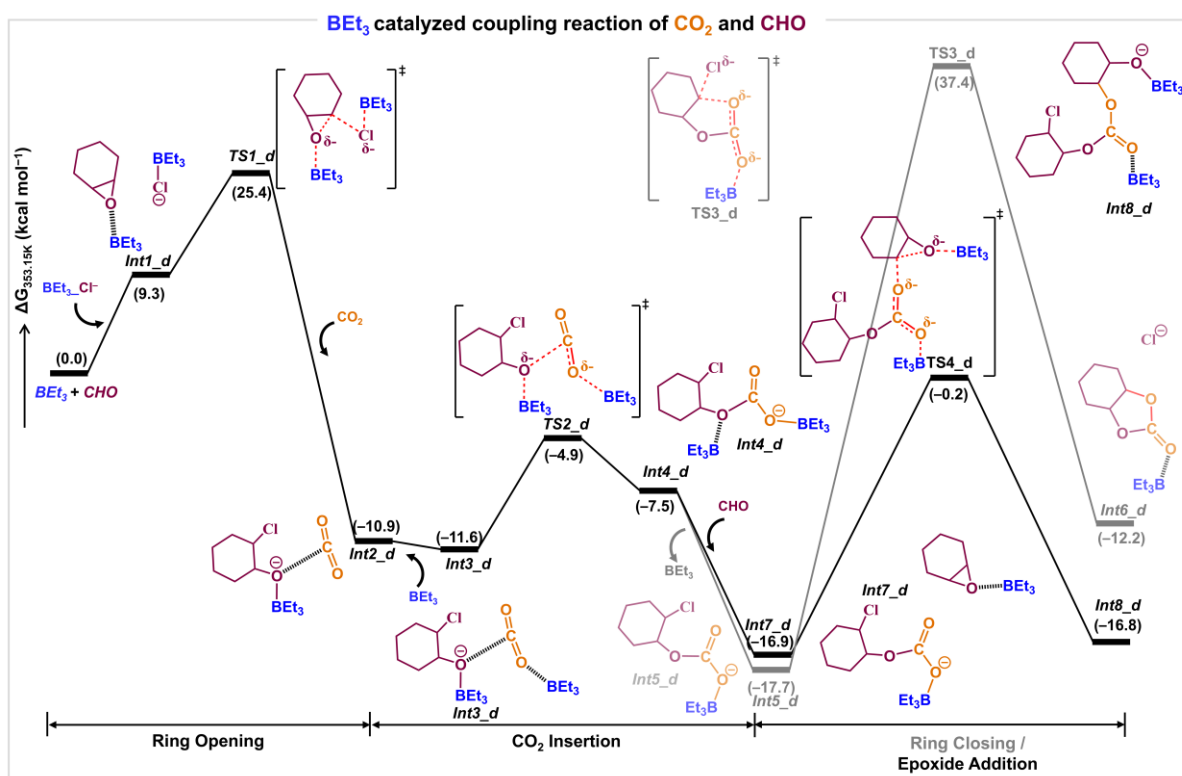


Fig. S5. Gibbs energy profile for BEt_3 catalyzed coupling reaction of CO_2 and CHO using M06-2X/def2-TZVP//M06-2X/def2-SVP level of DFT. Values in the parentheses are the Gibbs energies (relative to $\text{BEt}_3 + \text{CHO}$) at 353.15 K in kcal/mol.

The process begins with the ring-opening step via **TS1_d**, requiring an activation barrier of $\Delta G^\ddagger = 25.4$ kcal/mol. This is followed by CO_2 insertion, which proceeds through an additional BEt_3 molecule coordinated transition state, **TS2_d** ($\Delta G^\ddagger = 6.7$ kcal/mol). After CO_2 insertion, the reaction can lead to cyclic-carbonate (CC) formation via the ring-closing transition state **TS3_d** ($\Delta G^\ddagger = 55.1$ kcal/mol) or to poly-carbonate (PC) formation via epoxide addition transition state **TS4_d** ($\Delta G^\ddagger = 16.7$ kcal/mol). The much lower activation barrier for **TS4_d** (38.4 kcal/mol lower than **TS3_d**) makes PC formation the preferred pathway, consistent with experimental observations.

The three-dimensional structures of the optimized transition states for the BEt_3 -catalyzed CO_2 and CHO coupling reaction are illustrated in **Fig. S6**.

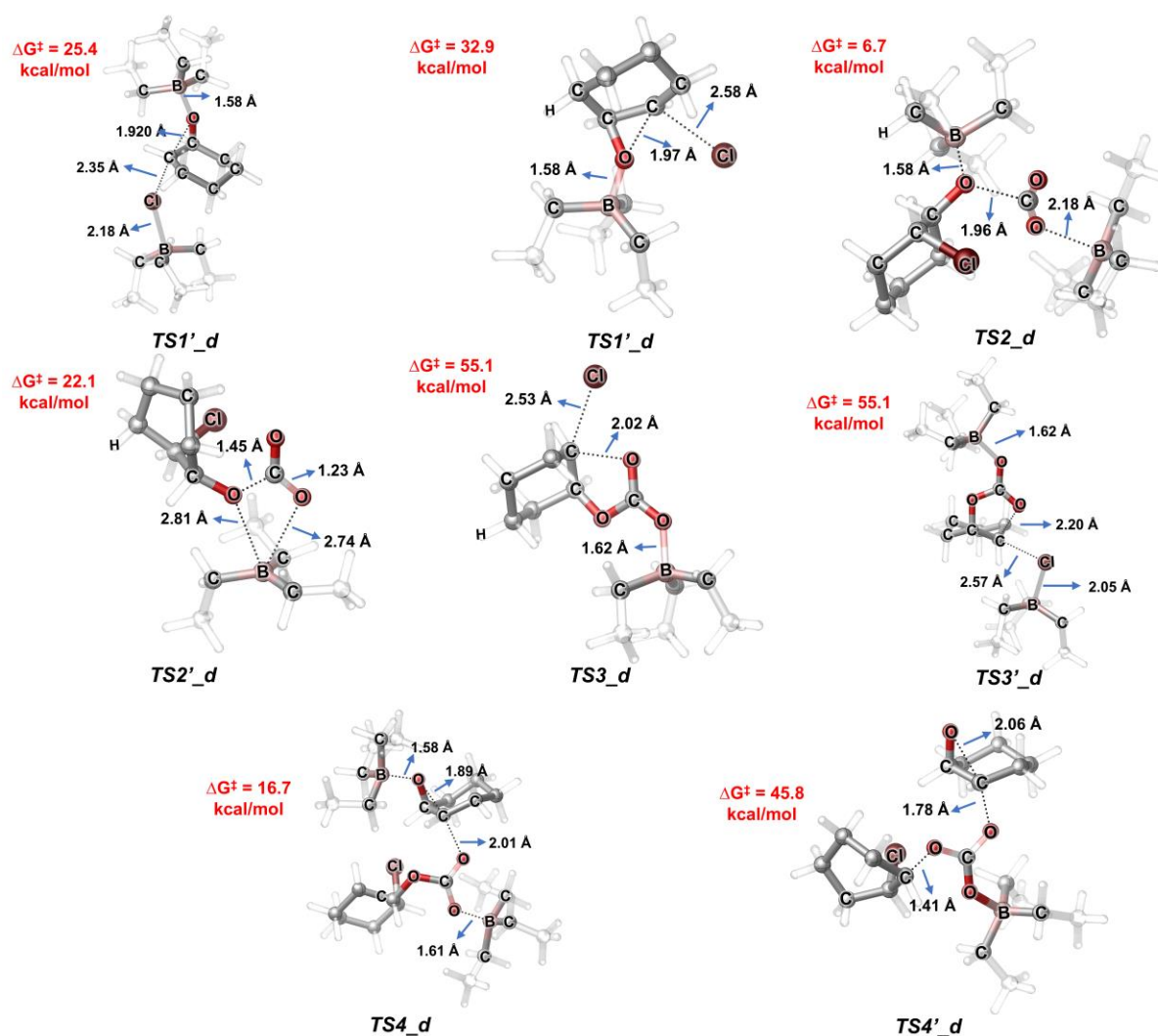


Fig. S6. Optimized geometries of the transition state structures involved in the BEt₃ catalyzed coupling reaction of CO₂ and cyclohexene oxide (CHO).

The DIA of the selectivity determining transition states of the BEt₃ catalyzed coupling reaction of CO₂ and cyclohexene oxide (CHO) is illustrated in **Fig. S7**. The total distortion energy and interaction energy are higher in the ring-closing transition state **TS3_d** ($\Delta E_{\text{dist}} = 86.6$ kcal/mol, $\Delta E_{\text{int}} = -40.0$ kcal/mol) compared to the epoxide addition transition state **TS4_d** ($\Delta E_{\text{dist}} = 28.1$ kcal/mol, $\Delta E_{\text{int}} = -12.4$ kcal/mol). The significantly higher distortion energy in **TS3_d** makes the ring-closing step less favorable than epoxide addition, leading to a preference for poly-carbonate formation.

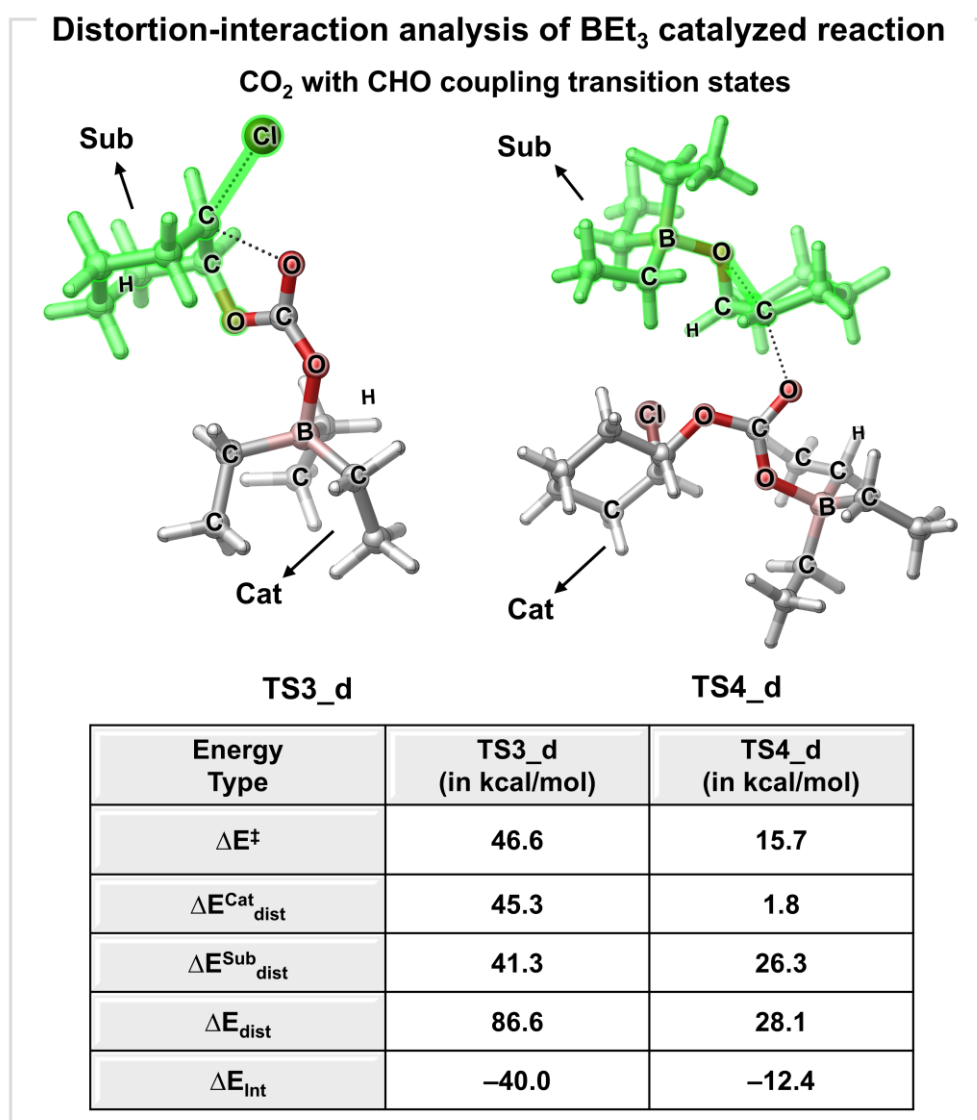


Fig. S7. Distortion/Interaction Analysis (DIA) of selectivity determining transition states of BEt₃ catalyzed CO₂ and cyclohexene oxide (CHO) coupling reaction.

In addition, non-covalent interaction (NCI) analysis was conducted to further investigate the differences between the ring-closing transition states in the BEt₃-catalyzed coupling reactions of CO₂ and PO (TS3_c), and CO₂ and CHO (TS3_d), respectively. The NCI plots (Fig. S8) for TS3_c and TS3_d reveal a significant increase in steric repulsion around the five-membered ring formation when the substrate changes from PO to the bulkier CHO. The enhanced red isosurfaces in TS3_d indicate pronounced steric hindrance during the ring-closing step, making this transition state energetically less favorable. These findings strongly suggest that the high activation barrier observed for the ring-closing step in the CO₂ and CHO system is a direct consequence of increased steric repulsion. Furthermore, this conclusion is consistent with our DIA results, which showed significantly higher distortion energy for TS3_c compared to TS3_d.

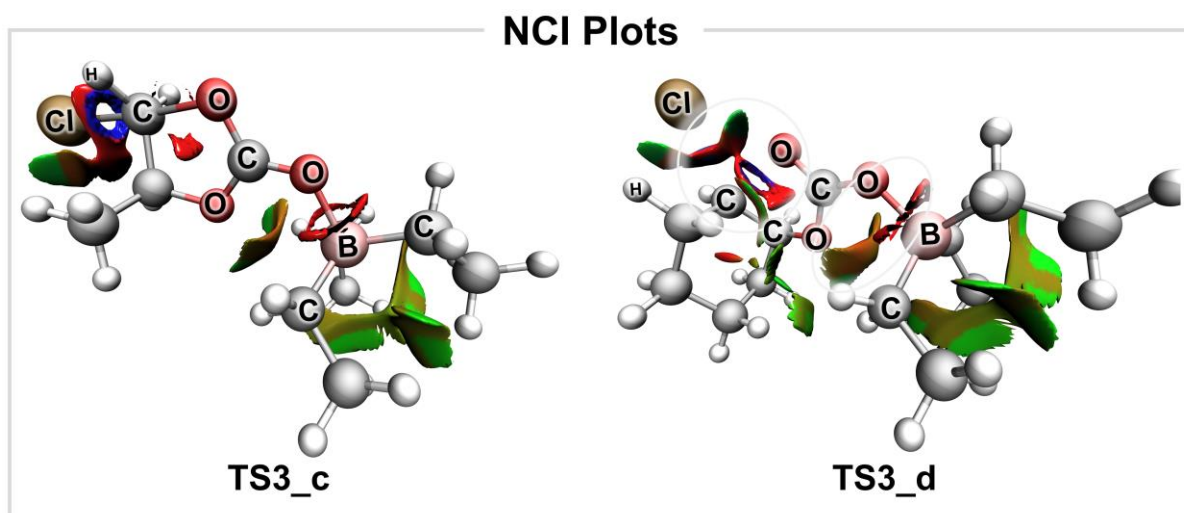


Fig. S8. NCI plots for BPh_3 catalyzed coupling reaction of CO_2 with PO (**TS3_c**) and CO_2 with CHO (**TS3_d**) ring closing transition state structures. Blue, green, and red isosurfaces represent strong attractions, weak van der Waals interaction, and steric repulsions, respectively.

S6. Electronic energies and Gibbs free energies

Total electronic energies and Gibbs free energies (373.15 K) of the optimized structures involved in BPh_3 catalyzed coupling reaction of CO_2 and PO at M06-2X/def2-TZVP//M06-2X/def2-SVP level are given below:

Molecule	E_{tot} [au]	$G_{373.15}$ [au]	Imaginary Frequency
CO_2	-188.5970	-188.6118	
PO	-193.0980	-193.0464	
BPh_3	-719.7681	-719.5438	
Cl^-	-460.2560	-460.2755	
$\text{BPh}_3\text{--Cl}^-$	-1180.0880	-1179.8668	
$\text{BPh}_3\text{--PO}$	-1373.1778	-1372.8746	
$\text{BPh}_3\text{--CO}_2$	-1368.6774	-1368.4465	
Int1_a	-2092.9955	-2092.4381	
TS1_a	-2092.9710	-2092.4137	<i>i510</i>
TS1'_a	-1373.1230	-1372.8225	<i>i645</i>
Int2_a	-1561.8291	-1561.5179	
TS2'_a	-1561.7728	-1561.4595	<i>i40</i>
Int3_a	-2281.6156	-2281.0486	
TS2_a	-2281.5980	-2281.0285	<i>i128</i>

TS2_conc_a	-1561.7680	-1561.4533	<i>i537</i>
Int4_a	-2281.6145	-2281.0411	
Int5_a	-1561.8338	-1561.5198	
TS3_a	-1561.7967	-1561.4817	<i>i529</i>
TS3'_a	-2281.5854	-2281.0123	<i>i516</i>
Int6_a	-1561.8149	-1561.4989	
Int7_a	-2474.7379	-2474.0847	
TS4_a	-2474.7154	-2474.0626	<i>i562</i>
TS4'_a	-1754.8681	-1754.4741	<i>i495</i>
Int8_a	-2474.7531	-2474.0970	

Total electronic energies and Gibbs free energies (333.15 K) of the optimized structures involved in BPh₃ catalyzed coupling reaction of CO₂ and CHO at M06-2X/def2-TZVP//M06-2X/def2-SVP level are given below:

Molecule	E_{tot} [au]	G_{333.15} [au]	Imaginary Frequency
CO₂	-188.5970	-188.6084	
CHO	-309.8294	-309.7104	
BPh₃	-719.7681	-719.5359	
Cl⁻	-460.2560	-460.2731	
BPh₃_ Cl⁻	-1180.0880	-1179.8584	
BPh₃_CHO	-1489.9032	-1489.5275	
BPh₃_CO₂	-1368.6774	-1368.4373	
Int1_b	-2209.7295	-2209.0938	
TS1_b	-2209.7045	-2209.0691	<i>i467</i>
TS1'_b	-1489.8629	-1489.4894	<i>i422</i>
Int2_b	-1678.5563	-1678.1718	
TS2'_b	-1678.5042	-1678.1155	<i>i30</i>
Int3_b	-2398.3433	-2397.6958	
TS2_b	-2398.3259	-2397.6748	<i>i174</i>
Int4_b	-2398.3327	-2397.6797	
Int5_b	-1678.5541	-1678.1644	
TS3_b	-1678.4653	-1678.0776	<i>i508</i>
TS3'_b	-2398.2804	-2397.6332	<i>i127</i>

Int6_b	-1678.5367	-1678.1465	
Int7_b	-2708.2147	-2707.4139	
TS4_b	-2708.1890	-2707.3888	<i>i568</i>
TS4'_b	-1988.3155	-1987.7814	<i>i346</i>
Int8_b	-2708.2131	-2707.4100	

Total electronic energies and Gibbs free energies (333.15 K) of the optimized structures involved in BEt₃ catalyzed coupling reaction of CO₂ and PO at M06-2X/def2-TZVP//M06-2X/def2-SVP level are given below:

Molecule	E_{tot} [au]	G_{333.15} [au]	Imaginary Frequency
CO₂	-188.5970	-188.6084	
PO	-193.0980	-193.0419	
BEt₃	-262.4825	-262.3207	
Cl⁻	-460.2560	-460.2731	
BEt₃_Cl⁻	-722.7874	-722.6269	
BEt₃_PO	-915.8776	-915.6357	
BEt₃_CO₂	-911.3821	-911.2110	
Int1_c	-1178.4058	-1177.9748	
TS1_c	-1178.3838	-1177.9529	<i>i504</i>
TS1'_c	-915.8247	-915.5846	<i>i534</i>
Int2_c	-1104.5269	-1104.2767	
TS2'_c	-1104.4923	-1104.2401	<i>i77</i>
Int3_c	-1367.0241	-1366.5865	
TS2_c	-1367.0175	-1366.5776	<i>i144</i>
TS2_conc_c	-1104.4821	-1104.2262	<i>i522</i>
Int4_c	-1367.0311	-1366.5851	
Int5_c	-1104.5420	-1104.2874	
TS3_c	-1104.5017	-1104.2460	<i>i520</i>
TS3'_c	-1366.9974	-1366.5526	<i>i519</i>
Int6_c	-1104.5260	-1104.2689	
Int7_c	-1560.1651	-1559.6413	
TS4_c	-1560.1356	-1559.6111	<i>i572</i>
TS4'_c	-1297.5825	-1297.2497	<i>i503</i>

Int8_c	-1560.1620	-1559.6349
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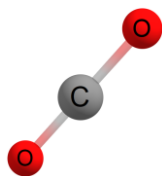
Total electronic energies and Gibbs free energies (353.15 K) of the optimized structures involved in BEt₃ catalyzed coupling reaction of CO₂ and CHO at M06-2X/def2-TZVP//M06-2X/def2-SVP level are given below:

Molecule	E_{tot} [au]	G_{353.15} [au]	Imaginary Frequency
CO₂	-188.5970	-188.6101	
CHO	-309.8294	-309.7130	
BEt₃	-262.4825	-262.3238	
Cl⁻	-460.2560	-460.2743	
BEt₃_Cl⁻	-722.7874	-722.6302	
BEt₃_CHO	-1032.6108	-1032.3097	
BEt₃_CO₂	-911.3821	-911.2148	
Int1_d	-1295.1412	-1294.6522	
TS1_d	-1295.1153	-1294.6265	<i>i498</i>
TS1'_d	-1032.5579	-1032.2587	<i>i508</i>
Int2_d	-1221.2482	-1220.9386	
TS2'_d	-1221.2150	-1220.9034	<i>i69</i>
Int3_d	-1483.7593	-1483.2635	
TS2_d	-1483.7513	-1483.2528	<i>i150</i>
Int4_d	-1483.7608	-1483.2569	
Int5_d	-1221.2640	-1220.9493	
TS3_d	-1221.1740	-1220.8615	<i>i477</i>
TS3'_d	-1483.6849	-1483.1840	<i>i356</i>
Int6_d	-1221.2563	-1220.9406	
Int7_d	-1793.6308	-1792.9849	
TS4_d	-1793.6058	-1792.9583	<i>i530</i>
TS4'_d	-1531.0362	-1530.5786	<i>i568</i>
Int8_d	-1793.6358	-1792.9847	

S7. Cartesian coordinates of the optimized structures

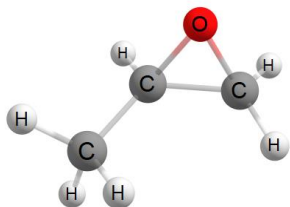
DFT optimization method: M06-2X/def2-SVP

CO₂



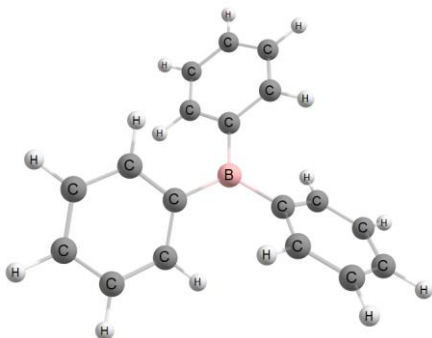
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O	0.000000000	0.000000000	1.156087000
O	0.000000000	0.000000000	-1.156087000

PO



O	6.976900000	-1.602020000	-5.198603000
C	7.325411000	-2.786054000	-5.878329000
H	6.803232000	-2.920864000	-6.834486000
C	8.782181000	-3.157270000	-5.867889000
H	8.919276000	-4.214855000	-6.134253000
H	9.340715000	-2.545772000	-6.590589000
C	6.509796000	-2.814866000	-4.657066000
H	5.429496000	-2.981207000	-4.725981000
H	6.974662000	-3.124166000	-3.713881000
H	9.206629000	-2.982855000	-4.869920000

BPh₃



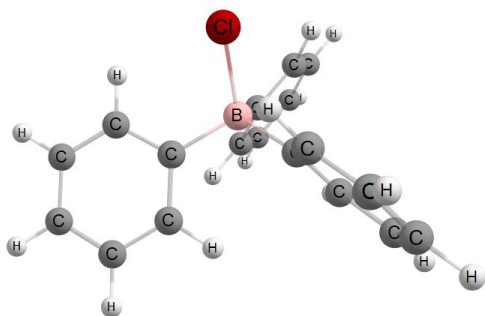
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C	1.922667000	2.011932000	0.265969000
C	4.455165000	1.570260000	-0.806089000
C	3.016466000	2.724363000	0.753956000
C	4.286518000	2.498542000	0.221948000
H	3.492120000	0.165978000	-2.121316000
H	0.933502000	2.187612000	0.695802000
H	5.448233000	1.388006000	-1.220197000
H	2.881106000	3.453213000	1.554785000
H	5.146974000	3.047100000	0.609490000
C	-0.357990000	-0.100669000	-0.386726000
C	-1.684135000	-0.171955000	-0.855119000
C	-0.130815000	-0.399615000	0.970390000
C	-2.736582000	-0.511146000	-0.007091000
C	-1.174481000	-0.767030000	1.817595000
C	-2.481048000	-0.816389000	1.330255000
H	-1.892890000	0.055039000	-1.903351000
H	0.887729000	-0.353842000	1.363491000
H	-3.758131000	-0.543960000	-0.389497000
H	-0.971056000	-1.010401000	2.861759000
H	-3.302044000	-1.093448000	1.994087000
C	0.769566000	-0.100312000	-2.862464000
C	1.356205000	0.714957000	-3.849420000
C	0.130540000	-1.280305000	-3.289289000
C	1.295300000	0.377870000	-5.200232000
C	0.089622000	-1.637755000	-4.635555000
C	0.666744000	-0.803972000	-5.594083000
H	1.859175000	1.637493000	-3.549572000
H	-0.333503000	-1.934302000	-2.547040000
H	1.743295000	1.034230000	-5.948160000
H	-0.397931000	-2.565184000	-4.940554000
H	0.626400000	-1.075779000	-6.650480000

Cl⁻



C1	1.010882000	-1.388100000	-0.936840000
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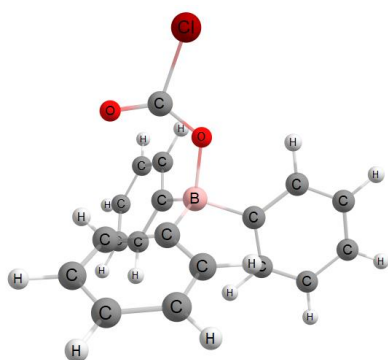
BPh₃ Cl⁻



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C	4.524581000	1.559499000	-0.600963000
C	2.665127000	2.899779000	0.125487000
C	4.035478000	2.762994000	-0.086961000
H	4.040378000	-0.428667000	-1.284945000
H	0.727422000	1.968285000	0.007010000
H	5.597852000	1.435156000	-0.768221000
H	2.265914000	3.832385000	0.532914000
H	4.718014000	3.583014000	0.149234000
C	-0.148549000	-0.497512000	-0.286218000
C	-1.309478000	0.097928000	-0.804885000
C	-0.218165000	-0.958593000	1.040522000
C	-2.475745000	0.235137000	-0.045515000
C	-1.374553000	-0.829917000	1.808097000
C	-2.514170000	-0.228442000	1.267911000
H	-1.301795000	0.461758000	-1.836515000
H	0.665169000	-1.444369000	1.463028000
H	-3.360275000	0.703056000	-0.485745000
H	-1.391187000	-1.202638000	2.835781000
H	-3.423364000	-0.127111000	1.865560000
C	0.953126000	-0.537024000	-2.743661000
C	1.035498000	0.649900000	-3.489430000
C	0.529439000	-1.685176000	-3.436184000
C	0.707752000	0.697071000	-4.847921000

C	0.201548000	-1.652925000	-4.790718000
C	0.287652000	-0.456595000	-5.507019000
H	1.370517000	1.564871000	-2.992088000
H	0.475493000	-2.627513000	-2.885151000
H	0.786645000	1.640514000	-5.394526000
H	-0.121939000	-2.567370000	-5.295179000
H	0.033512000	-0.427008000	-6.569369000
Cl	2.101382000	-2.265894000	-0.722419000

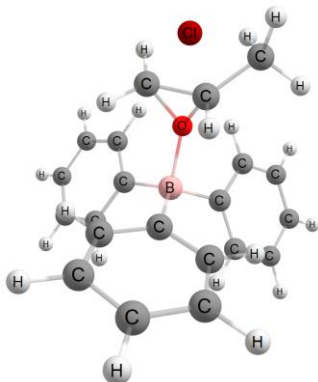
BPh₃_CO₂



B	1.091753000	-0.448611000	-1.154268000
C	2.078072000	0.769152000	-0.708368000
C	3.336854000	0.556535000	-0.126965000
C	1.679865000	2.105924000	-0.883949000
C	4.157628000	1.620271000	0.259874000
C	2.489209000	3.175026000	-0.504280000
C	3.738701000	2.936104000	0.073137000
H	3.676417000	-0.470827000	0.021916000
H	0.703413000	2.311892000	-1.333956000
H	5.133075000	1.417903000	0.709951000
H	2.145587000	4.201210000	-0.657269000
H	4.377741000	3.769664000	0.373736000
C	-0.237316000	-0.423053000	-0.210200000
C	-1.378306000	0.322723000	-0.546965000
C	-0.258993000	-1.077134000	1.032784000
C	-2.481834000	0.412947000	0.304180000
C	-1.356550000	-1.001850000	1.889854000
C	-2.477454000	-0.252767000	1.529279000
H	-1.408272000	0.839093000	-1.511235000
H	0.614793000	-1.660912000	1.338589000

H	-3.352985000	1.001938000	0.006228000
H	-1.337745000	-1.530476000	2.846143000
H	-3.340236000	-0.190675000	2.196454000
C	0.770229000	-0.428135000	-2.757777000
C	1.635364000	0.197381000	-3.670605000
C	-0.358815000	-1.068783000	-3.299263000
C	1.394069000	0.191071000	-5.046580000
C	-0.614448000	-1.079146000	-4.671039000
C	0.262646000	-0.446623000	-5.553378000
H	2.523854000	0.708711000	-3.289708000
H	-1.044635000	-1.582540000	-2.621849000
H	2.091289000	0.688898000	-5.725258000
H	-1.501859000	-1.588218000	-5.055273000
H	0.065448000	-0.452622000	-6.628155000
O	1.906213000	-1.734609000	-0.818453000
C	1.427178000	-2.905972000	-0.940537000
O	0.392944000	-3.321693000	-1.350764000
Cl	2.657641000	-4.116116000	-0.305055000

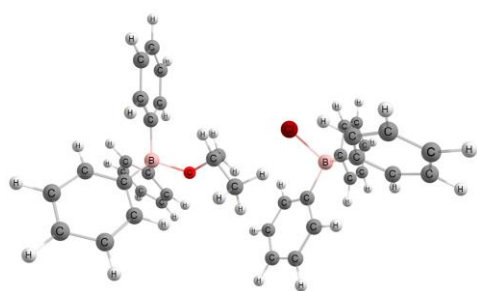
BPh₃_PO



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C	2.988612000	0.516605000	0.131476000
C	1.987250000	2.171748000	-1.295958000
C	3.877223000	1.479680000	0.612607000
C	2.869854000	3.139566000	-0.812226000
C	3.826028000	2.792891000	0.141906000
H	3.031158000	-0.503038000	0.537610000
H	1.242307000	2.458379000	-2.045263000

H	4.611584000	1.198880000	1.370998000
H	2.811073000	4.166522000	-1.181472000
H	4.522490000	3.543871000	0.522293000
C	-0.285654000	-0.361521000	-0.309384000
C	-1.450495000	0.398369000	-0.504514000
C	-0.204822000	-1.138357000	0.861740000
C	-2.503320000	0.379828000	0.411539000
C	-1.260546000	-1.167024000	1.775644000
C	-2.413471000	-0.412270000	1.556351000
H	-1.536777000	1.021627000	-1.400480000
H	0.697745000	-1.726700000	1.082945000
H	-3.396134000	0.983646000	0.230598000
H	-1.169576000	-1.783808000	2.672569000
H	-3.235290000	-0.435794000	2.276038000
C	0.548019000	-0.222468000	-2.917956000
C	1.414255000	0.305007000	-3.892713000
C	-0.632020000	-0.825824000	-3.387630000
C	1.122605000	0.240154000	-5.256347000
C	-0.935074000	-0.901341000	-4.749085000
C	-0.057387000	-0.364811000	-5.690432000
H	2.346517000	0.775763000	-3.568408000
H	-1.336180000	-1.241141000	-2.660998000
H	1.819703000	0.662105000	-5.984039000
H	-1.861715000	-1.378667000	-5.076011000
H	-0.290739000	-0.417977000	-6.756127000
O	1.761709000	-1.640795000	-1.118440000
C	2.477900000	-2.452739000	-2.060578000
H	2.279523000	-2.136673000	-3.090781000
C	3.895576000	-2.753016000	-1.676877000
H	4.265116000	-3.589185000	-2.289192000
H	4.526819000	-1.873583000	-1.869674000
C	1.317370000	-2.985701000	-1.314505000
H	0.358672000	-3.048557000	-1.838223000
H	1.508429000	-3.574272000	-0.404488000
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Cl	2.789925000	-3.194463000	1.546685000

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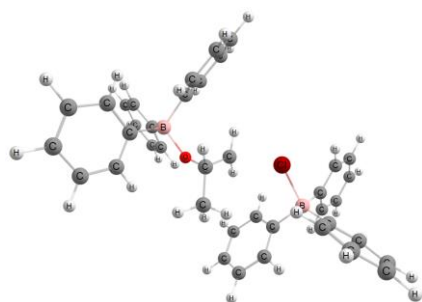


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C	2.662610000	0.874744000	-2.192271000
C	4.530451000	-1.066000000	-2.856324000
C	3.825767000	1.234449000	-2.871560000
C	4.770146000	0.262026000	-3.204135000
H	3.186428000	-2.466104000	-1.932845000
H	1.938566000	1.652041000	-1.929442000
H	5.259754000	-1.837826000	-3.112013000
H	3.999465000	2.279008000	-3.139658000
H	5.685733000	0.538497000	-3.730856000
C	0.592191000	0.130263000	0.133520000
C	-0.741903000	0.269215000	0.556093000
C	1.563088000	0.825713000	0.875670000
C	-1.091128000	1.048602000	1.660081000
C	1.228316000	1.608374000	1.981959000
C	-0.103711000	1.722401000	2.378243000
H	-1.530234000	-0.246505000	0.000103000
H	2.612231000	0.752541000	0.574977000
H	-2.137588000	1.129579000	1.961468000
H	2.010404000	2.129772000	2.537624000
H	-0.370737000	2.331797000	3.243903000
C	-0.176619000	-1.073373000	-2.193406000
C	-0.925315000	0.013657000	-2.675451000
C	-0.450065000	-2.330763000	-2.754670000
C	-1.901556000	-0.142262000	-3.658840000
C	-1.431405000	-2.500646000	-3.733830000
C	-2.163143000	-1.405801000	-4.190581000

H	-0.742305000	1.009950000	-2.261751000
H	0.121865000	-3.201260000	-2.423163000
H	-2.464704000	0.725446000	-4.009761000
H	-1.622000000	-3.494791000	-4.144098000
H	-2.930642000	-1.534753000	-4.956412000
O	1.272903000	-2.319708000	-0.511343000
C	0.528154000	-2.964538000	0.564570000
H	-0.202108000	-2.280097000	1.005984000
C	0.101324000	-4.369910000	0.290783000
H	-0.037464000	-4.878417000	1.256070000
H	-0.836594000	-4.391605000	-0.280620000
C	1.931757000	-2.603193000	0.747299000
H	2.175158000	-1.712843000	1.329799000
H	2.687665000	-3.384734000	0.658034000
H	0.887425000	-4.909200000	-0.257361000
Cl	1.822164000	-4.250742000	3.393348000
B	2.250807000	-6.170785000	3.291942000
C	2.446194000	-6.485414000	1.703838000
C	3.454099000	-5.820398000	0.979950000
C	1.642318000	-7.378976000	0.981612000
C	3.629850000	-6.004302000	-0.390805000
C	1.811170000	-7.580849000	-0.392994000
C	2.799350000	-6.887420000	-1.088669000
H	4.110702000	-5.131184000	1.521456000
H	0.851598000	-7.923244000	1.505174000
H	4.418061000	-5.462894000	-0.920468000
H	1.159789000	-8.279317000	-0.923886000
H	2.929767000	-7.035888000	-2.162685000
C	1.012736000	-7.008651000	3.935959000
C	1.197166000	-8.366464000	4.255183000
C	-0.272955000	-6.486064000	4.143483000
C	0.159704000	-9.162324000	4.740482000
C	-1.320261000	-7.271211000	4.632951000
C	-1.110688000	-8.616198000	4.932355000
H	2.188279000	-8.810803000	4.122219000
H	-0.446600000	-5.429456000	3.927500000
H	0.343849000	-10.213257000	4.976944000

H	-2.306969000	-6.826240000	4.784536000
H	-1.926372000	-9.232797000	5.316636000
C	3.619486000	-6.402390000	4.140798000
C	4.582983000	-7.343476000	3.743122000
C	3.859682000	-5.728591000	5.350791000
C	5.722809000	-7.606519000	4.508752000
C	4.993473000	-5.978417000	6.121762000
C	5.933957000	-6.923158000	5.704308000
H	4.440877000	-7.882658000	2.801545000
H	3.135929000	-4.978055000	5.678347000
H	6.451260000	-8.345028000	4.164699000
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TS1_a

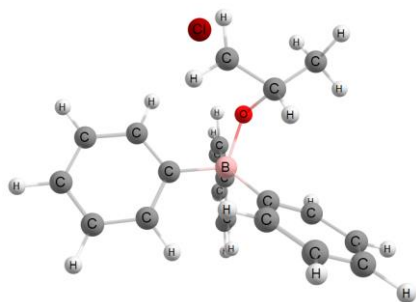


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C	2.446542000	0.821484000	-2.424187000
C	4.589596000	-0.848168000	-2.979462000
C	3.522908000	1.299948000	-3.168595000
C	4.605431000	0.463011000	-3.450462000
H	3.502009000	-2.346484000	-1.871430000
H	1.606359000	1.490891000	-2.212739000
H	5.429440000	-1.514015000	-3.193252000
H	3.520377000	2.330198000	-3.532823000
H	5.452297000	0.832142000	-4.033182000
C	0.951706000	-0.156874000	0.321750000
C	-0.266036000	-0.093357000	1.022641000
C	2.054752000	0.466571000	0.933014000
C	-0.379214000	0.535634000	2.264504000

C	1.957084000	1.101574000	2.172434000
C	0.736221000	1.136259000	2.846624000
H	-1.158779000	-0.546065000	0.580407000
H	3.020362000	0.447431000	0.419679000
H	-1.342004000	0.555362000	2.780064000
H	2.838740000	1.570068000	2.615799000
H	0.654894000	1.627599000	3.818432000
C	-0.204181000	-1.010000000	-2.011466000
C	-1.091760000	0.076273000	-2.082891000
C	-0.459432000	-2.087375000	-2.877578000
C	-2.182472000	0.085012000	-2.955447000
C	-1.549907000	-2.096519000	-3.747956000
C	-2.421178000	-1.007002000	-3.788993000
H	-0.927906000	0.940278000	-1.432138000
H	0.229853000	-2.936478000	-2.869927000
H	-2.852265000	0.947968000	-2.981676000
H	-1.717900000	-2.954478000	-4.403537000
H	-3.276210000	-1.007728000	-4.468518000
O	1.443507000	-2.488111000	-0.725558000
C	0.593416000	-3.237899000	0.119177000
H	-0.281211000	-2.664305000	0.457115000
C	0.240940000	-4.604831000	-0.407758000
H	-0.182131000	-5.214074000	0.403844000
H	-0.494713000	-4.520006000	-1.218633000
C	1.756277000	-3.120929000	1.003900000
H	1.903479000	-2.187789000	1.546601000
H	2.611630000	-3.755448000	0.780032000
H	1.143895000	-5.110013000	-0.781887000
Cl	1.282629000	-4.244333000	2.949399000
B	2.052514000	-6.153159000	3.122342000
C	2.395024000	-6.598701000	1.603862000
C	3.500015000	-6.048320000	0.927646000
C	1.624412000	-7.532803000	0.895306000
C	3.800028000	-6.377904000	-0.393731000
C	1.920692000	-7.882484000	-0.424993000
C	3.004545000	-7.299353000	-1.078728000
H	4.144414000	-5.341957000	1.461366000

H	0.766879000	-7.997293000	1.388835000
H	4.656885000	-5.918317000	-0.891173000
H	1.296730000	-8.611174000	-0.947263000
H	3.233246000	-7.562294000	-2.113440000
C	0.849500000	-7.000281000	3.800637000
C	1.149932000	-8.068329000	4.662123000
C	-0.508508000	-6.792142000	3.503543000
C	0.154920000	-8.892538000	5.191777000
C	-1.511669000	-7.605948000	4.029937000
C	-1.183696000	-8.664987000	4.877314000
H	2.192877000	-8.257777000	4.929320000
H	-0.784271000	-5.959588000	2.851865000
H	0.427911000	-9.713375000	5.858997000
H	-2.556812000	-7.410334000	3.779371000
H	-1.966327000	-9.303249000	5.293013000
C	3.350084000	-6.022404000	4.079587000
C	4.429193000	-6.908777000	3.924154000
C	3.420990000	-5.122613000	5.155919000
C	5.522826000	-6.902119000	4.793339000
C	4.510751000	-5.101030000	6.025657000
C	5.569062000	-5.993856000	5.849136000
H	4.413382000	-7.624167000	3.096969000
H	2.602392000	-4.414635000	5.304803000
H	6.343889000	-7.606414000	4.640729000
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TS1'_a

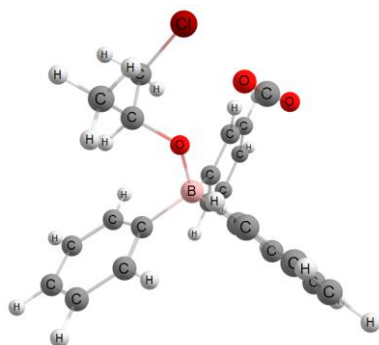


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C	2.021964000	0.907813000	-0.773499000
C	3.036465000	0.682197000	0.173766000

C	1.791862000	2.234564000	-1.169464000
C	3.791609000	1.739005000	0.686265000
C	2.544042000	3.295717000	-0.661547000
C	3.553054000	3.050002000	0.269930000
H	3.227706000	-0.342065000	0.514365000
H	1.003791000	2.442659000	-1.901005000
H	4.574223000	1.535015000	1.421375000
H	2.341984000	4.317573000	-0.993438000
H	4.146633000	3.875128000	0.671272000
C	-0.197517000	-0.404277000	-0.314356000
C	-1.398950000	0.266348000	-0.597944000
C	-0.099777000	-1.023469000	0.947319000
C	-2.465901000	0.291214000	0.303393000
C	-1.163590000	-1.009882000	1.851044000
C	-2.356263000	-0.357834000	1.532374000
H	-1.503391000	0.792774000	-1.551461000
H	0.835974000	-1.520851000	1.231156000
H	-3.385920000	0.821799000	0.044689000
H	-1.053163000	-1.505280000	2.818761000
H	-3.188037000	-0.345789000	2.240775000
C	0.741690000	-0.235263000	-2.902370000
C	1.682385000	0.288141000	-3.807582000
C	-0.423236000	-0.786406000	-3.464895000
C	1.474043000	0.274042000	-5.187945000
C	-0.647494000	-0.806996000	-4.843925000
C	0.302529000	-0.272342000	-5.713665000
H	2.604847000	0.720166000	-3.408988000
H	-1.177120000	-1.218991000	-2.800236000
H	2.229226000	0.692168000	-5.858050000
H	-1.567050000	-1.243942000	-5.241134000
H	0.132782000	-0.283448000	-6.792732000
O	2.017154000	-1.559778000	-1.116957000
C	1.988541000	-2.704174000	-1.934530000
H	1.303292000	-2.610107000	-2.792223000
C	3.386983000	-3.124876000	-2.326870000
H	3.370576000	-4.099825000	-2.836805000
H	3.819027000	-2.374129000	-3.002534000

C	1.432242000	-3.344087000	-0.747891000
H	0.407634000	-3.076722000	-0.483148000
H	1.919347000	-4.145404000	-0.202012000
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Cl	3.067587000	-2.987296000	1.334702000

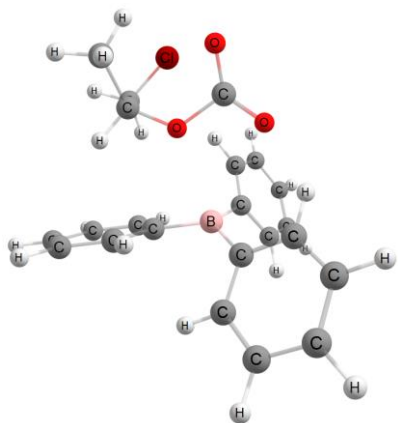
Int2_a



B	0.544107000	-0.139757000	-1.708232000
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C	2.988490000	0.809375000	-1.366538000
C	1.226365000	2.146767000	-0.469005000
C	3.931197000	1.748593000	-0.942553000
C	2.156460000	3.097731000	-0.043957000
C	3.518056000	2.903851000	-0.277840000
H	3.321584000	-0.096625000	-1.880828000
H	0.166576000	2.313169000	-0.256861000
H	4.994568000	1.577388000	-1.130667000
H	1.816297000	3.993694000	0.482137000
H	4.249499000	3.642572000	0.058593000
C	-0.778275000	-0.179171000	-0.730880000
C	-1.851370000	0.720738000	-0.865571000
C	-0.849314000	-1.068935000	0.355603000
C	-2.934428000	0.731476000	0.016424000
C	-1.929052000	-1.075644000	1.241726000
C	-2.981127000	-0.174153000	1.076496000
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H	-0.024385000	-1.768602000	0.511730000
H	-3.747671000	1.448124000	-0.126127000
H	-1.944835000	-1.786717000	2.071813000

H	-3.827017000	-0.175098000	1.768187000
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C	-1.108713000	-0.133101000	-3.833817000
C	0.744838000	1.083025000	-5.492068000
C	-1.423664000	0.098684000	-5.174729000
C	-0.494100000	0.712059000	-6.014395000
H	2.017123000	1.152056000	-3.761912000
H	-1.855296000	-0.614655000	-3.194514000
H	1.484557000	1.567562000	-6.134705000
H	-2.399440000	-0.201329000	-5.565716000
H	-0.733355000	0.900360000	-7.063727000
O	1.293896000	-1.446239000	-1.676132000
C	0.935542000	-2.531628000	-2.456646000
H	0.236723000	-2.231667000	-3.263320000
C	2.176081000	-3.129072000	-3.113637000
H	1.920227000	-3.991537000	-3.749331000
H	2.653626000	-2.358779000	-3.735382000
C	0.144783000	-3.571113000	-1.665688000
H	-0.747152000	-3.117293000	-1.218663000
H	-0.141126000	-4.421197000	-2.299128000
H	2.890562000	-3.446132000	-2.342295000
Cl	1.093331000	-4.264480000	-0.292707000
C	3.034602000	-1.806915000	0.310076000
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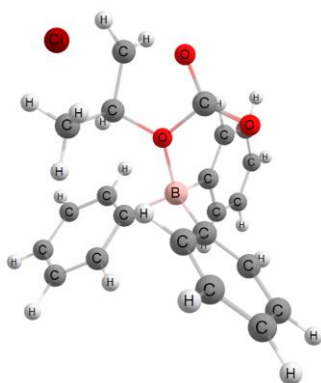
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C	3.207873000	2.571361000	0.435940000
C	2.466726000	3.836334000	-1.477539000
C	3.266052000	3.730385000	-0.341464000
H	2.312727000	0.607010000	0.676325000
H	1.007026000	2.875655000	-2.730486000
H	3.836208000	2.480693000	1.324710000
H	2.499216000	4.739663000	-2.090882000
H	3.933982000	4.548467000	-0.061433000
C	-0.596997000	0.111525000	-0.320182000
C	-1.210245000	1.149580000	0.398129000
C	-1.033028000	-1.200662000	-0.069658000
C	-2.241416000	0.898474000	1.307878000
C	-2.049579000	-1.458483000	0.845635000
C	-2.665498000	-0.408746000	1.532576000
H	-0.872398000	2.178462000	0.244095000
H	-0.534517000	-2.028605000	-0.573102000
H	-2.704334000	1.726621000	1.849460000
H	-2.354096000	-2.490977000	1.029569000
H	-3.463608000	-0.613133000	2.249934000
C	0.096522000	0.286281000	-2.954058000
C	1.052891000	0.474875000	-3.968975000
C	-1.190700000	-0.109690000	-3.349261000
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C	-1.512539000	-0.316654000	-4.693034000
C	-0.545184000	-0.126448000	-5.678591000
H	2.067893000	0.764617000	-3.686845000
H	-1.954593000	-0.263505000	-2.582422000
H	1.508723000	0.414364000	-6.077441000
H	-2.521968000	-0.627679000	-4.970900000
H	-0.791835000	-0.289233000	-6.730059000
O	1.529920000	-1.861253000	-1.824267000
C	1.360542000	-2.734212000	-2.907178000
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C	0.035187000	-3.484368000	-2.806792000
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H	-0.150701000	-4.065994000	-3.720139000
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C	2.223596000	-2.234230000	-0.574787000
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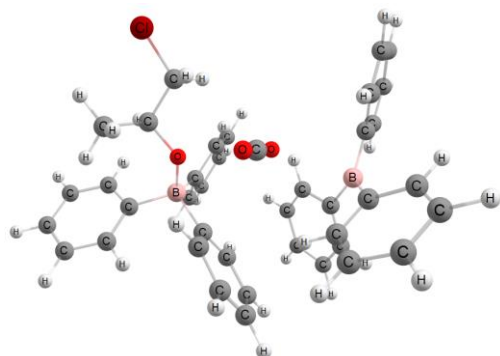


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C	4.427460000	2.356575000	-0.655352000
C	2.577978000	3.659976000	0.155139000
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H	3.971108000	0.350800000	-1.270485000
H	0.669313000	2.674799000	0.201656000
H	5.491052000	2.254088000	-0.883187000
H	2.179030000	4.588500000	0.570598000
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C	-0.207742000	0.088631000	-0.147644000

C	-1.193772000	1.027029000	-0.506389000
C	-0.562644000	-0.841486000	0.839422000
C	-2.446981000	1.058396000	0.102254000
C	-1.819162000	-0.829174000	1.450895000
C	-2.766426000	0.126347000	1.091200000
H	-0.973333000	1.745236000	-1.302319000
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H	-3.182819000	1.805732000	-0.203774000
H	-2.055709000	-1.574294000	2.213605000
H	-3.748319000	0.139934000	1.568916000
C	0.959839000	-0.039933000	-2.540888000
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C	-0.063156000	-0.875335000	-3.028155000
C	1.451073000	0.532377000	-4.872668000
C	-0.310043000	-1.032529000	-4.390753000
C	0.451616000	-0.326834000	-5.323184000
H	2.481682000	1.354751000	-3.177265000
H	-0.687417000	-1.421802000	-2.314686000
H	2.046480000	1.102372000	-5.589673000
H	-1.101423000	-1.706240000	-4.725382000
H	0.261496000	-0.442652000	-6.392409000
O	2.037706000	-1.222353000	-0.437945000
C	2.187146000	-2.438582000	-1.224384000
H	1.274599000	-2.539189000	-1.812343000
C	3.412470000	-2.347184000	-2.106184000
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H	3.144622000	-4.234794000	-0.207723000
H	1.391533000	-3.892840000	0.321513000

H	4.311249000	-2.215697000	-1.483874000
Cl	1.550335000	-5.118679000	-1.860552000
O	2.553680000	-0.383034000	1.622515000
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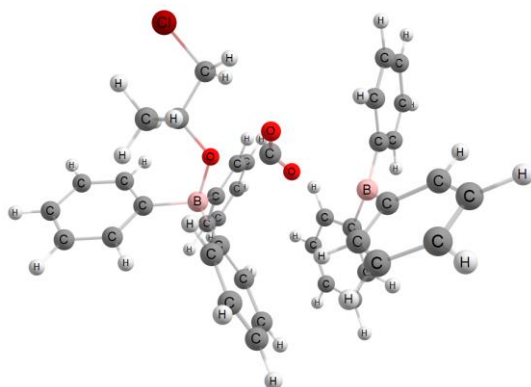


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C	2.356875000	1.051275000	0.468981000
C	4.944602000	0.504626000	-0.378747000
C	3.423009000	1.829606000	0.930264000
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H	4.054025000	-1.106435000	-1.503149000
H	1.346974000	1.278399000	0.821497000
H	5.957627000	0.279661000	-0.724042000
H	3.232415000	2.644400000	1.632749000
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C	-0.910466000	0.330485000	-0.297856000
C	-0.502639000	-1.866299000	0.534724000
C	-2.118755000	0.383186000	0.398026000
C	-1.713580000	-1.835535000	1.233490000
C	-2.533213000	-0.708974000	1.164889000
H	-0.618193000	1.184062000	-0.918003000
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C	-0.189122000	-0.561027000	-3.305893000
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C	-0.441942000	-0.176154000	-4.623141000
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H	2.903426000	0.756401000	-2.926549000
H	-0.965578000	-1.108549000	-2.762821000
H	2.469635000	1.458459000	-5.244830000
H	-1.392958000	-0.437191000	-5.094310000
H	0.324693000	0.853314000	-6.367368000
O	1.846961000	-2.277853000	-1.203481000
C	1.307971000	-3.221481000	-2.072045000
H	0.240132000	-3.017884000	-2.285900000
C	2.084850000	-3.290978000	-3.384172000
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C	1.372770000	-4.553713000	-1.321556000
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O	2.510724000	-2.709599000	1.544159000
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C	2.213678000	-0.631063000	3.964689000
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C	2.763116000	0.622991000	4.284859000
C	0.152214000	0.502120000	3.313944000
C	2.013300000	1.791760000	4.161697000
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H	0.449010000	-1.621401000	3.196772000
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C	5.518554000	-2.694092000	4.517050000
C	5.070340000	-1.127422000	2.740287000
C	6.879033000	-2.655366000	4.214333000
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H	0.877081000	-2.223141000	5.826856000
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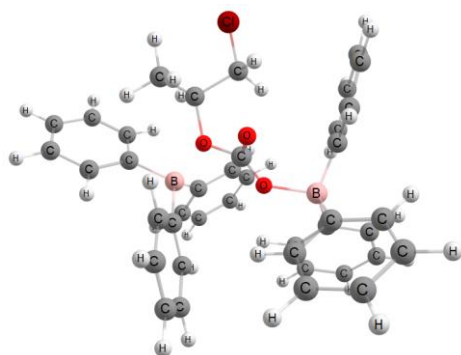
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C	2.398138000	1.148229000	0.553632000
C	4.935939000	0.695298000	-0.486774000
C	3.464388000	1.973848000	0.921646000
C	4.737171000	1.761465000	0.391904000
H	4.043735000	-0.967378000	-1.515102000
H	1.417746000	1.324760000	1.004586000
H	5.930473000	0.497368000	-0.894378000
H	3.296305000	2.779782000	1.639625000
H	5.570979000	2.406769000	0.677582000
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C	0.995821000	-0.517923000	-2.480756000
C	1.832137000	0.230989000	-3.325165000
C	-0.212531000	-0.965322000	-3.051015000
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C	-0.548748000	-0.723903000	-4.382377000
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H	2.185668000	1.080274000	-5.278645000
H	-1.493526000	-1.099541000	-4.782162000
H	0.057093000	0.206057000	-6.241266000
O	1.870696000	-2.328294000	-0.767343000
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H	0.843000000	-3.073949000	-2.361792000
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H	2.837083000	-4.111894000	-3.468497000
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C	1.500856000	-4.665788000	-1.127437000
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O	3.763073000	-3.403454000	0.311871000
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B	2.913671000	-1.937209000	3.704296000
C	2.160656000	-0.554728000	3.851430000
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C	0.801008000	1.914270000	3.999474000
H	0.256908000	-1.344745000	3.205710000
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C	4.476316000	-1.939814000	3.461099000
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C	6.722135000	-2.743443000	3.975629000
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C	7.263325000	-1.868472000	3.034853000
H	4.923162000	-3.483729000	4.904258000
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C	2.216093000	-3.276618000	4.188937000
C	1.263249000	-3.284310000	5.218517000
C	2.555392000	-4.512226000	3.607190000
C	0.676157000	-4.472781000	5.659501000
C	1.960460000	-5.699701000	4.026949000
C	1.020664000	-5.682813000	5.060735000

H	0.973923000	-2.337210000	5.681281000
H	3.294958000	-4.530882000	2.800644000
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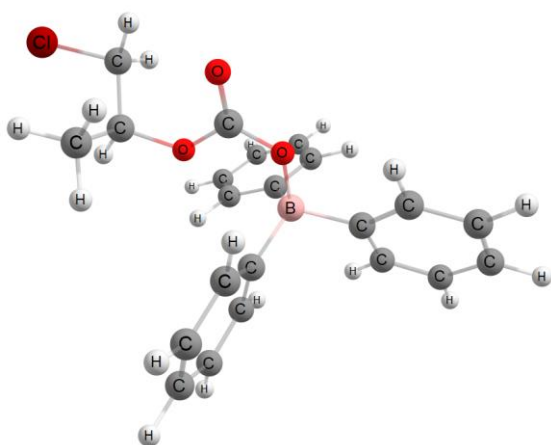


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C	5.054788000	0.585087000	-1.060664000
C	3.788959000	2.274752000	0.092892000
C	5.006450000	1.817510000	-0.409316000
H	3.956795000	-1.140951000	-1.709263000
H	1.692675000	1.882293000	0.353300000
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H	3.740837000	3.226346000	0.626013000
H	5.915018000	2.408766000	-0.277896000
C	0.039946000	-0.277766000	-0.020065000
C	-0.644392000	0.929476000	-0.250413000
C	-0.472103000	-1.110271000	0.985043000
C	-1.754047000	1.305840000	0.505556000
C	-1.590584000	-0.751862000	1.740073000
C	-2.232066000	0.463134000	1.510493000
H	-0.297082000	1.592807000	-1.049209000
H	0.033093000	-2.050168000	1.215523000
H	-2.251511000	2.257979000	0.307097000
H	-1.947115000	-1.421011000	2.525975000
H	-3.097296000	0.752896000	2.110028000

C	0.871919000	-0.775310000	-2.508418000
C	1.678047000	-0.358712000	-3.580948000
C	-0.390266000	-1.301350000	-2.843238000
C	1.272011000	-0.499806000	-4.910399000
C	-0.803393000	-1.460096000	-4.165533000
C	0.033147000	-1.063461000	-5.209358000
H	2.649547000	0.094988000	-3.375855000
H	-1.074386000	-1.586910000	-2.038249000
H	1.928194000	-0.163591000	-5.716274000
H	-1.786127000	-1.884400000	-4.382008000
H	-0.285553000	-1.179937000	-6.247343000
O	1.849219000	-2.157248000	-0.452564000
C	1.454996000	-3.403932000	-1.090921000
H	0.442717000	-3.197741000	-1.458056000
C	2.378131000	-3.758867000	-2.239047000
H	2.038505000	-4.705876000	-2.680986000
H	2.347946000	-2.977288000	-3.009548000
C	1.343740000	-4.507897000	-0.036417000
H	2.314646000	-4.943164000	0.219181000
H	0.866871000	-4.145849000	0.885231000
H	3.403461000	-3.876656000	-1.864948000
Cl	0.316023000	-5.828908000	-0.683113000
C	2.819086000	-2.270975000	0.626677000
O	3.732825000	-3.023123000	0.459304000
O	2.452791000	-1.548311000	1.593843000
B	2.905360000	-1.857508000	3.079811000
C	2.092197000	-0.786273000	3.984861000
C	1.442840000	0.331871000	3.441882000
C	2.037944000	-0.939795000	5.380561000
C	0.761196000	1.247028000	4.248581000
C	1.366666000	-0.030430000	6.196588000
C	0.719449000	1.070324000	5.630617000
H	1.459437000	0.479676000	2.359794000
H	2.531662000	-1.803119000	5.838723000
H	0.253339000	2.098219000	3.788518000
H	1.343263000	-0.181432000	7.278743000
H	0.185395000	1.782407000	6.263999000

C	4.497122000	-1.592124000	3.201531000
C	5.295153000	-2.194171000	4.185384000
C	5.118023000	-0.650409000	2.364598000
C	6.649815000	-1.882036000	4.325669000
C	6.469479000	-0.334330000	2.490630000
C	7.244699000	-0.950965000	3.474912000
H	4.846646000	-2.932754000	4.857567000
H	4.522627000	-0.149697000	1.594847000
H	7.244755000	-2.370814000	5.101283000
H	6.916690000	0.400211000	1.815715000
H	8.304455000	-0.706790000	3.578509000
C	2.395969000	-3.394190000	3.310625000
C	1.044291000	-3.646299000	3.609317000
C	3.203502000	-4.512948000	3.045157000
C	0.516105000	-4.939232000	3.617342000
C	2.689288000	-5.812320000	3.057513000
C	1.339284000	-6.030461000	3.334117000
H	0.388791000	-2.797346000	3.827711000
H	4.253832000	-4.353434000	2.789017000
H	-0.541839000	-5.096788000	3.840144000
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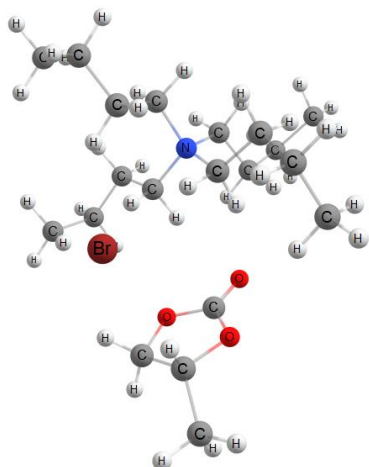


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C	2.909697000	2.554172000	-1.009110000
C	0.600444000	3.164769000	-0.915199000

C	3.272983000	3.871174000	-0.714906000
C	0.948958000	4.482847000	-0.622933000
C	2.293935000	4.844642000	-0.521265000
H	3.683516000	1.796718000	-1.151816000
H	-0.459286000	2.897483000	-0.977823000
H	4.329934000	4.138692000	-0.634168000
H	0.168737000	5.232863000	-0.469755000
H	2.574123000	5.875111000	-0.290391000
C	-0.012037000	0.065930000	-0.483755000
C	0.030775000	0.409649000	0.877805000
C	-1.032133000	-0.819766000	-0.870680000
C	-0.883721000	-0.097569000	1.803709000
C	-1.959122000	-1.329661000	0.039995000
C	-1.888569000	-0.969859000	1.386662000
H	0.806790000	1.100738000	1.219752000
H	-1.090177000	-1.124944000	-1.918948000
H	-0.813830000	0.192263000	2.855238000
H	-2.739185000	-2.015044000	-0.301482000
H	-2.610839000	-1.366571000	2.104172000
C	0.679176000	0.641641000	-3.084690000
C	1.590693000	0.328807000	-4.107082000
C	-0.606517000	1.030917000	-3.494824000
C	1.241107000	0.382336000	-5.457091000
C	-0.970776000	1.093370000	-4.841394000
C	-0.047511000	0.764023000	-5.833482000
H	2.611185000	0.039504000	-3.836796000
H	-1.351543000	1.283121000	-2.734139000
H	1.980031000	0.128062000	-6.221565000
H	-1.983579000	1.397346000	-5.118032000
H	-0.327635000	0.806806000	-6.888437000
O	1.426857000	-2.027725000	-2.038676000
C	1.453795000	-3.363588000	-2.512847000
H	0.394578000	-3.581250000	-2.716561000
C	2.250794000	-3.502854000	-3.800724000
H	2.147675000	-4.524949000	-4.190165000
H	1.865230000	-2.791744000	-4.544606000
C	1.896927000	-4.314926000	-1.402250000

H	2.977569000	-4.274610000	-1.242156000
H	1.368398000	-4.068533000	-0.473413000
H	3.310344000	-3.287539000	-3.612734000
Cl	1.463740000	-6.010140000	-1.831579000
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O	2.419509000	-0.184118000	-1.353039000

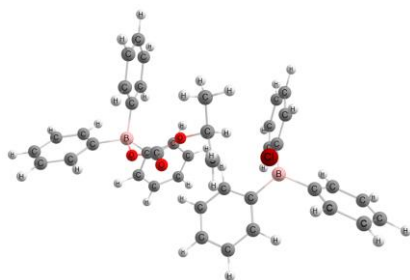
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C	2.957712000	1.877005000	0.044361000
C	1.792692000	4.319764000	-0.576849000
C	3.514343000	3.058543000	0.534494000
C	2.930511000	4.288922000	0.228635000
H	0.370989000	3.174210000	-1.718030000
H	3.425559000	0.919599000	0.287000000
H	1.329648000	5.276334000	-0.831304000
H	4.409958000	3.021236000	1.159626000
H	3.362564000	5.216422000	0.611085000
C	0.108471000	-0.059874000	-0.129333000
C	0.296365000	-1.262034000	0.566343000
C	-1.015475000	0.704855000	0.230427000
C	-0.588719000	-1.689167000	1.559458000
C	-1.909974000	0.289942000	1.215301000
C	-1.700226000	-0.915931000	1.887497000
H	1.161328000	-1.888035000	0.333533000

H	-1.190061000	1.658939000	-0.277054000
H	-0.407506000	-2.633213000	2.078795000
H	-2.773437000	0.911190000	1.465039000
H	-2.396046000	-1.246801000	2.661504000
C	0.459891000	0.649311000	-2.751204000
C	1.246054000	1.147993000	-3.804746000
C	-0.854262000	0.274241000	-3.066119000
C	0.755725000	1.256374000	-5.106842000
C	-1.363368000	0.391302000	-4.361634000
C	-0.557453000	0.878622000	-5.390604000
H	2.273415000	1.460836000	-3.591919000
H	-1.490446000	-0.136347000	-2.277629000
H	1.397728000	1.640637000	-5.903101000
H	-2.391821000	0.087994000	-4.572168000
H	-0.948744000	0.961946000	-6.406833000
O	1.160680000	-2.118848000	-2.388297000
C	1.330810000	-3.167706000	-3.368864000
H	0.612727000	-3.948235000	-3.108217000
C	1.073026000	-2.597710000	-4.747510000
H	1.153552000	-3.418563000	-5.470938000
H	0.076809000	-2.137079000	-4.789642000
C	2.743290000	-3.718607000	-3.210554000
H	3.457361000	-3.656980000	-4.022994000
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Cl	2.122664000	-5.741849000	-4.299754000
C	2.318759000	-1.577619000	-2.063386000
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O	3.347142000	-2.191158000	-2.430920000

TS3'_a

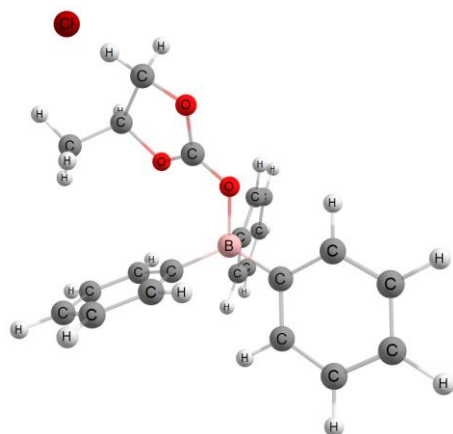


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C	0.938551000	0.631282000	-0.191612000
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C	-0.120924000	1.554565000	-0.156569000
C	2.058379000	1.999548000	1.498048000
C	-0.101866000	2.669532000	0.678515000
C	0.993981000	2.898287000	1.514407000
H	2.865661000	0.184397000	0.656095000
H	-0.988285000	1.389137000	-0.803745000
H	2.921599000	2.165620000	2.147532000
H	-0.944079000	3.365741000	0.679713000
H	1.015125000	3.770296000	2.171851000
C	-0.422433000	-1.599369000	-0.885226000
C	-0.952685000	-1.666007000	0.415300000
C	-1.019176000	-2.436083000	-1.845902000
C	-2.007916000	-2.519734000	0.745903000
C	-2.076789000	-3.291664000	-1.531597000
C	-2.575241000	-3.339456000	-0.229260000
H	-0.523152000	-1.027852000	1.192379000
H	-0.633085000	-2.428404000	-2.867937000
H	-2.386850000	-2.546404000	1.770306000
H	-2.503029000	-3.933423000	-2.306649000
H	-3.396598000	-4.013311000	0.023554000
C	0.970183000	-0.093007000	-2.736326000
C	2.222276000	0.202589000	-3.303690000
C	-0.155715000	0.179870000	-3.528458000
C	2.350857000	0.711404000	-4.595529000
C	-0.042855000	0.693571000	-4.822801000
C	1.213579000	0.955305000	-5.367488000
H	3.126678000	0.031935000	-2.710138000
H	-1.151685000	-0.026295000	-3.126511000
H	3.342827000	0.922105000	-5.003006000
H	-0.942993000	0.884833000	-5.411875000
H	1.306485000	1.350868000	-6.381168000
O	1.802271000	-2.894018000	-2.550080000
C	2.448821000	-3.823384000	-3.414019000
H	1.654877000	-4.506757000	-3.733941000

C	3.046528000	-3.103285000	-4.607474000
H	3.461888000	-3.842704000	-5.306401000
H	2.269986000	-2.512890000	-5.111672000
C	3.493696000	-4.600187000	-2.619760000
H	4.549398000	-4.506711000	-2.857029000
H	3.212872000	-5.133641000	-1.714163000
H	3.843781000	-2.420654000	-4.277875000
Cl	3.402053000	-6.472204000	-3.809055000
C	2.606209000	-2.417373000	-1.597352000
O	2.171860000	-1.456956000	-0.899000000
O	3.715925000	-2.953251000	-1.469434000
B	1.477532000	-7.348934000	-3.285934000
C	1.760521000	-8.923292000	-3.505038000
C	2.986400000	-9.557744000	-3.237069000
C	0.703656000	-9.747527000	-3.927821000
C	3.147639000	-10.936519000	-3.374845000
C	0.851753000	-11.128875000	-4.061811000
C	2.077732000	-11.731519000	-3.785736000
H	3.840326000	-8.952362000	-2.925163000
H	-0.262378000	-9.294387000	-4.164375000
H	4.117089000	-11.392769000	-3.162154000
H	0.005615000	-11.735695000	-4.391698000
H	2.201021000	-12.810985000	-3.895302000
C	0.441416000	-6.722379000	-4.350529000
C	-0.916773000	-6.606899000	-4.003531000
C	0.790392000	-6.363437000	-5.663366000
C	-1.873767000	-6.145538000	-4.909872000
C	-0.155599000	-5.892155000	-6.573701000
C	-1.494693000	-5.778455000	-6.199929000
H	-1.233335000	-6.878176000	-2.992525000
H	1.834636000	-6.444042000	-5.973423000
H	-2.918372000	-6.063363000	-4.601673000
H	0.155248000	-5.610516000	-7.582072000
H	-2.236204000	-5.403190000	-6.907816000
C	1.327295000	-6.852549000	-1.759822000
C	1.948034000	-7.548678000	-0.707777000
C	0.675946000	-5.651234000	-1.423909000

C	1.949626000	-7.057422000	0.598093000
C	0.670416000	-5.145397000	-0.122100000
C	1.316992000	-5.848724000	0.894026000
H	2.450232000	-8.495529000	-0.919819000
H	0.170280000	-5.064303000	-2.194133000
H	2.449742000	-7.620128000	1.389565000
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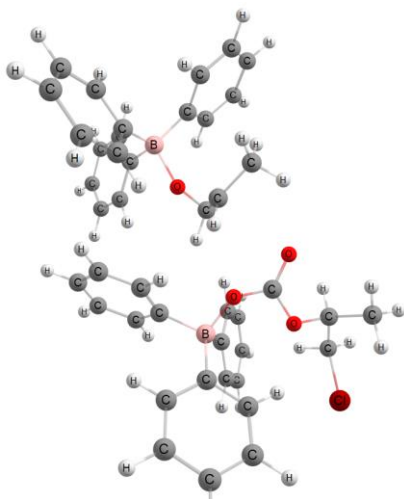


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C	1.270719000	3.172503000	-0.961450000
C	3.006122000	1.838755000	0.005816000
C	1.849740000	4.325616000	-0.429486000
C	3.598710000	2.984901000	0.537007000
C	3.020741000	4.236480000	0.322995000
H	0.363180000	3.262230000	-1.566245000
H	3.472121000	0.865760000	0.180040000
H	1.388904000	5.299755000	-0.609245000
H	4.517982000	2.901636000	1.121656000
H	3.481443000	5.136011000	0.736911000
C	0.090163000	-0.019692000	-0.179072000
C	0.393088000	-1.121449000	0.632910000
C	-1.127699000	0.634865000	0.074334000

C	-0.473753000	-1.561523000	1.635676000
C	-2.002438000	0.207190000	1.071442000
C	-1.679202000	-0.899662000	1.858513000
H	1.337319000	-1.654212000	0.490196000
H	-1.397617000	1.505821000	-0.530967000
H	-0.204456000	-2.427131000	2.245012000
H	-2.942039000	0.739228000	1.237230000
H	-2.361596000	-1.241467000	2.639358000
C	0.446926000	0.751676000	-2.790096000
C	1.178428000	1.422112000	-3.785854000
C	-0.789476000	0.207563000	-3.169371000
C	0.706881000	1.541808000	-5.094051000
C	-1.279185000	0.331012000	-4.470962000
C	-0.529953000	0.996997000	-5.440618000
H	2.144598000	1.863404000	-3.522725000
H	-1.374994000	-0.342682000	-2.428343000
H	1.304141000	2.064091000	-5.844873000
H	-2.244926000	-0.106842000	-4.733536000
H	-0.905809000	1.087751000	-6.461910000
O	1.079836000	-2.130900000	-2.387879000
C	1.342174000	-3.264203000	-3.299625000
H	0.771679000	-4.125904000	-2.947685000
C	0.951394000	-2.858783000	-4.698684000
H	1.142425000	-3.743134000	-5.322833000
H	-0.109641000	-2.578978000	-4.737793000
C	2.842245000	-3.478116000	-3.085401000
H	3.394907000	-3.627760000	-4.014103000
H	3.068485000	-4.298292000	-2.398597000
H	1.551722000	-1.998794000	-5.037631000
Cl	2.077489000	-5.995930000	-4.304334000

C	2.200896000	-1.559213000	-2.094812000
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O	3.258367000	-2.207514000	-2.479308000

Int7_a

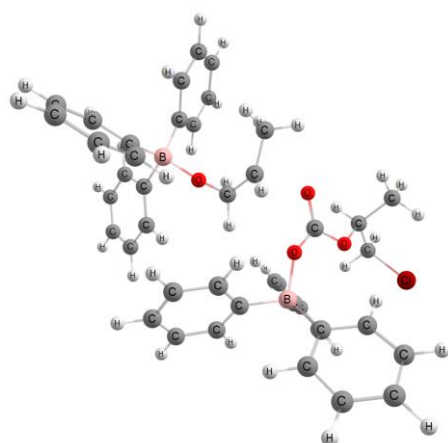


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C	3.406848000	1.254022000	-1.575544000
C	5.028842000	-0.363538000	-0.000628000
C	4.605397000	1.756708000	-1.058684000
C	5.419722000	0.951430000	-0.264245000
H	3.518186000	-1.873028000	-0.284150000
H	2.779214000	1.903598000	-2.192505000
H	5.668990000	-1.009554000	0.604657000
H	4.904039000	2.784861000	-1.278832000
H	6.362458000	1.334424000	0.131629000
C	0.461212000	-0.610819000	-0.537052000
C	0.793997000	-0.101506000	0.729057000
C	-0.852891000	-1.096967000	-0.686776000
C	-0.116273000	-0.088057000	1.790244000
C	-1.769338000	-1.091037000	0.364371000
C	-1.404391000	-0.587819000	1.614371000
H	1.796615000	0.300029000	0.895990000
H	-1.169738000	-1.475981000	-1.659394000
H	0.185931000	0.316891000	2.759208000

H	-2.778975000	-1.477103000	0.202510000
H	-2.119912000	-0.580698000	2.440013000
C	0.978699000	0.184555000	-3.103250000
C	1.649755000	0.058267000	-4.334408000
C	-0.128597000	1.044964000	-3.084197000
C	1.244090000	0.739776000	-5.481300000
C	-0.549008000	1.737156000	-4.224967000
C	0.134572000	1.588523000	-5.430930000
H	2.521846000	-0.600643000	-4.397704000
H	-0.685426000	1.169634000	-2.152286000
H	1.795397000	0.613625000	-6.416176000
H	-1.420901000	2.393115000	-4.170068000
H	-0.190716000	2.127724000	-6.323250000
O	-0.010918000	-2.417258000	-3.363267000
C	-0.618652000	-2.886811000	-4.553422000
H	0.165756000	-3.002374000	-5.320474000
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H	-2.056137000	-4.124412000	-3.533468000
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C	7.632514000	0.821605000	-3.263037000

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H	4.173044000	-1.569132000	-3.390354000
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TS4_a

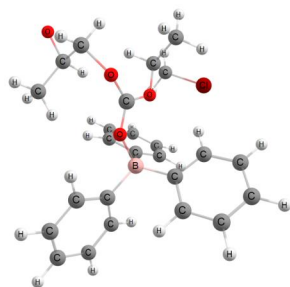


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C	-0.172565000	0.976961000	-3.174591000

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C	4.250709000	-5.160681000	-3.173316000
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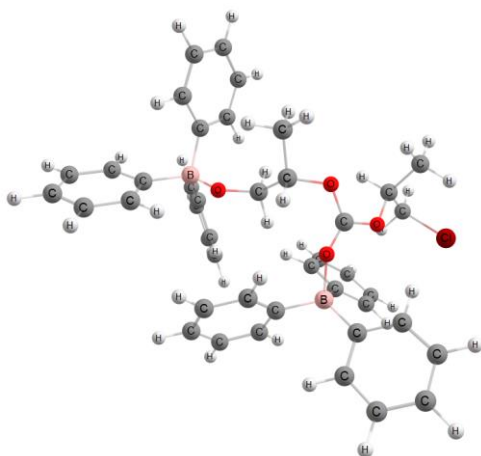
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C	1.550659000	-3.610761000	-2.553688000
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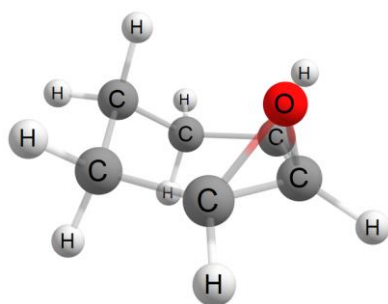
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C	0.333701000	0.980935000	-3.275931000
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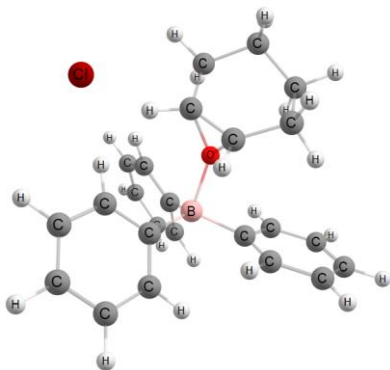
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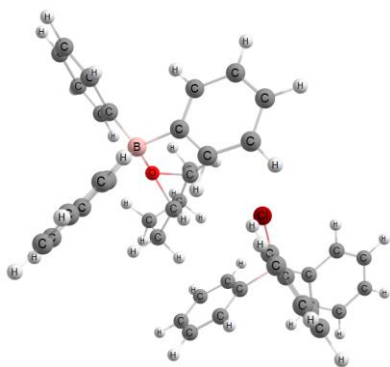
BPh₃_CHO



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C	2.047783000	2.120351000	-1.334354000
C	3.922937000	1.313542000	0.542315000
C	2.967475000	3.043064000	-0.831756000
C	3.916759000	2.639211000	0.106819000
H	3.024198000	-0.617704000	0.457351000
H	1.306978000	2.455684000	-2.067002000
H	4.636375000	0.977249000	1.297756000
H	2.940327000	4.081119000	-1.172630000
H	4.638327000	3.356536000	0.504992000
C	-0.260508000	-0.410503000	-0.347762000
C	-1.543656000	0.124506000	-0.560235000
C	-0.010947000	-0.966081000	0.923562000
C	-2.543672000	0.066665000	0.413506000
C	-1.011305000	-1.047796000	1.892921000
C	-2.286134000	-0.539434000	1.642018000
H	-1.767167000	0.620246000	-1.508246000
H	0.984026000	-1.321772000	1.219933000
H	-3.526233000	0.499601000	0.209811000
H	-0.766907000	-1.499457000	2.856768000
H	-3.066441000	-0.595886000	2.404694000
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C	1.387132000	0.376900000	-3.961333000
C	-0.708665000	-0.679567000	-3.516822000

C	1.124834000	0.338809000	-5.331393000
C	-0.985961000	-0.723860000	-4.885551000
C	-0.068652000	-0.210549000	-5.801303000
H	2.334730000	0.794633000	-3.612305000
H	-1.435962000	-1.108434000	-2.823183000
H	1.858588000	0.734836000	-6.037285000
H	-1.920713000	-1.166700000	-5.237360000
H	-0.279084000	-0.242685000	-6.872584000
Cl	2.977421000	-2.559118000	2.200844000
C	2.063074000	-2.872147000	-0.809689000
H	0.031160000	-2.923453000	-1.657911000
C	1.094200000	-2.934833000	-1.923469000
O	1.739144000	-1.695491000	-1.616178000
H	1.731174000	-2.816995000	0.232921000
C	3.485278000	-3.340242000	-0.987487000
H	4.116723000	-2.437847000	-0.982581000
H	3.750727000	-3.878402000	-0.066757000
H	3.292192000	-5.172453000	-2.125371000
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H	3.340845000	-2.480087000	-3.598295000
H	0.968211000	-2.924174000	-4.055435000
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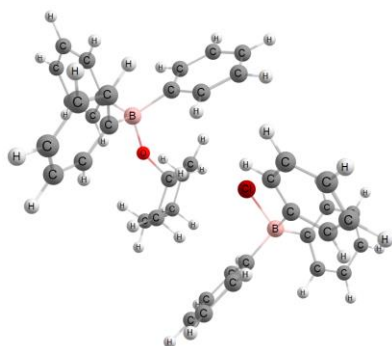
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C	4.334689000	1.892131000	-2.712921000
C	2.446504000	3.365915000	-2.489222000
C	3.789725000	3.169214000	-2.818869000
H	3.989652000	-0.172106000	-2.210239000
H	0.618870000	2.464416000	-1.802439000
H	5.382605000	1.722671000	-2.970862000
H	2.004363000	4.361419000	-2.571415000
H	4.403543000	4.006424000	-3.157325000
C	0.544216000	0.008625000	-0.007760000
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C	-0.508359000	-0.803946000	0.453233000
C	0.604309000	1.026632000	2.219706000
C	-0.983438000	-0.724980000	1.763783000
C	-0.427228000	0.194697000	2.652329000
H	1.904538000	1.571935000	0.596079000
H	-0.967434000	-1.528033000	-0.227959000
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C	0.696323000	-1.287561000	-3.801683000
C	-1.138427000	-0.231277000	-2.684888000
C	-0.127134000	-1.598419000	-4.882284000
C	-1.971271000	-0.525596000	-3.767373000
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H	1.753308000	-1.569714000	-3.838853000
H	-1.550987000	0.306995000	-1.827223000
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H	-3.018995000	-0.217728000	-3.746910000
H	-2.120572000	-1.458609000	-5.711246000
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C	1.774406000	-2.861408000	-1.088976000
O	2.216748000	-1.495471000	-1.335117000

H	2.086952000	-1.760508000	0.774277000
C	4.084690000	-2.440836000	0.026394000
H	4.609660000	-1.525034000	-0.292389000
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C	4.538162000	-3.659651000	-0.781552000
H	5.634502000	-3.654721000	-0.873013000
C	3.877978000	-3.726399000	-2.158937000
H	4.270155000	-4.584337000	-2.724395000
H	4.109668000	-2.816611000	-2.740768000
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C	0.723657000	-6.963131000	-0.905599000
C	3.420669000	-7.436591000	-1.378271000
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H	4.483727000	-7.620225000	-1.554174000
H	0.414845000	-7.542156000	-2.965532000
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C	-2.727150000	-6.471031000	1.781984000
C	-2.213201000	-4.203088000	1.173103000
C	-3.161412000	-5.197534000	1.415113000
H	-1.040812000	-7.747883000	2.174114000
H	-0.119613000	-3.687486000	1.128022000
H	-3.456145000	-7.259068000	1.986400000
H	-2.541201000	-3.200696000	0.884318000
H	-4.227625000	-4.979551000	1.323116000
C	1.551683000	-7.228822000	2.804374000

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C	1.967152000	-7.693222000	5.171363000
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H	1.688329000	-5.724970000	4.336354000
H	1.919407000	-10.591400000	3.394964000
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TS1_b

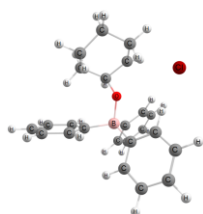


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C	1.606995000	2.212188000	-1.988168000
C	4.284169000	1.943807000	-2.660092000
C	2.340433000	3.332012000	-2.374759000
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H	5.338153000	1.827225000	-2.924896000
H	1.860091000	4.312742000	-2.413951000
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C	1.276608000	0.664191000	0.977351000
C	-0.445338000	-0.917487000	0.483286000
C	0.857535000	0.716449000	2.307760000
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H	2.128974000	1.273558000	0.664071000
H	-0.976494000	-1.565183000	-0.222528000
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H	-0.540875000	-0.040311000	3.776464000
C	0.173899000	-0.651328000	-2.632594000
C	0.548423000	-1.338986000	-3.799877000
C	-1.143095000	-0.166796000	-2.585194000
C	-0.342271000	-1.556870000	-4.850656000
C	-2.044081000	-0.369547000	-3.633425000
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H	1.577864000	-1.699789000	-3.884388000
H	-1.475548000	0.383407000	-1.700027000
H	-0.015598000	-2.100515000	-5.740418000
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C	2.595634000	-2.600677000	0.156973000
H	0.778270000	-2.947489000	-0.992806000
C	1.867814000	-2.845502000	-1.105467000
O	2.273238000	-1.535996000	-1.441062000
H	2.090522000	-1.972452000	0.891663000
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H	4.238090000	-2.817903000	-2.621755000
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C	-2.317658000	-4.205590000	0.989040000
C	-3.246945000	-5.201880000	1.286449000
H	-1.081961000	-7.711715000	2.058781000
H	-0.237208000	-3.673934000	0.857746000
H	-3.507819000	-7.250975000	1.917863000
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H	1.179715000	-5.405455000	4.114801000
H	2.415620000	-10.192334000	3.681665000
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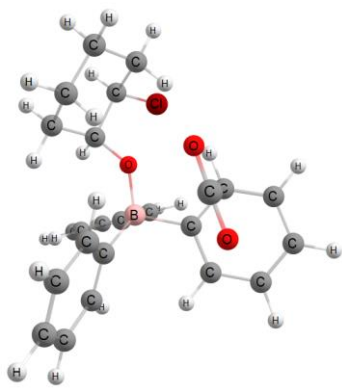
TS1'_b



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H	2.636991000	4.244297000	-1.265340000
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H	-1.533374000	0.974591000	-1.376707000
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C	0.527621000	-0.166974000	-2.973527000
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C	1.191625000	0.145992000	-5.314439000
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C	-0.044463000	-0.333088000	-5.755467000
H	2.440408000	0.587978000	-3.616065000
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C	1.279981000	-2.793222000	-1.729250000
O	1.875399000	-1.570965000	-1.397110000
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C	3.487397000	-3.801378000	-0.985968000
H	4.011918000	-2.834931000	-0.891768000
H	3.893779000	-4.420002000	-0.175831000
H	3.238619000	-5.357265000	-2.486914000
C	3.683821000	-4.350217000	-2.406216000
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H	3.499155000	-2.423699000	-3.371386000
H	1.063495000	-2.595157000	-3.864740000
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Int2_b

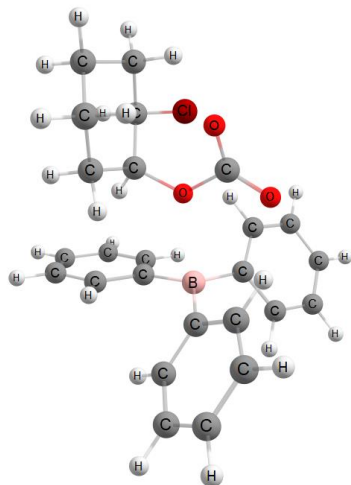


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C	1.456353000	2.371067000	-1.854886000
C	3.847960000	1.689950000	-0.628802000
C	2.351116000	3.371637000	-1.469699000
C	3.556913000	3.035686000	-0.852983000
H	3.178261000	-0.349498000	-0.844161000
H	0.521963000	2.659053000	-2.347046000
H	4.788177000	1.408154000	-0.147288000
H	2.107774000	4.421233000	-1.655074000
H	4.261739000	3.814196000	-0.551753000

C	-0.379637000	-0.348333000	-0.705180000
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C	-0.770600000	-1.623378000	-0.259835000
C	-1.758176000	0.592022000	1.089467000
C	-1.618685000	-1.795321000	0.838865000
C	-2.114713000	-0.686036000	1.523064000
H	-0.617676000	1.759723000	-0.305936000
H	-0.388724000	-2.493833000	-0.799088000
H	-2.137365000	1.471691000	1.616069000
H	-1.895963000	-2.803151000	1.160003000
H	-2.773365000	-0.814630000	2.385428000
C	-0.220814000	0.147088000	-3.357615000
C	0.335698000	0.847294000	-4.443013000
C	-1.530518000	-0.329312000	-3.535398000
C	-0.363697000	1.062916000	-5.632934000
C	-2.244537000	-0.122260000	-4.717056000
C	-1.663887000	0.578425000	-5.774536000
H	1.354991000	1.236496000	-4.351987000
H	-2.000787000	-0.886369000	-2.720388000
H	0.108041000	1.610961000	-6.452878000
H	-3.261409000	-0.511129000	-4.814234000
H	-2.219185000	0.744552000	-6.700900000
C	1.798333000	-1.302081000	1.361303000
O	1.448710000	-0.369159000	1.946473000
O	2.200171000	-2.254453000	0.836297000
Cl	-0.330195000	-3.740049000	-3.404542000
C	1.462376000	-3.528180000	-3.357972000
H	1.400646000	-1.539288000	-4.162099000
C	1.827652000	-2.038670000	-3.273485000
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H	1.823300000	-3.936439000	-4.314220000
C	2.050127000	-4.308757000	-2.193124000
H	1.661804000	-3.866058000	-1.262561000
H	1.725396000	-5.358976000	-2.243185000
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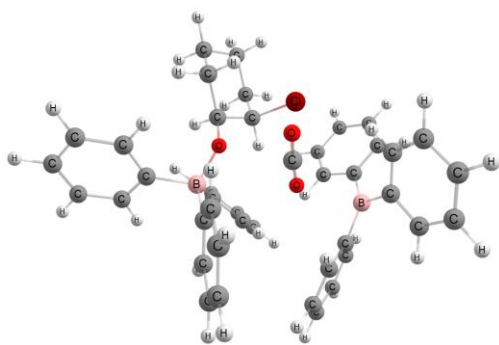
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C	2.485003000	3.736998000	-1.626092000
C	3.336353000	3.567036000	-0.535957000
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H	0.905253000	2.886275000	-2.809584000
H	3.903823000	2.268143000	1.093054000
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C	-1.260407000	-1.111531000	-0.149814000
C	-2.174616000	1.011684000	1.408305000
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H	-2.631954000	-2.330478000	0.974954000
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C	-0.112312000	0.275912000	-3.024032000
C	0.782453000	0.515384000	-4.084060000
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H	1.159787000	0.436279000	-6.207585000
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O	1.436707000	-1.672876000	-1.540482000
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H	4.618100000	-5.103822000	-3.154201000
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H	5.070767000	-2.705627000	-3.729535000
H	4.492520000	-2.872857000	-2.046510000
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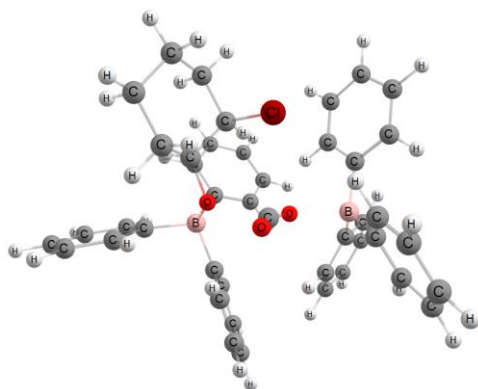


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H	0.552357000	0.700903000	-1.308962000
H	5.403382000	1.644995000	-1.706998000
H	1.525154000	1.214657000	-3.529968000
H	3.969128000	1.676864000	-3.749860000
C	2.723503000	-0.254473000	2.266777000
C	3.726820000	-1.137363000	1.828068000
C	2.577938000	-0.139037000	3.662817000
C	4.537449000	-1.850737000	2.716042000
C	3.356846000	-0.868091000	4.564632000
C	4.347607000	-1.730188000	4.093137000
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H	1.828920000	0.552473000	4.061702000
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H	4.971826000	-2.293449000	4.790773000
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C	4.495465000	-3.950997000	-0.777014000
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C	4.775672000	-2.773069000	-1.494811000
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C	6.002049000	-2.123579000	-1.369109000
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C	2.469485000	-5.035115000	-4.689339000
C	0.322848000	-4.919281000	-3.589959000
C	1.076354000	-5.036839000	-4.758783000
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C	2.689996000	-4.680956000	1.677637000
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H	-3.565624000	-0.897325000	3.011171000
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TS2_b



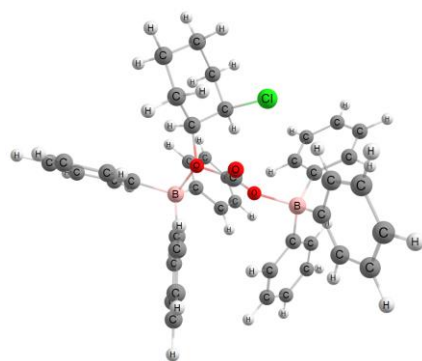
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C	4.010535000	1.305284000	-2.597739000
H	4.536123000	1.104372000	0.757475000
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H	5.711887000	1.699961000	-1.326218000
H	2.135739000	0.865138000	-3.575523000
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C	2.512973000	-0.207200000	3.741031000
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H	2.840398000	2.348794000	2.989342000
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C	5.304328000	-4.300711000	-0.259985000

C	4.615978000	-2.334498000	-1.451422000
C	6.636261000	-3.884049000	-0.327985000
C	5.941222000	-1.906740000	-1.517153000
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H	3.824395000	-4.180652000	-3.357329000
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H	0.034293000	-0.191257000	2.760823000
C	-0.191685000	-0.907550000	1.949429000
O	0.668843000	-0.605545000	0.881754000
H	1.125986000	-2.450345000	2.739741000

C	-0.730001000	-2.372456000	3.903539000
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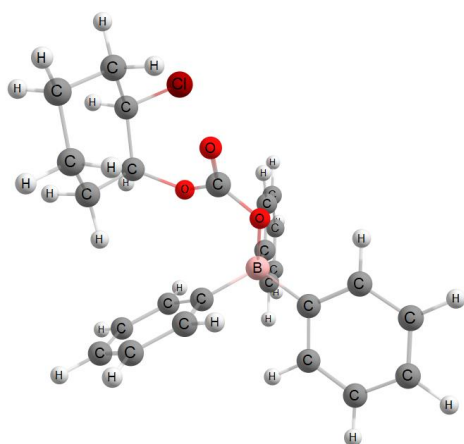


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C	4.101696567	1.396616572	-2.613659418
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H	1.089871346	0.271801493	-1.525955565
H	5.796005969	1.826315221	-1.344380664
H	2.243167604	0.894856336	-3.592733265
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C	2.934181189	-0.418613497	2.327060799
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C	2.569174593	-0.409447334	3.686398300
C	4.811177174	-1.865656234	2.952215129

C	3.284295975	-1.117306029	4.655092002
C	4.415552439	-1.847239096	4.289282793
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H	2.961212836	-1.092357508	5.698429098
H	4.981715423	-2.401232128	5.041096729
C	1.293800513	1.687772414	1.652374311
C	1.793123913	2.507950912	2.676050612
C	0.180628267	2.174698468	0.943379768
C	1.194958489	3.728537697	3.002275766
C	-0.434104704	3.382390121	1.267236571
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O	1.997586431	-2.411072089	-0.009102907
B	2.596271806	-3.771398823	-0.623318351
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C	5.193298126	-4.244095234	-0.290349777
C	4.582213386	-2.246477521	-1.456744214
C	6.546347682	-3.923813845	-0.439051261
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C	1.983139468	-4.688149198	-4.423923496

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C	0.630305175	-5.015378576	-4.440274530
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C	1.873530099	-6.167929619	0.328722710
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C	1.662827602	-7.070902339	1.376702212
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C	-0.045615095	-2.287247971	2.593213624
H	0.036834033	-0.184622156	2.598007968
C	-0.200491689	-0.957340558	1.852836794
O	0.791262771	-0.730180373	0.831824134
H	1.010811677	-2.486410617	2.814084719
C	-0.899180692	-2.223697982	3.859050427
H	-0.802169291	-3.173726688	4.403131151
H	-0.478086908	-1.431436101	4.502081587
H	-2.938651165	-1.804767583	4.462407430
C	-2.365158085	-1.925324434	3.530699299
H	-2.783583298	-2.796435391	3.004020354
C	-2.519625561	-0.680133196	2.650537285
H	-2.245136548	0.216606107	3.234037237
H	-3.573166492	-0.554162478	2.359516696
H	-1.941157142	-1.536390837	0.716299636
C	-1.635000297	-0.731134227	1.397972252
H	-1.695354478	0.216621603	0.849139253

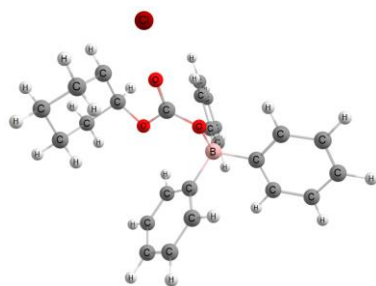
Int5_b



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C	1.197427000	3.215781000	-1.694182000
C	2.829569000	3.606489000	0.513270000
C	1.520438000	4.513097000	-1.289804000
C	2.340301000	4.715159000	-0.179897000
H	2.889823000	1.453326000	0.642767000
H	0.573372000	3.076228000	-2.582942000
H	3.479938000	3.750396000	1.380107000
H	1.137490000	5.370558000	-1.849298000
H	2.601205000	5.727143000	0.138809000
C	-0.127289000	0.149253000	-0.639586000
C	-1.296014000	0.917909000	-0.782232000
C	-0.209823000	-0.957359000	0.219543000
C	-2.482829000	0.599139000	-0.122099000
C	-1.389490000	-1.286390000	0.891354000
C	-2.535863000	-0.510974000	0.722696000
H	-1.273074000	1.799931000	-1.430324000
H	0.667738000	-1.591732000	0.359662000
H	-3.369957000	1.222151000	-0.262644000
H	-1.412097000	-2.160701000	1.546880000
H	-3.461161000	-0.766789000	1.244358000
C	1.106826000	0.441050000	-3.064096000
C	2.206558000	0.801390000	-3.863462000
C	-0.021535000	-0.054049000	-3.735378000

C	2.188598000	0.672682000	-5.253603000
C	-0.057645000	-0.181718000	-5.126750000
C	1.049744000	0.180859000	-5.894482000
H	3.102848000	1.193863000	-3.372695000
H	-0.890949000	-0.361058000	-3.147087000
H	3.064756000	0.959302000	-5.840728000
H	-0.954265000	-0.572202000	-5.615100000
H	1.026714000	0.080233000	-6.982075000
C	2.682712000	-1.493675000	-1.424684000
O	2.421538000	-0.310022000	-0.981251000
O	3.766692000	-2.031216000	-1.382182000
Cl	1.441179000	-4.663119000	-0.401789000
C	2.064893000	-4.559727000	-2.088448000
H	0.525283000	-3.375906000	-2.945569000
C	1.599160000	-3.247255000	-2.747594000
O	1.581299000	-2.097956000	-1.929175000
H	1.536071000	-5.356576000	-2.634664000
C	3.555296000	-4.871491000	-2.130129000
H	4.082263000	-4.180113000	-1.464259000
H	3.700348000	-5.899582000	-1.763216000
H	3.606083000	-5.487543000	-4.207616000
C	4.081933000	-4.726185000	-3.561014000
H	5.162794000	-4.934191000	-3.575618000
C	3.794137000	-3.334302000	-4.126090000
H	4.154667000	-3.266243000	-5.164827000
H	4.332096000	-2.583073000	-3.534281000
H	2.072440000	-2.011103000	-4.431481000
C	2.293183000	-3.038421000	-4.102825000
H	1.793980000	-3.712329000	-4.821749000

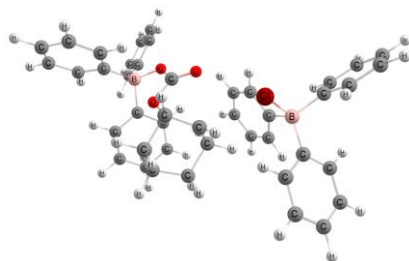
TS3_b



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C	1.283529000	3.326112000	-1.541153000
C	2.723812000	3.479846000	0.824371000
C	1.507841000	4.567989000	-0.943599000
C	2.232769000	4.650865000	0.245020000
H	2.875676000	1.333505000	0.682432000
H	0.730884000	3.281841000	-2.484894000
H	3.295217000	3.530322000	1.754670000
H	1.120775000	5.476553000	-1.411826000
H	2.416000000	5.619944000	0.714910000
C	0.060770000	0.081776000	-0.976727000
C	-1.177460000	0.673888000	-1.281939000
C	0.029136000	-1.000208000	-0.080034000
C	-2.378257000	0.202021000	-0.751421000
C	-1.166762000	-1.492741000	0.448653000
C	-2.380270000	-0.894283000	0.113830000
H	-1.200805000	1.530759000	-1.963316000
H	0.942326000	-1.509462000	0.247330000
H	-3.319595000	0.689819000	-1.017378000
H	-1.123493000	-2.354328000	1.119052000
H	-3.319035000	-1.273599000	0.524098000
C	1.431883000	0.737320000	-3.267012000
C	2.493798000	1.371972000	-3.933144000
C	0.456111000	0.134284000	-4.075429000
C	2.586536000	1.400709000	-5.325871000
C	0.529064000	0.161683000	-5.469791000
C	1.598811000	0.795258000	-6.103355000
H	3.269811000	1.859644000	-3.335138000
H	-0.378446000	-0.383149000	-3.593799000
H	3.430342000	1.901211000	-5.807540000
H	-0.251587000	-0.317428000	-6.066482000
H	1.661386000	0.818593000	-7.193874000
C	2.640823000	-1.485246000	-1.347707000
O	2.621133000	-0.229294000	-1.175329000
O	3.339077000	-2.282280000	-0.719847000

Cl	1.848523000	-4.175178000	0.890204000
C	2.696837000	-4.061455000	-1.551705000
H	0.676816000	-3.424100000	-1.460493000
C	1.531146000	-3.337162000	-2.146590000
O	1.835236000	-1.966809000	-2.317383000
H	2.410626000	-5.010152000	-1.103283000
C	3.954537000	-4.144895000	-2.363322000
H	4.360823000	-3.156170000	-2.605710000
H	4.722357000	-4.707767000	-1.816295000
H	3.195558000	-5.874172000	-3.463197000
C	3.557764000	-4.853613000	-3.675787000
H	4.453056000	-4.956497000	-4.307052000
C	2.465713000	-4.057426000	-4.393539000
H	2.209529000	-4.530441000	-5.353399000
H	2.837820000	-3.045196000	-4.620288000
H	0.456967000	-3.297193000	-3.993053000
C	1.216173000	-3.938379000	-3.522487000
H	0.764815000	-4.930658000	-3.363877000

TS3'_b



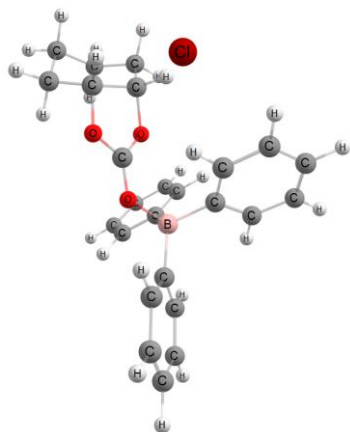
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C	2.172264000	2.904488000	-2.210708000
C	0.877780000	4.094748000	-0.064710000
C	2.470445000	4.223962000	-1.863939000
C	1.822585000	4.826245000	-0.786298000
H	-0.155981000	2.214917000	0.147438000
H	2.709382000	2.439997000	-3.043837000
H	0.368926000	4.552701000	0.786978000
H	3.220042000	4.780952000	-2.431320000
H	2.056639000	5.855490000	-0.505495000

C	-0.456037000	0.694684000	-2.984708000
C	-0.369109000	1.435619000	-4.177330000
C	-1.686694000	0.068433000	-2.733351000
C	-1.425678000	1.515895000	-5.083877000
C	-2.757716000	0.146324000	-3.626844000
C	-2.629844000	0.863666000	-4.814893000
H	0.553551000	1.982787000	-4.393595000
H	-1.831427000	-0.485664000	-1.801976000
H	-1.313852000	2.100501000	-6.000139000
H	-3.700884000	-0.351720000	-3.389016000
H	-3.463597000	0.926514000	-5.517381000
C	2.126323000	-0.143527000	-2.541488000
C	3.117512000	-0.555934000	-1.631227000
C	2.370783000	-0.414467000	-3.895791000
C	4.275821000	-1.218684000	-2.037454000
C	3.539808000	-1.055683000	-4.322302000
C	4.496220000	-1.468546000	-3.395427000
H	2.971847000	-0.355748000	-0.564980000
H	1.623932000	-0.130431000	-4.641452000
H	5.008411000	-1.532655000	-1.288430000
H	3.696789000	-1.244887000	-5.387155000
H	5.405393000	-1.976001000	-3.725322000
C	0.166923000	-1.296027000	-0.457853000
O	0.375408000	-0.053120000	-0.637651000
O	-0.095264000	-1.867390000	0.578697000
Cl	0.183214000	-4.659238000	2.359490000
C	0.742901000	-4.064080000	-0.394750000
H	-1.134832000	-3.532884000	-1.256797000
C	-0.057244000	-3.387954000	-1.427736000
O	0.264189000	-2.047933000	-1.609207000
H	0.352069000	-5.013164000	-0.021498000
C	2.163758000	-3.822227000	-0.313609000
H	2.428827000	-2.755991000	-0.353856000
H	2.630228000	-4.315818000	0.544828000
H	2.533252000	-5.601525000	-1.560441000
C	2.653222000	-4.510004000	-1.653442000
H	3.729864000	-4.294831000	-1.701683000

C	1.918414000	-3.970478000	-2.873803000
H	2.260832000	-4.493181000	-3.779413000
H	2.152752000	-2.904168000	-3.001759000
H	-0.144881000	-3.656477000	-3.546203000
C	0.408394000	-4.128733000	-2.722153000
H	0.111354000	-5.187708000	-2.668681000
B	1.933401000	-4.756992000	3.319469000
C	2.645193000	-6.159709000	2.899027000
C	2.409021000	-6.848734000	1.699351000
C	3.630264000	-6.704305000	3.743448000
C	3.120576000	-7.996741000	1.343606000
C	4.351920000	-7.848455000	3.401820000
C	4.102712000	-8.501598000	2.194106000
H	1.621053000	-6.487457000	1.032627000
H	3.830932000	-6.213667000	4.700608000
H	2.899932000	-8.505494000	0.401745000
H	5.109594000	-8.237687000	4.085973000
H	4.661463000	-9.400126000	1.924214000
C	1.561308000	-4.723808000	4.897150000
C	2.175554000	-3.837183000	5.792869000
C	0.642817000	-5.640964000	5.438942000
C	1.893458000	-3.861164000	7.162706000
C	0.349048000	-5.671250000	6.799744000
C	0.977752000	-4.778193000	7.672093000
H	2.891118000	-3.105377000	5.408325000
H	0.141210000	-6.339409000	4.762837000
H	2.389765000	-3.154776000	7.832387000
H	-0.373852000	-6.393482000	7.186814000
H	0.750801000	-4.798011000	8.740355000
C	2.786957000	-3.461435000	2.825661000
C	4.162489000	-3.524897000	2.550186000
C	2.155231000	-2.221839000	2.618344000
C	4.869396000	-2.419282000	2.064831000
C	2.845840000	-1.114529000	2.127392000
C	4.211555000	-1.209751000	1.843418000
H	4.693608000	-4.470736000	2.689802000
H	1.080595000	-2.139962000	2.788477000

H	5.937552000	-2.507476000	1.850967000
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Int6_b

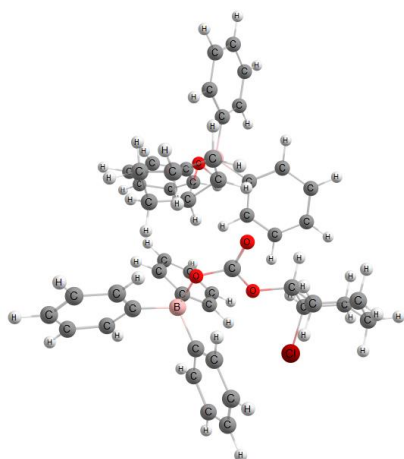


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C	2.427537000	2.139169000	0.268933000
C	1.421864000	3.369247000	-1.521423000
C	2.756508000	3.332138000	0.911706000
C	1.737148000	4.570560000	-0.882604000
C	2.410647000	4.556888000	0.337874000
H	2.696564000	1.187090000	0.733516000
H	0.907475000	3.397531000	-2.486741000
H	3.281973000	3.307479000	1.869346000
H	1.460000000	5.521943000	-1.343124000
H	2.663900000	5.493317000	0.839925000
C	-0.048973000	0.152630000	-0.989324000
C	-1.267069000	0.813650000	-1.230086000
C	-0.101057000	-0.975285000	-0.156187000
C	-2.470571000	0.358848000	-0.692058000
C	-1.300975000	-1.455796000	0.373717000
C	-2.494006000	-0.787189000	0.107705000
H	-1.272059000	1.708016000	-1.862343000

H	0.782911000	-1.558269000	0.125763000
H	-3.397877000	0.897845000	-0.902907000
H	-1.250498000	-2.370822000	0.969886000
H	-3.438520000	-1.153682000	0.516735000
C	1.312070000	0.798319000	-3.289606000
C	2.408096000	1.369304000	-3.959441000
C	0.292513000	0.260418000	-4.089006000
C	2.489479000	1.401267000	-5.352140000
C	0.355756000	0.293928000	-5.483793000
C	1.456985000	0.864326000	-6.122261000
H	3.217560000	1.805901000	-3.366231000
H	-0.566570000	-0.207246000	-3.600921000
H	3.357800000	1.851300000	-5.839452000
H	-0.457285000	-0.132812000	-6.076062000
H	1.510765000	0.890852000	-7.213028000
C	2.460406000	-1.492951000	-1.534684000
O	2.493504000	-0.289780000	-1.260953000
O	3.272654000	-2.338861000	-0.966612000
Cl	1.023069000	-4.155990000	0.890162000
C	3.055247000	-3.652434000	-1.544082000
H	0.928180000	-3.666326000	-1.373417000
C	1.666407000	-3.470140000	-2.171503000
O	1.656783000	-2.030459000	-2.404612000
H	2.957917000	-4.346373000	-0.696188000
C	4.193593000	-3.932066000	-2.523688000
H	4.489182000	-2.977307000	-2.989852000
H	5.070283000	-4.302494000	-1.973175000
H	3.516359000	-5.879342000	-3.206454000
C	3.775767000	-4.895597000	-3.634711000
H	4.623616000	-5.059363000	-4.316344000

C	2.568936000	-4.334711000	-4.386602000
H	2.313255000	-4.970521000	-5.247246000
H	2.816741000	-3.336826000	-4.786449000
H	0.504297000	-3.760526000	-3.928765000
C	1.372769000	-4.229811000	-3.444182000
H	1.058228000	-5.239941000	-3.135837000

Int7_b



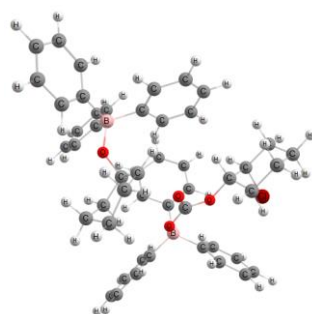
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C	1.456806000	-2.051940000	1.307845000
C	2.123059000	-2.855752000	2.246655000
C	0.526851000	-1.129681000	1.817513000
C	1.887764000	-2.740665000	3.619300000
C	0.279021000	-1.006635000	3.184141000
C	0.963005000	-1.812954000	4.096122000
H	2.850209000	-3.587994000	1.885129000
H	-0.012700000	-0.483094000	1.118259000
H	2.428805000	-3.381399000	4.320313000
H	-0.449614000	-0.275329000	3.542418000
H	0.775363000	-1.717946000	5.167926000
C	0.444952000	-3.125381000	-0.875986000
C	0.523827000	-4.526899000	-0.923739000
C	-0.768274000	-2.553461000	-1.286933000
C	-0.528089000	-5.313984000	-1.390056000
C	-1.832900000	-3.328034000	-1.753207000
C	-1.715100000	-4.715437000	-1.816211000

H	1.444058000	-5.019178000	-0.591945000
H	-0.878428000	-1.465280000	-1.259824000
H	-0.422106000	-6.401440000	-1.424304000
H	-2.757362000	-2.843557000	-2.077077000
H	-2.540246000	-5.325684000	-2.189982000
C	1.865135000	-0.778352000	-1.059682000
C	1.499061000	-0.570311000	-2.402411000
C	2.466607000	0.310935000	-0.403449000
C	1.711028000	0.652522000	-3.044770000
C	2.722034000	1.527192000	-1.042763000
C	2.333661000	1.705141000	-2.371079000
H	1.026891000	-1.389585000	-2.951803000
H	2.745052000	0.204200000	0.648987000
H	1.391702000	0.782414000	-4.082681000
H	3.229504000	2.334531000	-0.508007000
H	2.525698000	2.654576000	-2.876468000
C	3.512962000	-3.540671000	-1.479069000
O	3.009795000	-3.009588000	-0.418906000
O	4.563354000	-4.154513000	-1.515467000
Cl	0.579862000	-3.565868000	-4.602952000
C	2.354333000	-3.374033000	-4.905847000
H	4.219898000	-3.777875000	-3.967389000
C	3.154037000	-3.999904000	-3.771062000
O	2.761417000	-3.349830000	-2.581356000
H	2.527399000	-2.291355000	-4.907830000
C	2.723526000	-4.013953000	-6.239092000
H	2.123727000	-3.558676000	-7.040346000
H	3.781622000	-3.768168000	-6.435851000
H	2.866073000	-5.966817000	-7.166104000
C	2.545722000	-5.532466000	-6.206786000
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C	9.475537000	1.072943000	-2.894930000
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H	11.338645000	1.789965000	-3.712244000
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C	6.071887000	2.646550000	-2.192764000
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H	5.192747000	4.607033000	-2.402907000

H	5.987911000	3.295853000	1.620998000
H	5.113996000	5.027727000	0.053292000
C	6.556323000	-0.272079000	-3.282786000
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C	4.626254000	-0.552940000	-4.764901000
C	5.399108000	-1.277134000	-5.673001000
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H	4.563368000	0.501417000	-2.903451000
H	7.360200000	-2.083506000	-6.087212000
H	3.573914000	-0.342686000	-4.967065000
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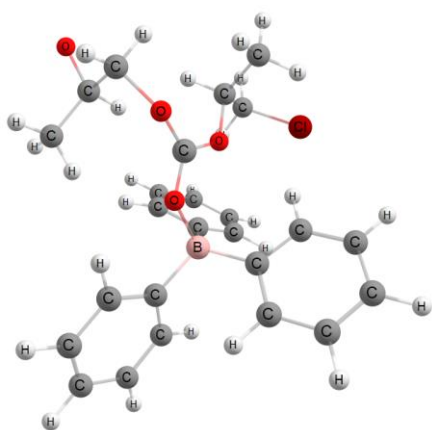
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C	5.597666000	-1.308894000	-0.459980000
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H	8.542275000	-1.271192000	-3.843148000
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TS4'_b

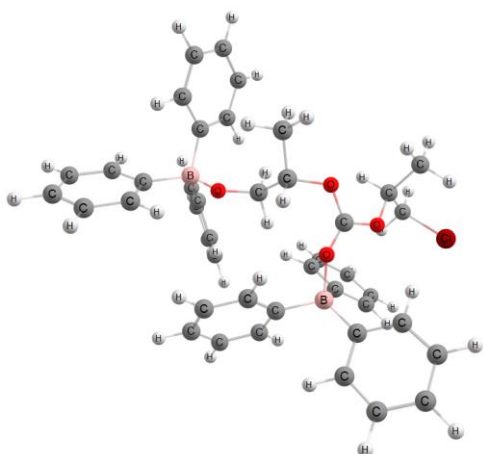


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H	1.789386000	0.729167000	1.540197000
H	1.673197000	2.771968000	-2.238148000
H	2.838742000	2.710695000	2.586370000
H	2.677993000	4.773592000	-1.190309000
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H	-3.411114000	1.557688000	0.173094000
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H	-3.895186000	-0.527765000	1.457617000
C	0.913652000	0.271015000	-2.692703000
C	2.104332000	0.372935000	-3.436264000
C	-0.279605000	0.163566000	-3.422620000
C	2.107567000	0.369979000	-4.832400000
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H	3.057746000	0.454179000	-2.904894000
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H	3.054098000	0.444886000	-5.372332000
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H	0.898226000	0.271586000	-6.625210000
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C	0.724923000	-3.502077000	-2.718629000

O	0.905993000	-2.416613000	-1.809338000
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C	2.816800000	-3.641203000	-4.210310000
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H	1.199650000	-2.162289000	-4.318617000
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C	4.601085000	-2.585542000	-0.968665000
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H	5.593740000	-1.783662000	2.266007000
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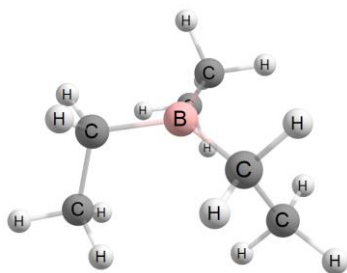
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C	-1.884300000	-3.575956000	-1.358750000
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H	1.591587000	-4.977311000	-0.406008000
H	-1.051850000	-1.632189000	-0.963314000
H	-0.211737000	-6.519797000	-1.070771000
H	-2.865402000	-3.175089000	-1.623372000
H	-2.455415000	-5.633633000	-1.703779000
C	1.730414000	-0.785367000	-1.082643000
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C	1.478614000	0.450546000	-3.181080000

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H	2.480756000	2.367731000	-3.304925000
C	3.491441000	-3.187767000	-1.503207000
O	3.037825000	-2.868814000	-0.393336000
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C	2.497808000	-3.465430000	-6.217323000
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H	4.178108000	-1.599355000	1.104840000
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H	4.931161000	-0.891884000	-1.032526000
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C	9.371526000	1.278580000	-2.674404000
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C	6.239976000	1.992963000	-0.082344000
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C	5.688676000	3.237088000	0.229890000
C	5.320288000	4.115547000	-0.790837000
H	6.188566000	2.195342000	-3.461241000
H	5.233557000	4.406199000	-2.929072000
H	5.549354000	3.526310000	1.274572000
H	4.888006000	5.090373000	-0.554427000
C	6.664442000	-0.516676000	-3.142371000
C	7.526860000	-1.260764000	-3.968259000
C	5.344976000	-0.360195000	-3.612369000
C	7.116014000	-1.800811000	-5.189729000
C	4.924953000	-0.868924000	-4.844954000
C	5.812744000	-1.593274000	-5.644084000
H	8.562563000	-1.407264000	-3.646793000

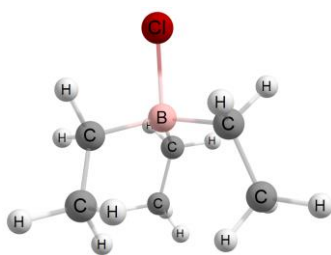
H	4.628181000	0.214200000	-3.017080000
H	7.823831000	-2.363891000	-5.803123000
H	3.901144000	-0.679084000	-5.184031000
H	5.503092000	-1.974705000	-6.620962000
H	6.549544000	1.320723000	0.722074000

BEt₃



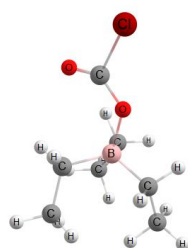
B	-0.660493000	1.976126000	0.089339000
C	0.915098000	1.940853000	-0.037191000
H	1.347272000	0.979189000	0.282516000
H	1.335346000	2.719955000	0.623914000
C	-1.459022000	0.643541000	0.383677000
H	-1.068367000	0.204439000	1.319339000
H	-2.536350000	0.817443000	0.535217000
C	-1.445694000	3.317651000	-0.200446000
H	-2.118121000	3.518220000	0.653015000
H	-0.779379000	4.189700000	-0.297178000
C	1.335538000	2.251057000	-1.484715000
H	0.949203000	3.228677000	-1.810619000
H	2.428845000	2.272558000	-1.598546000
H	0.948631000	1.495685000	-2.186349000
C	-2.302097000	3.166934000	-1.470191000
H	-3.006579000	2.326439000	-1.378061000
H	-2.891646000	4.071625000	-1.676827000
H	-1.677292000	2.974737000	-2.356288000
C	-1.245211000	-0.368528000	-0.755587000
H	-0.176430000	-0.589683000	-0.897001000
H	-1.757074000	-1.321448000	-0.558900000
H	-1.629272000	0.016773000	-1.712994000

BEt₃_Cl⁻



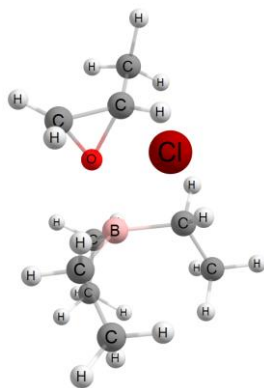
B	-0.571348000	1.784390000	0.318827000
C	0.959213000	1.741157000	-0.273776000
H	1.394259000	0.734688000	-0.113583000
H	1.572510000	2.423957000	0.340433000
C	-1.412178000	0.393393000	0.089308000
H	-1.043187000	-0.343308000	0.824693000
H	-2.477931000	0.553303000	0.347226000
C	-1.404348000	3.138465000	-0.090751000
H	-2.138210000	3.332349000	0.711417000
H	-0.724300000	4.013277000	-0.081261000
C	1.130021000	2.141165000	-1.743590000
H	0.778968000	3.173591000	-1.907308000
H	2.181242000	2.100220000	-2.082720000
H	0.547103000	1.498165000	-2.423026000
C	-2.158415000	3.094774000	-1.424563000
H	-2.903941000	2.282270000	-1.422304000
H	-2.702862000	4.031503000	-1.643313000
H	-1.487781000	2.904939000	-2.278390000
C	-1.314644000	-0.236196000	-1.304735000
H	-0.267368000	-0.482836000	-1.546192000
H	-1.896125000	-1.171633000	-1.397455000
H	-1.669341000	0.443597000	-2.096518000
Cl1	-0.341947000	1.914565000	2.297878000

BEt₃_CO₂



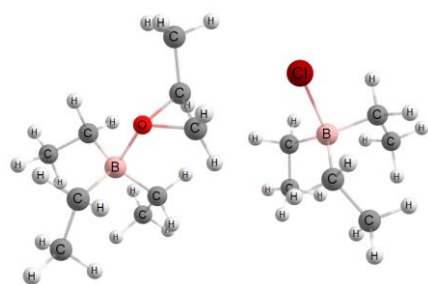
B	-0.559116000	1.785589000	0.402943000
C	0.974378000	1.735105000	-0.175122000
H	1.408801000	0.729303000	-0.033751000
H	1.589886000	2.409492000	0.451282000
C	-1.412969000	0.402316000	0.194940000
H	-1.052380000	-0.336707000	0.931970000
H	-2.480405000	0.576333000	0.435275000
C	-1.381813000	3.142224000	-0.003316000
H	-2.103955000	3.337955000	0.810407000
H	-0.699358000	4.014865000	-0.004423000
C	1.144552000	2.167724000	-1.634307000
H	0.788314000	3.200213000	-1.783880000
H	2.195563000	2.134757000	-1.971508000
H	0.565543000	1.530579000	-2.322431000
C	-2.152934000	3.099135000	-1.324980000
H	-2.897576000	2.286339000	-1.315403000
H	-2.698623000	4.036029000	-1.535032000
H	-1.491147000	2.911105000	-2.185789000
C	-1.301666000	-0.237701000	-1.191687000
H	-0.252361000	-0.487839000	-1.417472000
H	-1.884319000	-1.171405000	-1.282311000
H	-1.646739000	0.437597000	-1.991378000
O	-0.427159000	1.973854000	2.002726000
C	0.233086000	1.187647000	2.728598000
O	0.869267000	0.199559000	2.533814000
Cl	0.138696000	1.776355000	4.504359000

BEt₃_PO



C	0.163883000	2.597600000	2.788029000
C	-0.540207000	1.324512000	2.982349000
O	0.426745000	1.479418000	1.931829000
H	-1.576796000	1.376240000	2.618217000
H	-0.460081000	3.383037000	2.344815000
B	0.230704000	1.263501000	0.202998000
C	1.659013000	0.545106000	-0.111131000
H	1.649190000	-0.510310000	0.224668000
H	2.438351000	1.044189000	0.494518000
C	-1.074366000	0.306282000	0.138694000
H	-1.016660000	-0.422520000	0.972608000
H	-1.980098000	0.912730000	0.318976000
C	0.060054000	2.764760000	-0.369042000
H	-0.627090000	3.310825000	0.298199000
H	1.030178000	3.301948000	-0.381823000
C	2.084336000	0.611335000	-1.581160000
H	2.171649000	1.658691000	-1.911325000
H	3.056985000	0.124565000	-1.768771000
H	1.346076000	0.131937000	-2.243332000
C	-0.587972000	2.829068000	-1.756977000
H	-1.619033000	2.447578000	-1.696995000
H	-0.651752000	3.862380000	-2.136951000
H	-0.051673000	2.233869000	-2.515347000
C	-1.208224000	-0.499908000	-1.157434000
H	-0.346767000	-1.173902000	-1.301088000
H	-2.116063000	-1.126350000	-1.170845000
H	-1.255132000	0.153448000	-2.042437000
Cl	-2.875011000	3.221331000	1.695718000
C	-0.157377000	0.315449000	4.024026000
H	0.908084000	0.403505000	4.280512000
H	-0.760089000	0.468689000	4.930664000
H	-0.345683000	-0.703069000	3.655216000
H	1.025554000	2.860255000	3.410408000

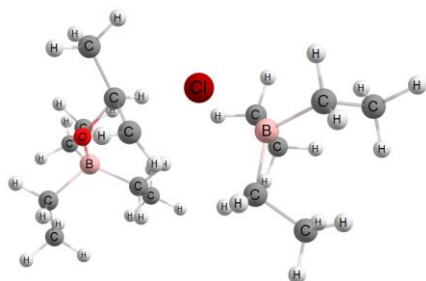
Int1_c



C	-0.866509000	2.604288000	2.780701000
C	0.102266000	1.576489000	3.134576000
O	0.050547000	2.092967000	1.782884000
H	-0.283372000	0.554839000	3.200309000
H	-1.909951000	2.320059000	2.634823000
B	-0.385168000	1.153291000	0.454300000
C	0.874027000	0.122398000	0.398705000
H	0.745847000	-0.697714000	1.131533000
H	1.777856000	0.673359000	0.721279000
C	-1.828954000	0.486933000	0.804298000
H	-1.888124000	0.207565000	1.873374000
H	-2.646405000	1.217626000	0.653314000
C	-0.418623000	2.289540000	-0.706334000
H	-0.898660000	3.192933000	-0.284742000
H	0.610305000	2.598285000	-0.970963000
C	1.158099000	-0.476987000	-0.981810000
H	1.376983000	0.317596000	-1.712673000
H	2.021052000	-1.162953000	-0.976254000
H	0.295819000	-1.040594000	-1.370454000
C	-1.180968000	1.900867000	-1.976178000
H	-2.232322000	1.667453000	-1.745147000
H	-1.184078000	2.704726000	-2.730613000
H	-0.752979000	1.006247000	-2.455389000
C	-2.142194000	-0.779093000	-0.001043000
H	-1.391059000	-1.561273000	0.192270000
H	-3.127161000	-1.200724000	0.254579000
H	-2.136431000	-0.589855000	-1.085916000
Cl	-1.425641000	2.755707000	5.819399000
C	1.342937000	1.883136000	3.911400000

H	1.686399000	2.902662000	3.690708000
H	1.081605000	1.822732000	4.976856000
H	2.145057000	1.170358000	3.675300000
H	-0.668958000	3.637975000	3.066549000
B	-3.319123000	2.015853000	5.654406000
C	-3.130821000	0.556832000	4.935663000
H	-2.773821000	-0.184109000	5.676891000
H	-2.316066000	0.634841000	4.194785000
C	-3.836118000	1.932811000	7.203111000
H	-2.985784000	1.603340000	7.825468000
H	-4.094121000	2.944866000	7.570785000
C	-4.093538000	3.135292000	4.743990000
H	-3.714658000	4.129513000	5.038744000
H	-3.823151000	3.023573000	3.674674000
C	-4.364014000	0.006160000	4.211240000
H	-4.681371000	0.691574000	3.407942000
H	-4.179837000	-0.975976000	3.741869000
H	-5.225356000	-0.111584000	4.888167000
C	-5.621383000	3.151576000	4.867170000
H	-5.923785000	3.350088000	5.908196000
H	-6.091666000	3.927945000	4.238766000
H	-6.072397000	2.187596000	4.582486000
C	-5.009917000	0.980567000	7.458814000
H	-4.741929000	-0.051051000	7.177560000
H	-5.318055000	0.956891000	8.518943000
H	-5.901215000	1.247771000	6.868833000

TS1_c

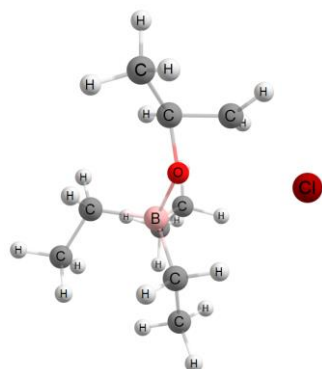


C	-0.837735000	2.747431000	3.247108000
C	0.163625000	1.694331000	3.086346000
O	0.145616000	2.217518000	1.781848000

H	-0.247703000	0.676067000	3.149401000
H	-1.857130000	2.551652000	2.920039000
B	-0.364866000	1.328546000	0.570323000
C	0.682593000	0.057982000	0.536583000
H	0.400101000	-0.711526000	1.282934000
H	1.670442000	0.438292000	0.862181000
C	-1.921574000	0.894762000	0.867743000
H	-2.044678000	0.633537000	1.937299000
H	-2.593811000	1.761114000	0.702010000
C	-0.197487000	2.362405000	-0.688007000
H	-0.498954000	3.361564000	-0.320925000
H	0.874047000	2.461635000	-0.950204000
C	0.870547000	-0.619437000	-0.823882000
H	1.233523000	0.104937000	-1.570627000
H	1.597927000	-1.449103000	-0.794059000
H	-0.074281000	-1.030040000	-1.213121000
C	-1.004449000	2.058703000	-1.952610000
H	-2.084251000	2.039082000	-1.733029000
H	-0.850188000	2.807717000	-2.748662000
H	-0.750311000	1.075743000	-2.380633000
C	-2.440456000	-0.304344000	0.068287000
H	-1.842480000	-1.203379000	0.288281000
H	-3.490623000	-0.548200000	0.301026000
H	-2.375284000	-0.136435000	-1.018006000
C1	-1.447871000	2.830445000	5.468718000
C	1.479203000	1.835064000	3.809533000
H	1.880707000	2.846820000	3.655503000
H	1.322724000	1.668497000	4.884506000
H	2.205051000	1.106046000	3.423955000
H	-0.485429000	3.774611000	3.292789000
B	-3.384026000	1.898496000	5.463200000
C	-3.034361000	0.383577000	5.002250000
H	-2.579280000	-0.180012000	5.838023000
H	-2.260694000	0.421067000	4.216030000
C	-3.808371000	2.091545000	7.019212000
H	-2.914826000	1.939074000	7.648960000
H	-4.131387000	3.132923000	7.205637000

C	-4.207761000	2.794059000	4.385309000
H	-3.886507000	3.846205000	4.475796000
H	-3.967004000	2.487735000	3.349027000
C	-4.229431000	-0.394152000	4.438358000
H	-4.631515000	0.108016000	3.543789000
H	-3.958818000	-1.419520000	4.137439000
H	-5.054727000	-0.471806000	5.164237000
C	-5.729959000	2.742002000	4.566382000
H	-6.018407000	3.117851000	5.561039000
H	-6.262971000	3.352007000	3.818449000
H	-6.119005000	1.714719000	4.485475000
C	-4.895479000	1.121578000	7.498125000
H	-4.555452000	0.078088000	7.401480000
H	-5.165725000	1.279833000	8.555763000
H	-5.821579000	1.210764000	6.908707000

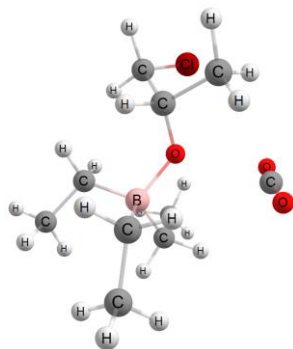
TS1'_c



C	-1.411316000	1.618485000	3.001279000
C	-0.165344000	0.874473000	2.800342000
O	0.063669000	1.838534000	1.809342000
H	-0.293487000	-0.141126000	2.389508000
H	-2.339117000	1.239734000	2.581163000
B	0.050771000	1.408494000	0.288672000
C	1.290984000	0.317216000	0.168003000
H	0.974442000	-0.697204000	0.487868000
H	2.080932000	0.623093000	0.882194000
C	-1.418144000	0.755888000	-0.050430000
H	-1.711867000	0.072236000	0.773147000
H	-2.171260000	1.564565000	-0.043397000

C	0.340152000	2.834917000	-0.454375000
H	-0.232877000	3.579369000	0.124528000
H	1.408679000	3.108317000	-0.340017000
C	1.932174000	0.216563000	-1.219107000
H	2.323277000	1.197180000	-1.533815000
H	2.771517000	-0.500787000	-1.259692000
H	1.203037000	-0.091991000	-1.984825000
C	-0.061169000	2.960070000	-1.925880000
H	-1.143397000	2.790272000	-2.046301000
H	0.152742000	3.960947000	-2.341333000
H	0.453087000	2.227571000	-2.571402000
C	-1.509149000	-0.061489000	-1.342109000
H	-0.832998000	-0.932338000	-1.305755000
H	-2.525105000	-0.449473000	-1.534894000
H	-1.216716000	0.529695000	-2.223629000
Cl	-2.364755000	3.654552000	1.999592000
C	0.881630000	0.908886000	3.892470000
H	0.999597000	1.940522000	4.253751000
H	0.601761000	0.258586000	4.735965000
H	1.846535000	0.571124000	3.488542000
H	-1.494189000	2.304023000	3.841679000

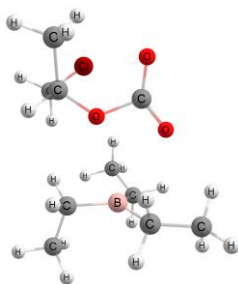
Int2_c



C	0.804196000	0.590093000	2.673446000
C	0.594939000	1.940398000	1.982601000
C	0.618342000	3.093049000	2.986395000
H	1.539339000	3.092214000	3.591820000
H	0.540068000	4.046551000	2.447288000
O	-0.572579000	1.953635000	1.258023000
H	1.485378000	2.050078000	1.323646000

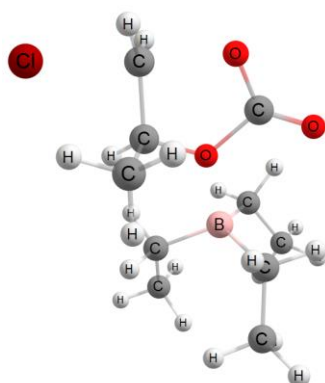
H	0.750152000	-0.213055000	1.931380000
B	-0.519350000	1.766157000	-0.260479000
C	0.245218000	0.339805000	-0.610483000
H	-0.263659000	-0.494978000	-0.089257000
H	1.279110000	0.358453000	-0.207956000
C	-2.099136000	1.722056000	-0.710557000
H	-2.569677000	2.692546000	-0.450332000
H	-2.198903000	1.653262000	-1.810516000
C	0.285497000	3.061395000	-0.923774000
H	0.181780000	3.909322000	-0.219937000
H	1.374793000	2.858464000	-0.989680000
C	0.330008000	0.016525000	-2.102831000
H	0.912469000	0.784677000	-2.637389000
H	0.802846000	-0.958161000	-2.320665000
H	-0.672740000	0.002813000	-2.562075000
C	-0.204642000	3.530457000	-2.297249000
H	-1.256600000	3.853087000	-2.244609000
H	0.375801000	4.378315000	-2.704893000
H	-0.165374000	2.721264000	-3.045203000
C	-2.881456000	0.582380000	-0.053639000
H	-2.686286000	0.565523000	1.030028000
H	-3.974145000	0.648778000	-0.203596000
H	-2.560096000	-0.393758000	-0.454802000
Cl	-0.481993000	0.238298000	3.889093000
C	-2.421654000	3.556444000	1.995843000
O	-1.939529000	4.488719000	1.502569000
O	-3.006001000	2.724526000	2.549723000
H	-0.243277000	2.996339000	3.664923000
H	1.761786000	0.548245000	3.211620000

TS2'_c



C	-0.300756000	0.539635000	3.035370000
C	0.508304000	1.763198000	2.608096000
C	0.951984000	2.617691000	3.795849000
H	1.673051000	2.042041000	4.400286000
H	1.435002000	3.532654000	3.430223000
O	-0.105442000	2.414909000	1.539885000
H	1.424354000	1.317034000	2.168219000
H	-0.556290000	-0.055578000	2.149997000
B	-0.575057000	1.890745000	-1.166793000
C	0.592675000	0.858040000	-0.814898000
H	0.354981000	0.285886000	0.094889000
H	1.535239000	1.394599000	-0.614513000
C	-2.073640000	1.374205000	-1.205542000
H	-2.751470000	2.238881000	-1.213064000
H	-2.195693000	0.867747000	-2.188052000
C	-0.129730000	3.241225000	-1.868615000
H	0.461357000	3.767985000	-1.098104000
H	0.596125000	2.987183000	-2.668234000
C	0.781935000	-0.114416000	-1.988898000
H	0.993478000	0.422320000	-2.928456000
H	1.611339000	-0.821495000	-1.824750000
H	-0.128898000	-0.711074000	-2.159126000
C	-1.234699000	4.155143000	-2.388265000
H	-1.871313000	4.443904000	-1.540261000
H	-0.840788000	5.070310000	-2.860305000
H	-1.864809000	3.644168000	-3.135341000
C	-2.462345000	0.424603000	-0.073398000
H	-2.346456000	0.940959000	0.891723000
H	-3.506700000	0.080934000	-0.148292000
H	-1.823547000	-0.475184000	-0.057315000
Cl	-1.861419000	0.947669000	3.821912000
C	-1.103487000	3.470413000	1.694382000
O	-1.691333000	3.633933000	0.624760000
O	-1.173094000	4.010574000	2.788392000
H	0.094834000	2.919371000	4.404791000
H	0.265497000	-0.075151000	3.749066000

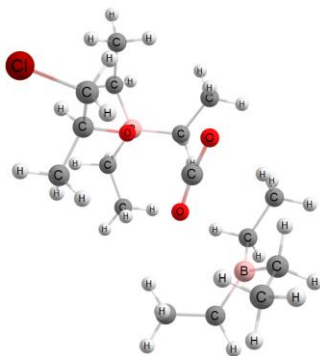
TS2_conc_c



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H	1.451774000	-2.481125000	-2.057069000
C	3.544113000	-1.944904000	-1.906088000
H	3.853868000	-2.747775000	-2.588361000
H	3.443038000	-1.004120000	-2.460825000
C	2.353282000	-3.670517000	-0.537331000
H	3.308436000	-4.169330000	-0.439079000
H	1.474706000	-4.139358000	-0.106571000
H	4.299126000	-1.818457000	-1.115201000
Cl	2.085391000	-4.964961000	-2.410223000
O	2.175099000	-0.662903000	1.745916000
C	2.260372000	-1.565995000	0.962796000
O	2.738465000	-2.727107000	1.049377000
C	0.564763000	-0.146020000	-2.427197000
H	1.430253000	-0.204573000	-3.113492000
H	0.068388000	-1.131062000	-2.479459000
C	-0.438774000	0.874135000	-2.980062000
H	-0.051451000	1.903119000	-2.944106000
H	-1.369748000	0.860416000	-2.392505000
H	-0.711188000	0.661790000	-4.026927000

C	2.225329000	1.209641000	-0.675553000
H	2.291036000	1.488892000	0.388666000
H	3.179268000	0.696483000	-0.894052000
C	2.164035000	2.473293000	-1.539101000
H	1.244917000	3.051887000	-1.353271000
H	2.176806000	2.227270000	-2.613551000
H	3.014873000	3.149541000	-1.351239000
C	-0.271523000	0.316142000	0.107161000
H	-1.131464000	-0.269028000	-0.271753000
H	-0.017419000	-0.103654000	1.091286000
C	-0.703608000	1.770844000	0.324428000
H	-0.994075000	2.268281000	-0.614982000
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Int3_c

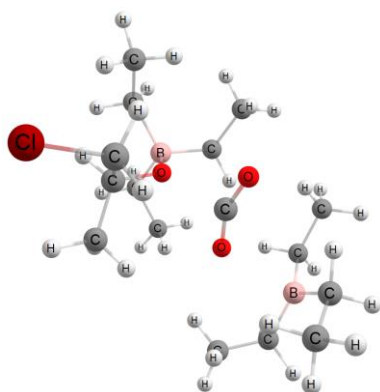


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H	2.174473000	-2.635432000	-3.072460000
C	3.757486000	-3.404496000	-1.829435000
H	4.201568000	-4.045106000	-2.606004000
H	4.297659000	-2.449535000	-1.795763000
C	1.508317000	-4.480567000	-2.211742000
H	1.696859000	-5.119379000	-1.338033000
H	0.434692000	-4.280483000	-2.287032000

H	3.876930000	-3.894254000	-0.849248000
Cl	1.978363000	-5.436563000	-3.671204000
C	1.655153000	-3.502895000	1.201386000
O	0.630596000	-4.017593000	1.044927000
O	2.684838000	-3.065479000	1.513968000
B	3.048891000	-2.288484000	4.060385000
C	2.775082000	-0.111532000	-1.386593000
H	3.350573000	-0.478813000	-2.260654000
H	2.545219000	0.945186000	-1.625622000
C	3.652432000	-0.174531000	-0.135437000
H	3.776006000	-1.221532000	0.187948000
H	3.174683000	0.358215000	0.704123000
H	4.659065000	0.263004000	-0.264612000
C	0.469164000	-0.668895000	-2.640744000
H	-0.075973000	0.280651000	-2.471026000
H	1.135970000	-0.452254000	-3.499324000
C	-0.534179000	-1.741929000	-3.081574000
H	-1.115269000	-2.133622000	-2.232496000
H	-0.023373000	-2.604371000	-3.540177000
H	-1.255901000	-1.376416000	-3.834035000
C	0.556414000	-0.520427000	0.095578000
H	1.153257000	-0.852972000	0.968402000
H	0.538040000	0.585384000	0.169780000
C	-0.870225000	-1.053384000	0.236315000
H	-0.889277000	-2.150463000	0.133865000
H	-1.522360000	-0.644063000	-0.553170000
H	-1.340682000	-0.803210000	1.204936000
C	4.624913000	-2.077365000	4.119357000
H	4.856044000	-1.012673000	4.290765000
H	5.037977000	-2.634486000	4.980382000
C	5.348028000	-2.534404000	2.840063000
H	4.999560000	-1.966242000	1.966619000
H	5.158713000	-3.595786000	2.625147000
H	6.436490000	-2.395553000	2.925521000
C	2.407194000	-3.677546000	4.471320000
H	2.179006000	-3.527372000	5.549257000
H	1.417013000	-3.809120000	4.003652000

C	3.253511000	-4.938154000	4.297642000
H	4.245227000	-4.827205000	4.762887000
H	3.420036000	-5.147539000	3.230187000
H	2.777030000	-5.826933000	4.738327000
C	2.139996000	-1.030782000	3.766961000
H	2.409736000	-0.259614000	4.514738000
H	2.506124000	-0.611008000	2.810055000
C	0.625689000	-1.219201000	3.715425000
H	0.234790000	-1.598870000	4.673499000
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TS2_c

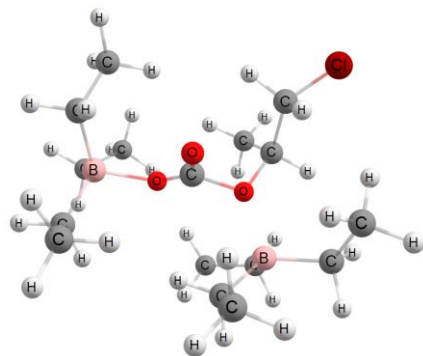


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H	2.235580000	-2.766969000	-2.812183000
C	3.867450000	-3.364861000	-1.537946000
H	4.321971000	-4.037448000	-2.280114000
H	4.363264000	-2.386948000	-1.584933000
C	1.667006000	-4.572748000	-1.812565000
H	1.940383000	-5.175493000	-0.936409000
H	0.581990000	-4.429900000	-1.824146000
H	4.031064000	-3.780414000	-0.531664000
Cl	2.105363000	-5.541008000	-3.269113000
C	1.718422000	-3.107626000	0.991739000
O	0.730918000	-3.741205000	1.020259000
O	2.722717000	-2.680619000	1.442846000
B	2.972206000	-2.386314000	3.879218000

C	2.752282000	-0.081408000	-1.484378000
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H	2.474673000	0.918429000	-1.871346000
C	3.658337000	0.078819000	-0.263041000
H	3.882505000	-0.902772000	0.184551000
H	3.155529000	0.666817000	0.522370000
H	4.617203000	0.580872000	-0.482942000
C	0.445562000	-0.882951000	-2.595858000
H	-0.135137000	0.058799000	-2.546520000
H	1.085256000	-0.763344000	-3.492673000
C	-0.519738000	-2.047460000	-2.849682000
H	-1.031682000	-2.363840000	-1.927835000
H	0.011407000	-2.931819000	-3.237755000
H	-1.298175000	-1.806757000	-3.594745000
C	0.569983000	-0.343516000	0.084633000
H	1.160652000	-0.549998000	0.998476000
H	0.564163000	0.761390000	0.003669000
C	-0.867464000	-0.824221000	0.299090000
H	-0.911961000	-1.920782000	0.394817000
H	-1.506841000	-0.547623000	-0.555631000
H	-1.333104000	-0.397051000	1.204907000
C	4.557775000	-2.227314000	3.976850000
H	4.813774000	-1.180109000	4.212275000
H	4.897134000	-2.829961000	4.841649000
C	5.353280000	-2.658188000	2.736038000
H	5.097309000	-2.031311000	1.871642000
H	5.127813000	-3.695418000	2.450255000
H	6.438382000	-2.582139000	2.908045000
C	2.286014000	-3.791126000	4.145066000
H	2.049537000	-3.764301000	5.230629000
H	1.303664000	-3.836488000	3.646984000
C	3.093749000	-5.047078000	3.823542000
H	4.085584000	-5.026845000	4.302660000
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H	2.585419000	-5.967746000	4.148822000
C	2.099128000	-1.064215000	3.850246000
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H	2.482122000	-0.453434000	3.011593000
C	0.582033000	-1.210088000	3.754753000
H	0.177581000	-1.763579000	4.617522000
H	0.286624000	-1.762653000	2.849286000
H	0.071373000	-0.236014000	3.712308000

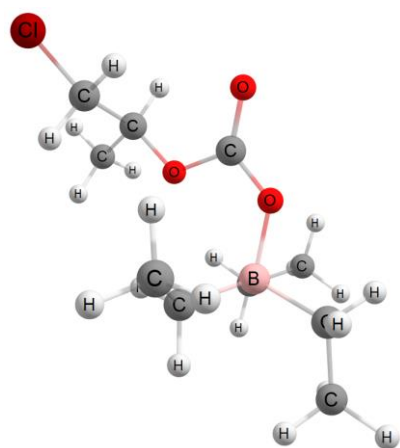
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H	2.371742000	-2.949974000	-2.352124000
C	3.978523000	-3.447378000	-0.990843000
H	4.450146000	-4.162156000	-1.679570000
H	4.468806000	-2.469668000	-1.085470000
C	1.767697000	-4.668829000	-1.215507000
H	2.056499000	-5.220268000	-0.311970000
H	0.685230000	-4.514746000	-1.208009000
H	4.113032000	-3.798682000	0.041787000
Cl	2.176623000	-5.699642000	-2.629200000
C	1.651404000	-2.724278000	0.891425000
O	0.655372000	-3.347459000	1.138440000
O	2.621221000	-2.316253000	1.580340000
B	2.786837000	-2.435454000	3.190324000
C	2.830746000	-0.100467000	-1.459765000
H	3.415458000	-0.733201000	-2.156502000
H	2.599518000	0.809155000	-2.047892000
C	3.683410000	0.271293000	-0.246839000
H	3.872374000	-0.609128000	0.386632000
H	3.158315000	0.998144000	0.392554000
H	4.654568000	0.715121000	-0.521535000

C	0.546656000	-1.101728000	-2.489200000
H	-0.047508000	-0.179654000	-2.636099000
H	1.203491000	-1.148830000	-3.378531000
C	-0.399064000	-2.310674000	-2.505826000
H	-0.833752000	-2.504055000	-1.513544000
H	0.128426000	-3.228186000	-2.812389000
H	-1.231662000	-2.186754000	-3.217234000
C	0.587687000	-0.115581000	0.072242000
H	1.130406000	-0.232674000	1.028305000
H	0.640981000	0.971123000	-0.135709000
C	-0.880892000	-0.503631000	0.267916000
H	-0.981135000	-1.564825000	0.541390000
H	-1.462893000	-0.343775000	-0.654829000
H	-1.360613000	0.084837000	1.066865000
C	4.388710000	-2.177643000	3.434940000
H	4.567915000	-1.092102000	3.554756000
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C	5.361457000	-2.696207000	2.372834000
H	5.194749000	-2.183594000	1.413414000
H	5.232374000	-3.773672000	2.184020000
H	6.418846000	-2.538931000	2.647978000
C	2.262702000	-3.905505000	3.662986000
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H	2.989227000	-5.052577000	1.951885000
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C	1.927071000	-1.205878000	3.830025000
H	2.268210000	-1.081119000	4.876528000
H	2.231629000	-0.273207000	3.316483000
C	0.402032000	-1.322524000	3.810687000
H	0.063311000	-2.207320000	4.372792000
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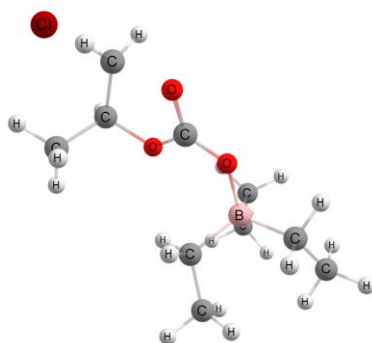
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C	-4.414336000	3.816804000	1.533296000
H	-4.943515000	2.943348000	1.112046000
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C	-5.391005000	2.833744000	3.862819000
H	-6.320362000	3.406928000	3.677592000
H	-5.542804000	1.857662000	3.367962000
C	-4.934552000	5.979901000	4.049658000
H	-5.736269000	5.527819000	4.657233000
H	-4.656773000	6.933151000	4.533230000
H	-5.385608000	6.231450000	3.075150000
C	-5.212823000	2.620985000	5.366859000
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H	-6.029436000	2.041979000	5.833849000
H	-4.269354000	2.088209000	5.569549000
C	-3.162147000	4.091527000	0.699220000
H	-3.377452000	4.294910000	-0.365033000
H	-2.602762000	4.956307000	1.091861000
H	-2.467845000	3.234806000	0.728140000
O	-3.504711000	1.089496000	2.064561000
C	-3.225716000	-0.133267000	1.419603000
H	-2.648350000	-0.785929000	2.092439000
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H	-5.127862000	-0.071405000	0.411220000
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H	-2.891044000	0.825547000	-0.498140000
H	-1.427786000	0.656241000	0.538976000
H	-5.144984000	-0.936530000	1.966489000
Cl	-1.894146000	-1.323125000	-0.676738000
C	-2.508871000	1.631556000	2.849305000
O	-2.830030000	2.753869000	3.360400000
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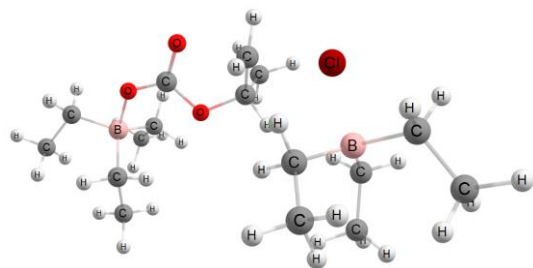
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H	-2.244321000	5.140044000	1.625568000
H	-3.036035000	4.523083000	0.181507000
C	-4.842831000	2.656589000	1.318172000
H	-4.218870000	1.971851000	0.710224000
H	-5.391783000	2.005547000	2.021734000
C	-5.859017000	4.588764000	3.621791000
H	-6.512346000	3.759142000	3.306797000
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H	-6.061002000	5.429345000	2.938928000
C	-5.842541000	3.337907000	0.379512000
H	-5.323050000	3.940497000	-0.382868000
H	-6.484228000	2.617013000	-0.155755000
H	-6.511361000	4.023055000	0.924975000

C	-4.067878000	6.167604000	1.143999000
H	-4.208639000	6.592722000	2.151086000
H	-3.596749000	6.950729000	0.525082000
H	-5.073803000	5.991081000	0.730974000
O	-3.465142000	1.105268000	3.457872000
C	-3.205064000	-0.254519000	3.841165000
H	-3.766066000	-0.424004000	4.763860000
C	-3.663089000	-1.187177000	2.738166000
H	-3.501669000	-2.218673000	3.074985000
H	-4.724808000	-1.019413000	2.515250000
C	-1.718495000	-0.404628000	4.141713000
H	-1.086356000	-1.046685000	3.540539000
H	-1.292720000	0.042124000	5.033955000
H	-3.078588000	-0.997615000	1.824713000
Cl	-2.070200000	-2.316026000	5.429418000
C	-2.380088000	1.702424000	2.961252000
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TS3'_c

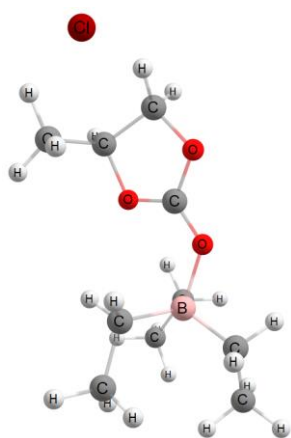


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C	-3.479131000	-1.520225000	1.864438000
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B	-3.041877000	-3.368945000	6.263217000
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H	-5.569013000	-2.121931000	6.988396000
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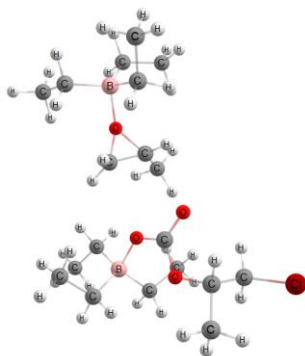
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H	-6.076106000	5.499429000	2.903141000

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H	-5.305151000	3.972559000	-0.408234000
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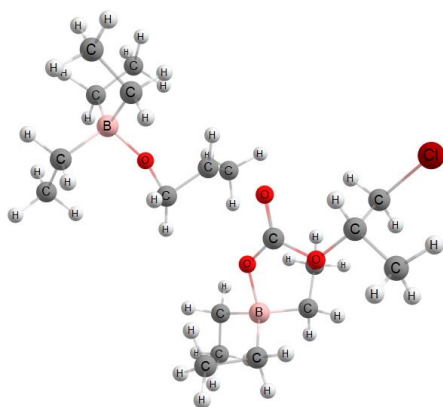
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C	-9.045769000	11.525482000	-0.109118000
H	-8.167368000	11.832285000	-0.709372000
H	-9.331629000	10.529076000	-0.497371000
C	-9.739837000	10.621257000	2.357155000
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H	-7.537525000	13.885131000	0.308499000
C	-9.834942000	9.118907000	2.083701000
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C	-6.681183000	9.925240000	2.327815000
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C	-5.636694000	8.794814000	-0.637421000
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O	-5.092057000	9.290303000	-1.895238000
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C	-3.195443000	10.501980000	-3.130444000

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H	-7.032104000	7.723172000	3.910919000
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TS4_c

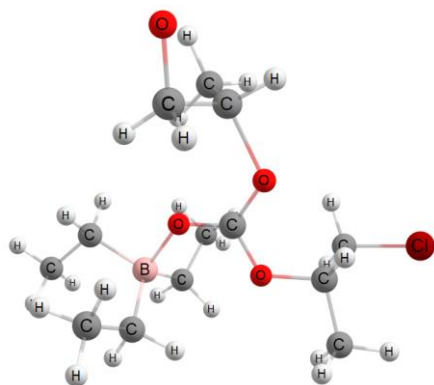


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C	-9.943996000	9.269035000	2.077135000
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H	-10.701378000	8.759688000	2.696934000
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H	-5.970451000	9.903346000	6.465781000
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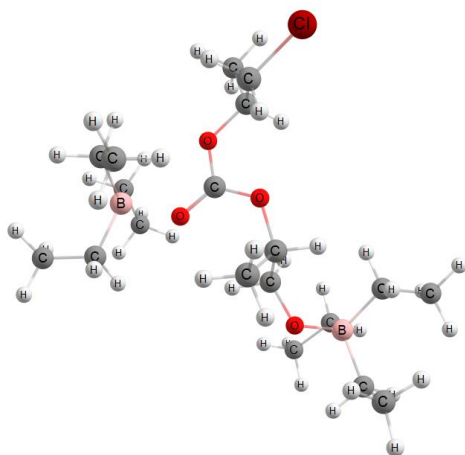
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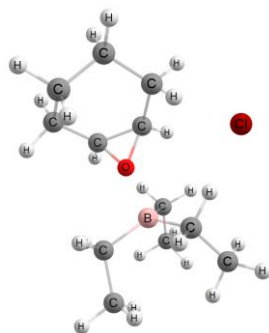


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H	-2.900791000	8.603152000	-0.067591000
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C	-3.397770000	8.137395000	-3.691612000
H	-3.972639000	8.716700000	-4.437878000
H	-2.358263000	8.106019000	-4.071852000
C	-3.442471000	11.382943000	-3.327737000
H	-3.445986000	10.983354000	-4.354638000
H	-4.499410000	11.510151000	-3.042243000
H	-2.982311000	12.386466000	-3.368060000
C	-3.964170000	6.718114000	-3.636079000
H	-3.349550000	6.065162000	-2.993124000
H	-4.976686000	6.732985000	-3.199883000
H	-4.034808000	6.225584000	-4.622633000
C	-1.318081000	7.728303000	-1.237001000
H	-1.172080000	7.164171000	-2.173128000
H	-0.718334000	8.648040000	-1.328252000
H	-0.876231000	7.129024000	-0.420837000
H	-5.071710000	7.934253000	0.244689000
C	-5.898342000	10.784571000	5.176974000
H	-6.886274000	11.024473000	5.595546000
H	-5.270586000	10.343271000	5.960520000
H	-5.434886000	11.712960000	4.819919000
H	-6.840942000	7.856165000	3.535568000
C	-7.140703000	7.972468000	-0.359420000
H	-6.903811000	7.555351000	-1.347484000
H	-7.436436000	7.156297000	0.316545000
H	-7.971726000	8.681976000	-0.469318000
H	-6.178678000	10.469227000	-1.034920000

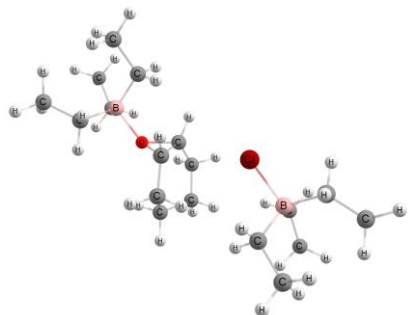
BEt₃_CHO



C	0.026891000	2.747833000	4.944152000
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C	-0.969376000	1.858218000	2.790246000
C	-0.142411000	0.644388000	2.961578000
C	0.881737000	0.548998000	4.065347000
C	1.272615000	1.928265000	4.601373000
H	0.310437000	3.686457000	5.443912000
H	-1.824727000	3.412677000	3.923220000
H	0.442224000	-0.057314000	4.875740000
H	1.858890000	2.458844000	3.834027000
H	-0.365916000	3.850449000	3.091793000
H	-0.578641000	2.176745000	5.671022000
H	1.921181000	1.809126000	5.482970000
H	1.762571000	0.001722000	3.693108000
O	0.183446000	1.595980000	1.950399000
H	-0.521999000	-0.297964000	2.554885000
H	-1.913571000	1.839326000	2.232586000
B	0.082719000	1.306227000	0.260898000
C	1.376596000	0.331351000	0.074453000
H	1.138326000	-0.712986000	0.360778000
H	2.166410000	0.665070000	0.774899000
C	-1.372732000	0.630715000	0.006784000
H	-1.619936000	-0.087737000	0.813862000
H	-2.151884000	1.413188000	0.055354000
C	0.227578000	2.825835000	-0.273996000
H	-0.426509000	3.448834000	0.363534000
H	1.266367000	3.192273000	-0.153119000
C	1.964750000	0.346170000	-1.339716000
H	2.270876000	1.367255000	-1.616410000
H	2.849233000	-0.305258000	-1.444416000
H	1.227887000	0.022139000	-2.090904000
C	-0.243834000	3.050445000	-1.713908000
H	-1.320497000	2.833065000	-1.788534000
H	-0.107879000	4.095948000	-2.036533000
H	0.282032000	2.411351000	-2.443977000
C	-1.471034000	-0.139621000	-1.314683000
H	-0.757489000	-0.980454000	-1.344759000

H	-2.477105000	-0.559017000	-1.481559000
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Cl	-3.060469000	3.732407000	1.408230000

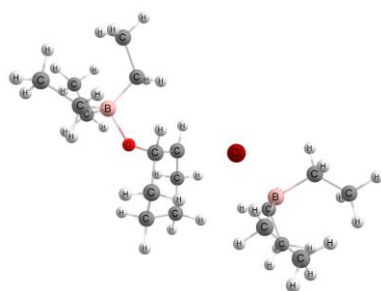
Int1_d



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C	-1.115156000	1.027335000	2.498867000
C	-0.597349000	0.905779000	3.902947000
C	-0.096603000	2.248457000	4.435297000
H	-0.878081000	4.253872000	4.755913000
H	-2.599408000	3.982504000	2.797506000
H	-1.448561000	0.565029000	4.514121000
H	0.814747000	2.550139000	3.892237000
H	-0.901028000	4.277415000	2.345607000
H	-2.083403000	2.951960000	4.823660000
H	0.175990000	2.137203000	5.495215000
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O	-0.281985000	1.813280000	1.613156000
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B	0.201601000	1.325829000	0.087946000
C	1.202266000	0.100312000	0.472304000
H	0.630610000	-0.824466000	0.682620000
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C	-1.144811000	0.904337000	-0.727370000
H	-1.864934000	0.400694000	-0.055271000
H	-1.673074000	1.802030000	-1.101822000
C	0.916118000	2.686229000	-0.442484000
H	0.282300000	3.542563000	-0.142129000

H	1.881140000	2.838352000	0.076512000
C	2.288691000	-0.202774000	-0.563723000
H	2.929879000	0.678589000	-0.723427000
H	2.945536000	-1.033281000	-0.257381000
H	1.861921000	-0.469037000	-1.543154000
C	1.128467000	2.766534000	-1.956800000
H	0.167428000	2.701895000	-2.491417000
H	1.610681000	3.707833000	-2.267610000
H	1.756295000	1.941196000	-2.327934000
C	-0.887437000	-0.046894000	-1.901189000
H	-0.435307000	-0.987318000	-1.549039000
H	-1.812016000	-0.309454000	-2.439922000
H	-0.192068000	0.386856000	-2.636358000
Cl	-4.132471000	1.488035000	3.582084000
B	-4.777448000	1.624736000	5.507868000
C	-4.874498000	3.235900000	5.784156000
H	-5.793433000	3.634498000	5.312543000
H	-4.043758000	3.740217000	5.259251000
C	-6.225047000	0.865481000	5.489319000
H	-6.726349000	1.117391000	4.538535000
H	-6.077044000	-0.231495000	5.461151000
C	-3.623230000	0.833327000	6.359216000
H	-3.334884000	-0.057257000	5.771024000
H	-2.705001000	1.450159000	6.440267000
C	-4.827997000	3.666005000	7.254803000
H	-3.876963000	3.359296000	7.720882000
H	-4.912243000	4.759459000	7.382321000
H	-5.634712000	3.207618000	7.848738000
C	-4.032885000	0.357005000	7.757570000
H	-4.880906000	-0.343633000	7.693150000
H	-3.218036000	-0.168059000	8.285769000
H	-4.355582000	1.188833000	8.403337000
C	-7.175539000	1.224197000	6.637258000
H	-7.404127000	2.302527000	6.629924000
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H	-6.743031000	0.998838000	7.625322000

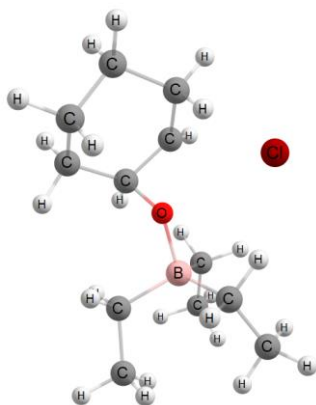
TS1_d



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C	-0.933986000	1.149504000	2.552625000
C	-0.312002000	1.034791000	3.930626000
C	0.060129000	2.410614000	4.483175000
H	-0.906836000	4.313344000	4.926008000
H	-2.728990000	4.024827000	3.146884000
H	-1.051366000	0.550277000	4.589497000
H	0.851304000	2.845829000	3.852003000
H	-1.086414000	4.138416000	2.479741000
H	-1.935281000	2.885732000	5.142389000
H	0.465490000	2.308621000	5.501456000
H	0.570374000	0.380827000	3.861906000
O	-0.182698000	1.924993000	1.655094000
H	-1.246368000	0.178015000	2.143748000
H	-2.496478000	2.196969000	1.448828000
B	0.155220000	1.370192000	0.216203000
C	1.081104000	0.036740000	0.497229000
H	0.450547000	-0.843555000	0.734707000
H	1.668457000	0.235519000	1.414538000
C	-1.255604000	1.036519000	-0.561627000
H	-1.968829000	0.560696000	0.140172000
H	-1.742580000	1.980665000	-0.880307000
C	0.976134000	2.629219000	-0.436199000
H	0.462953000	3.549899000	-0.097976000
H	1.989384000	2.683190000	0.007756000
C	2.065613000	-0.344555000	-0.612040000
H	2.762134000	0.485184000	-0.813619000

H	2.676385000	-1.228501000	-0.359378000
H	1.552570000	-0.565588000	-1.561196000
C	1.085905000	2.681544000	-1.961863000
H	0.086877000	2.719873000	-2.425917000
H	1.642449000	3.564554000	-2.321117000
H	1.591850000	1.792614000	-2.371416000
C	-1.141635000	0.099257000	-1.767842000
H	-0.748122000	-0.882410000	-1.458767000
H	-2.110892000	-0.080711000	-2.263188000
H	-0.452681000	0.491753000	-2.531536000
Cl	-3.832912000	1.364961000	3.457610000
B	-4.644128000	1.596477000	5.464575000
C	-4.781852000	3.205245000	5.622518000
H	-5.662515000	3.566510000	5.059817000
H	-3.912800000	3.699419000	5.157476000
C	-6.040367000	0.792844000	5.265545000
H	-6.441188000	1.025624000	4.264620000
H	-5.863140000	-0.298472000	5.271073000
C	-3.534467000	0.850384000	6.384773000
H	-3.162895000	-0.027875000	5.829266000
H	-2.652203000	1.494192000	6.559734000
C	-4.869107000	3.679482000	7.078382000
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H	-4.980112000	4.773516000	7.160173000
H	-5.718875000	3.224710000	7.611774000
C	-4.071184000	0.363000000	7.736947000
H	-4.886814000	-0.363166000	7.593426000
H	-3.294700000	-0.134312000	8.341416000
H	-4.478114000	1.187303000	8.343809000
C	-7.115690000	1.146019000	6.301456000
H	-7.367613000	2.217563000	6.252650000
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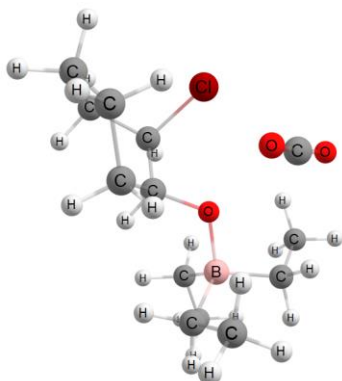
TS1'_d



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C	-0.219778000	0.949770000	2.765895000
C	0.923853000	0.723502000	3.747634000
C	1.277295000	1.997685000	4.508394000
H	0.271376000	3.454505000	5.780605000
H	-1.950436000	3.356628000	4.524455000
H	0.623073000	-0.063474000	4.462856000
H	1.675525000	2.736234000	3.794535000
H	-0.606178000	3.765620000	3.486605000
H	-0.394058000	1.817504000	5.867742000
H	2.063245000	1.796203000	5.253084000
H	1.781342000	0.339567000	3.174530000
O	0.052232000	1.897677000	1.778746000
H	-0.563502000	-0.009466000	2.348688000
H	-2.358676000	1.522879000	3.040364000
B	0.043339000	1.456198000	0.261624000
C	1.307298000	0.387925000	0.169226000
H	1.017559000	-0.611230000	0.557810000
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C	-1.416868000	0.793276000	-0.102916000
H	-1.799332000	0.210388000	0.759200000
H	-2.152435000	1.605988000	-0.224985000
C	0.309161000	2.876618000	-0.501994000
H	-0.311766000	3.610890000	0.041093000
H	1.363233000	3.194707000	-0.368665000

C	1.936970000	0.220767000	-1.216604000
H	2.319104000	1.187774000	-1.581036000
H	2.782969000	-0.489958000	-1.226304000
H	1.206535000	-0.131616000	-1.961051000
C	-0.062131000	2.944725000	-1.985227000
H	-1.130766000	2.714645000	-2.123972000
H	0.110337000	3.943577000	-2.424157000
H	0.503353000	2.222282000	-2.597854000
C	-1.442456000	-0.138664000	-1.317990000
H	-0.773510000	-1.004364000	-1.174235000
H	-2.449819000	-0.539496000	-1.529017000
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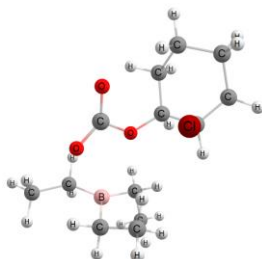
Int2_d



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C	0.213140000	1.574425000	2.101292000
C	0.696722000	2.902653000	2.754766000
C	0.261419000	3.086719000	4.209768000
H	-0.002327000	1.814993000	5.944662000
H	1.788617000	0.446539000	3.917815000
H	1.798902000	2.949504000	2.702472000
H	-0.831525000	3.174218000	4.236418000
H	0.602529000	-0.268808000	5.020531000
H	1.690667000	2.122865000	5.550680000
H	0.663498000	4.032561000	4.606564000

H	0.311479000	3.723198000	2.135561000
O	-0.771342000	1.721153000	1.155818000
H	1.113487000	1.112611000	1.648392000
H	-0.200163000	-0.455597000	2.685696000
B	-0.383700000	1.565009000	-0.325416000
C	0.406491000	0.126367000	-0.557148000
H	-0.126456000	-0.678722000	-0.012254000
H	1.426435000	0.153899000	-0.124415000
C	-1.812907000	1.580267000	-1.127799000
H	-2.363547000	2.503785000	-0.866167000
H	-1.645611000	1.642938000	-2.221640000
C	0.591531000	2.826133000	-0.750860000
H	1.461570000	2.853630000	-0.061776000
H	1.027561000	2.659855000	-1.754878000
C	0.541034000	-0.276056000	-2.028063000
H	1.060037000	0.507677000	-2.604354000
H	1.100925000	-1.216427000	-2.180707000
H	-0.447430000	-0.405034000	-2.497406000
C	-0.108556000	4.186054000	-0.730657000
H	-0.642465000	4.333132000	0.223462000
H	0.572066000	5.045901000	-0.868254000
H	-0.870690000	4.244516000	-1.524894000
C	-2.695542000	0.373529000	-0.801980000
H	-2.788410000	0.265153000	0.289441000
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H	-2.249124000	-0.560456000	-1.183965000
Cl	-1.884860000	0.745371000	3.765491000
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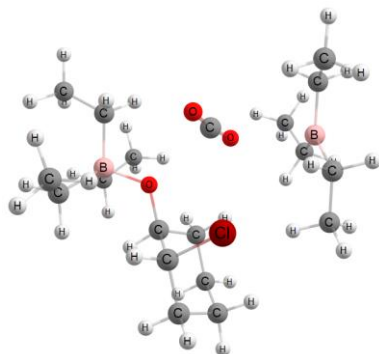
TS2'_d



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C	0.508165000	1.740819000	2.634255000
C	1.119911000	2.680820000	3.703768000
C	0.374838000	2.635485000	5.036045000
H	-0.567704000	1.086989000	6.226146000
H	1.455168000	-0.093878000	4.287059000
H	2.171889000	2.382260000	3.862965000
H	-0.643628000	2.988547000	4.832737000
H	-0.036522000	-0.814313000	4.913426000
H	1.196533000	1.066052000	6.325081000
H	0.832528000	3.336588000	5.751681000
H	1.111833000	3.700158000	3.303875000
O	-0.166763000	2.319048000	1.565947000
H	1.359683000	1.220104000	2.154245000
H	-0.328467000	-0.245472000	2.528337000
B	-0.596007000	1.885661000	-1.185587000
C	0.548783000	0.836757000	-0.809659000
H	0.268273000	0.265123000	0.088577000
H	1.492073000	1.357730000	-0.574267000
C	-2.093845000	1.377654000	-1.291880000
H	-2.768177000	2.245252000	-1.273800000
H	-2.193941000	0.922159000	-2.301427000
C	-0.121115000	3.255647000	-1.827431000
H	0.471146000	3.746627000	-1.034578000
H	0.609973000	3.016375000	-2.627151000
C	0.762683000	-0.128575000	-1.985119000
H	1.015207000	0.412519000	-2.912119000
H	1.574904000	-0.850086000	-1.799091000
H	-0.150865000	-0.709143000	-2.192077000
C	-1.205846000	4.203112000	-2.329435000
H	-1.854076000	4.467328000	-1.482146000
H	-0.793251000	5.130584000	-2.759574000
H	-1.829361000	3.728705000	-3.105412000
C	-2.508334000	0.375890000	-0.214875000
H	-2.383012000	0.834811000	0.777322000

H	-3.559382000	0.059203000	-0.312994000
H	-1.888326000	-0.536076000	-0.244161000
Cl	-2.010408000	0.946655000	3.602047000
C	-1.139265000	3.387047000	1.719643000
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O	-1.185473000	3.938150000	2.813625000

Int3_d

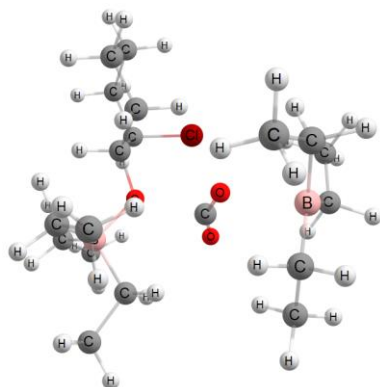


B	0.518862000	-1.527543000	3.020610000
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O	2.455999000	-4.340395000	1.624256000
O	3.489363000	-2.514046000	0.652723000
B	5.154859000	-2.910101000	-1.226017000
Cl	0.658504000	-3.617389000	-0.983778000
C	-0.517730000	-2.399780000	-0.296685000
H	-0.602680000	-0.701829000	0.911689000
C	0.221918000	-1.348884000	0.540185000
O	0.913984000	-1.913220000	1.583554000
H	-1.160489000	-2.993046000	0.365129000
C	-1.297937000	-1.778563000	-1.448582000
H	-1.790625000	-2.568102000	-2.035868000
H	-2.094166000	-1.157821000	-1.001324000
H	-1.007888000	-0.437366000	-3.126777000
C	-0.405595000	-0.908375000	-2.333684000
H	0.333004000	-1.558231000	-2.830599000
C	0.324329000	0.152106000	-1.506395000
H	-0.418227000	0.860249000	-1.095932000
H	0.994639000	0.740831000	-2.153197000
H	1.934363000	-1.097045000	-0.728806000

C	1.108752000	-0.472483000	-0.351156000
H	1.559843000	0.303473000	0.284206000
C	4.133762000	-3.598609000	-2.223902000
H	4.727401000	-4.304881000	-2.838879000
H	3.472819000	-4.257588000	-1.630826000
C	3.297663000	-2.685534000	-3.116869000
H	3.935127000	-2.051695000	-3.753578000
H	2.670398000	-2.018473000	-2.507261000
H	2.619579000	-3.251140000	-3.773899000
C	5.426199000	-1.353485000	-1.315595000
H	5.932026000	-1.193866000	-2.290439000
H	4.455573000	-0.840102000	-1.424357000
C	6.233896000	-0.723840000	-0.183374000
H	6.393607000	0.354785000	-0.331684000
H	7.224113000	-1.195007000	-0.081011000
H	5.706752000	-0.852172000	0.773928000
C	6.071050000	-3.822655000	-0.305388000
H	7.080878000	-3.771798000	-0.763349000
H	6.194165000	-3.333257000	0.675368000
C	5.650614000	-5.281560000	-0.128959000
H	5.564968000	-5.795530000	-1.098511000
H	4.667272000	-5.357457000	0.360190000
H	6.363567000	-5.851314000	0.486155000
C	-1.034615000	-2.021336000	3.285744000
H	-1.401866000	-1.641862000	4.258347000
H	-1.708385000	-1.557011000	2.536176000
C	-1.199303000	-3.542836000	3.235123000
H	-2.249977000	-3.882277000	3.189947000
H	-0.744693000	-4.016948000	4.120409000
H	-0.667447000	-3.959782000	2.362070000
C	1.578096000	-2.325577000	3.985762000
H	1.493920000	-3.413301000	3.816607000
H	2.613676000	-2.061996000	3.689195000
C	1.393189000	-2.033225000	5.475042000
H	0.377197000	-2.310737000	5.804027000
H	1.505007000	-0.956379000	5.686711000
H	2.105042000	-2.570886000	6.126155000

C	0.663175000	0.108035000	3.202106000
H	0.063028000	0.632631000	2.430938000
H	0.214702000	0.424486000	4.163363000
C	2.110285000	0.602608000	3.132134000
H	2.208144000	1.701379000	3.070105000
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TS2_d

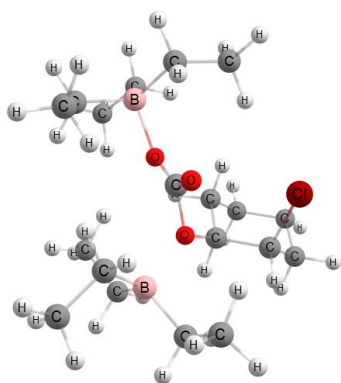


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B	5.021017000	-2.908576000	-0.776593000
Cl	-0.041656000	-3.039341000	-1.682704000
C	-0.872618000	-1.935884000	-0.497139000
H	-0.477907000	-0.570400000	1.029959000
C	0.150339000	-1.199200000	0.370140000
O	0.874946000	-2.075546000	1.168240000
H	-1.459213000	-2.608755000	0.140425000
C	-1.758260000	-0.961698000	-1.265766000
H	-2.456700000	-1.521205000	-1.905709000
H	-2.362199000	-0.415358000	-0.520186000
H	-1.599363000	0.752989000	-2.581266000
C	-0.932315000	0.030612000	-2.084926000
H	-0.406266000	-0.524705000	-2.878034000
C	0.093942000	0.752840000	-1.208783000
H	-0.438470000	1.379201000	-0.470197000
H	0.700223000	1.437183000	-1.822136000

H	1.602939000	-0.811546000	-1.187961000
C	0.996723000	-0.238434000	-0.470735000
H	1.695123000	0.282478000	0.199742000
C	4.600960000	-4.227741000	-1.565701000
H	5.547327000	-4.744495000	-1.826051000
H	4.086302000	-4.916460000	-0.874226000
C	3.751170000	-4.023035000	-2.819061000
H	4.279205000	-3.414101000	-3.569699000
H	2.819056000	-3.491768000	-2.567812000
H	3.471613000	-4.973479000	-3.299608000
C	5.186175000	-1.542768000	-1.580453000
H	6.054689000	-1.684110000	-2.256171000
H	4.320276000	-1.413358000	-2.251011000
C	5.378414000	-0.287415000	-0.731574000
H	5.471961000	0.625938000	-1.340214000
H	6.279293000	-0.359632000	-0.102491000
H	4.521315000	-0.153607000	-0.053791000
C	5.723303000	-3.045984000	0.647323000
H	6.808286000	-2.888675000	0.478506000
H	5.410238000	-2.192134000	1.272593000
C	5.495845000	-4.357082000	1.399686000
H	5.865640000	-5.220023000	0.823365000
H	4.423314000	-4.528632000	1.581061000
H	5.998780000	-4.371804000	2.379010000
C	-0.712059000	-2.144185000	3.206349000
H	-0.831078000	-1.879707000	4.273894000
H	-1.406516000	-1.461513000	2.675758000
C	-1.158410000	-3.591391000	2.983475000
H	-2.245201000	-3.747618000	3.100752000
H	-0.655009000	-4.270358000	3.690435000
H	-0.868774000	-3.934091000	1.975276000
C	1.880799000	-2.954464000	3.359679000
H	1.583267000	-3.979793000	3.083912000
H	2.887466000	-2.813430000	2.917722000
C	1.993098000	-2.856152000	4.882042000
H	1.012776000	-3.024571000	5.358914000
H	2.325861000	-1.852674000	5.195534000

H	2.697559000	-3.586132000	5.315815000
C	1.314636000	-0.322797000	3.053469000
H	0.702843000	0.403399000	2.481609000
H	1.099642000	-0.086035000	4.112662000
C	2.797835000	-0.069650000	2.767462000
H	3.082410000	0.996701000	2.794967000
H	3.077519000	-0.469825000	1.778014000
H	3.433544000	-0.594458000	3.499251000

Int4_d

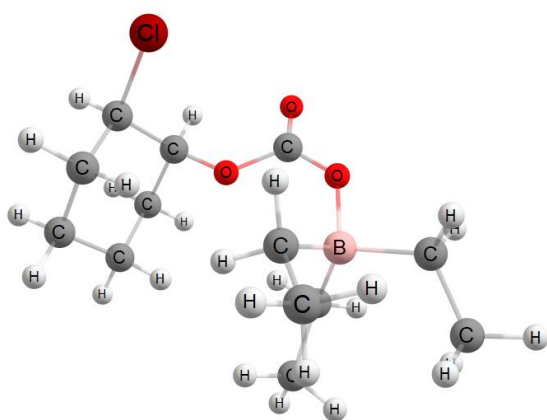


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O	3.124023000	-2.266909000	0.090703000
B	4.549053000	-2.747119000	-0.524881000
Cl1	-0.314740000	-3.221280000	-1.554108000
C	-0.827240000	-1.925560000	-0.405059000
H	-0.045193000	-0.486670000	0.906528000
C	0.382471000	-1.226309000	0.213476000
O	1.115539000	-2.109754000	1.059837000
H	-1.382496000	-2.448838000	0.381750000
C	-1.705504000	-0.912333000	-1.133689000
H	-2.552706000	-1.436619000	-1.598844000
H	-2.121040000	-0.230048000	-0.371171000
H	-1.562181000	0.640270000	-2.637568000
C	-0.911667000	-0.112397000	-2.166253000
H	-0.579066000	-0.798978000	-2.960797000
C	0.308816000	0.552205000	-1.526788000
H	-0.030536000	1.308092000	-0.796001000

H	0.892429000	1.090538000	-2.287921000
H	1.633012000	-1.172180000	-1.552699000
C	1.206693000	-0.468951000	-0.822400000
H	2.055947000	0.015947000	-0.323212000
C	4.314031000	-4.059818000	-1.458312000
H	5.309879000	-4.383834000	-1.820197000
H	3.925059000	-4.893544000	-0.851650000
C	3.384956000	-3.846285000	-2.654060000
H	3.777819000	-3.078816000	-3.340645000
H	2.391748000	-3.502851000	-2.319696000
H	3.221963000	-4.762758000	-3.246950000
C	5.000924000	-1.433433000	-1.383902000
H	5.882398000	-1.705222000	-1.996568000
H	4.206662000	-1.176134000	-2.110325000
C	5.327432000	-0.194618000	-0.549632000
H	5.577691000	0.692067000	-1.157936000
H	6.178910000	-0.381585000	0.123895000
H	4.475297000	0.077610000	0.094703000
C	5.508571000	-3.013246000	0.768719000
H	6.564878000	-2.926940000	0.444914000
H	5.359210000	-2.189331000	1.492860000
C	5.310946000	-4.353743000	1.481478000
H	5.571717000	-5.194030000	0.818223000
H	4.258385000	-4.501170000	1.769870000
H	5.924899000	-4.452165000	2.393518000
C	-0.593082000	-2.267812000	3.041984000
H	-0.820990000	-2.042683000	4.100363000
H	-1.243021000	-1.571765000	2.474502000
C	-0.972226000	-3.717759000	2.728239000
H	-2.061046000	-3.894374000	2.726480000
H	-0.532036000	-4.402761000	3.469210000
H	-0.566960000	-4.030377000	1.750877000
C	2.022630000	-2.988684000	3.385428000
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H	3.034283000	-2.818928000	2.972823000
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H	2.418820000	-1.890373000	5.238116000
H	2.781709000	-3.624092000	5.353097000
C	1.373900000	-0.376100000	3.069867000
H	0.713888000	0.333200000	2.535317000
H	1.154078000	-0.186172000	4.137693000
C	2.837847000	-0.040048000	2.778351000
H	3.063666000	1.035200000	2.865670000
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H	3.508200000	-0.572908000	3.471018000

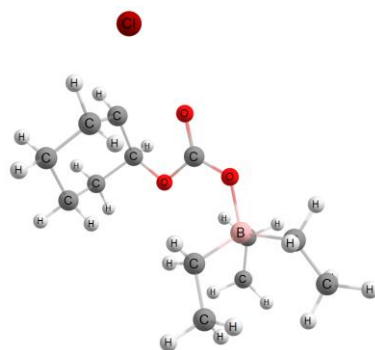
Int5_d



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Cl	4.966280000	-3.360587000	-1.565094000
C	3.363940000	-3.920557000	-2.168760000
H	2.462536000	-3.810798000	-0.204278000
C	2.253810000	-3.460019000	-1.224113000
O	2.203273000	-2.056684000	-1.232800000
H	3.407185000	-5.020038000	-2.150010000
C	3.134862000	-3.413460000	-3.584414000
H	3.170346000	-2.313936000	-3.548711000
H	3.948501000	-3.761264000	-4.238010000
H	1.775465000	-4.980308000	-4.208205000
C	1.769658000	-3.879600000	-4.101137000
H	1.596956000	-3.465512000	-5.106293000
C	0.641369000	-3.468708000	-3.152622000
H	-0.326354000	-3.841677000	-3.521954000
H	0.578473000	-2.369141000	-3.112504000

H	0.124439000	-3.642712000	-1.042682000
C	0.907851000	-3.981087000	-1.737031000
H	0.913974000	-5.085305000	-1.720875000
B	1.656980000	0.708326000	-1.369707000
C	1.876565000	2.245755000	-0.830839000
H	2.938942000	2.537857000	-0.947540000
H	1.702093000	2.220845000	0.260241000
C	2.509924000	0.367096000	-2.738720000
H	3.530773000	0.061425000	-2.438691000
H	2.078297000	-0.519715000	-3.239042000
C	0.067319000	0.287503000	-1.474187000
H	-0.010947000	-0.805113000	-1.316913000
H	-0.499374000	0.746550000	-0.640370000
C	0.983136000	3.334239000	-1.430578000
H	-0.081280000	3.106803000	-1.254094000
H	1.174116000	4.333299000	-0.999447000
H	1.110892000	3.425348000	-2.521226000
C	-0.623238000	0.621108000	-2.799420000
H	-0.108261000	0.131658000	-3.643346000
H	-1.679201000	0.298115000	-2.833763000
H	-0.609087000	1.702628000	-3.009526000
C	2.618339000	1.498676000	-3.763984000
H	3.077507000	2.396893000	-3.320036000
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H	1.626407000	1.802565000	-4.137738000

TS3_d

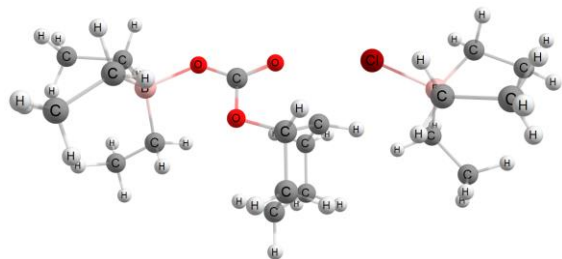


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Cl	4.614964000	-4.811841000	0.177692000
C	2.882177000	-3.987422000	-1.474049000
H	0.896145000	-3.802526000	-0.689260000
C	1.468041000	-3.475947000	-1.573015000
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H	2.888987000	-5.043078000	-1.212044000
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H	4.761430000	-4.104665000	-2.424055000
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C	1.708539000	-3.658583000	-4.074156000
H	1.251061000	-4.057052000	-4.992531000
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C	0.849056000	-4.023938000	-2.863734000
H	0.760323000	-5.118513000	-2.770687000
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C	2.321523000	2.183387000	-1.165902000
H	3.232327000	2.273879000	-1.789263000
H	2.689423000	2.075477000	-0.129557000
C	1.554441000	0.416103000	-3.128839000
H	2.536079000	-0.049831000	-3.349808000
H	0.802056000	-0.361668000	-3.353746000
C	0.046181000	0.689781000	-0.834078000
H	-0.184835000	-0.376888000	-0.662910000
H	0.066280000	1.156567000	0.169700000
C	1.516281000	3.482423000	-1.251051000
H	0.648074000	3.449028000	-0.572776000
H	2.109597000	4.370355000	-0.972113000
H	1.121620000	3.663666000	-2.263544000
C	-1.102971000	1.290443000	-1.649153000
H	-1.182394000	0.798245000	-2.632253000
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H	-0.953697000	2.364316000	-1.843940000
C	1.361864000	1.590495000	-4.091762000

H	2.134178000	2.360890000	-3.937545000
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H	0.387250000	2.082318000	-3.941285000

TS3'_d

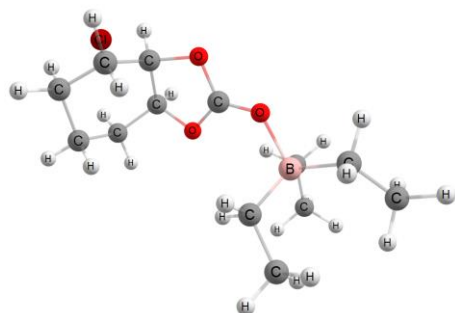


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C1	5.404314000	-3.106018000	1.394741000
C	3.426414000	-3.196364000	-0.243091000
H	1.733125000	-2.607415000	0.907944000
C	2.033825000	-2.680865000	-0.149459000
O	1.862978000	-1.457276000	-0.804715000
H	3.565039000	-4.073639000	0.385024000
C	4.047595000	-3.298081000	-1.582774000
H	4.025522000	-2.343768000	-2.123884000
H	5.084713000	-3.640442000	-1.486129000
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C	3.170981000	-4.340543000	-2.327580000
H	3.550922000	-4.434710000	-3.355148000
C	1.698887000	-3.925282000	-2.322115000
H	1.088659000	-4.680662000	-2.838909000
H	1.582474000	-2.975755000	-2.868258000
H	0.143521000	-3.370148000	-0.889780000
C	1.181553000	-3.731671000	-0.895689000
H	1.211968000	-4.678009000	-0.332735000
B	1.621079000	1.122740000	-2.039567000
C	2.307081000	2.517018000	-2.551195000
H	3.057615000	2.305797000	-3.337762000
H	2.885867000	2.917807000	-1.699586000
C	1.373127000	0.022424000	-3.237307000
H	2.335359000	-0.492298000	-3.437257000

H	0.678917000	-0.767547000	-2.896601000
C	0.334938000	1.342020000	-1.050065000
H	0.266078000	0.481127000	-0.361230000
H	0.502753000	2.226832000	-0.406281000
C	1.357296000	3.614614000	-3.037102000
H	0.655916000	3.906003000	-2.238385000
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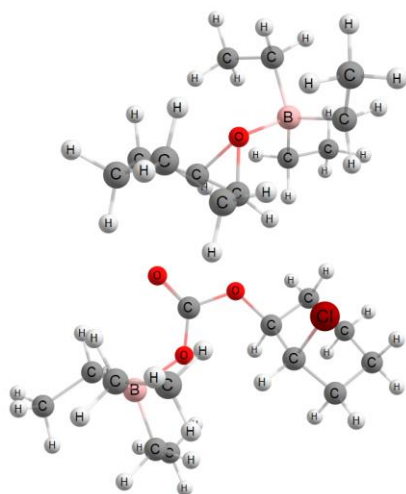
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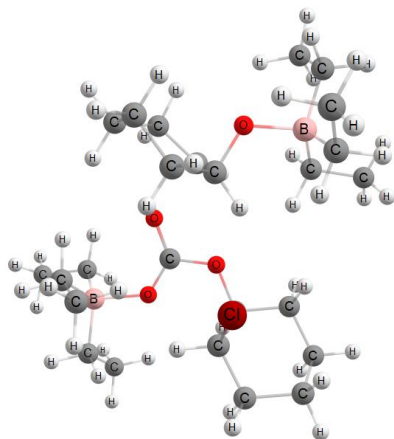


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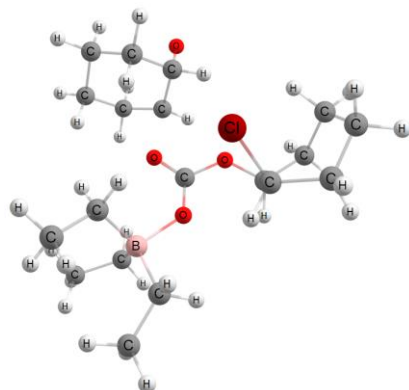
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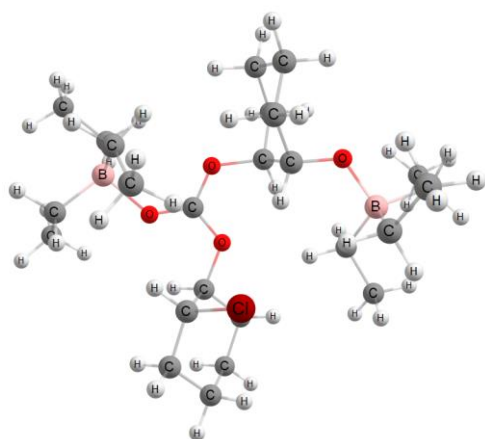
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Int8_d



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H	-10.649968000	10.658228000	-1.049089000

H	-11.110678000	12.351634000	-1.078191000
C	-9.263172000	10.591752000	1.578885000
H	-9.423736000	10.607491000	2.668582000
H	-10.135237000	10.089852000	1.127662000
H	-8.392486000	9.931271000	1.415462000
C	-10.227103000	11.647164000	-2.923533000
H	-9.995971000	12.651494000	-3.313062000
H	-9.417082000	10.982067000	-3.266424000
H	-11.157088000	11.312076000	-3.411888000
C	-9.108735000	14.647138000	-1.021169000
H	-10.057507000	14.537852000	-1.571606000
H	-9.370928000	14.801346000	0.037739000
H	-8.627878000	15.572865000	-1.376925000
Cl	-7.486172000	7.152701000	0.653911000
C	-6.827068000	10.518201000	-0.640294000
O	-6.149404000	11.296983000	0.122963000
O	-7.944623000	10.808771000	-1.082889000
C	-4.752026000	12.981961000	2.093799000
C	-4.091339000	12.167156000	0.979777000
C	-4.848671000	10.886933000	0.686468000
C	-5.065869000	10.042588000	1.956647000
C	-5.761471000	10.884434000	3.034258000
C	-4.941621000	12.133268000	3.353196000
H	-4.142735000	13.873582000	2.309784000
H	-3.986593000	12.759003000	0.056922000
H	-6.768158000	11.175825000	2.689629000
H	-3.958687000	11.809899000	3.730317000
H	-3.089093000	11.843249000	1.297761000
H	-5.734704000	13.343050000	1.743239000
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H	-5.882733000	10.251305000	3.925556000
O	-3.822734000	9.631352000	2.382546000
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B	-3.426993000	8.160695000	2.211599000
C	-1.862245000	8.091630000	2.702239000
H	-1.536446000	7.040162000	2.828304000
H	-1.801020000	8.545504000	3.708925000

C	-4.402890000	7.239300000	3.172357000
H	-5.461117000	7.372177000	2.865673000
H	-4.193784000	6.163221000	3.020349000
C	-3.597879000	7.742214000	0.621282000
H	-4.649239000	7.904623000	0.320182000
H	-2.996321000	8.430142000	-0.007533000
C	-0.887719000	8.821808000	1.777782000
H	-1.245379000	9.847714000	1.588011000
H	0.139018000	8.896797000	2.179066000
H	-0.814771000	8.323982000	0.795996000
C	-3.208354000	6.301517000	0.289142000
H	-3.275122000	6.055010000	-0.787687000
H	-2.172196000	6.090115000	0.603112000
H	-3.852287000	5.586044000	0.825966000
C	-4.271983000	7.564480000	4.661618000
H	-3.277408000	7.279084000	5.041083000
H	-4.367913000	8.650901000	4.825138000
H	-5.021145000	7.060187000	5.298016000
H	-4.336933000	10.272668000	-0.063463000