Electronic Supplementary Information for

Unique Catalytic Role of Intermolecular Electric Fields that Emanate from the Lewis Acids in a Ring Closing Carbonyl Olefin Metathesis Reaction

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Table S1. Intermolecular electric fields (EFs) in a.u. for Lewis acid (LA) attached to reactant complex (**RC-LA)** in ring-closing carbonyl-olefin metathesis (RCCOM) reaction as a function of distances[-a-]

Distance(Å)	**RC-LA** ($AlCl_3$)	**RC-LA** ($[AlCl_2]^+$ $[SbF_6]^-$)
d	-0.0658	-0.0507
d+0.25	-0.0475	-0.0361
d+0.50	-0.0355	-0.0262
d+0.75	-0.0272	-0.0192
d+1.00	-0.0213	-0.0141

[-a-]The 'd' is the distance between the aluminium (Al) of the LA and the carbonyl oxygen (O_d) of the reactant complex (**RC)**. (0.001 a.u. = 51.4 mV/Å)

Table S2. Energies of **RC-LA**, transition states **TS1-LA**, and **TS2-LA** for carbonyl-ene and [2+2] cycloaddition reaction with distances[-a-]

Distance(Å)	**RC-LA**	**TS1-LA**	**TS2-LA**	$\Delta E_1 = [E_{(TS1\text{-}LA)} - E_{(RC\text{-}LA)}]$	$\Delta E_2 = [E_{(TS2\text{-}LA)} - E_{(RC\text{-}LA)}]$
d	-3620.2804	-3620.2593	-3620.2585	13.27	13.73
d+0.25	-3620.2662	-3620.2444	-3620.2402	13.65	16.28
d+0.50	-3620.2435	-3620.2202	-3620.2106	14.61	20.61
d+0.75	-3620.2237	-3620.1976	-3620.1830	16.35	25.54
d+1.00	-3620.2081	-3620.1794	-3620.1609	18.02	29.61

[-a-]The 'd' is the distance between Al of the LA ($[AlCl_2]^+[SbF_6]^-$) and the carbonyl oxygen (O_d) of the **RC**. ΔE_1 energy barrier for carbonyl-ene reaction and ΔE_2 energy barrier for [2+2] cycloaddition reaction. Energies of **RC**s and transition states (**TS**s) are provided in Hartree and ΔE energies are given in kcal/mol.

Table S3. The relative energy changes of **RC**, **TS1**, and **TS2**, compared to their corresponding zero-field energies (Δ**RC**, Δ**TS1**, and Δ**TS2**), in kcal/mol for carbonyl-ene and [2+2] cycloaddition reaction with oriented external EFs (0.001 a.u. = 51.4 mV/Å)

Field (a.u.)	**ΔRC**	**ΔTS1**	**ΔTS2**
0.020	-26.89	-21.47	-3.71
0.018	-21.36	-16.17	0.12
0.016	-16.48	-11.59	3.16
0.014	-12.22	-7.71	5.40
0.012	-8.60	-4.54	6.87
0.010	-5.60	-2.06	7.58
0.008	-3.23	-0.27	7.54
0.006	-1.48	0.82	6.75
0.004	-0.36	1.23	5.23
0.002	0.13	0.96	2.98
0	0.00	0.00	0.00
-0.002	-0.77	-1.64	-3.70
-0.004	-2.18	-3.98	-8.12
-0.006	-4.25	-7.00	-13.25
-0.008	-6.97	-10.71	-19.11
-0.010	-10.37	-15.12	-25.68
-0.012	-14.46	-20.23	-32.96
-0.014	-19.25	-26.04	-40.97
-0.016	-24.78	-32.57	-49.70
-0.018	-31.07	-39.82	-59.16
-0.020	-38.15	-47.80	-69.36

Table S4. The **RC**, **TS1**, and **TS2** dipole moments in Debye for carbonyl-ene and [2+2] cycloaddition reaction with oriented external EFs (0.001 a.u. = 51.4 mV/Å)

Field (a.u.)	RC	TS1	TS2
0.020	-11.83	-11.45	-8.61
0.018	-10.53	-10.00	-6.95
0.016	-9.25	-8.56	-5.33
0.014	-7.97	-7.13	-3.75
0.012	-6.70	-5.72	-2.20
0.010	-5.43	-4.32	-0.67
0.008	-4.17	-2.92	0.84
0.006	-2.90	-1.52	2.34
0.004	-1.63	-0.13	3.82
0.002	-0.36	1.25	5.30
0	0.91	2.64	6.76
-0.002	2.21	4.03	8.22
-0.004	3.51	5.42	9.68
-0.006	4.84	6.81	11.13
-0.008	6.19	8.22	12.57
-0.010	7.57	9.63	14.02
-0.012	8.98	11.05	15.48
-0.014	10.44	12.49	16.94
-0.016	11.95	13.94	18.41
-0.018	13.52	15.42	19.91
-0.020	15.16	16.92	21.43

Table S5. Energies of **RC**, **TS1**, and **TS2** in Hartree for carbonyl-ene and [2+2] cycloaddition reaction with oriented external EFs. Barrier energies (ΔE) are in kcal/mol

Field (a.u.)	**RC**	**TS1**	**TS2**	ΔE = (E_{TS1}-E_{RC})	ΔE = (E_{TS2} -E_{RC})
0.020	-1617.2707	-1617.2142	-1617.1557	35.46	72.16
0.018	-1617.2619	-1617.2058	-1617.1496	35.24	70.47
0.016	-1617.2542	-1617.1985	-1617.1448	34.93	68.62
0.014	-1617.2474	-1617.1923	-1617.1412	34.55	66.61
0.012	-1617.2416	-1617.1872	-1617.1389	34.11	64.46
0.010	-1617.2368	-1617.1833	-1617.1377	33.59	62.17
0.008	-1617.2330	-1617.1804	-1617.1378	33.00	59.76
0.006	-1617.2303	-1617.1787	-1617.1391	32.35	57.22
0.004	-1617.2285	-1617.1780	-1617.1415	31.64	54.58
0.002	-1617.2277	-1617.1785	-1617.1451	30.87	51.83
0	-1617.2279	-1617.1800	-1617.1498	30.04	48.98
-0.002	-1617.2291	-1617.1826	-1617.1557	29.17	46.05
-0.004	-1617.2314	-1617.1863	-1617.1628	28.25	43.05
-0.006	-1617.2347	-1617.1912	-1617.1710	27.29	39.97
-0.008	-1617.2390	-1617.1971	-1617.1803	26.30	36.84
-0.010	-1617.2444	-1617.2041	-1617.1908	25.29	33.67
-0.012	-1617.2509	-1617.2122	-1617.2024	24.27	30.47
-0.014	-1617.2586	-1617.2215	-1617.2151	23.26	27.27
-0.016	-1617.2674	-1617.2319	-1617.2290	22.26	24.07
-0.018	-1617.2774	-1617.2435	-1617.2441	21.30	20.89
-0.020	-1617.2887	-1617.2562	-1617.2604	20.39	17.77

Table S6. The NBO charges of the carbonyl oxygen-atoms (O_d) and the ene carbon-atoms (C_a) in **RC**, **TS1**, and **TS2** with oriented external EFs (0.001 a.u. = 51.4 mV/Å)

Field (a.u.)	O_d-**RC**	C_a-**RC**	O_d-**TS1**	C_a-**TS1**	O_d-**TS2**	C_a-**TS2**
0.020	-0.489	-0.032	-0.575	0.039	-0.615	0.377
0.018	-0.497	-0.028	-0.587	0.051	-0.635	0.395
0.016	-0.504	-0.024	-0.598	0.063	-0.655	0.412
0.014	-0.511	-0.020	-0.609	0.075	-0.674	0.428
0.012	-0.519	-0.015	-0.620	0.086	-0.693	0.443
0.010	-0.526	-0.010	-0.631	0.098	-0.711	0.459
0.008	-0.533	-0.005	-0.642	0.111	-0.728	0.475
0.006	-0.541	-0.000	-0.653	0.122	-0.745	0.489
0.004	-0.548	0.005	-0.663	0.133	-0.761	0.503
0.002	-0.555	0.010	-0.674	0.144	-0.777	0.516
0	-0.563	0.015	-0.684	0.155	-0.792	0.528
-0.002	-0.571	0.021	-0.695	0.166	-0.805	0.540
-0.004	-0.578	0.027	-0.705	0.177	-0.819	0.551
-0.006	-0.586	0.034	-0.715	0.187	-0.832	0.560
-0.008	-0.594	0.041	-0.726	0.198	-0.844	0.569
-0.010	-0.603	0.048	-0.736	0.208	-0.854	0.577
-0.012	-0.612	0.056	-0.746	0.218	-0.864	0.584
-0.014	-0.621	0.065	-0.756	0.228	-0.873	0.590
-0.016	-0.631	0.075	-0.765	0.237	-0.881	0.595
-0.018	-0.641	0.085	-0.775	0.247	-0.888	0.599
-0.020	-0.652	0.097	-0.785	0.256	-0.891	0.603

Table S7. The lowest unoccupied molecular orbital (LUMO) energies of carbonyl (C=O) and highest occupied molecular orbital (HOMO) energies of ene (C=C) for **RC** with oriented external EFs. Energies are in eV (0.001 a.u. = 51.4 mV/Å)

Field (a.u.)	LUMO(C=O)	HOMO(C=C)	LUMO(C=O) − HOMO(C=C)
0.020	-0.1778	-0.3099	0.1771
0.018	-0.1757	-0.2982	0.1695
0.016	-0.1733	-0.2866	0.1617
0.014	-0.1707	-0.2749	0.1538
0.012	-0.1680	-0.2633	0.1458
0.010	-0.1652	-0.2517	0.1377
0.008	-0.1624	-0.2402	0.1295
0.006	-0.1596	-0.2287	0.1212
0.004	-0.1584	-0.2172	0.1129
0.002	-0.1624	-0.2057	0.1045
0	-0.1664	-0.1943	0.0960
-0.002	-0.1704	-0.1829	0.0874
-0.004	-0.1744	-0.1716	0.0787
-0.006	-0.1785	-0.1603	0.0700
-0.008	-0.1826	-0.1491	0.0612
-0.010	-0.1867	-0.1378	0.0524
-0.012	-0.1908	-0.1267	0.0434
-0.014	-0.1947	-0.1155	0.0344
-0.016	-0.1960	-0.1044	0.0254
-0.018	-0.1947	-0.0934	0.0163
-0.020	-0.1932	-0.0824	0.0071

Table S8. The energies of **RC**, **TS**s, intermediates (**I**s), and product (**PD)** for RCCOM in Hartree at the B2 level of theory

	With ($[AlCl_2]^+$ $[SbF_6]^-$)	With $[AlCl_3]$	Pristine reaction
RC	-3620.2816	-3240.6512	-1617.2279
TS1	-3620.2589	-3240.6259	-1617.1800
TS2	-3620.2586	-3240.6239	-1617.1498
I1	-3620.2719	-3240.6429	-1617.2243
TS3	-3620.2455	-3240.6125	-1617.1375
I2	-3620.2724	-3240.6415	-1617.2127
TS4	-3620.2584	-3240.6254	-1617.1434
PD	-3620.2876	-3240.6579	-1617.2359

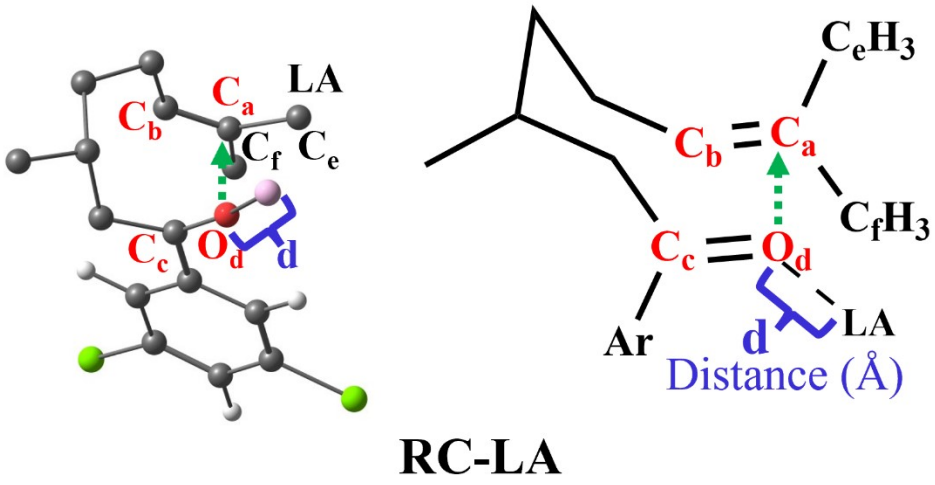

Fig. S1 Details of the calculation of intermolecular EF and direction in **RC**.

The intermolecular EF is projected along the O_d to C_a direction, which is taken as the reaction axis as shown in Fig. S1. We used TITAN code to calculate the intermolecular electric field. TITAN determines the intermolecular EF between two points using Coulomb's law, treating the LA as a collection of point charges.[46] Following the TITAN manual, we assigned O_d as atom 1 and C_a as atom 2 to define the EF direction. Next, we identified the atoms corresponding to the LA to calculate the EF. The necessary inputs, including NBO charges and atomic distances, were used to compute the field as described in TITAN manual.

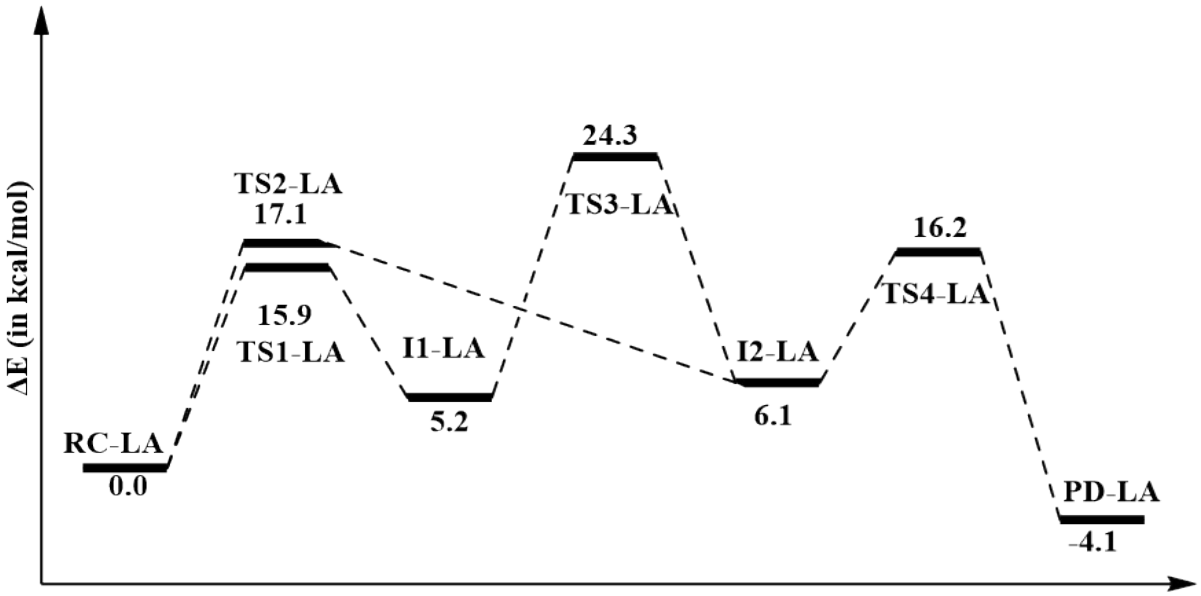

Fig. S2 Energy profile for the LA ($AlCl_3$) catalyzed RCCOM reaction.

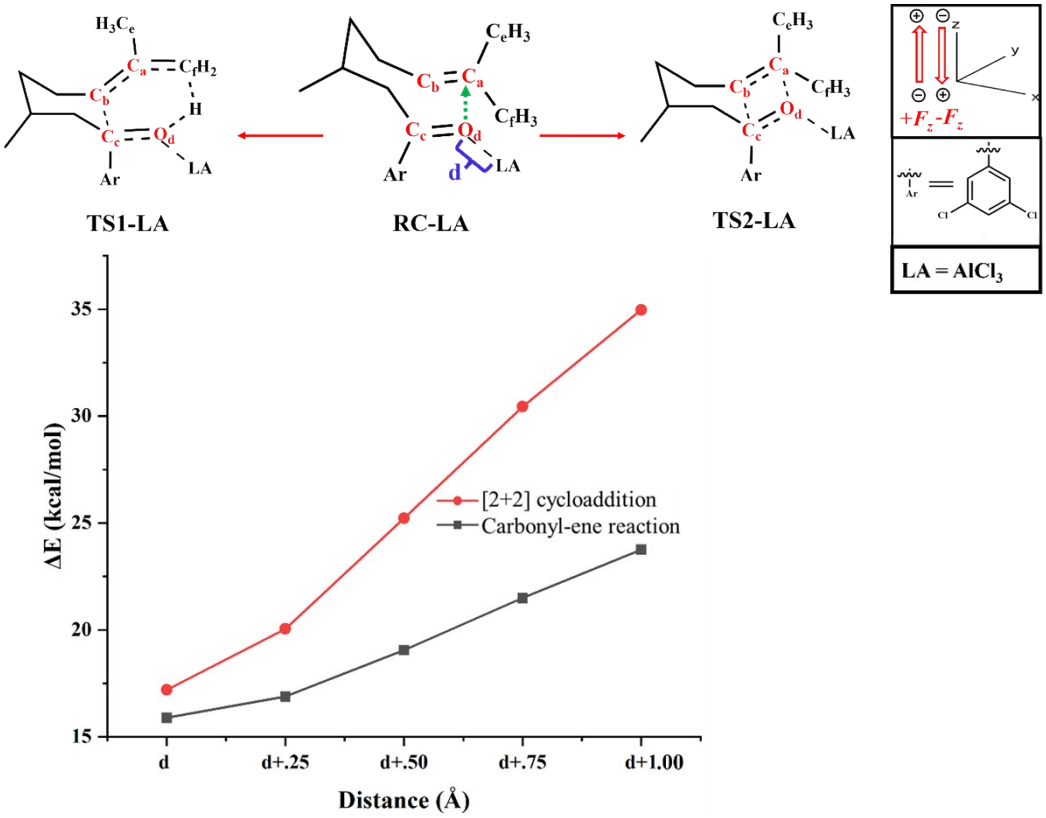

Fig. S3 The relationship between the Energy barrier (ΔE) and distance. ΔE as a function of LA ([$AlCl_3$]) distances are plotted. The black line shows ΔE for the carbonyl-ene reaction ($\Delta E = E_{(TS1\text{-}LA)} - E_{(RC\text{-}LA)}$), and the red line represents ΔE for the [2+2] cycloaddition reaction (ΔE =

$E_{(TS2\text{-}LA)} - E_{(RC\text{-}LA)}$). The 'd' is the distance between the Al of the LA and the carbonyl oxygen (O_d) of the **RC**.

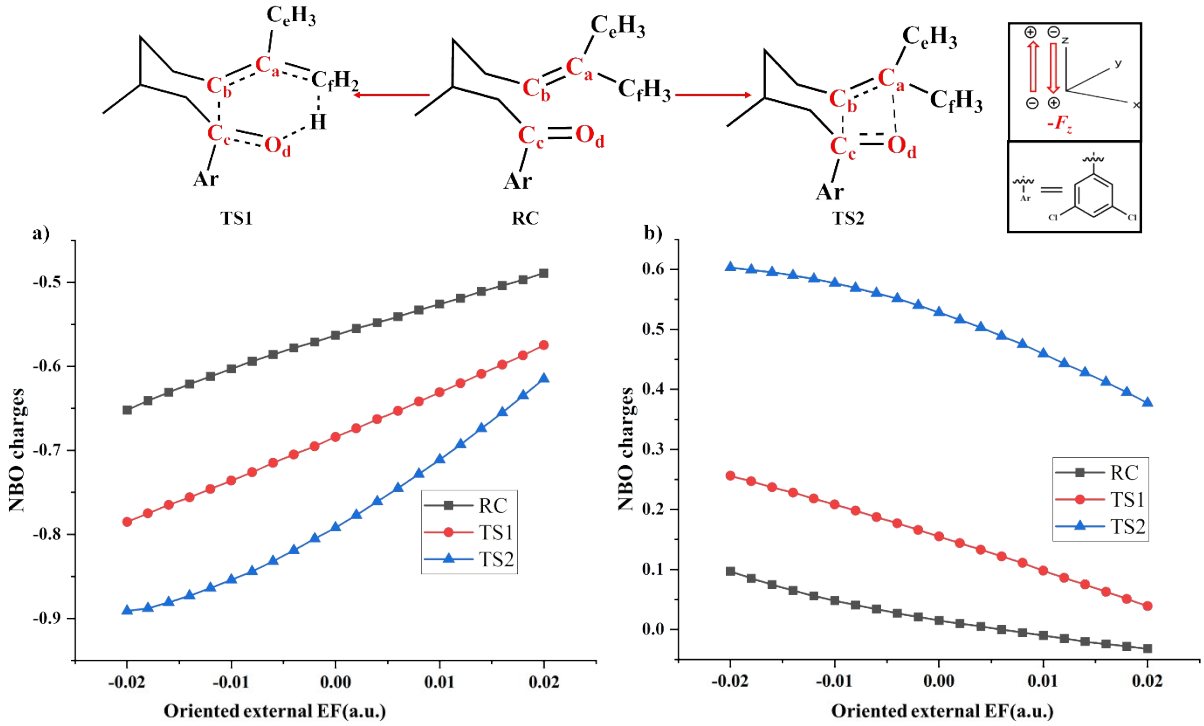

Fig. S4 The charge difference in atoms in the presence of oriented external EF. **a)** Changes in NBO charges for the O_d-atom in the presence of oriented external EF for **RC** (in black), **TS1** (in red), and **TS2** (in blue). **b)** Changes in NBO charges for the C_a-atom in the presence of an oriented external EF are shown for **RC** (in black), **TS1** (in red), and **TS2** (in blue).

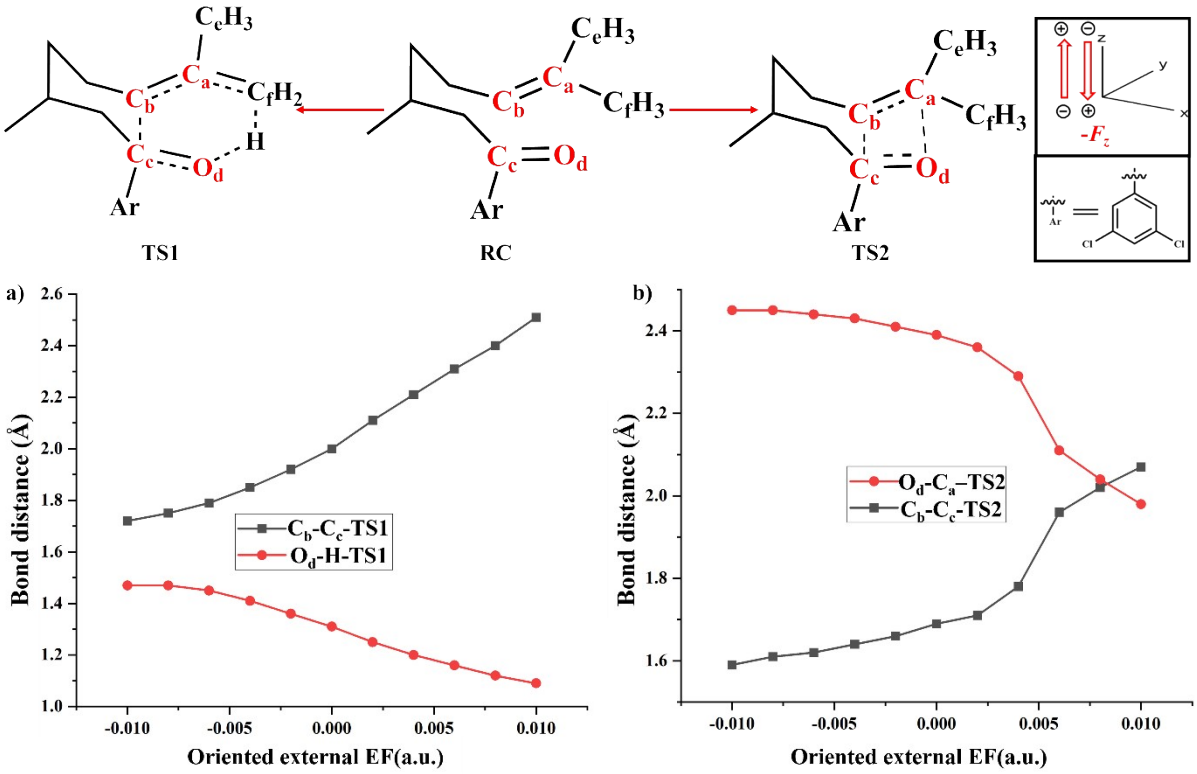

Fig. S5 The relation between the bond distance and the oriented external EF. **a)** The Change in bond distances in the presence of oriented external EF for **TS1**. The black line represents the bond distance between the C_b-C_c bond, while the red line shows the bond distance between the O_d-H bond. **b)** The change in bond distances in the presence of oriented external EF for **TS3**. The black line represents the bond distance between the C_b-C_c, and the red line shows the bond distance between the O_d-C_a.

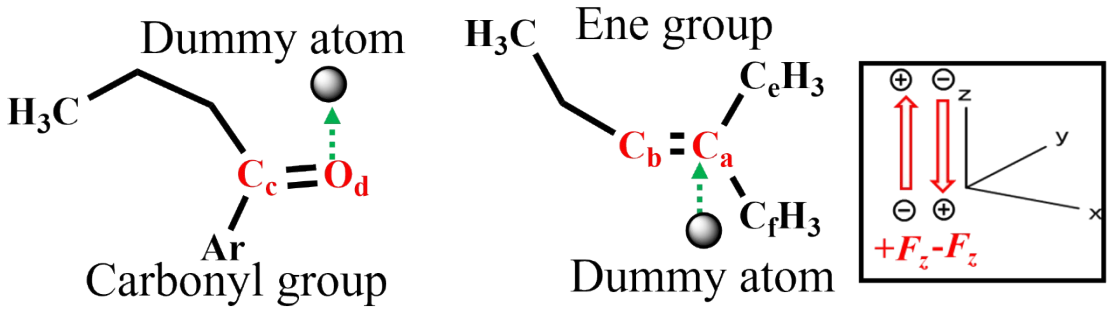

Fig. S6 Fragmentation of the reactants into carbonyl and ene groups, along with positioning a dummy atom to maintain the direction of the oriented external EFs between these groups, even in the absence of either the carbonyl or ene group.

Full citation of Gaussian 16: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A.V. Marenich, J. Bloino, B.G. Janesko, R. Gomperts, B. Mennucci, H.P. Hratchian, J.V. Ortiz, A.F. Izmaylov, J.L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V.G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, Jr., J.A. Montgomery, J.E. Peralta, F. Ogliaro, M.J. Bearpark, J.J. Heyd, E.N. Brothers, K.N. Kudin, V.N. Staroverov, T.A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A.P. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, J.M. Millam, M. Klene, C.Adamo, R.Cammi, J.W. Ochterski, R.L. Martin, K. Morokuma, O. Farkas, J.B. Foresman and D.J. Fox, *Gaussian 16, Revision A.03*; Gaussian, Inc.: Wallingford, CT, 2016.

Coordinates of the optimized geometries for the RCCOM reaction

The Cartesian coordinates of the saddle points and their corresponding energies in Hartree calculated at the B1 level of theory using the SMD model with 1,2-dichloroethane as a solvent. The associated imaginary frequencies are provided in cm^{-1}

RC-LA ($[AlCl_2]^+[SbF_6]^-$)				**I1-LA ($[AlCl_2]^+[SbF_6]^-$)**			
Energy = -3618.0378				Energy = -3618.0304			
Imaginary frequency = 0				Imaginary frequency = 0			
C	-1.815139	-0.711479	-0.514075	C	-1.947387	-0.363843	-0.409936
C	-2.091111	0.736950	-0.513041	C	-1.399955	1.035751	-0.117529
C	-2.774666	-1.693974	-1.113032	C	-1.272184	-0.988619	-1.641656
C	-2.660337	-3.176656	-0.705064	C	-1.844414	-2.348659	-2.073584
C	-3.285811	-3.470661	0.670628	C	-3.361162	-2.222262	-2.282015
C	-2.647040	-2.749081	1.873612	C	-4.043818	-1.745508	-0.993338
H	-3.210815	-4.561771	0.839547	H	-3.782414	-3.197733	-2.592278
H	-4.368778	-3.229770	0.626517	H	-3.557179	-1.501226	-3.102942
C	-2.984378	-1.285141	1.969316	C	-3.512289	-0.371274	-0.528933

H	-1.556249	-2.913372	1.868126	H	-3.871488	-2.498806	-0.202448
H	-3.025974	-3.241639	2.795228	H	-5.137848	-1.659086	-1.127723
C	-2.188630	-0.269135	2.412303	C	-4.146147	0.132640	0.768313
O	-0.624194	-1.081761	-0.247947	O	-1.617390	-1.257959	0.754929
C	-3.318552	-4.043747	-1.789901	C	-1.105110	-2.848109	-3.319519
H	-1.591171	-3.455927	-0.658899	H	-1.678453	-3.074258	-1.255160
H	-3.246310	-5.115849	-1.526704	H	-1.246436	-2.144663	-4.164751
H	-2.828438	-3.890294	-2.770784	H	-1.482002	-3.841364	-3.631452
H	-4.391727	-3.787675	-1.896050	H	-0.018729	-2.932280	-3.123053
C	-1.001432	1.632581	-0.400225	C	-0.871556	1.394860	1.133110
C	-1.240332	3.011797	-0.432484	C	-0.365671	2.690559	1.326055
C	-2.541051	3.530647	-0.552684	C	-0.389671	3.655385	0.309721
C	-3.612379	2.622352	-0.639480	C	-0.954311	3.283569	-0.921420
C	-3.408960	1.238399	-0.630837	C	-1.456682	1.995713	-1.146772
H	0.014604	1.253057	-0.308515	H	-0.840933	0.696151	1.971722
Cl	0.108630	4.118168	-0.309089	Cl	0.320050	3.109718	2.883568
Cl	-5.245980	3.244260	-0.740367	Cl	-1.020607	4.463916	-2.217061
H	-4.271090	0.569408	-0.679279	H	-1.889377	1.747665	-2.120392
C	-0.731238	-0.416379	2.753551	C	-4.484373	1.599841	0.833046
H	-0.363592	-1.454216	2.705529	H	-4.899128	1.880620	1.818195
H	-0.539766	-0.026398	3.774145	H	-5.231455	1.838983	0.048053
H	-0.119230	0.208499	2.071418	H	-3.599049	2.228611	0.622295
C	-2.738997	1.121578	2.583711	C	-4.362208	-0.695794	1.819143
H	-3.788822	1.204118	2.250780	H	-4.209160	-1.782902	1.759645
H	-2.122983	1.855327	2.026339	H	-4.771728	-0.304282	2.760927
H	-2.682889	1.420771	3.651492	H	-1.406138	-0.273901	-2.472583
H	-3.816122	-1.350488	-1.013409	H	-0.183987	-1.046517	-1.471954
H	-2.532426	-1.602865	-2.198354	Cl	0.412357	-3.901189	0.461454
Cl	1.202123	-2.388592	-2.500027	F	1.126585	-0.784429	0.696868
F	2.057453	-1.086779	0.350340	F	2.981363	1.199379	1.025421
F	1.853106	1.520923	1.213056	F	3.787373	-1.361103	0.560523
F	4.132545	0.127285	1.698961	Al	0.006893	-2.009975	1.316801
Al	0.818290	-2.140224	-0.425223	Sb	2.798461	-0.040115	-0.437677

Sb	3.208879	0.694709	0.106692	Cl	-0.127281	-1.876315	3.432357
Cl	0.853829	-3.894953	0.785310	F	2.292860	-1.413055	-1.705807
F	4.373052	-0.411890	-0.958891	F	1.519478	1.143674	-1.265312
F	2.079722	0.966135	-1.443661	F	4.303265	0.595158	-1.446440
F	4.228419	2.304143	-0.137656	H	0.014299	4.659515	0.469920
H	-2.717987	4.610781	-0.567096	H	-3.716873	0.362452	-1.330098
H	-4.031864	-1.032537	1.737945	H	-2.297425	-1.094089	1.466964

I2-LA ($[AlCl_2]^+[SbF_6]^-$)				**PD-LA ($[AlCl_2]^+[SbF_6]^-$)**			
Energy = -3618.0352				Energy = -3618.0450			
Imaginary frequency = 0				Imaginary frequency = 0			
C	-1.575851	1.134647	-0.430221	C	3.528381	-0.466756	0.754572
C	-0.329893	1.893382	-0.006500	C	1.857650	-2.359676	0.540277
C	-1.438672	0.439955	-1.782946	H	2.717754	-1.650393	-1.839851
C	-2.718516	-0.287491	-2.213741	C	2.237025	-0.997169	0.997816
C	-3.905862	0.695262	-2.365106	C	0.378197	-2.632211	0.319432
C	-3.843668	1.948509	-1.446256	C	0.093040	-3.878385	-0.538267
H	-4.846997	0.139132	-2.198544	C	0.950823	-5.053672	-0.039755
H	-3.939361	1.050259	-3.413374	C	2.450759	-4.726251	-0.142189
C	-2.937666	1.867822	-0.209470	H	0.720915	-5.972715	-0.612933
H	-4.858706	2.236811	-1.114664	H	0.686745	-5.254506	1.019424
H	-3.462153	2.802470	-2.036381	C	2.784117	-3.331821	0.325311
C	-3.271725	0.891562	0.952008	H	2.789852	-4.833523	-1.197316
O	-1.963988	0.120390	0.633173	H	3.054411	-5.459323	0.430933
C	-2.472509	-1.096125	-3.493043	C	-1.404625	-4.207582	-0.540753
H	-2.959348	-1.008140	-1.413659	H	0.407927	-3.649076	-1.579110
H	-3.391545	-1.629344	-3.805498	H	-1.621289	-5.073050	-1.197634
H	-1.671876	-1.844063	-3.334835	H	-2.001782	-3.344631	-0.889189
H	-2.163853	-0.429065	-4.323096	H	-1.745157	-4.461218	0.483499
C	0.264197	1.713094	1.254907	C	1.283825	-0.173476	1.644334
C	1.444027	2.404627	1.570671	C	1.629310	1.127686	2.038210
C	2.042670	3.299415	0.672068	C	2.901207	1.670980	1.792398
C	1.410014	3.492120	-0.567148	C	3.834895	0.841620	1.150031

C	0.239549	2.804946	-0.918410	H	0.273811	-0.540397	1.839852
H	-0.167242	1.041032	1.998222	Cl	0.436623	2.109454	2.868085
Cl	2.190621	2.137240	3.134291	Cl	5.439077	1.480985	0.804453
Cl	2.119181	4.613453	-1.715254	H	4.284513	-1.064528	0.238729
H	-0.211931	2.973270	-1.900196	H	-0.121055	-2.746300	1.303281
C	-3.149241	1.508071	2.332915	H	-0.095680	-1.747739	-0.140148
H	-2.238348	2.124744	2.417492	H	3.151811	2.694422	2.086570
H	-3.146952	0.728139	3.114319	H	3.847383	-3.117436	0.502853
H	-4.029266	2.161112	2.486066	C	2.467957	0.473141	-2.068615
C	-4.459892	-0.040089	0.838525	O	1.260669	0.447559	-1.693610
H	-4.516517	-0.551460	-0.133115	C	3.203373	1.750006	-2.239219
H	-5.378614	0.559912	0.974620	H	2.623265	2.623143	-1.902286
H	-1.186153	1.218112	-2.526747	H	3.455266	1.841231	-3.317320
H	-0.581829	-0.251592	-1.753618	H	4.172399	1.689226	-1.708422
Cl	-2.107277	-3.158932	0.185977	C	3.109070	-0.812564	-2.443359
F	0.420006	-1.209851	0.643388	H	4.208414	-0.747786	-2.403866
F	3.117397	-0.761763	0.846676	H	2.813154	-0.994070	-3.500974
F	2.162715	-3.282790	0.427202	Cl	-1.243834	1.433095	-3.324134
Al	-1.257049	-1.490216	1.183148	F	-1.050290	0.598189	-0.204298
Sb	2.136941	-1.630246	-0.566376	F	-2.751523	1.288654	1.893381
Cl	-1.266565	-1.552781	3.309154	F	-3.524707	1.585818	-0.693032
F	0.839787	-2.391354	-1.785498	Al	-0.206850	1.538512	-1.474209
F	1.835444	0.099511	-1.373771	Sb	-3.043592	0.082978	0.421465
F	3.665904	-2.050566	-1.650139	Cl	0.236648	3.459588	-0.686973
H	2.966078	3.828209	0.926775	F	-3.008067	-1.052648	-1.142213
H	-2.786195	2.885308	0.184902	F	-2.204508	-1.318037	1.454733
H	-4.424033	-0.792214	1.649102	F	-4.837629	-0.386488	0.920000
TS1-LA ($[AlCl_2]^+[SbF_6]^-$)				**TS2-LA ($[AlCl_2]^+[SbF_6]^-$)**			
Energy = -3618.0192				Energy = -3618.0149			
Imaginary frequency = -1024.84				Imaginary frequency = -140.66			
C	1.906596	0.900267	0.295560	C	-1.638901	-0.924184	-0.381698
C	2.271324	-0.546043	-0.068818	C	-2.030421	0.527895	-0.055755
C	2.693938	1.889433	-0.591254	C	-0.945630	-0.900921	-1.758837

C	2.467310	3.371042	-0.258977	C	-0.752427	-2.266384	-2.428520
C	2.849169	3.616252	1.209939	C	-2.129685	-2.936816	-2.554557
C	2.022542	2.723999	2.143035	C	-2.702715	-3.208421	-1.158206
H	2.684374	4.678533	1.473101	H	-2.045733	-3.895297	-3.101681
H	3.931503	3.407422	1.339474	H	-2.805747	-2.280071	-3.141394
C	2.217893	1.219030	1.847629	C	-2.881698	-1.928800	-0.311473
H	0.958878	2.992627	2.016156	H	-2.002666	-3.899656	-0.659950
H	2.285247	2.901065	3.202443	H	-3.681106	-3.721498	-1.214851
C	1.310913	0.299896	2.613041	C	-2.929171	-2.151922	1.171001
O	0.494258	1.089927	0.142214	O	-0.810414	-1.457274	0.638473
C	3.253627	4.260240	-1.228344	C	-0.041342	-2.099311	-3.775897
H	1.389092	3.606866	-0.370241	H	-0.121033	-2.895384	-1.771094
H	3.095820	5.331072	-0.995167	H	0.115677	-3.080175	-4.265849
H	2.935804	4.081953	-2.273939	H	0.944384	-1.615866	-3.637791
H	4.339659	4.049100	-1.157743	H	-0.642457	-1.466017	-4.459538
C	1.285259	-1.467228	-0.459955	C	-1.317933	1.255615	0.909644
C	1.653413	-2.789497	-0.759889	C	-1.624692	2.609056	1.121366
C	2.983933	-3.226913	-0.681827	C	-2.643423	3.261145	0.411181
C	3.952080	-2.286894	-0.287018	C	-3.350070	2.507872	-0.543556
C	3.616054	-0.960155	0.016918	C	-3.054232	1.160180	-0.789520
H	0.234730	-1.182862	-0.513920	H	-0.520444	0.789289	1.488619
Cl	0.405601	-3.925671	-1.239452	Cl	-0.696130	3.512284	2.305495
Cl	5.627839	-2.795222	-0.163642	Cl	-4.634787	3.284421	-1.455911
H	4.395088	-0.262051	0.337587	H	-3.613786	0.610790	-1.553985
C	-0.048329	0.585488	2.654447	C	-3.529092	-1.134315	2.048357
H	-0.407629	1.624629	2.674145	H	-3.807297	-0.196347	1.549108
H	-0.736333	-0.168748	3.054704	H	-2.883676	-0.964968	2.932209
H	0.029443	0.666280	1.284479	H	-4.446149	-1.620858	2.456065
C	1.839045	-1.014200	3.079494	C	-2.575824	-3.439868	1.790041
H	2.620589	-1.417773	2.413130	H	-1.680474	-3.895020	1.335301
H	1.033489	-1.752426	3.237893	H	-3.421476	-4.120987	1.532780
H	2.328922	-0.821814	4.059926	H	-1.540189	-0.264765	-2.441020
H	3.767014	1.665005	-0.454343	H	0.017647	-0.384193	-1.606603

H	2.447133	1.669465	-1.644668	Cl	1.854140	-3.358790	0.281078
Cl	0.082044	1.633144	-3.108539	F	1.730917	-0.209269	0.910051
F	-1.853747	0.317361	-1.022931	F	2.936819	2.236950	0.982099
F	-3.316219	-1.994475	-1.175582	F	4.349302	0.050488	0.153426
F	-1.663892	-1.612481	0.952185	Al	0.804449	-1.745758	1.220541
Al	-0.657083	1.676080	-1.110875	Sb	2.787448	0.988537	-0.479493
Sb	-3.225758	-0.705372	0.251716	Cl	0.731265	-1.890803	3.363244
Cl	-1.628174	3.459611	-0.469071	F	2.455088	-0.453215	-1.731466
F	-2.881815	0.761018	1.468602	F	1.072887	1.751746	-0.945269
F	-4.577084	0.356989	-0.617979	F	3.756807	2.067309	-1.743698
F	-4.451282	-1.611941	1.420838	H	-2.876038	4.315743	0.588301
H	3.258968	-4.259764	-0.916895	H	-3.794301	-1.386211	-0.619806
H	3.273359	0.938779	2.001906	H	-2.488648	-3.372760	2.886389
TS3-LA ($[AlCl_2]^+[SbF_6]^-$)				**TS4-LA ($[AlCl_2]^+[SbF_6]^-$)**			
Energy = -3618.0049				Energy = -3618.0154			
Imaginary frequency = -681.21				Imaginary frequency = -211.43			
C	-1.868324	0.482385	-0.144310	C	-1.970863	1.708735	0.492136
C	-0.857537	1.594906	0.169985	C	-3.112260	0.808963	0.600946
C	-1.599529	-0.173012	-1.520827	C	-1.034056	1.884878	1.628310
C	-2.763629	-1.068372	-1.966332	C	0.384661	2.330212	1.230568
C	-3.978214	-0.180980	-2.334347	C	0.361353	3.598785	0.357368
C	-3.981499	1.166775	-1.574178	C	-0.831833	3.651115	-0.632666
H	-4.914669	-0.740765	-2.161628	H	1.319720	3.651057	-0.188871
H	-3.944595	0.045925	-3.417922	H	0.317558	4.488851	1.014596
C	-3.398026	1.133584	-0.149312	C	-1.671641	2.374484	-0.738925
H	-5.000693	1.593304	-1.532300	H	-0.504481	3.959008	-1.638610
H	-3.366721	1.890769	-2.136203	H	-1.548548	4.426204	-0.297878
C	-4.230045	0.482638	0.914933	C	-0.898620	0.965879	-1.680464
O	-1.797598	-0.530008	0.853028	O	-0.421082	0.006413	-0.825881
C	-2.347120	-1.990368	-3.117586	C	1.268918	2.512723	2.467301
H	-3.031809	-1.704045	-1.100293	H	0.796438	1.511137	0.625069
H	-3.196370	-2.621681	-3.445696	H	2.304653	2.754708	2.163659
H	-1.516357	-2.653408	-2.810788	H	1.302327	1.590006	3.074680

H	-2.009117	-1.393263	-3.988476	H	0.889609	3.339479	3.101658
C	-0.135368	1.604829	1.375169	C	-4.328022	1.121806	-0.062397
C	0.825955	2.603361	1.599398	C	-5.404777	0.232236	0.023170
C	1.077399	3.615995	0.662512	C	-5.298058	-0.984961	0.720929
C	0.313503	3.608770	-0.516879	C	-4.079505	-1.289887	1.356330
C	-0.645867	2.620440	-0.773019	C	-2.994139	-0.406644	1.324312
H	-0.302893	0.845458	2.142181	H	-4.436104	2.063005	-0.608187
Cl	1.745378	2.577596	3.093924	Cl	-6.913206	0.630240	-0.767389
Cl	0.585081	4.866401	-1.711962	Cl	-3.923239	-2.810088	2.204645
H	-1.211856	2.644912	-1.708949	H	-2.050338	-0.689103	1.796343
C	-3.752473	0.555758	2.227548	C	0.218453	1.610221	-2.490185
H	-2.826399	-0.218411	1.762550	H	0.628088	0.808536	-3.138272
H	-4.324020	0.076963	3.035265	H	1.027046	1.975668	-1.837811
H	-3.085614	1.387374	2.505686	H	-0.148898	2.421993	-3.140211
C	-5.361916	-0.417149	0.570486	C	-2.040225	0.434685	-2.538467
H	-5.896418	-0.771414	1.467456	H	-1.633558	-0.394600	-3.147877
H	-4.981020	-1.283672	-0.005107	H	-2.442758	1.213974	-3.209100
H	-1.424105	0.609708	-2.277904	H	-2.854525	0.023784	-1.917191
H	-0.658224	-0.741500	-1.451307	H	-1.520096	2.689199	2.236355
Cl	-1.009406	-3.663066	0.164204	H	-1.019913	1.003832	2.294749
F	0.936194	-1.173624	0.672641	H	-6.142710	-1.680195	0.765970
F	1.718506	0.682830	-1.248680	H	-2.543379	2.524836	-1.390845
F	3.374624	0.041201	0.805202	Al	0.470064	-1.485476	-0.987233
Al	-0.639318	-1.844525	1.214251	Cl	0.282419	-2.470211	-2.893063
Sb	2.583548	-0.938554	-0.653843	Cl	0.152710	-2.763411	0.698978
Cl	-0.559632	-2.006882	3.344300	Sb	3.676265	-0.124372	0.262122
F	3.184704	-2.604322	0.109903	F	4.856456	-0.173359	-1.261645
F	1.510029	-1.927299	-1.926672	F	2.239992	-0.999306	-1.014396
F	4.094462	-0.746225	-1.827736	F	3.001436	1.581261	-0.363942
H	1.837275	4.382430	0.843214	F	2.259298	-0.236512	1.576356
H	-3.251089	2.174560	0.185457	F	4.930698	0.708608	1.460085
H	-6.059025	0.112657	-0.108002	F	4.204814	-1.921683	0.718113
RC-LA($AlCl_3$)				**I1-LA($AlCl_3$)**			

Energy = -3239.0347			
Imaginary frequency = 0			
C	0.141114	-0.585875	-0.495556
C	-1.278819	-0.171662	-0.486397
C	0.600996	-1.834539	-1.187834
C	1.989674	-2.389983	-0.806149
C	1.972516	-3.196325	0.505449
C	1.557509	-2.413656	1.767543
H	2.993931	-3.593444	0.660373
H	1.306212	-4.075517	0.377658
C	0.076600	-2.158801	1.870807
H	2.134759	-1.474233	1.821981
H	1.861072	-3.016986	2.650588
C	-0.553684	-1.070385	2.394039
O	0.995861	0.263834	-0.110044
C	2.519522	-3.253521	-1.961589
H	2.682734	-1.539068	-0.672931
H	3.511210	-3.674969	-1.709560
H	2.620730	-2.654730	-2.887381
H	1.830651	-4.097150	-2.168131
C	-1.578237	1.185436	-0.213591
C	-2.913182	1.608249	-0.228440
C	-3.966057	0.716344	-0.496974
C	-3.646170	-0.629428	-0.751446
C	-2.322808	-1.085583	-0.757293
H	-0.772235	1.897193	-0.013558
Cl	-3.285071	3.285794	0.104186
Cl	-4.943766	-1.766367	-1.050691
H	-2.119367	-2.142037	-0.945923
C	0.150778	0.170832	2.869429
H	1.249770	0.088722	2.868034
H	-0.182219	0.430151	3.895229
H	-0.135315	1.029712	2.225970

Energy = -3239.0286			
Imaginary frequency = 0			
C	0.262195	-0.952179	0.165261
C	-1.111466	-0.340971	-0.125712
C	0.855386	-1.650601	-1.070536
C	2.167534	-2.414242	-0.818585
C	1.975205	-3.401692	0.342833
C	1.530652	-2.665265	1.612108
H	2.920187	-3.946115	0.533201
H	1.211755	-4.155733	0.057895
C	0.194331	-1.919450	1.404935
H	2.318941	-1.945435	1.900913
H	1.403747	-3.365822	2.458244
C	-0.294810	-1.171810	2.645209
O	1.200282	0.141285	0.543116
C	2.630868	-3.102820	-2.107079
H	2.943177	-1.687024	-0.516233
H	1.873022	-3.832870	-2.456992
H	3.580787	-3.647318	-1.941467
H	2.793501	-2.363615	-2.915736
C	-1.412325	0.997787	0.179587
C	-2.714630	1.479731	-0.033400
C	-3.735063	0.665660	-0.546783
C	-3.411005	-0.669672	-0.839984
C	-2.121797	-1.180775	-0.636147
H	-0.663331	1.675116	0.595937
Cl	-3.076180	3.150687	0.357914
Cl	-4.660024	-1.727744	-1.472130
H	-1.917500	-2.233649	-0.851966
C	-1.770034	-1.249147	2.946550
H	-2.039255	-0.644301	3.831631
H	-2.051043	-2.305856	3.137058
H	-2.378018	-0.916597	2.084424

C	-2.054978	-1.033403	2.518891	C	0.552588	-0.453051	3.420277
H	-2.535949	-1.918760	2.065728	H	1.641670	-0.453739	3.269152
H	-2.462805	-0.119805	2.042045	H	0.173347	0.116861	4.280288
H	-2.347994	-0.981451	3.588838	H	0.099153	-2.374042	-1.423212
H	-0.162055	-2.628468	-1.139234	H	0.971956	-0.901770	-1.875315
H	0.624540	-1.506385	-2.253369	Cl	4.166220	0.798747	-0.673089
Cl	3.069490	1.061404	-2.352599	Al	2.152413	1.493965	-0.408736
Al	2.496811	1.294631	-0.285312	Cl	1.985367	3.051043	1.074460
Cl	3.984930	0.591103	1.104495	H	-4.745017	1.054278	-0.709769
H	-5.006432	1.056890	-0.500402	H	-0.570831	-2.664202	1.119363
H	-0.563133	-2.996252	1.547155	H	1.022580	0.379601	1.492190
Cl	1.814289	3.288625	0.188196	Cl	1.128251	1.893820	-2.247870
I2-LA($AlCl_3$)				**PD-LA($AlCl_3$)**			
Energy = -3239.0315				Energy = -3239.0403			
Imaginary frequency = 0				Imaginary frequency = 0			
C	-0.066549	0.998184	0.204815	C	0.413484	2.389185	-0.402572
C	1.343536	0.448860	0.074650	C	2.352484	0.923378	0.299307
C	-0.510467	1.844377	-0.988499	H	1.747939	0.187697	-2.077128
C	-1.915479	2.437428	-0.800950	C	0.993204	1.481833	0.518031
C	-1.979088	3.373778	0.433392	C	2.640657	-0.456344	0.871529
C	-0.962855	3.044421	1.562197	C	3.854962	-1.147760	0.223744
H	-3.012054	3.367279	0.827598	C	5.038349	-0.166280	0.163831
H	-1.784302	4.412363	0.101817	C	4.685649	1.073874	-0.676108
C	-0.395870	1.618555	1.598573	H	5.935708	-0.664888	-0.251122
H	-1.396006	3.276024	2.553222	H	5.287887	0.145102	1.199565
H	-0.084251	3.707091	1.451142	C	3.300889	1.602311	-0.399072
C	-1.311680	0.404260	1.906085	H	4.754068	0.827745	-1.759889
O	-1.055170	-0.110674	0.467285	H	5.428158	1.882321	-0.516456
C	-2.383062	3.148579	-2.076555	C	4.206030	-2.443056	0.964591
H	-2.601368	1.588842	-0.630529	H	3.574916	-1.402380	-0.821007
H	-3.392495	3.582344	-1.936026	H	5.035755	-2.978863	0.462970
H	-2.426134	2.443620	-2.929643	H	3.331974	-3.121913	1.014123
H	-1.690831	3.972933	-2.342644	H	4.521554	-2.220905	2.004272

C	1.632686	-0.920825	0.208903	C	0.229478	1.076436	1.638769
C	2.964447	-1.356254	0.111969	C	-1.054876	1.601060	1.839762
C	4.025627	-0.465128	-0.108698	C	-1.643648	2.501715	0.936308
C	3.711825	0.899606	-0.225280	C	-0.881303	2.877715	-0.181065
C	2.392375	1.367464	-0.137978	H	0.638419	0.364542	2.360598
H	0.844695	-1.650809	0.403941	Cl	-1.957465	1.124479	3.266433
Cl	3.311629	-3.068187	0.277315	Cl	-1.588383	3.982724	-1.355199
Cl	5.011914	2.049384	-0.488225	H	0.965548	2.698791	-1.294431
H	2.187706	2.439009	-0.226580	H	2.809143	-0.374487	1.967307
C	-0.714910	-0.573694	2.902749	H	1.744267	-1.091892	0.755556
H	0.341632	-0.790704	2.669530	H	-2.656542	2.884359	1.091599
H	-1.290998	-1.514560	2.931947	H	3.065973	2.598346	-0.801105
H	-0.761054	-0.097942	3.900945	C	-0.371681	-0.141048	-2.116036
C	-2.789689	0.632696	2.139315	O	-0.365426	-0.974453	-1.170400
H	-3.249890	1.266204	1.368034	C	-1.632354	0.460230	-2.622818
H	-2.900468	1.132529	3.119621	H	-2.471415	0.330202	-1.921807
H	0.227111	2.661122	-1.101157	H	-1.862139	-0.064655	-3.576510
H	-0.456817	1.229429	-1.904355	H	-1.479048	1.523373	-2.877818
Cl	-3.926307	-0.894566	-0.909157	C	0.917889	0.136662	-2.804953
Al	-1.867775	-1.439510	-0.578223	H	0.868735	1.042186	-3.430236
Cl	-1.680109	-3.229835	0.609637	H	1.111410	-0.740423	-3.460401
H	5.058632	-0.818882	-0.182843	Cl	-2.006029	-3.587989	-1.684285
H	0.484019	1.609581	2.262317	Al	-1.558138	-2.067366	-0.222606
H	-3.323254	-0.333692	2.186559	Cl	-3.293484	-0.938510	0.365151
Cl	-0.734569	-1.521301	-2.405595	Cl	-0.417485	-2.802606	1.447283
TS1-LA($AlCl_3$)				**TS2-LA($AlCl_3$)**			
Energy = -3239.0131				Energy = -3239.0078			
Imaginary frequency = -913.85				Imaginary frequency = -165.94			
C	0.253406	-0.912273	0.166799	C	0.046786	-0.827385	0.080552
C	-1.154106	-0.354787	-0.110401	C	-1.389939	-0.285926	-0.040798
C	0.758515	-1.755580	-1.029603	C	0.355230	-1.587881	-1.228239
C	2.089230	-2.487089	-0.797829	C	1.618729	-2.457649	-1.203998
C	1.964166	-3.395264	0.434741	C	1.486169	-3.458909	-0.045389

C	1.578209	-2.580934	1.674039	C	1.439996	-2.704958	1.288188
H	2.923225	-3.916635	0.618972	H	2.345386	-4.156529	-0.037618
H	1.198482	-4.175188	0.239168	H	0.568123	-4.066794	-0.189626
C	0.222352	-1.863760	1.495485	C	0.252288	-1.722877	1.390808
H	2.372260	-1.836788	1.861727	H	2.391993	-2.155917	1.374714
H	1.507678	-3.226880	2.569251	H	1.385743	-3.403020	2.144909
C	-0.165940	-0.941149	2.602813	C	0.424531	-0.634298	2.408363
O	1.150244	0.139741	0.458933	O	0.942847	0.235469	0.335988
C	2.488536	-3.266341	-2.056443	C	1.823364	-3.142060	-2.559847
H	2.871824	-1.734017	-0.587713	H	2.496594	-1.814088	-0.996848
H	3.451335	-3.792292	-1.904997	H	0.956154	-3.787269	-2.807869
H	2.597928	-2.588543	-2.925526	H	1.934201	-2.391563	-3.366705
H	1.719428	-4.024656	-2.307870	H	2.731148	-3.776593	-2.549911
C	-1.438674	1.009285	0.079366	C	-1.612578	1.096376	-0.157668
C	-2.747400	1.478465	-0.120943	C	-2.926838	1.571737	-0.299267
C	-3.792982	0.627636	-0.509437	C	-4.032831	0.708325	-0.325789
C	-3.485233	-0.731243	-0.690963	C	-3.781421	-0.670586	-0.210092
C	-2.189233	-1.230277	-0.497299	C	-2.481532	-1.176759	-0.072630
H	-0.662464	1.709387	0.397801	H	-0.771168	1.793125	-0.115960
Cl	-3.088760	3.181944	0.130115	Cl	-3.198465	3.302090	-0.434970
Cl	-4.765785	-1.834930	-1.166822	Cl	-5.140752	-1.784331	-0.237112
H	-1.999841	-2.299327	-0.630769	H	-2.322209	-2.256876	0.012935
C	0.771723	-0.000709	3.043833	C	1.704528	-0.383469	3.086437
H	1.833884	-0.282095	3.117467	H	1.688739	0.535843	3.694447
H	0.437635	0.785148	3.735895	H	2.559283	-0.396456	2.388224
H	0.935263	0.368563	1.785920	H	1.853258	-1.262842	3.756570
C	-1.594308	-0.863075	3.013858	C	-0.752516	0.092602	2.915302
H	-2.285395	-1.063755	2.176878	H	-1.709042	-0.200228	2.461813
H	-1.836241	0.091278	3.513398	H	-0.571894	1.182939	2.827322
H	-1.746865	-1.684591	3.749676	H	-0.776251	-0.099851	4.012026
H	-0.013043	-2.511288	-1.260604	H	-0.503079	-2.244757	-1.464749
H	0.824532	-1.077257	-1.899739	H	0.409060	-0.819454	-2.021985
Cl	1.355626	1.680213	-2.411169	Cl	2.056804	3.133871	0.625220

Al	2.139177	1.387765	-0.420411	Al	2.270431	1.188682	-0.331677
Cl	4.209046	0.751512	-0.428302	Cl	2.171201	1.352087	-2.497835
H	-4.808234	1.006181	-0.663413	H	-5.052432	1.091557	-0.431476
H	-0.574906	-2.602813	1.308298	H	-0.685517	-2.267663	1.610070
Cl	1.871796	3.121218	0.859234	Cl	4.168256	0.270524	0.260464
TS3-LA($AlCl_3$)				**TS4-LA ($AlCl_3$)**			
Energy = -3238.9992				Energy = -3239.0066			
Imaginary frequency = -509.34				Imaginary frequency = -97.38			
C	0.254894	-0.791623	0.137543	C	1.074899	1.305899	0.198798
C	-1.232078	-0.408546	0.048302	C	-0.359126	1.309801	0.008198
C	0.783043	-1.471763	-1.150718	C	1.694818	1.876705	1.417222
C	2.132143	-2.165974	-0.916019	C	2.746219	2.983627	1.033404
C	1.906288	-3.436299	-0.059292	C	3.828747	2.367280	0.132305
C	0.683282	-3.307735	0.879591	C	3.231898	1.709609	-1.119463
H	2.823766	-3.667354	0.510922	H	4.402242	1.628756	0.718071
H	1.727655	-4.299041	-0.730950	H	4.539238	3.158807	-0.175757
C	0.405319	-1.891152	1.411550	C	2.008329	0.792754	-0.845278
H	0.772503	-4.000036	1.737713	H	3.992295	1.109497	-1.651560
H	-0.224444	-3.611597	0.329628	H	2.896159	2.496110	-1.820105
C	1.335571	-1.352563	2.443265	C	2.341303	-0.721000	-0.395922
O	1.031884	0.343826	0.400226	O	1.228540	-1.130989	0.377321
C	2.847645	-2.479295	-2.233882	C	2.051094	4.202355	0.409742
H	2.763599	-1.455064	-0.349266	H	3.209285	3.290921	1.989046
H	3.797513	-3.018624	-2.048260	H	2.786349	5.009147	0.226776
H	3.080430	-1.549451	-2.786813	H	1.264485	4.595653	1.082199
H	2.213908	-3.119903	-2.880138	H	1.571943	3.950015	-0.556786
C	-1.661741	0.863580	0.469419	C	-0.929932	1.215015	-1.294573
C	-3.026688	1.187200	0.414241	C	-2.317705	1.227102	-1.446920
C	-3.990378	0.276418	-0.046466	C	-3.177119	1.283848	-0.334435
C	-3.538887	-0.992116	-0.448165	C	-2.609794	1.348409	0.952824
C	-2.182136	-1.345983	-0.405565	C	-1.226969	1.380036	1.138743
H	-0.944761	1.600403	0.840065	H	-0.302347	1.172364	-2.186194
Cl	-3.546348	2.782363	0.934574	Cl	-3.006658	1.153967	-3.049904

Cl	-4.711656	-2.166693	-1.024273	Cl	-3.667916	1.395126	2.340313
H	-1.877899	-2.349145	-0.717978	H	-0.825530	1.405225	2.153609
C	1.011654	-0.100241	2.998932	C	3.607391	-0.867001	0.457349
H	-0.052029	0.182993	3.052261	H	3.713837	-1.941208	0.699885
H	1.242199	0.367292	1.862154	H	3.540848	-0.319688	1.412943
H	1.674997	0.326034	3.765129	H	4.509325	-0.535953	-0.087457
C	2.668590	-1.960296	2.684994	C	2.501524	-1.554472	-1.677440
H	2.562163	-3.053675	2.821652	H	2.717887	-2.604384	-1.405178
H	3.182284	-1.506888	3.548877	H	3.334732	-1.168617	-2.294559
H	0.053247	-2.208910	-1.525782	H	1.568866	-1.526817	-2.268770
H	0.856283	-0.682034	-1.920420	H	0.961704	2.292292	2.122761
H	-5.050841	0.543015	-0.091036	H	2.251814	1.063526	1.920744
H	-0.593567	-1.881069	1.879288	H	-4.264200	1.272656	-0.465315
H	3.290978	-1.829760	1.776742	H	1.467701	0.668202	-1.792230
Al	1.684517	1.747690	-0.531875	Al	0.001468	-2.388901	0.302737
Cl	1.655780	3.326467	0.959051	Cl	-1.305299	-2.033596	2.017592
Cl	0.425065	2.178371	-2.237436	Cl	0.921628	-4.366908	0.447251
Cl	3.716517	1.291291	-1.145305	Cl	-1.175727	-2.270512	-1.542523
RC				**I1**			
Energy = -1616.1686				Energy = -1616.1663			
Imaginary frequency = 0				Imaginary frequency = 0			
C	-1.079529	-0.038513	-1.142055	C	-1.140147	-0.254202	-0.452015
C	0.370819	0.219121	-0.781796	C	0.372353	0.031409	-0.376334
C	-2.101487	1.062503	-0.873408	C	-1.849198	0.936166	-1.143311
C	-3.575389	0.610923	-0.911928	C	-3.381835	0.805611	-1.178970
C	-4.055911	0.006090	0.425589	C	-3.917264	0.619820	0.251473
C	-3.234168	-1.170700	0.996431	C	-3.267006	-0.587787	0.939720
H	-5.101842	-0.329367	0.281154	H	-5.018415	0.497574	0.229439
H	-4.091416	0.816275	1.185570	H	-3.703743	1.540767	0.835057
C	-1.950042	-0.747853	1.668836	C	-1.729305	-0.456444	1.005363
H	-3.039215	-1.914083	0.201182	H	-3.527949	-1.503023	0.376832
H	-3.871641	-1.683942	1.749773	H	-3.655903	-0.712750	1.968419
C	-0.773668	-1.418277	1.727589	C	-1.050887	-1.620511	1.722608

O	-1.386638	-1.078314	-1.714902	O	-1.409180	-1.398413	-1.253121
C	-4.482354	1.790003	-1.301813	C	-4.014218	2.015884	-1.876981
H	-3.659760	-0.171256	-1.690937	H	-3.625873	-0.109493	-1.753956
H	-5.545317	1.479837	-1.332071	H	-3.781088	2.949575	-1.325261
H	-4.209871	2.192212	-2.297425	H	-5.116699	1.916533	-1.925590
H	-4.391608	2.614280	-0.565048	H	-3.631538	2.128639	-2.910708
C	1.310023	-0.783702	-1.101904	C	1.297435	-0.843994	-0.971484
C	2.655777	-0.604688	-0.763271	C	2.673408	-0.585944	-0.854224
C	3.108986	0.563201	-0.124848	C	3.165785	0.532254	-0.164400
C	2.159504	1.554832	0.173042	C	2.221589	1.400010	0.412482
C	0.801418	1.401219	-0.144208	C	0.843382	1.166652	0.316199
H	0.967382	-1.693398	-1.603407	H	0.946050	-1.720124	-1.523574
Cl	3.810317	-1.878636	-1.124814	Cl	3.818295	-1.696940	-1.595296
Cl	2.690475	3.021279	0.981865	Cl	2.795010	2.812858	1.289864
H	0.097843	2.195659	0.116952	H	0.141093	1.856459	0.794224
C	-0.527369	-2.761109	1.085704	C	0.079565	-1.274947	2.662692
H	-1.324968	-3.063086	0.386109	H	0.482999	-2.173363	3.166276
H	-0.437626	-3.546828	1.866359	H	-0.271876	-0.560020	3.435341
H	0.437511	-2.755951	0.540304	H	0.905758	-0.769713	2.126475
C	0.406708	-0.859884	2.487031	C	-1.423414	-2.904837	1.518252
H	0.188552	0.129403	2.931106	H	-2.268708	-3.174066	0.870245
H	1.285740	-0.759759	1.819055	H	-0.899277	-3.728238	2.025377
H	0.712455	-1.550965	3.301755	H	-1.583053	1.864165	-0.603040
H	-1.884366	1.578940	0.078402	H	-1.443283	1.023820	-2.169712
H	-1.914432	1.814915	-1.671066	H	4.240022	0.723011	-0.079412
H	4.163598	0.692427	0.137662	H	-1.494958	0.473052	1.557017
H	-2.001277	0.217277	2.199978	H	-1.127755	-2.180961	-0.742559
I2				**PD**			
Energy = -1616.1583				Energy = -1616.1741			
Imaginary frequency = 0				Imaginary frequency = 0			
C	-0.928715	0.088425	0.194028	C	-0.994506	-1.586332	0.001788
C	0.588410	-0.017493	0.145643	C	1.372903	-0.819206	-0.494051
C	-1.510171	-0.860245	1.257128	H	1.832846	1.101316	2.708760

C	-3.045788	-0.827989	1.264823	C	-0.103012	-0.631336	-0.549108
C	-3.634227	-1.297107	-0.091424	C	2.248723	0.421413	-0.611479
C	-2.746561	-1.023261	-1.342249	C	3.687287	0.208291	-0.102775
H	-4.630646	-0.832385	-0.217316	C	4.261726	-1.088699	-0.697204
H	-3.812837	-2.389603	-0.038022	C	3.417002	-2.305974	-0.282346
C	-1.634625	0.024660	-1.197726	H	5.313566	-1.228718	-0.380461
H	-3.382201	-0.751671	-2.207144	H	4.263717	-0.996527	-1.803433
H	-2.241249	-1.966979	-1.623682	C	1.932636	-2.050212	-0.353403
C	-1.958392	1.529076	-0.949558	H	3.670623	-2.603715	0.760107
O	-1.382894	1.452156	0.405686	H	3.668269	-3.190012	-0.903619
C	-3.622294	-1.640077	2.431514	C	4.562724	1.428139	-0.411441
H	-3.324198	0.231890	1.414189	H	3.633345	0.080292	0.999275
H	-4.730082	-1.604383	2.430882	H	5.583428	1.303179	0.000733
H	-3.266230	-1.250415	3.405721	H	4.126072	2.351408	0.018365
H	-3.318003	-2.704098	2.356541	H	4.652179	1.573676	-1.507320
C	1.399411	1.042497	0.587758	C	-0.650637	0.537443	-1.130909
C	2.796034	0.903521	0.541099	C	-2.040481	0.715861	-1.175590
C	3.413599	-0.263649	0.062874	C	-2.935037	-0.231320	-0.655757
C	2.577798	-1.306830	-0.374650	C	-2.376863	-1.378411	-0.064997
C	1.179996	-1.201678	-0.339118	H	0.001608	1.310121	-1.545132
H	0.933604	1.963636	0.949686	Cl	-2.688730	2.192870	-1.876886
Cl	3.808735	2.232740	1.091922	Cl	-3.457042	-2.568684	0.651886
Cl	3.315477	-2.780901	-0.989703	H	-0.610133	-2.478323	0.505135
H	0.554532	-2.029607	-0.690486	H	2.284723	0.743811	-1.675066
C	-1.126675	2.477187	-1.816016	H	1.784560	1.260021	-0.061258
H	-0.064467	2.170458	-1.821038	H	-4.017070	-0.072097	-0.684675
H	-1.196782	3.511374	-1.425861	H	1.285512	-2.936135	-0.285946
H	-1.501567	2.468676	-2.858256	C	-0.101407	1.770437	1.985431
C	-3.419575	1.962217	-0.912006	O	0.355851	2.708166	1.345039
H	-4.035238	1.290935	-0.292377	C	-1.594687	1.558161	2.150168
H	-3.835780	1.975615	-1.937366	H	-2.159159	2.245320	1.497214
H	-1.144012	-1.886522	1.055348	H	-1.867991	1.740350	3.210089
H	-1.112883	-0.556828	2.245958	H	-1.860622	0.507398	1.927306

H	4.503398	-0.357148	0.027707	C	0.791515	0.738836	2.653890
H	-0.922542	-0.104435	-2.031335	H	0.764518	-0.189577	2.049454
H	-3.490610	2.987465	-0.499096	H	0.414002	0.479174	3.661867
TS1				**TS2**			
Energy = -1616.1234				Energy = -1616.0895			
Imaginary frequency = -1187.45				Imaginary frequency = -717.84			
C	-1.117178	-0.279675	-0.602699	C	1.094397	-0.282898	0.473432
C	0.363267	0.075424	-0.464159	C	-0.417219	0.033153	0.288276
C	-1.989298	0.899158	-1.081504	C	1.710325	0.927091	1.240436
C	-3.505064	0.670523	-1.018386	C	3.242459	0.994046	1.173223
C	-3.955961	0.532805	0.443740	C	3.670692	1.112489	-0.299553
C	-3.257369	-0.632264	1.153890	C	3.269974	-0.140671	-1.088868
H	-5.052328	0.378128	0.480794	H	4.767878	1.250940	-0.370041
H	-3.745419	1.483736	0.978013	H	3.200876	2.017740	-0.740735
C	-1.748881	-0.460288	1.296099	C	1.751553	-0.400023	-1.088785
H	-3.476692	-1.559269	0.595708	H	3.801158	-0.996555	-0.638142
H	-3.678872	-0.760465	2.172414	H	3.615190	-0.065795	-2.139519
C	-0.920348	-1.576418	1.618690	C	1.317705	-1.786096	-1.323041
O	-1.371775	-1.434495	-1.167422	O	1.339265	-1.468627	1.049853
C	-4.249471	1.806614	-1.732469	C	3.782772	2.150362	2.023674
H	-3.721124	-0.285318	-1.535999	H	3.637411	0.035294	1.568020
H	-5.345120	1.645715	-1.700397	H	3.403911	3.121996	1.645218
H	-3.941734	1.883355	-2.793975	H	3.463299	2.052911	3.080315
H	-4.035166	2.780205	-1.245999	H	4.890334	2.185303	1.998756
C	1.322981	-0.860334	-0.896289	C	-1.344445	-0.836280	0.887803
C	2.688097	-0.582332	-0.733762	C	-2.718115	-0.581936	0.756933
C	3.140747	0.613372	-0.154350	C	-3.206692	0.524736	0.044622
C	2.165142	1.535479	0.264516	C	-2.257718	1.385762	-0.537784
C	0.793961	1.286759	0.118160	C	-0.879708	1.157918	-0.424275
H	0.989049	-1.798528	-1.349112	H	-0.960941	-1.702819	1.436021
Cl	3.874100	-1.771721	-1.259799	Cl	-3.873278	-1.687178	1.500139
Cl	2.690151	3.041786	1.009455	Cl	-2.831103	2.788547	-1.439399
H	0.070926	2.022040	0.483165	H	-0.171182	1.845861	-0.898644

C	-1.204733	-2.832576	1.013440	C	2.249516	-2.929140	-1.203501
H	-2.248668	-3.183754	0.990304	H	1.730200	-3.901778	-1.255036
H	-0.467158	-3.637666	1.165007	H	2.821864	-2.830974	-0.263585
H	-1.180328	-2.324054	-0.222580	H	2.982580	-2.860427	-2.038725
C	0.410939	-1.362258	2.286616	C	-0.019341	-2.054907	-1.903218
H	0.681129	-0.294741	2.355863	H	-0.673779	-1.171893	-1.950811
H	1.215460	-1.911518	1.761032	H	-0.516014	-2.898191	-1.386822
H	0.360780	-1.773057	3.317422	H	0.172183	-2.408560	-2.943040
H	-1.745038	1.812065	-0.509595	H	1.304041	1.889464	0.869517
H	-1.680288	1.086311	-2.130800	H	1.372049	0.805460	2.290119
H	4.208467	0.819179	-0.031009	H	-4.280298	0.713139	-0.053388
H	-1.446925	0.498546	1.745776	H	1.222674	0.303000	-1.757142
TS3				**TS4**			
Energy = -1616.0787				Energy = -1616.0829			
Imaginary frequency = -792.04				Imaginary frequency = -668.42			
C	0.897343	-0.372449	0.284822	C	-0.939333	-0.350525	-0.062775
C	-0.624363	-0.118982	0.167050	C	0.512652	-0.187796	-0.070917
C	1.446391	0.621854	1.369037	C	-1.564518	-1.693241	0.046331
C	2.976810	0.665756	1.385966	C	-2.670748	-1.977483	-1.004894
C	3.477203	1.419912	0.130396	C	-3.734036	-0.870024	-0.913738
C	2.533749	1.269753	-1.092413	C	-3.111288	0.513453	-1.132841
H	4.506411	1.096141	-0.116728	H	-4.206839	-0.918537	0.085753
H	3.548556	2.499593	0.371455	H	-4.530164	-1.044132	-1.664425
C	1.655260	0.004791	-1.139815	C	-1.869244	0.806951	-0.253308
H	3.109097	1.354940	-2.034941	H	-3.858824	1.308817	-0.961501
H	1.822154	2.115400	-1.091166	H	-2.800636	0.601466	-2.192240
C	2.317455	-1.299757	-1.428787	C	-2.135935	1.157392	1.339881
O	1.193789	-1.666811	0.600520	O	-1.770286	0.071747	2.083195
C	3.530668	1.283910	2.675569	C	-2.076033	-2.135921	-2.413431
H	3.310354	-0.389308	1.335222	H	-3.138276	-2.938065	-0.715224
H	4.638265	1.331736	2.652824	H	-2.867248	-2.369874	-3.152819
H	3.229918	0.693121	3.563311	H	-1.329917	-2.954154	-2.435045
H	3.150500	2.317633	2.808166	H	-1.564311	-1.209213	-2.739070

C	-1.518810	-1.133389	0.550410	C	1.124135	0.935174	-0.693130
C	-2.901322	-0.907282	0.462683	C	2.519218	1.050734	-0.712017
C	-3.430158	0.304450	-0.010843	C	3.353331	0.095170	-0.107604
C	-2.514523	1.302608	-0.392374	C	2.737577	-1.007005	0.517483
C	-1.128864	1.111236	-0.304890	C	1.350640	-1.167995	0.533772
H	-1.109198	-2.083180	0.909482	H	0.521557	1.702798	-1.183837
Cl	-4.015677	-2.183046	0.952446	Cl	3.252844	2.431678	-1.507992
Cl	-3.138829	2.836591	-0.996785	Cl	3.752093	-2.209420	1.294059
H	-0.444004	1.912586	-0.603217	H	0.916091	-2.027182	1.050913
C	1.476781	-2.349829	-1.991804	C	-3.580661	1.598563	1.647615
H	0.702314	-1.977624	-2.685736	H	-3.652535	1.813616	2.732319
H	0.944527	-2.579948	-1.002666	H	-4.295390	0.788558	1.413465
H	2.019164	-3.235785	-2.363035	H	-3.874142	2.509163	1.088463
C	3.763742	-1.552307	-1.255205	C	-1.181288	2.350281	1.640142
H	4.236335	-0.956453	-0.463005	H	-1.269563	2.595849	2.716435
H	4.231928	-1.250226	-2.222322	H	-1.434211	3.244719	1.036788
H	1.045544	1.644689	1.223846	H	-0.131432	2.068419	1.439572
H	1.051360	0.236393	2.328854	H	-0.828390	-2.512648	0.066472
H	-4.510076	0.466946	-0.083820	H	-2.063211	-1.595156	1.046619
H	0.877739	0.155604	-1.909762	H	4.442277	0.203819	-0.121379
H	3.971222	-2.629681	-1.125979	H	-1.363289	1.672995	-0.703367