Mechanism of Alkoxy Groups Substitution by Grignard Reagents on Aromatic Rings and Experimental Verification of Theoretical Predictions of Anomalous Reactions.

Gonzalo Jiménez-Osés,[†] Anthony J. Brockway,[‡] Jared T. Shaw,[‡,] and K. N. Houk[†,*]*

† Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, California 90095-1569, United States.

‡ Department of Chemistry, One Shields Ave, University of California, Davis, California 95616, United States.

SUPPORTING INFORMATION

CONTENTS:

Figure S1. Stoichiometry and structure of methyl Grignard–substrate (**1a**) reactant complexes calculated at the B3LYP/6-31G(d) level. Relative free energies (in kcal mol^{-1}) include implicit solvation corrections calculated using the SMD polarizable continuum model and the internally stored parameters for tetrahydrofuran as implemented in Gaussian 09. Both explicitly solvated and unsolvated (energies in parentheses) CH_3MgCl dimers have been considered as starting materials. The isolated reactants have been arbitrarily chosen as the zero level in the relative energies calculations. Both monomer (eq. 1) and dimer (eq. 2) states of the Grignard reagent in the reactant complex have been considered. As can be seen, monomer **1a·CH3MgCl (a)** is the most stable species.

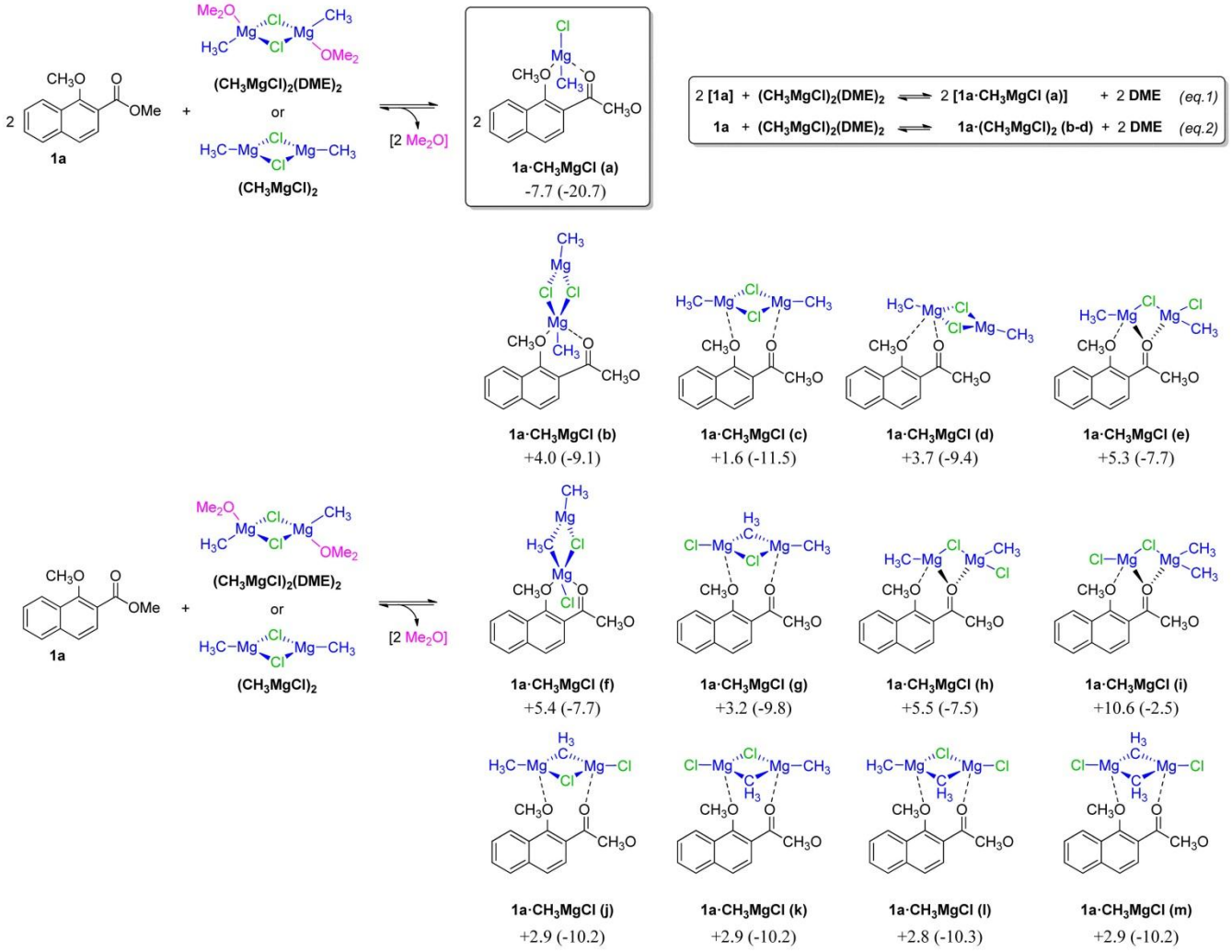
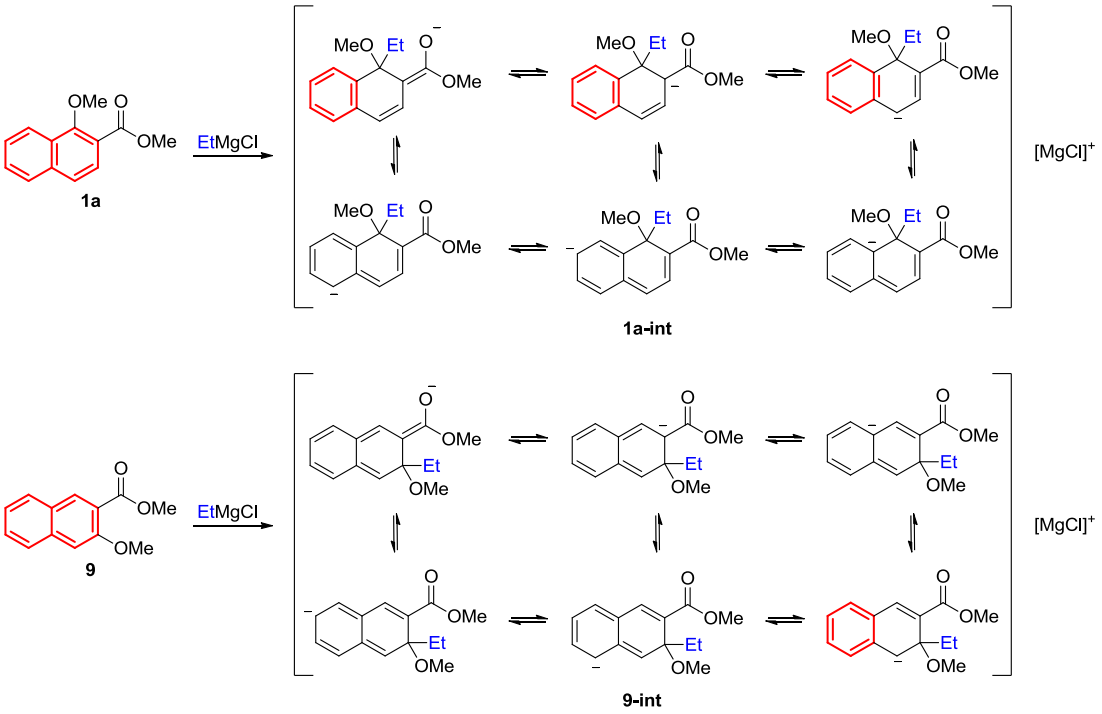
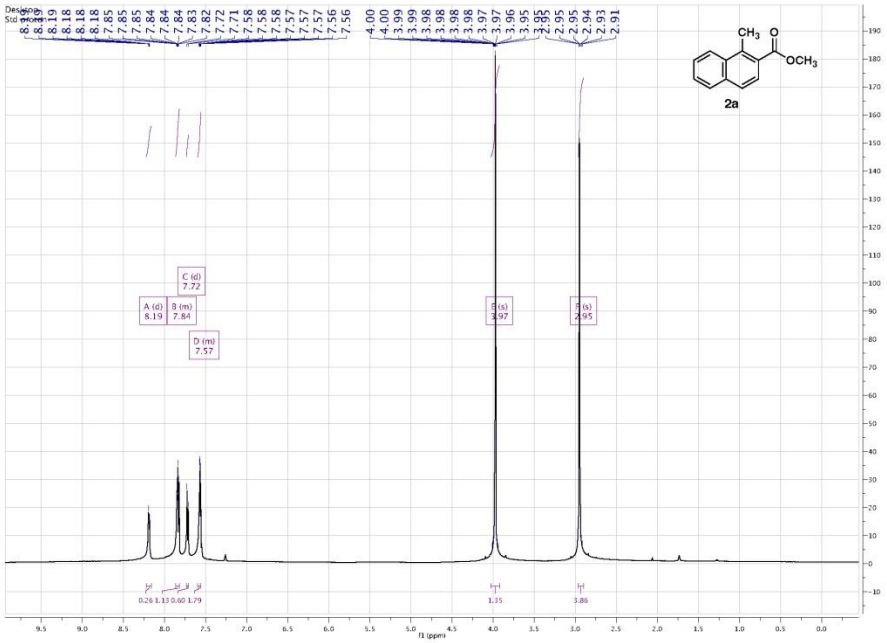
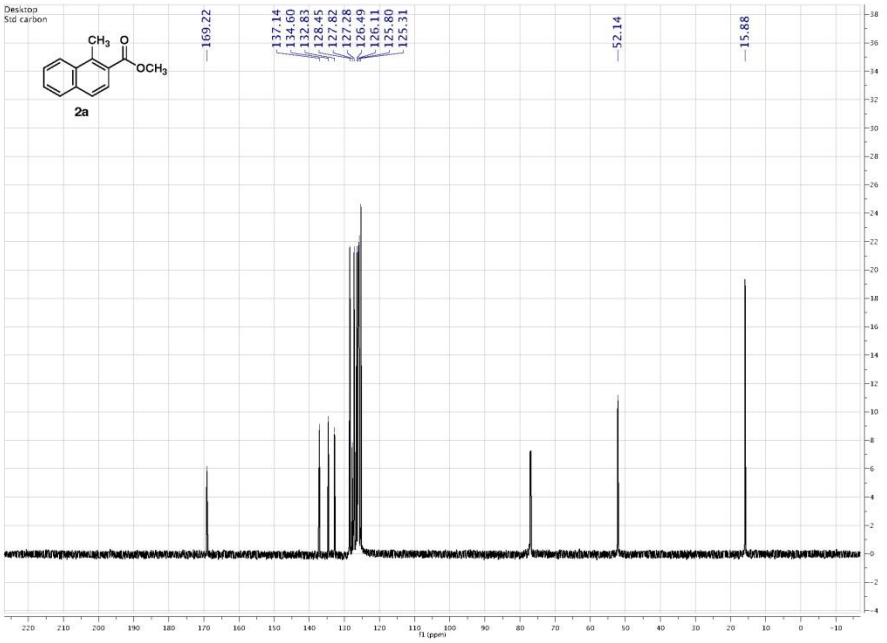


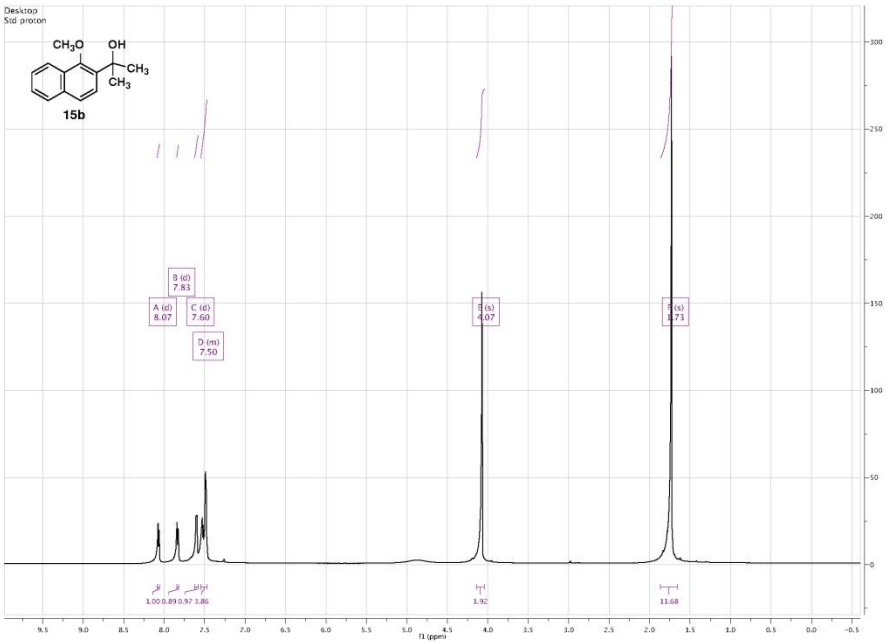
Figure S2. Resonance structures of the enolates derived from the reaction of methyl 1- and 3-methoxy-2-naphthoate (**1a** and **9**, respectively) with Grignard reagents (EtMgCl). The lack of enough resonance structures in **9-int** to preserve the aromaticity of one fused benzene ring (in red) precludes the formation of stable adducts after 1,4-addition , and drives the concerted elimination of the methoxy group in order to recover naphthalene aromaticity. On contrary, **1a-int** is stable enough to be located as an stationary point in the Potential Energy Surface of this reaction.

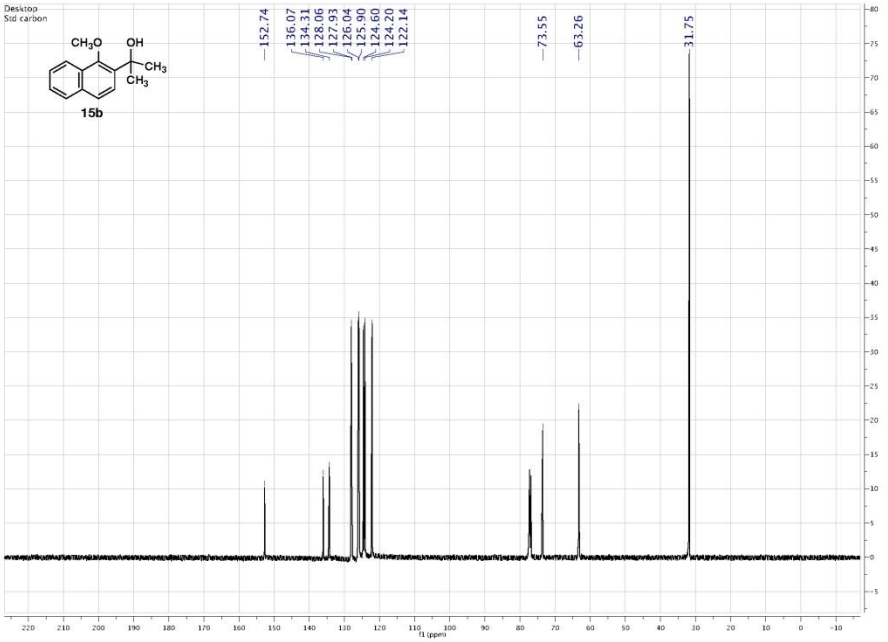


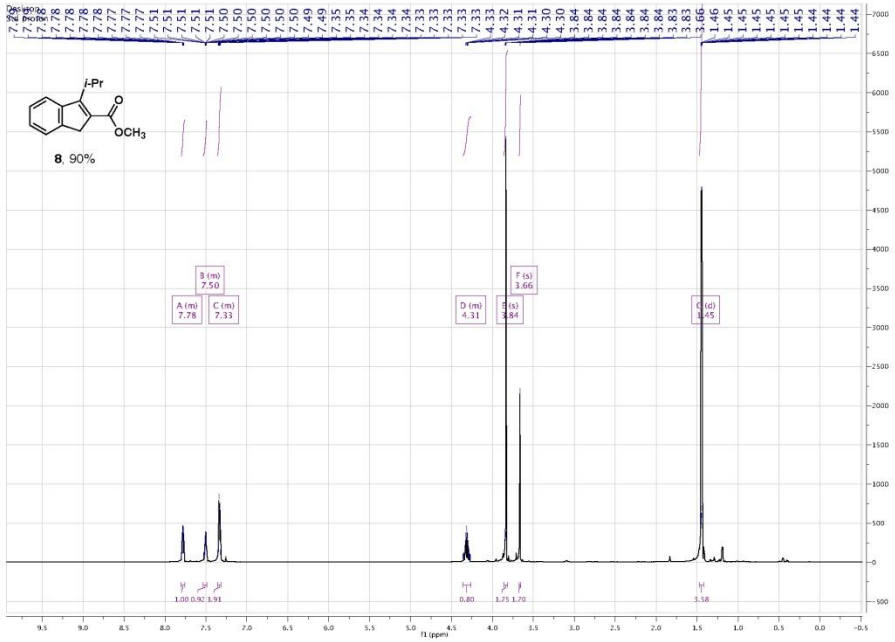
^{1}H and ^{13}C NMR Spectra

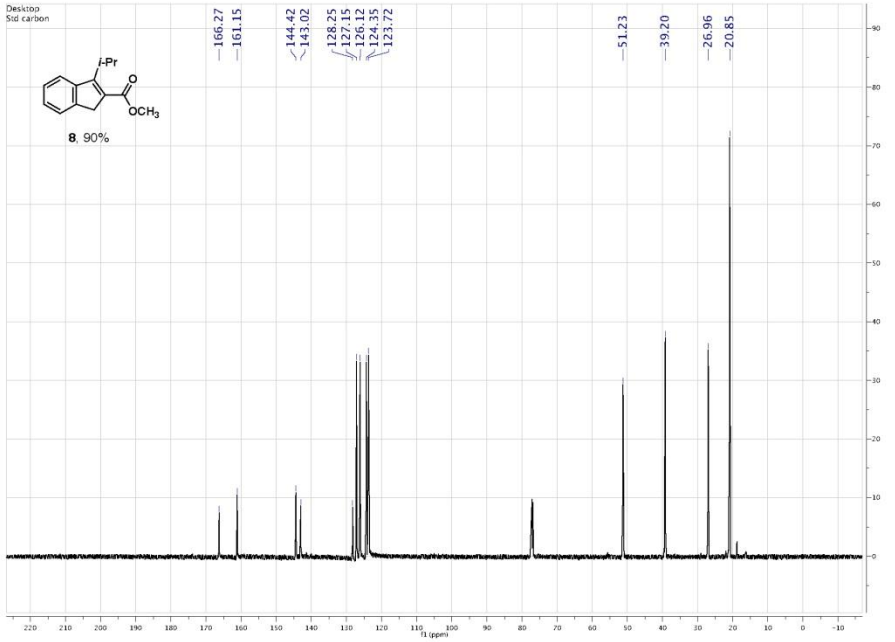


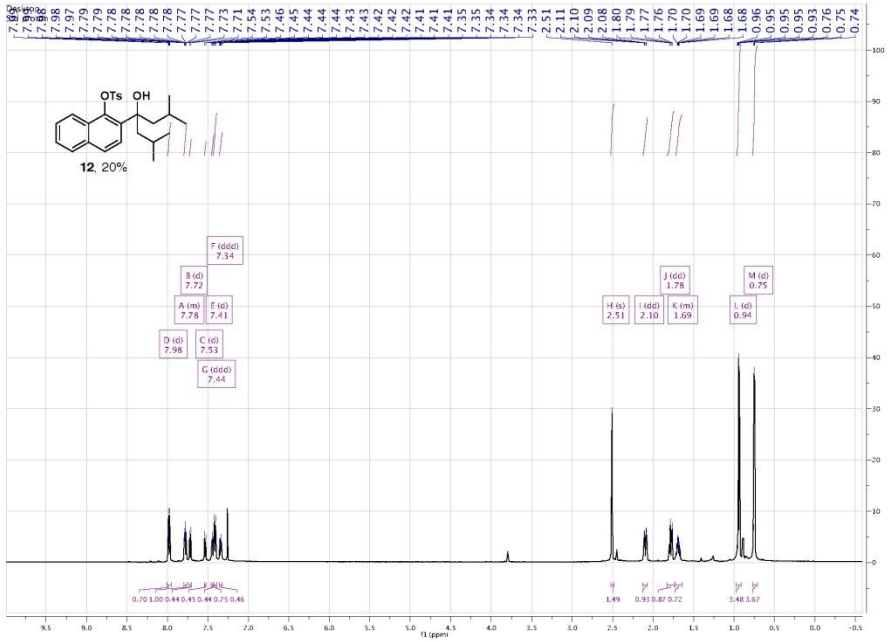



Desktop
Std proton
CH3O
OH
CH3
CH3
15b
B (d)
7.83
A (d)
8.07
C (d)
7.60
D (m)
7.50
E (s)
4.07
F (s)
1.73
1.00 0.89 0.97 3.86
1.92
11.68
f1 (ppm)


Desktop
Std carbon
CH3O
OH
CH3
CH3
15b
152.74
136.07
134.31
128.06
127.93
126.04
125.90
124.60
124.20
122.14
73.55
63.26
31.75
f1 (ppm)


i-Pr
OCH3
8, 90%
B (m)
7.50
A (m)
7.78
C (m)
7.33
D (m)
4.31
E (s)
3.84
F (s)
3.66
G (d)
1.45
f1 (ppm)


Desktop
Std carbon
i-Pr
OCH3
8, 90%
166.27
161.15
144.42
143.02
128.25
127.15
126.12
124.35
123.72
51.23
39.20
26.96
20.85
f1 (ppm)


OTs OH
12, 20%
F (ddd) 7.34
B (d) 7.72
A (m) 7.78
E (d) 7.41
D (d) 7.98
C (d) 7.53
G (ddd) 7.44
J (dd) 1.78
M (d) 0.75
H (s) 2.51
I (dd) 2.10
K (m) 1.69
L (d) 0.94
f1 (ppm)

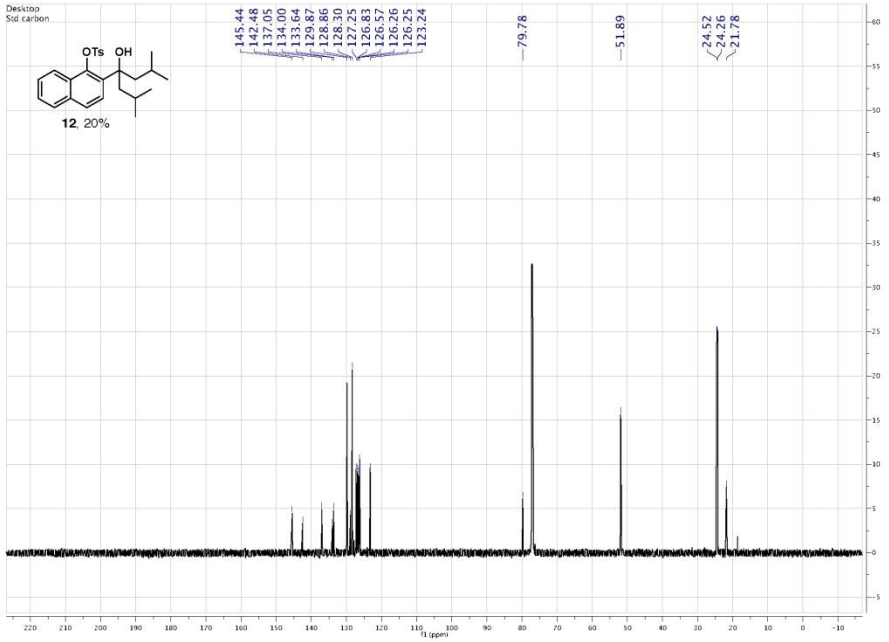

Desktop
Std carbon
OTs OH
12, 20%
145.44
142.48
137.05
134.00
133.64
129.87
128.86
128.30
127.25
126.83
126.57
126.26
126.25
123.24
79.78
51.89
24.52
24.26
21.78
f1 (ppm)

Table S1. B3LYP/6-31+G(d,p) absolute energies, enthalpies, free energies, entropies and lowest frequencies of the structures considered in this work

Structure	E_{elec} (Hartree)[a]	E_{elec} + ZPE (Hartree)[a]	E (Hartree)[a]	H (Hartree)[b]	S (cal mol^{-1} K^{-1})[b]	G (Hartree)[b]	Lowest freq. (cm^{-1})	AGsolv (kcal mol^{-1})[c]
Et_2O	–155.025044	–154.946956	–154.944544	–154.943926	58.7	–154.962195	223.9	–1.4
$(MeMgCl)_2$	–1400.586188	–1400.538562	–1400.532126	–1400.531508	98.7	–1400.559382	19.3	–16.2
(MeMgCl)2$(DME)_2$	–1710.698959	–1710.479171	–1710.466912	–1710.466294	142.3	–1710.505691	8.2	–11.6
$(EtMgCl)_2$	–1479.199125	–1479.095526	–1479.087822	–1479.087204	113.5	–1479.117858	8.3	–17.8
(EtMgCl)2$(DME)_2$_I	–1789.311451	–1789.035082	–1789.021477	–1789.020859	154.0	–1789.062239	14.2	–12.7
(EtMgCl)2$(DME)_2$_II	–1789.331403	–1789.034803	–1789.021226	–1789.020608	152.5	–1789.068032	10.2	–12.5
1a_I	–728.285253	–728.075262	–728.068579	–728.067961	98.9	–728.097798	37.5	–8.4
1a_II	–728.284542	–728.074964	–728.068280	–728.067662	99.3	–728.097451	26.0	–8.7
1a·CH_3MgCl (a)	–1428.600921	–1428.368648	–1428.358611	–1428.357993	124.5	–1428.394148	27.4	–18.3
1a·CH_3MgCl (b)	–2128.909540	–2128.643884	–2128.630031	–2128.629413	154.8	–2128.672448	14.3	–20.4
1a·CH_3MgCl (c)	–2128.917530	–2128.646903	–2128.633516	–2128.632898	147.2	–2128.675314	14.5	–17.6
1a·CH_3MgCl (d)	–2128.911145	–2128.645166	–2128.631478	–2128.630860	156.3	–2128.673401	4.5	–20.4
1a·CH_3MgCl (e)	–2128.907697	–2128.641049	–2128.627738	–2128.627120	146.9	–2128.669353	22.6	–20.3
1a·CH_3MgCl (f)	–2128.903897	–2128.642534	–2128.629021	–2128.628403	154.9	–2128.670630	7.2	–23.6
1a·CH_3MgCl (g)	–2128.910601	–2128.644642	–2128.631328	–2128.630710	147.6	–2128.672866	13.0	–20.6
1a·CH_3MgCl (h)	–2128.903211	–2128.640687	–2128.627289	–2128.626671	147.6	–2128.669065	25.6	–22.8
1a·CH_3MgCl (i)	–2128.895174	–2128.633402	–2128.619816	–2128.619198	152.2	–2128.661711	9.2	–23.0
1a·CH_3MgCl (j)	–2128.910705	–2128.644826	–2128.631544	–2128.630926	146.5	–2128.673192	17.2	–20.7
1a·CH_3MgCl (k)	–2128.910796	–2128.645059	–2128.631762	–2128.631144	147.0	–2128.673336	15.4	–20.8
1a·CH_3MgCl (l)	–2128.911465	–2128.644720	–2128.631626	–2128.631008	144.2	–2128.673035	20.4	–20.3
1a·CH_3MgCl (m)	–2128.907482	–2128.645130	–2128.632432	–2128.631814	142.2	–2128.673055	–60.0	–22.9
1a–TSOMe	–1428.566735	–1428.329010	–1428.319950	–1428.319332	114.9	–1428.354013	–371.5	–14.7
1a–TSCO	–1428.567427	–1428.329825	–1428.320921	–1428.320303	114.0	–1428.354581	–341.1	–15.0
1a–intOMe	–1428.612061	–1428.374654	–1428.365541	–1428.364923	116.6	–1428.399514	27.0	–16.9
1a–intCO	–1428.621287	–1428.381764	–1428.373249	–1428.372631	111.3	–1428.405978	46.3	–16.2
1a–TS2OMe	–1428.611586	–1428.374371	–1428.365402	–1428.364784	115.5	–1428.399200	–194.6	–16.4
1a–TS2CO	–1428.618548	–1428.380121	–1428.371185	–1428.370567	114.2	–1428.404901	–60.3	–15.4
1a–prodOMe	–1428.646092	–1428.408150	–1428.397941	–1428.397323	129.3	–1428.433710	12.8	–16.0
1a–prodCO	–1428.631944	–1428.400628	–1428.390389	–1428.389771	127.6	–1428.426098	22.3	–19.5
1a–TSOMe (b)	–2128.880444	–2128.608767	–2128.596077	–2128.595459	144.1	–2128.636514	–387.1	–16.7
1a–TSOMe (k)	–2128.861478	–2128.596804	–2128.584017	–2128.583399	144.7	–2128.624656	–379.3	–21.1
1a–TSOMe (l)	–2128.855381	–2128.590884	–2128.578122	–2128.577504	144.5	–2128.618807	–356.6	–21.1
1a–TSCO (b)	–2128.878040	–2128.608108	–2128.595622	–2128.595004	143.1	–2128.635535	–341.7	–18.1
1a–TSCO (k)	–2128.869300	–2128.606992	–2128.594503	–2128.593885	141.6	–2128.634434	–307.3	–23.1
1a–TSCO (l)	–2128.862086	–2128.593806	–2128.581392	–2128.580774	139.7	–2128.621356	–404.7	–19.2
1a·CH_3MgCl(DME) (d)_I	–2283.964335	–2283.613123	–2283.596446	–2283.595828	175.6	–2283.643619	8.1	–18.4
1a·CH_3MgCl(DME) (d)_II	–2283.959935	–2283.611617	–2283.594938	–2283.594320	174.4	–2283.642103	13.3	–20.2
1a·CH_3MgCl(DME) (d')_I	–2283.956372	–2283.606636	–2283.590053	–2283.589435	172.4	–2283.637273	16.0	–19.6
1a·CH_3MgCl(DME) (d')_II	–2283.952315	–2283.607740	–2283.591391	–2283.590773	169.4	–2283.638216	16.6	–23.1
1a–TS'OMe_I	–2283.910844	–2283.561659	–2283.546236	–2283.545618	161.6	–2283.591585	–517.4	–20.1
1a–TS'OMe_II	–2283.911547	–2283.560984	–2283.545510	–2283.544892	163.4	–2283.590832	–518.9	–19.3
1a–TS'CO_I	–2283.917410	–2283.568223	–2283.552705	–2283.552087	162.5	–2283.598214	–506.4	–20.1

1a–TS'CO_II	–2283.917853	–2283.568722	–2283.553187	–2283.552569	164.7	–2283.598649	–507.0	–20.2
1a·EtMgCl (a)_I	–1467.907719	–1467.646655	–1467.636133	–1467.635515	127.1	–1467.672581	30.6	–18.6
1a·EtMgCl (a)_II	–1467.907540	–1467.646870	–1467.636258	–1467.635640	128.5	–1467.672778	27.5	–18.8
1a–TSOMe–I	–1467.878281	–1467.612207	–1467.602453	–1467.601835	119.7	–1467.637781	–309.2	–15.0
1a–TSOMe–II	–1467.876416	–1467.609840	–1467.600116	–1467.599498	119.4	–1467.635401	–310.0	–14.8
1a–TSOMe–III	–1467.877525	–1467.611488	–1467.601660	–1467.601042	120.8	–1467.637057	–312.4	–15.0
1a–TSCO_I	–1467.876340	–1467.609864	–1467.600373	–1467.599755	118.0	–1467.635025	–294.6	–15.2
1a–TSCO_II	–1467.875984	–1467.608893	–1467.599310	–1467.598692	118.7	–1467.634187	–258.2	–14.7
1a–TSCO_III	–1467.875875	–1467.609414	–1467.599794	–1467.599176	119.2	–1467.634731	–284.3	–15.1
1a–intOMe–I	–1467.925354	–1467.658894	–1467.649103	–1467.648485	120.9	–1467.684388	29.6	–16.7
1a–intCO–I	–1467.935909	–1467.667866	–1467.658541	–1467.657923	116.0	–1467.692984	49.1	–16.2
1a–intCO–II	–1467.929919	–1467.661752	–1467.652616	–1467.651998	114.9	–1467.686579	46.4	–16.4
1a–TS2OMe–I	–1467.924755	–1467.658578	–1467.648920	–1467.648302	120.0	–1467.684087	–192.1	–16.3
1a–TS2OMe–II	–1467.916555	–1467.650544	–1467.640768	–1467.640150	121.4	–1467.676108	–249.4	–16.3
1a–TS2CO_I	–1467.932451	–1467.665118	–1467.655433	–1467.654815	119.7	–1467.690508	–84.0	–15.3
1a–TS2CO_II	–1467.931003	–1467.663670	–1467.654040	–1467.653422	119.1	–1467.689118	–70.4	–15.4
1a–prodOMe–I	–1467.956157	–1467.690448	–1467.679241	–1467.678623	138.7	–1467.716649	12.2	–16.5
1a–prodOMe–II	–1467.956157	–1467.690451	–1467.679244	–1467.678626	138.7	–1467.716652	12.3	–16.5
1a–prodCO–I	–1467.944757	–1467.684524	–1467.673645	–1467.673027	131.9	–1467.710548	29.2	–19.6
1a–prodCO–II	–1467.944545	–1467.684792	–1467.673908	–1467.673290	132.0	–1467.710818	29.1	–19.9
1a–prodCO–III	–1467.946260	–1467.686369	–1467.675497	–1467.674879	131.3	–1467.712496	29.0	–19.6
7_I	–690.168161	–689.963480	–689.956908	–689.956290	97.7	–689.985905	55.7	–7.9
7_II	–690.164662	–689.961232	–689.954664	–689.954045	97.9	–689.983551	44.1	–8.6
7·EtMgCl_I	–1429.787806	–1429.534535	–1429.524112	–1429.523494	128.0	–1429.560095	21.6	–19.7
7·EtMgCl_II	–1429.787332	–1429.534328	–1429.523844	–1429.523226	129.3	–1429.559920	19.7	–19.9
7·EtMgCl_III	–1429.787752	–1429.533743	–1429.523273	–1429.522655	128.3	–1429.559483	21.5	–19.2
7·EtMgCl_IV	–1429.788019	–1429.533734	–1429.523227	–1429.522609	130.1	–1429.559375	13.1	–18.9
7–TSOMe–I	–1429.762365	–1429.502958	–1429.493230	–1429.492612	119.9	–1429.528411	–273.0	–15.2
7–TSOMe–II	–1429.760011	–1429.500605	–1429.490860	–1429.490242	119.8	–1429.526099	–274.1	–15.2
7–TSCO–I	–1429.750954	–1429.491745	–1429.482193	–1429.481575	118.7	–1429.516918	–320.7	–15.5
7–TSCO–II	–1429.750303	–1429.491192	–1429.481469	–1429.480851	120.1	–1429.516602	–306.9	–15.3
7–intOMe–I	–1429.819581	–1429.558117	–1429.548456	–1429.547838	120.2	–1429.583516	26.2	–16.0
7–intOMe–II	–1429.816225	–1429.555074	–1429.545435	–1429.544817	120.1	–1429.580453	25.9	–16.3
7–intCO–I	–1429.793207	–1429.534222	–1429.524675	–1429.524057	120.7	–1429.559409	19.2	–17.7
7–intCO–II	–1429.798925	–1429.540425	–1429.530871	–1429.530253	119.9	–1429.565643	30.0	–18.0
7–intCO–III	–1429.813738	–1429.550814	–1429.541364	–1429.540746	117.4	–1429.576057	39.1	–15.0
7–intCO–IV	–1429.807341	–1429.542895	–1429.533432	–1429.532814	118.1	–1429.567978	35.6	–14.1
7'_I	–689.587851	–689.458155	–689.451723	–689.451105	96.4	–689.480558	60.5	–45.6
7'_II	–689.586781	–689.457585	–689.451133	–689.450515	96.5	–689.479978	49.0	–45.9
7'·EtMgCl_I	–1429.246932	–1429.049029	–1429.038744	–1429.038126	125.5	–1429.074788	28.1	–45.3
7'·EtMgCl_II	–1429.246892	–1429.049211	–1429.038867	–1429.038249	126.6	–1429.074965	24.7	–45.4
7'·EtMgCl_III	–1429.249471	–1429.050003	–1429.039593	–1429.038975	128.0	–1429.075764	17.1	–44.3
7'·EtMgCl_IV	–1429.249405	–1429.049809	–1429.039414	–1429.038796	127.8	–1429.075510	19.7	–44.2
7'–TSCO–I	–1429.194984	–1428.996791	–1428.987435	–1428.986817	117.4	–1429.021805	–371.2	–44.8
7'–TSCO–II	–1429.193084	–1428.995746	–1428.986341	–1428.985723	117.7	–1429.020950	–364.0	–45.3
7'–TSOMe–I	–1429.177080	–1428.979475	–1428.969976	–1428.969358	117.7	–1429.004854	–467.8	–44.4
7'–TSOMe–II	–1429.174419	–1428.977388	–1428.967830	–1428.967212	118.4	–1429.002796	–470.2	–44.9

9_I	–728.288062	–728.079483	–728.072881	–728.072263	99.7	–728.101925	18.0	–9.5
9_II	–728.287357	–728.079448	–728.072807	–728.072189	99.3	–728.102019	31.2	–9.8
9·EtMgCl_I	–1467.910982	–1467.651151	–1467.640600	–1467.639982	130.3	–1467.676993	15.0	–19.5
9·EtMgCl_II	–1467.911371	–1467.650861	–1467.640394	–1467.639776	128.3	–1467.676674	19.8	–19.2
9·EtMgCl_III	–1467.911132	–1467.651035	–1467.640534	–1467.639916	128.5	–1467.676864	22.3	–19.4
9–TSOMe–I	–1467.867755	–1467.602408	–1467.592708	–1467.592090	119.6	–1467.627955	–353.1	–15.3
9–TSOMe–II	–1467.866575	–1467.601445	–1467.591686	–1467.591068	120.6	–1467.626957	–363.2	–15.4
9–TSCO–I	–1467.882813	–1467.616643	–1467.607212	–1467.606594	118.0	–1467.641794	–287.0	–15.6
9–TSCO–II	–1467.881576	–1467.615802	–1467.606218	–1467.605600	119.5	–1467.641091	–281.2	–15.7
9–intOMe–I	–1467.960744	–1467.695414	–1467.684366	–1467.683748	136.8	–1467.721596	9.2	–16.7
9–intOMe–II	–1467.963896	–1467.697833	–1467.686979	–1467.686361	135.2	–1467.723843	8.8	–16.5
9–intOMe–III	–1467.960434	–1467.696223	–1467.685166	–1467.684548	136.6	–1467.722453	11.3	–17.4
9–intCO–I	–1467.926629	–1467.662326	–1467.652666	–1467.652048	121.4	–1467.687562	23.5	–18.4
9–intCO–II	–1467.928505	–1467.663668	–1467.654098	–1467.653480	120.4	–1467.688926	25.1	–18.2
9–intCO–III	–1467.923996	–1467.659167	–1467.649508	–1467.648890	122.1	–1467.684296	22.7	–18.2
9·iPrMgCl_I	–1507.221396	–1506.933408	–1506.922262	–1506.921644	134.2	–1506.959626	16.8	–19.7
9·iPrMgCl_II	–1507.221653	–1506.933303	–1506.922130	–1506.921512	134.6	–1506.959464	15.1	–19.4
9·iPrMgCl_III	–1507.221398	–1506.933342	–1506.922192	–1506.921574	134.7	–1506.959538	12.2	–19.6
9'–TSOMe–I	–1507.178714	–1506.885379	–1506.875037	–1506.874419	124.1	–1506.911255	–306.4	–15.5
9'–TSOMe–II	–1507.175644	–1506.880684	–1506.870386	–1506.869768	123.3	–1506.906586	–266.1	–14.7
9'–TSOMe–III	–1507.174060	–1506.880130	–1506.869874	–1506.869256	123.1	–1506.906039	–258.3	–15.2
9'–TSCO–I	–1507.192325	–1506.898277	–1506.888092	–1506.887474	123.4	–1506.923882	–242.8	–15.7
9'–TSCO–II	–1507.191522	–1506.895752	–1506.885631	–1506.885013	122.2	–1506.921469	–210.0	–14.9
9'–TSCO–III	–1507.190166	–1506.895568	–1506.885557	–1506.884939	121.7	–1506.921121	–234.4	–15.5
11_I	–1276.873145	–1276.659426	–1276.651270	–1276.650652	111.3	–1276.683382	18.4	–12.2
11_II	–1276.869240	–1276.657820	–1276.649661	–1276.649043	110.7	–1276.681684	31.9	–13.6
11_III	–1276.865113	–1276.656267	–1276.648116	–1276.647498	111.0	–1276.680137	27.3	–15.2
11_IV	–1276.868075	–1276.657418	–1276.649300	–1276.648682	110.1	–1276.681307	35.3	–14.1
11·EtMgCl_I								
11·EtMgCl_II	–2016.485776	–2016.218943	–2016.206760	–2016.206142	139.8	–2016.246117	30.0	–20.6
11·EtMgCl_III	–2016.485439	–2016.219160	–2016.206910	–2016.206292	140.9	–2016.246362	27.5	–20.9
11·EtMgCl (b)_I	–2016.486634	–2016.225440	–2016.213346	–2016.212728	141.0	–2016.252493	14.8	–24.3
11·EtMgCl (b)_II	–2016.486953	–2016.225462	–2016.213397	–2016.212779	140.2	–2016.252464	17.6	–24.2
11·EtMgCl (b)_III	–2016.488330	–2016.219952	–2016.208046	–2016.207428	139.0	–2016.246854	11.5	–19.9
11·EtMgCl(DME)_I	–2171.531901	–2171.180513	–2171.165271	–2171.164653	162.6	–2171.210013	20.0	–19.3
11·EtMgCl(DME)_II	–2171.532221	–2171.182186	–2171.166807	–2171.166189	164.1	–2171.211624	19.8	–20.0
11·EtMgCl(DME)_III	–2171.532609	–2171.182395	–2171.167187	–2171.166569	162.3	–2171.211736	17.2	–20.0
11·EtMgCl(DME)_IV	–2171.532680	–2171.182843	–2171.167412	–2171.166794	166.0	–2171.212269	13.4	–20.0
11·EtMgCl(DME)_IX	–2171.529094	–2171.180399	–2171.165101	–2171.164483	163.4	–2171.209734	20.2	–20.9
11·EtMgCl(DME)_V	–2171.526400	–2171.178738	–2171.163625	–2171.163007	161.0	–2171.208098	15.9	–21.8
11·EtMgCl(DME)_VI	–2171.519341	–2171.178571	–2171.163042	–2171.162424	169.1	–2171.207896	7.4	–25.7
11·EtMgCl(DME)_VII	–2171.524006	–2171.178552	–2171.163376	–2171.162758	161.1	–2171.208098	18.8	–22.9
11·EtMgCl(DME)_VIII	–2171.526768	–2171.179871	–2171.164521	–2171.163903	167.0	–2171.209147	8.7	–22.1
11·EtMgCl(DME)_X	–2171.527742	–2171.180013	–2171.164751	–2171.164133	163.9	–2171.209226	15.6	–21.6
11·EtMgCl(DME)_XI	–2171.529025	–2171.181619	–2171.166161	–2171.165543	167.5	–2171.210991	11.7	–21.6
11–TSOMe–I	–2016.454759	–2016.185103	–2016.173759	–2016.173141	132.0	–2016.211689	–330.6	–18.4
11–TSOMe–II	–2016.449768	–2016.180188	–2016.168840	–2016.168222	132.0	–2016.206882	–343.6	–18.5
11–TSOMe–III	–2016.450466	–2016.182258	–2016.170832	–2016.170214	133.5	–2016.208858	–341.9	–19.3
11–TSOMe–IV	–2016.454776	–2016.185127	–2016.173794	–2016.173176	131.9	–2016.211705	–328.9	–18.4

11–TSOMe–V	–2016.451583	–2016.182836	–2016.171540	–2016.170922	131.7	–2016.209401	–344.6	–19.1
11–TSCO–I	–2016.448920	–2016.180194	–2016.169052	–2016.168434	130.2	–2016.206656	–269.9	–19.3
11–TSCO–II	–2016.448645	–2016.180508	–2016.169199	–2016.168581	132.0	–2016.207143	–254.4	–19.5
11–TSCO–III	–2016.459516	–2016.191262	–2016.180366	–2016.179748	127.9	–2016.217708	–235.7	–19.9
11–TSCO–IV	–2016.449699	–2016.178123	–2016.166944	–2016.166326	130.5	–2016.204789	–296.2	–17.5
11–TSCO–V	–2016.449116	–2016.180954	–2016.169698	–2016.169080	131.5	–2016.207516	–246.9	–19.5
11–TSCO–VI	–2016.458218	–2016.188867	–2016.177894	–2016.177276	128.6	–2016.215371	–195.2	–19.2
11–TSCO–VII	–2016.449880	–2016.177218	–2016.166090	–2016.165472	130.0	–2016.203832	–263.0	–16.9
11–TSCO–VIII	–2016.457860	–2016.190425	–2016.179446	–2016.178828	128.8	–2016.216839	–235.4	–20.3
11–TSCO–IX	–2016.449754	–2016.178325	–2016.167236	–2016.166618	129.8	–2016.204822	–301.8	–17.7
13a_I	–653.051910	–652.849176	–652.843041	–652.842423	94.6	–652.871070	41.7	–9.4
13a_II	–653.053878	–652.851290	–652.845206	–652.844588	94.2	–652.873188	43.1	–9.6
13a·EtMgCl_I	–1392.674490	–1392.421946	–1392.411919	–1392.411301	124.0	–1392.447299	28.2	–20.4
13a·EtMgCl_II	–1392.674714	–1392.421553	–1392.411593	–1392.410975	123.2	–1392.446898	29.8	–20.0
13a·EtMgCl_III	–1392.674714	–1392.421555	–1392.411593	–1392.410975	123.2	–1392.446898	29.6	–20.0
13a–TSOMe–I	–1392.651525	–1392.392020	–1392.382847	–1392.382229	115.5	–1392.417011	–284.9	–15.8
13a–TSOMe–II	–1392.649772	–1392.390185	–1392.380974	–1392.380356	115.8	–1392.415286	–291.6	–15.8
13a–TSCO–I	–1392.650210	–1392.390569	–1392.381591	–1392.380973	114.6	–1392.415120	–203.5	–16.1
13a–TSCO–II	–1392.651246	–1392.391531	–1392.382594	–1392.381976	114.0	–1392.416182	–222.5	–16.1
13a·MeMgCl	–1353.367691	–1353.143612	–1353.134136	–1353.133518	119.8	–1353.168614	34.6	–19.8
13a'–TS'OMe	–1353.340005	–1353.109123	–1353.100601	–1353.099983	111.0	–1353.133579	–345.5	–15.6
13a–TS'CO	–1353.341783	–1353.110943	–1353.102682	–1353.102064	109.2	–1353.135029	–282.6	–16.0
13a_I	–770.993528	–770.706898	–770.698675	–770.698057	111.7	–770.730834	22.6	–10.7
13a_II	–770.995244	–770.708915	–770.700721	–770.700103	111.3	–770.732839	21.9	–10.9
13a_III	–770.992028	–770.704709	–770.696606	–770.695988	111.2	–770.728435	17.7	–10.5
13a_IV	–770.993603	–770.707025	–770.698827	–770.698209	112.0	–770.730889	21.8	–10.9
13a·EtMgCl_I	–1510.616114	–1510.279415	–1510.267315	–1510.266697	140.2	–1510.306610	23.3	–21.5
13a·EtMgCl_II	–1510.616293	–1510.279175	–1510.267036	–1510.266418	141.0	–1510.306319	19.3	–21.2
13a·EtMgCl_III	–1510.615807	–1510.279483	–1510.267218	–1510.266600	143.8	–1510.306647	15.8	–21.5
13a·EtMgCl_IV	–1510.615109	–1510.278354	–1510.266289	–1510.265671	140.9	–1510.305405	20.0	–21.7
13a·EtMgCl_V	–1510.615176	–1510.277777	–1510.265730	–1510.265112	140.7	–1510.304843	20.0	–21.3
13a·EtMgCl_VI	–1510.614687	–1510.278320	–1510.266140	–1510.265522	143.0	–1510.305421	18.7	–21.8
13a·EtMgCl_VII	–1510.614053	–1510.276518	–1510.264479	–1510.263861	140.4	–1510.303447	21.9	–21.2
13a·EtMgCl_VIII	–1510.614235	–1510.275888	–1510.263911	–1510.263293	139.5	–1510.302825	23.8	–20.8
13a·EtMgCl_IX	–1510.613877	–1510.276122	–1510.264090	–1510.263472	140.2	–1510.303121	25.1	–21.1
13a–TSOMe–I	–1510.592059	–1510.248664	–1510.237362	–1510.236744	132.6	–1510.275446	–284.1	–17.0
13a–TSOMe–II	–1510.590341	–1510.246612	–1510.235298	–1510.234680	132.9	–1510.273408	–292.6	–16.9
13a–TSOMe–III	–1510.591964	–1510.248392	–1510.237134	–1510.236516	133.3	–1510.275064	–280.8	–17.1
13a–TSOMe–IV	–1510.590070	–1510.246477	–1510.235167	–1510.234549	133.9	–1510.273226	–292.1	–17.1
13a–TSOMe–V	–1510.592463	–1510.248494	–1510.237268	–1510.236650	132.1	–1510.275193	–287.8	–16.9
13a–TSOMe–VI	–1510.590910	–1510.247105	–1510.235833	–1510.235215	133.3	–1510.273808	–289.4	–17.0
13a–TSCO–I	–1510.590974	–1510.246596	–1510.235548	–1510.234930	130.2	–1510.272949	–214.0	–16.9
13a–TSCO–II	–1510.589895	–1510.245776	–1510.234670	–1510.234052	131.2	–1510.272150	–219.2	–17.0
13a–TSCO–III	–1510.590935	–1510.246758	–1510.235709	–1510.235091	130.4	–1510.273196	–197.2	–17.1
13a–TSCO–IV	–1510.591606	–1510.247442	–1510.236380	–1510.235762	130.4	–1510.273921	–211.3	–17.1
13a–TSCO–V	–1510.583028	–1510.238230	–1510.227332	–1510.226714	128.7	–1510.264585	–204.4	–16.9
13a–TSCO–VI	–1510.584547	–1510.240469	–1510.229510	–1510.228892	129.4	–1510.266855	–221.8	–17.2

13c_I	–613.731930	–613.555803	–613.550366	–613.549748	89.6	–613.577098	45.2	–8.5
13c_II	–613.734256	–613.559088	–613.553660	–613.553042	89.1	–613.580459	75.5	–9.1
13c–TSCO_I	–1353.330949	–1353.099774	–1353.091309	–1353.090691	111.7	–1353.123947	–186.7	–16.2
13c–TSCO_II	–1353.331207	–1353.100592	–1353.092023	–1353.091405	112.9	–1353.124887	–187.8	–16.4
13c–TSOMe_I	–1353.330269	–1353.098308	–1353.089926	–1353.089308	110.3	–1353.122616	–273.8	–15.5
13c–TSOMe_II	–1353.328361	–1353.096169	–1353.087758	–1353.087140	110.6	–1353.120501	–278.7	–15.4
13c·EtMgCl_I	–1353.350566	–1353.124676	–1353.115431	–1353.114813	118.9	–1353.149365	27.8	–19.5
13c·EtMgCl_II	–1353.350875	–1353.124387	–1353.115200	–1353.114582	118.1	–1353.149116	27.4	–19.2
13c·EtMgCl_III	–1353.350199	–1353.124527	–1353.115240	–1353.114622	119.6	–1353.149343	24.4	–19.6
1a·$CH_3MgCl(DME)$_I	–1583.635798	–1583.316029	–1583.302988	–1583.302370	145.0	–1583.343778	24.5	–15.0
1a·$CH_3MgCl(DME)$_II	–1583.632625	–1583.314132	–1583.301113	–1583.300495	144.9	–1583.341722	24.9	–15.8
1'a·$CH_3MgCl(DME)$_I	–1583.638093	–1583.320296	–1583.307006	–1583.306388	150.2	–1583.348306	13.7	–16.0
1'a·$CH_3MgCl(DME)$_II	–1583.637845	–1583.319847	–1583.306588	–1583.305970	152.3	–1583.347780	4.5	–15.8
1a–TSOMe(DME)	–1583.589527	–1583.269486	–1583.257730	–1583.257112	133.0	–1583.296380	–398.0	–14.8
1a–TSCO(DME)–I	–1583.605122	–1583.285198	–1583.273180	–1583.272562	137.3	–1583.312358	–334.8	–14.9
1a–TSCO(DME)–II	–1583.602937	–1583.285558	–1583.273426	–1583.272808	139.4	–1583.312654	–343.3	–16.3
16	–500.415689	–500.246815	–500.242535	–500.241917	80.7	–500.266897	80.7	–7.5
16·$CH_3MgCl(DME)$	–1355.758349	–1355.482285	–1355.471270	–1355.470652	133.1	–1355.508292	15.8	–15.2
16–TSOMe(DME)	–1355.688449	–1355.416753	–1355.406650	–1355.406032	124.1	–1355.442108	–480.4	–17.1
17	–613.772898	–613.595791	–613.590430	–613.589812	89.8	–613.617129	45.9	–8.7
17·$CH_3MgCl(DME)$	–1469.127337	–1468.841038	–1468.829132	–1468.828514	141.0	–1468.867911	10.5	–15.4
17–TSCO(DME)	–1469.090257	–1468.806020	–1468.795151	–1468.794533	131.5	–1468.832095	–347.5	–16.7

[a] 1 Hartree = 627.51 kcal mol^{-1}. [b] Thermal corrections at 195.15 K. [c] Calculated trough the SMD method using tetrahydrofuran as solvent.

Cartesian coordinates of the structures considered in this work

Structure Et2O [B3LYP/6-31G(d)]

C	1.17086800	-0.19527900	0.00000000
H	2.02182000	0.49126400	0.00000000
H	1.23229100	-0.83971400	0.89294700
H	1.23229100	-0.83971400	-0.89294700
C	-1.17087300	-0.19535800	0.00000000
H	-2.02183600	0.49120500	0.00000000
H	-1.23226900	-0.83961100	-0.89302200
H	-1.23226900	-0.83961100	0.89302200
O	0.00000000	0.59000000	0.00000000

Structure (MeMgCl)2 [B3LYP/6-31G(d)]

Cl	-1.72060400	0.00000000	-0.00147100
Mg	0.00000000	1.69693000	-0.00135800
Mg	0.00000000	-1.69693000	-0.00135800
C	0.00000000	3.77670400	0.00329000
H	0.00000000	4.17633800	1.02582000
H	0.88472100	4.18403400	-0.50213000
H	-0.88472100	4.18403400	-0.50213000
Cl	1.72060400	0.00000000	-0.00147100
C	0.00000000	-3.77670400	0.00329000
H	-0.88472100	-4.18403400	-0.50213000
H	0.88472100	-4.18403400	-0.50213000
H	0.00000000	-4.17633800	1.02582000

Structure (MeMgCl)2(DME)2 [B3LYP/6-31G(d)]

Cl	0.13198000	0.09381500	1.73567200
C	2.37141700	2.77784100	-0.26923800
H	1.64175900	3.56704000	-0.50264500
H	2.85053900	3.08151200	0.67382600
H	3.14441100	2.84438400	-1.05021700
Cl	-0.13197400	-0.09380900	-1.73568500
C	-2.37140900	-2.77783100	0.26925700
H	-3.14440000	-2.84435500	1.05024100
H	-2.85053800	-3.08151800	-0.67379900
H	-1.64175600	-3.56703100	0.50267500
O	-2.97001400	0.61654100	0.19609500
O	2.97001200	-0.61654600	-0.19610100
C	-2.72658700	2.02218000	0.34705300
H	-1.79183400	2.12622300	0.89824100
H	-2.64224800	2.50165100	-0.63510600
H	-3.54491400	2.47750900	0.91691900
C	4.21973000	-0.32735800	0.44497700
H	5.04394700	-0.74128700	-0.14748000
H	4.30691800	0.75881800	0.49409200
H	4.23713600	-0.75352300	1.45542000
C	2.72657300	-2.02218400	-0.34706300
H	2.64220000	-2.50165100	0.63509500
H	1.79183400	-2.12621600	-0.89827700
H	3.54491100	-2.47752300	-0.91690400
C	-4.21974900	0.32733700	-0.44494400
H	-4.23718900	0.75349800	-1.45538800
H	-4.30692600	-0.75884000	-0.49405300
H	-5.04395200	0.74125900	0.14753700
Mg	-1.48260300	-0.87490800	0.17726600
Mg	1.48261600	0.87491500	-0.17727700

Structure (EtMgCl)2 [B3LYP/6-31G(d)]

Cl	0.32968500	-1.69173400	0.00003000
Mg	-1.66678300	-0.32565300	-0.00133300
Mg	1.66677400	0.32557500	-0.00004700
C	-3.72438800	-0.74030800	-0.00204300
H	-3.94149100	-1.37089700	-0.87744200
H	-3.94046500	-1.37921400	0.86754500
Cl	-0.32967400	1.69167900	-0.00144700
C	3.72434700	0.74038400	0.00095200
H	3.94127300	1.37523900	-0.87139700
H	3.94048900	1.37508400	0.87360800
C	4.67118900	-0.47540000	0.00125200
H	4.52211700	-1.11266300	-0.87982800
H	5.73082400	-0.17856900	0.00185400
H	4.52120500	-1.11298400	0.88194300
C	-4.67115600	0.47553000	0.00425400
H	-5.73080400	0.17875500	0.00320600
H	-4.52126300	1.10860900	0.88820800
H	-4.52192200	1.11726200	-0.87354500

Structure (EtMgCl)2(DME)2_I [B3LYP/6-31G(d)]

Cl	-0.11875900	0.00901700	-1.73902700
C	-3.05611800	2.03021500	0.14396000
H	-3.75195400	1.92984400	-0.70688100
H	-3.69676000	1.95100000	1.03851600
Cl	0.11876000	-0.00901600	1.73902600
C	3.05611700	-2.03021600	-0.14396000
H	3.69675700	-1.95100500	-1.03851700
H	3.75195500	-1.92984300	0.70688000
O	2.68845200	1.41988900	-0.19445600
O	-2.68845100	-1.41988900	0.19445400
C	2.06586800	2.69694600	-0.39856500
H	1.13041800	2.51578100	-0.92777300
H	1.86762300	3.18157200	0.56435800
H	2.71969100	3.33036800	-1.00921200
C	-3.97759000	-1.51674900	-0.42619100
H	-4.64785800	-2.11310000	0.20368100
H	-4.36366500	-0.50100100	-0.51983700
H	-3.88942500	-1.97879900	-1.41693700
C	-2.06586700	-2.69694600	0.39856200
H	-1.86762300	-3.18157200	-0.56436100
H	-1.13041600	-2.51578200	0.92776900
H	-2.71968800	-3.33036900	1.00921000
C	3.97759000	1.51674900	0.42619200
H	3.88942300	1.97879900	1.41693800
H	4.36366500	0.50100100	0.51983900
H	4.64785900	2.11310000	-0.20367900
Mg	1.67427100	-0.42423200	-0.13493900
Mg	-1.67427000	0.42423300	0.13493800
C	-2.45020500	3.44860700	0.10265400
H	-3.20869400	4.24819200	0.11085200
H	-1.79215000	3.63517400	0.96287200
H	-1.84326900	3.60572200	-0.80031400
C	2.45020200	-3.44860700	-0.10264800
H	3.20869000	-4.24819300	-0.11084600
H	1.84326700	-3.60571900	0.80032100
H	1.79214500	-3.63517500	-0.96286500

Structure (EtMgCl)2(DME)2_II [B3LYP/6-31G(d)]

Cl	-0.07530300	0.29235600	-1.71642900
C	3.07188800	-1.94288100	-0.53489000
H	2.51689600	-2.88386300	-0.68271700
H	3.55691600	-1.76427100	-1.51005300
Cl	0.07530400	-0.29235900	1.71643000
C	-3.07188300	1.94288100	0.53489400
H	-3.55691100	1.76427000	1.51005700
H	-2.51688900	2.88386200	0.68272300
O	-2.68848900	-1.43171000	-0.15044100
O	2.68848700	1.43171100	0.15044000
C	-2.11760100	-2.63238000	-0.68917300
H	-1.25742900	-2.33505800	-1.28903300
H	-1.80203300	-3.30008200	0.12097500
H	-2.85503400	-3.13712400	-1.32413000
C	3.88498500	1.66596400	-0.60478200
H	4.64128300	2.13494200	0.03521100
H	4.24055300	0.69297800	-0.94614100
H	3.67193600	2.31295800	-1.46432000
C	2.11759500	2.63238100	0.68916800
H	1.80202000	3.30007700	-0.12098300
H	1.25742700	2.33505800	1.28903200
H	2.85502700	3.13713200	1.32411900
C	-3.88499100	-1.66596100	0.60477600
H	-3.67194800	-2.31296000	1.46431100
H	-4.24055500	-0.69297400	0.94613900
H	-4.64128900	-2.13493200	-0.03522200
Mg	-1.68091000	0.39811300	0.12416900
Mg	1.68091200	-0.39811500	-0.12416800
C	4.16399500	-2.18581900	0.52774700
H	4.85245500	-3.00652800	0.26870700
H	4.79130800	-1.29646800	0.68869200
H	3.73032300	-2.43763000	1.50509900
C	-4.16399000	2.18582300	-0.52774200
H	-4.85244800	3.00653400	-0.26870000
H	-3.73031700	2.43763600	-1.50509300
H	-4.79130500	1.29647400	-0.68868800

Structure 1a_I [B3LYP/6-31G(d)]

C	-0.95170700	-0.35979100	0.04821400
C	-0.58073100	-1.71847400	0.27203200
C	0.73326800	-2.10399400	0.32598000
C	1.77392700	-1.15792400	0.12555000

C	1.42785700	0.20839100	-0.12091900
C	-2.39526300	0.00535600	-0.00942000
O	-2.87011500	1.11530300	0.13228800
O	-0.22507300	1.90414700	-0.41626300
C	-0.43086300	2.75745900	0.71827100
H	-1.37023600	-2.44791400	0.40707800
H	0.99284300	-3.14282500	0.51266300
H	-0.58108500	3.75963100	0.31155400
H	0.45226600	2.75436400	1.37022000
H	-1.32045900	2.45196000	1.27302600
C	0.04955400	0.59335700	-0.13547000
C	2.46292900	1.15300500	-0.35481700
C	3.78415700	0.76597500	-0.32423100
H	4.56798500	1.49610000	-0.50621300
C	4.12934500	-0.58186100	-0.06330700
H	5.17569500	-0.87453100	-0.04126500
C	3.14590500	-1.52138100	0.15283300
H	3.40650500	-2.55968100	0.34322400
H	2.18855300	2.17882700	-0.57325200
O	-3.17013600	-1.08567400	-0.24359600
C	-4.58090600	-0.83092000	-0.29327800
H	-5.04583100	-1.80112700	-0.47216500
H	-4.93086900	-0.40398500	0.65067000
H	-4.81759700	-0.13622400	-1.10359400

Structure 1a_II [B3LYP/6-31G(d)]

C	0.87971100	0.69988400	-0.00160500
C	0.27918900	1.98122700	0.17604100
C	-1.07952600	2.14097100	0.22879000
C	-1.94392700	1.02306200	0.07904000
C	-1.36897400	-0.27270800	-0.11436000
C	2.37237900	0.71330600	-0.06908200
O	3.02640800	1.74051300	-0.06236900
O	0.54410400	-1.68214100	-0.33624800
C	0.85065300	-2.41784200	0.85192300
H	0.94751700	2.82987900	0.26766600
H	-1.51186200	3.12758500	0.37387000
H	1.18634400	-3.40240100	0.51905500
H	-0.03939200	-2.52854800	1.48471500
H	1.65124700	-1.93294000	1.41856900
C	0.05574800	-0.41636200	-0.13141900
C	-2.22824000	-1.38952300	-0.29683900
C	-3.59629500	-1.23372000	-0.26799000
H	-4.24364400	-2.09443100	-0.41191100
C	-4.16656500	0.04472900	-0.05922400
H	-5.24748100	0.15484300	-0.03802800
C	-3.35759700	1.14697700	0.10639000
H	-3.79143500	2.13270700	0.25573300
H	-1.78406400	-2.36175000	-0.47796200
O	2.94889100	-0.50600300	-0.13629600
C	4.38222700	-0.49263900	-0.22787000
H	4.67775000	-1.54094000	-0.28242500
H	4.70514500	0.04497700	-1.12310300
H	4.82194300	-0.01211100	0.65035100

Structure 1a·CH3MgCl (a) [B3LYP/6-31G(d)]

C	0.10471500	1.38155400	-0.12962500
C	0.98718600	2.46776600	0.14054500
C	2.34282500	2.27585300	0.19230000
C	2.90692700	0.98626100	-0.00560000
C	2.03986300	-0.12088500	-0.27965900
C	-1.35881300	1.60551400	-0.12311800
O	-2.21596900	0.73313400	0.03738500
O	-0.18637700	-0.95024000	-0.68216100
Cl	-3.22696000	-2.56448700	-0.73323200
C	-0.32449500	-1.19189400	-2.11314800
H	0.56146800	3.44909200	0.31193700
H	3.00442600	3.11193300	0.40120300
H	-1.03812700	-2.00983000	-2.20277000
H	0.64984700	-1.45496400	-2.53269400
H	-0.71839900	-0.29533400	-2.60070100
Mg	-1.92888300	-1.26843700	0.65200500
C	-1.27112900	-1.33316100	2.65443600
H	-0.75438200	-2.27506300	2.89131800
H	-0.57535200	-0.52554100	2.93043700
H	-2.11007600	-1.26640400	3.36338100
C	0.64000600	0.11772200	-0.36133700
C	2.59639300	-1.41874700	-0.44168300
C	3.95715100	-1.60639500	-0.35544100
H	4.37393900	-2.60267500	-0.47000700
C	4.81880200	-0.51084900	-0.10621500
H	5.89074500	-0.67518100	-0.04327200
C	4.30469500	0.75441400	0.06922100
H	4.96293100	1.59451200	0.27458200
H	1.93252500	-2.26002200	-0.60623300
O	-1.69586700	2.88319300	-0.28814100
C	-3.10723100	3.18994400	-0.22733900
H	-3.16849300	4.26676100	-0.37947900
H	-3.64278100	2.65300400	-1.01283400
H	-3.51163000	2.90913300	0.74745600

Structure 1a·CH3MgCl (b) [B3LYP/6-31G(d)]

C	1.61033900	1.35759700	-0.23316800
C	2.77029000	2.12880800	0.07074000
C	3.98314500	1.52342000	0.26683000
C	4.11586500	0.10995700	0.18518800
C	2.96342000	-0.68412300	-0.12058600
C	0.30298900	2.02328100	-0.39141200
O	-0.79913600	1.46936100	-0.29998400
O	0.62720100	-0.79844900	-0.68706600
C	0.50443000	-1.04587200	-2.10813500
H	2.67025300	3.20454600	0.15221700
H	4.85994400	2.12061600	0.50129000
H	-0.34595400	-1.71576300	-2.22204100
H	1.41848300	-1.51340400	-2.48625000
H	0.31636800	-0.10810900	-2.64191800
Mg	-1.28863100	-0.27601500	0.76108200
C	-0.24650300	-0.68163200	2.54579900
H	0.52382100	-1.46036700	2.44193600
H	-0.92407900	-1.02563100	3.34100200
C	1.72242300	-0.02597100	-0.34752000
C	3.08448100	-2.09908300	-0.17193300
C	4.30227100	-2.70023000	0.05244400
H	4.38556400	-3.78264900	0.02174200
C	5.44730300	-1.91747300	0.33624300
H	6.40161200	-2.40657700	0.51019900
C	5.35466500	-0.54507100	0.40524900
H	6.22988500	0.05653200	0.63617300
H	2.19907900	-2.69493400	-0.36264900
O	0.39366300	3.32811900	-0.63279700
C	-0.85256800	4.05927500	-0.71017500
H	-0.55993100	5.10225000	-0.82389400
H	-1.43091900	3.72167200	-1.57281200
H	-1.43613100	3.90866500	0.19986700
Cl	-3.59542000	0.80416300	1.25785400
Cl	-2.57063300	-1.89228500	-0.66277700
Mg	-4.64882400	-0.86535300	-0.02498100
C	-6.61056900	-1.34791100	-0.55639900
H	-7.31879100	-0.55360100	-0.28586900
H	-6.71471000	-1.52031400	-1.63627400
H	0.26507900	0.20430200	2.95481700
H	-6.95294500	-2.26483400	-0.05727100

Structure 1a·CH3MgCl (c) [B3LYP/6-31G(d)]

C	1.10794100	0.40960000	-0.42045500
C	0.53210500	1.65849400	-0.19132200
C	1.36120200	2.71368200	0.29463300
C	2.69222200	2.51283600	0.54560800
C	3.29301900	1.24424200	0.33091300
C	4.66754600	1.00806500	0.58813500
C	5.22014100	-0.23431300	0.37088800
C	4.42078200	-1.29901900	-0.10990000
C	3.08335600	-1.10761100	-0.37341700
C	2.48628600	0.16651500	-0.16200200
C	-0.90811000	1.92492000	-0.40757000
O	-1.77917800	1.07136400	-0.59844800
O	0.36430900	-0.65439400	-0.91908400
Cl	-2.62861200	-2.21719900	-0.95587700
C	0.25486100	-0.68358300	-2.36643300
O	-1.20444000	3.22215800	-0.38443600
C	-2.59801900	3.58035800	-0.54410200
H	0.91050400	3.68165200	0.47318700
H	3.30450500	3.32795200	0.92118200
H	5.27611200	1.82646800	0.96350700
H	6.27367900	-0.40356900	0.57453600
H	4.86440100	-2.27801800	-0.26446100
H	2.47074800	-1.93385600	-0.71477600
H	-0.31421000	-1.57916800	-2.61237900
H	1.25500200	-0.72377600	-2.80692300
H	-0.28837100	0.19818800	-2.71275500
H	-2.61978100	4.66522000	-0.45030300
H	-3.20581700	3.10602300	0.22855100

H	-2.95118200	3.26847300	-1.52943000
Mg	-3.07026600	-0.23585100	0.41267400
Mg	-0.51633000	-2.31999800	0.27049400
C	-4.90880100	0.66235600	0.88372900
H	-5.60899500	-0.04514900	1.34979700
H	-4.80887100	1.49823000	1.59356000
H	-5.42209900	1.06187400	-0.00424600
Cl	-1.32645300	-0.88772800	2.04327300
C	0.79085100	-3.96170000	0.31562000
H	1.23462000	-4.20717900	-0.66159600
H	1.62632600	-3.82324300	1.01695800
H	0.26085500	-4.86822900	0.64165200

Structure 1a·CH3MgCl (d) [B3LYP/6-31G(d)]

C	-2.69438600	-0.10446700	0.37322300
C	-2.63977000	-0.53680800	-0.94980700
C	-3.34926200	-1.71494800	-1.32702400
C	-4.06740200	-2.42733600	-0.40381900
C	-4.10815900	-2.02447600	0.95943700
C	-3.39889200	-0.84689400	1.36212300
O	-2.05593200	1.05925700	0.75901100
C	-2.91318000	2.22814500	0.77865900
H	-3.30363700	-2.03803600	-2.36006100
H	-4.60421300	-3.32332100	-0.70293100
H	-2.28044800	3.04947500	1.10945700
H	-3.74481900	2.06849300	1.47078700
H	-3.29737400	2.42949400	-0.22696200
Mg	2.72492300	-0.87842300	-0.00281300
Mg	0.16055800	1.50822800	-0.00140500
Cl	0.69338500	-0.61134800	1.23491000
C	0.28673600	3.47720400	0.74959000
H	-0.27228100	4.21914300	0.15669900
H	-0.05089000	3.59398500	1.79155000
H	1.33213500	3.81872300	0.73577200
Cl	2.28625200	0.96531500	-1.40706700
C	-1.83678200	0.19156700	-1.95097700
O	-0.94356400	1.00834900	-1.70040800
C	4.23243100	-2.31948500	0.13085800
H	3.85006500	-3.33333700	-0.05146300
H	5.03732200	-2.14413800	-0.59516100
H	4.69550700	-2.33371000	1.12698800
O	-2.14022100	-0.12079900	-3.20798000
C	-1.33046600	0.49210400	-4.23899600
H	-0.27473000	0.27152500	-4.07026800
H	-1.68229500	0.05186100	-5.17109000
H	-1.48105800	1.57373100	-4.23893800
C	-3.40019500	-0.46581700	2.73108400
C	-4.09743400	-1.20751100	3.65762100
H	-4.08491300	-0.91666100	4.70390700
C	-4.82030400	-2.35758900	3.25894200
H	-5.36707600	-2.93161400	4.00169800
C	-4.82059700	-2.75928400	1.94158800
H	-5.36122000	-3.65133400	1.63626000
H	-2.81931100	0.39703600	3.03699600

Structure 1a·CH3MgCl (e) [B3LYP/6-31G(d)]

C	0.85946200	1.18479000	0.35433200
C	1.70845200	2.29790000	0.63013400
C	3.06685300	2.20011500	0.48904600
C	3.67456400	0.98215600	0.08045700
C	2.84505000	-0.15152100	-0.20071200
C	-0.60009400	1.32977300	0.55006900
O	-1.38476300	0.37288200	0.74259000
O	0.64318900	-1.10368500	-0.40532800
Cl	-2.55050200	-2.47222700	-0.16289200
C	0.36784700	-1.25871700	-1.84160000
H	1.25395500	3.22489600	0.95693400
H	3.69928600	3.05718400	0.70221600
H	-0.12036700	-2.22678300	-1.94243900
H	1.31551800	-1.24095700	-2.38306200
H	-0.30373400	-0.46409000	-2.17434200
Mg	-3.47862600	-0.17397100	-0.39256200
Mg	-0.75629800	-1.61024800	1.13231400
C	-5.07516200	0.33585000	0.87733900
H	-4.80240000	0.32680400	1.94412900
H	-5.49306100	1.33195400	0.66832300
H	-5.91117900	-0.37157300	0.77840700
Cl	-2.65336500	0.84255200	-2.30946400
C	0.15256000	-2.12915300	2.94511900
H	0.45256300	-3.18692500	2.96336100
H	1.05965400	-1.54488100	3.15827700
H	-0.51838600	-1.98606600	3.80381700
C	1.43499100	-0.00663900	-0.08142700
C	3.45214000	-1.38303500	-0.56961300
C	4.82100500	-1.47844100	-0.67578000
H	5.27714600	-2.42524900	-0.94908300
C	5.64160700	-0.35313400	-0.42137200
H	6.72002200	-0.44396500	-0.51354000
C	5.08085200	0.84747000	-0.04709800
H	5.70883900	1.70923800	0.16218500
H	2.82603300	-2.25106900	-0.74154100
O	-0.99651200	2.57915300	0.55626900
C	-2.40004200	2.89397500	0.76757800
H	-2.40655700	3.94246000	1.06248000
H	-2.92670900	2.75008600	-0.17730900
H	-2.82162100	2.25890800	1.54713000

Structure 1a·CH3MgCl (f) [B3LYP/6-31G(d)]

C	1.05739500	1.42512300	-0.42676200
C	1.93357500	1.89424300	-1.44897200
C	3.14604200	1.29357700	-1.66185800
C	3.55661200	0.17901400	-0.87951100
C	2.69307100	-0.30635600	0.15579200
C	-0.26432900	2.05445100	-0.24120600
O	-1.23428800	1.52623800	0.31404900
O	0.64067200	-0.08573000	1.40061800
Cl	-3.88887200	-0.05061200	-0.48482000
C	0.96975200	0.46848800	2.70374200
H	1.61690000	2.73196700	-2.05895500
H	3.80518000	1.65689800	-2.44532300
H	0.24644600	0.03529600	3.39273200
H	0.86267200	1.55789300	2.68150000
H	1.99493400	0.19869800	2.97335700
Mg	-2.72920200	-1.77514500	-1.61866500
Mg	-1.80107300	-0.37847000	0.88244900
C	-1.02334800	-2.19774900	-0.26286800
H	-0.47895000	-2.22626700	0.69222100
H	-1.41978500	-3.22814600	-0.31977600
H	-0.22935400	-2.14722600	-1.02448400
C	1.45200300	0.35711700	0.37699100
Cl	-2.28689600	-0.66697500	3.09493000
C	-3.01792200	-2.69639800	-3.47727600
H	-2.67971300	-3.74193500	-3.48817300
H	-4.07786900	-2.70049200	-3.76666100
H	-2.47611300	-2.18478700	-4.28578200
O	-0.35501100	3.27519700	-0.75533700
C	-1.65177200	3.91732900	-0.67422600
H	-1.53325600	4.85610200	-1.21335200
H	-2.41360500	3.28695500	-1.13639500
H	-1.91209800	4.09770800	0.37068600
C	3.08589700	-1.44153300	0.91547900
C	4.29235100	-2.05770600	0.67130100
H	4.58143700	-2.93002600	1.25002000
C	5.15667600	-1.56845000	-0.33753600
H	6.10652200	-2.06411200	-0.51682200
C	4.79474000	-0.47839000	-1.09748900
H	5.45125600	-0.10913800	-1.88094100
H	2.41131100	-1.82925200	1.67062200

Structure 1a·CH3MgCl (g) [B3LYP/6-31G(d)]

C	0.94682300	-0.56528000	0.41327000
C	0.28224600	-1.77383900	0.21999200
C	1.02389700	-2.89269200	-0.26313600
C	2.35918700	-2.78501700	-0.54762800
C	3.04675300	-1.55374400	-0.37865100
C	4.42508400	-1.41418600	-0.68032200
C	5.06058100	-0.20355600	-0.51577300
C	4.34425600	0.92420600	-0.04796600
C	3.00634000	0.82854900	0.26238000
C	2.32711300	-0.41269900	0.10876300
C	-1.16772000	-1.92714200	0.46705500
O	-1.98166400	-1.00557100	0.57298400
O	0.28504000	0.54249600	0.94099700
C	0.30641800	0.61623700	2.38967400
O	-1.54662200	-3.19916000	0.56880300
C	-2.96156200	-3.44892200	0.74086500
H	0.50409200	-3.83085800	-0.41178800
H	2.90757400	-3.64616600	-0.91926100
H	4.96898300	-2.27955400	-1.04964200
H	6.11603800	-0.10772600	-0.75457100
H	4.85122600	1.87862200	0.05737000
H	2.45766200	1.70721900	0.58593800

H	-0.12933200	1.57879600	2.65748200
H	1.33852800	0.56328300	2.74454600
H	-0.29150800	-0.19753200	2.80790100
H	-3.05390400	-4.53396400	0.76003400
H	-3.52761600	-3.02096200	-0.08873100
H	-3.30582000	-3.01343000	1.68133900
Mg	-3.06013100	0.47342100	-0.46040500
Mg	-0.72000500	2.15323000	-0.10496900
C	-2.69127600	2.25106000	0.91630900
H	-2.18357300	3.04609100	1.48905100
H	-3.54645100	2.78156900	0.46826100
H	-3.11133800	1.60852000	1.70859500
Cl	-1.22809400	0.93704000	-2.09332800
C	-4.99014900	-0.20389700	-0.94375400
H	-5.56662600	-0.50790900	-0.05635400
H	-5.59544600	0.55690100	-1.45694500
H	-4.96975900	-1.07534900	-1.61683900
Cl	0.73026600	3.86508100	0.25035000

Structure 1a·CH3MgCl (h) [B3LYP/6-31G(d)]

C	0.95640600	1.23234700	0.13707000
C	1.79960100	2.35759200	0.37715200
C	3.16303700	2.23459000	0.34069500
C	3.77889300	0.98155400	0.07459800
C	2.95406400	-0.16500400	-0.16787700
C	-0.51118500	1.39913200	0.20727500
O	-1.31492700	0.45589600	0.38016600
O	0.75723800	-1.11540000	-0.42433200
Cl	-2.42745300	-2.49455400	-0.21246100
C	0.51231300	-1.34676700	-1.84796100
H	1.33691500	3.31244000	0.59427300
H	3.79261700	3.09991100	0.52722800
H	-0.11870000	-0.55116100	-2.25069600
H	-0.01037000	-2.29980600	-1.90841400
H	1.47046000	-1.39005900	-2.37025400
Mg	-3.30846100	-0.22563000	-0.78547200
Mg	-0.75012400	-1.45973300	1.10110500
C	-2.82682500	0.49707300	-2.71578800
H	-1.95772100	1.17602900	-2.75616400
H	-2.61145500	-0.31067800	-3.43153900
H	-3.66321500	1.06456300	-3.15053400
Cl	-4.83189400	0.41951600	0.79633900
C	0.11167400	-1.72809600	2.98773400
H	0.62554400	-2.69695200	3.06973400
H	0.85407200	-0.95908900	3.24580400
H	-0.64435300	-1.71111100	3.78471700
C	1.54271300	0.00144800	-0.15045500
C	3.56605700	-1.42659300	-0.40268700
C	4.93744900	-1.54089200	-0.41440600
H	5.39775400	-2.50928300	-0.58620100
C	5.75509500	-0.40618500	-0.19364100
H	6.83582900	-0.51333100	-0.20825400
C	5.18836800	0.82497700	0.04971800
H	5.81370400	1.69483100	0.23150300
H	2.93999100	-2.29948600	-0.54883000
O	-0.90127900	2.64627000	0.09585700
C	-2.31916200	2.97064200	0.21002100
H	-2.33950000	4.03631500	0.43337900
H	-2.79873400	2.76643500	-0.74848400
H	-2.79017200	2.38139600	0.99697400

Structure 1a·CH3MgCl (i) [B3LYP/6-31G(d)]

C	0.84253500	1.31324800	0.28964200
C	1.74250400	2.37066000	0.61289200
C	3.09401700	2.21640700	0.45266500
C	3.64063900	0.99093500	-0.01456700
C	2.75760900	-0.08922700	-0.34264700
C	-0.60354600	1.49490000	0.53785700
O	-1.41851000	0.56695400	0.69530100
O	0.50495600	-0.90842000	-0.61232100
Cl	-2.73621900	-2.24162500	-0.55103200
C	0.27088400	-0.97079300	-2.05855100
H	1.33361400	3.29812200	0.99461400
H	3.76815800	3.03102800	0.70137700
H	-0.33627500	-1.85975200	-2.22188000
H	1.23194600	-1.05285800	-2.56892200
H	-0.27412900	-0.08161500	-2.38027200
Mg	-3.81577500	0.07943400	-0.99837200
Mg	-1.00701300	-1.42897900	0.77283200
C	-5.39002100	0.43886600	0.37018000
H	-5.10672100	0.24281100	1.41570300
H	-5.76965900	1.47199200	0.33851300
H	-6.25912300	-0.20690500	0.17332300
C	1.35855900	0.12129300	-0.21310100
C	3.30494000	-1.33280700	-0.76179000
C	4.66742400	-1.48818800	-0.87534400
H	5.07799800	-2.44517900	-1.18306800
C	5.54092800	-0.41359700	-0.58009200
H	6.61365400	-0.55203500	-0.67890600
C	5.03876300	0.79540900	-0.15409700
H	5.70738900	1.61631200	0.09049800
H	2.63951400	-2.16588300	-0.95737900
C	-2.79166300	1.03734700	-2.60947500
H	-2.43306800	0.33823500	-3.38088100
H	-3.45327800	1.74236000	-3.13638200
H	-1.91496400	1.63800600	-2.30974300
Cl	0.00384500	-2.14573900	2.63911000
O	-0.97423900	2.75559700	0.62482500
C	-2.36416300	3.03383500	0.94558300
H	-2.40177200	4.11138400	1.09648400
H	-2.99856900	2.73528200	0.10991700
H	-2.65502800	2.49566600	1.84878500

Structure 1a·CH3MgCl (j) [B3LYP/6-31G(d)]

C	1.17615500	-0.39098100	0.45783400
C	0.51129300	-1.59948700	0.25674600
C	1.24281700	-2.70354500	-0.27370000
C	2.56863800	-2.58583500	-0.59542500
C	3.25731900	-1.35657500	-0.41691700
C	4.62641300	-1.20406500	-0.75371600
C	5.26434100	0.00296100	-0.57394600
C	4.56001100	1.11487100	-0.05251800
C	3.23133100	1.00478900	0.29000100
C	2.54833300	-0.23178300	0.11905600
C	-0.93179500	-1.76346200	0.53481300
O	-1.72314100	-0.83833300	0.75741200
O	0.53594900	0.71498800	1.00960500
Cl	-4.74150900	-0.24091900	-0.77070700
C	0.52816000	0.73459300	2.45768400
O	-1.33219000	-3.02612500	0.52968700
C	-2.75035600	-3.27165000	0.73309500
H	0.72090000	-3.63938700	-0.42909600
H	3.10775100	-3.43632900	-1.00318700
H	5.16180300	-2.05749500	-1.16114800
H	6.31247700	0.10822100	-0.83920800
H	5.07079600	2.06520700	0.07071800
H	2.68899500	1.86547700	0.66500600
H	0.17628100	1.72385500	2.75140300
H	1.54224800	0.57387500	2.83363200
H	-0.15321900	-0.03075100	2.83705500
H	-2.87220200	-4.34014700	0.56215200
H	-3.34730900	-2.68189300	0.03477000
H	-3.02080000	-3.00986000	1.75846900
Mg	-2.71378400	0.64462300	-0.26711200
Mg	-0.43822800	2.43406700	-0.06104400
C	-2.46005300	2.47067400	0.98220700
H	-1.92106600	2.64881100	1.92688300
H	-2.68925700	3.46838200	0.57557900
H	-3.44446600	2.11652200	1.33850800
Cl	-1.02919400	1.05628500	-1.97806100
C	0.86043800	4.07616000	0.14245100
H	1.34234900	4.14751600	1.13039300
H	1.67236200	4.05721200	-0.59959100
H	0.33523900	5.03105800	-0.00501000

Structure 1a·CH3MgCl (k) [B3LYP/6-31G(d)]

C	-1.00236400	0.54798000	0.34769200
C	-0.41437800	1.79647900	0.16132100
C	-1.22773800	2.87965800	-0.28485200
C	-2.56013300	2.69906200	-0.54751500
C	-3.17226300	1.42768900	-0.38587200
C	-4.54714300	1.21510800	-0.66125000
C	-5.11068600	-0.03117300	-0.50192900
C	-4.32221400	-1.12338200	-0.06705000
C	-2.98530400	-0.95730400	0.21701300
C	-2.37920400	0.32182500	0.06898400
C	1.02924900	2.03688400	0.39256100
O	1.91995000	1.18842300	0.33332400
O	-0.25849100	-0.51680600	0.85122800
Cl	-0.63887900	-3.83512900	-0.05932300
C	-0.28911400	-0.63896300	2.30064700
O	1.30301700	3.31029300	0.66821300

C	2.70006800	3.65425900	0.82954800
H	-0.76623000	3.85004800	-0.42142200
H	-3.16487600	3.53329100	-0.89223900
H	-5.14634000	2.05421700	-1.00469900
H	-6.16430400	-0.18244300	-0.71905300
H	-4.77201000	-2.10646000	0.03416100
H	-2.38208200	-1.81005400	0.51156200
H	0.37904600	-1.46168300	2.55246300
H	-1.30906600	-0.85161100	2.62956600
H	0.07751000	0.28737100	2.75022600
H	2.70622000	4.73025000	0.99787200
H	3.26107000	3.39319400	-0.07000000
H	3.11770400	3.12394300	1.68788100
Mg	2.96683300	-0.23925300	-0.78959900
Mg	0.76527400	-2.06493700	-0.27534500
Cl	2.83634000	-1.98235100	0.94825900
C	4.65633500	0.62387800	-1.69381800
H	4.41426300	1.51148100	-2.29929000
H	5.39782700	0.94801500	-0.94760200
H	5.18372600	-0.06694900	-2.36702800
C	1.26413800	-1.01984700	-2.14717900
H	0.31060900	-1.45119400	-2.50151000
H	1.15970400	0.04257900	-2.42232400
H	2.00381300	-1.44474400	-2.84306800

Structure 1a·CH3MgCl (l) [B3LYP/6-31G(d)]

C	1.22239600	-0.37805000	0.39725700
C	0.61108200	-1.61948000	0.22058800
C	1.39977100	-2.71191600	-0.24872100
C	2.72876300	-2.55318600	-0.53918500
C	3.36487700	-1.29268000	-0.38482000
C	4.73654000	-1.09873300	-0.68865200
C	5.32314900	0.13728600	-0.53230800
C	4.56271400	1.23771100	-0.06864900
C	3.22962200	1.08794300	0.24006400
C	2.59837800	-0.17865000	0.09211300
C	-0.83157800	-1.83593500	0.47480500
O	-1.67196800	-0.94077000	0.61272300
O	0.51890500	0.71708200	0.88470400
C	0.45817300	0.79211500	2.33390700
O	-1.16895100	-3.11563900	0.54420600
C	-2.58043600	-3.41581400	0.72342500
H	0.91964900	-3.67339700	-0.38137300
H	3.31164500	-3.39576700	-0.90062800
H	5.31540900	-1.94407100	-1.05099500
H	6.37394300	0.27397300	-0.77138800
H	5.03326100	2.21063100	0.03679900
H	2.64418900	1.93914800	0.56774500
H	-0.10024800	1.69695700	2.56995800
H	1.47258900	0.84131400	2.73932200
H	-0.07503300	-0.07655200	2.72663300
H	-2.64442300	-4.49942700	0.63711300
H	-3.17850200	-2.91485900	-0.04038600
H	-2.89968000	-3.08563200	1.71425300
Mg	-2.68352500	0.49360800	-0.45360900
Mg	-0.43745000	2.33293800	-0.35835700
C	-1.18443700	1.04840100	-2.04008900
H	-1.78420100	0.27592400	-2.55194200
H	-0.15150900	0.69520300	-2.19870300
H	-1.30773600	1.92449600	-2.69697900
Cl	-2.46907800	2.37222400	1.04047400
C	0.92041100	3.92543700	-0.56282200
H	1.40532200	4.21011900	0.38405400
H	1.72841600	3.72308700	-1.28119600
H	0.40897400	4.83084500	-0.92105600
Cl	-4.57802800	-0.55473100	-1.13883600

Structure 1a·CH3MgCl (m) [B3LYP/6-31G(d)]

C	1.09342300	-0.52691100	0.38890800
C	0.42704800	-1.73241700	0.16960400
C	1.16857100	-2.84321600	-0.33219900
C	2.50542700	-2.73394100	-0.60914900
C	3.19486100	-1.50717400	-0.41642400
C	4.57436800	-1.36443000	-0.71148900
C	5.21066700	-0.15732900	-0.52519000
C	4.49417000	0.96396500	-0.04219900
C	3.15518300	0.86487100	0.26248200
C	2.47525900	-0.37337900	0.08800100
C	-1.02562800	-1.88776900	0.40657900
O	-1.82761500	-0.94949700	0.56704400
O	0.43953700	0.57903100	0.92954400
Cl	-4.73096500	-0.21125500	-1.09615500
Cl	0.86323200	3.89449600	0.07825400
C	0.43901400	0.62061900	2.38006800
O	-1.42632300	-3.15467300	0.42998500
C	-2.85300800	-3.39150500	0.57350100
H	0.64695200	-3.77749800	-0.49850400
H	3.05348700	-3.59008800	-0.99261800
H	5.11862800	-2.22431900	-1.09279600
H	6.26705600	-0.05904800	-0.75868400
H	5.00202500	1.91594600	0.07945000
H	2.60474800	1.73840700	0.59621800
H	-0.00204500	1.57666300	2.66142000
H	1.46598000	0.55806500	2.74853300
H	-0.16660900	-0.20028400	2.77192500
H	-2.97792100	-4.45587100	0.38022100
H	-3.41732900	-2.78441500	-0.13697700
H	-3.16063000	-3.14518400	1.59232400
Mg	-2.73865800	0.62967800	-0.40113400
Mg	-0.61897000	2.18429700	-0.12044600
C	-2.52458600	2.27266500	1.10661100
C	-1.15312600	1.12078000	-1.99335900
H	-1.99302700	3.14691300	1.52045400
H	-3.48068300	2.71215000	0.77608400
H	-2.76512600	1.66340300	1.99221400
H	-1.85360100	0.46316200	-2.53661500
H	-0.17817600	0.62751000	-2.13842500
H	-1.12533200	2.02674800	-2.61996200

Structure 1a-TSOMe [B3LYP/6-31G(d)]

C	-0.10976000	1.30032400	-0.08795100
C	0.79406600	2.39036400	0.11746400
C	2.13571300	2.19732600	0.26284000
C	2.69309400	0.87888500	0.17540400
C	1.83535000	-0.24229800	-0.02314000
C	-1.52480900	1.52045600	-0.08467600
O	-2.39343000	0.61224000	0.04788700
O	-0.30998800	-1.03584600	-0.84775000
Cl	-3.27656000	-2.99059900	0.42013100
C	-0.23674200	-0.85026700	-2.27867900
H	0.37509400	3.38935900	0.16802600
H	2.80332500	3.03966500	0.41850700
H	-0.78191600	-1.68998700	-2.71226700
H	0.80848400	-0.87230200	-2.59652600
H	-0.69844300	0.09690200	-2.57036600
Mg	-1.85130400	-1.26296600	0.44309600
C	-0.15367500	-0.94647800	1.89702500
H	0.51569600	-1.81023700	1.91492000
H	0.32095000	-0.10138800	2.39455600
H	-1.03747500	-1.19936700	2.52646400
C	0.39059500	-0.04583800	-0.05382500
C	2.39865700	-1.52920000	-0.16859600
C	3.76861600	-1.71577900	-0.11501600
H	4.18621500	-2.71211800	-0.22730300
C	4.61842800	-0.61302000	0.09541900
H	5.69408100	-0.76021400	0.14392700
C	4.08894900	0.65576100	0.23824700
H	4.74497600	1.50895300	0.39257200
H	1.73791200	-2.37709500	-0.31787100
O	-1.92233100	2.79573800	-0.19207700
C	-3.33624800	3.04645100	-0.11491200
H	-3.43969000	4.12518100	-0.23272300
H	-3.86520400	2.52026300	-0.91317000
H	-3.73314700	2.72681300	0.85188100

Structure 1a-TSCO [B3LYP/6-31G(d)]

C	0.06343800	1.12676400	-0.16783600
C	0.90049000	2.26845000	-0.05233500
C	2.26565900	2.14135500	0.02945400
C	2.88280500	0.86362900	0.04987200
C	2.05945100	-0.30639000	-0.03681900
C	-1.44093300	1.26943000	-0.22389900
O	-2.13867400	0.50357500	-1.00026400
O	-0.14691400	-1.27615700	-0.28226900
Cl	-3.32569500	-2.84740800	0.53349600
C	-0.16009500	-1.88894200	-1.60703000
H	0.43444300	3.24600700	-0.04001300
H	2.89172100	3.02727100	0.09745400
H	-0.75194300	-2.80072000	-1.50734500
H	0.86065700	-2.12906200	-1.90890000
H	-0.62365700	-1.19945700	-2.31675200
Mg	-2.16496900	-0.94706300	0.31371900

C	-1.81301200	0.63641400	1.83796900
H	-1.38388000	-0.21753600	2.39961500
H	-1.27348000	1.51455300	2.18712000
H	-2.86733100	0.74823400	2.13515300
C	0.65775600	-0.12479400	-0.19171600
C	2.66965300	-1.58747100	0.06159900
C	4.03451600	-1.70225300	0.20050000
H	4.48721100	-2.68634100	0.28333900
C	4.85407900	-0.54846500	0.24825500
H	5.92997300	-0.65657600	0.35223900
C	4.28794300	0.70391800	0.18117500
H	4.90870800	1.59457300	0.23817000
H	2.04571400	-2.47458400	0.05668700
O	-1.80892400	2.56802500	-0.08867300
C	-3.18512200	2.86335600	-0.35309800
H	-3.28142900	3.94040900	-0.20952900
H	-3.45500600	2.58439800	-1.37365000
H	-3.83450500	2.33415000	0.35209400

Structure 1a-intOMe [B3LYP/6-31G(d)]

C	-0.17132100	1.25273700	0.18208400
C	0.73970200	2.33973600	-0.05274400
C	2.08239200	2.17534900	-0.15027600
C	2.67299000	0.86064800	-0.04137100
C	1.85801600	-0.27290600	0.20385000
C	-1.55034600	1.49015600	0.23460900
O	-2.48278000	0.59321200	0.30693700
O	-0.32107200	-1.12387300	-0.64252400
Cl	-3.59017900	-2.97977900	-0.51193200
C	0.04054600	-0.90428900	-2.01851800
H	0.30774100	3.32885200	-0.16110100
H	2.73499900	3.02382500	-0.33374900
H	-0.56822700	-1.58303000	-2.62274500
H	1.09712200	-1.13826800	-2.16549600
H	-0.14940100	0.13662100	-2.30357300
Mg	-2.25723500	-1.23810500	-0.18671000
C	-0.07598200	-0.76579200	1.73428500
H	0.14129300	-1.83738600	1.77934000
H	0.48367500	-0.27601000	2.53557000
H	-1.13603900	-0.59207400	1.95816300
C	0.35821300	-0.13943200	0.39359700
C	2.45171200	-1.54189200	0.28447000
C	3.82512000	-1.71141200	0.13466200
H	4.26046100	-2.70469800	0.19522700
C	4.63488800	-0.59239100	-0.09425500
H	5.70942700	-0.71037900	-0.20834700
C	4.06393500	0.66906300	-0.18188700
H	4.69014100	1.53847500	-0.36815500
H	1.82521800	-2.41500600	0.44461100
O	-1.95187200	2.78023500	0.18107500
C	-3.35932100	3.03406800	0.12329500
H	-3.44990000	4.12033600	0.07775000
H	-3.80784900	2.58278300	-0.76694000
H	-3.86658600	2.65030800	1.01231200

Structure 1a-intCO [B3LYP/6-31G(d)]

C	0.09509000	0.93763100	0.65837200
C	0.96972200	1.94423500	1.14699800
C	2.33697400	1.83420400	1.05025000
C	2.93629900	0.67438700	0.50173600
C	2.08790300	-0.36936200	0.00858800
C	-1.42380100	0.98993800	0.94810500
O	-1.81665200	-0.06846500	1.67781200
O	-0.13272000	-1.17154900	-0.51765000
Cl	-3.29971200	-2.91331900	-0.70550600
C	-0.14313600	-1.15708700	-1.97659900
H	0.54775600	2.82943000	1.60810500
H	2.97514500	2.63198200	1.42149500
H	-0.78792700	-1.98459500	-2.27847500
H	0.86878700	-1.30567300	-2.35537800
H	-0.54809400	-0.20275900	-2.32071300
Mg	-2.10614200	-1.24283300	0.19109100
C	-1.91255100	2.31529200	1.52372100
H	-1.45345500	2.45419300	2.50603000
H	-1.67591800	3.17833900	0.89312900
H	-2.99120000	2.26060700	1.68163400
C	0.68053900	-0.16585600	0.05421200
C	2.68671300	-1.56925400	-0.46897300
C	4.05598700	-1.70779600	-0.49285400
H	4.49726700	-2.63500500	-0.84778300
C	4.89630000	-0.65881100	-0.04596500
H	5.97515400	-0.78175200	-0.07820900
C	4.34562700	0.50135100	0.44614100
H	4.98175100	1.30275300	0.81379900
H	2.05243300	-2.39255900	-0.77889700
O	-2.05674300	0.77010100	-0.48436900
C	-3.27650000	1.43732200	-0.81447500
H	-3.60250400	1.03500500	-1.77757400
H	-4.06425000	1.25481600	-0.07257800
H	-3.11949200	2.51637800	-0.91743900

Structure 1a-TS2OMe [B3LYP/6-31G(d)]

C	-0.02641000	1.30138500	-0.16477900
C	-0.97120200	2.27951400	0.30249100
C	-2.29086000	2.00825200	0.46305400
C	-2.80509900	0.69442700	0.16864200
C	-1.93746100	-0.32434300	-0.30799300
C	1.34316700	1.63533100	-0.23439900
O	2.31930400	0.81100000	-0.38946300
O	0.32571800	-1.17304600	0.54190200
Cl	3.81083000	-2.61437100	0.17895800
C	-0.08467100	-1.07547400	1.90714600
H	-0.58702300	3.26560000	0.53961400
H	-2.97721500	2.76914000	0.82273100
H	0.53633100	-1.75501900	2.50083200
H	-1.13135300	-1.37710600	2.00695700
H	0.03050700	-0.04904800	2.27967700
Mg	2.22374400	-1.06667700	0.05184700
C	0.04156900	-0.61881900	-1.84807200
H	-0.03480400	-1.70832100	-1.90624100
H	-0.57434100	-0.20123700	-2.65013200
H	1.06948100	-0.30963600	-2.06539200
C	-0.47516700	-0.06408300	-0.51128100
C	-2.46776900	-1.59823700	-0.58312600
C	-3.81701400	-1.87631600	-0.40624300
H	-4.19949700	-2.87054600	-0.61844600
C	-4.67673100	-0.86762800	0.05222800
H	-5.73489800	-1.07423500	0.19036100
C	-4.17476700	0.39213400	0.33530600
H	-4.83730600	1.17502000	0.69688100
H	-1.80577100	-2.39171700	-0.91496600
O	1.65516900	2.93754300	-0.08748100
C	3.04540600	3.28202500	-0.01813000
H	3.06267200	4.36506400	0.10914300
H	3.52981400	2.79414700	0.83268700
H	3.56489700	2.99933800	-0.93689900

Structure 1a-TS2CO [B3LYP/6-31G(d)]

C	-0.26087100	1.27435400	-0.28988000
C	-1.27824100	2.26779100	-0.23812300
C	-2.60145000	1.94014200	-0.07500000
C	-3.00661000	0.58319600	-0.01840600
C	-2.00768000	-0.44410700	-0.06942400
C	1.12189700	1.67501200	-0.71763600
O	1.72506000	0.93138400	-1.54485600
O	0.33687400	-1.05512500	-0.01275500
Cl	3.63193700	-2.37759500	-0.56073000
C	0.39506100	-1.69812700	1.29921100
H	-0.99719500	3.30990900	-0.34212800
H	-3.35686900	2.71968400	-0.02686300
H	1.15286100	-2.47830800	1.20510200
H	-0.56876500	-2.13747400	1.55425100
H	0.68953000	-0.95897300	2.04738400
Mg	2.41307200	-0.50233700	-0.34585700
C	1.56325700	3.10894400	-0.57608700
H	1.12860500	3.70607600	-1.38888500
H	1.26215100	3.54494400	0.37916700
H	2.64908400	3.14251900	-0.67215500
C	-0.63756800	-0.05656100	-0.12166000
C	-2.42867200	-1.80373000	-0.12013700
C	-3.76517800	-2.12707300	-0.06853700
H	-4.07029200	-3.16794700	-0.12701400
C	-4.74858900	-1.11386400	0.04236300
H	-5.79895600	-1.38607400	0.09308800
C	-4.37532000	0.20968800	0.05754200
H	-5.12512900	0.99491300	0.11061700
H	-1.68741900	-2.58425900	-0.25077400
O	2.27665500	0.90418800	0.93965200
C	2.37681900	1.35525300	2.25112600
H	3.19801000	0.85444300	2.78876100
H	2.58278200	2.43876700	2.29170500
H	1.45196500	1.17985600	2.83199500

Structure 1a-prodOMe [B3LYP/6-31G(d)]

C	0.07572900	1.62016500	0.24959400
C	0.92731100	2.72820200	0.54090300
C	2.26078200	2.54106300	0.77189900
C	2.82051600	1.23639300	0.73494700
C	1.97928000	0.11562900	0.42257100
C	-1.36369900	1.90322100	0.10341600
O	-2.27589400	1.08672400	0.32034100
O	-2.63946400	-1.62364400	1.86081200
Cl	-4.81805200	1.50112300	2.56020200
C	-2.82444600	-2.82614500	2.53659800
H	0.49421400	3.72004600	0.59056600
H	2.90451500	3.38578900	1.00187000
H	-3.69352300	-2.81696500	3.21812400
H	-1.94347000	-3.08607500	3.15013900
H	-2.98055500	-3.66489500	1.83502900
Mg	-3.30823600	0.06361800	1.69728000
C	-0.27222300	-0.84871600	-0.29554700
H	0.32844300	-1.60412500	-0.80566000
H	-0.79646500	-1.32450000	0.54618800
H	-1.04805600	-0.52822800	-0.99341600
C	0.58336300	0.31688000	0.14304200
C	2.57593300	-1.17860300	0.42422000
C	3.91285600	-1.35216800	0.70471600
H	4.33731400	-2.35206500	0.70861300
C	4.73636100	-0.23967800	0.99152900
H	5.79135700	-0.38773700	1.20469900
C	4.19703700	1.02614800	1.00652700
H	4.81820000	1.88861400	1.23480600
H	1.96570200	-2.05143100	0.22679000
O	-1.64239400	3.14475500	-0.26746400
C	-3.04075800	3.52706500	-0.32496000
H	-3.02726600	4.59678900	-0.52915000
H	-3.53523600	2.98707700	-1.13556100
H	-3.53807200	3.30784600	0.62211700

Structure 1a-prodCO [B3LYP/6-31G(d)]

C	-0.18195200	1.20740600	-0.91258200
C	0.63564900	2.36037300	-1.11389100
C	1.97225000	2.35224400	-0.81341200
C	2.59190600	1.19069700	-0.27923000
C	1.80082700	0.01515800	-0.06856100
C	-1.63297100	1.27674400	-1.20576000
O	-2.44796800	0.47076600	-0.73640500
O	-0.30754100	-1.11751100	-0.26243600
Cl	-3.20731600	-2.87588700	0.33412400
C	-0.23083500	-2.04074900	-1.38669200
H	0.18268900	3.26850000	-1.49509300
H	2.57258500	3.24427900	-0.96893000
H	-0.87392100	-2.87808900	-1.11805100
H	0.80584600	-2.35670900	-1.52714400
H	-0.60614700	-1.55179200	-2.29052500
Mg	-2.17665600	-0.89941100	0.80296100
C	-2.16164600	2.38290400	-2.08978300
H	-2.16062400	3.33158600	-1.53795100
H	-1.55116200	2.51975700	-2.98758800
H	-3.19081900	2.14735200	-2.36473800
C	0.42458200	0.05090200	-0.41920900
C	2.40545800	-1.13830000	0.50240700
C	3.74233800	-1.13153900	0.82839500
H	4.19478300	-2.01223900	1.27449200
C	4.53179400	0.02156400	0.59924200
H	5.58608000	0.00999400	0.86071500
C	3.96803200	1.15760300	0.06258500
H	4.56847000	2.04882500	-0.09951800
H	1.79231100	-2.00929300	0.70408500
O	-1.72156800	0.14139200	2.22990300
C	-1.69542100	0.29741800	3.60409800
H	-0.66468800	0.42937300	3.98645400
H	-2.26152700	1.18994500	3.93243200
H	-2.12419000	-0.56197200	4.15338900

Structure 1a-TSOMe (b) [B3LYP/6-31G(d)]

Cl	-3.19100900	0.30747000	1.66459500
Cl	-2.68241900	-1.43828800	-1.23214300
Mg	-4.56426100	-0.93237000	0.16704300
C	-6.58928700	-1.41824400	0.06881500
H	-6.86863200	-2.14287300	0.84551800
H	-7.22842100	-0.53708700	0.21278900
H	-6.85984500	-1.86206900	-0.89796100
C	1.57407900	1.39978000	-0.13073000
C	2.83188600	1.98453100	0.21938300
C	3.93107700	1.22347600	0.48674000
C	3.86855200	-0.20504600	0.37632600
C	2.63542400	-0.83625600	0.04149900
C	0.41121400	2.21907900	-0.29266300
O	-0.77696900	1.78966300	-0.30449600
O	0.42984200	-0.61345800	-0.95476900
C	0.67950500	-0.49722100	-2.37265500
H	2.88716700	3.06612100	0.27656500
H	4.87628700	1.68833100	0.75151600
H	-0.14445200	-1.02255600	-2.85639000
H	1.63238100	-0.97308300	-2.61786500
H	0.69523600	0.55233600	-2.67932200
Mg	-1.19493100	-0.09322800	0.21440700
C	0.39475600	-0.62073800	1.76774000
H	0.60064300	-1.69522600	1.77543500
H	1.17857600	-0.10314500	2.32115400
H	-0.53197500	-0.44361000	2.35233600
C	1.42802200	-0.02876300	-0.09960400
C	2.59796900	-2.23748400	-0.12716100
C	3.73881200	-3.00419100	0.03376000
H	3.69348800	-4.08122300	-0.09976000
C	4.95526600	-2.38621900	0.38082100
H	5.84984200	-2.98875100	0.51449300
C	5.01552600	-1.01541500	0.54880200
H	5.95640600	-0.53598300	0.80788400
H	1.65426500	-2.70874700	-0.38220400
O	0.63173300	3.53728600	-0.40145300
C	-0.52511800	4.38691100	-0.47915200
H	-0.12885600	5.40050400	-0.54297900
H	-1.11749100	4.15140600	-1.36692900
H	-1.14897000	4.27360000	0.41085200

Structure 1a-TSOMe (k) [B3LYP/6-31G(d)]

C	-1.17975700	-1.89679300	-0.04517500
C	0.23642500	-1.73026100	-0.09006300
C	0.85525400	-0.44098900	0.04599700
O	-2.02759000	-0.97303100	0.10508200
Mg	-0.22943200	1.99511500	-0.49432200
Mg	-3.55425800	0.22713800	0.17354200
Cl	-2.62757300	2.25052400	-0.65182000
C	0.43102600	0.43845500	-1.94664000
H	-0.52904800	0.00016800	-2.24402000
H	1.23482600	-0.20281200	-2.30192200
H	0.58095000	1.39408700	-2.49903500
Cl	0.82757800	3.94449300	-0.08342600
C	-5.47979400	-0.21783900	0.84873700
H	-6.03735200	-0.83565000	0.13057900
H	-6.07509000	0.69026500	1.00916000
H	-5.47657800	-0.76744500	1.80029800
C	2.41818500	-2.77138700	-0.48614100
H	3.01745900	-3.64101700	-0.73990600
C	3.08606900	-1.54096600	-0.16289700
C	2.31826600	-0.38327900	0.14619000
C	1.06369500	-2.85878900	-0.42797600
H	0.56997000	-3.80037900	-0.63566400
O	-1.60590600	-3.16620200	-0.17841000
C	-3.01844100	-3.41079700	-0.17544500
H	-3.11940500	-4.49387500	-0.24630600
H	-3.49842000	-2.93617800	-1.03684100
H	-3.48060700	-3.04783200	0.74618300
C	2.98476100	0.80976300	0.49851500
C	4.36869200	0.86144700	0.54810300
H	4.86147200	1.79122800	0.81615700
C	5.12902700	-0.27928000	0.23858000
H	6.21425100	-0.23468000	0.27199600
C	4.49508000	-1.45782500	-0.11263000
H	5.07713000	-2.34465200	-0.35100700
H	2.41659600	1.70920500	0.71507900
O	0.18290200	0.54259200	0.84437900
C	0.18032300	0.32169800	2.27011200
H	1.20268100	0.19028900	2.63170100
H	-0.25869500	1.21850600	2.70993100
H	-0.42406500	-0.55737900	2.50814200

Structure 1a-TSOMe (l) [B3LYP/6-31G(d)]

C	-0.91684700	-1.77609700	-0.07739700
C	0.49539200	-1.57237100	-0.10587600
C	1.08384700	-0.27413500	0.05775200
O	-1.78713800	-0.87247300	0.07688800

Cl	-5.26170900	-0.17171800	0.62129700
Mg	0.14958800	2.25111200	-0.53084400
Mg	-3.19703900	0.41095900	0.02841500
Cl	-2.35055100	2.45179800	-0.65190000
C	1.09308900	4.10350400	-0.21354100
H	2.07069100	4.17706000	-0.71219900
H	1.27165000	4.32510100	0.85000300
H	0.48449000	4.93503100	-0.59698200
C	0.65819400	0.58887200	-1.98603100
H	-0.28435900	0.08622000	-2.22844400
H	1.48890700	-0.02684100	-2.32814900
H	0.72706000	1.51768600	-2.59493300
C	2.70282500	-2.56047700	-0.49378700
C	3.33968500	-1.32213700	-0.14271400
C	2.54186300	-0.18835700	0.18042300
C	4.74613100	-1.20922500	-0.07473500
C	5.35071400	-0.02644700	0.31122600
H	6.43415500	0.04063500	0.35897900
C	4.56186100	1.08883400	0.64246000
H	5.03196500	2.01976000	0.94539000
C	3.18042500	1.00712800	0.57456900
H	2.58752000	1.88350400	0.81581500
O	0.37565400	0.70373500	0.81920700
C	0.32759300	0.48536200	2.24469600
H	-0.15095600	1.37099900	2.66649000
H	1.33786200	0.37794700	2.64740900
H	-0.26443400	-0.40667800	2.46509500
C	1.34990200	-2.67805500	-0.44990100
H	0.87846600	-3.62676400	-0.67618200
H	3.32322000	-3.41260300	-0.75585000
H	5.34996800	-2.07769000	-0.32599200
O	-1.31566400	-3.04787300	-0.22326400
C	-2.72747700	-3.32145100	-0.23781000
H	-2.80278100	-4.40707900	-0.29611500
H	-3.20064500	-2.86680300	-1.11285500
H	-3.21095100	-2.95249800	0.66927500

Structure 1a-TSCO (b) [B3LYP/6-31G(d)]

Cl	-3.73663000	0.95007600	-0.22115900
Cl	-2.24455300	-2.07104200	0.25409300
Mg	-4.50015300	-1.24617100	0.27561400
C	-6.34530600	-2.15975700	0.60146100
H	-7.17839300	-1.54192100	0.24212900
H	-6.41656700	-3.13064100	0.09357700
H	-6.52114200	-2.34653600	1.66939400
C	1.59693000	1.27159000	-0.05879400
C	2.76778700	1.97088000	0.33648300
C	3.96339300	1.31361200	0.49619700
C	4.05633700	-0.09150100	0.31702800
C	2.88167100	-0.82379500	-0.05517900
C	0.27177900	1.97864600	-0.20499600
O	-0.53755600	1.64131400	-1.15691100
O	0.53199100	-0.80510000	-0.64793900
C	0.49132700	-1.15288800	-2.05856200
H	2.69640200	3.03942500	0.49919100
H	4.85544600	1.86615700	0.77992000
H	-0.35370400	-1.83444200	-2.17609600
H	1.41592600	-1.65921900	-2.34274300
H	0.35090200	-0.24553300	-2.65180700
Mg	-1.37057100	0.21067500	-0.09231800
C	-0.56756300	1.29741300	1.69011900
H	-0.74784500	0.28598900	2.11290800
H	0.30112400	1.67598900	2.22587000
H	-1.43110800	1.92931400	1.93336500
C	1.68251900	-0.09185200	-0.27760800
C	2.95681200	-2.23991600	-0.16245600
C	4.14898700	-2.89463100	0.05149000
H	4.19109100	-3.97756200	-0.02510700
C	5.31961900	-2.17023100	0.38294200
H	6.25375300	-2.70109900	0.54348900
C	5.26962000	-0.80168600	0.51884400
H	6.15997900	-0.24126900	0.79315600
H	2.05672600	-2.80253000	-0.38549800
O	0.38261700	3.29140100	0.12226200
C	-0.74112300	4.11758600	-0.20639400
H	-0.47584600	5.11613800	0.14405100
H	-0.91911700	4.12215400	-1.28387200
H	-1.64197500	3.76623800	0.30589500

Structure 1a-TSCO (k) [B3LYP/6-31G(d)]

C	-1.25487700	-0.20489400	-0.29223700
C	-0.65088100	-1.30870200	0.28533200
C	-1.47762200	-2.38805500	0.70187600
C	-2.83877400	-2.34327000	0.52589400
C	-3.47176900	-1.20018100	-0.02793700
C	-4.88090400	-1.11171700	-0.17788800
C	-5.46715300	0.03425800	-0.66459700
C	-4.66935600	1.15301700	-1.00742300
C	-3.29899000	1.10034600	-0.88879300
C	-2.66477700	-0.08296800	-0.42001400
C	0.84008700	-1.37642800	0.47367300
O	1.62267700	-0.91945700	-0.43543100
O	-0.46022800	0.88303900	-0.67525200
Cl	0.14612200	3.46313300	1.46327100
C	-0.21928500	1.00710300	-2.09973900
O	1.18762700	-2.50263300	1.13966000
C	2.56386700	-2.88349300	1.14702300
H	-1.00886200	-3.25523800	1.14920000
H	-3.45267400	-3.18702400	0.82971100
H	-5.48987300	-1.96425400	0.11180500
H	-6.54677000	0.09182300	-0.76973300
H	-5.14513400	2.06573000	-1.35424100
H	-2.69623400	1.97372100	-1.11158200
H	0.35604700	1.92444200	-2.23180100
H	-1.17252500	1.08263400	-2.62602100
H	0.34344000	0.13945800	-2.45177000
H	2.61468600	-3.77286400	1.77588700
H	3.18654300	-2.09592700	1.58585700
H	2.91478700	-3.12275700	0.13849500
Mg	3.40209600	-0.39284500	-1.04591400
Mg	0.96246900	1.46689500	0.76123000
Cl	3.13079900	1.83977700	-0.31016600
C	4.87730500	-1.46766400	-2.05837500
H	4.46803500	-2.32198400	-2.61457200
H	5.41154400	-0.83989300	-2.78381600
H	5.63835100	-1.86883400	-1.37457700
C	1.02983600	-0.12619200	2.34165100
H	0.86310400	0.85366800	2.83734600
H	0.29779300	-0.78803200	2.80378500
H	2.03444500	-0.44729800	2.63695400

Structure 1a-TSCO (l) [B3LYP/6-31G(d)]

C	1.34468000	0.12528700	-0.37031500
C	0.64313100	1.25477500	0.01532600
C	1.39817200	2.36808800	0.48381600
C	2.76931100	2.33175000	0.54141600
C	3.49250300	1.17488600	0.15397000
C	4.90916200	1.10634300	0.21832400
C	5.57581000	-0.04330900	-0.13856500
C	4.85138100	-1.18143500	-0.56799200
C	3.47725800	-1.14966700	-0.64741100
C	2.76330800	0.02998800	-0.30057400
C	-0.87133800	1.36453800	-0.08223700
O	-1.49802200	0.85873400	-1.09894900
O	0.64708200	-1.02732500	-0.76950400
C	0.46299800	-1.18722400	-2.20629800
O	-1.23921000	2.60367300	0.35560300
C	-2.50134600	3.13035100	-0.07919200
H	0.86233200	3.25765700	0.78605100
H	3.31911500	3.20088500	0.89297800
H	5.45744500	1.97976100	0.56182700
H	6.65975500	-0.08547200	-0.08309400
H	5.38528100	-2.09015700	-0.83066200
H	2.93024100	-2.03252000	-0.95900400
H	-0.03965100	-2.14469400	-2.34213100
H	1.44323400	-1.19429300	-2.68783100
H	-0.15825800	-0.37047700	-2.57206800
H	-2.53637000	4.14314700	0.32423600
H	-3.34199900	2.55028000	0.31461500
H	-2.55613200	3.15010200	-1.16995900
Mg	-2.91151000	-0.21386800	-0.28917000
Mg	-0.30621600	-1.90624100	0.84449100
Cl	-2.30474600	-2.52346300	-0.33529500
C	-1.52000800	0.35281500	1.67536600
H	-1.57276600	-0.65226700	2.14428900
H	-0.82862600	0.92112800	2.29888100
H	-2.51489800	0.78620300	1.87095600
Cl	-5.08242000	0.32236600	-0.10284300
C	0.77767200	-2.83694700	2.36269600
H	0.11860900	-3.25347600	3.13676500
H	1.37988000	-3.67342400	1.98037900
H	1.47238500	-2.15451200	2.87108800

Structure 1a·CH3MgCl(DME) (d)_I [B3LYP/6-31G(d)]

C	2.20800700	-0.18989800	0.38384400
C	1.97267900	-1.29685900	-0.42851700
C	2.75436900	-1.47337400	-1.60824800
C	3.72128100	-0.56712300	-1.95313600
C	3.95820500	0.58645700	-1.15606000
C	3.18061000	0.78785100	0.02949900
O	1.49469900	-0.00360400	1.55093200
C	2.14750500	-0.52158300	2.73391600
H	2.56211800	-2.33880500	-2.23067500
H	4.31045700	-0.71283300	-2.85429100
H	1.48863400	-0.27590500	3.56471500
H	3.12674600	-0.04924700	2.85859900
H	2.26464900	-1.60786000	2.65664800
Mg	-0.92871700	-0.41640700	1.55416200
Cl	-3.10480400	-1.27222600	0.50703900
C	-1.15722200	-0.10795800	3.63395300
H	-0.82723800	-0.96365600	4.24541600
H	-0.63286700	0.77613600	4.03065600
H	-2.21857900	0.03584600	3.88665800
Cl	-0.93261000	1.35121300	-0.20302800
C	0.90919300	-2.26538600	-0.09855100
O	0.00616500	-2.08972700	0.72635300
C	3.38488700	1.95942900	0.80704900
C	4.33744200	2.88165900	0.43702500
H	4.48120400	3.77983600	1.03056000
C	5.12369700	2.67454000	-0.72184800
H	5.87246600	3.41070900	-1.00069900
C	4.93451500	1.55562900	-1.50231300
H	5.52642500	1.40249900	-2.40097000
H	2.75896000	2.12652200	1.67627200
O	0.98142000	-3.39620900	-0.79614100
C	-0.09223600	-4.34570200	-0.59352300
H	0.09058300	-5.13518500	-1.32145700
H	-0.05406000	-4.73993100	0.42438000
H	-1.05752700	-3.86473900	-0.76214100
Mg	-2.96006000	0.42811600	-1.20797600
O	-4.38452500	1.79898700	-0.45086200
C	-4.35088500	2.31011100	0.88850900
H	-4.78588400	3.31665800	0.90748600
H	-4.90443800	1.64796400	1.56398800
H	-3.30300900	2.35406000	1.18525400
C	-5.70423700	1.76409600	-1.00505300
H	-6.35554000	1.11703500	-0.40428800
H	-6.11968000	2.77856400	-1.03805100
H	-5.61267700	1.36672400	-2.01675300
C	-3.31829000	0.14265200	-3.26606300
H	-2.48722100	-0.37959200	-3.76346300
H	-4.21590000	-0.46078800	-3.47237400
H	-3.44544500	1.08990400	-3.81305900

Structure 1a·CH3MgCl(DME) (d)_II [B3LYP/6-31G(d)]

C	-2.01984400	0.52279400	0.08995500
C	-1.54042800	0.85296600	-1.17566000
C	-2.14359200	0.26325700	-2.32545600
C	-3.17148800	-0.63282700	-2.19789900
C	-3.65201800	-1.01503300	-0.91479600
C	-3.06035800	-0.43585000	0.25373600
O	-1.49173600	1.11574100	1.21668200
C	-2.22570400	2.27297400	1.68198500
H	-1.76812000	0.53711200	-3.30423000
H	-3.62422300	-1.07488900	-3.08126500
H	-1.68754700	2.62621800	2.55929700
H	-3.25118000	1.98895100	1.93744200
H	-2.23627000	3.04978600	0.90969000
Mg	0.95237900	1.33728900	1.42807300
Cl	3.35428700	1.13100400	0.53109800
C	0.87249600	2.58328100	3.13276000
H	0.57090500	3.62083800	2.91423500
H	0.20794200	2.22872000	3.93655600
H	1.87225900	2.65727800	3.58540000
Cl	0.83357900	-1.15186400	1.34227000
C	-0.40396700	1.78143300	-1.33273400
O	0.40187200	2.08972600	-0.45061200
C	-3.50840000	-0.84485300	1.53846500
C	-4.51798000	-1.77296900	1.65902000
H	-4.84764300	-2.08939000	2.64426700
C	-5.12146100	-2.32987000	0.50601700
H	-5.91856300	-3.05968500	0.61715200
C	-4.69474400	-1.96277100	-0.75114600
H	-5.14694700	-2.40049000	-1.63739800
H	-3.02143700	-0.43843400	2.41764000
O	-0.28891700	2.27806100	-2.56474200
C	0.84759800	3.13933500	-2.80397800
H	0.81910600	3.35386400	-3.87175600
H	0.74920700	4.05843400	-2.22202200
H	1.77291100	2.63208200	-2.52440800
Mg	3.19829100	-1.26236700	0.75097500
O	2.89925700	-1.69854200	-1.33279300
C	2.28681300	-2.94680900	-1.67264400
H	1.83810700	-2.87900300	-2.67140000
H	3.02294000	-3.75978500	-1.65173100
H	1.50554100	-3.12778900	-0.93287800
C	3.90929700	-1.29509000	-2.26300400
H	4.73439200	-2.01805400	-2.27977200
H	3.47500800	-1.20902700	-3.26693400
H	4.26952500	-0.31961300	-1.93257000
C	4.61147200	-2.60903300	1.54041800
H	4.81944600	-2.40668000	2.60111600
H	4.28808900	-3.66034800	1.49133900
H	5.58484300	-2.56003000	1.02788900

Structure 1a·CH3MgCl(DME) (d')_I [B3LYP/6-31G(d)]

C	-1.92655500	0.18499300	-0.01654800
C	-1.37368500	0.60597700	-1.22279800
C	-1.36253600	-0.29563300	-2.32623900
C	-1.87070500	-1.56128000	-2.20135500
C	-2.40939800	-2.01608500	-0.96913800
C	-2.43348500	-1.12878100	0.15585900
O	-1.99609600	1.06026100	1.07065700
C	-3.27254400	1.73866700	1.21514600
H	-0.92008700	0.03276100	-3.25835200
H	-1.83830300	-2.24537100	-3.04390000
H	-3.17765700	2.36774400	2.10000500
H	-4.06705300	1.00016600	1.34443500
H	-3.46897200	2.35525400	0.33268400
Mg	-0.25013700	2.23162100	1.58246600
Cl	1.35597900	0.49987400	1.83476200
C	-0.77806500	3.74833300	2.93819300
H	-1.48531500	4.48475000	2.52654700
H	-1.23264500	3.36224700	3.86333300
H	0.10247400	4.32395200	3.25871800
Cl	1.71545600	-2.53006800	-0.65207400
C	-0.75470100	1.94080300	-1.36790100
O	-0.33991600	2.64124000	-0.43188300
C	-2.93825400	-1.59536000	1.40064700
C	-3.41747400	-2.87950300	1.51704100
H	-3.78914500	-3.23306200	2.47437200
C	-3.41344300	-3.75245400	0.40187000
H	-3.79191200	-4.76462300	0.51204200
C	-2.91616900	-3.33134800	-0.81021800
H	-2.89046000	-4.00550400	-1.66179700
H	-2.90964700	-0.93935800	2.26354100
O	-0.66145300	2.34759200	-2.62315600
C	0.06135900	3.57962000	-2.86793200
H	-0.03721800	3.75039900	-3.93907400
H	-0.38526300	4.39686500	-2.29874400
H	1.10735800	3.44234200	-2.58750600
Mg	2.45763100	-0.36581600	-0.27183100
O	4.32622000	-0.84250400	0.65080700
C	4.31915700	-1.67326800	1.82121100
H	4.07364700	-2.70628600	1.55194100
H	5.30100800	-1.62637800	2.30794500
H	3.55608700	-1.27252200	2.48897500
C	5.33987700	-1.22770000	-0.28592500
H	6.32754200	-1.14684700	0.18433400
H	5.17122300	-2.25389900	-0.63340700
H	5.27377900	-0.53480800	-1.12625100
C	2.71963300	1.19205500	-1.69571200
H	1.95326000	1.16643900	-2.48645900
H	2.67128000	2.18834800	-1.22853500
H	3.68357300	1.15409900	-2.22678800

Structure 1a·CH3MgCl(DME) (d')_II [B3LYP/6-31G(d)]

C	1.96101300	-0.43544500	-0.03928700
C	1.26655900	-0.64269400	-1.22553400
C	1.40126000	0.30764500	-2.27817300
C	2.20050000	1.41066000	-2.12778700
C	2.90186200	1.64826100	-0.91506100
C	2.77345000	0.71220700	0.16247400
O	1.86348800	-1.35496800	1.00826100

C	2.92227100	-2.34838700	1.04076900
H	0.83330900	0.15085700	-3.18643100
H	2.28680200	2.13355900	-2.93389700
H	2.71661400	-2.97457500	1.90873400
H	3.88934700	-1.84954400	1.13969200
H	2.89766500	-2.94978800	0.12696800
Mg	-0.11121100	-2.08991700	1.53499300
Cl	-1.27484600	-0.04802900	1.90114000
C	0.07047300	-3.71393700	2.85775400
H	0.53088400	-4.60581300	2.40549600
H	0.66550800	-3.47552500	3.75268900
H	-0.91026600	-4.04047200	3.23348300
Cl	-2.45663400	-0.05838000	-1.77162800
C	0.35714900	-1.79934400	-1.40471700
O	-0.15685800	-2.44722000	-0.48024300
C	3.43942900	0.96973200	1.39182600
C	4.21631200	2.09605300	1.53791900
H	4.71250900	2.29142800	2.48408400
C	4.36192500	3.01274800	0.46850800
H	4.97764300	3.89778200	0.60084000
C	3.71524300	2.79578800	-0.72707600
H	3.80918300	3.50654400	-1.54363500
H	3.30287600	0.28474900	2.22121800
O	0.14940900	-2.11202900	-2.66857800
C	-0.88372700	-3.08936200	-2.94362500
H	-0.86955100	-3.21148900	-4.02578400
H	-0.65490000	-4.03067300	-2.44033100
H	-1.84026800	-2.68772300	-2.60465300
Mg	-2.15182500	1.41364800	0.03262700
O	-4.12916400	1.46020600	0.80984200
C	-4.93642100	2.61233100	0.55333100
H	-5.53052000	2.47080500	-0.35858000
H	-5.60464600	2.79584600	1.40387500
H	-4.25474500	3.45417100	0.42671200
C	-4.89445700	0.26372000	0.98693500
H	-5.59638000	0.39479300	1.81974800
H	-5.43931300	0.01826000	0.06810800
H	-4.18774400	-0.53220500	1.22169000
C	-1.40778400	3.39179400	-0.00921800
H	-1.54093800	3.92683500	0.94405000
H	-0.32783600	3.42284600	-0.21988200
H	-1.87899400	4.01498100	-0.78581800

Structure 1a-TS'OMe_I [B3LYP/6-31G(d)]

C	-1.65923300	0.03477900	0.11638700
C	-1.85510300	0.98245700	-0.93992400
C	-2.72800700	0.64292200	-2.02472400
C	-3.45356700	-0.51016500	-2.03288900
C	-3.38565200	-1.42370400	-0.92800200
C	-2.51896200	-1.14382300	0.16671300
O	-1.27567700	0.55694900	1.39813400
C	-2.40813000	1.09089500	2.14609700
H	-2.79819400	1.33799800	-2.85359900
H	-4.11332500	-0.74228600	-2.86396000
H	-1.99105400	1.50092200	3.06517800
H	-3.11702500	0.29022000	2.36369600
H	-2.89903200	1.88073700	1.57014700
Mg	0.41363300	1.91172400	1.62047500
C	0.35255400	-0.90762500	-0.22221600
H	0.00198200	-1.56625900	-1.00532900
H	0.67411800	0.09433700	-0.47573500
H	0.27679600	-1.23044000	0.80928000
Cl	2.64655200	0.86649500	1.52476600
C	0.11201500	3.18977900	3.26468600
H	-0.76896100	3.84305100	3.16889200
H	0.00163800	2.65939100	4.22294400
H	0.97499800	3.85931500	3.39599100
Cl	3.70216600	-3.02142700	0.70596800
C	-1.04710700	2.16547200	-1.01086700
O	-0.08462200	2.45011400	-0.24824700
C	-2.47363700	-2.04039800	1.25599300
C	-3.26340200	-3.17688000	1.27726700
H	-3.21205800	-3.85704100	2.12248300
C	-4.12227200	-3.45556100	0.19762100
H	-4.73856100	-4.35037900	0.21225000
C	-4.17734700	-2.59503200	-0.88301500
H	-4.83837700	-2.80762600	-1.71970400
H	-1.79763500	-1.83547700	2.08071100
O	-1.34352300	3.00073300	-2.02081600
C	-0.53555000	4.18131700	-2.15091000
H	-0.94282000	4.70985400	-3.01312400
H	-0.60820800	4.80086700	-1.25357800
H	0.51125400	3.91800300	-2.32289000
Mg	2.57603200	-1.13070900	0.15846900
O	3.60889900	-0.47927800	-1.55137400
C	4.90812400	0.10511900	-1.34208800
H	5.64151900	-0.67492700	-1.10974800
H	5.20854800	0.65271600	-2.24240600
H	4.81300300	0.79551800	-0.50315200
C	3.58564200	-1.37994200	-2.67189100
H	3.88467400	-0.84110600	-3.57801500
H	4.25219100	-2.23024800	-2.49357600
H	2.55753000	-1.73127600	-2.77758400

Structure 1a-TS'OMe_II [B3LYP/6-31G(d)]

C	1.61530800	0.16375100	0.15045600
C	2.13277800	-0.80853000	-0.76447000
C	3.05160200	-0.38633600	-1.77876900
C	3.53138800	0.88828000	-1.83264600
C	3.14660300	1.85476500	-0.84488200
C	2.21665200	1.49327800	0.17158200
O	1.16709900	-0.31262900	1.42957400
C	2.27156200	-0.55933800	2.34869000
H	3.35959000	-1.11761800	-2.51722400
H	4.23157900	1.18317500	-2.60875200
H	1.81974400	-0.95709000	3.25667200
H	2.79759400	0.37531200	2.55117400
H	2.96118400	-1.29170500	1.91904100
Mg	-0.25895000	-1.95397700	1.59226600
C	-0.47841800	0.62995800	-0.53828500
H	-0.15494900	1.28268100	-1.33773900
H	-0.52492500	-0.43627000	-0.72064700
H	-0.64652300	1.03177200	0.45251700
Cl	-2.60478700	-1.36332200	1.11596800
C	0.00316400	-2.95432800	3.42569200
H	-0.74515200	-3.75360200	3.53262500
H	0.98490600	-3.43926300	3.53890000
H	-0.12620800	-2.30884600	4.30837200
Cl	-3.79257500	-0.10563400	-2.65824700
C	1.58403300	-2.13521000	-0.79826800
O	0.60624100	-2.54486100	-0.11624800
C	1.86368100	2.44522300	1.15209400
C	2.41338600	3.71559200	1.14405900
H	2.13121100	4.43478100	1.90783500
C	3.33218600	4.07643500	0.14042700
H	3.76080400	5.07495700	0.13122800
C	3.68633600	3.16269100	-0.83449800
H	4.39548200	3.43766500	-1.61144600
H	1.14279500	2.16967200	1.91600800
O	2.16019500	-2.97077000	-1.67471700
C	1.59609600	-4.28865200	-1.79019800
H	2.20158400	-4.78987500	-2.54543200
H	1.65671900	-4.81869100	-0.83651900
H	0.55241900	-4.23462900	-2.10934400
Mg	-2.71839900	0.25803500	-0.69163300
O	-3.84317000	1.74845600	0.24293800
C	-4.81190100	2.54038200	-0.46782200
H	-5.79928700	2.40932900	-0.01081900
H	-4.52174400	3.59714400	-0.43464400
H	-4.82606900	2.17515500	-1.49467700
C	-3.76476000	2.07679100	1.63580600
H	-3.43336800	3.11482100	1.75919400
H	-4.74569300	1.94206500	2.10578200
H	-3.04945000	1.39255100	2.09287800

Structure 1a-TS'CO_I [B3LYP/6-31G(d)]

O	-0.19654300	2.12241800	0.76024000
Mg	-0.22544500	2.08249600	-1.22275000
C	-1.27851600	-0.31524600	1.47931300
H	-1.29581600	-0.92530100	2.37501500
H	-0.63791700	-0.61938700	0.66369700
H	-1.95699100	0.52302600	1.38899000
Cl	-1.69091800	0.21214500	-1.89675200
C	-0.24627500	3.78860800	-2.45487600
H	-1.27139700	4.08617500	-2.72110800
H	0.27363100	3.63630100	-3.41339700
H	0.21329700	4.67386400	-1.98903300
Cl	-2.80343500	-3.49049700	-0.42983700
C	1.46124500	0.40534300	1.27835400
C	1.89720900	-0.53097900	2.26149800
C	2.90721900	-1.41935800	2.00828500
C	3.53576500	-1.46806600	0.73348100

C	3.11821600	-0.54419000	-0.27612100
H	1.39602400	-0.52229300	3.22205700
H	3.22604900	-2.11736100	2.77791200
C	0.28925300	1.29491100	1.59808200
C	2.10592400	0.40872100	0.05072500
O	1.79129000	1.35598000	-0.93998900
C	2.71782100	2.47759600	-0.96445700
H	2.39962700	3.11659200	-1.78829700
H	2.66002100	3.02286200	-0.01796900
H	3.73264400	2.10869500	-1.12893600
C	3.71423700	-0.61688800	-1.56374500
C	4.69282400	-1.54997300	-1.83006100
H	5.13171700	-1.60223900	-2.82244800
C	5.12226400	-2.44900200	-0.82654100
H	5.89592900	-3.17780100	-1.05086600
C	4.55056300	-2.40970500	0.42604700
H	4.86332200	-3.10800400	1.19826400
H	3.36995300	0.05143100	-2.34542200
O	0.28417600	1.61625200	2.91869200
C	-0.74917100	2.50132500	3.34866000
H	-0.56332200	2.67678300	4.40927600
H	-0.72015900	3.44174000	2.79337600
H	-1.72978900	2.02864500	3.21600400
Mg	-2.57847400	-1.24907900	-0.15051200
O	-4.54870700	-0.55109000	-0.07718000
C	-5.66155600	-1.43540900	0.14757400
H	-6.19892900	-1.12994800	1.05316300
H	-6.33600600	-1.40354600	-0.71557500
H	-5.25106200	-2.43886800	0.25940700
C	-4.95259600	0.80182200	-0.32471800
H	-5.61598900	0.83894100	-1.19626800
H	-5.47008900	1.20564600	0.55370500
H	-4.05199600	1.37951200	-0.53348900

Structure 1a-TS'CO_II [B3LYP/6-31G(d)]

O	0.13649100	-2.37814800	0.43778900
Mg	0.18227800	-2.05500800	-1.51846200
C	1.43211300	-0.19419800	1.52116800
H	1.48297400	0.30357800	2.48288100
H	0.86575400	0.26607100	0.72560700
H	2.01646700	-1.09333600	1.36695100
Cl	1.71522700	-0.15778100	-1.91385600
C	0.00236700	-3.51857400	-3.01766800
H	0.98768200	-3.83770900	-3.38689900
H	-0.54624300	-3.16597500	-3.90502200
H	-0.50584300	-4.43482500	-2.68022400
Cl	5.21539400	0.11792300	0.28868000
C	-1.35970700	-0.62244500	1.23326500
C	-1.70861700	0.19158300	2.35101400
C	-2.63953500	1.19011300	2.24966200
C	-3.27057800	1.47798300	1.00752800
C	-2.93999800	0.68013600	-0.13341600
H	-1.20753800	-0.00552100	3.29136700
H	-2.89623600	1.78819000	3.12027100
C	-0.27636400	-1.65471800	1.40042500
C	-2.00935800	-0.39184300	0.03027000
O	-1.78394800	-1.20290200	-1.09394000
C	-2.78731700	-2.24550000	-1.24843700
H	-2.53764400	-2.77094800	-2.16998000
H	-2.73888300	-2.93068600	-0.39723900
H	-3.77865800	-1.79120700	-1.31533700
C	-3.54065300	0.98589300	-1.38408000
C	-4.44193800	2.02304800	-1.49330600
H	-4.88816700	2.25026400	-2.45744100
C	-4.78534100	2.79932800	-0.36223900
H	-5.50090800	3.61063000	-0.46200400
C	-4.20670900	2.53307400	0.85949800
H	-4.45731700	3.13249200	1.73129100
H	-3.26324900	0.40762700	-2.25863000
O	-0.30734100	-2.17597400	2.65342100
C	0.63765700	-3.21200200	2.93196800
H	0.42545200	-3.53419300	3.95226600
H	0.52539800	-4.04486100	2.23434100
H	1.65890400	-2.81868500	2.87012100
Mg	3.00099600	0.55143100	0.04216300
O	2.90670900	2.61761400	-0.24315600
C	1.75353500	3.31266000	-0.73377200
H	1.41754000	4.05040500	0.00450600
H	1.99429000	3.81385000	-1.67827900
H	0.97388100	2.57086000	-0.90810700
C	4.03756500	3.48117100	-0.03043600
H	4.29415800	3.98795300	-0.96771600
H	3.79648900	4.22182200	0.74112700
H	4.86382300	2.84572100	0.28817600

Structure 1a·EtMgCl (a)_I [B3LYP/6-31G(d)]

C	0.22114400	1.27948400	-0.35051700
C	1.15962200	2.33311600	-0.14669100
C	2.49350700	2.06546300	0.01480300
C	2.97840800	0.72945200	0.00050400
C	2.05450400	-0.34653300	-0.20264100
C	-1.22141200	1.59334100	-0.46559900
O	-2.14430000	0.79203200	-0.29405100
O	-0.19584800	-1.08187400	-0.64646100
Cl	-3.30845200	-2.54774800	-0.63899800
C	-0.28207900	-1.47633500	-2.04691700
H	0.79327500	3.35196300	-0.11358400
H	3.19753300	2.87794500	0.17162500
H	-1.04059600	-2.25728600	-2.08200600
H	0.69231300	-1.84146400	-2.38145400
H	-0.59513500	-0.62011100	-2.65157100
Mg	-2.02276800	-1.11091100	0.60917200
C	-1.47985100	-0.89135800	2.65451700
H	-0.51354400	-1.39343400	2.83252400
H	-2.19800600	-1.47005900	3.25769900
C	0.68099100	-0.03383200	-0.40035700
C	2.52971700	-1.68609100	-0.18284300
C	3.86745100	-1.94544700	0.01119000
H	4.22137400	-2.97190700	0.03453500
C	4.78617500	-0.88344500	0.19228200
H	5.83896900	-1.10478700	0.34276400
C	4.35044700	0.42275900	0.19117200
H	5.05147000	1.23917300	0.34352700
H	1.82085700	-2.49862800	-0.29621800
O	-1.46080000	2.86876900	-0.76267900
C	-2.84905200	3.26736300	-0.81910800
H	-2.82781300	4.32930100	-1.06044600
H	-3.37187800	2.70122300	-1.59261600
H	-3.32866800	3.09548800	0.14679300
C	-1.40140300	0.53654700	3.23012700
H	-0.66098000	1.15619400	2.70183000
H	-2.36349800	1.06290000	3.14931300
H	-1.12018700	0.56782300	4.29619000

Structure 1a·EtMgCl (a)_II [B3LYP/6-31G(d)]

C	0.20945200	1.46816600	-0.00781200
C	1.18798900	2.42065100	0.40076600
C	2.51681400	2.08936900	0.44314200
C	2.95647400	0.78292600	0.09634500
C	1.99173200	-0.19028500	-0.32183400
C	-1.22565700	1.83083200	0.02101900
O	-2.16467500	1.03146200	0.06734300
O	-0.29430900	-0.74170300	-0.84252700
Cl	-3.46393600	-2.06165200	-1.06928700
C	-0.44129200	-0.78418900	-2.29188400
H	0.85703700	3.41158200	0.68718000
H	3.25192600	2.82408000	0.75967700
H	-1.21984100	-1.52136100	-2.48377200
H	0.51092000	-1.07193500	-2.74487700
H	-0.75567900	0.19755600	-2.65785600
Mg	-2.06844900	-1.04568900	0.44763500
C	-1.41675000	-1.37625500	2.44311100
C	0.62420700	0.19450200	-0.38743800
C	2.42174100	-1.50837600	-0.63579800
C	3.75477300	-1.84119100	-0.55468800
H	4.07434800	-2.85321300	-0.78503000
C	4.71336300	-0.87635100	-0.16093400
H	5.76184500	-1.15457100	-0.10360400
C	4.32222700	0.40420400	0.16050400
H	5.05453500	1.14267600	0.47602800
H	1.68281900	-2.25232000	-0.91139500
O	-1.43700700	3.14546600	0.01871000
C	-2.81319500	3.57718300	0.11589700
H	-2.76881100	4.66542200	0.10275200
H	-3.38680300	3.19903600	-0.73268000
H	-3.25627700	3.21525300	1.04612700
H	-0.83920600	-0.50770300	2.80496200
H	-2.30139900	-1.40698500	3.10072200
C	-0.58627400	-2.65283200	2.68869300
H	-0.29195900	-2.79131500	3.74277700
H	-1.13682700	-3.55782800	2.39760000
H	0.34597600	-2.65394400	2.10490500

Structure 1a-TSOMe-I [B3LYP/6-31G(d)]

C	-0.05148200	1.30630400	-0.09725600
C	0.86305300	2.40284700	0.01149700
C	2.21009000	2.21217400	0.08427900
C	2.75968400	0.88786200	0.03621200
C	1.89060700	-0.23730800	-0.07833700
C	-1.46645100	1.53255800	-0.04137500
O	-2.33279700	0.62815000	0.12330500
O	-0.27336200	-1.03533400	-0.84427400
Cl	-3.24114800	-2.96831500	0.38539900
C	-0.21327400	-0.87947800	-2.28012700
H	0.44757500	3.40396300	0.04565900
H	2.88662700	3.05803500	0.16436800
H	-0.78347400	-1.71353100	-2.69189300
H	0.82735200	-0.93205500	-2.60927400
H	-0.65598800	0.07339100	-2.58307300
Mg	-1.79587200	-1.25678300	0.45566600
C	-0.10981700	-0.96288000	1.95758300
H	0.76883700	-1.60808400	1.91470800
H	-0.91375800	-1.60464100	2.39370800
C	0.44711500	-0.03877700	-0.07628700
C	2.44737000	-1.53112900	-0.19155100
C	3.81799000	-1.72028900	-0.18039200
H	4.22866200	-2.72228000	-0.26487000
C	4.67805100	-0.61305200	-0.05097000
H	5.75441300	-0.76209600	-0.03663700
C	4.15651200	0.66257600	0.05503000
H	4.81944800	1.51960200	0.14579300
H	1.78011600	-2.38235300	-0.28226200
O	-1.86312500	2.80852700	-0.14177400
C	-3.27333100	3.06374500	-0.02344300
H	-3.37778000	4.14159600	-0.14812300
H	-3.82799500	2.53126700	-0.79977200
H	-3.64056500	2.75437300	0.95832800
C	0.08393100	0.24382200	2.85956300
H	0.12474900	-0.03096600	3.92339500
H	1.01412600	0.77019800	2.62267700
H	-0.73257800	0.97166200	2.75127100

Structure 1a-TSOMe-II [B3LYP/6-31G(d)]

C	-0.01083300	1.30599600	-0.14508100
C	0.87094600	2.41559200	0.05463600
C	2.22145500	2.25594100	0.15079700
C	2.81417600	0.95829400	-0.00534700
C	1.97919700	-0.18077100	-0.20541900
C	-1.42999300	1.48807800	-0.09304400
O	-2.26971500	0.55473300	0.05648900
O	-0.18279700	-1.04411100	-0.88279600
Cl	-3.00207500	-3.04980900	0.62288000
C	-0.22902400	-0.86868800	-2.31752300
H	0.42791200	3.40134600	0.14510100
H	2.87042700	3.11256400	0.30760100
H	-0.76474400	-1.73735400	-2.70313000
H	0.78846800	-0.84296600	-2.71489000
H	-0.75804700	0.05240000	-2.57586500
Mg	-1.63079800	-1.28115300	0.50513700
C	0.06018800	-0.84351000	1.95102900
H	-0.87048000	-0.61724800	2.51895900
C	0.53256000	-0.02398700	-0.15055000
C	2.57243500	-1.43950800	-0.44654300
C	3.94998300	-1.58352000	-0.47306100
H	4.39024500	-2.55843700	-0.66125700
C	4.77556900	-0.46709000	-0.24853200
H	5.85622100	-0.58136300	-0.26185800
C	4.21617000	0.77743800	-0.02048800
H	4.85396400	1.64393800	0.13612300
H	1.93150300	-2.29827500	-0.61501400
O	-1.86441400	2.75342200	-0.18056100
C	-3.28071700	2.96587400	-0.05348800
H	-3.41659500	4.04229000	-0.15930100
H	-3.82278300	2.43149200	-0.83735900
H	-3.63624800	2.62924000	0.92367900
C	0.61331800	-2.21359800	2.33888500
H	-0.08759300	-3.03267700	2.13029900
H	1.54210200	-2.42774300	1.79792300
H	0.85412300	-2.26856200	3.41207500
H	0.74082600	-0.04191100	2.23378600

Structure 1a-TSOMe-III [B3LYP/6-31G(d)]

C	-0.15942900	1.09161200	0.00762400
C	0.68781300	2.19776500	0.34538400
C	2.03734400	2.06108100	0.46296200
C	2.66256300	0.79068300	0.22698300
C	1.86479400	-0.33925600	-0.11436000
C	-1.58478300	1.24518200	-0.00618700
O	-2.41046100	0.29070900	-0.06745800
O	-0.20855100	-1.10651600	-1.11943800
Cl	-3.14641300	-3.34289500	-0.36218600
C	-0.06932300	-0.71513400	-2.50407500
H	0.21578800	3.15915500	0.51559100
H	2.66100600	2.91284300	0.71820300
H	-0.55664400	-1.49990400	-3.08471300
H	0.99093000	-0.65684900	-2.76161200
H	-0.55332200	0.24920500	-2.68211300
Mg	-1.79445700	-1.59663400	0.01479700
C	-0.23861300	-1.45072400	1.67075900
C	0.41021100	-0.21563900	-0.15373900
C	2.49563600	-1.57083500	-0.39522100
C	3.87323700	-1.69511700	-0.33789800
H	4.34165100	-2.65108400	-0.55375200
C	4.66371400	-0.58365800	0.00913200
H	5.74483700	-0.68185700	0.05923600
C	4.06698200	0.63242200	0.28628700
H	4.67603500	1.49399000	0.54899300
H	1.88119000	-2.42878600	-0.64965700
O	-2.04245300	2.50170900	0.08203100
C	-3.46921000	2.67328100	0.13141600
H	-3.62319400	3.75074100	0.19167300
H	-3.93779500	2.26795800	-0.76866400
H	-3.88766000	2.17672000	1.01037500
H	0.82321800	-1.65806600	1.77879100
C	-0.76022300	-0.52417800	2.76058100
H	-0.49705000	0.52166600	2.55043800
H	-1.85255500	-0.56682800	2.86192500
H	-0.33896600	-0.76211400	3.74777300
H	-0.72049700	-2.45216500	1.74249700

Structure 1a-TSCO_I [B3LYP/6-31G(d)]

C	0.05722200	1.15526700	-0.22975600
C	0.89400700	2.30282800	-0.18099200
C	2.26050500	2.18433500	-0.10782100
C	2.88186400	0.91150100	-0.02930500
C	2.06108800	-0.26354400	-0.05136100
C	-1.44331400	1.29507700	-0.28914600
O	-2.14926300	0.50236700	-1.02731200
O	-0.14219800	-1.25032100	-0.23860700
Cl	-3.29725300	-2.81790300	0.54538900
C	-0.15303500	-1.92874200	-1.53227800
H	0.42594500	3.27868500	-0.21560500
H	2.88376300	3.07461100	-0.09026900
H	-0.74803800	-2.83221500	-1.38846500
H	0.86821800	-2.18459500	-1.81873100
H	-0.61344300	-1.27437700	-2.27648700
Mg	-2.15125600	-0.90356100	0.33846900
C	-1.92339800	0.73322300	1.85956600
H	-2.01737200	-0.24363500	2.39282100
H	-2.93079500	1.17193600	1.88205000
C	0.65808300	-0.09405900	-0.20376000
C	2.67620900	-1.53699100	0.10419400
C	4.04230700	-1.64118800	0.23695100
H	4.49864700	-2.61875800	0.36465500
C	4.85889900	-0.48412800	0.22089200
H	5.93592500	-0.58434200	0.32098600
C	4.28867200	0.76193000	0.09752900
H	4.90716500	1.65592700	0.10581300
H	2.05494400	-2.42481400	0.14921600
O	-1.81342500	2.59468300	-0.18250700
C	-3.16932500	2.89918100	-0.53370200
H	-3.26628800	3.97663300	-0.39425600
H	-3.37171300	2.62372500	-1.57076900
H	-3.86891000	2.37288100	0.12262000
C	-0.94647100	1.57863400	2.66733500
H	-0.84993700	2.58055700	2.23476500
H	-1.26726200	1.70580400	3.71112000
H	0.05404100	1.13026100	2.68910500

Structure 1a-TSCO_II [B3LYP/6-31G(d)]

C	0.18513400	1.17327100	-0.26708600
C	1.06236700	2.27068300	-0.05213400
C	2.41639000	2.08204700	0.07720700
C	2.98250300	0.78067700	0.04726600

C	2.11793800	-0.34774600	-0.13572700
C	-1.30442800	1.38137900	-0.38081800
O	-2.00725000	0.67152700	-1.20931000
O	-0.11668900	-1.20936200	-0.50537200
Cl	-3.39383000	-2.65900300	0.15950300
C	-0.11876000	-1.75047000	-1.86076600
H	0.63563700	3.26503400	-0.00646100
H	3.07352300	2.93608300	0.21976600
H	-0.74686800	-2.64250000	-1.82401600
H	0.90000900	-2.01423700	-2.14955400
H	-0.53761500	-1.00697600	-2.54298000
Mg	-2.13499600	-0.81027200	0.05506700
C	-1.80102000	0.70771100	1.67881200
H	-2.89389800	0.62828600	1.84384800
C	0.73109100	-0.09951400	-0.33072000
C	2.67331600	-1.65630000	-0.08837700
C	4.02631200	-1.83484100	0.09388700
H	4.43652900	-2.83992000	0.13621600
C	4.88776900	-0.72048300	0.23825500
H	5.95366100	-0.87835100	0.37605900
C	4.37383200	0.55604700	0.22152400
H	5.02629000	1.41578900	0.35224400
H	2.01592800	-2.51525500	-0.16772800
O	-1.62153800	2.69568400	-0.23135000
C	-2.96799700	3.05950300	-0.55511700
H	-3.02278500	4.13661400	-0.39049400
H	-3.19963100	2.81653600	-1.59409100
H	-3.67662600	2.54660000	0.10350500
C	-1.03988100	-0.30198200	2.55786700
H	-1.36420600	-1.34567400	2.41984900
H	0.03824700	-0.26903900	2.35882500
H	-1.17461200	-0.09098500	3.62890100
H	-1.53209600	1.72162600	1.96758500

Structure 1a-TSCO_III [B3LYP/6-31G(d)]

C	-0.25178000	-1.10369700	-0.29615100
C	-1.07379100	-2.24954100	-0.12006000
C	-2.42905800	-2.12919200	0.06699700
C	-3.04940000	-0.85467200	0.13599400
C	-2.24018000	0.31927900	-0.01063400
C	1.24185600	-1.24365700	-0.46865300
O	1.88890000	-0.46547300	-1.27390100
O	-0.06187400	1.29955400	-0.41070600
Cl	3.13476900	2.87503600	0.20595700
C	-0.13649700	1.91905800	-1.72967300
H	-0.60374100	-3.22486200	-0.14700600
H	-3.04372800	-3.01841200	0.18063200
H	0.46093500	2.83009900	-1.66392200
H	-1.17528600	2.16002700	-1.96178700
H	0.27979000	1.23407800	-2.47220200
Mg	1.98073900	0.95933400	0.07444500
C	1.70894500	-0.60574100	1.64930800
C	-0.85328100	0.14519200	-0.26966100
C	-2.84746000	1.59739900	0.13369800
C	-4.19881400	1.70555200	0.37343600
H	-4.64885000	2.68744700	0.48999600
C	-5.00706300	0.54784900	0.48156800
H	-6.07271800	0.65078700	0.66551300
C	-4.44148500	-0.70186100	0.37188100
H	-5.05211300	-1.59546700	0.47431400
H	-2.22986500	2.48744200	0.08251200
O	1.62858600	-2.54061400	-0.36758900
C	2.89172600	-2.87687500	-0.95967200
H	3.03443500	-3.93600800	-0.74034200
H	2.86838500	-2.70923800	-2.03918100
H	3.70341200	-2.28966700	-0.52445600
H	1.07295500	-1.43458400	1.95740000
C	3.15414600	-0.83000200	2.11433100
H	3.23448700	-0.89012800	3.21004500
H	3.54849400	-1.77087000	1.71474900
H	3.84443100	-0.03111700	1.80341400
H	1.26696500	0.28056100	2.15704600

Structure 1a-intOMe-I [B3LYP/6-31G(d)]

C	-0.02852900	1.30211500	-0.02978600
C	0.94931000	2.29388900	-0.38670300
C	2.27295400	2.02351600	-0.50909900
C	2.77147900	0.68268000	-0.30792800
C	1.88692100	-0.36176000	0.06156700
C	-1.38673400	1.64426600	0.02105500
O	-2.38026400	0.83163700	0.18991500
O	-0.37410000	-1.11980000	-0.62808400
Cl	-3.75522200	-2.72162200	-0.16656900
C	-0.06443300	-1.03845600	-2.03163500
H	0.58564200	3.29896300	-0.57168800
H	2.97646600	2.80294200	-0.78664600
H	-0.72876000	-1.73814600	-2.54677000
H	0.97320900	-1.33433900	-2.20013100
H	-0.22148700	-0.01901400	-2.40100000
Mg	-2.29017300	-1.05875700	-0.08263000
C	-0.02576400	-0.59149200	1.70064000
H	0.16171000	-1.66766500	1.78541300
H	-1.10503700	-0.42825500	1.84602200
C	0.40853400	-0.10209100	0.29243800
C	2.38968400	-1.66305200	0.21838000
C	3.73890900	-1.94818500	0.03029100
H	4.10222900	-2.96448600	0.15252400
C	4.61817200	-0.91526200	-0.31741100
H	5.67510700	-1.12362300	-0.46247100
C	4.13769700	0.37517200	-0.48501600
H	4.81650300	1.17701700	-0.76608200
H	1.70870900	-2.47131300	0.46960400
O	-1.69445700	2.95030500	-0.14900800
C	-3.08098100	3.30044000	-0.20987500
H	-3.09431900	4.38154600	-0.35586900
H	-3.57940400	2.80267200	-1.04716900
H	-3.59575700	3.03885600	0.71831900
C	0.68685300	0.15058000	2.83765500
H	0.32200300	-0.20588500	3.80657700
H	1.76724300	-0.01533400	2.79669100
H	0.50293100	1.22743900	2.77588200

Structure 1a-intCO-I [B3LYP/6-31G(d)]

C	-0.17696600	1.08778000	0.08076800
C	-1.11962200	2.13960200	0.22832800
C	-2.47515600	1.90898300	0.25517600
C	-2.99129500	0.60328700	0.07250500
C	-2.07253600	-0.48604900	-0.08092600
C	1.32578700	1.36904300	-0.15410600
O	1.75281200	0.78597300	-1.28342500
O	0.20544900	-1.30968800	-0.01534300
Cl	3.44496400	-2.78661600	-0.51086900
C	0.17239200	-2.13014000	1.18735300
H	-0.75787400	3.15624900	0.32486700
H	-3.16740300	2.73672600	0.38581700
H	0.88864000	-2.93592600	1.01751200
H	-0.82725100	-2.53628100	1.34299500
H	0.46894200	-1.53049600	2.05223900
Mg	2.23317700	-0.90092000	-0.51214900
C	1.78850900	2.82950000	-0.02510300
H	1.36029000	3.30678300	0.86545000
H	2.87159900	2.77679200	0.13268300
C	-0.67934300	-0.20701300	0.01066600
C	-2.59269400	-1.78199200	-0.36049300
C	-3.95077000	-1.99257800	-0.43500200
H	-4.32976800	-2.98402500	-0.66680400
C	-4.85974100	-0.92591100	-0.22953400
H	-5.92884500	-1.11092700	-0.28250800
C	-4.38706000	0.34291200	0.01009000
H	-5.07577000	1.17406000	0.14007300
H	-1.90742900	-2.59768100	-0.56346400
O	2.08940500	0.56159100	0.95051700
C	1.93569200	0.89255400	2.32356600
H	2.44725900	0.12178500	2.90651700
H	2.39405400	1.86288100	2.54630500
H	0.87640200	0.92157000	2.61158100
C	1.51417700	3.66514600	-1.28155400
H	0.44424900	3.77667400	-1.48669800
H	1.94123200	4.66802300	-1.17050400
H	1.96959300	3.18354800	-2.14990500

Structure 1a-intCO-II [B3LYP/6-31G(d)]

C	-0.20429300	1.08345900	-0.17983500
C	-1.12029400	2.14312300	-0.43086800
C	-2.48207700	1.96203700	-0.39973900
C	-3.04326000	0.68261700	-0.16949000
C	-2.15791600	-0.42350300	0.03372900
C	1.31726200	1.29212700	-0.41650900
O	1.70428000	0.61998800	-1.52259100
O	0.08340100	-1.28297900	0.26595100
Cl	3.18114000	-2.93354900	-0.49753100
C	0.18386500	-1.71840200	1.65363400

H	-0.73589500	3.12726200	-0.66543500
H	-3.14563000	2.80353600	-0.58171900
H	0.82707700	-2.60011200	1.64376800
H	-0.80819000	-1.97474300	2.02811200
H	0.62861800	-0.91771600	2.24766100
Mg	1.94857100	-1.06891000	-0.63327700
C	1.77427200	2.75967500	-0.42039600
H	2.84278000	2.74411400	-0.65627500
H	1.30618800	3.23200000	-1.29125400
C	-0.75761000	-0.16636200	0.06082000
C	-2.71291700	-1.72753900	0.16364300
C	-4.07684200	-1.91400400	0.14212500
H	-4.48434200	-2.91693100	0.23417400
C	-4.95433100	-0.81346500	-0.01264900
H	-6.02817800	-0.97728800	-0.02122000
C	-4.44530600	0.45418700	-0.17375500
H	-5.10938300	1.30260600	-0.31951400
H	-2.05101800	-2.58225300	0.24718200
O	1.99787900	0.55767800	0.78539800
C	3.39106700	0.83553100	1.00376900
H	3.77517300	0.02779500	1.63258800
H	3.95443400	0.85091500	0.06207400
H	3.53313300	1.78733000	1.52338200
C	1.51840000	3.58619700	0.84757200
H	1.98240600	4.57435700	0.75297500
H	0.45276000	3.73891400	1.03999000
H	1.93324700	3.10591400	1.73850200

Structure 1a-TS2OMe-I [B3LYP/6-31G(d)]

C	-0.00566300	1.29497500	0.00450400
C	0.93111200	2.27154300	-0.48170100
C	2.24890000	2.00150000	-0.66049200
C	2.76674900	0.68827400	-0.37513800
C	1.90752600	-0.32823800	0.12266800
C	-1.37644500	1.63239000	0.07969000
O	-2.35500100	0.81469400	0.23984500
O	-0.37301300	-1.19252900	-0.67377000
Cl	-3.86371200	-2.61018000	-0.24601600
C	0.01972400	-1.11602800	-2.04499900
H	0.54237000	3.25557900	-0.71958100
H	2.92837700	2.76134300	-1.03512900
H	-0.61932000	-1.79222500	-2.62361800
H	1.06016900	-1.43429500	-2.15797300
H	-0.08581700	-0.09229800	-2.42796800
Mg	-2.26117600	-1.07461700	-0.16043500
C	-0.04936000	-0.61932500	1.71180700
H	0.11348800	-1.70045000	1.75517900
H	-1.12712500	-0.44160800	1.82632400
C	0.45111800	-0.06532300	0.36008400
C	2.44149900	-1.60700700	0.37304800
C	3.78383700	-1.88910500	0.15770300
H	4.16744200	-2.88651500	0.35219800
C	4.63567400	-0.88055300	-0.31698600
H	5.68879000	-1.09061100	-0.48522200
C	4.13092800	0.38183500	-0.57986000
H	4.78561800	1.16381000	-0.95735600
H	1.78599200	-2.40143800	0.71538600
O	-1.68353400	2.93531000	-0.07174700
C	-3.07295400	3.28458600	-0.13697500
H	-3.08669400	4.36691500	-0.27048300
H	-3.56276200	2.79320300	-0.98255400
H	-3.58919900	3.00907300	0.78580500
C	0.63595700	0.05525900	2.90955700
H	0.47126200	1.13714100	2.89583100
H	0.23081900	-0.34189700	3.84634900
H	1.71457800	-0.12576000	2.89823300

Structure 1a-TS2OMe-II [B3LYP/6-31G(d)]

C	-0.06693700	1.38330300	-0.17061200
C	-1.01930700	2.40300400	0.17863800
C	-2.34514300	2.14941400	0.30927300
C	-2.84102800	0.80671200	0.16409800
C	-1.95508400	-0.25609600	-0.17077800
C	1.30728400	1.72835500	-0.23618200
O	2.29756200	0.91545100	-0.29474400
O	0.36367400	-1.08892900	0.71390300
Cl	3.93836800	-2.36290600	0.50220900
C	-0.06366000	-0.92484100	2.06236500
H	-0.63863600	3.40547800	0.33839100
H	-3.04295800	2.94052600	0.56732700
H	0.58738400	-1.51874600	2.71593900
H	-1.09139600	-1.28184400	2.18343300
H	-0.01827500	0.12972600	2.37002600
Mg	2.24982200	-0.93652500	0.26573000
C	0.03471500	-0.55418600	-1.78514900
H	1.04598400	-0.15837600	-1.93203000
C	-0.51394500	0.01039900	-0.45082200
C	-2.46794500	-1.56901500	-0.20877000
C	-3.81145200	-1.83444400	0.01852600
H	-4.17295400	-2.85845400	-0.00840000
C	-4.69217700	-0.77836600	0.29512700
H	-5.74704200	-0.97646900	0.46661100
C	-4.20773300	0.51565200	0.37405900
H	-4.87815600	1.33618900	0.61862100
H	-1.78950300	-2.39691300	-0.36718600
O	1.59466500	3.04208000	-0.18826300
C	2.97815500	3.41575100	-0.11446700
H	2.97476400	4.50557800	-0.07656600
H	3.44741500	3.00696500	0.78481300
H	3.52378500	3.06697200	-0.99439500
C	0.03645500	-2.05778700	-2.10846900
H	-0.96827300	-2.44074100	-2.29986000
H	0.62282600	-2.22126300	-3.01978400
H	0.47718900	-2.66636400	-1.31183600
H	-0.56268000	-0.04051600	-2.54960900

Structure 1a-TS2CO_I [B3LYP/6-31G(d)]

C	0.24579000	-1.15823800	-0.18578600
C	1.12054300	-2.27607300	-0.08160000
C	2.47947300	-2.12573700	0.04439600
C	3.06991900	-0.83849800	0.00203300
C	2.22030300	0.31103700	-0.10486400
C	-1.19589800	-1.38438500	-0.56569300
O	-1.70152100	-0.60513600	-1.43027700
O	-0.01235000	1.24808000	-0.04309600
Cl	-3.13370700	2.96692700	-0.53421900
C	0.06427100	1.97550400	1.22263000
H	0.70027700	-3.27453200	-0.11066400
H	3.12012400	-2.99861800	0.13598600
H	-0.58373000	2.84489700	1.09651900
H	1.08718600	2.29292500	1.42151500
H	-0.29930700	1.33461700	2.02912900
Mg	-2.14267400	0.96491300	-0.29701000
C	-1.80287200	-2.76044500	-0.36952100
H	-1.30133600	-3.43026200	-1.08532900
H	-1.55001300	-3.13012800	0.63001100
C	0.80867400	0.11421900	-0.10640600
C	2.82297000	1.59235400	-0.25935500
C	4.19214200	1.72977900	-0.25271100
H	4.63552700	2.71170800	-0.39129300
C	5.02977900	0.60010700	-0.08485800
H	6.10853300	0.72664100	-0.07028000
C	4.47848400	-0.65447400	0.03027600
H	5.11413900	-1.53100600	0.12682100
H	2.19342200	2.45761500	-0.43497100
O	-2.13812700	-0.40190000	1.04907200
C	-2.18204400	-0.79039100	2.38502200
H	-2.74735200	-0.06699700	2.99386600
H	-2.67601900	-1.76930600	2.50720100
H	-1.17347000	-0.87570600	2.82918500
C	-3.31169200	-2.80150400	-0.61106400
H	-3.55320200	-2.45757900	-1.62012700
H	-3.68459200	-3.82434700	-0.49469800
H	-3.82814300	-2.15453600	0.10237400

Structure 1a-TS2CO_II [B3LYP/6-31G(d)]

C	-0.22213700	1.11244900	-0.03053300
C	-1.15431800	2.16891600	0.17049500
C	-2.50430500	1.93720100	0.26647300
C	-3.02548200	0.63024300	0.09991000
C	-2.11595800	-0.45964000	-0.10060200
C	1.20299300	1.44570200	-0.37863800
O	1.75798500	0.76856700	-1.29712000
O	0.16344400	-1.27904900	-0.10034700
Cl	3.37286800	-2.78407800	-0.71789000
C	0.12104400	-2.11712600	1.09697500
H	-0.78592500	3.18559200	0.24076200
H	-3.19072300	2.76293900	0.43288800
H	0.81096500	-2.93949300	0.89844500
H	-0.88514600	-2.50041000	1.26264000
H	0.45304500	-1.53136200	1.95720000
Mg	2.28400200	-0.86465600	-0.29631200

C	1.77728800	2.81201300	-0.06407500
H	1.33356700	3.22310900	0.84796300
H	2.83951600	2.64813900	0.13425900
C	-0.71702500	-0.19026000	-0.07206700
C	-2.64936200	-1.75201700	-0.37318500
C	-4.00937500	-1.96029800	-0.39289800
H	-4.39979900	-2.94770100	-0.62216300
C	-4.90618900	-0.89487600	-0.13459400
H	-5.97685100	-1.07803900	-0.14258200
C	-4.42247100	0.37137200	0.09739100
H	-5.10409500	1.20132500	0.26542700
H	-1.97388600	-2.56432000	-0.61762500
O	2.20576400	0.37114700	1.16547800
C	2.25198100	0.63295700	2.53171600
H	2.95008200	-0.04600800	3.04675300
H	2.59504200	1.66151900	2.73482200
H	1.26507100	0.51716000	3.01669800
C	1.62608400	3.78520000	-1.24884100
H	0.57712800	3.99611500	-1.48412500
H	2.11730700	4.73585200	-1.01720800
H	2.09376500	3.36443700	-2.14352500

Structure 1a-prodOMe-I [B3LYP/6-31G(d)]

C	0.69868200	-1.01332300	0.14518200
C	1.45590600	-2.18252600	-0.17275900
C	2.78370400	-2.09919100	-0.48100800
C	3.44937300	-0.84668300	-0.45592200
C	2.70982700	0.33561200	-0.11528300
C	-0.73294700	-1.23839200	0.45206300
O	-1.64386300	-0.40966600	0.32028200
O	-2.82307100	2.34471000	-0.15113400
Cl	-4.76281000	-0.88567100	-1.10455700
C	-3.23104200	3.66287000	-0.29912000
H	0.95359900	-3.14181800	-0.18269700
H	3.34581800	-2.99206500	-0.74121800
H	-4.23505500	3.76386700	-0.74935200
H	-2.53739700	4.23338400	-0.94299500
H	-3.26531500	4.19024000	0.67133600
Mg	-3.22674200	0.59199200	-0.36880300
C	0.55686800	1.51872400	0.56537100
H	0.98863400	2.37247600	0.03678700
H	-0.48551600	1.49093500	0.25613400
C	1.29900100	0.25554300	0.16802000
C	3.43084600	1.56532400	-0.06725700
C	4.77702500	1.62371400	-0.35091500
H	5.29555400	2.57715400	-0.30489000
C	5.48910600	0.45454500	-0.70231400
H	6.55003900	0.51312700	-0.92883900
C	4.83405900	-0.75397200	-0.75170500
H	5.36968700	-1.66288200	-1.01400100
H	2.91932600	2.48026900	0.20361300
O	-0.98684400	-2.46330500	0.89687200
C	-2.36489200	-2.80957100	1.18001100
H	-2.33748000	-3.86741500	1.43793300
H	-2.72505100	-2.22006900	2.02684600
H	-2.99841200	-2.62987800	0.30916000
C	0.61412500	1.78134100	2.08397900
H	0.14058300	0.96574100	2.64210500
H	1.64505100	1.87630200	2.44315600
H	0.07700700	2.70515200	2.32179200

Structure 1a-prodOMe-II [B3LYP/6-31G(d)]

C	0.69870100	-1.01316800	0.14566300
C	1.45582800	-2.18248800	-0.17206400
C	2.78360400	-2.09929200	-0.48045800
C	3.44930200	-0.84678900	-0.45586800
C	2.70983500	0.33562600	-0.11549400
C	-0.73296300	-1.23810300	0.45257600
O	-1.64386900	-0.40952000	0.31996700
O	-2.82399400	2.34447600	-0.15033800
Cl	-4.76219500	-0.88634500	-1.10596000
C	-3.23263500	3.66243500	-0.29836700
H	0.95347200	-3.14175900	-0.18171800
H	3.34566100	-2.99226300	-0.74046000
H	-4.24074000	3.76269700	-0.73952900
H	-2.54472000	4.23087900	-0.95017800
H	-3.25768000	4.19243600	0.67093300
Mg	-3.22701000	0.59172900	-0.36918500
C	0.55716300	1.51891700	0.56569800
H	-0.48550600	1.49082900	0.25746500
C	1.29907800	0.25566000	0.16818400
C	3.43083600	1.56537200	-0.06817300
C	4.77695400	1.62366000	-0.35214500
H	5.29546300	2.57713900	-0.30669900
C	5.48899200	0.45434400	-0.70314800
H	6.54988500	0.51284000	-0.92987800
C	4.83394100	-0.75419400	-0.75192700
H	5.36951400	-1.66321100	-1.01397000
H	2.91933300	2.48044300	0.20230800
O	-0.98681000	-2.46269600	0.89826600
C	-2.36489600	-2.80900000	1.18121200
H	-2.33746200	-3.86679100	1.43934800
H	-2.72520100	-2.21936600	2.02789800
H	-2.99827300	-2.62953100	0.31021300
C	0.61588200	1.78228300	2.08413000
H	0.14285000	0.96698600	2.64313400
H	1.64714800	1.87739000	2.44229100
H	0.07904000	2.70624500	2.32199400
H	0.98829700	2.37249200	0.03629300

Structure 1a-prodCO-I [B3LYP/6-31G(d)]

C	0.25831000	1.36021200	-0.34216500
C	1.27313500	2.32068500	-0.04684800
C	2.57742000	1.94886100	0.14756800
C	2.96670700	0.58518800	0.06643100
C	1.97465800	-0.40416400	-0.23217700
C	-1.15127100	1.79558400	-0.48622200
O	-2.10369000	1.01426900	-0.34247100
O	-0.29593700	-0.94841800	-0.79414100
Cl	-3.47694200	-2.25558800	-0.87080700
C	-0.35008600	-1.27191200	-2.21330600
H	1.00074100	3.36522800	0.04941800
H	3.32970400	2.69765000	0.37921600
H	-1.14759900	-2.00738800	-2.31294200
H	0.61401900	-1.67705100	-2.53062100
H	-0.59204600	-0.37238600	-2.78707900
Mg	-2.11011400	-0.92811500	0.37968700
C	-1.48569700	3.24590100	-0.77639000
H	-0.66106000	3.75335000	-1.28444000
H	-2.34305700	3.23059300	-1.45708300
C	0.63711200	0.02059300	-0.45246000
C	2.34940200	-1.77533800	-0.27434000
C	3.65643600	-2.14465500	-0.05372300
H	3.93295100	-3.19460100	-0.07620000
C	4.64362700	-1.16604800	0.21723300
H	5.67127600	-1.47418700	0.38757400
C	4.30506000	0.16718500	0.28088500
H	5.05788700	0.91844300	0.50437600
H	1.58669100	-2.52501600	-0.45155900
O	-1.50898500	-0.77619600	2.09620700
C	-1.49582700	-1.30197200	3.37567400
H	-0.46903000	-1.53851000	3.71591500
H	-1.91096600	-0.59604300	4.12024900
H	-2.08006600	-2.23645700	3.47396100
C	-1.88143500	3.99676400	0.51328700
H	-1.05191400	4.04673300	1.22633200
H	-2.18469400	5.01952300	0.26935000
H	-2.71986500	3.49396000	1.00356600

Structure 1a-prodCO-II [B3LYP/6-31G(d)]

C	0.30620800	1.35826800	0.27172200
C	1.40348600	2.10622600	0.79691300
C	2.68258900	1.61522700	0.77425100
C	2.96192900	0.33238000	0.23254300
C	1.88512300	-0.44318300	-0.30654300
C	-1.07430400	1.89795600	0.36170900
O	-2.07023600	1.16147000	0.33264400
O	-0.44112100	-0.63391000	-0.87330500
Cl	-3.71147700	-1.63479100	-1.17342000
C	-0.57765800	-0.46920700	-2.31331200
H	1.21785900	3.07560900	1.24465000
H	3.49888800	2.20060700	1.18816200
H	-1.43328800	-1.08189500	-2.59511200
H	0.33839700	-0.80351100	-2.80674000
H	-0.77302500	0.58176400	-2.54653600
Mg	-2.19286700	-0.91013500	0.36467800
C	-1.30248600	3.39282800	0.47104100
H	-2.36737300	3.52736100	0.67654200
C	0.57674900	0.11042900	-0.29309200
C	2.15010100	-1.74562300	-0.81196000
C	3.43203600	-2.24571500	-0.80291500
H	3.62501200	-3.24587600	-1.17946800

C	4.50216900	-1.47122000	-0.29230200
H	5.50848100	-1.88030700	-0.29401700
C	4.27108300	-0.21346000	0.21816300
H	5.08794200	0.37652400	0.62528800
H	1.32489000	-2.34848000	-1.17360600
O	-1.50024300	-1.40297600	1.97793900
C	-1.47630300	-2.32568800	3.00809800
H	-0.46908000	-2.76334500	3.14944200
H	-1.75340700	-1.87245100	3.97898000
H	-2.16701300	-3.17609700	2.85335300
C	-0.90142800	4.14942300	-0.81052400
H	-1.12429400	5.21481700	-0.69702700
H	0.16632800	4.04604300	-1.02731200
H	-1.46445500	3.77967900	-1.67399500
H	-0.74931800	3.79410200	1.32841200

Structure 1a-prodCO-III [B3LYP/6-31G(d)]

C	0.21996700	1.42169100	-0.02432500
C	1.19316300	2.38508000	0.38023900
C	2.52554800	2.07332700	0.44898800
C	2.98720900	0.76907100	0.12702500
C	2.03836500	-0.21969300	-0.28916200
C	-1.22039900	1.78313000	-0.03793700
O	-2.11528100	0.92789100	-0.00822500
O	-0.22241800	-0.81274900	-0.83708300
Cl	-3.31679900	-2.30633200	-0.99022400
C	-0.34575200	-0.88741100	-2.28585800
H	0.86842500	3.38070900	0.65902800
H	3.24519600	2.82220300	0.76783900
H	-1.09095000	-1.65944500	-2.47422100
H	0.62295300	-1.14716200	-2.72010800
H	-0.69268700	0.07413400	-2.67559600
Mg	-1.96936900	-1.10467100	0.39947900
C	-1.61966600	3.24737200	-0.07520700
C	0.66866200	0.14795300	-0.37725000
C	2.48689800	-1.53825300	-0.57551200
C	3.82220400	-1.85464900	-0.47242700
H	4.15582100	-2.86686300	-0.68099600
C	4.76525700	-0.87292300	-0.08229100
H	5.81584900	-1.13867100	-0.00702100
C	4.35601800	0.40795300	0.21478100
H	5.07570600	1.15916100	0.52923500
H	1.75925700	-2.29547600	-0.84453600
O	-1.29086500	-1.16793900	2.09139900
C	-1.17608300	-1.87077100	3.27747700
H	-0.12029000	-2.09057700	3.52819600
H	-1.58480900	-1.30591900	4.13697000
H	-1.70297000	-2.84360400	3.26603000
H	-1.30869300	3.69609000	0.87984900
C	-3.11610700	3.46882100	-0.29468100
H	-3.44476800	3.04196700	-1.24688500
H	-3.70451900	2.99960300	0.49771900
H	-3.33606400	4.54087900	-0.30300400
H	-1.02262800	3.75485800	-0.84433100

Structure 7_I [B3LYP/6-31G(d)]

C	-0.75430100	-0.16613600	0.00811600
C	-2.20948600	-0.15463000	-0.11715400
O	-2.92937800	0.76752900	-0.47054100
O	0.03934400	2.20656100	-0.08048200
C	-1.14279300	2.87735500	0.38096300
H	-0.85405100	3.92610900	0.47287000
H	-1.43755000	2.48399700	1.35994200
H	-1.96753100	2.74915900	-0.31768900
C	0.14703600	0.87340500	-0.05024200
O	-2.72130000	-1.38454200	0.18159300
C	-4.13980300	-1.50775800	0.02590100
H	-4.37320200	-2.54202200	0.28305600
H	-4.66550300	-0.81999500	0.69441400
H	-4.43864700	-1.29188600	-1.00386600
C	1.45665600	-1.05200600	0.03878700
C	1.51660200	0.34694900	-0.04905800
C	2.73481700	1.02601400	-0.10727200
C	3.90757700	0.27052300	-0.08589900
H	4.87177500	0.76928700	-0.13482500
C	3.85549700	-1.12737200	0.00070600
H	4.78066100	-1.69741900	0.01788900
C	2.62949200	-1.79889800	0.06751300
H	2.76093800	2.10944700	-0.16919700
H	2.60021100	-2.88348800	0.13934800
C	0.01280200	-1.47784900	0.10291900
H	-0.25539600	-2.16295900	-0.71231500
H	-0.21561700	-2.01420400	1.03413000

Structure 7_II [B3LYP/6-31G(d)]

C	-0.66946200	-0.48320200	0.09830500
C	-2.08796000	-0.83643700	0.06670400
O	-2.50639800	-1.94443500	0.36174300
O	-0.29852700	1.99379500	-0.02996200
C	-1.52637900	2.47325700	0.52528800
H	-1.33756000	3.51769800	0.78387500
H	-1.78914900	1.90706000	1.42446300
H	-2.33853400	2.40017600	-0.19765300
C	0.03437800	0.69354300	-0.00338100
O	-2.91450000	0.14723100	-0.38642700
C	-4.30218300	-0.21224400	-0.44790900
H	-4.81772000	0.67417700	-0.82082700
H	-4.45183800	-1.05554000	-1.12722000
H	-4.67869500	-0.48765600	0.54125100
C	1.65970600	-0.97598200	0.04755900
C	1.47390300	0.41125200	-0.05701100
C	2.55356400	1.28829600	-0.17450000
C	3.83884100	0.74558100	-0.19719200
H	4.69987000	1.40158800	-0.29304900
C	4.03206000	-0.63873700	-0.09501200
H	5.04150700	-1.04103800	-0.11310000
C	2.94390800	-1.50949300	0.03229400
H	2.39110100	2.35912700	-0.24788500
H	3.10456900	-2.58155100	0.11655300
C	0.31499300	-1.63974400	0.18014400
H	0.12931800	-2.37959100	-0.60984100
H	0.21031100	-2.18372700	1.12886900

Structure 7·EtMgCl_I [B3LYP/6-31G(d)]

C	0.51663200	1.11837000	0.21900700
C	-0.76276100	1.78134500	0.26333700
O	-1.87815100	1.23253900	0.22297800
O	-0.29970700	-1.11497000	0.28662400
C	-0.08916800	-2.53787600	0.42837600
H	-1.08456400	-2.94727600	0.59874500
H	0.55115600	-2.73709900	1.28978900
H	0.33230300	-2.94664100	-0.49222000
C	-3.65781200	-1.81048600	0.81900400
C	0.72675800	-0.24042100	0.21901300
O	-0.65674200	3.11073900	0.36114600
C	-1.88990400	3.85834300	0.36499600
H	-1.58754500	4.90306700	0.43157800
H	-2.44727100	3.67375000	-0.55606300
H	-2.50233800	3.57718700	1.22477900
H	-4.70615900	-1.55341700	0.59358900
C	-3.44495200	-1.68037400	2.34104600
H	-2.42458500	-1.96139400	2.64467500
H	-3.59035300	-0.64636700	2.68387900
H	-4.12730200	-2.30656700	2.93985200
H	-3.58815600	-2.87618100	0.53975200
C	2.83355600	0.71477600	0.12288700
C	2.16818900	-0.53258900	0.15132300
C	2.91401400	-1.72092500	0.09688100
C	4.30380400	-1.64112500	0.02593500
H	4.88588000	-2.55688200	-0.01870300
C	4.95504700	-0.40307300	0.00715200
H	6.03920200	-0.36489100	-0.04829700
C	4.21917900	0.78308700	0.05272000
H	2.44665100	-2.69607300	0.09885900
H	4.72278500	1.74595800	0.02974300
C	1.83738600	1.84159000	0.16261000
H	1.91517800	2.48563400	-0.72360700
H	1.98576100	2.49493100	1.03287200
Mg	-2.41078900	-0.63116500	-0.43686200
Cl	-1.94083400	-0.63082800	-2.68462300

Structure 7·EtMgCl_II [B3LYP/6-31G(d)]

C	-0.62884000	1.10354100	-0.22621100
C	0.64079900	1.78617300	-0.27174800
O	1.76248500	1.24986600	-0.29978600
O	0.21528100	-1.10753400	-0.46994400
C	0.01869600	-2.50394200	-0.78703700
H	-0.66880800	-2.60398700	-1.62918500
H	-0.34315000	-3.03942300	0.09328700
H	1.00782000	-2.86678100	-1.06519300
C	3.55239600	-1.75623900	-1.05001600
H	3.11210300	-1.75779100	-2.06349600

H	3.56368100	-2.81837900	-0.75004500
C	-0.82069000	-0.25472000	-0.31172800
O	0.51616100	3.11725100	-0.28702500
C	1.74017900	3.88007800	-0.28142900
H	1.42403100	4.92279400	-0.27268900
H	2.32811200	3.64536000	0.60865600
H	2.32842600	3.66135700	-1.17553200
C	5.01666000	-1.28000700	-1.16450000
H	5.08140700	-0.24057300	-1.51673400
H	5.53070800	-1.31418200	-0.19423500
H	5.62305100	-1.88294600	-1.86094000
C	-2.25346200	-0.57469300	-0.21198600
C	-2.93525700	0.65653800	-0.07661700
C	-5.03320800	-0.50421900	0.04461600
H	-6.11492700	-0.48897600	0.14250800
C	-4.36438500	-1.72706100	-0.07699700
H	-4.93039500	-2.65387500	-0.06827700
C	-2.97721700	-1.77746400	-0.20480100
H	-2.49364400	-2.74168500	-0.28429200
C	-1.95654600	1.79974200	-0.07328900
H	-2.01135700	2.37866700	0.85845000
H	-2.14445600	2.50989700	-0.88969800
C	-4.31810100	0.69555800	0.04920000
H	-4.83530500	1.64563200	0.15460800
Mg	2.31767800	-0.63962300	0.27443300
Cl	1.86429500	-0.70682400	2.52523000

Structure 7·EtMgCl_III [B3LYP/6-31G(d)]

C	-0.63508900	1.19975600	0.01417200
C	0.59784000	1.95191700	0.02407700
O	1.74338100	1.47701500	0.08967700
O	0.30161600	-0.94372700	0.50698800
C	0.15492400	-2.15589600	1.29726600
H	-0.10024300	-2.99008200	0.64008400
H	-0.60495700	-2.00841500	2.06625900
H	1.13440600	-2.30958000	1.75143000
C	2.54380700	-0.95443900	-2.26452400
C	-0.75982300	-0.14694400	0.25643900
O	0.40374600	3.27287800	-0.04888800
C	1.58718300	4.09832200	-0.05905800
H	1.21829700	5.12142000	-0.12500800
H	2.16053000	3.95018800	0.85863700
H	2.21172900	3.85475700	-0.92157100
H	1.78034100	-0.39353700	-2.83187200
C	2.40518700	-2.45214500	-2.60709100
H	3.17733800	-3.05580900	-2.11116100
H	1.43548500	-2.85985900	-2.28320800
H	2.48422200	-2.66766200	-3.68607000
H	3.50295800	-0.59480500	-2.67290300
C	-2.91629000	0.61913800	-0.10102800
C	-2.17209100	-0.54851400	0.17829300
C	-2.81888600	-1.78856100	0.28226300
C	-4.20306900	-1.83638300	0.12451700
H	-4.71499400	-2.79105100	0.20171400
C	-4.93805500	-0.67415400	-0.13672300
H	-6.01621300	-0.73479200	-0.25450900
C	-4.29560400	0.56081700	-0.25686200
H	-2.27344500	-2.70459700	0.46948400
H	-4.86606200	1.46009700	-0.47395200
C	-1.99666100	1.80598800	-0.21944200
H	-2.22432200	2.58479400	0.52063100
H	-2.07569600	2.28542900	-1.20453900
Mg	2.43442900	-0.43692800	-0.20718500
Cl	3.50866400	-1.14271200	1.70392700

Structure 7·EtMgCl_IV [B3LYP/6-31G(d)]

C	0.49784500	1.09729400	-0.24407700
C	-0.79279100	1.73613300	-0.35126000
O	-1.89657700	1.16898000	-0.30550300
O	-0.26315300	-1.16823600	-0.30674500
C	-0.02238600	-2.49226900	-0.85800000
H	0.30817400	-3.16354800	-0.06232100
H	0.71548200	-2.43230400	-1.65937700
H	-0.98860900	-2.80836500	-1.25253500
C	-2.56578600	-0.88239000	2.42247900
H	-2.50203400	-1.94568700	2.70803200
H	-3.57439800	-0.57915200	2.74899300
C	0.73125600	-0.25654300	-0.23963900
O	-0.70678300	3.06069100	-0.51209400
C	-1.95338000	3.78029600	-0.61178000
H	-1.66837000	4.82431000	-0.73809300
H	-2.52763000	3.42740400	-1.47118200
H	-2.54163600	3.64635900	0.29889700
C	-1.52832700	-0.09125200	3.24469000
H	-0.49778600	-0.39822700	3.01140800
H	-1.58265300	0.98903900	3.04370700
H	-1.64466000	-0.20759500	4.33550300
C	2.17366300	-0.52273000	-0.13285700
C	2.82102200	0.73228700	-0.09507200
C	4.94627100	-0.36500100	0.10797500
H	6.02763900	-0.31576100	0.19848000
C	4.30835900	-1.61065900	0.08750200
H	4.89812000	-2.51901000	0.16814300
C	2.92252800	-1.70430200	-0.03031200
H	2.45516800	-2.68061500	-0.02985600
C	1.80664100	1.84295700	-0.16523300
H	1.95689500	2.48961900	-1.04001500
H	1.85909300	2.49844400	0.71460300
C	4.20281600	0.81490900	0.02294500
H	4.69811200	1.78187500	0.05362300
Mg	-2.44881800	-0.71238400	0.30780600
Cl	-3.43290400	-1.82482500	-1.45124100

Structure 7-TSOMe-I [B3LYP/6-31G(d)]

Cl	-3.73471500	-2.30748200	0.01163100
C	0.26337000	1.14537100	-0.30493600
C	-1.03320600	1.69954100	-0.28118100
O	-2.09274600	1.00451400	-0.20638500
O	-0.33067600	-1.16746700	-1.01323300
C	-0.20572700	-1.07146800	-2.45418100
H	-0.85146100	-1.85257700	-2.85687700
H	0.83328300	-1.25111900	-2.74234000
H	-0.53022400	-0.08666200	-2.80086800
Mg	-1.95545600	-0.94997900	0.21443000
C	-0.37001300	-1.04357500	1.82599100
H	0.59769200	-1.54305600	1.85620200
H	-1.09691600	-1.82206600	2.14055200
C	0.47209600	-0.24654000	-0.27817400
O	-1.10572200	3.04058600	-0.30332900
C	-2.41887600	3.61907600	-0.21915400
H	-2.25909000	4.69678600	-0.26126900
H	-3.04106800	3.29088300	-1.05563400
H	-2.90472100	3.34147400	0.71978800
C	-0.43209600	0.16121000	2.75207200
H	-1.46505600	0.45161500	2.98364900
H	0.07578400	-0.00954500	3.71269900
H	0.04844700	1.03946400	2.29580500
C	1.91249500	-0.49743900	-0.14961200
C	2.57181500	0.73912700	-0.02095600
C	2.61890100	-1.70268900	-0.14289700
H	2.09672200	-2.65004100	-0.24309700
C	4.00533700	-1.65664200	0.00419800
H	4.57787200	-2.57984700	0.01517400
C	4.66616700	-0.42881700	0.14187300
H	5.74642600	-0.41213300	0.25817700
C	3.95480000	0.77556400	0.12755500
H	4.47909700	1.72303400	0.22511300
C	1.57634100	1.87691100	-0.11153200
H	1.80736000	2.54342500	-0.95559200
H	1.58620000	2.50847300	0.78681700

Structure 7-TSOMe-II [B3LYP/6-31G(d)]

Cl	-3.72401200	-2.15853800	-0.15396400
C	0.24015300	1.33343100	-0.10015200
C	-1.05458400	1.87500600	0.01413500
O	-2.11610000	1.17751700	-0.02315800
O	-0.36394000	-0.84102500	-1.14794700
C	-0.29064300	-0.49938300	-2.55523200
H	-0.93406100	-1.21839000	-3.06336000
H	0.74139300	-0.60129700	-2.90057700
H	-0.64717200	0.52069800	-2.71945900
Mg	-1.95099100	-0.81313300	0.15745400
C	-0.34596100	-1.16054100	1.70373100
H	-1.21144000	-0.87348000	2.34025200
C	0.45034200	-0.04566200	-0.29500000
O	-1.12728700	3.20212200	0.21258500
C	-2.44072800	3.75934500	0.38569900
H	-2.28098500	4.82896700	0.52440100
H	-3.05855400	3.57571600	-0.49697700
H	-2.93215800	3.32970000	1.26247200
C	1.88699700	-0.32028900	-0.20696900
C	2.54215800	0.87084300	0.16070900

C	2.59802700	-1.50076000	-0.43692900
H	2.08305900	-2.40799500	-0.73772400
C	3.98336600	-1.48151500	-0.27170300
H	4.55953200	-2.38663000	-0.44174800
C	4.63813500	-0.30436200	0.11247600
H	5.71749400	-0.30851200	0.23795900
C	3.92316800	0.87931700	0.32621700
H	4.44433600	1.79113800	0.60736700
C	1.54460800	2.00414400	0.27795100
H	1.80031300	2.83814600	-0.39124400
H	1.52119300	2.42521500	1.29357500
H	0.49270900	-0.59825100	2.11310200
C	-0.10857200	-2.66838500	1.77912800
H	-0.96114400	-3.24896200	1.40354500
H	0.76874900	-2.95990200	1.18984100
H	0.07666000	-3.00947200	2.81030000

Structure 7-TSCO-I [B3LYP/6-31G(d)]

Cl	-3.59238500	-2.45595500	0.35292300
C	0.34239500	0.83205700	-0.38048700
C	-1.06394600	1.28526800	-0.54540800
O	-1.87849400	0.59798800	-1.28523700
O	-0.20041800	-1.50214200	-0.16282900
C	-0.10489300	-2.52439100	-1.19510000
H	-0.87921900	-3.25469500	-0.95896800
H	0.88227500	-2.98748600	-1.16883900
H	-0.28620800	-2.07020500	-2.17343400
Mg	-2.17649100	-0.73415400	0.10989400
C	-1.80453000	0.97248500	1.56282800
H	-2.13166400	0.06286600	2.12232000
H	-2.70578500	1.59356500	1.47288000
C	0.71706200	-0.46238300	-0.25185900
O	-1.13504100	2.64015200	-0.55608100
C	-2.37013100	3.20594900	-1.01430400
H	-2.22907900	4.28625000	-0.96018300
H	-2.58119500	2.89528200	-2.03979300
H	-3.20013200	2.90420800	-0.36840200
C	-0.75025600	1.66082500	2.42074000
H	0.15027100	1.04266800	2.52691500
H	-0.45173500	2.61496800	1.97133800
H	-1.10859400	1.88244900	3.43622200
C	2.16143400	-0.59503700	-0.06930000
C	2.69422200	0.71139700	-0.13290000
C	4.89498100	-0.18687200	0.21400900
H	5.96571300	-0.03894400	0.32282500
C	4.36223000	-1.47740100	0.29921000
H	5.02285000	-2.32085500	0.47952400
C	2.98944100	-1.69636200	0.16177200
H	2.58517800	-2.69977800	0.25528700
C	1.57068900	1.70843400	-0.31549300
H	1.67945700	2.31098000	-1.22733600
H	1.51711600	2.42018500	0.51828600
C	4.06015800	0.91785100	0.00416000
H	4.47768700	1.92072300	-0.04108700

Structure 7-TSCO-II [B3LYP/6-31G(d)]

Cl	-3.36724500	-2.57671000	0.22838700
C	0.43754100	0.88052100	-0.31570200
C	-0.98014700	1.28595400	-0.50542400
O	-1.75149700	0.59945100	-1.29191300
O	-0.00679100	-1.48531700	-0.28807700
C	0.14395600	-2.38784000	-1.41853900
H	-0.58235400	-3.18540900	-1.25955600
H	1.15819000	-2.79025100	-1.43829300
H	-0.06950200	-1.84726400	-2.34514400
Mg	-2.01267000	-0.79967300	0.04647400
C	-1.58942500	0.79250100	1.59517500
H	-1.25245900	-0.12276400	2.12976500
C	0.86454100	-0.40279000	-0.25879000
O	-1.10797700	2.63844700	-0.46944000
C	-2.29408000	3.18348600	-1.06529900
H	-2.21841700	4.26150900	-0.91491800
H	-2.33364800	2.94814100	-2.13159600
H	-3.19520500	2.79965200	-0.58136800
C	2.30021600	-0.48677800	0.00047900
C	2.77188000	0.84200700	0.08040000
C	4.98902200	0.01065500	0.48536600
H	6.04329800	0.19417700	0.67255800
C	4.51507500	-1.30395000	0.42593800
H	5.20424500	-2.13091000	0.57277800
C	3.16432100	-1.56818500	0.18565900
H	2.80199800	-2.59174500	0.16390600
C	1.61322300	1.80111600	-0.09376500
H	1.74972300	2.48823300	-0.93941400
H	1.46794100	2.43397000	0.79239200
H	-0.88814700	1.56308800	1.91516300
C	-3.02259900	1.16507500	1.99971500
H	-3.14249900	1.24371400	3.09075900
H	-3.30560000	2.13458000	1.57587900
H	-3.77697200	0.43622400	1.66535500
C	4.11595500	1.09346600	0.31862600
H	4.48784600	2.11312100	0.38385700

Structure 7-intOMe-I [B3LYP/6-31G(d)]

Cl	4.00122900	-2.26366900	0.27899900
C	-0.19068800	1.13235400	-0.03685200
C	1.05736600	1.69748700	-0.04406100
O	2.18452000	1.06948000	-0.26238400
O	0.43239200	-1.25702900	0.51667000
C	0.10885100	-1.26980400	1.91780600
H	0.88335300	-1.85759800	2.41878500
H	-0.86235300	-1.74476100	2.07450700
H	0.08781200	-0.24888600	2.31704100
Mg	2.34273200	-0.80095700	0.05699700
C	-0.03151400	-0.79984900	-1.78178800
H	-0.23332600	-1.87557900	-1.84637100
H	1.05326700	-0.67275600	-1.93592300
C	-0.43507900	-0.30117200	-0.37591100
O	1.12974100	3.02839600	0.22951800
C	2.43273000	3.60761800	0.32478400
H	2.26184500	4.66139000	0.55286900
H	3.01993600	3.14446300	1.12434600
H	2.98145300	3.51265400	-0.61656800
C	-0.73724900	-0.05538300	-2.91929600
H	-0.52191300	1.01637700	-2.87351900
H	-0.39675800	-0.43406700	-3.88862300
H	-1.82209300	-0.19027500	-2.86524300
C	-1.90188100	-0.48780700	-0.06813700
C	-2.48475200	0.71675100	0.34676600
C	-2.65766600	-1.65813400	-0.16588100
H	-2.19929400	-2.59121000	-0.48454500
C	-4.01332000	-1.61480700	0.16427000
H	-4.61557900	-2.51683600	0.09949100
C	-4.60039900	-0.41259300	0.57731600
H	-5.65731700	-0.38954000	0.82968800
C	-3.84163200	0.75694000	0.66782100
H	-4.30577800	1.68711100	0.98685400
C	-1.47229400	1.83955500	0.36095800
H	-1.41538400	2.32456800	1.34692000
H	-1.75960300	2.63510700	-0.34385500

Structure 7-intOMe-II [B3LYP/6-31G(d)]

Cl	3.96978600	-2.11233500	0.53258800
C	-0.22655900	1.22716700	-0.20302600
C	1.01399300	1.80281700	-0.22903000
O	2.16074100	1.17256000	-0.31302900
O	0.40377900	-1.08704500	0.57598800
C	0.07506200	-0.96115000	1.97274900
H	0.85426900	-1.48847800	2.53051900
H	-0.89153300	-1.42771600	2.17396300
H	0.04221800	0.09519100	2.26300400
Mg	2.33327500	-0.66112100	0.14243000
C	-0.01802100	-0.77544500	-1.78227400
H	1.01731500	-0.44514600	-1.96839400
C	-0.45645300	-0.24367700	-0.39413300
O	1.06065800	3.16044300	-0.12938400
C	2.35056100	3.76823500	-0.04595600
H	2.15773500	4.83998000	0.03210900
H	2.90046200	3.42490100	0.83645600
H	2.94908400	3.56048300	-0.93765500
C	-1.93211600	-0.40325000	-0.08710700
C	-2.53497300	0.84788800	0.10754700
C	-2.68201900	-1.57819900	0.02252600
H	-2.21278600	-2.55088800	-0.08756600
C	-4.04666600	-1.48933800	0.30575700
H	-4.63828300	-2.39601900	0.39831700
C	-4.65370600	-0.24013300	0.47387400
H	-5.71711300	-0.18232100	0.69090500
C	-3.90048200	0.93209800	0.37784000
H	-4.37330900	1.90048900	0.52327800
C	-1.53088900	1.97182200	-0.00614800
H	-1.53678300	2.61373100	0.88706400

H	-1.77671300	2.63679200	-0.84939500
H	-0.60932300	-0.21149200	-2.51212700
C	-0.14479300	-2.27713800	-2.06958500
H	0.37865200	-2.88908500	-1.32781500
H	-1.19171800	-2.59244000	-2.08993200
H	0.28311400	-2.50269800	-3.05269200

Structure 7-intCO-I [B3LYP/6-31G(d)]

Cl	-3.58256300	-2.93051700	0.53699300
C	0.29525000	0.79737600	-0.05774700
C	-1.07208700	1.48771600	-0.06730200
O	-2.11071900	0.61268600	-0.26712700
O	-0.29718800	-1.60582000	-0.08275300
C	-0.16811900	-2.43780000	-1.27477800
H	-0.87369500	-3.26097000	-1.14666000
H	0.84864600	-2.82130400	-1.35270300
H	-0.41036800	-1.84430100	-2.16249800
Mg	-2.28890800	-1.15440400	0.19400700
C	-1.36829700	2.25700900	1.26296500
H	-1.28741000	1.53470400	2.08675500
H	-2.43176800	2.51367800	1.19667200
C	0.60382400	-0.52179300	-0.04515900
O	-0.94195200	2.41291800	-1.16574500
C	-2.13947500	3.06987000	-1.55522700
H	-1.90951000	3.58954200	-2.48961800
H	-2.94967400	2.35380900	-1.72327000
H	-2.46698800	3.81309000	-0.81344300
C	-0.56240200	3.52015300	1.58538600
H	0.44218700	3.29796800	1.95892000
H	-0.46026700	4.15807100	0.70184000
H	-1.06858000	4.10017100	2.36569600
C	2.05110900	-0.75770800	0.02623200
C	2.67006100	0.50430000	-0.03723300
C	4.82051700	-0.55301600	0.12992700
H	5.90413600	-0.48374500	0.16697400
C	4.20270800	-1.80435100	0.22048800
H	4.81063100	-2.69749700	0.33609900
C	2.81063400	-1.92106200	0.17354500
H	2.34214700	-2.89558900	0.27853900
C	1.60311400	1.56769700	-0.10180800
H	1.63690100	2.15822800	-1.02688500
H	1.70168500	2.28600600	0.71896100
C	4.05382300	0.61261500	0.00922300
H	4.53729500	1.58547900	-0.03842600

Structure 7-intCO-II [B3LYP/6-31G(d)]

Cl	-3.29895100	-3.05541700	0.60900600
C	0.29261900	0.90666800	0.04784500
C	-1.10241000	1.55386000	0.00836800
O	-2.11730200	0.63843900	0.04796200
O	-0.18379000	-1.49973400	-0.19530600
C	-0.01390100	-2.24763900	-1.43215100
H	-0.67318100	-3.11386600	-1.35465000
H	1.02291700	-2.56871200	-1.53212400
H	-0.29246400	-1.61791800	-2.28280200
Mg	-2.14312100	-1.17480000	0.34062800
C	-1.24759500	2.58411300	1.15600300
H	-1.04149500	2.06316900	2.10112300
C	0.67134500	-0.38994400	-0.04889600
O	-1.14622500	2.36690600	-1.18943600
C	-1.33670800	1.66579900	-2.40129300
H	-1.36273200	2.42097900	-3.19189700
H	-0.50755100	0.96989900	-2.61482600
H	-2.28000100	1.10769800	-2.40510000
C	2.12309600	-0.56542300	0.08282800
C	2.67526300	0.72443400	0.19793900
C	4.86639400	-0.24273900	0.38122700
H	5.94078000	-0.12689700	0.49342600
C	4.31344200	-1.52396900	0.29238500
H	4.96148800	-2.39453300	0.34451800
C	2.93443200	-1.70055100	0.14629000
H	2.51440700	-2.70171900	0.11118400
C	1.55598400	1.73716300	0.19194400
H	1.62588600	2.45833600	-0.63356300
H	1.55173500	2.32995600	1.11608100
H	-0.48216700	3.35989200	1.03926000
C	-2.63338500	3.23002100	1.19972500
H	-2.69635900	3.94689200	2.02642600
H	-2.83774600	3.76112900	0.26578600
H	-3.41076400	2.47364200	1.33686900
C	4.04596000	0.89181600	0.34389100
H	4.47819000	1.88520800	0.43725400

Structure 7-intCO-III [B3LYP/6-31G(d)]

Cl	3.45185600	-2.63589800	-0.42538000
C	-0.38412300	0.92267500	-0.09569800
C	1.05765200	1.38090800	-0.29018500
O	1.60385300	0.82212400	-1.38079600
O	0.12699900	-1.43751800	-0.06703200
C	0.00692000	-2.40678900	1.00699600
H	0.84380600	-3.09413200	0.87847600
H	-0.93854500	-2.94386100	0.93167600
H	0.07195700	-1.89989900	1.97469200
Mg	2.13695100	-0.82039500	-0.52144200
C	1.27230000	2.89318000	-0.17278600
H	0.67551800	3.35414000	-0.97010700
C	-0.77495900	-0.37302900	-0.04486200
O	1.87832800	0.68379300	0.86804400
C	1.57940800	0.94131000	2.23186300
H	0.51445000	0.78198100	2.44770600
H	2.17545100	0.25082400	2.83525000
H	1.85129900	1.96822300	2.50394100
C	-2.23567700	-0.50966700	-0.07080500
C	-2.75817000	0.80112400	-0.09824600
C	-4.98843800	-0.08878200	-0.14417500
H	-6.06370900	0.06414100	-0.16798000
C	-4.47176800	-1.38760100	-0.14674500
H	-5.14965300	-2.23603500	-0.18081400
C	-3.09285900	-1.61278800	-0.11405000
H	-2.71305800	-2.62868500	-0.14891400
C	-1.61928900	1.79471400	-0.13567400
H	-1.65179500	2.50393000	0.70363200
H	-1.65500100	2.40272900	-1.05092100
H	0.85757300	3.25985600	0.77582000
C	2.73689000	3.30643900	-0.32362800
H	2.83288800	4.39735600	-0.30503400
H	3.35116100	2.89553100	0.48402700
H	3.13681200	2.93643500	-1.27101400
C	-4.12886600	1.01647500	-0.12892100
H	-4.53168100	2.02626300	-0.15192000

Structure 7-intCO-IV [B3LYP/6-31G(d)]

Cl	3.68061900	-2.36757300	-0.52711500
C	-0.41011200	0.85806000	0.01343600
C	1.00979500	1.40877400	-0.09902700
O	1.63318000	0.99397300	-1.20916600
O	0.20748800	-1.48010800	-0.18764800
C	0.18193400	-2.45489500	0.89419700
H	0.99360500	-3.15251500	0.68477700
H	-0.77584000	-2.97534300	0.90697800
H	0.34801400	-1.94297500	1.84630100
Mg	2.15938100	-0.72092200	-0.50219400
C	1.16786700	2.90775000	0.17866500
H	0.60802900	3.19280300	1.07851600
C	-0.73374200	-0.45309900	-0.07023200
O	1.71992800	0.56656600	1.09650300
C	2.78662200	1.15214200	1.84216900
H	2.41989800	1.95881200	2.48677600
H	3.20339800	0.36195100	2.47390900
H	3.58649700	1.54086900	1.19752600
C	-2.18163700	-0.67232400	-0.06043100
C	-2.77647200	0.59586300	0.09558700
C	-4.95052500	-0.42117900	0.02154100
H	-6.03285400	-0.33453800	0.05760600
C	-4.36088400	-1.67595300	-0.15940300
H	-4.99009200	-2.55466400	-0.27132300
C	-2.97109100	-1.81570700	-0.20665000
H	-2.52880400	-2.79205700	-0.37980800
C	-1.69475200	1.65141600	0.13916400
H	-1.71722700	2.23432000	1.07095200
H	-1.82214800	2.37233000	-0.67839600
H	2.22582700	3.09403600	0.38252500
C	0.77252900	3.78056500	-1.02095800
H	1.00575600	4.83063800	-0.81364500
H	1.33016400	3.46638900	-1.90658000
H	-0.29442600	3.72073800	-1.25562700
C	-4.15745100	0.72715300	0.14042700
H	-4.62016100	1.70416200	0.25837700

Structure 7'_I [B3LYP/6-31G(d)]

C	-0.75846700	-0.24494500	-0.04085000
C	-2.19880400	-0.15887300	-0.07729000

O	-2.90558800	0.84386800	-0.15494000
O	-0.13408700	2.17743700	-0.46221600
C	-0.66855200	2.88446600	0.64558000
H	-0.76204800	3.93360500	0.33562400
H	0.00342000	2.82842600	1.51670000
H	-1.65794900	2.50130000	0.91932400
C	0.15497900	0.84496100	-0.20252900
O	-2.80082100	-1.41087600	-0.00840700
C	-4.21798500	-1.38387800	-0.02565300
H	-4.53862800	-2.42829900	0.03894900
H	-4.62414100	-0.81596100	0.82027200
H	-4.60402400	-0.93149500	-0.94699900
C	1.35766900	-1.10576400	0.08669400
C	1.46036600	0.33826000	-0.13000500
C	2.73595500	0.94734600	-0.23258600
C	3.87438600	0.17479500	-0.11678400
H	4.85786700	0.63805800	-0.19294700
C	3.78276100	-1.23424600	0.10198200
H	4.69876000	-1.81860900	0.18826200
C	2.55567800	-1.85997100	0.20048100
H	2.80610200	2.02076500	-0.40442000
H	2.50245000	-2.93756000	0.36356800
C	-0.00057300	-1.44298500	0.13684700
H	-0.42232200	-2.42865800	0.29084800

Structure 7'_II [B3LYP/6-31G(d)]

C	-0.67478000	-0.61196300	-0.01747000
C	-2.09228900	-0.90201600	-0.01643200
O	-2.61959200	-2.00474100	0.09829900
O	-0.54743700	1.88628100	-0.43731500
C	-0.97215800	2.54947300	0.73904400
H	-1.32095500	3.54664300	0.43870300
H	-0.14691200	2.66078200	1.45946200
H	-1.79898300	2.01612800	1.22637000
C	0.00738200	0.63174200	-0.19981100
O	-2.88863600	0.22521000	-0.16078100
C	-4.28232900	-0.03960300	-0.18292700
H	-4.76938600	0.93232900	-0.30610200
H	-4.55372300	-0.70186900	-1.01345100
H	-4.62020900	-0.51360100	0.74647800
C	1.56920100	-1.04642000	0.08293000
C	1.38803900	0.38866600	-0.14190300
C	2.52095600	1.23109800	-0.26682000
C	3.78878100	0.69278400	-0.16516800
H	4.66325300	1.33617300	-0.26050700
C	3.97362200	-0.70515200	0.06106200
H	4.98606500	-1.10166500	0.13589800
C	2.89097400	-1.55486100	0.18022200
H	2.38228800	2.29654200	-0.44813400
H	3.04851900	-2.62135300	0.34806100
C	0.30067800	-1.63713500	0.15446900
H	0.06689300	-2.68377800	0.30842100

Structure 7'·EtMgCl_I [B3LYP/6-31G(d)]

C	-0.63696000	1.11679300	-0.19505800
C	0.63606900	1.75789300	-0.21444200
O	1.75353700	1.19568900	-0.11495300
O	0.19198100	-1.25042100	-0.25134900
C	0.16625300	-2.00363500	-1.47914700
H	1.03988800	-2.65735500	-1.46455800
H	0.21921400	-1.32533700	-2.33799700
H	-0.75347600	-2.59226200	-1.53590700
C	3.61550500	-1.73505800	-0.77201400
C	-0.83878700	-0.29767600	-0.15487500
O	0.59579900	3.10465800	-0.35350500
C	1.85487700	3.77864800	-0.30039500
H	1.61763100	4.84075900	-0.39226800
H	2.36615200	3.58332300	0.64672200
H	2.50571400	3.46403100	-1.12195000
H	4.58449600	-1.62784300	-0.25301800
C	3.80539900	-1.27931900	-2.23186600
H	2.88789200	-1.40521600	-2.82717700
H	4.05952400	-0.21089400	-2.29156200
H	4.60107200	-1.81825700	-2.78127600
H	3.43930700	-2.82673100	-0.76833200
C	-2.88050100	0.74229800	-0.06031800
C	-2.20768600	-0.55918100	-0.06680300
C	-2.98125900	-1.74894500	0.01975200
C	-4.35356000	-1.66260700	0.09842700
H	-4.94868100	-2.57087200	0.17483100
C	-5.01556600	-0.39615500	0.09782700
H	-6.10182900	-0.36677800	0.16334200
C	-4.29850000	0.77752100	0.02615200
H	-2.49119200	-2.72026400	0.05105200
H	-4.81242800	1.73839000	0.03647800
C	-1.91314000	1.74952300	-0.13822800
Mg	2.16063800	-0.72729500	0.45702300
Cl	2.22911800	-0.79035300	2.78323200
H	-2.07932100	2.81884100	-0.11322400

Structure 7'·EtMgCl_II [B3LYP/6-31G(d)]

C	-0.75122100	1.11502700	-0.19446200
C	0.50144700	1.79389600	-0.24171400
O	1.63706700	1.26034500	-0.22715800
O	0.13699100	-1.22255700	-0.41665900
C	0.08047300	-1.88826600	-1.69357800
H	0.11564700	-1.15152900	-2.50411400
H	-0.84319400	-2.46857000	-1.76826600
H	0.95109300	-2.54359600	-1.74770300
C	3.48231600	-1.59020400	-1.16864200
H	3.19532300	-1.34214800	-2.20724900
H	3.39288300	-2.69132300	-1.11671400
C	-0.91179800	-0.30514300	-0.21937100
O	0.41789000	3.14425100	-0.30753100
C	1.65944300	3.85152600	-0.27733300
H	1.38931000	4.90954700	-0.29787200
H	2.22234400	3.61970900	0.63144400
H	2.27687300	3.60186600	-1.14568800
C	4.97027400	-1.23016200	-0.98484500
H	5.14171400	-0.14877200	-1.09545600
H	5.32819400	-1.49645800	0.01952100
H	5.65306100	-1.72537800	-1.70195200
C	-2.26700400	-0.61181800	-0.08106200
C	-2.97441000	0.66649100	0.02634700
C	-5.06674000	-0.54291500	0.22304500
H	-6.14894700	-0.55009400	0.34094800
C	-4.37056000	-1.78698200	0.12450100
H	-4.93591100	-2.71559600	0.17956000
C	-3.00170000	-1.82751100	-0.02279800
H	-2.48334500	-2.78355000	-0.06751900
C	-2.04005300	1.70517300	-0.04378900
C	-4.38696800	0.65423700	0.18104400
H	-4.92630200	1.59722200	0.26695700
Mg	2.12219000	-0.67629500	0.23018700
Cl	2.31546300	-0.83755700	2.54428400
H	-2.23445400	2.76626900	0.04573700

Structure 7'·EtMgCl_III [B3LYP/6-31G(d)]

C	0.70013900	1.21564300	-0.03386300
C	-0.52343300	1.94837400	-0.00329500
O	-1.67858400	1.46244000	-0.05951000
O	-0.27883200	-1.00467000	-0.67391800
C	-0.23618200	-1.39436200	-2.06417300
H	0.64253900	-2.02117000	-2.24164900
H	-0.18637300	-0.50246300	-2.69776500
H	-1.15919500	-1.93961100	-2.26454000
C	-2.34436500	-1.04733400	2.29908700
C	0.79869000	-0.18841700	-0.28605100
O	-0.38412300	3.29183000	0.10414300
C	-1.59713100	4.04188200	0.19881600
H	-1.28531400	5.08429800	0.29332600
H	-2.21321200	3.90896200	-0.69533200
H	-2.18070200	3.73940400	1.07357700
H	-1.51825100	-0.59212400	2.87254900
C	-2.39070600	-2.55260000	2.62682400
H	-3.22260800	-3.05474600	2.11211100
H	-1.47261600	-3.06482000	2.30347600
H	-2.50786300	-2.78054300	3.70376100
H	-3.25638700	-0.57708400	2.70944200
C	2.89247600	0.62894000	0.17094200
C	2.13484300	-0.57742300	-0.16890100
C	2.81249700	-1.81937000	-0.30401100
C	4.17560700	-1.87203500	-0.11323500
H	4.69850400	-2.82221000	-0.20650000
C	4.92063700	-0.69880700	0.21949000
H	5.99652000	-0.77915700	0.36503200
C	4.29631300	0.52071600	0.36292500
H	2.25385200	-2.72467100	-0.53431200
H	4.87367600	1.40765100	0.62277100
C	2.00717100	1.71034000	0.24604300
Mg	-2.16791800	-0.51588100	0.23113100
Cl	-3.69639200	-1.13601000	-1.44572800

H	2.24408500	2.73094900	0.51854400

Structure 7'·EtMgCl_IV [B3LYP/6-31G(d)]

C	0.55805400	1.05915200	-0.38612000
C	-0.72839700	1.65781100	-0.53577200
O	-1.83202700	1.06718500	-0.45218300
O	-0.20893500	-1.33076000	-0.38840900
C	-0.14301600	-2.05075800	-1.63861900
H	0.79228100	-2.61638100	-1.68575400
H	-0.18913100	-1.34556700	-2.47542400
H	-1.00899300	-2.71321000	-1.66377500
C	-2.21919500	-0.69413800	2.55796300
H	-1.63007800	-1.52927700	2.97630700
H	-3.25399800	-0.90405900	2.88064200
C	0.78635400	-0.34639600	-0.25526700
O	-0.71617600	2.98919200	-0.78482400
C	-1.99525000	3.62283600	-0.86240500
H	-1.78372700	4.67902900	-1.04258300
H	-2.59088600	3.20943300	-1.68162800
H	-2.55166700	3.50053800	0.07159900
C	-1.75112600	0.61058300	3.23162100
H	-0.70834400	0.84725300	2.97766500
H	-2.35073900	1.47419400	2.90547100
H	-1.80727900	0.59731700	4.33703100
C	2.15139400	-0.56794000	-0.06168200
C	2.79313200	0.74841900	-0.06905000
C	4.93304700	-0.33078400	0.29849500
H	6.01050500	-0.27233100	0.44284300
C	4.30066400	-1.61234900	0.30227700
H	4.90874100	-2.50204000	0.45613200
C	2.93995800	-1.73501600	0.12711900
H	2.46728100	-2.71512900	0.15388700
C	1.81211700	1.72628200	-0.27040800
C	4.19940100	0.82171100	0.12179600
H	4.69176900	1.79384700	0.12673900
Mg	-2.12618000	-0.77672500	0.41777100
Cl	-3.59999400	-2.01435000	-0.93318100
H	1.95261000	2.79960700	-0.28469900

Structure 7'-TSCO-I [B3LYP/6-31G(d)]

Cl	-3.68016700	-2.34149900	0.46752400
C	0.37847100	0.82751000	-0.38795600
C	-1.02944200	1.26153500	-0.52174000
O	-1.85993000	0.56174000	-1.26687200
O	-0.17684100	-1.60733100	-0.17868700
C	-0.09888300	-2.46953200	-1.33392200
H	-0.85487200	-3.24994500	-1.20276000
H	0.89780000	-2.91478200	-1.38606400
H	-0.29232800	-1.88975300	-2.24291800
Mg	-2.05192800	-0.78922800	0.10280000
C	-1.75056600	1.01797000	1.49325500
H	-1.99072400	0.07583400	2.04890000
H	-2.70399900	1.56247200	1.43347400
C	0.75874900	-0.52784400	-0.21738000
O	-1.14086000	2.63348200	-0.58645600
C	-2.38441500	3.12981400	-1.06014800
H	-2.28856100	4.21937700	-1.04854400
H	-2.59479600	2.78013900	-2.07510200
H	-3.21460500	2.82921700	-0.40946600
C	-0.72935300	1.76838400	2.33740300
H	0.21016400	1.20919300	2.40412700
H	-0.49381300	2.73256700	1.87411400
H	-1.08048300	1.96562400	3.36312000
C	2.14754200	-0.62011700	-0.03109400
C	2.64438100	0.75307200	-0.11315600
C	4.89934400	-0.08150700	0.22666200
H	5.96812900	0.10180500	0.32805400
C	4.40847100	-1.41074800	0.31927600
H	5.10730200	-2.22704700	0.49797800
C	3.05589100	-1.68162200	0.19365800
H	2.69420700	-2.70548200	0.28659000
C	1.54271600	1.61868200	-0.31283700
C	4.03247700	0.97924800	0.01593100
H	4.41914300	1.99709300	-0.04567800
H	1.57216400	2.69769100	-0.39892400

Structure 7'-TSCO-II [B3LYP/6-31G(d)]

Cl	-3.46834000	-2.48109000	0.31699500
C	0.46933900	0.87721800	-0.30147100
C	-0.95743300	1.25341300	-0.44933800
O	-1.72827700	0.56454400	-1.26762900
O	0.02173900	-1.58750900	-0.28037900
C	0.16857100	-2.35894900	-1.49041100
H	-0.55072200	-3.18226600	-1.43541500
H	1.18670800	-2.75243200	-1.54720500
H	-0.03176800	-1.72572500	-2.36148300
Mg	-1.89062300	-0.86472900	0.02759000
C	-1.58219300	0.82750600	1.53733200
H	-1.36083200	-0.13598800	2.05687900
C	0.90764000	-0.46784000	-0.21395800
O	-1.14044900	2.62307600	-0.43322300
C	-2.26837600	3.10824000	-1.15029500
H	-2.26061900	4.19225400	-1.00127500
H	-2.19226000	2.87942500	-2.21845400
H	-3.20895600	2.69228500	-0.77550400
C	2.28934500	-0.51044800	0.03615800
C	2.71968400	0.88655700	0.08282700
C	4.99524100	0.13135900	0.47083400
H	6.04790000	0.35538800	0.63836300
C	4.56707800	-1.22191600	0.44191300
H	5.29598000	-2.01671400	0.59569700
C	3.23642800	-1.54328100	0.22816100
H	2.92125300	-2.58663400	0.22597100
C	1.58628700	1.71365700	-0.10662500
H	-0.80524700	1.49663900	1.90466300
C	-2.97826300	1.32769500	1.91711800
H	-3.12646700	1.40983200	3.00653900
H	-3.14772600	2.32641000	1.49783000
H	-3.78329100	0.67708700	1.54457200
C	4.08795000	1.16474000	0.29504100
H	4.42738000	2.20072000	0.32672800
H	1.56603500	2.79641400	-0.11174800

Structure 7'-TSOMe-I [B3LYP/6-31G(d)]

Cl	-3.87879400	-2.21471500	-0.02044800
C	0.24304600	1.15785500	-0.14751300
C	-1.02486000	1.71519500	-0.12866900
O	-2.14445700	1.05900300	-0.04970600
O	-0.36876200	-1.17324700	-0.99095400
C	-0.07969100	-0.97275100	-2.38136500
H	-0.74128100	-1.64536400	-2.93534200
H	0.96663500	-1.22346500	-2.57439600
H	-0.26139900	0.06797600	-2.67052600
Mg	-2.03598500	-0.87316400	0.06407200
C	-0.30374100	-1.15627700	1.61622100
H	0.34835400	-2.03120600	1.56112400
H	-1.29849000	-1.58692400	1.91833000
C	0.44670200	-0.30418500	-0.06444300
O	-1.10585900	3.08451500	-0.16300200
C	-2.41168700	3.63979700	-0.14445800
H	-2.26981500	4.72342600	-0.19307100
H	-3.00925300	3.30631100	-1.00107800
H	-2.95379800	3.37928400	0.77180000
C	0.12045800	-0.18556200	2.70955400
H	1.14738500	0.15000400	2.53354100
H	-0.51515200	0.70945200	2.71742300
H	0.07649100	-0.63361700	3.71388000
C	1.87260600	-0.49590500	-0.08593800
C	2.50958400	0.82768600	-0.07118600
C	2.64395800	-1.67007400	-0.10161800
H	2.14706800	-2.64064800	-0.12780000
C	4.02861900	-1.59813200	-0.08523700
H	4.63216300	-2.50288300	-0.10157000
C	4.66266300	-0.31729400	-0.03493700
H	5.75203900	-0.27292000	-0.00443200
C	3.94338700	0.85554900	-0.01982100
H	4.46114400	1.81397500	0.02269700
C	1.54124600	1.81510000	-0.11967400
H	1.68810400	2.88654500	-0.06804000

Structure 7'-TSOMe-II [B3LYP/6-31G(d)]

Cl	3.82129700	-2.13418200	0.08769800
C	-0.24288800	1.28931700	-0.03805600
C	1.02221900	1.84561400	-0.04094500
O	2.14678900	1.19332700	0.06578400
O	0.34983400	-0.93689500	1.07119700
C	0.09701000	-0.56437600	2.43503200
H	0.75388700	-1.18712000	3.04976900
H	-0.95063500	-0.75958400	2.67665600
H	0.31497000	0.49721300	2.59039400
Mg	2.02252600	-0.73843200	-0.01085100
C	0.30975000	-1.04953700	-1.58319700

H	1.29471000	-0.80796900	-2.05602700
C	-0.45377700	-0.17283200	0.07617800
O	1.10552100	3.20847400	-0.20155200
C	2.41101900	3.76173100	-0.22321500
H	2.27086100	4.83896200	-0.35418700
H	2.95228500	3.57150800	0.71135000
H	3.01093800	3.36508800	-1.05066300
C	-1.88239700	-0.36204400	0.11306300
C	-2.50660400	0.93124400	-0.19115400
C	-2.66359400	-1.50079900	0.36383100
H	-2.17922500	-2.44017500	0.63114700
C	-4.04898200	-1.43053200	0.29281900
H	-4.66046200	-2.30581900	0.49940400
C	-4.66729300	-0.19211900	-0.06011000
H	-5.75486700	-0.15228500	-0.13454500
C	-3.93779000	0.94967900	-0.30168100
H	-4.44536900	1.87917300	-0.55978200
C	-1.53512100	1.91331400	-0.28400600
H	-0.39081700	-0.46133200	-2.17765300
C	0.02885100	-2.54471300	-1.71247800
H	0.79375200	-3.16174900	-1.22227100
H	-0.93696700	-2.78401900	-1.25440800
H	-0.02518600	-2.87543500	-2.76279800
H	-1.67981000	2.96287700	-0.50696100

Structure 9_I [B3LYP/6-31G(d)]

C	4.27054400	0.17375800	0.07036100
C	3.21643600	1.06053500	0.05710100
C	1.87591500	0.59170100	0.01858600
C	1.64484400	-0.81917500	-0.00581800
C	2.75248200	-1.70850200	0.00840200
C	4.04040700	-1.22432900	0.04559100
H	0.95959000	2.53786100	0.00474400
H	5.29078900	0.54732100	0.10003400
H	3.39878600	2.13244300	0.07568900
C	0.76370500	1.47194100	-0.00171300
C	0.30776500	-1.27639300	-0.04200200
H	2.56283300	-2.77899300	-0.01085500
H	4.88347500	-1.90929500	0.05611600
C	-0.77722500	-0.41938100	-0.04684900
C	-0.53640700	0.99974000	-0.03536900
H	0.10431400	-2.34239500	-0.06529000
C	-2.11487400	-1.09228300	-0.06611200
O	-3.15531800	-0.28025100	0.20093100
O	-2.25286300	-2.28451700	-0.27603500
C	-4.43797000	-0.92388300	0.20666100
H	-4.64976500	-1.37266600	-0.76761800
H	-4.47457900	-1.70599400	0.96997800
H	-5.15608400	-0.13420900	0.43048700
O	-1.62300400	1.81211500	-0.07881200
C	-1.42144100	3.21618600	-0.08943000
H	-0.90929300	3.55683500	0.81990900
H	-0.84637100	3.53459200	-0.96885400
H	-2.41929600	3.65624500	-0.12946700

Structure 9_II [B3LYP/6-31G(d)]

C	-4.20092600	-0.26283300	0.00024500
C	-3.28151300	0.76285900	0.02114700
C	-1.88766600	0.48853000	0.00792200
C	-1.45983300	-0.87540100	-0.02738200
C	-2.43163100	-1.91083700	-0.04871800
C	-3.77583700	-1.61376700	-0.03484700
H	-1.25618200	2.54581300	0.07541100
H	-5.26388700	-0.03638800	0.01036600
H	-3.61328100	1.79813100	0.04820000
C	-0.91210700	1.51872000	0.03407000
C	-0.06947100	-1.14276900	-0.04225300
H	-2.09356700	-2.94413600	-0.07580800
H	-4.51360600	-2.41095000	-0.05093000
C	0.87869100	-0.13750000	-0.03350300
C	0.44046700	1.23241700	0.01459600
H	0.26619600	-2.17369100	-0.07058500
C	2.32799400	-0.48727500	-0.12028700
O	2.54996600	-1.76624600	0.29239600
O	3.21993500	0.22929800	-0.52026100
C	3.90881700	-2.20885900	0.17653500
H	4.24367100	-2.16679500	-0.86381900
H	4.57022600	-1.58500600	0.78384400
H	3.91274900	-3.23753200	0.53936200
O	1.41236400	2.17432200	0.06718200
C	1.03305300	3.53963800	0.12858300
H	0.45537200	3.83619500	-0.75659300
H	0.44688000	3.75506500	1.03183800
H	1.96708800	4.10277800	0.15752800

Structure 9·EtMgCl_I [B3LYP/6-31G(d)]

Cl	-4.13435000	-0.99126100	-1.38080000
C	0.59824300	0.76364500	-0.27115200
C	1.85192300	1.29294200	-0.00741800
C	3.00387200	0.48433000	0.10452400
C	2.86307200	-0.92797300	-0.07530100
C	1.58001000	-1.46515800	-0.35823500
C	-0.56451700	1.67450600	-0.34589200
O	-1.74639300	1.34477400	-0.22065100
O	-0.77932100	-1.14770200	-0.74866900
C	-0.88148500	-2.47420300	-1.31338300
H	1.94781200	2.36525800	0.12231500
H	-1.91789700	-2.55840200	-1.64108300
H	-0.65423000	-3.23139900	-0.55658100
H	-0.19940900	-2.56297200	-2.16355400
Mg	-2.64796800	-0.44988600	0.28669600
C	-2.47390500	-0.88587900	2.35953500
C	0.46900200	-0.65693500	-0.45082300
O	-0.22892500	2.94665500	-0.55230200
C	-1.31268000	3.90265500	-0.57993600
H	-0.83520700	4.86367800	-0.76682900
H	-2.01354100	3.65229400	-1.37861200
H	-1.83633100	3.90731700	0.37859800
H	-1.49625400	-0.53690600	2.73637000
H	1.49098700	-2.53623800	-0.49390900
C	4.01638500	-1.74773100	0.03713100
H	3.91520400	-2.82162200	-0.09626200
C	5.24567900	-1.19124800	0.31358100
H	6.12045600	-1.82991200	0.39851600
C	5.38527500	0.20818300	0.49018300
H	6.36304200	0.62775400	0.70743500
C	4.28599600	1.02863000	0.38798500
H	4.38128100	2.10305100	0.52292200
C	-3.57976200	-0.31859000	3.27419100
H	-3.62323900	0.77953300	3.23273600
H	-4.57444700	-0.67969000	2.97997400
H	-3.45141800	-0.58437900	4.33705400
H	-2.44277300	-1.98015800	2.49720200

Structure 9·EtMgCl_II [B3LYP/6-31G(d)]

Cl	-4.30539600	-1.07850000	-1.13196300
C	0.46244400	0.74476600	-0.30574700
C	1.72634400	1.29018800	-0.14231600
C	2.88973700	0.49329600	-0.07597200
C	2.74946800	-0.92537500	-0.19474400
C	1.45505500	-1.47998500	-0.37272600
C	-0.70868300	1.64682200	-0.34168400
O	-1.88090200	1.31398600	-0.15056800
O	-0.92657000	-1.19367300	-0.62062400
C	-1.04993000	-2.53936000	-1.13393000
H	1.82161400	2.36700000	-0.05816500
H	-2.10228200	-2.64123600	-1.40007700
H	-0.77374400	-3.26913100	-0.36652100
H	-0.41647100	-2.65247900	-2.01807000
Mg	-2.76495300	-0.45471900	0.45449700
C	-2.55777300	-0.77246300	2.54599900
C	0.33347400	-0.68246800	-0.42363800
O	-0.39306800	2.91576500	-0.59478200
C	-1.48352600	3.86417600	-0.59161600
H	-1.02250300	4.82352100	-0.82315000
H	-2.22031900	3.59154200	-1.34968300
H	-1.96026800	3.88772200	0.39078100
H	-2.50986000	-1.85566400	2.74925900
H	1.36607700	-2.55600000	-0.46101100
C	3.91448700	-1.73347400	-0.12875900
H	3.81389300	-2.81215200	-0.21603900
C	5.15453700	-1.15969400	0.04564500
H	6.03841400	-1.78946300	0.09570600
C	5.29350800	0.24607100	0.16193500
H	6.27982900	0.67930400	0.29890200
C	4.18295700	1.05548600	0.10263700
H	4.27778400	2.13472400	0.19161500
C	-1.36504100	-0.09027700	3.24590800
H	-0.40086300	-0.41583500	2.82803300
H	-1.39692800	1.00386700	3.13613000
H	-1.31430000	-0.28942600	4.32966300
H	-3.48692900	-0.45003700	3.04386000

Structure 9·EtMgCl_III [B3LYP/6-31G(d)]

Cl	-4.33339800	-0.52463000	-1.20826500
C	0.50928700	0.89402500	-0.11935000
C	1.79111200	1.34874400	0.14776900
C	2.92269500	0.50915600	0.05836400
C	2.72904000	-0.85297800	-0.33409800
C	1.41654300	-1.31137300	-0.62100200
C	-0.62844800	1.82666900	0.02987300
O	-1.80730800	1.50335600	0.19492000
O	-0.94980900	-0.88247200	-0.81717900
C	-1.12617200	-2.10480000	-1.56797500
H	1.92630000	2.38375600	0.44178700
H	-2.17839700	-2.10597900	-1.85360800
H	-0.89539400	-2.97231400	-0.94264700
H	-0.48655700	-2.08516700	-2.45477800
Mg	-2.73566200	-0.33108800	0.43165900
C	-2.44976600	-1.18237000	2.35948700
C	0.32701500	-0.47549400	-0.51666600
O	-0.27180600	3.10900300	-0.00897000
C	-1.32692000	4.07735700	0.18720900
H	-0.83592300	5.04690900	0.11411700
H	-2.08784300	3.96509100	-0.58756600
H	-1.78335900	3.94426200	1.17050100
H	1.28759200	-2.34470900	-0.91962100
C	3.86178700	-1.70370200	-0.42360200
H	3.72088800	-2.74012700	-0.71884800
C	5.12104800	-1.22401100	-0.13823100
H	5.97956100	-1.88603700	-0.20913000
C	5.31283300	0.12603300	0.24864100
H	6.31364800	0.48520400	0.46919100
C	4.23468200	0.97465800	0.34539900
H	4.36965200	2.01151100	0.64272900
H	-3.42326300	-1.25787500	2.86975700
H	-1.85846600	-0.50263100	2.99690000
C	-1.78191400	-2.57367800	2.38392200
H	-2.36741800	-3.31671200	1.82353800
H	-0.77883900	-2.55664400	1.93061400
H	-1.65203800	-2.98528500	3.39904900

Structure 9-TSOMe-I [B3LYP/6-31G(d)]

Cl	-4.65153400	-1.40738300	0.02332000
C	0.24217800	0.79172600	-0.18394600
C	1.53144300	1.32678100	-0.10030900
C	2.67582600	0.52303500	-0.06272300
C	2.50089100	-0.91066100	-0.12688400
C	1.21619200	-1.45233300	-0.23270500
C	-0.90799100	1.66638300	-0.12056700
O	-2.09526400	1.27202100	0.00372000
O	-1.03725600	-1.16214600	-1.05642000
C	-0.79490200	-1.06776700	-2.47448100
H	1.64042300	2.40592000	-0.05510000
H	-1.67195800	-1.50058700	-2.95869200
H	0.10125000	-1.63733400	-2.73165200
H	-0.66887400	-0.02403000	-2.78041700
Mg	-2.54446400	-0.66555500	0.15532600
C	-0.92353400	-1.27439000	1.64845700
H	-0.57678500	-2.30687100	1.54659100
H	-1.96350400	-1.36827500	2.05845600
C	0.04318200	-0.65955900	-0.19334800
O	-0.65427600	2.97605800	-0.17766700
C	-1.78168700	3.86579900	-0.06783800
H	-1.36032500	4.86726600	-0.15160300
H	-2.49685400	3.67905500	-0.87216800
H	-2.27897200	3.73660600	0.89632700
C	-0.11740800	-0.49311700	2.67494300
H	-0.19649100	-0.92161300	3.68344900
H	0.94514600	-0.48357600	2.40878700
H	-0.45021700	0.55126300	2.74342000
H	1.09529800	-2.52871600	-0.32420600
C	3.67873800	-1.72504800	-0.11326600
H	3.56547100	-2.80511800	-0.16470400
C	4.92522000	-1.15977900	-0.03088400
H	5.80500000	-1.79832900	-0.01754200
C	5.09233100	0.25452700	0.04264600
H	6.09089700	0.67587900	0.11023800
C	3.99037800	1.06978500	0.02629700
H	4.09936300	2.15088200	0.07905700

Structure 9-TSOMe-II [B3LYP/6-31G(d)]

Cl	4.61471100	-1.22297700	-0.02694200
C	-0.30603500	0.92146100	0.06770500
C	-1.60297100	1.39533000	-0.14476600
C	-2.72313800	0.55571900	-0.12050900
C	-2.51639500	-0.84375100	0.17713300
C	-1.22427900	-1.32351500	0.41125200
C	0.82058900	1.81746400	-0.05534700
O	2.02274600	1.44874400	-0.10153200
O	1.02330000	-0.88680700	1.16018200
C	0.78619700	-0.61999800	2.55674100
H	-1.74086700	2.45478200	-0.33782200
H	1.67428100	-0.97175000	3.08468000
H	-0.09743000	-1.16904400	2.88994400
H	0.64064000	0.45136300	2.72948900
Mg	2.50446200	-0.48963100	-0.11748100
C	0.88353500	-1.21696100	-1.54907600
H	1.76057000	-0.81637500	-2.11639500
C	-0.06997200	-0.51682400	0.24785100
O	0.53013900	3.11824100	-0.14344500
C	1.63495100	4.02445200	-0.32216400
H	1.18367700	5.01556800	-0.36246800
H	2.33050000	3.95113900	0.51699300
H	2.16494300	3.80470300	-1.25199500
H	-1.08264800	-2.36367900	0.68962000
C	-3.67388100	-1.68298300	0.25464300
H	-3.53793300	-2.73717000	0.48329200
C	-4.92896700	-1.17575400	0.03529200
H	-5.79199900	-1.83450600	0.09218400
C	-5.12631200	0.20244500	-0.27211200
H	-6.13066200	0.57774700	-0.44426400
C	-4.04484400	1.04219900	-0.34453800
H	-4.17686900	2.09783900	-0.57198500
H	0.03008000	-0.81071700	-2.09232900
C	0.91222900	-2.74200200	-1.59704000
H	0.06535000	-3.16365600	-1.04250000
H	0.83924800	-3.12588400	-2.62445400
H	1.83178200	-3.15929400	-1.16623900

Structure 9-TSCO-I [B3LYP/6-31G(d)]

Cl	-4.47170800	-1.60146400	-0.05516200
C	0.33163100	0.52433100	-0.29431900
C	1.55618700	1.15753100	-0.24220900
C	2.77843600	0.44605700	-0.13290800
C	2.73735700	-0.98016500	-0.07253700
C	-0.92908200	1.31932300	-0.49240500
O	-1.81103800	0.93264000	-1.35358900
O	-0.93844300	-1.51732500	-0.21553200
C	-1.01740100	-2.95658800	-0.20731100
H	1.58119400	2.23966000	-0.30168300
H	-2.08171500	-3.18936300	-0.24334100
H	-0.57436200	-3.35385300	0.71063500
H	-0.50648600	-3.36079500	-1.08563900
Mg	-2.64071100	-0.30040800	-0.09729000
C	-1.90278400	1.02132400	1.57004000
C	0.31209300	-0.90705900	-0.21508800
O	-0.70481100	2.64478000	-0.33036700
C	-1.71820500	3.52433000	-0.83352600
H	-1.35145700	4.53087300	-0.62834800
H	-1.86299500	3.37598400	-1.90566400
H	-2.66744600	3.35935500	-0.31476700
C	1.47411300	-1.63188300	-0.10889300
H	1.45439400	-2.71326900	-0.04674900
C	3.95602100	-1.69940300	0.02881800
H	3.92542900	-2.78534100	0.07523600
C	5.16157700	-1.03283500	0.06801200
H	6.08864800	-1.59414500	0.14561200
C	5.20352800	0.38095800	0.00746800
H	6.16134700	0.89240500	0.03905000
C	4.03559400	1.10421600	-0.09116900
H	4.05973200	2.19009400	-0.13865000
H	-2.58161300	0.25657500	2.01721200
C	-0.73484600	1.19905900	2.53307000
H	-1.06305600	1.47455400	3.54589900
H	-0.14053200	0.28148000	2.62631300
H	-0.06077600	1.99076100	2.18708500
H	-2.50372800	1.93889100	1.51667900

Structure 9-TSCO-II [B3LYP/6-31G(d)]

Cl	-4.28849800	-1.79968400	-0.05223700
C	0.42732000	0.50674300	-0.26149200
C	1.61827600	1.19349600	-0.15231000
C	2.86612100	0.53530400	-0.00273100

C	2.88719800	-0.89232600	0.03555900
C	-0.86550100	1.24740200	-0.48373800
O	-1.71023700	0.82666400	-1.36702100
O	-0.75225300	-1.59052500	-0.26965300
C	-0.76855200	-3.03064300	-0.28215200
H	1.59559500	2.27666500	-0.19191700
H	-1.81970700	-3.30889300	-0.35957300
H	-0.34297800	-3.42276900	0.64643300
H	-0.20889700	-3.40061500	-1.14583500
Mg	-2.50567900	-0.43719300	-0.11636800
C	-1.73956400	0.81263900	1.58212700
C	0.46876700	-0.92591400	-0.20501500
O	-0.70913800	2.58453100	-0.31880000
C	-1.64418600	3.42481100	-1.01209500
H	-1.55911500	3.28572700	-2.09262400
H	-2.67108400	3.21608800	-0.70447600
H	-1.36834200	4.44317200	-0.73447400
C	1.65745800	-1.59942500	-0.06366200
H	1.68450300	-2.68163800	-0.02013000
C	4.13202400	-1.55787400	0.17784200
H	4.14864700	-2.64472400	0.20771000
C	5.30365300	-0.83908500	0.27720100
H	6.25111500	-1.35969400	0.38606500
C	5.28403400	0.57593100	0.23833100
H	6.21558200	1.12911300	0.31742900
C	4.08960200	1.24782800	0.10087000
H	4.06658200	2.33434900	0.06979500
H	-0.81058000	1.22728500	1.97293500
C	-2.92736700	1.71313800	1.94376200
H	-2.78567300	2.72353400	1.54480800
H	-3.88896200	1.34154700	1.55824800
H	-3.05700700	1.81675700	3.03164800
H	-1.83972600	-0.17248000	2.08720100

Structure 9-intOMe-I [B3LYP/6-31G(d)]

Cl	-4.87525100	1.33507200	0.73809400
C	0.80986900	0.50116000	0.07726700
C	1.93572100	1.27491200	-0.18027700
C	3.23619300	0.73012200	-0.17604900
C	3.37996800	-0.66206600	0.11117700
C	2.21723400	-1.42984300	0.38267400
C	-0.50144000	1.17638000	-0.00059700
O	-1.59184600	0.59279200	-0.04492600
O	-3.29619200	-1.77213300	-0.96750100
C	-3.98712200	-2.86400600	-1.47713400
H	1.81403700	2.32952400	-0.40017100
H	-3.75082300	-3.79045600	-0.92303000
H	-3.72374600	-3.05352600	-2.53310200
H	-5.08508600	-2.74557200	-1.44077200
Mg	-3.43844000	-0.14993200	-0.16415000
C	-0.25525500	-1.78959800	0.70398600
H	-0.94285700	-1.82593500	-0.14969400
H	-0.82778000	-1.30727800	1.50840200
C	0.93930600	-0.90811200	0.37576300
O	-0.43431600	2.50338100	-0.03785000
C	-1.67304400	3.23772100	-0.18401900
H	-1.39120600	4.28402800	-0.07367800
H	-2.09470800	3.05963300	-1.17680700
H	-2.39571600	2.94011500	0.57725600
C	0.06341000	-3.22558900	1.13127100
H	-0.87180400	-3.74616900	1.35968900
H	0.56213100	-3.78891900	0.33446500
H	0.69627800	-3.26492500	2.02561100
H	2.35938300	-2.48069000	0.60967700
C	4.68318400	-1.22506000	0.12029400
H	4.79779200	-2.28374000	0.33874000
C	5.78566500	-0.44249600	-0.14327600
H	6.77821500	-0.88449200	-0.13356300
C	5.64142900	0.93904300	-0.42887900
H	6.52270000	1.53980800	-0.63427400
C	4.39189300	1.51365100	-0.44569400
H	4.27049900	2.57191900	-0.66337400

Structure 9-intOMe-II [B3LYP/6-31G(d)]

Cl	4.10654600	-2.10282500	-1.01448400
C	-0.88374900	0.27124900	-0.21952300
C	-1.98236100	1.12440800	-0.24592100
C	-3.30248900	0.65576100	-0.08438800
C	-3.50351700	-0.74623600	0.11094200
C	-2.36903000	-1.59617800	0.13605400
C	0.45034400	0.87506600	-0.43305300
O	1.49472800	0.21921500	-0.58052600
O	3.94072200	1.28207500	0.85931000
C	5.02546100	1.73487700	1.60954700
H	-1.82379900	2.18525600	-0.40248000
H	4.72923400	1.96832600	2.64711800
H	5.45347500	2.66068900	1.18567500
H	5.85039100	1.00379600	1.67022500
Mg	3.40581400	-0.16159700	-0.13605300
C	0.04893900	-2.16281000	0.07597700
C	-1.07263100	-1.14583600	-0.01898300
O	0.44631500	2.19796900	-0.48315300
C	1.70006500	2.88576700	-0.73647500
H	1.45785000	3.94210300	-0.62417100
H	2.46948100	2.56698400	-0.02372300
H	2.02028300	2.68169300	-1.76269200
H	-2.53451400	-2.66056900	0.28708000
C	-4.82818500	-1.23155500	0.27026800
H	-4.98437100	-2.29703900	0.41843300
C	-5.89840000	-0.36547800	0.23767000
H	-6.90811100	-0.74745100	0.36079300
C	-5.69879400	1.02531100	0.04340000
H	-6.55581200	1.69217000	0.02008000
C	-4.42756300	1.52564900	-0.11485800
H	-4.26477400	2.59007500	-0.26467000
H	0.78149600	-2.01637100	-0.71985900
C	0.76322700	-2.15767000	1.44129200
H	0.07281900	-2.42972300	2.24744200
H	1.59018600	-2.87539300	1.43759800
H	1.17037100	-1.16936800	1.68555400
H	-0.38726800	-3.15598300	-0.08027300

Structure 9-intOMe-III [B3LYP/6-31G(d)]

Cl	4.60731500	1.19564700	-1.36292500
C	-0.88379500	0.38127400	-0.14850900
C	-1.96359000	1.10731900	0.34311600
C	-3.28447000	0.61773100	0.28275100
C	-3.50608800	-0.65877100	-0.32319000
C	-2.39152100	-1.36809500	-0.83658200
C	0.45994500	0.97402900	0.01201400
O	1.51757500	0.33874800	-0.07934900
O	3.60725300	-1.36610900	1.36768900
C	4.41813600	-2.21447400	2.10776500
H	-1.78814000	2.07576300	0.79786700
H	4.21349800	-3.27649400	1.88140500
H	4.25337200	-2.08743600	3.19267600
H	5.49704700	-2.05434300	1.93034200
Mg	3.46079000	-0.12414300	0.06131700
C	0.00207600	-1.77443700	-1.35665600
H	0.79384100	-1.15948600	-1.79185800
C	-1.09246300	-0.90367000	-0.76580600
O	0.45005200	2.27454700	0.28681600
C	1.71735100	2.92853300	0.52394500
H	1.47045900	3.98262100	0.64385100
H	2.16882700	2.54257400	1.44310300
H	2.39473900	2.78037200	-0.31995200
H	-2.57471700	-2.32813600	-1.31462900
C	-4.83250100	-1.16104800	-0.39393200
H	-5.00420600	-2.13061900	-0.85439800
C	-5.88401900	-0.43191700	0.11455700
H	-6.89477300	-0.82631500	0.05663300
C	-5.66370600	0.83385900	0.71591800
H	-6.50637000	1.39415500	1.11049300
C	-4.39102300	1.34803700	0.79823700
H	-4.21310200	2.31751000	1.25690500
H	-0.44239400	-2.33790800	-2.18575200
C	0.60969400	-2.77610100	-0.35466800
H	-0.17279900	-3.40401800	0.08653100
H	1.31683500	-3.43586900	-0.87046000
H	1.15084800	-2.27975200	0.45615100

Structure 9-intCO-I [B3LYP/6-31G(d)]

Cl	-4.32537900	-2.17820100	-0.72794500
C	0.28145600	0.57341200	-0.02682000
C	1.54707600	1.03324900	-0.32843600
C	2.69987500	0.20564100	-0.31447200
C	2.55397300	-1.17194500	0.02924300
C	-0.93672300	1.53163800	-0.03875900
O	-1.98421800	1.01326500	-0.76633400
O	-1.12424700	-1.32411900	0.58693100
C	-1.22591100	-2.53913900	1.36122500
H	1.65379100	2.07963400	-0.58758600

H	-2.28296000	-2.65405300	1.60208800
H	-0.62685900	-2.44005400	2.26986200
H	-0.89697500	-3.40213000	0.77656400
Mg	-2.70663800	-0.66042000	-0.55619800
C	-1.39294400	1.85129600	1.41666200
C	0.16834000	-0.81445300	0.30424700
O	-0.44404600	2.73046300	-0.65312600
C	-1.42876000	3.68625000	-1.00966500
H	-0.90947400	4.44959700	-1.59574900
H	-2.22145600	3.23454800	-1.61308100
H	-1.87931300	4.16950000	-0.12984100
C	1.25477100	-1.65676500	0.33171600
H	1.14377600	-2.70788800	0.57229500
C	3.70189800	-2.00712900	0.04797600
H	3.58755900	-3.05687900	0.30837600
C	4.94276200	-1.49551200	-0.26097600
H	5.81595300	-2.14201800	-0.24464300
C	5.09070600	-0.12834000	-0.60101000
H	6.07577900	0.26123900	-0.84233000
C	3.99306200	0.70281700	-0.62712000
H	4.09964700	1.75262200	-0.88866000
H	-1.65804900	0.90422400	1.90617700
C	-0.38017500	2.61240500	2.27534300
H	-0.78589000	2.80429700	3.27530200
H	0.55086300	2.04710000	2.39399000
H	-0.12632300	3.57418700	1.81956400
H	-2.32532500	2.42309900	1.33242600

Structure 9-intCO-II [B3LYP/6-31G(d)]

Cl	-4.25891000	-2.16149300	-0.83076600
C	0.32476200	0.58476400	0.10004500
C	1.59045700	1.10789400	-0.07046600
C	2.76925700	0.31901000	-0.09361700
C	2.65073200	-1.09297900	0.07781700
C	-0.90460700	1.54902300	0.15127000
O	-1.97744200	1.05418100	-0.54673300
O	-1.03664600	-1.40609200	0.48843200
C	-1.11078400	-2.70436000	1.11847000
H	1.67452500	2.18381500	-0.18190200
H	-2.16629500	-2.87503500	1.33194000
H	-0.52330600	-2.69422700	2.03989900
H	-0.75221300	-3.48514000	0.44275400
Mg	-2.66542500	-0.64359800	-0.50232600
C	-1.24516000	1.84264500	1.63569000
C	0.24382300	-0.83238900	0.28387900
O	-0.50393700	2.82260900	-0.37220600
C	-0.54706300	2.94614100	-1.78665400
H	0.11469200	2.22315600	-2.28613000
H	-1.56318200	2.81582300	-2.16951400
H	-0.19646100	3.95816400	-2.00842400
C	1.35581100	-1.64208000	0.26753300
H	1.27070100	-2.71502100	0.39579500
C	3.82214700	-1.89481600	0.05383500
H	3.72898700	-2.97076500	0.18214300
C	5.05929400	-1.31814900	-0.12999700
H	5.95065800	-1.93927400	-0.14736700
C	5.17994400	0.08351800	-0.29640800
H	6.16256600	0.52447300	-0.43915500
C	4.05933200	0.88359300	-0.27833100
H	4.14574100	1.95978600	-0.40618600
H	-0.36124900	2.28808600	2.10760700
C	-2.45603700	2.76155200	1.80768500
H	-2.26812700	3.73136600	1.33909800
H	-3.34705100	2.33088700	1.33985700
H	-2.67034900	2.92507900	2.87005900
H	-1.42031400	0.88158200	2.14001500

Structure 9-intCO-III [B3LYP/6-31G(d)]

Cl	-4.37673300	-1.96105400	-0.86529800
C	0.33917300	0.62292400	0.02230400
C	1.61842000	1.12258300	-0.13826500
C	2.78073300	0.31319000	-0.18024500
C	2.63600500	-1.09993700	-0.05001500
C	-0.85060500	1.62895500	0.08909500
O	-2.00685100	1.15940000	-0.46676400
O	-1.05506300	-1.37474800	0.31244100
C	-1.14670900	-2.69590800	0.88964600
H	1.72740400	2.19511300	-0.24615000
H	-2.20600700	-2.86594400	1.08499800
H	-0.57000100	-2.72807400	1.81729600
H	-0.78728000	-3.45248700	0.18745200

Mg	-2.71013400	-0.52418600	-0.53093400
C	-1.07233900	2.09974300	1.55671100
C	0.23033500	-0.79891300	0.15190700
O	-0.36114600	2.76573600	-0.65637500
C	-1.32818600	3.73092000	-1.03125600
H	-2.16119100	3.27589500	-1.57538700
H	-1.72834200	4.28629800	-0.17005500
H	-0.80674800	4.43685000	-1.68413200
C	1.33022800	-1.62678100	0.11145200
H	1.22220600	-2.70185200	0.19338400
C	3.79275700	-1.92284700	-0.09273400
H	3.67929300	-3.00016100	0.00415400
C	5.04033100	-1.36373400	-0.25637700
H	5.92049000	-2.00013600	-0.28845300
C	5.18717600	0.04010900	-0.38431100
H	6.17821100	0.46631600	-0.51306600
C	4.08168600	0.85955800	-0.34724500
H	4.18730500	1.93699100	-0.44678300
H	-0.13881200	2.55265200	1.91055000
C	-1.53712600	1.03100900	2.54781500
H	-1.69729400	1.47099200	3.53851500
H	-2.49174900	0.58641700	2.23863800
H	-0.80232200	0.22576100	2.66358100
H	-1.82587500	2.89517900	1.52140700

Structure 9·iPrMgCl_I [B3LYP/6-31G(d)]

Cl	-3.97576900	-0.84787000	-1.78206900
C	0.68528500	0.79767400	-0.33068800
C	1.93533500	1.31568800	-0.02890700
C	3.08680400	0.50428200	0.06339600
C	2.94955400	-0.89939700	-0.17554900
C	1.67068000	-1.42467400	-0.49720000
C	-0.47597100	1.71133900	-0.37682800
O	-1.66029000	1.37548400	-0.29464400
O	-0.68251200	-1.09631700	-0.90941000
C	-0.76727000	-2.39892100	-1.53082300
H	2.02820900	2.38142000	0.14807800
H	-1.79274200	-2.46977900	-1.89416600
H	-0.56040900	-3.18549200	-0.79863500
H	-0.06181400	-2.45323700	-2.36452500
Mg	-2.61734500	-0.42472600	0.02255100
C	-2.68203000	-0.98170700	2.08887900
C	0.55988200	-0.61416400	-0.57222800
O	-0.13885400	2.99312000	-0.50284600
C	-1.22309000	3.94911200	-0.50156900
H	-0.74298200	4.91856100	-0.62847000
H	-1.90791900	3.74092700	-1.32583400
H	-1.76492200	3.90363700	0.44571400
H	1.58536100	-2.48929500	-0.67790700
C	4.10189800	-1.72268500	-0.08197700
H	4.00347600	-2.79028800	-0.26028700
C	5.32714200	-1.17725400	0.23219600
H	6.20138400	-1.81846700	0.30206500
C	5.46335500	0.21390500	0.46705700
H	6.43799700	0.62463400	0.71326000
C	4.36467000	1.03738900	0.38472900
H	4.45707400	2.10542400	0.56468000
C	-3.79696200	-0.24966500	2.86001400
H	-3.63489400	0.83934200	2.88210700
H	-4.78692300	-0.41482900	2.41377800
H	-3.86407700	-0.56951400	3.91683600
H	-2.93716200	-2.05619600	2.11557400
C	-1.34396700	-0.82670600	2.83403900
H	-0.53964400	-1.42596800	2.38286400
H	-0.99418300	0.21782400	2.84193300
H	-1.40825200	-1.13180000	3.89542200

Structure 9·iPrMgCl_II [B3LYP/6-31G(d)]

Cl	-4.17045700	-0.47807800	-1.60595800
C	0.63024500	0.88926400	-0.24472300
C	1.90729200	1.32508200	0.07373200
C	3.03015800	0.47086700	0.02652400
C	2.83378500	-0.88792900	-0.37548100
C	1.52696100	-1.32826500	-0.71181500
C	-0.49718700	1.84054900	-0.14546200
O	-1.69073600	1.53756800	-0.06915400
O	-0.82436500	-0.87381100	-0.99576800
C	-0.98091800	-2.09062700	-1.76123600
H	2.04497400	2.35765900	0.37456500
H	-2.01928700	-2.07925300	-2.09343800
H	-0.78676800	-2.96442500	-1.13204400

H	-0.30267100	-2.07274600	-2.61873900
Mg	-2.67460600	-0.26681300	0.12397500
C	-2.57416700	-1.04266500	2.11758200
C	0.44529900	-0.47823700	-0.64908100
O	-0.11597500	3.11613400	-0.12851100
C	-1.16341400	4.10047800	0.02331200
H	-0.65081100	5.06139400	0.00553400
H	-1.87496600	4.02181700	-0.80094800
H	-1.68399800	3.95376000	0.97214300
H	1.39595600	-2.36005500	-1.01473400
C	3.95761600	-1.75352100	-0.42382500
H	3.81440800	-2.78753100	-0.72634700
C	5.21138500	-1.29073800	-0.09028300
H	6.06329100	-1.96378700	-0.13027800
C	5.40606400	0.05607900	0.30629700
H	6.40249200	0.40167400	0.56502700
C	4.33629300	0.91873700	0.36401800
H	4.47341900	1.95325300	0.66831100
C	-1.62973600	-0.26400700	3.05104600
H	-1.91452800	0.79400100	3.14289700
H	-1.60695500	-0.67650400	4.07721600
H	-0.58711200	-0.28360100	2.69564800
H	-3.58971900	-0.94343900	2.53826100
C	-2.22996700	-2.54362900	2.15919600
H	-2.22190500	-2.95159300	3.18736100
H	-2.94403100	-3.14946400	1.58413500
H	-1.22837500	-2.74984400	1.74765800

Structure 9·iPrMgCl_III [B3LYP/6-31G(d)]

Cl	-4.04963500	-0.27639200	-1.71797400
C	0.74454200	0.92892500	-0.16515800
C	2.01141100	1.30711100	0.25140600
C	3.11620400	0.42979600	0.19658900
C	2.91268700	-0.88865100	-0.32034600
C	1.61674900	-1.26837400	-0.75783800
C	-0.36807800	1.89593500	-0.04873200
O	-1.56879900	1.61252100	-0.02885600
O	-0.70640200	-0.72978500	-1.12418300
C	-0.85307500	-1.87412900	-1.99550800
H	2.15506500	2.31016400	0.63757200
H	-1.87627200	-1.81149200	-2.36655500
H	-0.70406900	-2.80189400	-1.43504900
H	-0.13738600	-1.79999600	-2.81888100
Mg	-2.55929000	-0.20514500	0.02769300
C	-2.40543000	-1.12924600	1.95346500
C	0.55230700	-0.39805700	-0.68357700
O	0.03659800	3.16009200	0.05655200
C	-0.99675800	4.15547200	0.23228000
H	-0.46601500	5.10507900	0.28700600
H	-1.68201400	4.13888700	-0.61739400
H	-1.55128400	3.96497400	1.15378000
H	1.47911400	-2.26980900	-1.14749000
C	4.01848300	-1.77668800	-0.37717900
H	3.86930200	-2.78046200	-0.76628300
C	5.26201100	-1.37353000	0.05691100
H	6.09998600	-2.06336200	0.00937300
C	5.46386800	-0.06673200	0.56736500
H	6.45203100	0.23205200	0.90428400
C	4.41155900	0.81636500	0.63595100
H	4.55454800	1.82060700	1.02670100
H	-1.56677300	-0.63517000	2.47924000
C	-2.05056400	-2.62638700	1.87474300
H	-2.82428900	-3.20349700	1.34685600
H	-1.10111300	-2.80366800	1.34653300
H	-1.94701900	-3.09372800	2.87211000
C	-3.65410900	-0.93655400	2.83344900
H	-4.54979100	-1.37738600	2.37292900
H	-3.55144100	-1.41010700	3.82806800
H	-3.87933200	0.12505200	3.00942400

Structure 9'-TSOMe-I [B3LYP/6-31G(d)]

Cl	-4.64224700	-1.12196100	-0.28924800
C	0.30891000	0.94752100	-0.11940100
C	1.61059500	1.42741300	0.04915700
C	2.73364300	0.59512400	-0.02163900
C	2.52193900	-0.80577300	-0.30545200
C	1.22267000	-1.29055000	-0.49529600
C	-0.81398000	1.84441300	0.03652600
O	-2.01715500	1.47893900	0.07782800
O	-1.01409500	-0.83189900	-1.26398200
C	-0.75478000	-0.54422000	-2.65316900
H	1.74934900	2.48608500	0.24562100
H	-1.64046000	-0.87363300	-3.19930700
H	0.12535800	-1.10020300	-2.98414700
H	-0.59143400	0.52787700	-2.80424700
Mg	-2.52645000	-0.44299600	-0.03415700
C	-0.98630800	-1.28901600	1.46731100
H	-2.00596900	-1.03540800	1.86078100
C	0.06834400	-0.48609800	-0.32720200
O	-0.51950800	3.14105300	0.16168300
C	-1.62170300	4.04639400	0.36023200
H	-1.16727000	5.03482600	0.42393000
H	-2.31664900	3.99452700	-0.48103000
H	-2.15310400	3.80686800	1.28431800
C	-0.02594500	-0.74914900	2.51361000
H	-0.19839900	-1.20703200	3.49894800
H	1.01140200	-0.96685200	2.23209900
H	-0.11747300	0.33651700	2.63782000
H	1.08182200	-2.32639200	-0.78945600
C	3.67839200	-1.64129300	-0.42327400
H	3.53803500	-2.69676300	-0.64332100
C	4.93904200	-1.12841700	-0.25337000
H	5.80197100	-1.78389100	-0.34102200
C	5.14195700	0.25139600	0.04209100
H	6.15049100	0.63110700	0.17591900
C	4.06060900	1.08738600	0.15234200
H	4.19690100	2.14402100	0.37246300
C	-0.93271500	-2.80692200	1.33161900
H	0.04017300	-3.12640400	0.93919400
H	-1.05788300	-3.30593800	2.30476900
H	-1.70922700	-3.20400800	0.66503300

Structure 9'-TSOMe-II [B3LYP/6-31G(d)]

Cl	4.52056300	-1.09226300	0.35164800
C	-0.42336000	0.93985600	0.13356500
C	-1.72282400	1.38842500	-0.12699300
C	-2.82998100	0.53439500	-0.10711400
C	-2.61258000	-0.85397900	0.24163500
C	-1.32401700	-1.30746800	0.52270400
C	0.69160100	1.85026100	0.04206300
O	1.90068800	1.49797800	0.05616200
O	0.89991900	-0.82541900	1.30517500
C	0.63864300	-0.51168900	2.68760400
H	-1.87032900	2.44043700	-0.35159100
H	1.52046400	-0.83941100	3.24073100
H	-0.24788700	-1.05391000	3.02464300
H	0.48492600	0.56424800	2.81967300
Mg	2.39797600	-0.43674500	0.04926700
C	0.79670600	-1.27779500	-1.41634600
C	-0.17206200	-0.48967200	0.35836700
O	0.38709300	3.14649400	-0.07904300
C	1.48601200	4.06563900	-0.21930800
H	1.02363000	5.04965800	-0.29488300
H	2.14310100	4.01442900	0.65191800
H	2.06240900	3.84169100	-1.12023100
H	-1.17257400	-2.34159700	0.82017600
C	-3.76237100	-1.70750600	0.31219200
H	-3.61864700	-2.75182400	0.57852900
C	-5.01608300	-1.22581900	0.04088700
H	-5.87172000	-1.89455800	0.09369000
C	-5.22339000	0.14059600	-0.31549600
H	-6.22758300	0.49521300	-0.52784400
C	-4.15269600	0.99324200	-0.38330700
H	-4.29285500	2.03925200	-0.64761500
H	-0.21505400	-1.21517500	-1.81229300
C	1.17974100	-2.74970300	-1.24092300
H	0.51627500	-3.24964600	-0.52637800
H	1.10803100	-3.30102400	-2.19224200
H	2.21187900	-2.89172600	-0.88545400
C	1.69869600	-0.54719900	-2.44303000
H	2.78116700	-0.57722500	-2.21902300
H	1.61341100	-1.02490300	-3.43217900
H	1.41225000	0.50354700	-2.56620200

Structure 9'-TSOMe-III [B3LYP/6-31G(d)]

Cl	-4.54702600	-1.06886100	-0.70054200
C	0.37317800	0.85308100	-0.18636400
C	1.67565600	1.35611800	-0.09014000
C	2.80230700	0.52840300	-0.10013200
C	2.59635900	-0.89758300	-0.23279900
C	1.30181300	-1.40579600	-0.35430500
C	-0.75230500	1.74654900	-0.04847800

O	-1.94717800	1.37240300	0.08090200
O	-0.94075700	-1.02835700	-1.16131600
C	-0.69264600	-0.87037300	-2.57419100
H	1.80806200	2.42904000	0.00908100
H	-1.59158700	-1.23120700	-3.07644700
H	0.17495700	-1.46885800	-2.86172600
H	-0.51437000	0.18101000	-2.82178800
Mg	-2.47525000	-0.54051700	-0.00249200
C	-0.80682200	-1.30682800	1.56755700
C	0.14057800	-0.59324900	-0.26523200
O	-0.47143400	3.05274100	-0.03479200
C	-1.57638600	3.95821800	0.14354300
H	-1.13551500	4.95393100	0.09965600
H	-2.31309300	3.82668400	-0.65224200
H	-2.05555800	3.79297700	1.11157000
H	1.15912500	-2.47384900	-0.49905300
C	3.75826300	-1.73613600	-0.26605600
H	3.62176200	-2.80984800	-0.36956200
C	5.01612800	-1.20195000	-0.16373000
H	5.88246300	-1.85845700	-0.18661800
C	5.21360400	0.20421300	-0.02226200
H	6.22129600	0.60056500	0.06006600
C	4.12944500	1.04192900	0.00727200
H	4.26174400	2.11669400	0.11189900
C	-2.22670400	-1.55910700	2.16416400
H	-2.87458000	-2.21253300	1.55790300
H	-2.14368900	-2.07021800	3.13639200
H	-2.78306500	-0.63091400	2.38518900
C	0.01802100	-0.52260800	2.57527000
H	1.06511100	-0.44321300	2.26934100
H	-0.36848400	0.49812700	2.70805200
H	0.00255400	-0.99699600	3.56904500
H	-0.36267200	-2.28968800	1.38530200

Structure 9'-TSCO-I [B3LYP/6-31G(d)]

Cl	-4.22305600	-1.92755700	-0.10478700
C	0.45858500	0.42147600	-0.40392600
C	1.64525000	1.12305700	-0.33225000
C	2.89682400	0.48730700	-0.12998800
C	2.92959600	-0.93436000	0.00263300
C	-0.82953000	1.13722900	-0.68631800
O	-1.68475500	0.65310000	-1.52453700
O	-0.70252900	-1.68113100	-0.26947500
C	-0.70810100	-3.11959100	-0.18683000
H	1.61554900	2.20032700	-0.44796800
H	-1.75718500	-3.40932600	-0.24759400
H	-0.28103300	-3.44549800	0.76626400
H	-0.14383200	-3.54088100	-1.02350800
Mg	-2.46100600	-0.53704700	-0.19631000
C	-1.81966100	0.83082100	1.46862900
C	0.51259900	-1.00406300	-0.24945200
O	-0.68163300	2.48287300	-0.61376700
C	-1.58939700	3.27128500	-1.40039800
H	-1.33510400	4.30690300	-1.17035200
H	-1.44552100	3.06968300	-2.46496900
H	-2.62843700	3.06945900	-1.13502100
C	1.70548600	-1.65636700	-0.05600500
H	1.74041400	-2.73287900	0.06075900
C	4.17864900	-1.57805800	0.19612400
H	4.20434000	-2.66038400	0.29765400
C	5.34367700	-0.84381900	0.25528000
H	6.29470000	-1.34777500	0.40405100
C	5.31253900	0.56525600	0.12324600
H	6.23881200	1.13069500	0.17165600
C	4.11343200	1.21605000	-0.06573000
H	4.08139400	2.29794300	-0.16823200
H	-2.12166000	-0.14490200	1.92035000
C	-0.67978500	1.35203200	2.32923000
H	-1.01089400	1.57071300	3.35742800
H	0.14653700	0.63602100	2.40035200
H	-0.27472000	2.28531900	1.91809400
C	-3.03343100	1.76662900	1.50284600
H	-3.42592500	1.89654300	2.52440200
H	-2.75831900	2.76315500	1.13932500
H	-3.88415100	1.41989200	0.89409900

Structure 9'-TSCO-II [B3LYP/6-31G(d)]

Cl	-4.19552900	-1.74950100	-0.33487200
C	0.51364900	0.54808800	-0.34810500
C	1.70843700	1.21441300	-0.16742500
C	2.94510500	0.53564300	-0.01847300
C	2.95316400	-0.89216300	-0.06069600
C	-0.76754300	1.30909700	-0.55844300
O	-1.61444900	0.93020500	-1.46386300
O	-0.68454600	-1.53161100	-0.48980300
C	-0.71594300	-2.97019500	-0.55065400
H	1.69711700	2.29824700	-0.15167100
H	-1.76819900	-3.23350600	-0.65663800
H	-0.31111900	-3.39660100	0.37212900
H	-0.14418900	-3.31660900	-1.41604700
Mg	-2.42178900	-0.36795400	-0.26871800
C	-1.66497400	0.88356600	1.49408900
C	0.54197900	-0.88589300	-0.36529000
O	-0.58377600	2.64646000	-0.37388500
C	-1.46400500	3.52041000	-1.09313500
H	-1.35190800	3.38177800	-2.17142800
H	-2.50851800	3.35279400	-0.82078700
H	-1.15953000	4.52773700	-0.80454300
C	1.72017700	-1.57961500	-0.23090600
H	1.73578300	-2.66278700	-0.24603000
C	4.18766800	-1.57752600	0.07749000
H	4.19381500	-2.66447600	0.04597900
C	5.36235600	-0.87780900	0.24977700
H	6.30184600	-1.41347700	0.35471600
C	5.35592000	0.53732200	0.29123200
H	6.28966300	1.07556000	0.42736300
C	4.17176400	1.22819600	0.15925300
H	4.15921400	2.31493900	0.18906500
H	-0.90929300	1.60982400	1.78850000
C	-3.05284700	1.52512000	1.67097800
H	-3.12913000	2.47663300	1.13485000
H	-3.88884400	0.88950900	1.33035500
H	-3.26759900	1.73154500	2.73257000
C	-1.48839600	-0.36694100	2.37528000
H	-1.62231900	-0.11997400	3.44172400
H	-2.22124700	-1.16420200	2.16785300
H	-0.48699300	-0.80067300	2.27003900

Structure 9'-TSCO-III [B3LYP/6-31G(d)]

Cl	-4.35770300	-1.66551200	-0.09414300
C	0.42304200	0.49283100	-0.44046200
C	1.63506100	1.14078100	-0.30484900
C	2.85769600	0.44315300	-0.12903600
C	2.83421000	-0.98455000	-0.09554600
C	-0.83948400	1.26834400	-0.68117000
O	-1.73747100	0.83443100	-1.51142700
O	-0.82085400	-1.56622400	-0.45581100
C	-0.88308700	-3.00470400	-0.43470400
H	1.64993100	2.22330700	-0.35662400
H	-1.94202300	-3.25179300	-0.51132200
H	-0.47456100	-3.38876200	0.50496300
H	-0.33173400	-3.41187600	-1.28670100
Mg	-2.53362400	-0.36545400	-0.23136700
C	-1.75380500	0.96593800	1.44693600
C	0.42048200	-0.94059700	-0.37930500
O	-0.60438500	2.60406000	-0.64824900
C	-1.63994600	3.43965500	-1.17694100
H	-1.83169200	3.20541100	-2.22587800
H	-2.56668500	3.32075600	-0.60606700
H	-1.26706600	4.45953300	-1.07115100
C	1.58459000	-1.65196000	-0.21843500
H	1.57644800	-2.73446200	-0.17552100
C	4.05447800	-1.68929000	0.06821000
H	4.03638800	-2.77624200	0.09436800
C	5.24594800	-1.00797400	0.19279900
H	6.17447100	-1.55822800	0.31779200
C	5.27088700	0.40711100	0.15873200
H	6.21749100	0.93079200	0.25771100
C	4.10095700	1.11650700	0.00059000
H	4.11262900	2.20328800	-0.02745100
C	-1.44756200	-0.26948800	2.31577400
H	-1.70730300	-0.08682900	3.37078200
H	-1.99771400	-1.18004100	2.03202900
H	-0.37782700	-0.51316500	2.28729900
C	-1.14561100	2.20368600	2.08885300
H	-0.04920100	2.17613200	2.03568800
H	-1.47111900	3.13158000	1.61244700
H	-1.41398300	2.26985100	3.15527700
H	-2.85745200	1.12509500	1.42440500

Structure 11_I [B3LYP/6-31G(d)]

C	-0.54400400	-1.25430100	-0.14042600

C	0.08403900	-2.48258200	0.21698700
C	1.44609100	-2.58306200	0.33174400
C	2.28247400	-1.45917000	0.10328800
C	1.68100100	-0.20680600	-0.24447300
C	-2.02776400	-1.20635400	-0.28895700
O	-2.68338800	-0.29625600	-0.75978300
O	-0.27347000	1.06964600	-0.77943900
H	-0.54463600	-3.34600200	0.39295900
H	1.90214000	-3.53201000	0.60139100
C	0.26115000	-0.14155200	-0.36025000
C	2.51332100	0.92378300	-0.46795300
C	3.88073900	0.81296200	-0.35217900
H	4.50779200	1.68350100	-0.52221000
C	4.47801800	-0.42397900	-0.01058000
H	5.55886100	-0.49354400	0.07673100
C	3.69527800	-1.53415300	0.21254200
H	4.14762700	-2.48658900	0.47714500
H	2.05708400	1.87364800	-0.71887500
O	-2.60427400	-2.34724900	0.15647900
C	-4.03435100	-2.39617900	0.04576800
H	-4.32319400	-3.36725900	0.44873800
H	-4.49038400	-1.58844600	0.62403700
H	-4.34332500	-2.30498500	-0.99897100
S	-0.81561300	2.18171500	0.36548800
O	-1.22714000	1.46131300	1.56516200
O	0.18331300	3.24448100	0.44332100
C	-2.23460600	2.77358200	-0.55692400
H	-2.69629800	3.55436500	0.05143500
H	-1.87519000	3.18529800	-1.50112400
H	-2.89931200	1.92597100	-0.71651100

Structure 11_II [B3LYP/6-31G(d)]

C	0.29094400	1.45300600	-0.00357600
C	-0.56824800	2.52591400	0.36867900
C	-1.92915000	2.37499600	0.40870500
C	-2.53244600	1.13053100	0.08801500
C	-1.69449700	0.02356500	-0.26528100
C	1.74638300	1.79839900	-0.02628800
O	2.18666200	2.80594200	0.49139200
O	0.49375400	-0.86129000	-0.70718900
H	-0.09988300	3.47091900	0.61799200
H	-2.56429900	3.21130600	0.68852300
C	-0.28226700	0.22394000	-0.29948500
C	-2.29547000	-1.22622300	-0.57734300
C	-3.66439300	-1.36805500	-0.54306100
H	-4.11221100	-2.32848400	-0.78190700
C	-4.49449700	-0.27565100	-0.19576200
H	-5.57302500	-0.40535000	-0.17209000
C	-3.93922300	0.94518900	0.11344300
H	-4.57030500	1.78807800	0.38363500
H	-1.66290200	-2.06739100	-0.83174200
O	2.53140600	0.94189300	-0.71873500
C	3.91740100	1.32470900	-0.77035300
H	4.40394200	0.57536300	-1.39668600
H	4.02539100	2.31830300	-1.21166000
H	4.35131800	1.33139200	0.23275200
S	1.15061800	-1.87291100	0.46239800
O	1.60207200	-1.06699900	1.59096300
O	0.23926200	-2.99483500	0.66869000
C	2.54073700	-2.42046900	-0.53083100
H	3.09652100	-3.13890700	0.07528200
H	2.15272100	-2.89690200	-1.43208200
H	3.14594600	-1.54853900	-0.77252500

Structure 11_III [B3LYP/6-31G(d)]

C	-0.50424300	-1.22446400	-0.15083400
C	0.11795200	-2.42684100	0.28693000
C	1.47748400	-2.51340400	0.44634300
C	2.31343300	-1.40162500	0.16542600
C	1.71465000	-0.17355800	-0.26461700
C	-1.97986100	-1.20590700	-0.39735700
O	-2.56362700	-0.44067300	-1.13370800
O	-0.23078300	1.10528000	-0.80258700
H	-0.51479700	-3.28243300	0.48870800
H	1.93125900	-3.44233000	0.78135000
C	0.29375800	-0.11232000	-0.38606200
C	2.55576600	0.92993300	-0.57431300
C	3.92262800	0.82891800	-0.44239200
H	4.55397400	1.67747700	-0.69087900
C	4.51435900	-0.37716400	0.00392200
H	5.59404800	-0.44183800	0.10592600
C	3.72593700	-1.46669400	0.29601500
H	4.17428700	-2.39982400	0.62774700
H	2.10642000	1.84410600	-0.94421300
O	-2.60200400	-2.19809100	0.28109900
C	-4.02439800	-2.26164500	0.08860300
H	-4.36542100	-3.08758700	0.71354300
H	-4.49063400	-1.32309100	0.39809500
H	-4.26268200	-2.44812400	-0.96201400
S	-1.15943800	2.03980600	0.24762300
O	-2.03842100	2.81163200	-0.61149900
O	-1.64909900	1.20630500	1.33966400
C	0.11532500	3.13134500	0.90200800
H	-0.37774800	3.79934800	1.61197600
H	0.87406500	2.53073100	1.40548900
H	0.54295600	3.70159900	0.07652100

Structure 11_IV [B3LYP/6-31G(d)]

C	0.24810600	1.42778900	-0.00138500
C	-0.61223700	2.47898400	0.42090200
C	-1.97016500	2.31267800	0.49515000
C	-2.56743100	1.07479800	0.13951100
C	-1.72687200	-0.00862900	-0.27390400
C	1.70247700	1.78342900	-0.06785200
O	2.15963700	2.78911500	0.43835100
O	0.44051200	-0.89950300	-0.72400400
H	-0.14404900	3.42101800	0.68294600
H	-2.60675400	3.13115900	0.82039000
C	-0.31344600	0.19509500	-0.30727700
C	-2.32970000	-1.23873900	-0.65363100
C	-3.69702500	-1.39540900	-0.60600500
H	-4.14403400	-2.33876100	-0.90720200
C	-4.52720500	-0.33205800	-0.17821900
H	-5.60428500	-0.46983400	-0.14335400
C	-3.97246600	0.87512700	0.18144100
H	-4.60442900	1.70009900	0.50046500
H	-1.69850400	-2.04423900	-1.00996400
O	2.43475000	0.91275600	-0.78101000
C	3.84711600	1.17515600	-0.83037700
H	4.27412400	0.32518500	-1.36120400
H	4.04121000	2.10982300	-1.36325900
H	4.25436900	1.24444200	0.18098100
S	1.48165000	-1.67950400	0.34259500
O	2.59528600	-2.13802600	-0.47287500
O	1.66883800	-0.86068700	1.53456400
C	0.46569300	-3.10083700	0.77616200
H	1.05551800	-3.71056200	1.46442300
H	-0.44643600	-2.74988000	1.26062000
H	0.24361200	-3.65992500	-0.13367600

Structure 11·EtMgCl_I [B3LYP/6-31G(d)]

C	0.36651200	1.31821200	-0.70386600
C	1.36856200	2.27797900	-1.01440800
C	2.69011600	2.01473200	-0.75803000
C	3.09316600	0.78367000	-0.17630700
C	2.10349200	-0.21059700	0.12084600
C	-1.06218800	1.68026100	-0.86191500
O	-1.97222600	1.28145500	-0.12790700
O	-0.21987700	-0.89682400	0.06812700
Cl	-3.57228800	-1.39421900	1.52290600
H	1.06417000	3.22661800	-1.44073800
H	3.44783400	2.75795000	-0.98996000
Mg	-1.81121800	0.08257200	1.56136100
C	-0.59734300	0.91873800	3.08959800
H	-1.05882800	0.66395700	4.05702000
C	0.74734300	0.09051300	-0.17344900
C	2.50832800	-1.43895500	0.70740400
C	3.83488300	-1.67208300	0.98612800
H	4.13384800	-2.61115500	1.44231100
C	4.81651700	-0.69698600	0.68441900
H	5.86020800	-0.89951800	0.90709400
C	4.45301500	0.50264800	0.11694200
H	5.20200500	1.25588200	-0.11241700
H	1.75790700	-2.18313500	0.94429200
O	-1.28564600	2.53806700	-1.84537300
C	-2.65595700	2.96411700	-2.03428300
H	-2.62483800	3.63927400	-2.88816600
H	-3.28629200	2.09749700	-2.24117100
H	-3.01586600	3.47882000	-1.14089500
C	-0.36777900	2.44237300	3.04104500
H	-1.31333900	2.99943400	3.10258700
H	0.26724400	2.81645300	3.86113200

H	0.12036300	2.75702700	2.10692400
H	0.38310700	0.41499200	3.11304100
S	-0.57112000	-1.87323500	-1.35332300
O	-1.50939300	-1.10926100	-2.16511600
O	0.71488800	-2.29303100	-1.89284000
C	-1.38853800	-3.21969400	-0.50669600
H	-2.22031300	-2.81493300	0.08058800
H	-1.74645200	-3.88669100	-1.29510400
H	-0.65206400	-3.72264400	0.12117100

Structure 11·EtMgCl_II [B3LYP/6-31G(d)]

Cl	3.56290300	1.91574800	0.62834100
C	-0.33430000	-1.60878200	0.18045900
C	-1.33548700	-2.58330800	0.44206200
C	-2.66124900	-2.23160600	0.46655800
C	-3.06908800	-0.89180600	0.23247700
C	-2.07936200	0.10277600	-0.06409100
C	1.09473300	-1.98045700	0.30570900
O	1.98050600	-1.22593400	0.72108300
O	0.25253600	0.65740300	-0.42278100
H	-1.02810200	-3.60336400	0.64067400
H	-3.41913000	-2.98070700	0.67818900
Mg	1.76752700	0.71939400	1.42469700
C	0.50566600	0.88856300	3.12178700
H	1.14544000	0.77245600	4.01278400
C	-0.71858800	-0.30090700	-0.09369900
C	-2.48931800	1.44304600	-0.29451500
C	-3.82063100	1.78272100	-0.23124100
H	-4.12374700	2.81184300	-0.39941700
C	-4.80173100	0.80188600	0.05321300
H	-5.84896900	1.08718400	0.09540200
C	-4.43367700	-0.50453800	0.27898100
H	-5.18260600	-1.26005400	0.50094200
H	-1.73954500	2.19523100	-0.50625700
O	1.34550900	-3.24091600	-0.01236300
C	2.71759600	-3.68163300	0.12218200
H	2.71041400	-4.72325100	-0.19547100
H	3.36248900	-3.07933000	-0.52012200
H	3.04143500	-3.59092000	1.16114000
S	0.66626800	0.64889800	-2.13345400
O	1.60135900	-0.45081200	-2.33269500
O	-0.59375000	0.69967400	-2.86197600
C	1.50051100	2.23002800	-2.17483700
H	1.88710000	2.32933500	-3.19233100
H	0.76515300	3.00703300	-1.96244000
H	2.31159600	2.22280000	-1.43836400
C	-0.29134800	2.20075100	3.26711400
H	0.36796100	3.07936600	3.26743600
H	-1.00250900	2.34156200	2.44047100
H	-0.88244600	2.25239600	4.19652500
H	-0.19613800	0.03989600	3.17485400

Structure 11·EtMgCl_III [B3LYP/6-31G(d)]

Cl	3.62178300	-1.72436000	-0.60846500
C	-0.44135300	1.55841800	0.11994400
C	-1.45047700	2.54340400	-0.05831700
C	-2.75417700	2.17473100	-0.27381000
C	-3.13079900	0.80663500	-0.32474700
C	-2.13495300	-0.20475900	-0.11992500
C	0.97756800	1.97641300	0.21292700
O	1.92807200	1.33424500	-0.24568700
O	0.17381200	-0.76719400	0.35668400
H	-1.16552500	3.58884800	-0.03845500
H	-3.51743300	2.93407900	-0.41926900
Mg	1.85497800	-0.44135100	-1.32812300
C	0.68478300	-0.33062400	-3.09559500
H	0.19989000	0.65806200	-3.16113300
C	-0.79894500	0.21483500	0.11441800
C	-2.51294600	-1.57256100	-0.17567600
C	-3.81979200	-1.92245400	-0.42326800
H	-4.09791500	-2.97106600	-0.47215400
C	-4.80809600	-0.92669100	-0.61651500
H	-5.83622500	-1.22100800	-0.80681900
C	-4.47046700	0.40629600	-0.56842000
H	-5.22452400	1.17406400	-0.71987900
H	-1.75707600	-2.33485400	-0.03290300
O	1.14625700	3.15617400	0.78923800
C	2.50652900	3.64166000	0.88462800
H	2.42721500	4.60099900	1.39384600
H	3.10867600	2.93857300	1.46277700
H	2.93380300	3.76166400	-0.11314700
S	0.43056600	-1.07087000	2.06834800
O	1.28859500	-0.00089000	2.56105100
O	-0.88503300	-1.30078400	2.64923000
C	1.33610600	-2.60253400	1.89223100
H	1.63661300	-2.88241200	2.90509500
H	0.66211800	-3.34807900	1.46851800
H	2.20736900	-2.42899200	1.25093800
C	1.43568000	-0.60137100	-4.41548000
H	2.24501900	0.12317100	-4.58207300
H	1.90339200	-1.59484900	-4.42211700
H	0.78480200	-0.55304600	-5.30423500
H	-0.15488200	-1.04171300	-3.01968000

Structure 11·EtMgCl (b)_I [B3LYP/6-31G(d)]

Cl	-4.14638400	0.07261800	-1.56353500
C	0.89064600	1.38880400	0.00067100
C	1.76961100	2.49538600	-0.17526700
C	3.12928500	2.34586600	-0.09145800
C	3.70752900	1.08046300	0.18867900
C	2.84983300	-0.05373900	0.36395400
C	-0.57893900	1.61745400	-0.04002900
O	-1.41163700	0.78994400	0.32246100
O	0.66156700	-1.00681100	0.42589700
H	1.33434900	3.46624400	-0.37529500
H	3.78155100	3.20316400	-0.23190100
Mg	-3.03388200	-0.55992600	0.36126200
C	-3.62455300	-1.08463600	2.33041800
H	-2.74100700	-1.41484700	2.90336900
C	1.44429900	0.13456600	0.23803800
C	3.42900700	-1.31545200	0.67028800
C	4.79461800	-1.45029200	0.77729800
H	5.22496600	-2.41747600	1.02036300
C	5.64468900	-0.33480300	0.58390100
H	6.72050100	-0.45764700	0.66892400
C	5.11111500	0.90173800	0.30071600
H	5.75777700	1.76408200	0.16224900
H	2.78008300	-2.16441500	0.84987000
O	-0.90372400	2.82635400	-0.47022000
C	-2.31945500	3.15448200	-0.52420400
H	-2.35668200	4.13344700	-0.99990800
H	-2.86185100	2.40377900	-1.10332300
H	-2.71844600	3.20435900	0.49207400
S	-0.17360200	-1.67000600	-0.86279700
O	-1.51241800	-1.98017100	-0.33786100
O	0.01462100	-0.84622800	-2.04411800
C	0.67670700	-3.23960300	-1.03582500
H	0.14384100	-3.79552700	-1.81075300
H	1.70693900	-3.04476000	-1.33635300
H	0.62513200	-3.76579900	-0.08158400
C	-4.35471000	0.00620500	3.14077900
H	-3.73219600	0.90353400	3.27418700
H	-5.27505200	0.33692100	2.64005800
H	-4.64939300	-0.31816500	4.15351100
H	-4.27312700	-1.97553200	2.28720100

Structure 11·EtMgCl (b)_II [B3LYP/6-31G(d)]

Cl	-4.37889800	0.51719700	-1.21972400
C	0.84586900	1.43208900	0.20027100
C	1.75765000	2.52583100	0.18746100
C	3.11307800	2.32309400	0.19170500
C	3.65424700	1.01136400	0.22282700
C	2.76227100	-0.10987300	0.22924000
C	-0.61523300	1.70582900	0.25601200
O	-1.46316300	0.85473900	0.51302900
O	0.54322500	-0.99160100	0.20802300
H	1.35159700	3.52942600	0.17787100
H	3.79106700	3.17183500	0.17932100
Mg	-3.10822900	-0.46624900	0.43855000
C	-3.52204000	-1.36078400	2.31794800
H	-4.34346500	-2.08652700	2.20015300
C	1.36132200	0.13999700	0.19312200
C	3.30479100	-1.42271500	0.28669700
C	4.66733700	-1.61523700	0.31521000
H	5.06986900	-2.62265500	0.36796500
C	5.55053000	-0.50913100	0.28800600
H	6.62337700	-0.67722500	0.30847800
C	5.05331600	0.77348600	0.24725300
H	5.72613700	1.62685500	0.23766200
H	2.63160900	-2.27012600	0.34021400
O	-0.91371800	2.97706100	0.03821800
C	-2.31871600	3.34782100	0.09451300

H	-2.34161100	4.38823600	-0.22652600
H	-2.90876800	2.70832000	-0.56561300
H	-2.67685400	3.25387000	1.12279200
S	-0.35306700	-1.39461600	-1.14451300
O	-1.68497300	-1.75229200	-0.63353000
O	-0.17488400	-0.38178000	-2.17069500
C	0.43650400	-2.93285100	-1.61970900
H	-0.13936800	-3.32926800	-2.45918800
H	1.46292500	-2.71800900	-1.91957400
H	0.39642800	-3.61578300	-0.76993600
C	-2.34010100	-2.06376500	3.01495100
H	-1.93110800	-2.87850300	2.39958300
H	-1.50628700	-1.37237000	3.20576100
H	-2.60197900	-2.51162200	3.98894800
H	-3.93131500	-0.59987600	3.00360300

Structure 11·EtMgCl (b)_III [B3LYP/6-31G(d)]

Cl	2.95278500	-0.06277000	2.20108900
C	-0.73996300	1.45170100	-0.15507700
C	-1.56454700	2.56240100	0.18747200
C	-2.92810800	2.44163200	0.25325600
C	-3.56903000	1.20767200	-0.03496200
C	-2.76808000	0.07109700	-0.38549000
C	0.73336700	1.63504800	-0.23872700
O	1.52849900	0.75928400	-0.57213000
O	-0.59693900	-0.86921300	-0.81759800
H	-1.08608000	3.51082700	0.39555800
H	-3.53780700	3.30014400	0.52077200
Mg	2.97726700	-0.67406100	-0.06730400
C	4.49736200	-0.96394900	-1.51089000
H	4.08798500	-1.52943500	-2.36406000
C	-1.35213300	0.22621000	-0.41195000
C	-3.40682700	-1.15947500	-0.70326700
C	-4.77947300	-1.25743500	-0.65870500
H	-5.25930000	-2.19932400	-0.90742600
C	-5.57218000	-0.14128600	-0.29892800
H	-6.65368100	-0.23806600	-0.26873900
C	-4.97969700	1.06416000	0.00371600
H	-5.58441000	1.92631400	0.27202000
H	-2.80475400	-2.01423900	-0.98724800
O	1.11643800	2.86676100	0.07152400
C	2.54355000	3.13000700	0.08482800
H	2.62694000	4.19300400	0.30679700
H	3.01592500	2.52572100	0.86242400
H	2.97571200	2.90055200	-0.89134300
S	-0.04259200	-2.07025900	0.20318300
O	1.39976400	-2.15739500	-0.09153200
O	-0.85857700	-3.25074300	-0.02464500
C	-0.28109500	-1.45729700	1.87353100
H	-1.32728000	-1.17682600	2.00310900
H	-0.03108100	-2.30824900	2.51190500
H	0.42098100	-0.64133500	2.06622200
C	5.15452100	0.32556800	-2.04547400
H	4.41875700	0.99439400	-2.51718300
H	5.63495000	0.90230100	-1.24208200
H	5.93400700	0.14166800	-2.80378100
H	5.28658900	-1.61335500	-1.09971400

Structure 11·EtMgCl(DME)_I [B3LYP/6-31G(d)]

C	1.18993500	1.25615100	-0.51000700
C	1.95856100	2.40226500	-0.86754700
C	3.30595500	2.45649600	-0.62525100
C	3.98153200	1.36922700	-0.01150900
C	3.23901600	0.19413200	0.33630900
C	-0.27947000	1.30140700	-0.70816100
O	-1.10153900	0.65775700	-0.05744900
Cl	-2.73836000	-1.78362900	1.94606900
H	1.44909600	3.24241000	-1.32280300
H	3.87259200	3.34362100	-0.89448300
C	-3.69656500	2.16613700	1.61678600
H	-4.42340400	1.97449900	2.42325100
C	1.84123600	0.16612100	0.06149500
C	3.91406400	-0.89255300	0.95468900
C	5.26275000	-0.81681700	1.21548900
H	5.76812200	-1.65208500	1.69136400
C	5.99950700	0.34090600	0.86746500
H	7.06452600	0.38331400	1.07773200
C	5.37222700	1.40892000	0.26746400
H	5.93225200	2.30110200	-0.00023400
H	3.35207300	-1.77880200	1.21944100
O	-0.63030200	2.16781800	-1.65606300
C	-2.04014800	2.39523900	-1.87279300
H	-2.08560700	3.09357300	-2.70785600
H	-2.54223300	1.45903600	-2.12182800
H	-2.49287700	2.82917100	-0.97860100
H	-4.29852100	2.64226200	0.82003000
Mg	-2.88192100	0.31069500	0.94401500
O	-4.01479700	-0.30397700	-0.78946800
C	-3.62168200	-1.47918000	-1.51772800
H	-2.53796000	-1.44175400	-1.63344200
H	-3.90316800	-2.38059900	-0.96307900
H	-4.10396100	-1.47485500	-2.50326900
C	-5.43516800	-0.22461800	-0.60866700
H	-5.93164800	-0.18153900	-1.58597300
H	-5.79923800	-1.09285200	-0.04626900
H	-5.63426100	0.69080800	-0.04963500
O	1.14232500	-0.97371400	0.43146800
S	0.88599500	-2.16257200	-0.74408200
O	-0.06559500	-1.64893300	-1.72969200
O	2.18511900	-2.65610300	-1.19047300
C	0.09672700	-3.32834500	0.35755700
H	-0.19308500	-4.18073500	-0.26138800
H	0.82620400	-3.63196700	1.10951800
H	-0.77728400	-2.85464700	0.81771800
C	-2.67703500	3.20420300	2.13154600
H	-2.11042500	2.82032600	2.99101300
H	-1.92992700	3.46865700	1.36660400
H	-3.13235800	4.15461400	2.45673400

Structure 11·EtMgCl(DME)_II [B3LYP/6-31G(d)]

C	0.77252000	0.67342200	-1.34176800
C	1.45203400	1.70241700	-2.04914100
C	2.68787100	2.13303800	-1.63800100
C	3.32848200	1.54910800	-0.51302700
C	2.67930100	0.48050300	0.18817200
C	-0.60243200	0.30121700	-1.75623900
O	-1.55478600	0.12381300	-0.99508000
Cl	-3.08488900	-1.65817500	1.53994900
H	0.96747000	2.15152100	-2.90903500
H	3.19303500	2.93183400	-2.17410200
C	-1.03737200	1.85225900	2.11532200
H	-1.74481100	2.58932500	2.53615100
C	1.39484200	0.06567000	-0.26069800
C	3.32849600	-0.11444500	1.30225700
C	4.56306400	0.33656400	1.70893300
H	5.04920200	-0.12098800	2.56557100
C	5.20710400	1.39272600	1.02030600
H	6.18269300	1.73520900	1.35380000
C	4.60365800	1.98372800	-0.06609400
H	5.09464600	2.79380200	-0.59916900
H	2.83654700	-0.92329800	1.82753300
O	-0.73953300	0.23381200	-3.07448600
C	-2.03819600	-0.15482700	-3.57130200
H	-1.93406500	-0.16723700	-4.65555300
H	-2.29260800	-1.14628700	-3.19195100
H	-2.79693500	0.56744400	-3.26110600
H	-0.38034400	2.45163500	1.46054000
Mg	-2.14780200	0.40863600	1.00008300
O	-3.93252300	1.44087900	0.38783800
C	-5.18172800	0.81776600	0.07101800
H	-5.04459500	-0.25350300	0.21765900
H	-5.96620900	1.18817900	0.74275000
H	-5.45919200	1.03447500	-0.96915100
C	-3.97718500	2.86518600	0.30579900
H	-4.21472800	3.18199600	-0.71862100
H	-4.73455600	3.26218900	0.99360900
H	-2.99301900	3.23453100	0.59544200
O	0.75997500	-0.96952200	0.41964500
S	0.91178600	-2.51611400	-0.28227200
O	0.18083100	-2.50280100	-1.54819500
O	2.32293700	-2.88684100	-0.25976700
C	-0.00051700	-3.39452900	0.97878400
H	-0.04064600	-4.43501300	0.64774200
H	0.55002000	-3.30978300	1.91663700
H	-1.00379700	-2.96488600	1.06499500
C	-0.18846400	1.30624300	3.28262700
H	-0.80373000	0.75047900	4.00340600
H	0.58530300	0.60883500	2.93352700
H	0.33441200	2.09170100	3.85423100

Structure 11·EtMgCl(DME)_III [B3LYP/6-31G(d)]

C	0.83250100	0.51232500	-1.34543000

C	1.56752200	1.46305900	-2.10627900
C	2.79202900	1.90574600	-1.67488500
C	3.36317800	1.41728300	-0.46977600
C	2.65752400	0.42839500	0.29083600
C	-0.53327000	0.13905800	-1.78595600
O	-1.51357800	0.01182500	-1.04794500
Cl	-2.96279900	-1.49383000	1.79679000
H	1.13270600	1.84437200	-3.02330100
H	3.33948100	2.64444800	-2.25373500
C	-0.94263300	2.04173500	1.86966400
H	0.03023500	1.65210900	2.21274900
C	1.39134900	-0.00817900	-0.18628900
C	3.23339000	-0.06802700	1.49008000
C	4.45324900	0.40065700	1.92023800
H	4.88349100	0.02017700	2.84203500
C	5.15474100	1.37610900	1.17109300
H	6.11816900	1.73333400	1.52393100
C	4.62203800	1.87146900	0.00288300
H	5.15675500	2.62071600	-0.57508700
H	2.69533100	-0.81340800	2.06223800
O	-0.62957900	0.00987300	-3.10269900
C	-1.92230900	-0.35536000	-3.62948800
H	-1.77986600	-0.42298200	-4.70731200
H	-2.22773000	-1.31885900	-3.21663400
H	-2.66274700	0.40945700	-3.38334000
H	-1.45775600	2.31340200	2.80810600
Mg	-2.03298500	0.46655100	0.92940600
O	-3.88854300	1.33824100	0.25614400
C	-4.85297300	0.50922100	-0.40266700
H	-4.30134300	-0.13876300	-1.08408100
H	-5.39091700	-0.10707400	0.32536100
H	-5.55504700	1.13730900	-0.96601200
C	-4.49401700	2.26579000	1.16432300
H	-5.16431700	2.93904800	0.61551400
H	-5.05917100	1.73195200	1.93848000
H	-3.68472700	2.83574000	1.62111700
O	0.71037600	-0.97858300	0.54402700
S	0.88448100	-2.57679400	-0.03470600
O	0.13077900	-2.68086600	-1.28278600
O	2.30473200	-2.91035900	-0.01088000
C	0.01387800	-3.37138800	1.30838700
H	-0.04234600	-4.42980800	1.04309400
H	0.59711400	-3.23219100	2.21953900
H	-0.98319400	-2.92805500	1.40169900
C	-0.68507400	3.33269700	1.06544200
H	-0.10657300	3.13525600	0.15163200
H	-1.61985900	3.81211900	0.73656800
H	-0.12620300	4.10231000	1.62449200

Structure 11·EtMgCl(DME)_IV [B3LYP/6-31G(d)]

C	-0.86073900	0.30758700	1.42924900
C	-1.53522500	1.16951200	2.33692000
C	-2.73181500	1.74624100	1.99431300
C	-3.33667300	1.48302000	0.73653200
C	-2.69435100	0.58341900	-0.17581600
C	0.47877800	-0.21670700	1.79473900
O	1.46068700	-0.25176000	1.05078400
Cl	2.90869600	-1.33312600	-1.93799800
H	-1.07705800	1.37561700	3.29789100
H	-3.23211900	2.41696600	2.68746400
C	1.05868300	2.29624900	-1.35227400
H	0.06827400	1.99572600	-1.73314800
C	-1.45280100	0.00753000	0.21087000
C	-3.30465100	0.30943400	-1.42825000
C	-4.49753600	0.90674200	-1.76453000
H	-4.95472100	0.69555900	-2.72681100
C	-5.13630900	1.79535900	-0.86613000
H	-6.07908900	2.25660500	-1.14666300
C	-4.56906300	2.07546100	0.35603500
H	-5.05600500	2.75672200	1.04900400
H	-2.81386800	-0.37008700	-2.11375000
O	0.54886600	-0.60202900	3.06257700
C	1.80775700	-1.15415900	3.50317400
H	1.64969100	-1.42050900	4.54753900
H	2.04808000	-2.03657300	2.90713500
H	2.60409300	-0.41239700	3.40699800
Mg	2.11911000	0.53456700	-0.78179300
O	3.99060700	1.20526400	0.03305000
C	5.19393300	0.43330400	0.10697000
H	4.97621400	-0.52975300	-0.35430600
H	5.99676600	0.93807900	-0.44473200
H	5.49529300	0.30314800	1.15476600
C	4.14131700	2.53508400	0.53014600
H	4.40638800	2.51727700	1.59583300
H	4.92271600	3.06375000	-0.02998100
H	3.18470100	3.03908400	0.38824400
O	-0.83067900	-0.86700400	-0.67522200
S	-1.06073200	-2.52541000	-0.35554500
O	-0.34522200	-2.84478300	0.87875800
O	-2.48711300	-2.81313500	-0.46481000
C	-0.17176300	-3.12456200	-1.78542600
H	-0.14531500	-4.21240600	-1.68755200
H	-0.72653700	-2.83094700	-2.67751600
H	0.83691700	-2.69841600	-1.78497700
C	1.72933100	3.18239100	-2.42273400
H	1.13382600	4.06708100	-2.70544800
H	2.70775000	3.56387300	-2.09320300
H	1.91671600	2.62319900	-3.34958600
H	0.82142800	2.92543600	-0.47483300

Structure 11·EtMgCl(DME)_IX [B3LYP/6-31G(d)]

C	0.83603200	-0.65672800	1.29409200
C	1.55666000	-1.63954600	2.02749000
C	2.81045300	-2.02789800	1.63036700
C	3.42636100	-1.45232600	0.48756000
C	2.73255900	-0.43460900	-0.24513600
C	-0.55619900	-0.34341100	1.69369500
O	-1.50688700	-0.18095300	0.92723900
Cl	-0.75983900	-1.73189000	-2.18954700
H	1.08811800	-2.08814200	2.89612600
H	3.34751000	-2.78981500	2.18864200
C	-3.20295700	1.51806800	-1.57452600
C	1.43747600	-0.05467100	0.19875200
C	3.34914000	0.14250400	-1.38626900
C	4.59945100	-0.27085700	-1.78375600
H	5.05991800	0.17046000	-2.66283600
C	5.29162500	-1.27074200	-1.05867100
H	6.27959900	-1.58360700	-1.38481900
C	4.71746700	-1.84776100	0.05086300
H	5.24336200	-2.61821100	0.60876900
H	2.81515200	0.90024200	-1.94559500
O	-0.71427200	-0.31149700	3.01289700
C	-2.03882500	-0.01258900	3.50014000
H	-1.94643100	-0.00571200	4.58558200
H	-2.35652700	0.96394500	3.12963500
H	-2.74576900	-0.78018900	3.17591400
Mg	-2.17000600	-0.28877500	-1.05312500
O	-3.73918100	-1.68885200	-0.58839900
C	-3.66460000	-3.10801300	-0.76985500
H	-2.66875700	-3.32188300	-1.15766900
H	-3.82837700	-3.61861700	0.18834100
H	-4.42429100	-3.43290100	-1.49186000
C	-5.02499800	-1.24811900	-0.15446600
H	-5.79277300	-1.53661000	-0.88368700
H	-5.26975800	-1.68637200	0.82241400
H	-4.98508600	-0.16153700	-0.07795800
O	0.77089200	0.94944500	-0.50191400
S	0.87829100	2.50905000	0.14819000
O	0.04311300	2.56158400	1.34689100
O	2.28390900	2.89189200	0.21936600
C	0.06758300	3.32539700	-1.22346700
H	-0.01877600	4.37829100	-0.94618200
H	0.69274700	3.20776300	-2.10931000
H	-0.91571600	2.87664700	-1.36862900
H	-2.63884100	2.09078800	-2.33136600
C	-3.63264100	2.48150600	-0.44738300
H	-2.77709700	2.83925800	0.14296400
H	-4.17010700	3.37721900	-0.80234300
H	-4.30236200	1.99249000	0.27655300
H	-4.10916300	1.21493500	-2.12916300

Structure 11·EtMgCl(DME)_V [B3LYP/6-31G(d)]

C	0.74153400	1.31298200	-0.68878600
C	1.46824000	2.53388000	-0.72053700
C	2.74252000	2.60846800	-0.21840100
C	3.36973600	1.46847600	0.34852800
C	2.66560600	0.22059700	0.36998700
C	-0.66764000	1.30131600	-1.15884500
O	-1.58667600	0.67663500	-0.62851200
Cl	-0.70011400	0.75138000	2.75122700
H	0.98630400	3.41118300	-1.13615800
H	3.28289800	3.55072900	-0.23857800

C	-4.44983800	1.18290400	1.26777300
H	-4.56598500	1.74575500	2.20921500
C	1.35685100	0.17779300	-0.18594500
C	3.28505700	-0.91305800	0.96240700
C	4.55292900	-0.81948200	1.48956100
H	5.01095100	-1.68852000	1.95322400
C	5.26047300	0.40631600	1.44890700
H	6.26065500	0.46384600	1.86877000
C	4.67893600	1.52364000	0.89513900
H	5.21102200	2.47112000	0.87509000
H	2.72991800	-1.84183400	1.02709000
O	-0.85788800	2.08773900	-2.20994100
C	-2.20197200	2.15176400	-2.74034400
H	-2.14559200	2.86387300	-3.56277400
H	-2.49671100	1.16427800	-3.10157700
H	-2.90119400	2.48889300	-1.97330400
H	-5.18046600	0.35975900	1.35984500
Mg	-2.46534700	0.38722100	1.29000900
O	-2.60083100	-1.71784500	1.26332300
C	-1.72992600	-2.61509800	1.96502800
H	-1.06879400	-1.99366400	2.56957600
H	-2.32453500	-3.27625200	2.60849700
H	-1.15162200	-3.20744800	1.24872200
C	-3.52655000	-2.38552600	0.40175900
H	-2.98712400	-2.91753800	-0.38921700
H	-4.13786900	-3.08928500	0.98093100
H	-4.17096300	-1.61679000	-0.02829000
O	0.71142400	-1.06041900	-0.18263100
S	0.46942000	-1.87815900	-1.62204500
O	-0.46867600	-2.93275500	-1.26553300
O	0.18548000	-0.92274600	-2.68798900
C	2.08960800	-2.60014000	-1.92358700
H	2.02161000	-3.13135900	-2.87560300
H	2.82763600	-1.79912400	-1.98482200
H	2.32206100	-3.29072100	-1.11264600
C	-4.89742400	2.09342500	0.10878600
H	-4.23721000	2.96766200	0.00025800
H	-4.88216600	1.56580600	-0.85694300
H	-5.91895700	2.49564800	0.22213600

Structure 11·EtMgCl(DME)_VI [B3LYP/6-31G(d)]

C	-0.80063200	0.10246400	1.39324800
C	-1.38512000	0.90690600	2.40883600
C	-2.55936200	1.58052900	2.18390800
C	-3.21999000	1.49348700	0.92996600
C	-2.66316900	0.66493700	-0.09820300
C	0.52419500	-0.52466300	1.63969500
O	1.44911800	-0.55973900	0.83030000
Cl	3.63735800	-1.12814400	-1.83120300
H	-0.87713500	0.98599900	3.36356400
H	-2.99265800	2.19906000	2.96502500
C	0.94969400	1.98192800	-1.59046500
H	0.12575400	1.49256300	-2.13670200
C	-1.46100100	-0.04540900	0.18264600
C	-3.30939200	0.59895200	-1.36207900
C	-4.46740800	1.30726900	-1.59007300
H	-4.94564500	1.26180400	-2.56425300
C	-5.03311300	2.10894800	-0.56918200
H	-5.94836300	2.66053100	-0.76436600
C	-4.42057500	2.20184900	0.65973500
H	-4.84379900	2.82667800	1.44197500
H	-2.85604600	0.01252900	-2.15290700
O	0.64626200	-1.00330600	2.87153700
C	1.89974000	-1.65150600	3.18558500
H	1.78910300	-1.99741900	4.21254300
H	2.05965400	-2.48889500	2.50401700
H	2.72604500	-0.94256000	3.09860500
Mg	2.24695200	0.44102300	-0.87179000
O	3.71860100	1.47468900	0.33904400
C	5.05860900	1.01664600	0.55140400
H	5.12567900	0.02917700	0.09489600
H	5.76957500	1.69737400	0.06639800
H	5.27414900	0.96965900	1.62744900
C	3.50369000	2.81157000	0.78714100
H	3.66109700	2.88153600	1.87223000
H	4.18839800	3.50085700	0.27681700
H	2.47416100	3.06992500	0.53737400
O	-0.96405100	-0.87057100	-0.81840900
S	-1.01459500	-2.54982200	-0.62108600
O	-0.13223700	-3.05088600	-1.65475900
O	-0.82435400	-2.85539300	0.79477600
C	-2.72429200	-2.90774100	-1.05613400
H	-2.85946500	-3.98350300	-0.92261300
H	-3.38627100	-2.35377100	-0.38919600
H	-2.88246900	-2.62773400	-2.09793600
C	1.59345100	3.01957200	-2.53299700
H	0.88550100	3.77302300	-2.91957000
H	2.40099700	3.58259000	-2.04069200
H	2.04775700	2.53921600	-3.41017300
H	0.44032200	2.52189000	-0.77126700

Structure 11·EtMgCl(DME)_VII [B3LYP/6-31G(d)]

C	-1.34527600	-1.38614700	-0.17041700
C	-2.18489300	-2.53277900	-0.24566800
C	-3.52810500	-2.44750300	0.01429900
C	-4.12414800	-1.20757600	0.36541600
C	-3.30649400	-0.03279900	0.42740300
C	0.11696000	-1.53840800	-0.39572700
O	0.95831400	-0.76511700	0.05677000
Cl	3.79869100	0.26051500	-1.79165300
H	-1.73312400	-3.48177000	-0.50805400
H	-4.15298000	-3.33442100	-0.04286400
C	2.86628700	1.77633200	1.96202100
H	3.83046500	1.53598800	2.44715200
C	-1.91740300	-0.15675900	0.13659300
C	-3.90263700	1.20631200	0.78720000
C	-5.24961500	1.27988600	1.06129400
H	-5.69312200	2.23075300	1.34237600
C	-6.06206400	0.12282000	0.98859600
H	-7.12368400	0.19681500	1.20636000
C	-5.50976700	-1.09183700	0.65114600
H	-6.12747300	-1.98465100	0.60034600
H	-3.27704800	2.08761700	0.86816000
O	0.42214500	-2.61620700	-1.10021400
C	1.83205800	-2.84757400	-1.37520100
H	1.85018300	-3.76335600	-1.96454600
H	2.24985700	-2.00286000	-1.92699300
H	2.37660700	-2.96510700	-0.43681300
H	2.10990600	1.49425800	2.71803000
Mg	2.64998200	0.53753100	0.22939400
O	3.60829700	-1.30817700	1.21449600
C	5.03244800	-1.39532600	1.09669600
H	5.27257100	-1.15772700	0.06016600
H	5.51914900	-0.67574300	1.76798100
H	5.36765600	-2.41128300	1.34637200
C	3.16015900	-1.57706000	2.54193800
H	3.46624000	-2.58729700	2.84738400
H	3.56071700	-0.83985800	3.24781500
H	2.07074400	-1.51175200	2.53368200
O	-1.17378600	1.01487300	0.22050000
S	-0.41416600	1.64152900	-1.14801800
O	0.94881200	1.96303400	-0.73332800
O	-0.69404400	0.77132000	-2.28135700
C	-1.31503600	3.18608700	-1.30332400
H	-0.86368300	3.72661800	-2.13848800
H	-2.36248800	2.95986700	-1.50692100
H	-1.19385200	3.74623100	-0.37507000
C	2.80290100	3.30314700	1.76796300
H	3.58374900	3.65604100	1.07984900
H	1.84447000	3.61518900	1.32969300
H	2.92410600	3.88014300	2.70173700

Structure 11·EtMgCl(DME)_VIII [B3LYP/6-31G(d)]

C	0.94623900	-1.21963100	0.82545300
C	1.71787600	-2.40637300	0.96008900
C	2.96433700	-2.50677300	0.39734900
C	3.51793300	-1.42936700	-0.34226200
C	2.76949600	-0.21452600	-0.47397200
C	-0.43683200	-1.19470400	1.36341400
O	-1.37385500	-0.56679400	0.87183800
Cl	-1.13055700	-1.26967500	-2.50918300
H	1.28989300	-3.23913700	1.50519700
H	3.53754700	-3.42388500	0.50027300
C	-4.45785400	-1.41806600	-0.12462900
C	1.49291100	-0.13736400	0.15066300
C	3.31352300	0.85289000	-1.23907000
C	4.55098500	0.72956900	-1.82874000
H	4.95036500	1.54625400	-2.42330600
C	5.30239100	-0.46141600	-1.68130500
H	6.27772300	-0.54341000	-2.15243700
C	4.79408800	-1.51608400	-0.95826100
H	5.35967900	-2.43832800	-0.85452900

H	2.72354900	1.75081800	-1.38187200
O	-0.58952400	-1.97254500	2.42891400
C	-1.92279900	-2.04533300	2.98755300
H	-1.84852600	-2.76964200	3.79775100
H	-2.21245800	-1.06383800	3.36857100
H	-2.63799600	-2.37118700	2.22979900
Mg	-2.61355500	-0.62306700	-0.85043300
O	-2.82545300	1.43957600	-1.19879100
C	-2.01555800	2.20927200	-2.09763100
H	-1.41194800	1.49405900	-2.65716200
H	-2.66163400	2.77683100	-2.77938900
H	-1.37518000	2.89222400	-1.52967100
C	-3.67554800	2.24003400	-0.37193900
H	-3.07135300	2.88042200	0.27983200
H	-4.33596800	2.85358900	-0.99758700
H	-4.27554600	1.55073300	0.22444900
O	0.80868800	1.07091100	0.02479400
S	0.59737000	2.05906100	1.36147300
O	-0.47325600	2.96082200	0.96238300
O	0.51548700	1.24435200	2.56871300
C	2.15129300	2.96632300	1.39112800
H	2.10837400	3.63135600	2.25666000
H	2.97351900	2.25683800	1.49466900
H	2.23782200	3.54117700	0.46865400
H	-4.29736300	-2.48243000	0.12635700
C	-5.68612100	-1.32927700	-1.05253300
H	-5.50688100	-1.84025800	-2.00824300
H	-6.60244100	-1.77310000	-0.62664700
H	-5.93542500	-0.28715300	-1.30215600
H	-4.71640500	-0.95123900	0.84388900

Structure 11·EtMgCl(DME)_X [B3LYP/6-31G(d)]

C	0.94647300	-1.05422200	1.06475500
C	1.74907400	-2.19423200	1.34621600
C	2.93436900	-2.39331700	0.68589000
C	3.39580300	-1.46466200	-0.28449500
C	2.61999900	-0.29081100	-0.55755700
C	-0.37687500	-0.93031500	1.71725600
O	-1.41792100	-0.56216800	1.16685100
Cl	-1.10631500	-0.87641300	-2.39965100
H	1.39775700	-2.91024200	2.08062300
H	3.53498000	-3.27381100	0.89702900
C	-3.38570500	1.88090200	-0.38667100
C	1.40095600	-0.11473900	0.15046300
C	3.08220800	0.63877600	-1.52583200
C	4.26327400	0.41476200	-2.19440300
H	4.60514200	1.12682400	-2.93978900
C	5.03712300	-0.73926600	-1.92222800
H	5.96896600	-0.89910100	-2.45743600
C	4.61241100	-1.65731800	-0.98920600
H	5.20148000	-2.54646300	-0.77989500
H	2.48433700	1.51571700	-1.73907300
O	-0.36811500	-1.33015000	2.98297500
C	-1.61624000	-1.23690200	3.70327000
H	-1.38996300	-1.59301900	4.70748300
H	-1.95154600	-0.19826200	3.72382700
H	-2.37795500	-1.86166800	3.23107900
Mg	-2.27020600	0.06559200	-0.62576600
O	-3.79769700	-1.47653400	-0.57144900
C	-3.37984700	-2.84309400	-0.47765900
H	-2.67013800	-2.90090800	0.34870500
H	-4.24686500	-3.48092300	-0.26386800
H	-2.88950500	-3.15976300	-1.40446400
C	-4.77642300	-1.28634400	-1.60306400
H	-4.35684500	-1.55540700	-2.57947700
H	-5.66163800	-1.89838700	-1.39032000
H	-5.04776600	-0.22995900	-1.59128800
O	0.65974700	1.04157300	-0.08797600
S	0.89471000	2.30787300	1.01734800
O	0.26394100	1.92647000	2.27969300
O	2.29980100	2.69731400	0.98888300
C	-0.11301800	3.49776900	0.13895400
H	-0.12608000	4.40061800	0.75368600
H	0.35231600	3.69403500	-0.82757900
H	-1.11693500	3.08703400	0.02295800
H	-4.39523800	1.55181600	-0.07799500
H	-3.05434900	2.47579900	0.48259300
C	-3.54395300	2.81821000	-1.60180200
H	-2.58005900	3.22869600	-1.93596500
H	-3.95577800	2.28856900	-2.47209300
H	-4.20567900	3.68153400	-1.41819700

Structure 11·EtMgCl(DME)_XI [B3LYP/6-31G(d)]

C	-0.92693400	0.92792300	1.04209600
C	-1.60665900	2.12003400	1.41452400
C	-2.81125700	2.44495900	0.84577400
C	-3.42025500	1.59434300	-0.11421200
C	-2.77113000	0.36910000	-0.47699600
C	0.41284000	0.65609800	1.61341000
O	1.37823600	0.18873400	1.00585100
Cl	1.22507900	1.90623900	-1.98990400
H	-1.14289800	2.77794900	2.14033800
H	-3.31360100	3.36748900	1.12330500
C	2.75405000	-1.86386400	-1.56234700
C	-1.52243100	0.06836300	0.13069000
C	-3.38504700	-0.48735200	-1.42906300
C	-4.58802700	-0.14158400	-1.99962300
H	-5.04770000	-0.80005300	-2.73090100
C	-5.23387800	1.06686600	-1.64261600
H	-6.18445800	1.32353700	-2.10177400
C	-4.66284100	1.91403900	-0.72075300
H	-5.15366500	2.84346100	-0.44407000
H	-2.89052200	-1.41114100	-1.70192800
O	0.50502600	1.02071100	2.88828400
C	1.77664000	0.80792900	3.53299500
H	1.64857600	1.18721300	4.54620900
H	2.00919500	-0.25897400	3.54488700
H	2.56516500	1.35376400	3.00961900
Mg	2.20114900	0.10173400	-0.92051700
O	4.04148200	1.01156500	-0.28359800
C	5.07843800	0.22740900	0.30390900
H	4.69405900	-0.78805900	0.40847200
H	5.96418800	0.21750000	-0.34332600
H	5.35088300	0.63092600	1.28831500
C	4.43493100	2.36460900	-0.54279800
H	4.69874600	2.86610500	0.39769400
H	5.29810400	2.38050600	-1.22002300
H	3.58156100	2.85372400	-1.01271100
O	-0.89149700	-1.12356900	-0.22640200
S	-1.10581000	-2.42717900	0.83198100
O	-0.45583700	-2.10120900	2.10010800
O	-2.51086900	-2.81830300	0.81076600
C	-0.11653600	-3.59163600	-0.10050000
H	-0.10856800	-4.51563400	0.48210600
H	-0.59339900	-3.75116900	-1.06824800
H	0.89015300	-3.19128800	-0.22316300
H	2.98853700	-2.53938700	-0.71811600
C	3.92832000	-1.92024200	-2.56288500
H	4.85677700	-1.51328800	-2.13625200
H	4.17019700	-2.93881400	-2.91041100
H	3.71629000	-1.32603500	-3.46211200
H	1.88154300	-2.32571600	-2.05472700

Structure 11-TSOMe-I [B3LYP/6-31G(d)]

C	-0.05227400	1.38050900	-0.07446200
C	0.89969900	2.44616900	0.03379800
C	2.23951600	2.21339600	0.09200800
C	2.74725800	0.87378500	0.02638000
C	1.84571400	-0.22338900	-0.09666800
C	-1.45717000	1.65750000	0.01354600
O	-2.35442000	0.78626000	0.20367300
O	-0.34420400	-0.93751600	-0.91823200
Cl	-3.21811900	-2.92344100	0.01799300
H	0.51486300	3.45864900	0.07980900
H	2.94269600	3.03716700	0.17050800
Mg	-1.92529000	-1.11985700	0.34586700
C	-0.18310700	-0.98383800	1.84154800
H	0.64013200	-1.69472000	1.76887700
H	-1.04560800	-1.58250100	2.22735700
C	0.40998400	0.02397000	-0.08548600
C	2.36473400	-1.53111300	-0.21836700
C	3.72843600	-1.76179800	-0.21058600
H	4.10873800	-2.77505300	-0.30261200
C	4.62120100	-0.68151700	-0.07773100
H	5.69275600	-0.86187000	-0.06926300
C	4.13678800	0.60722100	0.03849400
H	4.82402300	1.44451700	0.13130100
H	1.67551500	-2.36446600	-0.31279700
O	-1.80762100	2.94311300	-0.07352800
C	-3.21020400	3.24771400	0.02352400
H	-3.27465900	4.32737900	-0.11101900
H	-3.76816200	2.72754600	-0.75820200

H	-3.60040500	2.96012800	1.00315400
C	0.08798600	0.14994800	2.81252600
H	0.12133700	-0.19731000	3.85489300
H	1.04698100	0.63170400	2.59696300
H	-0.68526300	0.92781500	2.75850100
S	-0.46252200	-0.67148900	-2.63153700
O	-1.70966100	0.05142300	-2.85500100
O	0.81264700	-0.16950400	-3.11752400
C	-0.68299600	-2.40293800	-3.06237700
H	-0.88126700	-2.42746200	-4.13665000
H	0.23833200	-2.93547900	-2.82464200
H	-1.53352300	-2.79864200	-2.50169500

Structure 11-TSOMe-II [B3LYP/6-31G(d)]

C	-0.09745600	1.64495500	-0.07155900
C	-1.09113300	2.67631800	-0.11285400
C	-2.41622000	2.39760800	-0.24897000
C	-2.87532800	1.03736800	-0.29010600
C	-1.93345300	-0.03249900	-0.24420100
C	1.28678000	1.97597300	-0.05512300
O	2.23175300	1.15643100	-0.29189900
O	0.32248400	-0.77239700	0.33440300
Cl	3.36329300	-2.21966000	-1.27242200
H	-0.74996200	3.70338900	-0.04733200
H	-3.14972600	3.19764500	-0.28346300
Mg	1.81189500	-0.62104700	-1.04627100
C	0.02887900	-0.18595700	-2.38046500
C	-0.50803200	0.27843700	-0.26814500
C	-2.40060900	-1.36389900	-0.20438200
C	-3.75831500	-1.64126100	-0.22623500
H	-4.09950500	-2.67137300	-0.18640200
C	-4.68803100	-0.59029800	-0.29650000
H	-5.75250400	-0.80815700	-0.31711400
C	-4.25165300	0.72269400	-0.32499300
H	-4.96991900	1.53812500	-0.35832700
H	-1.68755400	-2.17664000	-0.13326700
O	1.58959600	3.25549000	0.20316600
C	2.97657200	3.62598900	0.15459800
H	2.99383800	4.69032100	0.38948100
H	3.55376600	3.06329300	0.89249000
H	3.39225700	3.44741300	-0.84047600
S	0.27951400	-1.08398100	2.04915200
O	-0.24505800	0.09507600	2.71955800
O	-0.32880900	-2.39692400	2.19872900
C	2.05607100	-1.21475200	2.30173300
H	2.19322900	-1.48724200	3.35103900
H	2.45517900	-1.99407700	1.64793500
H	2.50853400	-0.24579600	2.08719100
H	-0.77232300	0.52045300	-2.58681000
C	-0.27529500	-1.56827500	-2.95406800
H	0.54091700	-2.28979000	-2.81267900
H	-1.17103400	-1.98922800	-2.48564000
H	-0.47158400	-1.52170400	-4.03603200
H	0.91904600	0.27804600	-2.86464500

Structure 11-TSOMe-III [B3LYP/6-31G(d)]

C	-0.11241400	1.50458300	0.34127700
C	-1.10842100	2.48719500	0.66265700
C	-2.43311700	2.26251600	0.46020000
C	-2.88699700	1.00305500	-0.06025100
C	-1.94510200	-0.01359200	-0.38740600
C	1.27245900	1.80297200	0.49506600
O	2.22344200	1.07365500	0.06889700
O	0.27216800	-0.94282200	0.08039300
Cl	3.42662200	-1.99824700	-1.61756300
H	-0.76579900	3.43124700	1.07108200
H	-3.16919000	3.02011100	0.71230600
Mg	1.87189200	-0.48220300	-1.08109500
C	0.16398800	0.29259400	-2.37887800
C	-0.51377600	0.26419600	-0.26689000
C	-2.40891200	-1.26133200	-0.85554800
C	-3.76383400	-1.50651200	-1.00300600
H	-4.10238600	-2.47447400	-1.36035600
C	-4.69662000	-0.50248400	-0.68943100
H	-5.75990400	-0.69374900	-0.80674100
C	-4.26269700	0.72685100	-0.22725300
H	-4.98155100	1.50246600	0.02513000
H	-1.69116000	-2.03877400	-1.09411400
O	1.56920800	2.95183200	1.11678100
C	2.95887800	3.29601600	1.23590700
H	2.97060600	4.24453400	1.77293400
H	3.50040100	2.53182300	1.79899300
H	3.41650500	3.40959800	0.24982900
S	0.06937700	-1.72608000	1.61950000
O	-0.50492500	-0.76924000	2.55226000
O	-0.55821500	-3.00770100	1.33786400
C	1.81452600	-1.98117200	1.97865200
H	1.85269800	-2.53581200	2.91945500
H	2.26665000	-2.56415900	1.17259000
H	2.29441900	-1.00706900	2.08347300
H	-0.87744500	0.11524300	-2.62825500
C	0.63092800	1.67963900	-2.79840000
H	0.31423300	2.43438500	-2.06544300
H	1.72260300	1.75693700	-2.89138700
H	0.20694700	1.97971900	-3.76627200
H	0.71030700	-0.51106700	-2.92326500

Structure 11-TSOMe-IV [B3LYP/6-31G(d)]

C	-0.17214800	1.49283100	0.27813200
C	-1.20917100	2.41512400	0.63497700
C	-2.52775900	2.09458500	0.52836100
C	-2.92416800	0.79621300	0.06643100
C	-1.93364300	-0.16660200	-0.28569100
C	1.19745900	1.92080100	0.26211100
O	2.14491500	1.28990700	-0.28923100
O	0.35487400	-0.92919000	0.11110500
Cl	3.30320300	-2.08931200	-1.63616800
H	-0.90830800	3.39540100	0.98685100
H	-3.29643500	2.80917900	0.80707700
Mg	1.85912200	-0.43768200	-1.16772100
C	0.01557300	0.10503300	-2.43058600
C	-0.52595600	0.20419000	-0.23968000
C	-2.34009800	-1.46032400	-0.68024700
C	-3.67930800	-1.80072400	-0.74028400
H	-3.97270800	-2.79990000	-1.04908200
C	-4.66042300	-0.84813200	-0.40576200
H	-5.71292600	-1.11389300	-0.45503300
C	-4.28653500	0.42210600	-0.01124600
H	-5.04145700	1.15675900	0.25764400
H	-1.58339900	-2.19222500	-0.94501200
O	1.45054300	3.09645100	0.84274300
C	2.81400000	3.55507300	0.82626700
H	2.80243100	4.49501200	1.37790600
H	3.46661600	2.82858000	1.31541000
H	3.15372100	3.71775200	-0.19978700
S	0.57589100	-1.35013700	1.78213700
O	1.79729500	-0.68168200	2.21726200
O	-0.68618300	-1.17497800	2.48261100
C	0.91378300	-3.08984100	1.47988000
H	1.20079100	-3.51867300	2.44301800
H	0.00253700	-3.55487300	1.10249100
H	1.73339600	-3.16679000	0.76109900
H	0.89862800	-0.18531600	-3.05236000
C	-0.43451700	1.49030000	-2.85494800
H	-1.41485700	1.73114700	-2.43193800
H	0.26436700	2.26752500	-2.51790000
H	-0.51535000	1.58308400	-3.94723200
H	-0.72928000	-0.66795400	-2.62204400

Structure 11-TSOMe-V [B3LYP/6-31G(d)]

C	0.11312900	1.49915300	-0.36164400
C	1.13054800	2.43713000	-0.73595000
C	2.45372400	2.16629900	-0.57813700
C	2.87834900	0.90161400	-0.04909600
C	1.91080600	-0.07717300	0.32429600
C	-1.26321500	1.86143800	-0.43825200
O	-2.21963100	1.18534200	0.05655800
O	-0.35512800	-0.92653800	-0.06681500
Cl	-3.47093400	-1.88755600	1.70171200
H	0.80861800	3.38788500	-1.14555600
H	3.20751900	2.89159600	-0.86959900
Mg	-1.88353900	-0.40342500	1.16365300
C	-0.06466400	0.27455700	2.38682400
H	0.69181000	-0.46875200	2.63803900
H	-0.95530300	-0.00430900	3.00587600
C	0.49029800	0.24786900	0.23996800
C	2.34782600	-1.34105400	0.77951000
C	3.69656300	-1.63308700	0.88227300
H	4.01300000	-2.61157600	1.23096400
C	4.65338800	-0.66294800	0.53313600
H	5.71252700	-0.89143700	0.61642300
C	4.24870700	0.57723400	0.07541400

H	4.98578800	1.32403400	-0.20905400
H	1.61234700	-2.09479500	1.03851800
O	-1.54197600	3.01729900	-1.05484000
C	-2.91799700	3.42889300	-1.09165100
H	-2.91669200	4.37262800	-1.63711700
H	-3.53018700	2.68790400	-1.61169600
H	-3.30726800	3.57250800	-0.08044800
C	0.33545800	1.69253200	2.74869600
H	0.37358100	1.84484300	3.83614500
H	1.32373200	1.93482800	2.34640500
H	-0.36947800	2.43101700	2.34386300
S	-0.23580400	-1.73246500	-1.60431100
O	0.34572300	-0.80815000	-2.56510100
O	0.35045800	-3.03488000	-1.32875700
C	-1.99990200	-1.92221000	-1.90450600
H	-2.08936700	-2.49629500	-2.83007200
H	-2.45125100	-2.46568400	-1.07078700
H	-2.44185200	-0.93147700	-2.01952800

Structure 11-TSCO-I [B3LYP/6-31G(d)]

C	0.02373400	1.24670100	-0.31791400
C	0.91307500	2.34572700	-0.17823800
C	2.26805300	2.16005500	-0.06109700
C	2.82587800	0.85889800	-0.01499300
C	1.95456900	-0.27475500	-0.12495800
C	-1.45930900	1.50183900	-0.40777000
O	-2.20904400	0.84161900	-1.21170600
O	-0.29459700	-1.15002900	-0.42582500
Cl	-3.48827300	-2.60836700	0.52320700
H	0.49237900	3.34291800	-0.17510300
H	2.92938000	3.01843900	0.02192300
Mg	-2.40580900	-0.69064800	-0.00243600
C	-2.05452300	0.71227000	1.73277700
H	-2.30400900	-0.27582500	2.17721800
H	-2.98453900	1.29682900	1.78707700
C	0.56936500	-0.03110500	-0.33713900
C	2.51463100	-1.57319600	0.01219200
C	3.86539400	-1.74345600	0.20853400
H	4.27130400	-2.74466700	0.32186600
C	4.73158600	-0.62552600	0.27140900
H	5.79737000	-0.77630900	0.41633500
C	4.21818600	0.64573400	0.16769600
H	4.86971900	1.51303000	0.23667900
H	1.86227300	-2.43647300	-0.00047600
O	-1.74332000	2.79515000	-0.14268000
C	-3.06870700	3.23407000	-0.47137700
H	-3.09354800	4.29154100	-0.20609200
H	-3.26782000	3.09608900	-1.53609000
H	-3.81219200	2.68329300	0.11203600
C	-0.98051200	1.34301000	2.61269300
H	-0.74074000	2.35942600	2.27966600
H	-1.29049700	1.41618900	3.66566400
H	-0.04842800	0.76389000	2.59499000
S	-0.42547900	-2.01221100	-1.94752500
O	-1.79479300	-1.75032600	-2.37699000
O	0.72821300	-1.68424600	-2.76495600
C	-0.36220600	-3.68715200	-1.30118600
H	-0.57447700	-4.33726100	-2.15372200
H	0.62895900	-3.88924300	-0.89775700
H	-1.15087100	-3.77418700	-0.54863100

Structure 11-TSCO-II [B3LYP/6-31G(d)]

C	-0.27295300	1.48472600	0.36829500
C	-1.09777000	2.63882200	0.45030900
C	-2.44794000	2.57101400	0.21409200
C	-3.06227400	1.35491800	-0.17521900
C	-2.25403700	0.17701600	-0.29923400
C	1.20954700	1.61772400	0.61410100
O	1.86809700	0.72643100	1.25706300
O	-0.06867200	-0.87612800	-0.12314300
Cl	3.12636900	-2.17347300	-1.34062300
H	-0.63122000	3.57890500	0.71495300
H	-3.06164200	3.46327400	0.30606200
Mg	2.10101900	-0.43855000	-0.31105800
C	1.74941800	1.33453700	-1.66406900
H	1.37576200	0.53864800	-2.33987800
C	-0.87551100	0.27752500	0.03637700
C	-2.86463300	-1.01371500	-0.77545000
C	-4.20710000	-1.04948100	-1.07463800
H	-4.65164100	-1.96809400	-1.44691900
C	-5.01373400	0.10162900	-0.90911500
H	-6.07397900	0.05557700	-1.14010500
C	-4.44815000	1.27749400	-0.47486600
H	-5.05212400	2.17446900	-0.36471900
H	-2.25574600	-1.89302700	-0.93921500
O	1.57353600	2.91465000	0.71873600
C	2.83626600	3.17297200	1.35262400
H	2.94209000	4.25842500	1.33992400
H	2.83477900	2.79751400	2.37841700
H	3.65550300	2.70886200	0.79898900
S	-0.02494900	-2.08915900	1.12909300
O	1.35583600	-2.03592100	1.60152000
O	-1.16338900	-1.89948800	2.00935200
C	-0.18669400	-3.55010500	0.09594900
H	-0.01974600	-4.39937400	0.76326400
H	-1.18567300	-3.58859000	-0.33582500
H	0.59933100	-3.50139600	-0.66243100
C	3.16267900	1.76415000	-2.08148100
H	3.50754900	2.61824400	-1.48627500
H	3.90785000	0.96323700	-1.97008400
H	3.21007400	2.07752500	-3.13605600
H	1.05157500	2.16227200	-1.79657800

Structure 11-TSCO-III [B3LYP/6-31G(d)]

C	-0.50494700	1.28572500	0.30331300
C	-1.26609600	2.45020600	0.59801100
C	-2.63671000	2.45011900	0.50541300
C	-3.34648000	1.29197700	0.09656000
C	-2.60830700	0.10883500	-0.23507700
C	0.98009600	1.29649900	0.54335200
O	1.51737400	0.36246400	1.24409400
O	-0.47408100	-0.95511000	-0.57518000
Cl	4.76123600	-0.85396000	-0.19492300
H	-0.73523900	3.34146600	0.90845000
H	-3.19629700	3.34978500	0.74759300
Mg	2.53267200	-0.52496500	-0.22336000
C	1.68035000	0.87832900	-1.75491900
H	1.91292800	-0.04226300	-2.33896300
C	-1.19419300	0.15089700	-0.09678300
C	-3.30812300	-1.04328200	-0.68800400
C	-4.68151300	-1.02500000	-0.78434900
H	-5.20715000	-1.90922200	-1.13312700
C	-5.41625300	0.13596800	-0.44122900
H	-6.49932400	0.13059500	-0.52377800
C	-4.76176900	1.26874000	-0.01440100
H	-5.31841700	2.16703500	0.23986500
H	-2.75184700	-1.93187500	-0.96477200
O	1.45323000	2.55355100	0.61522500
C	2.77328300	2.71126900	1.16635900
H	2.97065900	3.78259200	1.12842400
H	2.80389700	2.34500200	2.19468100
H	3.51005400	2.17175000	0.56437200
S	-0.00466000	-2.28933500	0.26963400
O	-0.77301900	-3.43303000	-0.18859800
O	1.46364000	-2.31302700	0.04292500
C	-0.34977100	-1.95592100	1.99887300
H	0.00763900	-2.83767300	2.53628400
H	0.20033600	-1.05812000	2.28455500
H	-1.42921200	-1.84582400	2.11626000
C	2.60564900	2.00351600	-2.21900800
H	2.39388400	2.93286100	-1.67639800
H	3.66388500	1.76023200	-2.06402700
H	2.48237400	2.23028600	-3.28934100
H	0.64486800	1.09360500	-2.02661400

Structure 11-TSCO-IV [B3LYP/6-31G(d)]

C	-0.14896600	1.41468500	0.45020900
C	-0.90013700	2.61064400	0.59879500
C	-2.24729400	2.64082800	0.33681200
C	-2.92835000	1.49212900	-0.14038400
C	-2.19588700	0.27235200	-0.31827200
C	1.35054800	1.43844400	0.63126700
O	1.98810200	0.40170200	1.08189300
O	-0.08184900	-0.92207200	-0.15831100
Cl	3.13582900	-2.16089800	-1.52147200
H	-0.38104300	3.50161900	0.92896900
H	-2.80729800	3.56194200	0.47601100
Mg	1.97008700	-0.43781900	-0.69067700
C	1.75340200	1.60305500	-1.55911000
H	1.28366700	0.96488700	-2.34325700
C	-0.81732200	0.26944400	0.03733500
C	-2.86879500	-0.85857100	-0.85583500

C	-4.20660500	-0.78796100	-1.17396600
H	-4.70421200	-1.65946700	-1.58954400
C	-4.93879700	0.40549300	-0.96968700
H	-5.99536100	0.43974700	-1.21974000
C	-4.30952900	1.52076200	-0.46695300
H	-4.85870900	2.44713800	-0.31874400
H	-2.32378400	-1.77881600	-1.02792700
O	1.78285900	2.66948400	1.00452900
C	3.05651200	2.73196600	1.66279200
H	3.22867200	3.79394200	1.84350800
H	3.02920200	2.18406800	2.60775300
H	3.85120000	2.32393800	1.03431800
S	-0.41427400	-2.25222400	0.98456300
O	-1.27155000	-1.69255800	2.01667000
O	-0.82473400	-3.36020700	0.13649500
C	1.22594700	-2.56800100	1.64419900
H	1.08633300	-3.36851900	2.37561400
H	1.87820600	-2.90000100	0.83201900
H	1.58574000	-1.65185800	2.11328800
C	3.20187100	1.94281100	-1.93095900
H	3.61473800	2.67894900	-1.23292700
H	3.87447600	1.07207400	-1.92166400
H	3.27970300	2.37704900	-2.93837600
H	1.13451200	2.49870200	-1.54681100

Structure 11-TSCO-V [B3LYP/6-31G(d)]

C	0.33934300	1.51163200	-0.35957300
C	1.28192400	2.57402400	-0.42346900
C	2.62381900	2.35242000	-0.24315600
C	3.11767200	1.06074700	0.06722800
C	2.19131600	-0.02758100	0.18073500
C	-1.12203000	1.80810200	-0.56482200
O	-1.88769600	1.01078500	-1.21905300
O	-0.10373000	-0.82732000	0.07472100
Cl	-3.39100700	-1.79063800	1.39717100
H	0.91208400	3.56877600	-0.63509000
H	3.32652600	3.17765600	-0.32304600
Mg	-2.24086400	-0.18180500	0.29040300
C	-1.73933700	1.55818900	1.67616200
C	0.81969400	0.23567000	-0.09039400
C	2.68710000	-1.29696000	0.58018100
C	4.02918800	-1.49109100	0.81389100
H	4.38553900	-2.46853200	1.12640200
C	4.94924200	-0.42726600	0.65815600
H	6.00689500	-0.59760200	0.83688800
C	4.49779100	0.82139400	0.29962100
H	5.19119100	1.65230300	0.19819500
H	1.99320500	-2.11214600	0.73687500
O	-1.33421500	3.14237700	-0.65617000
C	-2.65206700	3.54503700	-1.04799500
H	-2.61572100	4.63364700	-1.10460400
H	-2.91933700	3.11566000	-2.01539300
H	-3.38387600	3.23507200	-0.29461900
S	-0.35156600	-1.98832500	-1.18933000
O	-1.74985000	-1.76871500	-1.56049800
O	0.73627600	-1.90309600	-2.14561500
C	-0.29296700	-3.48847600	-0.20294300
H	-0.60463000	-4.29279900	-0.87399700
H	0.72112400	-3.65585600	0.15703200
H	-1.01504700	-3.36871500	0.60926800
C	-0.86694400	0.92691300	2.76677900
H	-1.09158600	-0.13606100	2.92299700
H	0.20046000	1.00517000	2.52223000
H	-1.00203300	1.42058600	3.74156200
H	-1.59821900	2.63880800	1.65984500
H	-2.81276600	1.41097600	1.91850600

Structure 11-TSCO-VI [B3LYP/6-31G(d)]

C	0.54197600	1.37415100	-0.19824500
C	1.36267900	2.52164400	-0.37832800
C	2.73146400	2.44139800	-0.29193700
C	3.38010600	1.21297700	-0.00471300
C	2.58134600	0.04206900	0.20875800
C	-0.94228700	1.48566100	-0.42307500
O	-1.52995400	0.66295200	-1.21655700
O	0.39376300	-0.93801000	0.44685000
Cl	-4.81096400	-0.54239100	0.11980800
H	0.87872800	3.46580300	-0.59470600
H	3.33711000	3.33083900	-0.44456100
Mg	-2.56883100	-0.31299700	0.18123200
C	-1.72037700	1.00455700	1.79211800
C	1.17149600	0.17189100	0.08227600
C	3.21977800	-1.18487000	0.53881700
C	4.59220900	-1.24777700	0.63017900
H	5.07091500	-2.18909200	0.88425800
C	5.38653600	-0.09744200	0.40388900
H	6.46779600	-0.16723500	0.48073500
C	4.79222400	1.10528900	0.09743500
H	5.39514800	1.99467300	-0.06670100
H	2.61784100	-2.06718000	0.72560600
O	-1.34519900	2.76889800	-0.35289100
C	-2.66698600	3.05694300	-0.83872400
H	-2.79906400	4.12840200	-0.68718400
H	-2.75284900	2.79994400	-1.89673200
H	-3.41717000	2.50129900	-0.26761500
S	-0.14542200	-2.15245200	-0.52787100
O	0.56579700	-3.37493200	-0.19862900
O	-1.61124300	-2.12271400	-0.28733300
C	0.20655600	-1.65962900	-2.21733600
H	-0.19387600	-2.46486200	-2.83811300
H	-0.30316000	-0.71321800	-2.40402100
H	1.28931000	-1.58712500	-2.33365100
C	-1.85963600	-0.14675700	2.81777600
H	-2.76191100	-0.76250000	2.67018100
H	-0.99511500	-0.82046700	2.79364300
H	-1.93800400	0.23691900	3.84687600
H	-0.83142200	1.58530600	2.04024800
H	-2.57298600	1.69416600	1.88128800

Structure 11-TSCO-VII [B3LYP/6-31G(d)]

C	0.20144100	1.44257600	-0.48119200
C	1.07152700	2.55485400	-0.63399900
C	2.42135600	2.43625100	-0.41578300
C	2.99056200	1.21234800	0.02012400
C	2.13757400	0.07490600	0.20568800
C	-1.28973700	1.62548300	-0.61628500
O	-2.04662000	0.66087300	-1.05224500
O	-0.09918300	-0.88071400	0.10971300
Cl	-3.43075900	-1.75046800	1.56022600
H	0.64152800	3.50160200	-0.93553900
H	3.07230800	3.29486800	-0.55901600
Mg	-2.07954200	-0.18104600	0.70795000
C	-1.66845400	1.85093800	1.54295500
C	0.75505900	0.22615600	-0.10280700
C	2.70179600	-1.12980400	0.70621300
C	4.04880000	-1.20751700	0.98175900
H	4.46281100	-2.13391100	1.36937700
C	4.89788300	-0.09576900	0.76967500
H	5.95916900	-0.17810100	0.98626100
C	4.37623400	1.08827700	0.30200500
H	5.01624300	1.95351300	0.14861300
H	2.06658100	-1.98917800	0.88391400
O	-1.59124900	2.89368200	-1.00107300
C	-2.94994500	3.13410400	-1.38430900
H	-2.98671600	4.18750800	-1.66533700
H	-3.23587100	2.50187500	-2.22726300
H	-3.62859200	2.94921400	-0.54521100
S	0.04287600	-2.22677000	-1.05382000
O	0.92830600	-1.75907900	-2.10763400
O	0.34827200	-3.38274000	-0.22531900
C	-1.64127900	-2.34489600	-1.66521200
H	-1.61655400	-3.14697900	-2.40775600
H	-2.30279900	-2.61024200	-0.83614700
H	-1.90673500	-1.38682600	-2.11311000
C	-0.90161100	1.20732900	2.71579500
H	-1.25964000	0.20140600	2.99381500
H	0.16803800	1.12034500	2.49227700
H	-0.99198300	1.80558400	3.63386300
H	-1.33671700	2.87801600	1.41014000
H	-2.75312700	1.90250300	1.75770300

Structure 11-TSCO-VIII [B3LYP/6-31G(d)]

C	0.46628200	1.29054800	-0.33245700
C	1.27571200	2.41880100	-0.64286100
C	2.64621100	2.35212800	-0.58735100
C	3.30950800	1.15990500	-0.19801200
C	2.52387800	0.01334800	0.15181800
C	-1.01865900	1.37902300	-0.52992600
O	-1.63234200	0.47924900	-1.20616900
O	0.34861900	-0.94840200	0.53812000
Cl	-4.84374000	-0.67689100	0.28742600
H	0.78074300	3.33580600	-0.93727000

H	3.24222300	3.22426500	-0.84279300
Mg	-2.60604900	-0.40307100	0.29775500
C	-1.82518900	1.04027900	1.80081300
H	-2.22505300	0.20825800	2.42458200
H	-2.63479500	1.78340600	1.76840600
C	1.10995100	0.12327900	0.04876800
C	3.17851500	-1.17145900	0.58720400
C	4.55325500	-1.21963900	0.64881900
H	5.04414100	-2.12852500	0.98450600
C	5.33397700	-0.09524500	0.28681800
H	6.41727800	-0.15272800	0.34193100
C	4.72420600	1.06836800	-0.12333900
H	5.31698300	1.93907700	-0.39144600
H	2.58765800	-2.03273300	0.87779000
O	-1.43152700	2.65706800	-0.55897700
C	-2.77099600	2.89238600	-1.02743200
H	-2.90555900	3.97271300	-0.97387000
H	-2.88716300	2.53495900	-2.05280500
H	-3.49663900	2.38872100	-0.38203800
C	-0.62758500	1.61351700	2.55255200
H	-0.24248400	2.51689100	2.06457000
H	-0.88124600	1.89507700	3.58552800
H	0.20074200	0.89701200	2.61627300
S	-0.18042600	-2.26277700	-0.30537500
O	0.56586100	-3.43440000	0.11711200
O	-1.64058100	-2.23851000	-0.03451600
C	0.12078000	-1.91969900	-2.04093900
H	-0.28304500	-2.78260900	-2.57613600
H	-0.40885400	-1.00128400	-2.29876600
H	1.19873100	-1.84315400	-2.19314900

Structure 11-TSCO-IX [B3LYP/6-31G(d)]

C	0.14333400	1.35250600	-0.51263200
C	0.97674200	2.47569500	-0.75753400
C	2.33312900	2.41420300	-0.55179600
C	2.94438600	1.24370300	-0.03717600
C	2.12997700	0.09429500	0.23261400
C	-1.35249700	1.47734100	-0.64777500
O	-2.07779400	0.47382800	-1.03332300
O	-0.06588300	-0.94879000	0.19821900
Cl	-3.33189800	-1.92916900	1.65436700
H	0.51449800	3.38551000	-1.11822300
H	2.95423300	3.28059600	-0.76370600
Mg	-2.05768000	-0.31891700	0.75755300
C	-1.83032000	1.75424900	1.54565100
H	-1.78657600	1.03871300	2.40268700
C	0.74268500	0.17840300	-0.07227700
C	2.73792600	-1.05753900	0.80341300
C	4.08857300	-1.07408600	1.06842200
H	4.53613100	-1.95919600	1.51122300
C	4.89945800	0.04836200	0.77472500
H	5.96478100	0.01361400	0.98423600
C	4.33627100	1.18196800	0.23681300
H	4.94676700	2.05479000	0.01969000
H	2.13236800	-1.92308500	1.04363800
O	-1.70504100	2.72126600	-1.05045500
C	-3.06063100	2.89251500	-1.48459900
H	-3.13860900	3.94234400	-1.76963200
H	-3.27906200	2.24482400	-2.33597100
H	-3.76004600	2.67237000	-0.67271300
S	0.13848000	-2.34762900	-0.89991600
O	1.01262200	-1.89514100	-1.96953000
O	0.48263400	-3.44772900	-0.01338600
C	-1.53510600	-2.56106400	-1.51552700
H	-1.47239600	-3.39623500	-2.21833800
H	-2.19248700	-2.81152900	-0.67848400
H	-1.83482700	-1.63795600	-2.01253700
C	-0.97226500	2.94813200	1.94237500
H	0.07277400	2.65870000	2.10077600
H	-0.98990200	3.71575000	1.16139500
H	-1.32327400	3.41927500	2.87100300
H	-2.88789600	2.04688000	1.45836500

Structure 13a_I [B3LYP/6-31G(d)]

C	-1.27343400	-0.50170500	0.01829800
C	-0.79512700	-1.82782400	0.24101600
C	0.54230500	-2.11899000	0.31811300
C	1.51310200	-1.09965200	0.13215600
C	1.06851100	0.23685000	-0.11907400
C	-2.74800500	-0.25521700	-0.07810400
O	-3.24918300	0.84383100	0.10622100
O	-0.69303900	1.80989000	-0.42774600
C	-0.96889000	2.64712900	0.70425900
H	-1.51494100	-2.62875000	0.37188900
H	0.87343400	-3.13629800	0.51009900
H	-1.17936800	3.63746500	0.29511000
H	-0.09518100	2.70174500	1.36654000
H	-1.84341200	2.28126500	1.24537400
C	-0.33427400	0.52065300	-0.14579400
C	2.03424800	1.25522300	-0.34163700
C	3.37991600	0.96702100	-0.29479100
H	4.10962600	1.75320600	-0.46799400
C	3.82120700	-0.35142000	-0.02791500
H	4.88601600	-0.56553000	0.00773700
C	2.90757800	-1.36121700	0.17693800
H	3.24201200	-2.37740000	0.37137700
H	1.68728300	2.25787800	-0.56376500
C	-3.64625900	-1.43810600	-0.42599300
H	-3.26499200	-2.00645600	-1.28112700
H	-3.72527100	-2.13061600	0.42156100
H	-4.64270400	-1.05275700	-0.64942800

Structure 13a_II [B3LYP/6-31G(d)]

C	-1.25922600	-0.61837400	-0.03131900
C	-0.71908400	-1.92725400	0.14582100
C	0.63032600	-2.15092900	0.20194800
C	1.54930600	-1.07424800	0.06473900
C	1.03909200	0.25114300	-0.11044700
C	-2.76025200	-0.53407900	-0.11588700
O	-3.42825300	-1.51286300	0.18892500
O	-0.83469200	1.74704200	-0.26098000
C	-0.92871500	2.47757800	0.96630600
H	-1.42957900	-2.74155600	0.23555500
H	1.01641300	-3.15793400	0.33861800
H	-1.28965800	3.47411900	0.70281100
H	0.04861300	2.55835900	1.45703400
H	-1.63592600	2.00107200	1.65710000
C	-0.37700400	0.45234700	-0.12483000
C	1.95202500	1.32557300	-0.28610200
C	3.31092100	1.10140300	-0.26611700
H	3.99951500	1.92964100	-0.40895200
C	3.81758700	-0.20532800	-0.06998900
H	4.89169600	-0.36896800	-0.05308800
C	2.95500400	-1.26779000	0.08656800
H	3.33997000	-2.27535400	0.22344000
H	1.55932800	2.32078800	-0.46341900
C	-3.45710600	0.71880500	-0.61621200
H	-3.46973200	1.49025100	0.16201300
H	-2.95582300	1.15210100	-1.48508600
H	-4.48850300	0.45096900	-0.85646100

Structure 13a·EtMgCl_I [B3LYP/6-31G(d)]

C	0.31274600	1.61977300	0.01412000
C	1.45490900	2.37860900	0.41268100
C	2.70772900	1.82488800	0.44381600
C	2.91266300	0.46500500	0.08651400
C	1.78884100	-0.32282200	-0.32398400
C	-1.03248600	2.24320800	0.05067900
O	-2.07187400	1.57201300	0.09893500
O	-0.55365200	-0.47243000	-0.83504100
C	-0.70744200	-0.47879500	-2.28442300
H	1.32300100	3.41142900	0.71488200
H	3.56070800	2.42059000	0.75672300
H	-1.59932600	-1.07314200	-2.47847800
H	0.18187400	-0.91970000	-2.74214800
H	-0.85266700	0.54446300	-2.64282400
Mg	-2.33238900	-0.48724700	0.47042600
C	-1.70437100	-0.92117800	2.45676800
C	0.50768300	0.29203300	-0.37271100
C	1.98096500	-1.69382900	-0.64922500
C	3.23769300	-2.25161600	-0.58932800
H	3.37505600	-3.30192200	-0.82864200
C	4.35355300	-1.46905300	-0.20531900
H	5.33903900	-1.92420100	-0.16489800
C	4.19353400	-0.14276800	0.12928800
H	5.04631300	0.45596400	0.43817700
H	1.12115800	-2.29758100	-0.91650200
Cl	-3.87561700	-1.27874700	-1.03433500
H	-1.03665700	-0.12607700	2.83108500
C	-1.01010800	-2.28331400	2.66067900
H	-1.65802400	-3.11823500	2.36056100
H	-0.09164200	-2.37039100	2.06149300

H	-0.71678600	-2.47589600	3.70658700
H	-2.58284000	-0.87587400	3.12099800
C	-1.15539100	3.75003400	0.06429300
H	-0.87657400	4.14078400	1.05133100
H	-0.50151100	4.22153300	-0.67587800
H	-2.19585500	4.01620600	-0.12813100

Structure 13a·EtMgCl_II [B3LYP/6-31G(d)]

C	0.26787200	1.37281000	-0.54774200
C	1.36230500	2.28213900	-0.42481800
C	2.63595300	1.84176900	-0.17829800
C	2.91199200	0.45606300	-0.02822900
C	1.83834700	-0.48392700	-0.15410000
C	-1.10416600	1.89755000	-0.75672200
O	-2.11428800	1.22434600	-0.51126800
O	-0.47755200	-0.92843600	-0.60821600
C	-0.59870100	-1.44669400	-1.96471300
H	1.17594700	3.34674700	-0.50951500
H	3.45078000	2.55379000	-0.08128700
H	-1.44904300	-2.12689400	-1.93861400
H	0.32534500	-1.96162900	-2.24019700
H	-0.79717900	-0.62304000	-2.65664100
Mg	-2.29054900	-0.55869000	0.59393200
C	-1.73960900	-0.15411800	2.61184900
H	-0.86956500	-0.77650200	2.88201200
C	0.53345000	0.00621200	-0.43582500
C	2.10164000	-1.86962800	0.02630700
C	3.37837500	-2.30351600	0.30160500
H	3.56979100	-3.36236400	0.44840900
C	4.44469500	-1.37786500	0.40726500
H	5.44677400	-1.73677100	0.62406700
C	4.21547800	-0.02907100	0.24983500
H	5.02989000	0.68441300	0.34363900
H	1.27932600	-2.57388800	-0.02910500
Cl	-3.72845600	-1.97288700	-0.50202100
C	-1.43789600	1.30643700	2.99851500
H	-2.30527000	1.96028700	2.82981500
H	-1.15466500	1.43287200	4.05702900
H	-0.60908400	1.72776800	2.40942800
H	-2.55021800	-0.52621500	3.25879700
C	-1.29311800	3.31080400	-1.25882000
H	-1.06533100	4.02650800	-0.45869500
H	-0.63531100	3.53662500	-2.10385400
H	-2.33684300	3.44058600	-1.54890900

Structure 13a·EtMgCl_III [B3LYP/6-31G(d)]

C	0.26829000	1.37259300	-0.54804100
C	1.36267100	2.28204200	-0.42505700
C	2.63627100	1.84189900	-0.17805300
C	2.91244100	0.45625000	-0.02752200
C	1.83890500	-0.48385600	-0.15347900
C	-1.10360000	1.89724600	-0.75758000
O	-2.11387200	1.22399800	-0.51265400
O	-0.47671700	-0.92889700	-0.60793400
C	-0.59824000	-1.44665400	-1.96457300
H	1.17625500	3.34661100	-0.51014200
H	3.45098900	2.55404000	-0.08099200
H	-1.44774200	-2.12788400	-1.93817300
H	0.32624700	-1.96033600	-2.24093600
H	-0.79829400	-0.62299600	-2.65605500
Mg	-2.29088400	-0.55842600	0.59307100
C	-1.74045900	-0.15322200	2.61106300
C	0.53399700	0.00605800	-0.43564700
C	2.10224600	-1.86949000	0.02718500
C	3.37895000	-2.30328000	0.30286600
H	3.57038200	-3.36210100	0.44979000
C	4.44514200	-1.37750700	0.40868100
H	5.44720900	-1.73624600	0.62582500
C	4.21585800	-0.02874900	0.25096900
H	5.03020100	0.68480500	0.34488200
H	1.28000500	-2.57382400	-0.02839100
Cl	-3.72763600	-1.97433200	-0.50211300
H	-0.86776300	-0.77237700	2.88015900
C	-1.44423100	1.30824600	2.99829300
H	-2.31440100	1.95867400	2.83076800
H	-1.16041500	1.43532300	4.05657500
H	-0.61771700	1.73327400	2.40859900
H	-2.54916700	-0.52894300	3.25829300
C	-1.29245300	3.31056800	-1.25954700
H	-1.06466200	4.02629800	-0.45945500
H	-0.63459000	3.53640100	-2.10455800
H	-2.33614200	3.44036900	-1.54975600

Structure 13a-TSOMe-I [B3LYP/6-31G(d)]

Cl	-3.97185900	-1.96537900	0.09937300
C	0.09415500	1.49161700	-0.30455300
C	1.25608700	2.32371700	-0.16062400
C	2.50744500	1.81055200	-0.00353800
C	2.71836700	0.39107600	0.00209200
C	1.60614800	-0.48612400	-0.15953900
C	-1.21655600	2.06836800	-0.31230800
O	-2.26573400	1.36069600	-0.18536100
O	-0.64299200	-0.75608000	-1.01019700
C	-0.52822200	-0.65176400	-2.44763200
H	1.12210400	3.40051300	-0.15805600
H	3.36568400	2.46732300	0.10584800
H	-1.25485800	-1.35712600	-2.85311800
H	0.48335100	-0.93023600	-2.75398200
H	-0.75779500	0.36488300	-2.77850800
Mg	-2.21964600	-0.57225100	0.24082100
C	-0.60882100	-0.62435300	1.84558300
H	0.09021200	-1.46227800	1.83712000
H	-1.55333400	-1.03007100	2.27702700
C	0.26548000	0.06561100	-0.25443800
C	1.83023300	-1.88021200	-0.22361500
C	3.10846800	-2.39943900	-0.11796700
H	3.26323100	-3.47346700	-0.16470000
C	4.20625900	-1.53585100	0.05834800
H	5.20881300	-1.94555800	0.14654500
C	4.01185600	-0.16803400	0.11633000
H	4.85928200	0.50125300	0.24268300
H	0.97996800	-2.54246800	-0.35010500
C	-0.13917400	0.53966900	2.69867600
H	-0.74340100	1.44202800	2.52887300
H	-0.19671700	0.31946600	3.77487400
H	0.89991000	0.80240000	2.47568200
C	-1.42533700	3.56474500	-0.41312900
H	-1.15746200	4.05785900	0.52960300
H	-0.81857400	4.01452700	-1.20509600
H	-2.48157500	3.75501200	-0.61154100

Structure 13a-TSOMe-II [B3LYP/6-31G(d)]

Cl	3.94399600	-1.80270300	0.08949900
C	-0.11965700	1.65670700	0.00820300
C	-1.26611300	2.40912700	-0.41675200
C	-2.49863300	1.84650400	-0.56055500
C	-2.71767500	0.46855100	-0.22330200
C	-1.62095000	-0.32817400	0.21903300
C	1.18349300	2.24340700	-0.01235700
O	2.24277600	1.53737100	0.03176100
O	0.61924100	-0.42196800	1.11756500
C	0.52821600	-0.02869100	2.50638600
H	-1.13301700	3.45832300	-0.65970500
H	-3.34228200	2.44216200	-0.89715100
H	1.23985700	-0.66195600	3.03784200
H	-0.48648000	-0.20852000	2.87039700
H	0.79332000	1.02512000	2.62494900
Mg	2.18414400	-0.43671500	-0.17289500
C	0.59465300	-0.70405800	-1.77098400
C	-0.28573200	0.24287300	0.22247600
C	-1.85691500	-1.65613900	0.63962500
C	-3.13311000	-2.19407300	0.60783700
H	-3.29872800	-3.21645300	0.93479300
C	-4.21107200	-1.41870200	0.14423600
H	-5.21011000	-1.84498700	0.11202500
C	-4.00488600	-0.11185300	-0.26177900
H	-4.84034200	0.49402900	-0.60373100
H	-1.02139700	-2.25182300	0.99061700
H	1.47203700	-0.32921700	-2.34055000
C	0.43388300	-2.21097200	-1.94491600
H	0.26085400	-2.48415100	-2.99807900
H	1.31595400	-2.77321000	-1.61237700
H	-0.42898000	-2.58356600	-1.38070300
H	-0.25273200	-0.15357500	-2.17635900
C	1.38149100	3.73761400	-0.14952800
H	1.29814600	4.03849300	-1.20212100
H	0.64916400	4.31402500	0.42243000
H	2.38896900	3.98589500	0.19062500

Structure 13a-TSCO-I [B3LYP/6-31G(d)]

Cl	-3.82359000	-2.00877600	0.11735600
C	0.19608400	1.30308200	-0.39610200

C	1.21702100	2.28311000	-0.23954000
C	2.53376100	1.93166800	-0.07128000
C	2.92273100	0.56960100	0.00477400
C	1.91676800	-0.44419800	-0.11428600
C	-1.24039500	1.70493800	-0.59967600
O	-1.98208300	0.99867400	-1.38655800
O	-0.40059200	-1.03253900	-0.46826100
C	-0.46408300	-1.68092900	-1.77496400
H	0.95041400	3.33305000	-0.27978300
H	3.29540700	2.70156600	0.02039600
H	-1.21741000	-2.46440600	-1.67829700
H	0.50908100	-2.11224200	-2.01594600
H	-0.76415500	-0.94543200	-2.52441900
Mg	-2.35272000	-0.31620700	0.03456100
C	-1.88491700	1.12424500	1.66619300
H	-2.97226400	1.20880800	1.85705700
H	-1.47529300	2.11314300	1.86570000
C	0.57819400	-0.03389600	-0.36210000
C	2.29197000	-1.80769800	0.04252900
C	3.60673300	-2.14899900	0.26535200
H	3.87874200	-3.19320100	0.39089100
C	4.60809100	-1.15059100	0.34438500
H	5.64174000	-1.43744400	0.51539000
C	4.26982800	0.17781900	0.22387300
H	5.02961200	0.95110200	0.30509600
H	1.52646600	-2.57514500	0.01372600
C	-1.23022300	0.09926000	2.60655300
H	-1.70467700	-0.89234900	2.56435100
H	-0.16763800	-0.03948200	2.36699800
H	-1.27745600	0.41400800	3.66053700
C	-1.61773800	3.16582600	-0.46794200
H	-1.34869200	3.67081300	-1.40605300
H	-2.70105700	3.23968900	-0.35379400
H	-1.13068900	3.68269700	0.36030200

Structure 13a-TSCO-II [B3LYP/6-31G(d)]

Cl	-3.54168500	-2.33841200	0.21279300
C	0.24405300	1.19617600	-0.48716300
C	1.18862500	2.25675800	-0.38965200
C	2.51754500	2.01698000	-0.13946900
C	2.99246100	0.69907200	0.08306100
C	2.06280000	-0.39018600	0.02357100
C	-1.20957100	1.47974200	-0.76829200
O	-1.87699100	0.65816700	-1.50315500
O	-0.19132800	-1.17193700	-0.35698400
C	-0.16059700	-1.93956500	-1.59855300
H	0.85271500	3.27670200	-0.53776600
H	3.22099000	2.84417900	-0.09341400
H	-0.87155900	-2.75509200	-1.45733600
H	0.84540800	-2.33054200	-1.76105000
H	-0.46955800	-1.29527200	-2.42444900
Mg	-2.19606200	-0.55016300	0.03345500
C	-1.87390700	1.04556100	1.54854200
H	-1.52506900	0.20226700	2.18041600
C	0.71284900	-0.10113600	-0.31337300
C	2.52004300	-1.70310400	0.32652600
C	3.84297000	-1.92819300	0.63253600
H	4.17808400	-2.93404000	0.86928000
C	4.77097800	-0.85841300	0.65316600
H	5.81256300	-1.05442400	0.89119900
C	4.35134800	0.42562200	0.39113300
H	5.05372700	1.25458500	0.42653900
H	1.80938600	-2.52195600	0.34174000
H	-1.16445200	1.84787700	1.75387800
C	-3.30069700	1.45340000	1.93698600
H	-3.37187500	1.79083800	2.98280200
H	-3.66770100	2.28038300	1.31532500
H	-4.02123000	0.63026600	1.82979100
C	-1.68240100	2.91574000	-0.75207200
H	-1.35664300	3.39566400	-1.68556600
H	-2.77355800	2.92719900	-0.74165000
H	-1.30227600	3.49576500	0.09075700

Structure 13a·MeMgCl [B3LYP/6-31G(d)]

C	0.22019600	1.49063400	-0.15606500
C	1.34409000	2.34906200	0.04061300
C	2.61564200	1.85074400	0.14912200
C	2.85928900	0.45282300	0.07588800
C	1.75441700	-0.43577300	-0.12918300
C	-1.14493600	2.06945400	-0.20992600
O	-2.15874200	1.39639900	0.01480800
O	-0.59521700	-0.75536800	-0.51897300
C	-0.78428400	-1.08248500	-1.92650000
H	1.18350600	3.41794600	0.12510400
H	3.45437500	2.52323000	0.30622200
H	-1.66494400	-1.72272800	-1.95758200
H	0.10469200	-1.59446200	-2.30378500
H	-0.96572300	-0.16624900	-2.49597100
Mg	-2.35167100	-0.54720000	0.81326600
C	-1.71049100	-0.55695500	2.82331000
C	0.45140000	0.11780800	-0.26462800
C	1.98710900	-1.83804200	-0.16814500
C	3.26314300	-2.33425200	-0.02894700
H	3.43134700	-3.40692700	-0.04887200
C	4.35945400	-1.45661900	0.15271900
H	5.36068100	-1.86422000	0.25937600
C	4.16090400	-0.09505600	0.20813900
H	4.99889400	0.57973400	0.36160100
H	1.14305700	-2.50911600	-0.28014500
Cl	-3.89795600	-1.66333800	-0.46798100
H	-0.83570100	0.08023500	3.02554900
H	-2.50211800	-0.21267900	3.50540000
C	-1.31819400	3.53991500	-0.51614100
H	-1.02786500	4.14109000	0.35505800
H	-0.69904600	3.85878300	-1.36037400
H	-2.37156600	3.72972100	-0.72776800
H	-1.43905900	-1.56702400	3.16447400

Structure 13a-TS'OMe [B3LYP/6-31G(d)]

Cl	3.96215900	-1.95784800	-0.24937200
C	-0.07995400	1.53580200	0.08505700
C	-1.23123500	2.35438000	-0.16849300
C	-2.47898900	1.83229600	-0.33183400
C	-2.70029300	0.42006900	-0.21124700
C	-1.59825700	-0.44530500	0.04730100
C	1.23181200	2.10489100	0.08101200
O	2.27873500	1.38822000	-0.01272700
O	0.65292200	-0.66918600	0.90908300
C	0.55388400	-0.46153500	2.33560600
H	-1.09244700	3.42707400	-0.25552100
H	-3.32825200	2.47996300	-0.52941000
H	1.27041700	-1.15207000	2.78246200
H	-0.45963200	-0.69768300	2.66979600
H	0.80695500	0.57015700	2.59414700
Mg	2.21507200	-0.55949200	-0.38414000
C	0.53636100	-0.68090300	-1.88290800
C	-0.25400300	0.10695300	0.10496400
C	-1.82975700	-1.82722800	0.22708000
C	-3.10956100	-2.34745000	0.15008100
H	-3.27200400	-3.41232000	0.28876300
C	-4.19882300	-1.49679800	-0.11849100
H	-5.20263600	-1.90759700	-0.18506900
C	-3.99538200	-0.14067400	-0.29616900
H	-4.83656000	0.51843200	-0.49609100
H	-0.98459700	-2.48002800	0.41906800
H	1.44854000	-0.74960300	-2.51503200
H	-0.11689200	0.03624600	-2.37863100
C	1.44859500	3.60244900	0.11504400
H	1.27327800	4.03595900	-0.87810200
H	0.78218900	4.10622900	0.82093400
H	2.48718000	3.79650700	0.38979100
H	0.06725500	-1.66790100	-1.87096100

Structure 13a-TS'CO [B3LYP/6-31G(d)]

Cl	-3.88495700	-2.01549400	0.36747900
C	0.13031900	1.30099000	-0.24939500
C	1.15633300	2.28081300	-0.14816400
C	2.47854100	1.92808500	-0.02748500
C	2.86548300	0.56622700	0.05474200
C	1.85317900	-0.44628000	-0.01260200
C	-1.31929600	1.70570500	-0.38965000
O	-2.07811300	1.00911200	-1.16492300
O	-0.47614000	-1.03345100	-0.28216500
C	-0.57342800	-1.69999000	-1.57814800
H	0.88853600	3.33062600	-0.18739600
H	3.24515200	2.69671800	0.02435700
H	-1.32369700	-2.48210300	-1.45142300
H	0.39313800	-2.13405100	-1.83932600
H	-0.89280500	-0.97440600	-2.32949200
Mg	-2.41775300	-0.32322000	0.25405700
C	-1.90084300	1.15192600	1.81880900
H	-1.78646500	0.25514400	2.45986300

C	0.50802500	-0.03536500	-0.21822300
C	2.22994900	-1.80834600	0.15301800
C	3.55077000	-2.15050500	0.33403500
H	3.82420800	-3.19335200	0.46736600
C	4.55722500	-1.15422900	0.36014000
H	5.59556700	-1.44193700	0.49809700
C	4.21885100	0.17307800	0.23064400
H	4.98333400	0.94486500	0.27186800
H	1.46168900	-2.57352500	0.16470500
H	-1.11954400	1.83696400	2.14664600
C	-1.68059200	3.16645800	-0.22085900
H	-1.37684300	3.70005900	-1.13225800
H	-1.20628700	3.64216900	0.63908200
H	-2.76499300	3.25192800	-0.13345000
H	-2.87675800	1.60624600	2.04107700

Structure 13b_I [B3LYP/6-31G(d)]

C	0.11443000	-0.16011600	-0.28317300
C	-0.13904100	-1.53668600	-0.56111000
C	-1.40213300	-2.06866500	-0.52045900
C	-2.51142000	-1.26416800	-0.14879600
C	-2.28814400	0.11384400	0.16434600
C	1.52111500	0.36058800	-0.32263500
O	1.77838500	1.53667000	-0.53214200
O	-0.81007100	1.96840300	0.41261100
C	-0.85734400	2.91309400	-0.66628200
H	0.69218500	-2.17799400	-0.83376300
H	-1.56537200	-3.11613400	-0.76062600
H	-0.77087600	3.89749500	-0.20143600
H	-1.81323000	2.84318200	-1.20149200
H	-0.01969600	2.75493300	-1.34824900
C	-0.96640600	0.65426200	0.06396900
C	-3.38726800	0.91507600	0.57558500
C	-4.65470900	0.38165100	0.64864900
H	-5.48759700	1.00328300	0.96564200
C	-4.88032400	-0.97662800	0.31942000
H	-5.88550300	-1.38512200	0.38008100
C	-3.83113700	-1.78074500	-0.06641100
H	-3.99787500	-2.82759400	-0.30857000
H	-3.20234000	1.94872700	0.84487700
C	2.65461700	-0.63860200	-0.07515900
H	2.39630700	-1.26731600	0.78821600
H	2.70285600	-1.32700000	-0.93297000
C	4.01629400	0.03108000	0.12315900
H	4.23878400	0.65811300	-0.74820000
H	3.95902100	0.71874100	0.97676800
C	5.14826700	-0.97983600	0.34548000
H	5.19881000	-1.66658100	-0.51201200
H	4.91607700	-1.60412100	1.22033800
C	6.51268200	-0.31168700	0.54384500
H	7.30301200	-1.05420200	0.70265900
H	6.78938100	0.28935700	-0.33089300
H	6.50268400	0.35688100	1.41330100

Structure 13b_II [B3LYP/6-31G(d)]

C	-0.01355300	0.87024200	0.19517600
C	-0.75199700	2.09139100	0.18080500
C	-2.11288000	2.11288400	0.03273700
C	-2.84261600	0.90362200	-0.13162100
C	-2.13223400	-0.33843700	-0.11610200
C	1.48256600	1.01383700	0.32412200
O	1.94144500	2.09708800	0.66202300
O	-0.06822400	-1.54290000	0.12340400
C	-0.05730600	-2.16328000	1.41337500
H	-0.18393600	3.00787400	0.29577000
H	-2.65090500	3.05751200	0.02548500
H	0.46040900	-3.11705900	1.29038900
H	-1.07620100	-2.34212500	1.77711000
H	0.47941200	-1.54537400	2.14450200
C	-0.71496700	-0.32459400	0.07892500
C	-2.85110100	-1.54762700	-0.31615500
C	-4.21603000	-1.52991100	-0.50078700
H	-4.75381500	-2.46045100	-0.66025700
C	-4.92316200	-0.30411600	-0.49398200
H	-6.00027900	-0.30334800	-0.63752300
C	-4.24937000	0.88429000	-0.31831500
H	-4.78677300	1.82944300	-0.32598900
H	-2.30232900	-2.48246300	-0.34833400
C	2.42135500	-0.13836700	-0.01641200
H	2.35591500	-0.88468600	0.78772500
H	2.05110300	-0.65671100	-0.90863100
C	3.87479200	0.31111900	-0.19219800
H	4.20324600	0.83727500	0.71165100
H	3.93028500	1.05040200	-1.00234100
C	4.82248000	-0.85665800	-0.49269900
H	4.76665600	-1.59159200	0.32372100
H	4.48311600	-1.38272900	-1.39661900
C	6.27703100	-0.41216800	-0.67761800
H	6.93329500	-1.26506700	-0.88560100
H	6.37215800	0.29335700	-1.51202900
H	6.65482300	0.08886800	0.22204600

Structure 13b_III [B3LYP/6-31G(d)]

C	0.39645000	-0.48732600	-0.87209500
C	-0.12565800	-1.80933200	-0.96102300
C	-1.41468400	-2.10110700	-0.58974500
C	-2.25561500	-1.09262200	-0.04948400
C	-1.74346200	0.23757400	0.08468200
C	1.80768200	-0.20351800	-1.31105100
O	2.08496000	0.77154400	-1.99172100
O	0.06238200	1.79538200	-0.17897200
C	-0.15461000	2.70547300	-1.27030400
H	0.50449700	-2.59753600	-1.36214600
H	-1.80118600	-3.11175400	-0.69338200
H	0.23088700	3.67011300	-0.93300500
H	-1.22498300	2.79756100	-1.49420600
H	0.39561200	2.37095800	-2.15214800
C	-0.41643000	0.52190900	-0.36449800
C	-2.56364100	1.23778900	0.67261300
C	-3.84462300	0.94177800	1.08140600
H	-4.46279100	1.71412000	1.53089300
C	-4.36199100	-0.36741800	0.92741400
H	-5.37531000	-0.58701900	1.25268900
C	-3.58275700	-1.36114200	0.37917300
H	-3.97101700	-2.37111400	0.27172100
H	-2.15316000	2.23226400	0.80747600
C	2.89987100	-1.15373700	-0.83336500
H	3.82058200	-0.85962800	-1.34757200
H	2.66343300	-2.18343500	-1.13133100
C	3.09486400	-1.10594800	0.69848200
H	2.17478400	-1.44351100	1.19392000
H	3.87381700	-1.83299100	0.96573700
C	3.48464100	0.28098200	1.22840900
H	2.69723700	1.00478500	0.98116800
H	4.38862500	0.62493200	0.70672000
C	3.72814500	0.28615700	2.74078700
H	4.53754000	-0.40140900	3.01694300
H	4.00428300	1.28536100	3.09582800
H	2.82931900	-0.02417200	3.28782900

Structure 13b_IV [B3LYP/6-31G(d)]

C	0.14665800	1.19153200	0.18809900
C	-0.66882900	2.18434600	-0.43306700
C	-1.96479000	1.93312200	-0.79670600
C	-2.54486900	0.65462800	-0.57253700
C	-1.75732600	-0.35921700	0.05979100
C	1.55952700	1.61513500	0.50724800
O	1.81323500	2.81126600	0.56428200
O	0.29938700	-1.04625700	1.08959500
C	0.11472600	-1.08688100	2.50934200
H	-0.21615600	3.15503600	-0.60276500
H	-2.56310800	2.70685600	-1.27123800
H	0.69240000	-1.94102800	2.86957300
H	-0.94223100	-1.22229300	2.76786700
H	0.48447900	-0.16760000	2.98129100
C	-0.41648000	-0.05163600	0.45195700
C	-2.32206200	-1.64744700	0.26096800
C	-3.61571500	-1.91478100	-0.12914300
H	-4.03430800	-2.90578600	0.02334000
C	-4.40250300	-0.90768400	-0.73713800
H	-5.42272600	-1.12995400	-1.03800100
C	-3.87579200	0.34582500	-0.95675600
H	-4.47273600	1.11914800	-1.43406000
H	-1.70717900	-2.42360100	0.70328600
C	2.68532700	0.60168100	0.65605000
H	2.45733700	-0.11868300	1.44627100
H	3.56748900	1.17717300	0.95489800
C	2.97159700	-0.16714800	-0.65001000
H	2.08388800	-0.74121500	-0.94140800
H	3.16379300	0.55259700	-1.45797400
C	4.16924800	-1.11678800	-0.51870700
H	5.05524200	-0.54494300	-0.20923200

H	3.97081000	-1.83586000	0.28855200
C	4.47508700	-1.87362100	-1.81520300
H	5.33170300	-2.54615400	-1.69236900
H	3.61745100	-2.47963100	-2.13189300
H	4.71005400	-1.18052600	-2.63227200

Structure 13b·EtMgCl_I [B3LYP/6-31G(d)]

C	0.04120700	-1.14039600	0.07257500
C	-0.28558600	-2.46562500	0.49210500
C	-1.57888600	-2.91819900	0.49623700
C	-2.64784700	-2.07616200	0.08809600
C	-2.35447800	-0.74328600	-0.34600800
C	1.45022500	-0.66926400	0.13467200
O	1.73478500	0.53468100	0.17878400
O	-0.73495100	0.96038800	-0.84103400
C	-0.57896400	1.04738100	-2.28664500
H	0.50626500	-3.12244700	0.83310100
H	-1.80240600	-3.92851800	0.82754600
H	-0.32367000	2.08726200	-2.48645000
H	-1.51479900	0.75753200	-2.77151200
H	0.23537200	0.39176000	-2.60887200
Mg	0.50050200	2.21611500	0.48531700
C	-0.29673800	2.15487300	2.45727500
C	-0.99790100	-0.31598400	-0.36326700
C	-3.42249800	0.11693200	-0.72232700
C	-4.72232500	-0.33426500	-0.68781500
H	-5.53337500	0.33211200	-0.96615600
C	-5.01275600	-1.65844800	-0.27922800
H	-6.04395000	-1.99934500	-0.25893900
C	-3.99889500	-2.50789900	0.10402600
H	-4.22027100	-3.52028100	0.43149500
H	-3.20055000	1.13869200	-1.00854100
Cl	1.13121700	3.82418700	-1.03114800
H	-0.19061200	1.14205600	2.88285100
C	-1.76470100	2.60227600	2.61148100
H	-1.91437100	3.63246300	2.26003900
H	-2.45067100	1.97095900	2.02764600
H	-2.12702600	2.57227800	3.65305200
H	0.32912100	2.79013400	3.10530000
C	2.57301800	-1.68999600	0.16954000
H	2.51782000	-2.20862000	1.13950500
H	2.37159600	-2.46331200	-0.58439800
C	3.97023500	-1.09059600	-0.01629800
H	4.14099200	-0.32654300	0.75048200
H	4.01527900	-0.56576600	-0.97906500
C	5.07460300	-2.15331500	0.04915000
H	4.89460300	-2.91887600	-0.71942900
H	5.02291600	-2.67459700	1.01596300
C	6.47565700	-1.56255300	-0.13735000
H	7.24469100	-2.34123800	-0.08702900
H	6.56862500	-1.06276000	-1.10892600
H	6.69881500	-0.82089200	0.63873700

Structure 13b·EtMgCl_II [B3LYP/6-31G(d)]

C	-0.12167400	-1.04727500	-0.03057000
C	-0.50082400	-2.37661500	0.32831700
C	-1.81472300	-2.76313100	0.36416700
C	-2.85353300	-1.84743000	0.04700800
C	-2.50838100	-0.50804400	-0.32457200
C	1.31314400	-0.65553300	-0.01418100
O	1.66590800	0.52829900	0.06921700
O	-0.82606300	1.14513900	-0.77610000
C	-0.70248300	1.31942000	-2.21652300
H	0.26820300	-3.09114500	0.59785600
H	-2.07729000	-3.77791400	0.65004900
H	-0.43251600	2.36512000	-2.35784300
H	-1.65521400	1.07745200	-2.69487600
H	0.09170300	0.67186900	-2.59950100
Mg	0.53334000	2.22596800	0.58491600
C	-0.13193700	2.01465200	2.59752700
H	-1.23043300	1.91306500	2.61372300
C	-1.13318800	-0.14692600	-0.37107700
C	-3.54439300	0.42203100	-0.61383600
C	-4.86333800	0.03325400	-0.55380100
H	-5.64898300	0.75206100	-0.76711000
C	-5.20601100	-1.29522100	-0.20371300
H	-6.25180600	-1.58590700	-0.16112000
C	-4.22326000	-2.21276800	0.09401200
H	-4.48333600	-3.22966900	0.37581900
H	-3.28176500	1.44549600	-0.85657700
Cl	1.13408900	3.94484600	-0.81411900
C	0.47866700	0.87677300	3.43797300
H	1.56988100	0.97527900	3.52613500
H	0.08635300	0.82987500	4.46782100
H	0.28913700	-0.11277900	2.99480900
H	0.05914300	2.96982700	3.11266900
C	2.37720400	-1.73498800	-0.08853800
H	2.33500800	-2.30742800	0.85101700
H	2.10002000	-2.44908100	-0.87625200
C	3.79651400	-1.20177800	-0.30551100
H	4.05284700	-0.51273700	0.50712500
H	3.82386300	-0.60504200	-1.22612200
C	4.83543800	-2.32788800	-0.38460200
H	4.56868900	-3.01637000	-1.19938900
H	4.80141200	-2.92233600	0.53985500
C	6.25892900	-1.80576300	-0.60281800
H	6.98036900	-2.62880500	-0.65183400
H	6.33398800	-1.23884700	-1.53842300
H	6.56547000	-1.14008400	0.21268700

Structure 13b·EtMgCl_III [B3LYP/6-31G(d)]

C	-0.17464700	-1.12753800	0.09946200
C	-0.58776600	-2.39965300	0.59937000
C	-1.91182400	-2.74340300	0.67855600
C	-2.92643800	-1.83738700	0.26890500
C	-2.54625100	-0.55546800	-0.24449800
C	1.26986100	-0.77409100	0.07470000
O	1.65356700	0.40219000	0.05088900
O	-0.81814200	0.98473800	-0.88747900
C	-0.71381600	0.98500500	-2.34079000
H	0.16333100	-3.10245900	0.94125000
H	-2.20096700	-3.71474300	1.07015500
H	-0.37706300	1.98631500	-2.60615000
H	-1.69005500	0.75494900	-2.77545000
H	0.02664400	0.24407500	-2.65614800
Mg	0.58065000	2.20095600	0.31503200
C	-0.13536000	2.30960700	2.31480700
C	-1.16191600	-0.24179800	-0.33559100
C	-3.55717900	0.36878000	-0.62608700
C	-4.88615000	0.02727400	-0.51980700
H	-5.65248200	0.74257100	-0.80349200
C	-5.26390900	-1.24698300	-0.03127000
H	-6.31719900	-1.50145800	0.04487700
C	-4.30576000	-2.15611700	0.35818000
H	-4.59307700	-3.12985100	0.74604200
H	-3.26667100	1.35337300	-0.97454900
Cl	1.28113500	3.66237600	-1.31458000
H	-0.55460200	1.33478400	2.61896600
C	0.88106000	2.75917800	3.38462200
H	1.28960700	3.75472100	3.16444700
H	0.45446200	2.81386700	4.40051900
H	1.74156900	2.07712600	3.44644500
H	-0.99634300	2.99814100	2.34360700
C	2.30551200	-1.88346700	0.09679400
H	2.25912700	-2.36192100	1.08754900
H	2.00160900	-2.66278500	-0.61561800
C	3.73487500	-1.40918900	-0.18233600
H	4.01431000	-0.64805700	0.55487900
H	3.76750500	-0.90875100	-1.15839000
C	4.74752400	-2.56151100	-0.15502200
H	4.45779900	-3.32209100	-0.89438800
H	4.70912300	-3.05884900	0.82486300
C	6.17961200	-2.09579400	-0.43565000
H	6.88239800	-2.93591500	-0.41229500
H	6.25586900	-1.62292000	-1.42204500
H	6.51006000	-1.36207200	0.30904800

Structure 13b·EtMgCl_IV [B3LYP/6-31G(d)]

C	0.55949900	-0.64802000	0.53805600
C	0.73994600	-1.93109600	1.13870000
C	-0.19433100	-2.92469000	1.00393400
C	-1.38574000	-2.71050400	0.26081100
C	-1.59520200	-1.43777200	-0.36185600
C	1.56550900	0.42614600	0.75214200
O	1.26866600	1.62500500	0.65101200
O	-0.80018800	0.76900800	-0.87364100
C	-0.34120900	0.79801300	-2.25527000
H	1.62620700	-2.11663200	1.73432700
H	-0.03733800	-3.88901400	1.47922200
H	-0.53913600	1.81019700	-2.60555500
H	-0.89029600	0.05237900	-2.83635000
H	0.73268800	0.59220700	-2.29025100

Mg	-0.60923600	2.54756600	0.41618700
C	-1.77568100	2.25809200	2.17264100
C	-0.59454100	-0.43754300	-0.21970000
C	-2.79967200	-1.20439900	-1.08109800
C	-3.74547200	-2.19795900	-1.19160300
H	-4.66726000	-2.00881400	-1.73369100
C	-3.53207000	-3.46330900	-0.59268800
H	-4.28832500	-4.23697300	-0.69019100
C	-2.38062000	-3.71192600	0.12040100
H	-2.22030700	-4.67793300	0.59189100
H	-2.97261100	-0.22672600	-1.51632500
Cl	-0.38970100	4.13997200	-1.22618600
H	-1.38360200	1.40809100	2.75724700
C	-3.28846700	2.04981600	1.95560300
H	-3.74363400	2.89883100	1.42737100
H	-3.49760800	1.15654000	1.34858100
H	-3.85517600	1.92565600	2.89401200
H	-1.63670700	3.13052400	2.83197600
C	3.00126400	0.07119400	1.07789800
H	3.04285800	-0.59570600	1.94799400
H	3.49711500	1.00532800	1.35615500
C	3.73412400	-0.58832100	-0.11212200
H	3.22609500	-1.52069600	-0.39090300
H	3.66988100	0.07718100	-0.98367600
C	5.20806200	-0.87834700	0.20065500
H	5.70881200	0.05810100	0.48080700
H	5.26917000	-1.53423900	1.08062500
C	5.94677300	-1.52507500	-0.97523500
H	6.99489800	-1.72018800	-0.72378700
H	5.48763000	-2.48059600	-1.25645200
H	5.93154400	-0.87573600	-1.85869400

Structure 13b·EtMgCl_V [B3LYP/6-31G(d)]

C	0.31364900	-0.71097700	0.45870500
C	0.25214000	-1.99814400	1.07479000
C	-0.86721500	-2.78384000	0.98878500
C	-2.01781800	-2.33968900	0.28456900
C	-1.98911300	-1.05654500	-0.35122800
C	1.52522700	0.13715200	0.61832900
O	1.48171000	1.36761200	0.47764500
O	-0.78340600	0.93628600	-0.93390900
C	-0.38214900	0.85327100	-2.33107000
H	1.10398300	-2.35404400	1.64202000
H	-0.89015700	-3.75547200	1.47442700
H	-0.37263500	1.88150100	-2.69043900
H	-1.10025600	0.23817300	-2.87990600
H	0.62031100	0.42082000	-2.40111500
Mg	-0.17061300	2.65495600	0.31126100
C	-1.25687900	2.63234300	2.14366700
H	-2.26195100	2.21231000	1.96813200
C	-0.80173600	-0.27870800	-0.26299500
C	-3.14866100	-0.59109700	-1.03044300
C	-4.27918900	-1.37356300	-1.09025700
H	-5.16406600	-1.00665700	-1.60189700
C	-4.30304000	-2.65060800	-0.47862900
H	-5.20322300	-3.25590600	-0.53595800
C	-3.19892800	-3.12039700	0.19677400
H	-3.21870200	-4.09425600	0.67881600
H	-3.13770700	0.39735800	-1.47546000
Cl	0.25879000	4.15718300	-1.37231200
C	-0.62180200	1.90199400	3.34260600
H	0.35006300	2.33641400	3.61620600
H	-1.24228500	1.92831000	4.25425300
H	-0.43871300	0.83807200	3.12888400
H	-1.44751100	3.67837000	2.43299800
C	2.86608300	-0.49613000	0.92484000
H	2.78721100	-1.18342800	1.77533600
H	3.53507300	0.31758100	1.21860400
C	3.44796100	-1.24727700	-0.29448900
H	2.76138800	-2.04775600	-0.60062800
H	3.51643200	-0.55057800	-1.14083000
C	4.83378000	-1.83977900	-0.00665100
H	5.51031300	-1.03640000	0.31467400
H	4.76062300	-2.53658100	0.84025000
C	5.43260000	-2.56207600	-1.21747200
H	6.41829500	-2.97748500	-0.98137000
H	4.79168900	-3.38970600	-1.54511300
H	5.55385700	-1.87898000	-2.06659300

Structure 13b·EtMgCl_VI [B3LYP/6-31G(d)]

C	0.36686400	-0.73378800	0.51973700
C	0.39293100	-1.97623200	1.22368700
C	-0.66856100	-2.84226900	1.19186300
C	-1.84358900	-2.52933000	0.45820100
C	-1.90249100	-1.29351500	-0.26362500
C	1.51575000	0.20502000	0.62034100
O	1.38475600	1.41873600	0.40920300
O	-0.83652900	0.73615600	-0.97833700
C	-0.43358000	0.58741400	-2.37006300
H	1.26437800	-2.23197200	1.81510000
H	-0.62625300	-3.77727400	1.74355900
H	-0.48892900	1.58928000	-2.79392500
H	-1.11207300	-0.10636200	-2.87344300
H	0.59435500	0.21599400	-2.41724700
Mg	-0.33824700	2.59145700	0.12333000
C	-1.47602800	2.67181400	1.91823500
C	-0.77268000	-0.43028500	-0.22918400
C	-3.08932600	-0.95744200	-0.97135900
C	-4.16180900	-1.81972800	-0.97759200
H	-5.06831800	-1.55122100	-1.51191300
C	-4.09797400	-3.05130800	-0.28138400
H	-4.95296100	-3.72119500	-0.29718800
C	-2.96657600	-3.39539700	0.42388100
H	-2.92022100	-4.33343400	0.97078800
H	-3.14639700	-0.00247900	-1.48123800
Cl	0.06310600	3.96638500	-1.67569500
H	-1.56437900	1.66475200	2.36138100
C	-0.96527600	3.64068300	3.00478400
H	-0.91287100	4.67405200	2.63593700
H	-1.59937100	3.66290200	3.90728000
H	0.04776600	3.38009600	3.34411900
H	-2.51233900	2.95078900	1.66446400
C	2.89726600	-0.31178100	0.96336800
H	2.86696900	-0.91114600	1.88137600
H	3.51502800	0.56776100	1.16531100
C	3.51883800	-1.14743700	-0.17824400
H	2.89038900	-2.02395900	-0.38357900
H	3.52799300	-0.54528800	-1.09682800
C	4.94762000	-1.60276400	0.14763200
H	5.56810200	-0.72085900	0.35632600
H	4.93638500	-2.19578600	1.07307500
C	5.58129500	-2.42182500	-0.98091900
H	6.59923600	-2.73122500	-0.72022500
H	5.00053100	-3.32851500	-1.19004900
H	5.63729400	-1.84105900	-1.90930500

Structure 13b·EtMgCl_VII [B3LYP/6-31G(d)]

C	0.01106900	-1.06654600	-0.65994500
C	-0.34680500	-2.43935100	-0.49215900
C	-1.62613200	-2.81517700	-0.17696300
C	-2.64926900	-1.84544800	-0.00239200
C	-2.32909400	-0.46023300	-0.17697500
C	1.42276300	-0.69573500	-0.93507400
O	1.85567300	0.44366600	-0.70390500
O	-0.72901800	1.23681500	-0.74312800
C	-0.99535500	1.69617800	-2.10001900
H	0.41664400	-3.20111800	-0.59610200
H	-1.86956600	-3.86598500	-0.04660700
H	-0.70033600	2.74463400	-2.11289100
H	-2.05779100	1.57011500	-2.32416300
H	-0.38634900	1.12606200	-2.80757100
Mg	0.99474900	2.03213900	0.37144800
C	0.80541600	1.47244800	2.41710300
C	-0.99643400	-0.10760800	-0.52610200
C	-3.34096700	0.51860200	0.02527000
C	-4.61783000	0.13627500	0.36798700
H	-5.38219900	0.89009700	0.53174400
C	-4.94109800	-1.23379900	0.52166300
H	-5.95410100	-1.51868900	0.79122600
C	-3.97767100	-2.20161700	0.34432300
H	-4.21986500	-3.25308000	0.47432000
H	-3.08517000	1.56801500	-0.06638900
Cl	1.33579300	3.96651100	-0.82095000
H	0.83840900	0.37387800	2.51990400
C	-0.45244700	1.99601400	3.14022900
H	-0.50237600	3.09337600	3.12405000
H	-1.37801400	1.63493500	2.66790700
H	-0.50850100	1.69643000	4.20055900
H	1.69361200	1.82607200	2.96592300
C	2.39409900	-1.72362600	-1.47791500
H	3.09110500	-1.17741500	-2.12226400
H	1.87018300	-2.45962800	-2.09556600

C	3.20539500	-2.45075700	-0.37014900
H	2.52112600	-2.96276900	0.31976800
H	3.78529800	-3.23948200	-0.86746100
C	4.15605400	-1.54990800	0.42892800
H	4.83045400	-1.03153400	-0.26574300
H	3.58739700	-0.76618700	0.94257600
C	4.97614100	-2.34156900	1.45299700
H	5.58676100	-3.11241700	0.96656200
H	5.65116200	-1.68240600	2.00894100
H	4.32640400	-2.84196200	2.18147000

Structure 13b·EtMgCl_VIII [B3LYP/6-31G(d)]

C	-0.12878600	-0.91179800	-0.70905600
C	-0.49214400	-2.29178400	-0.64541200
C	-1.76288100	-2.68464000	-0.31631000
C	-2.77059400	-1.72645100	-0.02556100
C	-2.44429300	-0.33331800	-0.09367500
C	1.27445600	-0.52647300	-1.01055900
O	1.73256500	0.57772500	-0.67928200
O	-0.84413000	1.39510200	-0.56342300
C	-1.14149700	1.97397800	-1.86665100
H	0.26154100	-3.04598700	-0.83964100
H	-2.01114400	-3.74110200	-0.26460500
H	-0.83235300	3.01611700	-1.79691200
H	-2.21150900	1.88036800	-2.07004800
H	-0.56071100	1.46035500	-2.63837200
Mg	0.92240900	2.05994100	0.57123500
C	0.78644200	1.35858900	2.57814700
H	-0.27433700	1.35622200	2.88238000
C	-1.12049800	0.03886900	-0.45615600
C	-3.44049100	0.63087600	0.22287800
C	-4.70844100	0.22869900	0.57579500
H	-5.46077600	0.97063100	0.82663800
C	-5.03806500	-1.14754400	0.62647000
H	-6.04375800	-1.44806900	0.90623600
C	-4.08956600	-2.10265400	0.33590000
H	-4.33626000	-3.15989800	0.38594700
H	-3.17919000	1.68291000	0.20859500
Cl	1.24805800	4.09601700	-0.44109700
C	1.39840100	-0.01064000	2.93048900
H	2.47802400	-0.03922500	2.72391000
H	1.27988900	-0.28751100	3.99172300
H	0.94712100	-0.82903000	2.34935200
H	1.24927500	2.12267100	3.22356300
C	2.19733700	-1.49754300	-1.71738400
H	2.84821100	-0.89377100	-2.35903400
H	1.62217200	-2.17054300	-2.36053100
C	3.08332800	-2.32702600	-0.74761600
H	2.44954400	-2.86096700	-0.02687500
H	3.57992100	-3.09867100	-1.35075200
C	4.14338500	-1.51438400	0.00652900
H	4.76969500	-0.97913700	-0.71986300
H	3.65998600	-0.74551200	0.61956300
C	5.02351600	-2.39802300	0.89689400
H	5.54798200	-3.16219400	0.30978800
H	5.77929900	-1.80036800	1.41745800
H	4.42635200	-2.91389700	1.65861800

Structure 13b·EtMgCl_IX [B3LYP/6-31G(d)]

C	-0.25730400	-1.01067400	-0.67528100
C	-0.70515400	-2.35892700	-0.52572900
C	-1.98327900	-2.65172400	-0.12837000
C	-2.91416700	-1.61691800	0.15477400
C	-2.50227900	-0.25313800	0.00525900
C	1.15379800	-0.73484000	-1.05039100
O	1.68778400	0.36084600	-0.82171200
O	-0.82314900	1.34279900	-0.62413400
C	-1.16361500	1.87199100	-1.93895700
H	-0.01105600	-3.16996200	-0.71162900
H	-2.29602700	-3.68604900	-0.01530000
H	-0.80159300	2.89917000	-1.94029300
H	-2.24628200	1.82231800	-2.08100600
H	-0.65044600	1.29248600	-2.71178900
Mg	1.04701400	1.98055400	0.35618500
C	1.01871200	1.39302400	2.40145500
C	-1.17562800	0.01398600	-0.43237200
C	-3.41899500	0.78836400	0.31776200
C	-4.69336400	0.48776800	0.74136300
H	-5.38401700	1.28862900	0.98828600
C	-5.10896400	-0.85987300	0.86988700
H	-6.11886600	-1.08008700	1.20394400
C	-4.23765800	-1.88795000	0.58701400
H	-4.54956700	-2.92313200	0.69766200
H	-3.09093200	1.81900600	0.24426300
Cl	1.43839100	3.91343800	-0.82364900
H	0.51274600	0.41839300	2.51411100
C	2.38901200	1.31584100	3.10551700
H	2.91436200	2.28015500	3.07942800
H	2.32319100	1.02363400	4.16727000
H	3.05813000	0.58607100	2.62548000
H	0.38168900	2.09804500	2.96084500
C	1.99867900	-1.81207700	-1.69883700
H	2.68196400	-1.29693000	-2.38221800
H	1.37278700	-2.48597400	-2.29189800
C	2.83689300	-2.63396500	-0.68116100
H	2.17297500	-3.10865000	0.05397300
H	3.30578600	-3.45233300	-1.24351700
C	3.92343800	-1.83608800	0.05118600
H	4.57716500	-1.35478700	-0.68850200
H	3.46912200	-1.02360900	0.63008000
C	4.75949900	-2.71968800	0.98323500
H	5.26261800	-3.52239000	0.42989000
H	5.52992800	-2.13186200	1.49322200
H	4.13470300	-3.18708700	1.75413700

Structure 13b-TSOMe-I [B3LYP/6-31G(d)]

Cl	0.90503000	4.31003300	0.03452500
C	0.07624500	-0.97772000	-0.11900000
C	-0.28218800	-2.35491300	0.07657200
C	-1.57662900	-2.77198600	0.14615100
C	-2.65352100	-1.83493400	0.00277400
C	-2.36179700	-0.45655700	-0.21420500
C	1.44622700	-0.56003200	-0.03658400
O	1.76535400	0.66781600	0.04570500
O	-0.75832400	1.15890600	-1.03445800
C	-0.66335500	0.91089300	-2.45539200
H	0.51258300	-3.08421900	0.19131700
H	-1.81274000	-3.82135000	0.29775500
H	-0.53788700	1.89046000	-2.91874100
H	-1.58573400	0.44071100	-2.80575200
H	0.19505200	0.27083900	-2.67706900
Mg	0.44783500	2.12589300	0.26281200
C	-0.94848200	1.21631900	1.81042500
H	-2.01735200	1.40537400	1.69701700
H	-0.52226100	2.16200900	2.21969000
C	-0.97951600	-0.00625500	-0.21576400
C	-3.42668300	0.44892800	-0.42360500
C	-4.74087700	0.01601600	-0.40721600
H	-5.54776500	0.72562800	-0.56567400
C	-5.03147800	-1.34214500	-0.17706900
H	-6.06430300	-1.67945500	-0.15938200
C	-4.00578400	-2.24744500	0.02336100
H	-4.22693300	-3.29848500	0.19206000
H	-3.19885300	1.49636800	-0.59183100
C	-0.64007600	0.08439600	2.77347200
H	0.41317200	-0.22477500	2.71892500
H	-0.83395100	0.36157200	3.82012600
H	-1.24620300	-0.80046300	2.55412500
C	2.58078300	-1.57419500	0.00949900
H	2.53036400	-2.10214900	0.97396800
H	2.40566600	-2.34365500	-0.75384800
C	3.97529500	-0.96367900	-0.16787100
H	4.13869400	-0.20029300	0.60110200
H	4.02266400	-0.43559800	-1.12921500
C	5.08877300	-2.01648200	-0.10148000
H	5.03586000	-2.54333900	0.86227300
H	4.91994600	-2.78034100	-0.87437100
C	6.48656100	-1.41433300	-0.27673300
H	6.69897100	-0.67377000	0.50365900
H	7.26265200	-2.18616500	-0.22520400
H	6.58159200	-0.90921600	-1.24558900

Structure 13b-TSOMe-II [B3LYP/6-31G(d)]

Cl	-0.65183400	4.27044000	0.09055700
C	-0.22384000	-1.04738600	-0.10411700
C	0.07971500	-2.37587500	-0.55638000
C	1.35526800	-2.84621100	-0.64824900
C	2.46460400	-2.04038400	-0.22424100
C	2.22834800	-0.71491700	0.24419300
C	-1.55989400	-0.53777200	-0.17547800
O	-1.80216800	0.71122600	-0.11484500
O	0.66750300	0.91281600	1.10708200

C	0.38255800	0.53031500	2.47208000
H	-0.73956300	-3.01565200	-0.86638000
H	1.54801200	-3.85296600	-1.00768600
H	0.30252900	1.46508600	3.02876400
H	1.20593100	-0.07401100	2.86107800
H	-0.55601400	-0.02727800	2.52657600
Mg	-0.35758800	2.06632600	-0.20538300
C	1.03724600	1.16813900	-1.75533400
C	0.88172200	-0.17162400	0.18820700
C	3.30940900	0.04268100	0.74754700
C	4.59191600	-0.48069600	0.77340900
H	5.41224600	0.11402700	1.16452300
C	4.83100400	-1.77766800	0.28515300
H	5.83874700	-2.18404800	0.29835000
C	3.78518600	-2.54134200	-0.20307100
H	3.96604900	-3.55063100	-0.56459800
H	3.12152500	1.04490500	1.11691900
H	0.18349300	1.54930700	-2.35618900
C	2.22986400	2.11549800	-1.84169700
H	2.59236200	2.22129500	-2.87659400
H	1.99611700	3.12617600	-1.48283300
H	3.07499000	1.74135200	-1.25237000
H	1.25934300	0.19172600	-2.18306600
C	-2.75171400	-1.45987400	-0.38296300
H	-2.82015500	-1.68552700	-1.45920600
H	-2.56795300	-2.41975500	0.11315000
C	-4.08449100	-0.86872000	0.09543600
H	-4.26171200	0.08507300	-0.41287900
H	-4.01392500	-0.63299100	1.16617300
C	-5.26504800	-1.81822600	-0.14404300
H	-5.33185000	-2.05206900	-1.21637700
H	-5.07639000	-2.77493000	0.36419900
C	-6.60006700	-1.24048200	0.33636100
H	-6.83343400	-0.30124400	-0.17928800
H	-7.42549000	-1.93711500	0.15173000
H	-6.57602300	-1.02920400	1.41236000

Structure 13b-TSOMe-III [B3LYP/6-31G(d)]

Cl	-0.16362300	4.59545700	-0.36265100
C	0.40134200	-0.69067100	0.32941500
C	0.34957100	-2.07837900	0.70003000
C	-0.78960700	-2.81919800	0.61426000
C	-2.00506300	-2.23669300	0.12342600
C	-2.01302100	-0.87093200	-0.28411500
C	1.57319200	0.10028100	0.57367100
O	1.55601500	1.36953500	0.47033800
O	-0.71100900	0.99638000	-1.09368200
C	-0.25004500	0.60703900	-2.40693400
H	1.25203400	-2.54768400	1.07534500
H	-0.79152700	-3.86539000	0.90656900
H	-0.26983700	1.51739300	-3.00771100
H	-0.92965200	-0.13957100	-2.82585200
H	0.76610700	0.20663200	-2.35400100
Mg	-0.09154500	2.42300700	0.19357300
C	-1.50318700	1.37467000	1.63532600
H	-2.53730700	1.22798000	1.31970100
H	-1.42888000	2.44729900	1.92893900
C	-0.81158700	-0.06889900	-0.13079000
C	-3.19484100	-0.32154000	-0.83159500
C	-4.33971600	-1.08754200	-0.96174500
H	-5.24109100	-0.64891800	-1.37990000
C	-4.33826300	-2.43219300	-0.54436000
H	-5.24004500	-3.03050400	-0.64233400
C	-3.19160100	-2.99319600	-0.01310800
H	-3.18488700	-4.03395200	0.30128800
H	-3.19452800	0.71781300	-1.14317600
C	-1.10509300	0.51028500	2.81680500
H	-0.01453400	0.48129700	2.95399500
H	-1.53283700	0.87164300	3.76349300
H	-1.43770500	-0.52411400	2.68283300
C	2.90916500	-0.50814500	0.95192800
H	2.79282000	-1.36030900	1.62887800
H	3.46346700	0.26724500	1.49021200
C	3.71482600	-0.94236100	-0.29289500
H	3.15749400	-1.71574400	-0.83939700
H	3.80794300	-0.08328900	-0.97083100
C	5.11120900	-1.46859300	0.06238900
H	5.65879100	-0.69243600	0.61445900
H	5.01343300	-2.32129300	0.74915800
C	5.91998300	-1.89076700	-1.16833700
H	6.06440100	-1.04855500	-1.85570100
H	6.91086400	-2.26178200	-0.88387200
H	5.41197000	-2.68894400	-1.72336200

Structure 13b-TSOMe-IV [B3LYP/6-31G(d)]

Cl	0.91005800	4.46841600	0.33991900
C	-0.61601200	-0.59559400	-0.41609100
C	-0.75721300	-1.91847200	-0.95757700
C	0.25605800	-2.82931300	-0.94837500
C	1.51328300	-2.51992900	-0.33002900
C	1.71185800	-1.22980500	0.24303500
C	-1.64510200	0.38609800	-0.58478800
O	-1.42404300	1.62704100	-0.39239200
O	0.74397500	0.80550100	1.10178000
C	0.14936800	0.47535200	2.37768200
H	-1.70288700	-2.19299600	-1.41165900
H	0.11456500	-3.81633600	-1.37928000
H	0.33710900	1.33638700	3.02063600
H	0.63279700	-0.41597400	2.78568200
H	-0.92540100	0.30821200	2.26885400
Mg	0.41242800	2.34262300	-0.17764700
C	1.58347900	1.08931700	-1.66408400
C	0.67631400	-0.22155200	0.09998300
C	2.91449600	-0.95928300	0.93407900
C	3.90392100	-1.92283000	1.04082400
H	4.82238900	-1.69948900	1.57575600
C	3.72130000	-3.18603500	0.44977400
H	4.50186400	-3.93807600	0.52727200
C	2.54656000	-3.47702300	-0.22121200
H	2.39647900	-4.45897200	-0.66312100
H	3.05380700	0.01805000	1.38305300
H	1.01401800	1.78916600	-2.31243700
C	3.03455600	1.53556200	-1.51550700
H	3.55859600	1.55142800	-2.48446300
H	3.12758400	2.54212900	-1.08781700
H	3.59372000	0.84826700	-0.87004200
H	1.50135300	0.12373700	-2.16017000
C	-3.05913000	0.01873500	-0.99112200
H	-3.06099700	-0.71007200	-1.80937300
H	-3.52247000	0.93553900	-1.36854500
C	-3.88766300	-0.53233100	0.18982600
H	-3.41414800	-1.44461800	0.57707000
H	-3.87074900	0.20072700	1.00803600
C	-5.34129300	-0.83145200	-0.19845800
H	-5.80537300	0.08351500	-0.59150600
H	-5.35326700	-1.55856300	-1.02285000
C	-6.17348000	-1.36771500	0.97050800
H	-6.20975500	-0.64602800	1.79552400
H	-7.20473100	-1.57258700	0.66231500
H	-5.75187800	-2.30070700	1.36428800

Structure 13b-TSOMe-V [B3LYP/6-31G(d)]

Cl	-0.06506000	4.58379200	0.32936200
C	0.30463500	-0.67461000	-0.61168300
C	0.32159700	-2.11134100	-0.58216400
C	-0.78702700	-2.85181300	-0.30531700
C	-2.04661500	-2.21384700	-0.05107900
C	-2.13299200	-0.79145100	-0.08601200
C	1.51828700	0.07287800	-0.76304000
O	1.57118600	1.32231000	-0.52050100
O	-1.18387200	1.26908200	-0.92580200
C	-1.39916900	1.23585700	-2.35490100
H	1.26099300	-2.62119900	-0.76614500
H	-0.73715900	-3.93674800	-0.28762700
H	-1.59965100	2.26762700	-2.64678200
H	-2.26194800	0.60332400	-2.57889200
H	-0.51060100	0.85935300	-2.86906900
Mg	0.06368400	2.34544200	0.24356000
C	-0.66746600	0.92945700	1.86625700
H	-1.74616800	0.84591900	2.00925100
H	-0.37712100	1.89565100	2.34026200
C	-0.93128800	-0.00509500	-0.30617800
C	-3.39002000	-0.17178000	0.09830500
C	-4.52780300	-0.92681400	0.32202400
H	-5.48547800	-0.43505000	0.46600500
C	-4.44178300	-2.33116600	0.37172700
H	-5.33546600	-2.92223000	0.55271700
C	-3.22378600	-2.95945900	0.18820900
H	-3.15645900	-4.04421000	0.21702000
H	-3.44969000	0.91133200	0.06982500
C	0.11393700	-0.19336500	2.52246900
H	1.16232000	-0.20796200	2.19358600

H	0.12789000	-0.10817700	3.61916500
H	-0.31330600	-1.17115300	2.27795000
C	2.83255300	-0.57300200	-1.15335800
H	3.36680900	0.15990200	-1.76832700
H	2.67491900	-1.46461400	-1.76828300
C	3.70275800	-0.92328400	0.07421100
H	3.17289400	-1.65126800	0.70378300
H	3.83140300	-0.01838800	0.68174400
C	5.07583300	-1.48363500	-0.31693200
H	5.60042800	-0.74853100	-0.94284600
H	4.93938000	-2.37675100	-0.94330900
C	5.94209400	-1.83664300	0.89654200
H	6.91587800	-2.23259600	0.58753100
H	6.12380200	-0.95542800	1.52331000
H	5.45715600	-2.59502800	1.52320900

Structure 13b-TSOMe-VI [B3LYP/6-31G(d)]

Cl	0.03058500	4.45725900	0.15513200
C	0.40571000	-0.82390300	-0.54427300
C	0.43020000	-2.23522500	-0.27826200
C	-0.68436300	-2.93545500	0.07365800
C	-1.96650700	-2.29303300	0.12760100
C	-2.06033700	-0.89560200	-0.13836400
C	1.61808800	-0.09293000	-0.74862300
O	1.66207500	1.17778300	-0.64370200
O	-1.06225800	1.09026600	-1.07904900
C	-1.14792200	0.96221100	-2.51711300
H	1.38079200	-2.75500800	-0.33095200
H	-0.62459500	-4.00023300	0.28001600
H	-1.36677500	1.96410200	-2.88896900
H	-1.95889300	0.27612100	-2.77421200
H	-0.20100900	0.60197700	-2.92751000
Mg	0.14601500	2.21730300	0.09646500
C	-0.57707400	0.87398700	1.77822500
C	-0.84473300	-0.13268700	-0.35887800
C	-3.33337100	-0.28367400	-0.17685900
C	-4.48233300	-1.02109100	0.05803400
H	-5.45372600	-0.53648300	0.02389400
C	-4.38889000	-2.39409400	0.34846200
H	-5.29053900	-2.96942000	0.54045500
C	-3.15308100	-3.01610600	0.38120300
H	-3.08089800	-4.08088200	0.58865500
H	-3.39996800	0.77665100	-0.39472600
H	0.35732000	1.32150500	2.18030200
C	-1.80601900	1.55476900	2.37151700
H	-1.84656500	1.44028800	3.46655300
H	-1.83562800	2.63212900	2.16406900
H	-2.73026200	1.11518900	1.97871200
H	-0.51916600	-0.17794700	2.05339100
C	2.94237300	-0.77119200	-1.03320400
H	3.46232600	-0.14336900	-1.76632300
H	2.80185700	-1.75693800	-1.48729100
C	3.81811900	-0.88535100	0.23387500
H	3.30303900	-1.50441400	0.98170000
H	3.92484100	0.11390100	0.67454900
C	5.20449000	-1.47534600	-0.05345800
H	5.71307800	-0.85260300	-0.80249500
H	5.09097100	-2.46967700	-0.50848800
C	6.07583300	-1.58331000	1.20191000
H	7.05983600	-2.00444200	0.96752400
H	6.23404900	-0.59944400	1.65970700
H	5.60813700	-2.22823500	1.95590500

Structure 13b-TSCO-I [B3LYP/6-31G(d)]

Cl	1.49815500	3.95513200	0.13734500
C	-0.27599500	-0.95149300	-0.29242400
C	-0.67565600	-2.30243300	-0.08372400
C	-1.99739800	-2.65400600	0.04131000
C	-3.02093800	-1.67243500	0.01817400
C	-2.65421300	-0.29796200	-0.15340000
C	1.18025400	-0.58016400	-0.44200800
O	1.49191400	0.37133100	-1.26527500
O	-0.93423800	1.36054200	-0.50883400
C	-1.14675700	1.88526300	-1.85418300
H	0.08141000	-3.07666800	-0.04557000
H	-2.27243600	-3.69703800	0.17473800
H	-0.91280200	2.94960100	-1.79636100
H	-2.18901000	1.73822800	-2.14252500
H	-0.47276600	1.37642900	-2.54671100
Mg	1.08240400	1.75235200	0.06755900
C	1.32842700	0.32558300	1.76719700
H	2.24032000	0.91188500	1.99387800
H	1.57324100	-0.70085600	2.03483700
C	-1.27994400	0.00909900	-0.35186900
C	-3.66946500	0.69710400	-0.09256700
C	-4.98696700	0.34072600	0.08673800
H	-5.75125700	1.11099400	0.13891200
C	-5.35556000	-1.02056000	0.21597700
H	-6.40047100	-1.28475700	0.35142500
C	-4.39145300	-2.00207800	0.18943100
H	-4.66350600	-3.04763400	0.31049300
H	-3.39211300	1.74325400	-0.15956500
C	0.14284000	0.81542600	2.61232800
H	-0.05592400	1.89124700	2.49790200
H	-0.78227700	0.28639700	2.35195300
H	0.31024500	0.65098500	3.68773900
C	2.22005000	-1.67853700	-0.25734100
H	2.09908200	-2.34794900	-1.12557200
H	2.00468500	-2.28198600	0.62978300
C	3.66611500	-1.17366800	-0.22648000
H	3.85396900	-0.57963900	-1.12733200
H	3.79610100	-0.49461300	0.62650000
C	4.68804500	-2.31375700	-0.12834400
H	4.55354000	-2.99833800	-0.97831400
H	4.48988000	-2.90803000	0.77531300
C	6.13558300	-1.81273000	-0.10191900
H	6.84513700	-2.64518300	-0.03532300
H	6.37292100	-1.24240400	-1.00803400
H	6.31131600	-1.15463400	0.75774800

Structure 13b-TSCO-II [B3LYP/6-31G(d)]

Cl	1.42245400	3.94889500	0.11169100
C	-0.39774800	-0.94119400	-0.26195900
C	-0.80478100	-2.28423900	-0.02103800
C	-2.12658200	-2.62054900	0.14196800
C	-3.14069600	-1.62938800	0.12643800
C	-2.76478600	-0.26190600	-0.07804500
C	1.06327700	-0.58305500	-0.42895500
O	1.37264400	0.35846100	-1.26201500
O	-1.04010000	1.37530500	-0.49468100
C	-1.26617300	1.88156000	-1.84435700
H	-0.05351800	-3.06414500	0.01968400
H	-2.40803100	-3.65806300	0.30238200
H	-1.01934000	2.94389500	-1.80662700
H	-2.31415700	1.74216200	-2.11562800
H	-0.60809100	1.35483800	-2.53884000
Mg	0.98111700	1.75053100	0.06752100
C	1.10102900	0.32378100	1.78837600
H	0.23469900	0.93733800	2.11649100
C	-1.39314700	0.02826600	-0.31326900
C	-3.76829200	0.74459400	-0.01047200
C	-5.08430800	0.40509400	0.20764000
H	-5.83951800	1.18394000	0.26449100
C	-5.46297200	-0.94990500	0.37044300
H	-6.50677100	-1.20075300	0.53642400
C	-4.50981900	-1.94178700	0.33724400
H	-4.78928900	-2.98217100	0.48330600
H	-3.48234900	1.78634600	-0.10413600
H	0.82205600	-0.69209500	2.06741200
C	2.37505200	0.75630300	2.52928400
H	2.23563200	0.75068000	3.62159500
H	3.20980400	0.08061300	2.31268500
H	2.70697600	1.77087400	2.26751100
C	2.09509200	-1.68578000	-0.22647100
H	1.86447500	-2.46369700	-0.97321900
H	1.97178200	-2.15791800	0.75377200
C	3.54263600	-1.23119700	-0.43948600
H	3.64111500	-0.82034100	-1.45010900
H	3.77629500	-0.40812500	0.24679700
C	4.55160700	-2.36889100	-0.23592200
H	4.30988900	-3.19764100	-0.91723700
H	4.44952500	-2.77303700	0.78161900
C	6.00033900	-1.92675800	-0.46583000
H	6.28285300	-1.12189400	0.22359200
H	6.69988400	-2.75658900	-0.31439800
H	6.14223300	-1.55161400	-1.48652400

Structure 13b-TSCO-III [B3LYP/6-31G(d)]

Cl	0.45486600	4.48879500	-0.28760700
C	0.12791400	-0.71937400	0.09378900
C	0.05583700	-2.06970900	0.54193200
C	-1.13028500	-2.76121900	0.56680000

C	-2.34889300	-2.13768600	0.19510500
C	-2.32244000	-0.76653500	-0.21977900
C	1.43852800	0.02555500	0.05492400
O	1.63581200	0.88789900	-0.88928200
O	-1.05454700	1.23442900	-0.68682800
C	-1.13127900	1.45070200	-2.12827700
H	0.96446500	-2.57243400	0.85126700
H	-1.14796100	-3.79883400	0.88990100
H	-1.18517000	2.53243000	-2.26131700
H	-2.02951700	0.97121100	-2.52134100
H	-0.23200900	1.04661700	-2.59775400
Mg	0.63880000	2.28297200	0.08098600
C	0.94442300	1.28987300	2.05131300
H	1.68389000	2.08404700	2.27420900
H	1.33535200	0.38927300	2.52234800
C	-1.06174800	-0.11371000	-0.29882400
C	-3.55199600	-0.11234800	-0.51084900
C	-4.74300600	-0.79834800	-0.43509600
H	-5.67529900	-0.28528600	-0.65361600
C	-4.76673100	-2.16474000	-0.06364800
H	-5.71483400	-2.69257800	-0.01399700
C	-3.59549200	-2.81497400	0.25130800
H	-3.60748300	-3.85753100	0.55914200
H	-3.54518100	0.94138700	-0.76638100
C	-0.43332200	1.62478200	2.64361800
H	-0.81558400	2.60535900	2.32344300
H	-1.18353300	0.87584000	2.35701700
H	-0.41748300	1.64924900	3.74422900
C	2.69041400	-0.62815400	0.61920200
H	2.47488300	-1.23032500	1.50704600
H	3.35917500	0.17985700	0.93378200
C	3.40907400	-1.47795700	-0.44993700
H	2.74955900	-2.28582300	-0.79762000
H	3.60635400	-0.84290200	-1.32141400
C	4.72191400	-2.08032700	0.06693800
H	5.37897500	-1.26967900	0.41153300
H	4.51760900	-2.70272000	0.95006700
C	5.45049900	-2.91633200	-0.99009700
H	6.38508600	-3.33024000	-0.59509900
H	4.83106900	-3.75592300	-1.32891400
H	5.69872300	-2.31180500	-1.87068300

Structure 13b-TSCO-IV [B3LYP/6-31G(d)]

Cl	0.66877300	4.41646600	-0.38334700
C	-0.04402400	-0.73680500	0.08029700
C	-0.20276300	-2.07509100	0.54191700
C	-1.43971100	-2.66240400	0.64618500
C	-2.62111100	-1.93680300	0.34836800
C	-2.50320200	-0.57428800	-0.07898900
C	1.32388400	-0.10699300	-0.03660200
O	1.54280300	0.73203900	-0.99365200
O	-1.10247400	1.30706200	-0.64627900
C	-1.25148200	1.52314100	-2.08191600
H	0.67682800	-2.65262500	0.79966300
H	-1.52561500	-3.69378100	0.97807700
H	-1.20876400	2.60437400	-2.22239100
H	-2.21540100	1.13090900	-2.41116700
H	-0.42806300	1.03177000	-2.60445700
Mg	0.70783100	2.20824400	0.02265300
C	1.00655600	1.20372400	1.98812000
H	0.05462600	1.70146200	2.26554200
C	-1.19922000	-0.03349300	-0.24499000
C	-3.68789700	0.18360000	-0.29541900
C	-4.92623600	-0.39632900	-0.13787500
H	-5.82295800	0.19503900	-0.30003200
C	-5.04369900	-1.75487900	0.24483700
H	-6.02865400	-2.19847900	0.35919300
C	-3.91528900	-2.50355100	0.48927900
H	-3.99744200	-3.54041900	0.80541900
H	-3.60640000	1.23201400	-0.55983300
H	0.93502400	0.21224700	2.43619000
C	2.20806700	1.97424900	2.55178200
H	2.20316300	2.01185500	3.65232400
H	3.15934300	1.50927100	2.26032200
H	2.24488400	3.01751900	2.20785700
C	2.53650800	-0.85929700	0.48059100
H	2.31697400	-1.40372200	1.40413700
H	3.29894700	-0.11142200	0.71858600
C	3.10612800	-1.81129900	-0.59423900
H	2.35649800	-2.56651000	-0.86917500
H	3.30501800	-1.22822200	-1.50117100
C	4.38956800	-2.51393500	-0.13309400
H	5.13929200	-1.75620800	0.13379100
H	4.18735300	-3.08011000	0.78751900
C	4.96742800	-3.45487000	-1.19530900
H	5.88439600	-3.93885200	-0.84084600
H	4.25297400	-4.24505600	-1.45703000
H	5.21119900	-2.91076600	-2.11566600

Structure 13b-TSCO-V [B3LYP/6-31G(d)]

Cl	0.43101800	4.54699600	0.19868000
C	0.09780900	-0.64541900	-0.55940400
C	0.12864100	-2.06851800	-0.58014900
C	-1.00270600	-2.82067200	-0.37658800
C	-2.24730500	-2.20462400	-0.09174600
C	-2.31579000	-0.77382300	-0.05455700
C	1.34523000	0.17215300	-0.79863700
O	1.22971800	1.24027200	-1.52220900
O	-1.22865600	1.36402400	-0.34091300
C	-1.80347900	1.92730600	-1.55968300
H	1.06320600	-2.57216600	-0.79427400
H	-0.95066600	-3.90532800	-0.42285400
H	-1.85628700	3.00411300	-1.39048400
H	-2.80162200	1.51513000	-1.71734600
H	-1.14743800	1.69965900	-2.40266500
Mg	0.64728900	2.32045400	0.00734000
C	1.47921000	0.89754300	1.49589900
H	2.38784200	1.50252200	1.66458400
H	1.76512000	-0.13652200	1.66478900
C	-1.13559400	-0.03690100	-0.34906800
C	-3.54856600	-0.15329700	0.29276900
C	-4.66450000	-0.91507400	0.55536900
H	-5.59686200	-0.42899400	0.82850000
C	-4.60700700	-2.32851800	0.48382300
H	-5.49861900	-2.91441900	0.68814800
C	-3.42271300	-2.95628000	0.17350800
H	-3.36565200	-4.04125400	0.13544000
H	-3.59262900	0.92677100	0.37870900
C	0.37226800	1.25982700	2.51004900
H	0.07733400	2.32019300	2.48808500
H	-0.53555700	0.66655100	2.34165400
H	0.69200400	1.06035400	3.54433900
C	2.70434100	-0.52118300	-0.93146500
H	3.40010400	0.27821800	-1.20426100
H	2.59889300	-1.13321400	-1.84374600
C	3.32976000	-1.38308900	0.17843300
H	2.58992600	-2.04865200	0.63963100
H	3.69461200	-0.73230400	0.98041500
C	4.50204900	-2.22407600	-0.34939900
H	5.23161500	-1.56249000	-0.83712000
H	4.13994600	-2.90483500	-1.13368900
C	5.19904300	-3.03295400	0.74875600
H	6.02644700	-3.62523000	0.34241500
H	5.60939000	-2.37609200	1.52522700
H	4.50145800	-3.72515400	1.23638100

Structure 13b-TSCO-VI [B3LYP/6-31G(d)]

Cl	0.65874600	4.48820600	0.20396400
C	-0.08156500	-0.65036500	-0.57404600
C	-0.18841500	-2.06864800	-0.64988300
C	-1.37287000	-2.72054400	-0.40703400
C	-2.53331000	-2.00443600	-0.01936600
C	-2.46362000	-0.57614000	0.06848500
C	1.22753800	0.05183800	-0.85328500
O	1.18985500	1.13249700	-1.55919500
O	-1.20910000	1.46182500	-0.24101200
C	-1.81556400	2.10005600	-1.40723500
H	0.67937600	-2.64729300	-0.94162100
H	-1.42720600	-3.80218500	-0.49835300
H	-1.75477500	3.17316100	-1.21937700
H	-2.85591900	1.78353200	-1.49808500
H	-1.24540400	1.82988900	-2.29910600
Mg	0.74603100	2.25182400	0.00167000
C	1.51394100	0.79758000	1.47459600
H	0.69300900	1.19902700	2.10430500
C	-1.24073600	0.06000600	-0.27982800
C	-3.60689300	0.14234000	0.51779400
C	-4.77098600	-0.52231500	0.82999000
H	-5.63316600	0.03675400	1.18239900
C	-4.85280500	-1.93105500	0.70724600
H	-5.78128600	-2.43931800	0.95136200
C	-3.75582500	-2.65366800	0.29783300

H	-3.80483600	-3.73690600	0.22048900
H	-3.54170700	1.21750000	0.64306100
H	1.50906700	-0.27074000	1.68271200
C	2.85379700	1.44067200	1.86179100
H	3.16099400	1.19432000	2.89052000
H	3.66741200	1.11325000	1.20125000
H	2.82759400	2.53816400	1.80496400
C	2.51458900	-0.75999000	-0.98721100
H	3.29476200	-0.02618300	-1.21362700
H	2.37512700	-1.32598800	-1.92458600
C	3.01082400	-1.71952000	0.10864500
H	2.18912100	-2.30939900	0.53014300
H	3.42321200	-1.13975700	0.94015500
C	4.09603800	-2.67012700	-0.41986200
H	4.90900600	-2.07958900	-0.86510700
H	3.68302500	-3.27976200	-1.23685300
C	4.66562200	-3.58752600	0.66651000
H	5.43606400	-4.25361100	0.26241900
H	5.11963800	-3.00557800	1.47763800
H	3.88121800	-4.21420300	1.10867100

Structure 13c_I [B3LYP/6-31G(d)]

C	1.40615800	0.86649100	-0.03475100
C	0.70725800	2.09712400	0.14090100
C	-0.65898600	2.15684900	0.20679200
C	-1.43154100	0.97042300	0.07842800
C	-0.76123400	-0.28317500	-0.09754000
C	2.87046100	0.96997000	-0.19276500
O	3.67255100	0.06438200	-0.33625500
O	1.23014800	-1.54363500	-0.33929300
C	1.97547300	-2.12343000	0.74269100
H	1.29519800	3.00927200	0.21660700
H	-1.16745600	3.10731300	0.34460000
H	2.22824700	-3.13286200	0.41238600
H	1.35436600	-2.17864000	1.64528100
H	2.89082600	-1.56148300	0.93268000
C	0.66874300	-0.31958500	-0.13516700
C	-1.53343200	-1.46887600	-0.22997500
C	-2.90850800	-1.41753600	-0.18658300
H	-3.48959200	-2.32957000	-0.29089800
C	-3.57263200	-0.18018900	-0.00825700
H	-4.65848800	-0.15258000	0.02456700
C	-2.85001700	0.98514000	0.12094500
H	-3.35776800	1.93711000	0.25499800
H	-1.01395100	-2.40883200	-0.37543000
H	3.22655500	2.02505900	-0.18871400

Structure 13c_II [B3LYP/6-31G(d)]

C	-1.54772600	-0.47881300	-0.10148400
C	-1.11316900	-1.81682800	0.11728800
C	0.21900100	-2.11602100	0.22210300
C	1.20528900	-1.09569400	0.09405600
C	0.79055100	0.25706900	-0.13268900
C	-2.99497600	-0.20439200	-0.23369900
O	-3.85887600	-1.05527000	-0.10444400
O	-1.00694200	1.83882000	-0.42554100
C	-1.20823100	2.61419000	0.76159000
H	-1.87816400	-2.58265400	0.19716500
H	0.54409100	-3.13892400	0.39418300
H	-1.48119200	3.61740100	0.42783100
H	-0.29322100	2.66212300	1.36455500
H	-2.01947900	2.19680400	1.37141300
C	-0.60662700	0.53801000	-0.20714000
C	1.77335100	1.26937300	-0.29257700
C	3.11330600	0.96172300	-0.21025400
H	3.85875700	1.74166500	-0.33816900
C	3.52690000	-0.36984900	0.03219100
H	4.58694900	-0.59982400	0.09645700
C	2.59416700	-1.37382200	0.17628900
H	2.91112200	-2.39900300	0.35106600
H	1.44828900	2.28284500	-0.50177400
H	-3.26162200	0.84149500	-0.47689300

Structure 13c-TSCO_I [B3LYP/6-31G(d)]

Cl	-4.00638200	-1.56639600	0.30421100
C	0.18797700	1.34248000	-0.66684300
C	1.23843200	2.29747800	-0.60527600
C	2.53139400	1.91036200	-0.35494900
C	2.84705200	0.54900500	-0.09685900
C	1.79610700	-0.42879500	-0.09933600
C	-1.19178900	1.80094900	-0.96059200
O	-2.03721000	1.10238700	-1.60918400
O	-0.56705800	-0.91204000	-0.38752100
C	-0.69791700	-1.75504600	-1.57231800
H	1.00179500	3.34342100	-0.78272100
H	3.33075300	2.64620700	-0.33600700
H	-1.52152300	-2.43661200	-1.35583400
H	0.22993800	-2.30751800	-1.73175900
H	-0.93302300	-1.12709900	-2.43451300
Mg	-2.46215900	0.04542600	0.05015200
C	-1.92265200	1.69634100	1.43268000
H	-2.99500300	1.75050200	1.70646000
H	-1.61469100	2.73837500	1.31756800
C	0.48567000	0.00759600	-0.42775700
C	2.10141100	-1.77377600	0.24824300
C	3.39482700	-2.14134900	0.54170500
H	3.61575400	-3.17015400	0.81127300
C	4.44076200	-1.18713800	0.50599600
H	5.45695700	-1.49494900	0.73512300
C	4.16958300	0.12736800	0.20093300
H	4.96551600	0.86767700	0.19413300
H	1.29957900	-2.50169100	0.30523900
C	-1.10818500	1.02534900	2.54549700
H	-1.48970900	0.02740400	2.80324200
H	-0.05618500	0.90104600	2.25509900
H	-1.10803200	1.60957200	3.47905400
H	-1.32960200	2.88972800	-0.91288200

Structure 13c-TSCO_II [B3LYP/6-31G(d)]

Cl	3.70028700	-2.01306600	-0.33022800
C	-0.22679300	1.23648600	0.67494200
C	-1.18330100	2.28687500	0.65499800
C	-2.50031300	2.03564000	0.36020900
C	-2.93058900	0.72761000	0.00938700
C	-1.97296100	-0.34132100	-0.02882000
C	1.18537200	1.54791800	1.00726400
O	1.94507000	0.74567000	1.62833200
O	0.32618100	-1.05878400	0.27664500
C	0.35486500	-1.97568100	1.41285200
H	-0.85604200	3.29434300	0.89851000
H	-3.22918400	2.84144500	0.37322700
H	1.12014900	-2.71433600	1.17193800
H	-0.62215900	-2.44974300	1.52327700
H	0.62516500	-1.42093300	2.31396800
Mg	2.30632800	-0.26193800	-0.10924000
C	2.02773300	1.51525900	-1.39464300
H	1.92893300	0.85190200	-2.27681700
C	-0.63815400	-0.04990000	0.35459300
C	-2.38904700	-1.62838800	-0.46889000
C	-3.70210800	-1.85666900	-0.81166000
H	-4.00803300	-2.84197300	-1.15142200
C	-4.65809400	-0.81430700	-0.73577100
H	-5.69158700	-1.01272600	-1.00486800
C	-4.27768200	0.44827700	-0.34144100
H	-5.00353000	1.25649600	-0.30337200
H	-1.65506900	-2.42196100	-0.55554500
H	1.19582300	2.21877700	-1.48484400
C	3.37424500	2.25139000	-1.43508700
H	3.49236100	2.87521500	-2.33509600
H	3.49680600	2.91805000	-0.57044500
H	4.22952800	1.56139900	-1.42367200
H	1.44699600	2.61520500	0.96250400

Structure 13c-TSOMe_I [B3LYP/6-31G(d)]

Cl	-4.18665900	-1.39676900	0.18048500
C	0.15534000	1.61475100	-0.52218900
C	1.36422600	2.38535600	-0.47246900
C	2.57547200	1.80678500	-0.24865700
C	2.68022000	0.38508900	-0.06519300
C	1.50970600	-0.43058400	-0.13069100
C	-1.08893400	2.28904600	-0.58074300
O	-2.22199900	1.75219000	-0.40486500
O	-0.76372900	-0.62250800	-0.96234400
C	-0.64126300	-0.72087700	-2.40190100
H	1.28397000	3.46259900	-0.60123200
H	3.48119000	2.40515200	-0.21334200
H	-1.44512400	-1.38561000	-2.72043600
H	0.33109800	-1.15014000	-2.65609600
H	-0.75352000	0.26423000	-2.86305200
Mg	-2.33265300	-0.13600600	0.22964500
C	-0.75738200	-0.13448400	1.87198200
H	-0.12263900	-1.01727400	1.96585200
H	-1.72933100	-0.41066500	2.34021800

C	0.21885200	0.19775000	-0.31617700
C	1.63400200	-1.83399500	-0.01323700
C	2.87180500	-2.42153200	0.17580900
H	2.95212500	-3.50057000	0.26951200
C	4.02633700	-1.61918300	0.25497000
H	4.99705600	-2.08270000	0.40835600
C	3.92967000	-0.24468900	0.13600500
H	4.82234900	0.37354000	0.18858300
H	0.73847100	-2.44481400	-0.06467300
C	-0.19555500	1.09020900	2.56881200
H	-0.70191200	2.01372300	2.25223800
H	-0.30014700	1.03450100	3.66245200
H	0.86948200	1.21917700	2.35012300
H	-1.06717300	3.37669000	-0.74274500

Structure 13c-TSOMe_II [B3LYP/6-31G(d)]

Cl	4.15340800	-1.20204200	0.14718900
C	-0.20784700	1.83722300	-0.05078700
C	-1.40768400	2.50466100	-0.46385900
C	-2.59541700	1.84799300	-0.57251700
C	-2.69540900	0.45815800	-0.21944100
C	-1.53529000	-0.24952700	0.22090300
C	1.02458100	2.52512000	-0.13449600
O	2.17072100	1.98603300	-0.07474100
O	0.71996300	-0.12789100	1.10136300
C	0.60338100	0.27884100	2.48668800
H	-1.33868900	3.56046700	-0.71657100
H	-3.49169100	2.36903900	-0.89623200
H	1.38592100	-0.26438900	3.01778000
H	-0.38156700	-0.00294900	2.86701500
H	0.75420200	1.35733800	2.58198100
Mg	2.28648200	-0.00740500	-0.19325800
C	0.74061500	-0.48309800	-1.79274400
C	-0.25535600	0.42574800	0.21144600
C	-1.66273200	-1.58817400	0.65668500
C	-2.89231900	-2.22436900	0.63915300
H	-2.97569000	-3.25342300	0.97608900
C	-4.03104500	-1.53901800	0.17770400
H	-4.99376100	-2.04249300	0.15744300
C	-3.93231700	-0.22346500	-0.24061800
H	-4.81624700	0.31065500	-0.57997800
H	-0.77984100	-2.11192300	1.00699100
H	1.58860500	-0.06457700	-2.37571300
C	0.68713700	-2.00073100	-1.92230200
H	0.53461400	-2.31547100	-2.96715000
H	1.60715200	-2.48817900	-1.57532500
H	-0.14763700	-2.41880300	-1.34752800
H	-0.14552500	-0.00238900	-2.20414700
H	0.98717600	3.60936200	-0.31564200

Structure 13c·EtMgCl_I [B3LYP/6-31G(d)]

C	0.38288100	1.76935300	-0.02376100
C	1.55540000	2.49717600	0.33501400
C	2.78024000	1.88623600	0.38207400
C	2.91065800	0.50101100	0.08501700
C	1.74843100	-0.25301800	-0.29038500
C	-0.89463800	2.47628300	0.02352000
O	-2.01713600	1.96480100	0.00635900
O	-0.60835100	-0.28453400	-0.80319100
C	-0.73404900	-0.35504900	-2.25699400
H	1.45574400	3.55026700	0.58517800
H	3.66669700	2.44992300	0.65848000
H	-1.66650200	-0.88688700	-2.44075600
H	0.12611600	-0.88751600	-2.66994300
H	-0.79053300	0.65710700	-2.66747900
Mg	-2.45150000	-0.07328900	0.42172800
C	-1.92388400	-0.40299500	2.45631600
C	0.50130100	0.42018300	-0.36476800
C	1.87398900	-1.64480300	-0.55630600
C	3.10234500	-2.25857400	-0.47310600
H	3.18974300	-3.32356500	-0.66623100
C	4.25504100	-1.51269800	-0.12492000
H	5.21802100	-2.01179700	-0.06595700
C	4.16022400	-0.16676200	0.15135200
H	5.04243800	0.40234600	0.43188600
H	0.98504800	-2.21723500	-0.79659000
Cl	-3.98754300	-0.83570000	-1.09877500
H	-1.15710500	0.32453800	2.77387300
C	-1.43766900	-1.82179300	2.81354900
H	-2.19087700	-2.58318300	2.56952900
H	-0.52683200	-2.09588200	2.26105100
H	-1.20078000	-1.94810300	3.88344600
H	-2.80054400	-0.16690900	3.08136200
H	-0.82213200	3.57382600	0.11564600

Structure 13c·EtMgCl_II [B3LYP/6-31G(d)]

C	0.30589600	1.26542000	-1.01076100
C	1.43121100	2.12611400	-1.17350200
C	2.68456900	1.73246800	-0.78701200
C	2.89303600	0.45399800	-0.19853500
C	1.78029700	-0.43774300	-0.03461100
C	-1.00748900	1.79092700	-1.37715300
O	-2.10100500	1.29687400	-1.08937100
O	-0.56201800	-0.89639800	-0.38722600
C	-0.66013900	-1.82921200	-1.50703900
H	1.27133500	3.11295500	-1.60014900
H	3.53424100	2.39731400	-0.91336200
H	-1.55116300	-2.42345000	-1.30946600
H	0.24059100	-2.44671900	-1.54406100
H	-0.77881600	-1.26916000	-2.43894700
Mg	-2.43524800	-0.08079500	0.48502500
C	-1.97588000	0.96127800	2.28635000
H	-1.16712600	0.43430000	2.81992400
C	0.50147700	-0.01115700	-0.47913200
C	1.98406400	-1.70307400	0.58247400
C	3.24004600	-2.07605600	1.00194700
H	3.38694300	-3.03875700	1.48238400
C	4.34394300	-1.20689300	0.82272500
H	5.32954400	-1.51682600	1.15807500
C	4.17326800	0.02929300	0.24000600
H	5.01784400	0.70154800	0.11463600
H	1.13178500	-2.35418400	0.74172800
Cl	-3.88204900	-1.72371600	-0.19111500
C	-1.61232000	2.45328700	2.18161000
H	-2.43017700	3.04147800	1.74270800
H	-1.37949100	2.91862400	3.15392300
H	-0.72954000	2.62281400	1.54590700
H	-2.85149600	0.85902200	2.94719500
H	-0.99434500	2.73804900	-1.94327000

Structure 13c·EtMgCl_III [B3LYP/6-31G(d)]

C	0.44251700	1.36158600	-0.98253700
C	1.56138900	2.24307500	-1.04633700
C	2.79520600	1.85303500	-0.59769800
C	2.98802800	0.55696100	-0.04374100
C	1.88185900	-0.35565700	0.01981800
C	-0.85473200	1.88203600	-1.40851200
O	-1.95736200	1.37724400	-1.18407600
O	-0.42681600	-0.83234500	-0.49329300
C	-0.43980200	-1.72502600	-1.64963600
H	1.41206800	3.24232800	-1.44718800
H	3.64018700	2.53377300	-0.64829200
H	-1.33276600	-2.33698100	-1.53096800
H	0.47095700	-2.32874100	-1.65169600
H	-0.50859600	-1.13272100	-2.56645900
Mg	-2.37202800	-0.09111300	0.29924400
C	-2.00892400	0.81116600	2.19076500
C	0.62573800	0.06914300	-0.48636400
C	2.06795400	-1.63984700	0.60254500
C	3.30198900	-2.01066400	1.08420000
H	3.43486500	-2.98819200	1.53801200
C	4.40079500	-1.12041300	1.00368800
H	5.36915600	-1.42900300	1.38704000
C	4.24611100	0.13383700	0.45635200
H	5.08600800	0.82161100	0.40685500
H	1.21799100	-2.30788500	0.68648000
Cl	-3.75504900	-1.68309200	-0.60078200
H	-1.16003500	1.51311300	2.11959700
H	-0.82021300	2.83981600	-1.95617500
C	-3.20410900	1.54848400	2.82812600
H	-4.06327900	0.88007500	2.97384800
H	-2.97413100	1.98305100	3.81544400
H	-3.55787700	2.37718600	2.19834300
H	-1.66485400	0.03299500	2.89247200

Structure 1a·CH3MgCl(DME)_I [B3LYP/6-31G(d)]

C	0.84782000	1.87068200	0.04041600
C	2.05589900	2.47726400	0.48764800
C	3.23705400	1.78347200	0.51816600
C	3.29265500	0.42449800	0.10879500
C	2.09305100	-0.21118200	-0.34693700
O	-0.25344000	-0.10828900	-0.83969800

C	-0.50372000	0.05517800	-2.26143200
H	2.00135400	3.51234400	0.80473300
H	4.14689000	2.26709400	0.86340600
H	-1.45398100	-0.43992600	-2.45759700
H	0.31317600	-0.40452600	-2.82523800
H	-0.58587000	1.11749100	-2.50105200
C	0.88831800	0.54892200	-0.38004500
C	2.14032400	-1.57543800	-0.74495500
C	3.32573300	-2.27461500	-0.70156800
H	3.35116200	-3.31715000	-1.00631400
C	4.51485700	-1.64581100	-0.25954000
H	5.44288300	-2.20990100	-0.23154300
C	4.49597600	-0.32801700	0.13818400
H	5.40486200	0.15739300	0.48436300
H	1.22513000	-2.05862600	-1.06893400
Mg	-1.87403600	-0.47522700	0.57115800
O	-1.44636900	-2.60908400	0.61304000
C	-0.61595100	-3.14973200	1.64379800
H	-0.22897000	-2.30787100	2.21740300
H	-1.20454300	-3.80211400	2.30113600
H	0.21133200	-3.72234500	1.20470700
C	-2.09277600	-3.61946700	-0.16829300
H	-1.34515500	-4.21801200	-0.70572100
H	-2.68478300	-4.27590400	0.48182400
H	-2.75134100	-3.10464600	-0.86743400
C	-0.36273600	2.75236100	0.07820900
O	-1.52575500	2.12043700	-0.19669500
O	-0.30395700	3.93711900	0.33636400
C	-2.70992200	2.95288400	-0.15512300
H	-2.84570500	3.35232400	0.85210300
H	-2.60740000	3.77801100	-0.86316100
H	-3.52639000	2.28792900	-0.43186900
C	-1.43347100	0.12306800	2.55223400
H	-0.36003000	0.17826900	2.79511600
H	-1.83370900	1.12580300	2.76767100
H	-1.88044900	-0.53965800	3.30973900
Cl	-3.71191400	-0.55877200	-0.85756900

Structure 1a·CH3MgCl(DME)_II [B3LYP/6-31G(d)]

C	0.41224700	1.91649600	-0.03535800
C	1.45871600	2.69232300	0.53905100
C	2.73437200	2.20535000	0.65228600
C	3.05346700	0.89435700	0.20996100
C	2.01961800	0.08793000	-0.36562800
O	-0.26134600	-0.18529300	-1.05607900
C	-0.41167000	-0.02216500	-2.48892400
H	1.20072600	3.68507500	0.88902300
H	3.51659800	2.81754100	1.09298300
H	-1.19437000	-0.71778700	-2.78952100
H	0.53528900	-0.26116200	-2.98151400
H	-0.71712800	1.00134600	-2.71483500
C	0.71126200	0.63961300	-0.48581700
C	2.33009700	-1.23271400	-0.79163200
C	3.60937400	-1.72618600	-0.66466000
H	3.83518600	-2.73689400	-0.99328300
C	4.63543200	-0.92653300	-0.10560500
H	5.64024900	-1.32880500	-0.01205200
C	4.36065100	0.35209200	0.32374800
H	5.14256300	0.96763500	0.76112200
H	1.54017000	-1.84934100	-1.20577300
Mg	-1.96781800	-0.94216300	0.07633200
O	-0.96477700	-2.79663200	0.54593600
C	-0.16495800	-3.02402800	1.71452700
H	-0.19776400	-2.10554900	2.29983500
H	-0.58694000	-3.85053900	2.29936600
H	0.86533100	-3.26395600	1.42273800
C	-1.12512900	-3.96693400	-0.25596800
H	-0.15138700	-4.31363000	-0.62748000
H	-1.59409400	-4.76709900	0.33044200
H	-1.77297800	-3.69755600	-1.09030500
C	-0.92973000	2.58280600	-0.06414100
O	-1.92162100	1.83733100	-0.60370300
O	-1.10915000	3.70902000	0.34979000
C	-3.23277600	2.44243800	-0.54657300
H	-3.52064100	2.59696800	0.49507900
H	-3.23023500	3.39786400	-1.07568300
H	-3.89608100	1.72593900	-1.02908700
Cl	-1.91120200	-0.01704600	2.19117700
C	-3.44995000	-1.48593400	-1.34573400
H	-3.98415700	-0.62128600	-1.77016100
H	-3.10781200	-2.06754300	-2.21867700
H	-4.22926900	-2.10436800	-0.87295500

Structure 1'a·CH3MgCl(DME)_I [B3LYP/6-31G(d)]

C	0.92263500	0.32251900	0.15807700
C	0.76540000	-1.04706000	0.52946400
C	1.84056000	-1.89443600	0.56569000
C	3.13408500	-1.44704900	0.18344000
C	3.30841500	-0.08411500	-0.21913100
C	-0.31572300	1.13037800	0.11865200
O	-1.43476500	0.62028100	0.00285400
Cl	-2.68613100	-2.09037400	1.66923300
H	-0.22226700	-1.40025400	0.81147400
H	1.70761100	-2.92656500	0.87785200
C	-4.58671800	1.48656400	1.09266100
H	-4.31142800	1.95672900	2.05038900
H	-5.63153000	1.16440100	1.22186700
C	2.18676300	0.80084500	-0.19146400
C	4.58982400	0.35207000	-0.65309600
C	5.65926700	-0.51482800	-0.65771300
H	6.63384200	-0.17284700	-0.99463300
C	5.49523100	-1.85557700	-0.23342200
H	6.34792600	-2.52905000	-0.23920100
C	4.26053300	-2.31067400	0.17238800
H	4.12766700	-3.34336900	0.48452200
H	4.70336800	1.37273200	-1.00070400
O	-0.16134800	2.44606200	0.22247900
C	-1.35994100	3.25136700	0.15254300
H	-1.02160600	4.27330200	0.32012600
H	-1.81600200	3.15473000	-0.83567200
H	-2.07898500	2.94320000	0.91325600
H	-4.61530700	2.30808800	0.35708400
Mg	-3.29610200	-0.12324900	0.59873600
O	-3.88702600	-0.87474600	-1.29801300
C	-3.54985100	-2.17093300	-1.80671000
H	-2.98377000	-2.67630200	-1.02412700
H	-4.46513700	-2.73453900	-2.02568400
H	-2.94954900	-2.07245500	-2.72005800
C	-4.71829100	-0.11712700	-2.17847300
H	-4.19409500	0.08086800	-3.12246600
H	-5.64774900	-0.66282700	-2.38394200
H	-4.94773200	0.82030700	-1.67050200
O	2.38650800	2.09477200	-0.59897000
C	2.80465400	3.00284500	0.42895100
H	2.03181800	3.10433300	1.19681600
H	3.74315400	2.67093500	0.88898200
H	2.95922000	3.96424900	-0.06510600

Structure 1'a·CH3MgCl(DME)_II [B3LYP/6-31G(d)]

C	1.05987700	0.17116100	-0.03574500
C	1.02733100	-1.25462500	-0.11143900
C	2.17766100	-1.99150700	-0.19741100
C	3.44794400	-1.35486200	-0.22353900
C	3.50839500	0.07321600	-0.15134000
C	-0.25790000	0.84509600	0.01653900
O	-1.31541200	0.21709900	0.15614700
Cl	-4.11976200	0.73227600	-1.74087400
H	0.06024800	-1.74477000	-0.11551400
H	2.12707400	-3.07502200	-0.25953700
C	-2.36336100	-2.88231500	-0.95183100
H	-1.75919800	-2.95703900	-1.86921200
H	-3.23352000	-3.53557600	-1.12176800
C	2.29651800	0.82322000	-0.04431000
C	4.77462500	0.71734000	-0.19656600
C	5.93153900	-0.02249700	-0.29378800
H	6.89461900	0.47868000	-0.33200200
C	5.87442800	-1.43577000	-0.35285200
H	6.79500500	-2.00781000	-0.43001000
C	4.66035500	-2.08547200	-0.32160400
H	4.61257800	-3.17003200	-0.37608100
H	4.80800000	1.80057200	-0.17222000
O	-0.24232500	2.16503200	-0.09533700
C	-1.52165300	2.84635000	-0.08999100
H	-1.27928600	3.88765600	-0.29963300
H	-2.18618400	2.42947000	-0.84914900
H	-1.98551000	2.75112500	0.89559900
H	-1.76907800	-3.37725000	-0.16512700
Mg	-2.94304600	-0.88162900	-0.55077500
O	-4.04810900	-0.90502400	1.26989600
C	-5.02401500	0.06941400	1.65455500
H	-5.05597100	0.81111900	0.85612600
H	-6.00727600	-0.40607000	1.75821500

H	-4.73856000	0.53299400	2.60783700
C	-3.95200400	-2.00342900	2.17827500
H	-3.61667700	-1.65478400	3.16364700
H	-4.92576500	-2.49933200	2.27711900
H	-3.22682100	-2.70005200	1.75666100
O	2.42014700	2.18555300	0.00790700
C	2.37983000	2.76359300	1.31587800
H	1.41225600	2.58974300	1.79830500
H	3.18362300	2.36123700	1.94528500
H	2.52612400	3.83632600	1.17578400

Structure 1a-TSOMe(DME) [B3LYP/6-31G(d)]

C	-0.93055500	1.78779800	-0.00755100
C	-2.18737200	2.39161500	-0.30235700
C	-3.33583500	1.66457000	-0.44257200
C	-3.30975300	0.24635800	-0.25616800
C	-2.07565600	-0.41002200	0.02783100
O	0.14458500	-0.17701300	1.00641700
Cl	4.02609700	-0.21790100	-0.13089500
C	-0.12374500	0.15093000	2.38431200
H	-2.19371500	3.47097600	-0.41605100
H	-4.28122600	2.15169600	-0.66228100
H	0.66637300	-0.32464600	2.96952100
H	-1.09863100	-0.25129900	2.67116500
H	-0.10774500	1.23264600	2.53726000
C	0.08304300	-0.30926000	-1.75469400
H	-0.24679700	-1.34704300	-1.83760200
H	1.06208400	-0.21840900	-2.28922800
C	-0.83132400	0.36276100	0.05039700
C	-2.06949600	-1.80372600	0.25669900
C	-3.23951800	-2.54086700	0.21196400
H	-3.21601100	-3.61256400	0.38926000
C	-4.45992000	-1.89837000	-0.07582400
H	-5.37976300	-2.47617000	-0.11676300
C	-4.48994800	-0.53700700	-0.30630000
H	-5.43192500	-0.03912200	-0.52375600
H	-1.12262900	-2.29545400	0.45611400
H	-0.58668300	0.33655100	-2.32049700
Mg	1.72960100	-0.16983400	-0.21421200
O	1.72258200	-2.39040100	-0.16325600
C	2.12515000	-2.96566600	1.08537200
H	1.55509200	-2.46176400	1.86807100
H	1.88195500	-4.03514900	1.09638200
H	3.19860200	-2.81946400	1.24840700
C	2.33271500	-3.06239200	-1.27496900
H	2.06584100	-4.12590300	-1.25186400
H	1.93169600	-2.60929200	-2.18287600
H	3.42049100	-2.94022100	-1.24610000
C	0.21495200	2.67195200	0.02144500
O	0.19934700	3.88730800	0.03504900
O	1.47027000	2.00846800	-0.00802800
C	2.59713200	2.92839900	-0.02757500
H	3.48405700	2.29981900	-0.03610200
H	2.54309000	3.55580200	-0.91871500
H	2.56349400	3.56199700	0.85990400

Structure 1a-TSCO(DME)-I [B3LYP/6-31G(d)]

C	-0.69627400	0.29856500	0.59899500
C	-0.84619800	-0.87223800	1.39508000
C	-2.01926100	-1.58457300	1.42574200
C	-3.12472400	-1.18884300	0.62866500
C	-3.00009600	-0.01773800	-0.18466800
C	0.65148000	0.97474900	0.66053900
O	1.58584300	0.42655100	1.36982300
Cl	4.96277900	0.55748300	-0.28272200
H	-0.00137000	-1.16810800	2.00702600
H	-2.11304900	-2.46092400	2.06244700
C	1.22117200	0.65872900	-1.48867100
H	0.93216300	-0.32415400	-1.89157400
H	2.10837000	1.01490600	-2.04911400
C	-1.78275800	0.73457600	-0.15236000
C	-4.08749600	0.35754400	-1.01983400
C	-5.25344800	-0.37499900	-1.02631400
H	-6.07497700	-0.07991000	-1.67338800
C	-5.38791200	-1.51749700	-0.20080500
H	-6.31519000	-2.08392700	-0.21200100
C	-4.34426200	-1.91634800	0.60325700
H	-4.43637600	-2.80085200	1.22916700
H	-3.97169100	1.21773100	-1.66950700
O	0.53846500	2.32774300	0.66737900
C	1.74553700	3.06579900	0.88104500
H	1.45311900	4.11660100	0.85932000
H	2.19857500	2.81270100	1.84198600
H	2.46276800	2.86747600	0.07498100
H	0.42225100	1.35621100	-1.72858800
Mg	2.78387100	-0.05462100	-0.08381000
O	2.83310200	-2.11805900	-0.34945800
C	4.04929400	-2.85308000	-0.57893300
H	4.17294500	-3.61095800	0.20335000
H	4.00680500	-3.33606800	-1.56215000
H	4.86574000	-2.13214600	-0.54549300
C	1.66743700	-2.95205600	-0.38238600
H	1.57479200	-3.42605900	-1.36673500
H	1.74006200	-3.72320100	0.39363500
H	0.80053400	-2.31978800	-0.19144000
O	-1.71153200	1.85368200	-0.94878100
C	-2.21688700	3.05861400	-0.35848900
H	-3.27358500	2.94941300	-0.08470800
H	-1.62918600	3.33138600	0.52179500
H	-2.11705100	3.83134600	-1.12390100

Structure 1a-TSCO(DME)-II [B3LYP/6-31G(d)]

C	0.79429800	0.16923100	-0.53844100
C	0.95035500	-1.04065100	-1.27181100
C	2.14754500	-1.70908700	-1.31763600
C	3.27279800	-1.22658800	-0.60077000
C	3.13979600	-0.01970500	0.15696000
C	-0.57781200	0.79350100	-0.56232300
O	-1.51548200	0.21833100	-1.25150900
Cl	-2.96397400	-2.82527700	0.63979400
H	0.09176100	-1.41374500	-1.81806100
H	2.24172500	-2.62262800	-1.89891000
C	-1.05886800	0.45800700	1.59353600
H	-0.72018100	-0.48226700	2.05782700
H	-1.97442600	0.79924200	2.11635100
C	1.89284800	0.68042900	0.14579500
C	4.24902500	0.43898300	0.91900700
C	5.44290900	-0.24665800	0.90402800
H	6.28107000	0.11213900	1.49531900
C	5.58454100	-1.42456600	0.13098100
H	6.53322300	-1.95450800	0.12575900
C	4.52077700	-1.90467100	-0.59867300
H	4.61719700	-2.81824400	-1.18038900
H	4.12938300	1.32500700	1.53235700
O	-0.52520100	2.15200600	-0.56473400
C	-1.76228600	2.83716800	-0.74815700
H	-1.52339200	3.89907000	-0.66784600
H	-2.19212300	2.62150700	-1.73005600
H	-2.47697100	2.55850200	0.03469100
H	-0.29796300	1.20776800	1.79609700
Mg	-2.38465400	-0.67323400	0.24484300
O	-4.26830600	0.24950800	0.14733800
C	-5.25381400	-0.08186600	1.14017000
H	-6.03634300	0.68559400	1.14452800
H	-5.68225600	-1.06893400	0.93934400
H	-4.74625400	-0.09594400	2.10586700
C	-4.82634800	0.35104100	-1.17356400
H	-5.28111300	-0.60191200	-1.46866800
H	-5.58112700	1.14572900	-1.19251300
H	-4.00177200	0.59874900	-1.84280800
O	1.80605400	1.83124100	0.89798400
C	2.24752100	3.02472400	0.24138700
H	3.29485600	2.93819800	-0.07328600
H	1.61686500	3.24503600	-0.62441700
H	2.15502200	3.82571800	0.97863700

Structure 16 [B3LYP/6-31G(d)]

C	1.71482200	1.18332300	0.00001700
C	0.85050400	2.30645500	0.00002700
C	-0.51412000	2.15387400	-0.00000800
C	-1.08759200	0.85187400	-0.00002200
C	-0.23260300	-0.29572600	-0.00003300
O	1.93043300	-1.23783400	-0.00001200
C	3.34336700	-1.12126800	0.00000100
H	1.28860500	3.30104800	0.00003100
H	-1.17079400	3.01987200	-0.00002500
H	3.72866000	-2.14256800	-0.00019000
H	3.70309600	-0.59636000	0.89473600
H	3.70312700	-0.59613500	-0.89460200
C	1.18663800	-0.09294500	-0.00001800
C	-0.80825100	-1.59214900	0.00000200
C	-2.17729900	-1.75122600	0.00002900

H	-2.60728000	-2.74926100	0.00007400
C	-3.02789900	-0.62109000	0.00000300
H	-4.10615700	-0.75766100	0.00001600
C	-2.49328300	0.64810000	-0.00001500
H	-3.14403000	1.51950500	-0.00002100
H	-0.15106000	-2.45447200	0.00005800
H	2.78666800	1.34337400	0.00012500

Structure 16·CH3MgCl(DME) [B3LYP/6-31G(d)]

C	-0.18890700	-1.22058900	-1.70432800
C	-1.43837700	-1.84232100	-1.93978800
C	-2.57050800	-1.38409800	-1.30665900
C	-2.50975800	-0.28945700	-0.40225600
C	-1.24955100	0.34731500	-0.14944500
O	1.13617300	0.44398000	-0.60509200
Cl	2.78680300	2.20112700	1.72366200
C	1.41494600	1.56575200	-1.47866100
H	-1.49377900	-2.68395700	-2.62392500
H	-3.53138000	-1.85933300	-1.48687100
H	2.30692300	2.05122400	-1.08393000
H	0.57715200	2.26765400	-1.45732700
H	1.57616300	1.20229400	-2.49830000
C	1.58731200	-1.75044100	2.08836700
H	2.32459200	-2.19738100	2.77341900
H	1.29157700	-2.54978000	1.39077500
C	-0.11061500	-0.15957000	-0.83608900
C	-1.18668700	1.43351100	0.76518100
C	-2.32856000	1.87227900	1.39859500
H	-2.26953600	2.69936700	2.10027000
C	-3.57631800	1.25192700	1.14896800
H	-4.46636200	1.61065000	1.65849000
C	-3.66284200	0.19587200	0.27051300
H	-4.61819400	-0.28732000	0.08069200
H	-0.23234900	1.90945000	0.97161000
H	0.71073400	-1.57454800	-2.19865000
H	0.69660500	-1.54844400	2.70120800
Mg	2.30871100	0.00206400	1.16016000
O	4.14054900	-0.51846000	0.18259100
C	5.26915200	0.34390400	-0.01160100
H	4.95826600	1.34151100	0.29858000
H	6.10889800	0.00608400	0.60804700
H	5.56785600	0.33912800	-1.06768500
C	4.42608800	-1.89079900	-0.10351000
H	4.67959400	-2.01162000	-1.16451600
H	5.26178800	-2.24067100	0.51501400
H	3.52928800	-2.46104400	0.14051700

Structure 16-TSOMe(DME) [B3LYP/6-31G(d)]

C	0.94700200	-2.16148600	-0.05939100
C	2.24410800	-2.65715800	-0.26282700
C	3.34296500	-1.82732400	-0.36305500
C	3.16263700	-0.42390700	-0.22440700
C	1.85084700	0.12394000	-0.03517600
O	-0.38541400	-0.37687800	0.97296600
Cl	-2.60894100	2.57993400	-0.07794000
C	0.02775400	-0.49494900	2.34582000
H	2.37704100	-3.73574100	-0.32737000
H	4.34249300	-2.22758700	-0.50403900
H	-0.84516400	-0.26166000	2.96054700
H	0.83581600	0.20968600	2.55806800
H	0.36915200	-1.51529400	2.53629500
C	-0.37460900	-0.37678500	-1.66232400
H	-0.85899500	0.55165600	-2.06773800
H	-1.02968500	-1.23703300	-1.87122600
C	0.68743800	-0.76816100	-0.05776100
C	1.70621300	1.52278700	0.11026400
C	2.79721200	2.37155600	0.08907300
H	2.65700000	3.44269400	0.20376400
C	4.09088800	1.83687900	-0.09054100
H	4.95275600	2.49948900	-0.11015900
C	4.26219400	0.47819200	-0.24595900
H	5.25926100	0.06607700	-0.38627900
H	0.71448100	1.95000100	0.24901700
H	0.10699200	-2.85039000	-0.00490200
H	0.49732200	-0.47814000	-2.30461100
Mg	-1.73228600	0.50724200	-0.11789400
O	-3.36844200	-0.75270100	-0.09068500
C	-4.70136300	-0.31883500	-0.42459300
H	-4.65988500	0.76423800	-0.53945300
H	-5.02198900	-0.79637600	-1.35739900
H	-5.38608400	-0.58616100	0.38768800
C	-3.27681900	-2.16519000	0.15022100
H	-3.53619600	-2.72036300	-0.75836600
H	-2.24680600	-2.37617300	0.43823700
H	-3.95603000	-2.44542500	0.96332800

Structure 17 [B3LYP/6-31G(d)]

C	1.00325500	0.02928800	0.00000800
C	0.66028800	1.40983800	0.00000600
C	-0.65932000	1.79243200	0.00000200
C	-1.70506500	0.82886200	0.00000000
C	-1.36049300	-0.56314000	0.00000200
C	2.41701700	-0.43965900	0.00001200
O	2.76042600	-1.60614200	-0.00000100
H	1.45062300	2.15152100	0.00000800
H	-0.92157900	2.84772100	0.00000100
C	0.00739200	-0.92927000	0.00000500
C	-2.40125500	-1.53184000	-0.00000100
C	-3.72179300	-1.14481300	-0.00000400
H	-4.50983000	-1.89272700	-0.00000600
C	-4.06185700	0.23095100	-0.00000500
H	-5.10828300	0.52402400	-0.00000800
C	-3.07721700	1.19383800	-0.00000300
H	-3.33889500	2.24931000	-0.00000400
H	-2.13355300	-2.58559600	0.00000100
O	3.30038700	0.58711600	0.00000000
C	4.68302800	0.20283400	-0.00001300
H	5.24610300	1.13674200	-0.00002200
H	4.91775900	-0.38833500	0.88925500
H	4.91774100	-0.38834100	-0.88928100
H	0.28952600	-1.97802400	0.00000700

Structure 17·CH3MgCl(DME) [B3LYP/6-31G(d)]

C	1.12422900	1.28477600	-0.10954400
C	2.15370100	2.27006300	-0.17337100
C	3.47082200	1.88677400	-0.17597600
C	3.83885300	0.51282100	-0.11239000
C	2.80297900	-0.47587800	-0.04614000
C	-0.29871000	1.66475000	-0.10493900
O	-1.24557900	0.87271200	-0.05420200
Cl	-1.20622900	-2.58680900	0.39234700
H	1.88481800	3.31895300	-0.21872100
H	4.25636000	2.63676000	-0.22486200
C	-3.40028400	0.18326900	2.47531900
H	-2.71724400	0.27335000	3.33404800
H	-4.23765800	-0.43619400	2.83218400
C	1.45015800	-0.06115500	-0.04977100
C	3.15373300	-1.85235800	0.02303700
C	4.47635200	-2.23339300	0.02386900
H	4.74080300	-3.28552300	0.07877800
C	5.50068200	-1.25677800	-0.04433400
H	6.54065200	-1.57225400	-0.04264800
C	5.19085400	0.08473600	-0.11044600
H	5.97979300	0.83120600	-0.16068600
H	2.35686300	-2.58917800	0.07922400
O	-0.50663000	2.98179900	-0.17321700
C	-1.87670300	3.42705600	-0.13663900
H	-1.82231200	4.51536200	-0.13709300
H	-2.41300000	3.06924700	-1.01928800
H	-2.37158700	3.06127700	0.76563700
H	0.66843900	-0.81499500	-0.00181700
H	-3.81541100	1.19410800	2.32320200
Mg	-2.41421200	-0.63597000	0.78747900
O	-3.83987800	-0.76746400	-0.78890300
C	-3.71215900	-1.60086600	-1.94719500
H	-2.73360400	-2.07693800	-1.88685800
H	-4.49545000	-2.36873700	-1.94350400
H	-3.79560300	-0.99361400	-2.85761400
C	-5.12197200	-0.14748400	-0.67666400
H	-5.29541500	0.52535500	-1.52676800
H	-5.91062300	-0.90993400	-0.64879700
H	-5.12189200	0.41478100	0.25763500

Structure 17-TSCO(DME) [B3LYP/6-31G(d)]

C	-0.93835100	-1.00982700	-0.05798900
C	-1.76096100	-1.89633000	0.69161700
C	-3.09547500	-1.62509400	0.86857400
C	-3.69012400	-0.45903500	0.31257500
C	-2.86634600	0.43236400	-0.44801400
C	0.52173500	-1.29416900	-0.26602700
O	1.21432000	-0.56907900	-1.09244200
Cl	1.88525300	2.84496900	0.64119400

H	-1.32323300	-2.79385300	1.11399300
H	-3.71899600	-2.30801000	1.44098500
C	1.17355200	-0.76427400	1.77807100
H	0.60356800	0.04284900	2.26087800
H	2.21088200	-0.74413100	2.17125800
C	-1.49178800	0.12369400	-0.61848300
C	-3.45162900	1.59850500	-1.01113300
C	-4.78857400	1.87241100	-0.82941100
H	-5.22449700	2.76899800	-1.26156600
C	-5.60275200	0.99043300	-0.07723200
H	-6.65666700	1.21775700	0.05910300
C	-5.06507000	-0.14862800	0.48031400
H	-5.68856600	-0.82660100	1.05860700
H	-2.82201800	2.27452700	-1.58442700
O	0.75255500	-2.63673300	-0.22438300
C	2.07333400	-3.06976600	-0.53021800
H	2.06735700	-4.15322200	-0.39880600
H	2.34325900	-2.82005900	-1.56006100
H	2.79700900	-2.61868100	0.16010000
H	-0.87144200	0.78912000	-1.21150600
H	0.75333000	-1.70913800	2.11586900
Mg	1.97676300	0.62235300	0.23755000
O	4.01201700	0.31803900	-0.12228500
C	4.99722500	1.11117200	0.56138900
H	5.92060500	0.53023700	0.66739500
H	5.18816500	2.03647800	0.00829500
H	4.59219400	1.35936500	1.54243000
C	4.42824400	-0.07168000	-1.44102100
H	4.65330600	0.81632000	-2.04371600
H	5.31831700	-0.70805500	-1.37361100
H	3.59771700	-0.62308500	-1.88133000