Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Gas phase models of hydride transfer from divalent alkaline earth metals to CO_2 and CH_2O

Christian Sant Gjermestad[1], Mauritz Johan Ryding[2] and Einar Uggerud[2]

[1] *Department of Chemistry, University of Bergen, Allégaten 41, NO-5007 Bergen, Norway.*
[2] *Department of Chemistry and Hylleraas Centre for Quantum Molecular Sciences, University of Oslo, PO Box 1033, Blindern, NO-0135 Oslo, Norway.*

SUPPLEMENTARY INFORMATION

Electrospray solutions used in experiments

Table S1. Solutions used in the experiment in order to produce the desired ions during electrospray ionization.

Ion to produce	**Solution used**
CH_3OMg^+	2 mM $MgCl_2$ in MeOH or MeOH/H_2O 1:1
$CH_3OMgCl_2^-$	2 mM $MgCl_2$ in MeOH with 5 µL/mL Et_3N
HCO_2Mg^+	2 mM $MgCl_2$ and 4 mM HCOOH in MeOH or MeOH/H_2O 1:1
$HCO_2MgCl_2^-$	2 mM $MgCl_2$ and 4 mM HCOOH in MeOH

Source conditions used in experiments

Table S2. Source conditions used in experiments when producing the indicated ions on the QTOF 2 instrument.

Parameter	**CH_3OMg^+**	**HCO_2Mg^+**	**$CH_3OMgCl_2^-$**	**$HCO_2MgCl_2^-$**
Capillary voltage	3.5 kV	3.5 kV	3.5 kV	3.5 kV
Cone voltage	30 V	35 V	30 V	18 V
Extractor voltage	4 V	4 V	0 V	0
Solution flow	20 µL min^{-1}	20 µL min^{-1}	20 µL min^{-1}	20 µL min^{-1}
Nebulizer gas	on	on	on	on
Desolvation gas	425 L h^{-1}	350 L h^{-1}	275 L h^{-1}	200 L h^{-1}
Cone gas	off	off	off	off

Computational method evaluation

Table S3. Energies (E + ZPE, kJ mol^{-1}) of the structures, **TS2A**, **5A** and **6A**, relative to $MeOMg^+$ (**4A**) using various selected quantum chemical methods. Geometries were fully optimized with each method.

Method	**Basis set**	**TS2A**	**5A**	**6A**
CCSD(T)	aug-cc-pVTZ	100	−28	165
MP2	aug-cc-pVTZ	116	−8	184
M11	aug-cc-pVTZ	89	−25	185
wb97xd	aug-cc-pVTZ	95	−22	174
G4	–	97	−35	164
B3LYP	cc-pVDZ	87	−60	147
	cc-pVTZ	86	−48	148
	cc-pVQZ	87	−46	149
	aug-cc-pVDZ	87	−48	144
	aug-cc-pVTZ	87	−46	147
	daug-cc-pVTZ	87	−46	147
	aug-cc-pVQZ	88	−45	149
	LANL2DZ	151	–	195

Detailed Gaussian Settings

Intermediates:
 # opt=(tight,calcfc,maxcycle=300) freq int=ultrafine nosymm

Transition states:
 # opt=(tight,calcfc,ts,noeigentest,maxcycle=300) freq int=ultrafine nosymm

Intrinsic Reaction Coordinate:
 # irc=(calcfc, tight, forward, stepsize=10, maxpoints=300, maxcycles=1000) int=ultrafine nosymm

For low absolute values of the imaginary frequency, the *stepsize* was increased. In some cases, the local quadratic approximation was also employed in the predictor step in (*irc=LQA*).

Extracted threshold energies

Table S4. Threshold energies (E_T, kJ mol^{-1}) extracted from appearance curves at different collision gas pressures (P_{Ar}, 10^{-4} mbar).

CH_3OMg^+		HCO_2Mg^+		$CH_3OMgCl_2^-$		$HCO_2MgCl_2^-$	
P_{Ar}	E_T	P_{Ar}	E_T	P_{Ar}	E_T	P_{Ar}	E_T
1.01	133	1.03	192	1.04	176	1.03	183
2.03	118	2.03	182	2.04	153	2.09	160
3.03	119	3.08	179	2.86	153	3.07	155
3.87	112	4.06	174	3.82	146	4.17	145
5.10	104	4.97	163	5.14	132	5.15	136

Table S5. Extrapolation of threshold energies in Table S4 to zero pressure using linear regression.

Parameter	CH_3OMg^+	HCO_2Mg^+	$CH_3OMgCl_2^-$	$HCO_2MgCl_2^-$
E_T (P_{Ar} = 0) [kJ mol^{-1}]	136	198	181	189
Slope [kJ mol^{-1} mbar^{-1}]	-6.35×10^4	$-6.62\text{E}\times10^4$	$-9.63\text{E}\times10^4$	-1.06×10^5
R^2	0.905	0.964	0.905	0.938

Supplementary Experiments

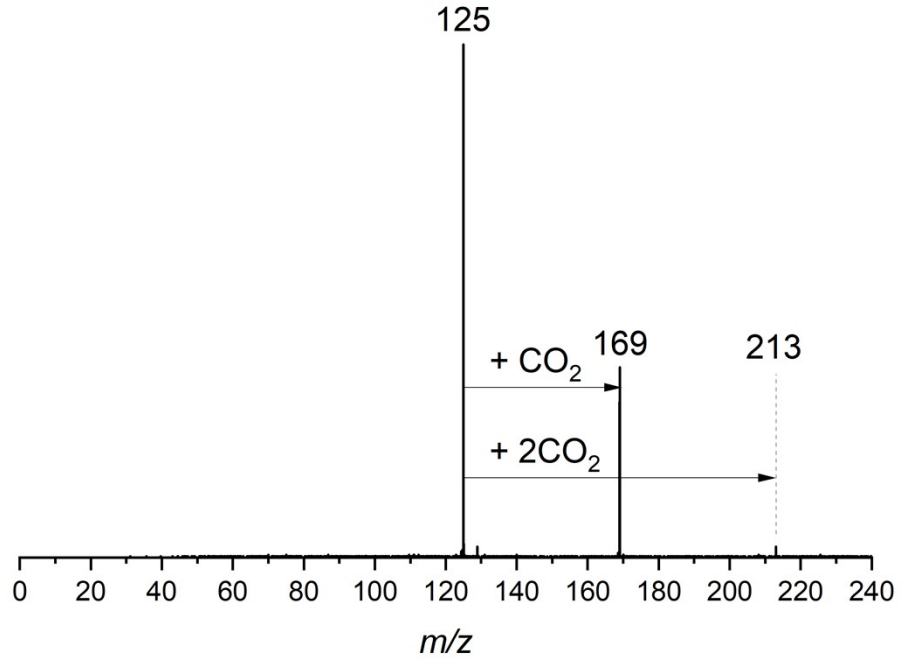

Figure S1. Reaction of $CH_3OMgCl_2^-$ (*m/z* 125) with CO_2 ($P_{nom} = 4.8\times10^{-4}$ mbar, E_{CoM} = 70 kJ mol^{-1}).

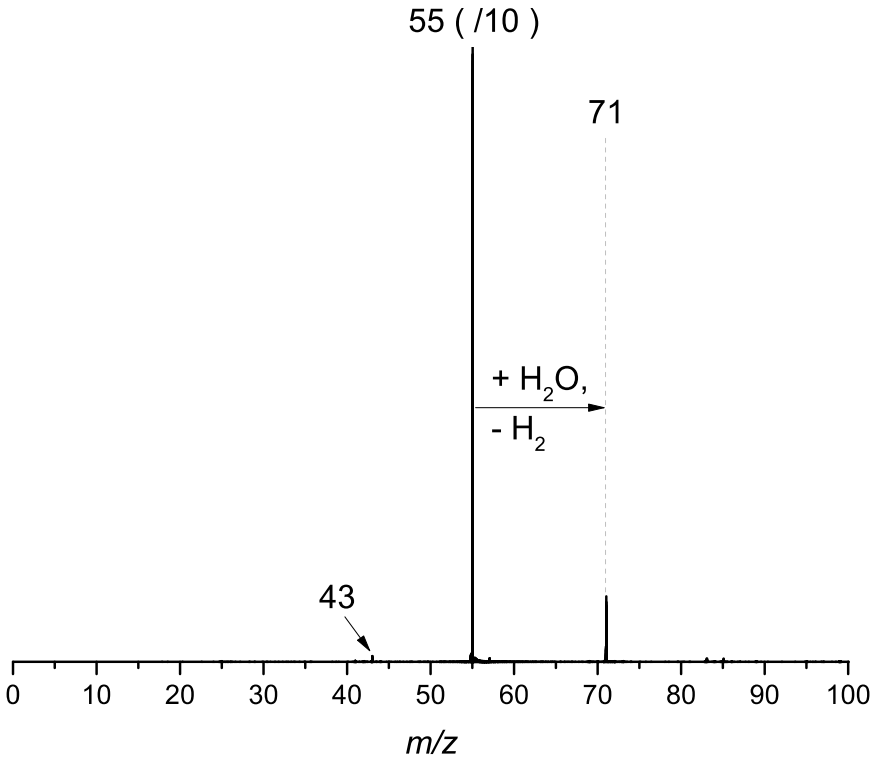

Figure S2. Reaction of CH_3OMg^+ (*m/z* 55) with H_2O (P_{nom} = 2.3×10^{-4} mbar, E_{CoM} = 19 kJ mol^{-1}). Note that the intensity of the reactant peak is scaled down a factor of ten.

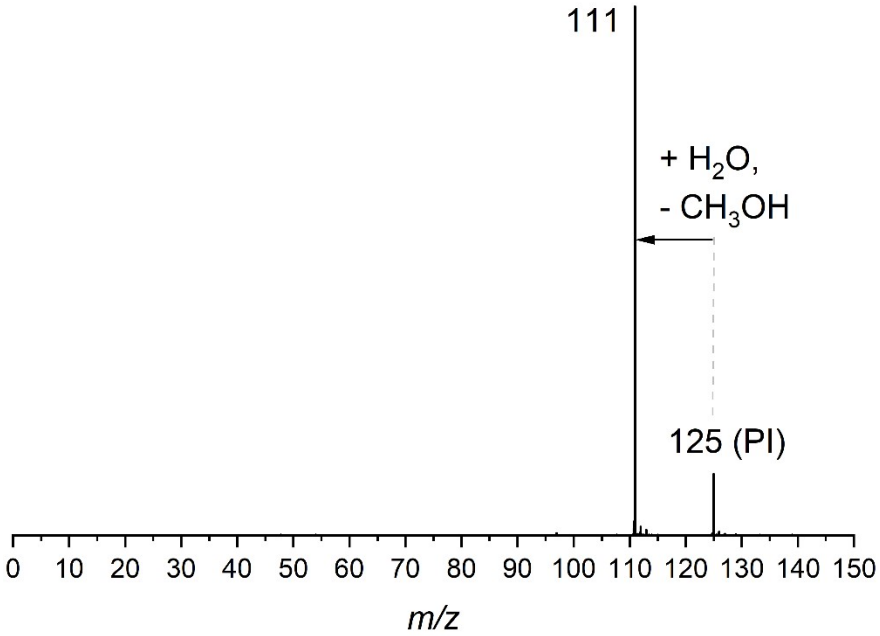

Figure S3. Reaction of $CH_3OMgCl_2^-$ (*m/z* 125) with H_2O (P_{nom} = 3.0×10^{-4} mbar, E_{CoM} = 20 kJ mol^{-1}).

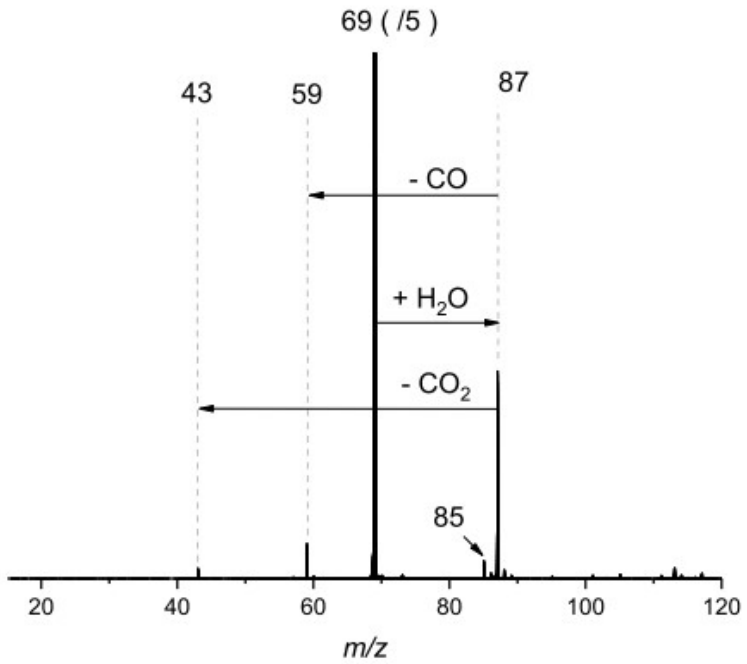

Figure S4. Reaction of HCO_2Mg^+ (*m/z* 69) with H_2O (P_{nom} = 1.1×10^{-3} mbar, E_{CoM} = 20 kJ mol^{-1}). Note that the intensity of the reactant peak is scaled down a factor of five.

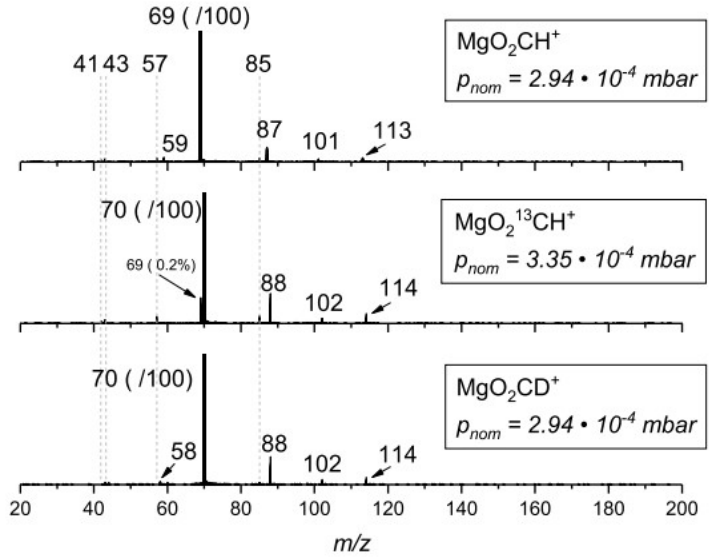

Figure S5. Isotope labelling experiments for the reaction of magnesium formate with H_2O. E_{CoM} = 22 kJ mol^{-1} in all three experiments.

Supplementary computations

Table S6. Computed reaction energies for loss of formate from $HCO_2MCl_2^-$, M = Be, Mg, Ca, Sr, Ba. B3LYP/LANL2DZ energies in kJ mol^{-1}.

	$BeCl_2$	**$MgCl_2$**	**$CaCl_2$**	**$SrCl_2$**	**$BaCl_2$**
ΔE_r^0	333	371	384	375	359

As seen in Table S6, there appears to be no clear trend within the group 2 metals with regards to the binding energies of formate to MCl_2. Table 2 and Table 4 of the main text show that the effect of the metal is muted by the presence of a single chloride ligand, and more so in the presence of two; in this case, the computational method may not be able to sufficiently reproduce the expected trend. Please note that loss of formate is less favourable compared to decarboxylation for all metal dichlorides (*cf.* main text Table 2); it is most competitive in the case of $HCO_2BaCl_2^-$, being less favourable by only 53 kJ mol^{-1}.

Table S7. Computed trends in complexation energy ($\Delta E_{complex}$) for $M^{2+} + CH_3O^-$ with M = Be, Mg, Ca, Sr, Ba. B3LYP/LANL2DZ energies in kJ/mol.

	Be	**Mg**	**Ca**	**Sr**	**Ba**
$\Delta E_{complex}$	−2143	−1576	−1267	−1169	−1079

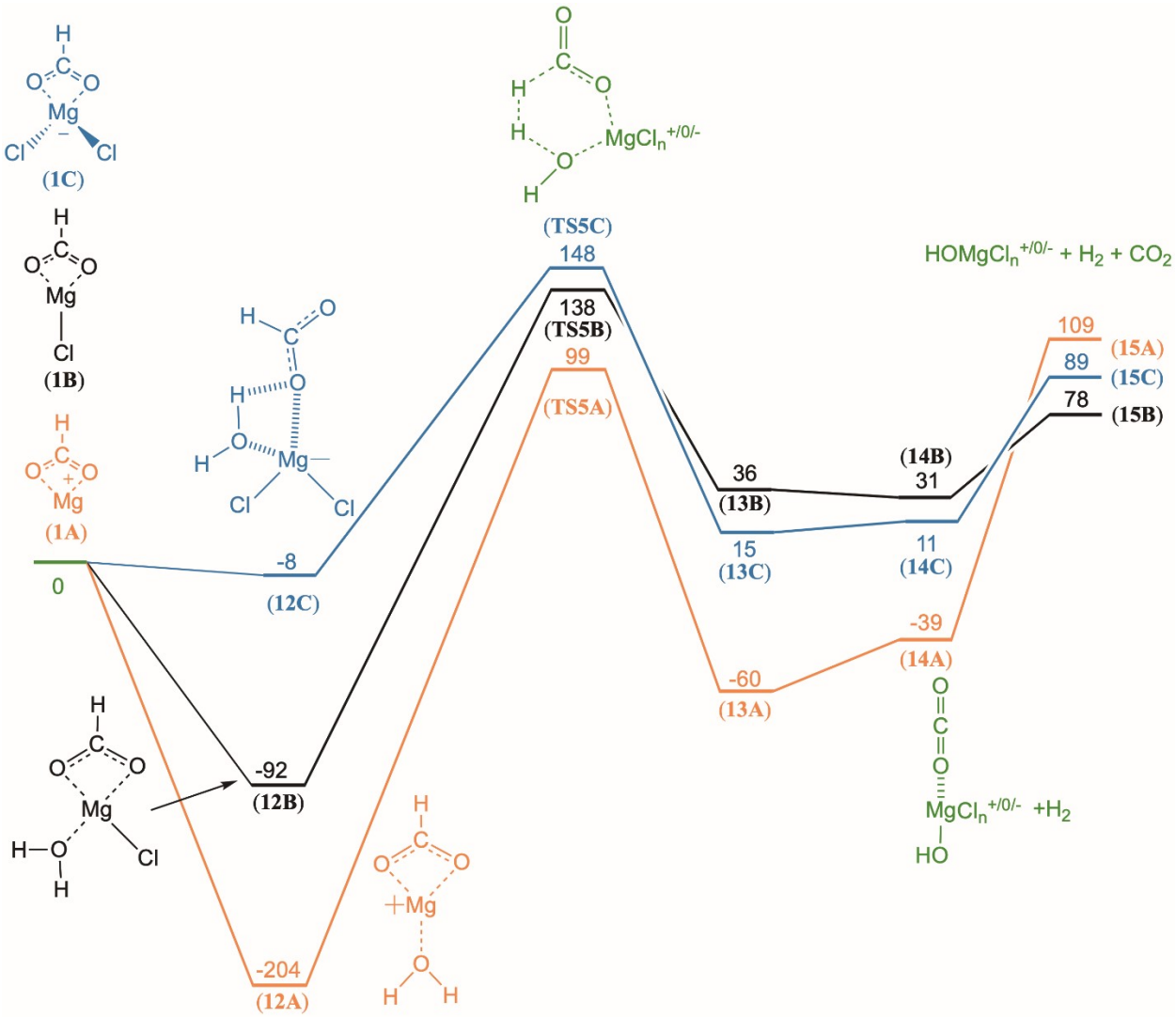

Figure S6. Potential energy diagram for reaction between H_2O and HCO_2Mg^+ (orange), HCO_2MgCl (black) and $HCO_2MgCl_2^-$ (blue), based on quantum chemical computations (G4, 0K). Relative energies given in kJ mol^{-1}.

Absolute energies

Table S8. Absolute energies of the structures in Fig. 1 of the main text concerning the thermochemistry of hydride transfer to CO_2 and CH_2O from $HMgCl_n$. Energies in Hartree at 298 K unless otherwise noted.

	G4 (0 K)	G4 Energy	G4 Enthalpy	G4 Free Energy
H-	-0.514955	-0.513539	-0.512595	-0.524955
Mg2+	-199.079467	-199.078050	-199.077106	-199.093956
MgCl+	-659.764700	-659.762141	-659.761196	-659.786833
MgCl2	-1120.241218	-1120.236915	-1120.235971	-1120.266650
CO2	-188.535267	-188.532654	-188.53171	-188.55596
HCO2-	-189.147026	-189.144052	-189.143108	-189.170822
HCO2MgCl2- (1C)	-1309.516913	-1309.509179	-1309.508235	-1309.550969
HCO2MgCl (1B)	-849.269016	-849.263306	-849.262362	-849.299350
HCO2Mg2+ (1A)	-388.812061	-388.808289	-388.807345	-388.838331
HMgCl2- (3C)	-1120.901001	-1120.896201	-1120.895257	-1120.929933
HMgCl (3B)	-660.660238	-660.656842	-660.655898	-660.683050
HMg+ (3A)	-200.206834	-200.204472	-200.203527	-200.224676
CH2O	-114.453193	-114.450324	-114.449379	-114.4748
CH3O-	-115.043175	-115.040278	-115.039334	-115.065397
CH3OMgCl2- (4C)	-1235.434370	-1235.426211	-1235.425267	-1235.470025
CH3OMgCl (4B)	-775.189309	-775.183080	-775.182135	-775.219673
CH3OMg+ (4A)	-314.722500	-314.718011	-314.717067	-314.749131

Table S9. Absolute energies of the structures in Fig. 4 of the main text, involving decarboxylation of magnesium formates. Energies in Hartree at 298 K unless otherwise noted.

	G4 (0 K)	G4 Energy	G4 Enthalpy	G4 Free Energy
CO2	-188.535267	-188.532654	-188.53171	-188.55596
1A	-388.812061	-388.808289	-388.807345	-388.838331
1B	-849.269016	-849.263306	-849.262362	-849.299350
1C	-1309.516913	-1309.509179	-1309.508235	-1309.550969
TS1primeA	-388.738457	-388.734712	-388.733768	-388.764980
TS1A	-388.737291	-388.733371	-388.732427	-388.763873
TS1B	-849.195323	-849.189416	-849.188471	-849.226069
TS1C	-1309.442643	-1309.434634	-1309.433690	-1309.478217
2A	-388.788280	-388.782849	-388.781905	-388.810128
2B	-849.208156	-849.201251	-849.200307	-849.240765
2C	-1309.443240	-1309.434328	-1309.433383	-1309.481062
3A	-200.206834	-200.204472	-200.203527	-200.224676
3B	-660.660238	-660.656842	-660.655898	-660.683050
3C	-1120.901001	-1120.896201	-1120.895257	-1120.929933

Table S10. Absolute energies of the structures in Fig. 6 of the main text, involving deformylation of magnesium methoxides. Energies in Hartree at 298 K unless otherwise noted.

	G4 (0 K)	G4 Energy	G4 Enthalpy	G4 Free Energy
CH2O	-114.453193	-114.450324	-114.449379	-114.4748
4A	-314.722500	-314.718011	-314.717067	-314.749131
4B	-775.189309	-775.183080	-775.182135	-775.219673
4C	-1235.434370	-1235.426211	-1235.425267	-1235.470025
TS2A	-314.685742	-314.682000	-314.681056	-314.711151
TS2B	-775.125964	-775.119884	-775.118940	-775.156271
TS2C	-1235.360257	-1235.352446	-1235.351502	-1235.394163
5A	-314.735854	-314.730219	-314.729274	-314.762991
5B	-775.141764	-775.135127	-775.134183	-775.172365
5C	-1235.368379	-1235.359596	-1235.358652	-1235.403736
6A	-200.206834	-200.204472	-200.203527	-200.224676
6B	-660.660238	-660.656842	-660.655898	-660.683050
6C	-1120.901001	-1120.896201	-1120.895257	-1120.929933

Table S11. Absolute energies of the structures referenced in Table 1 of the main text, involving substitution of Cl with other halides. B3LYP/LANL2DZ energies in Hartree.

	E(0K) = E + ZPE	E(298K) = E + Sum of thermal energies	H(298K) = E + Sum of thermal enthalpies	G(298K) = E + Sum of thermal free energies
CH2O	-114.456963	-114.454094	-114.453149	-114.478670
CO2	-188.529226	-188.526548	-188.525604	-188.549995
HCO2MgF	-289.946018	-289.940432	-289.939488	-289.975498
HCO2MgCl	-205.043324	-205.037483	-205.036538	-205.073931
HCO2MgBr	-203.258163	-203.252176	-203.251231	-203.289935
HCO2MgI	-201.472504	-201.466431	-201.465487	-201.505090
TS_HCO2MgF	-289.868306	-289.862553	-289.861608	-289.898121
TS_HCO2MgCl	-204.965644	-204.959625	-204.958681	-204.996582
TS_HCO2MgBr	-203.180336	-203.174157	-203.173213	-203.212474
TS_HCO2MgI	-201.394513	-201.388241	-201.387297	-201.427477
HMgF	-101.334435	-101.331142	-101.330198	-101.356134
HMgCl	-16.432154	-16.428690	-16.427746	-16.455079
HMgBr	-14.647265	-14.643703	-14.642759	-14.671420
HMgI	-12.861590	-12.857978	-12.857034	-12.886560
HCO2MgF2	-389.954495	-389.947313	-389.946369	-389.986399
HCO2MgCl2	-220.164898	-220.157090	-220.156146	-220.199096
HCO2MgBr2	-216.596201	-216.588024	-216.587079	-216.632880
HCO2MgI2	-213.026577	-213.018201	-213.017257	-213.064982
TS_HCO2MgF2	-389.865458	-389.857872	-389.856928	-389.900223
TS_HCO2MgCl2	-220.079055	-220.070713	-220.069769	-220.117596
TS_HCO2MgBr2	-216.511463	-216.502918	-216.501974	-216.550849
TS_HCO2MgI2	-212.942805	-212.934073	-212.933129	-212.983906
HMgF2	-201.325870	-201.321701	-201.320757	-201.351631
HMgCl2	-31.542071	-31.537311	-31.536367	-31.570353
HMgBr2	-27.976143	-27.971056	-27.970112	-28.007618
HMgI2	-24.408400	-24.403114	-24.402170	-24.440959
MeOMgF	-215.880152	-215.874245	-215.873301	-215.909132
MeOMgCl	-130.979480	-130.973344	-130.972399	-131.009579
MeOMgBr	-129.195188	-129.188931	-129.187987	-129.226397
MeOMgI	-127.410329	-127.404005	-127.403061	-127.442324
TS_MeOMgF	-215.805075	-215.799116	-215.798172	-215.834793
TS_MeOMgCl	-130.903388	-130.897261	-130.896316	-130.933857
TS_MeOMgBr	-129.118205	-129.111917	-129.110973	-129.149937
TS_MeOMgI	-127.332453	-127.326059	-127.325115	-127.365089
MeOMgF2	-315.877709	-315.870100	-315.869156	-315.912983
MeOMgCl2	-146.092474	-146.084263	-146.083319	-146.129616
MeOMgBr2	-142.525117	-142.516544	-142.515600	-142.564801

MeOMgI2	-138.956915	-138.948152	-138.947208	-138.998284
TS_MeOMgF2	-315.791731	-315.784656	-315.783712	-315.824285
TS_MeOMgCl2	-146.004502	-145.996865	-145.995921	-146.038119
TS_MeOMgBr2	-142.437956	-142.429946	-142.429002	-142.474180
TS_MeOMgI2	-138.870373	-138.862160	-138.861216	-138.908368

Table S12. Absolute energies of the structures referenced in Table 2 of the main text, involving substitution of Mg with other earth alkali metals in formate complexes. B3LYP/LANL2DZ energies in Hartree.

	E(0K) = E + ZPE	**E(298K) = E + Sum of thermal energies**	**H(298K) = E + Sum of thermal enthalpies**	**G(298K) = E + Sum of thermal free energies**
HCO2Be	-203.551483	-203.547947	-203.547003	-203.576633
HCO2Mg	-189.716447	-189.712568	-189.711624	-189.742857
HCO2Ca	-225.492190	-225.488059	-225.487114	-225.519615
HCO2Sr	-219.390665	-219.386391	-219.385447	-219.419251
HCO2Ba	-214.198691	-214.194296	-214.193351	-214.228109
TS_HCO2Be	-203.480391	-203.476838	-203.475893	-203.505725
TS_HCO2Mg	-189.640015	-189.636010	-189.635066	-189.666702
TS_HCO2Ca	-225.412901	-225.408515	-225.407571	-225.440706
TS_HCO2Sr	-219.308506	-219.303926	-219.302982	-219.337547
TS_HCO2Ba	-214.111420	-214.106654	-214.105710	-214.141356
HBe	-14.940525	-14.938164	-14.937220	-14.956602
HMg	-1.112764	-1.110402	-1.109457	-1.130604
HCa	-36.871681	-36.869309	-36.868365	-36.890642
HSr	-30.765515	-30.763137	-30.762193	-30.785714
HBa	-25.564989	-25.562603	-25.561659	-25.585977
HCO2BeCl	-218.936289	-218.931156	-218.930212	-218.965183
HCO2CaCl	-240.770972	-240.764657	-240.763712	-240.803229
HCO2SrCl	-234.647725	-234.641117	-234.640173	-234.681492
HCO2BaCl	-229.435150	-229.428339	-229.427395	-229.470062
TS_HCO2BeCl	-218.865710	-218.860530	-218.859586	-218.894804
TS_HCO2CaCl	-240.687193	-240.680571	-240.679627	-240.719824
TS_HCO2SrCl	-234.559824	-234.552973	-234.552029	-234.593739
HBeCl	-30.341556	-30.338730	-30.337786	-30.362736
HCaCl	-52.143767	-52.139971	-52.139027	-52.161953
HSrCl	-46.012234	-46.008248	-46.007304	-46.039401
HBaCl	-40.792548	-40.788424	-40.787480	-40.820951
HCO2BeCl2	-234.056156	-234.048807	-234.047863	-234.091206
HCO2CaCl2	-255.891992	-255.883653	-255.882709	-255.927840
HCO2SrCl2	-249.764956	-249.756233	-249.755289	-249.802262
HCO2BaCl2	-244.546175	-244.537160	-244.536215	-244.584872

TS_HCO2BeCl2	-233.978232	-233.970834	-233.969890	-234.014795
TS_HCO2CaCl2	-255.796283	-255.787762	-255.786818	-255.832861
TS_HCO2SrCl2	-249.665585	-249.656699	-249.655755	-249.703406
TS_HCO2BaCl2	-244.442275	-244.433105	-244.432161	-244.481141
HBeCl2	-45.441499	-45.437472	-45.436528	-45.468128
HCaCl2	-67.255811	-67.250509	-67.249565	-67.286199
HSrCl2	-61.124400	-61.118778	-61.117834	-61.156187
HBaCl2	-55.900454	-55.894607	-55.893663	-55.933334

Table S13. Absolute energies of the structures referenced in Table 3 of the main text, involving decomposition of reaction energies. B3LYP/LANL2DZ energies in Hartree.

	E(0K) = E + ZPE	**E(298K) = E + Sum of thermal energies**	**H(298K) = E + Sum of thermal enthalpies**	**G(298K) = E + Sum of thermal free energies**
Be(0)	-14.670226	-14.66881	-14.667866	-14.683329
Mg(0)	-0.819916	-0.8185	-0.817555	-0.834405
Ca(0)	-36.550702	-36.549286	-36.548341	-36.565914
Sr(0)	-30.433996	-30.43258	-30.431636	-30.450325
Ba(0)	-25.215875	-25.214458	-25.213514	-25.232841
Be(2+)	-13.652907	-13.651491	-13.650547	-13.66601
Mg(2+)	0	0.001416	0.00236	-0.014489
Ca(2+)	-35.881534	-35.880118	-35.879174	-35.896746
Sr(2+)	-29.81157	-29.810154	-29.809209	-29.827898
Ba(2+)	-24.651771	-24.650355	-24.649411	-24.668737

Table S14. Absolute energies of the structures referenced in Table 4 of the main text, involving substitution of Mg with other earth alkali metals in methoxy complexes. B3LYP/LANL2DZ energies in Hartree.

	E(0K) = E + ZPE	**E(298K) = E + Sum of thermal energies**	**H(298K) = E + Sum of thermal enthalpies**	**G(298K) = E + Sum of thermal free energies**
MeOBe	-129.523356	-129.519441	-129.518497	-129.547605
MeOMg	-115.654048	-115.649652	-115.648708	-115.680209
MeOCa	-151.418115	-151.413770	-151.412826	-151.444751
MeOSr	-145.310574	-145.306098	-145.305154	-145.338421
MeOBa	-140.116593	-140.112153	-140.111208	-140.144953
TS_MeOBe	-129.466766	-129.463480	-129.462536	-129.490717
TS_MeOMg	-115.596698	-115.592976	-115.592032	-115.622124
TS_MeOCa	-151.362715	-151.358612	-151.357667	-151.389260
TS_MeOSr	-145.256106	-145.251752	-145.250807	-145.283946
TS_MeOBa	-140.057467	-140.052723	-140.051778	-140.086496
MeOBeCl	-144.908912	-144.903489	-144.902545	-144.937423
MeOCaCl	-166.691461	-166.685046	-166.684102	-166.722914

MeOSrCl	-160.563293	-160.556653	-160.555708	-160.596183
MeOBaCl	-155.348236	-155.341454	-155.340510	-155.382193
TS_MeOBeCl	-144.803337	-144.798271	-144.797327	-144.831468
TS_MeOCaCl	-166.625004	-166.618354	-166.617410	-166.657014
TS_MeOSrCl	-160.497820	-160.490879	-160.489935	-160.531286
TS_MeOBaCl	-155.279201	-155.272094	-155.271150	-155.313739
MeOBeCl2	-159.999404	-159.992437	-159.991493	-160.032004
MeOCaCl2	-181.807420	-181.798894	-181.797950	-181.846640
MeOSrCl2	-175.676280	-175.667421	-175.666477	-175.716432
MeOBaCl2	-170.455070	-170.445988	-170.445044	-170.495978
TS_MeOBeCl2	-159.895883	-159.889018	-159.888074	-159.929596
TS_MeOCaCl2	-181.728328	-181.720078	-181.719134	-181.763220
TS_MeOSrCl2	-175.598785	-175.590163	-175.589218	-175.634958
TS_MeOBaCl2	-170.376601	-170.367691	-170.366747	-170.413922

Table S15. Absolute energies of the structures in Fig. 9 of the main text, involving reaction of magnesium methoxides with carbon dioxide. Energies in Hartree at 298 K unless otherwise noted.

	G4 (0 K)	**G4 Energy**	**G4 Enthalpy**	**G4 Free Energy**
7A	-503.313533	-503.305196	-503.304252	-503.348113
7B	-963.749960	-963.741458	-963.740514	-963.784939
7C	-1423.978740	-1423.966283	-1423.965339	-1424.022965
7Cprime	-1424.00469	-1423.99417	-1423.99323	-1424.04359
TS3A	-503.259001	-503.252746	-503.251802	-503.289620
TS3B	-963.703806	-963.695613	-963.694669	-963.738327
TS3C	-1423.950360	-1423.940049	-1423.939105	-1423.988619
8A	-503.346961	-503.338980	-503.338036	-503.381061
8B	-963.753249	-963.743765	-963.742821	-963.789350
8C	-1423.977068	-1423.965399	-1423.964455	-1424.017451

Table S16. Absolute energies of the structures in Fig. 10 of the main text, involving reaction of magnesium methoxides with water. Energies in Hartree at 298 K unless otherwise noted.

	G4 (0 K)	**G4 Energy**	**G4 Enthalpy**	**G4 Free Energy**
H2O	-76.397253	-76.394418	-76.393474	-76.415555
9A	-391.201266	-391.193517	-391.192573	-391.234962
9B	-851.620445	-851.611837	-851.610893	-851.654991
9C	-1311.855775	-1311.845314	-1311.844370	-1311.894451
TS4A	-391.133429	-391.127497	-391.126553	-391.162322
TS4B	-851.559099	-851.550876	-851.549932	-851.593332
TS4C	-1311.789680	-1311.780040	-1311.779096	-1311.825484

10A	-391.180219	-391.171224	-391.170280	-391.213668
10B	-851.585933	-851.575369	-851.574425	-851.622647
10C	-1311.812293	-1311.800232	-1311.799288	-1311.851587
11A	-390.005535	-389.997971	-389.997026	-390.037123
11B	-850.419729	-850.411901	-850.410957	-850.452341
11C	-1310.645494	-1310.635685	-1310.634741	-1310.681760

Table S17. Absolute energies of the structures in Fig. S6, involving reaction of magnesium formates and H_2O. Energies in Hartree at 298 K unless otherwise is noted.

	G4 (0 K)	**G4 Energy**	**G4 Enthalpy**	**G4 Free Energy**
H2	-1.16802	-1.16566	-1.164715	-1.179507
12A	-465.287074	-465.280165	-465.279220	-465.318409
12B	-925.701153	-925.692416	-925.691472	-925.735642
12C	-1385.917158	-1385.906259	-1385.905315	-1385.956164
TS5A	-465.171475	-465.165295	-465.164350	-465.201319
TS5B	-925.613718	-925.605329	-925.604385	-925.648133
TS5C	-1385.857663	-1385.847432	-1385.846487	-1385.895435
13A	-465.232320	-465.223674	-465.222729	-465.265615
13B	-925.652682	-925.641751	-925.640807	-925.690912
13C	-1385.908480	-1385.896923	-1385.895979	-1385.949024
14A	-464.056270	-464.049051	-464.048107	-464.087045
14B	-924.486403	-924.478327	-924.477382	-924.520481
14C	-1384.741919	-1384.732938	-1384.731994	-1384.778682
15A	-275.464411	-275.461253	-275.460308	-275.486790
15B	-735.933112	-735.928119	-735.927175	-735.959564
15C	-1196.176982	-1196.170727	-1196.169783	-1196.208304

Table S18. Absolute energies of the structures in Table S3, where the choice of computational method is evaluated. Energies in Hartree at 298 K unless otherwise is noted.

	Sum(E + ZPE)	**Sum(E + therm. energies)**	**Sum(E + therm. enthalpies)**	**Sum(E + therm. free energies)**
CH2O_CCSD(T)_augccpVTZ	-114.31629	-114.31343	-114.31248	-114.31813
CH2O_B3LYP_ccpVDZ	-114.481281	-114.478412	-114.477468	-114.502953
CH2O_B3LYP_ccpVTZ	-114.522890	-114.520023	-114.519079	-114.544541
CH2O_B3LYP_ccpVQZ	-114.533153	-114.530286	-114.529341	-114.554802
CH2O_B3LYP_augccpVDZ	-114.494118	-114.491248	-114.490304	-114.515790
CH2O_B3LYP_augccpVTZ	-114.525656	-114.522788	-114.521844	-114.547309
CH2O_B3LYP_augccpVQZ	-114.534080	-114.531213	-114.530268	-114.555731
CH2O_MP2	-114.289578	-114.286710	-114.285766	-114.311243

CH2O_M11	-114.476066	-114.473199	-114.472255	-114.497719
4A_CCSD(T)_augccpVTZ	-314.32127	-314.31676	-314.31581	-314.33187
4A_B3LYP_augccpVDZ	-314.927519	-314.923082	-314.922138	-314.954043
4A_B3LYP_augccpVQZ	-314.980677	-314.976200	-314.975256	-315.007291
4A_B3LYP_augccpVTZ	-314.969579	-314.965112	-314.964168	-314.996155
4A_B3LYP_ccpVDZ	-314.915619	-314.911195	-314.910250	-314.942065
4A_B3LYP_ccpVQZ	-314.979498	-314.975026	-314.974082	-315.006102
4A_B3LYP_ccpVTZ	-314.967159	-314.962706	-314.961762	-314.993711
4A_M11	-314.908504	-314.904145	-314.903201	-314.934579
4A_MP2	-314.291518	-314.287021	-314.286077	-314.318045
4A_wb97xd	-314.910293	-314.905844	-314.904900	-314.936666
TS2A_CCSD(T)_augccpVTZ	-314,28327	-314,27953	-314,27859	-314,28883
TS2A_B3LYP_augccpVDZ	-314,28327	-314,27953	-314,27859	-314,28883
TS2A_B3LYP_augccpVQZ	-314.947115	-314.943384	-314.942440	-314.972512
TS2A_B3LYP_augccpVTZ	-314.936280	-314.932544	-314.931600	-314.961686
TS2A_B3LYP_ccpVDZ	-314.882618	-314.878852	-314.877908	-314.908073
TS2A_B3LYP_ccpVQZ	-314.946255	-314.942527	-314.941583	-314.971651
TS2A_B3LYP_ccpVTZ	-314.934246	-314.930514	-314.929570	-314.959651
TS2A_M11	-314.874483	-314.870752	-314.869808	-314.899885
TS2A_MP2	-314.247493	-314.243746	-314.242801	-314.272922
TS2A_wb97xd	-314.874120	-314.870394	-314.869450	-314.899513
5A_CCSD(T)_augccpVTZ	-314,33201	-314,32768	-314,32673	-314,33488
5A_B3LYP_augccpVDZ	-314.945878	-314.940226	-314.939282	-314.973143
5A_B3LYP_augccpVQZ	-314.997834	-314.992171	-314.991227	-315.025075
5A_B3LYP_augccpVTZ	-314.986979	-314.981298	-314.980354	-315.014221
5A_B3LYP_ccpVDZ	-314.938379	-314.932714	-314.931769	-314.965741
5A_B3LYP_ccpVQZ	-314.996875	-314.991197	-314.990253	-315.024111
5A_B3LYP_ccpVTZ	-314.985390	-314.979711	-314.978767	-315.012658
5A_M11	-314.917879	-314.912277	-314.911333	-314.944890
5A_MP2	-314.294553	-314.288844	-314.287900	-314.321929
5A_wb97xd	-314.918624	-314.912929	-314.911985	-314.945895
6A_CCSD(T)_ccpVTZ	-199,94198	-199,93961	-199,93867	-314,34395
6A_B3LYP_augccpVDZ	-200.378602	-200.376239	-200.375295	-200.396448
6A_B3LYP_augccpVQZ	-200.389936	-200.387573	-200.386629	-200.407770
6A_B3LYP_augccpVTZ	-200.388116	-200.385753	-200.384809	-200.405953
6A_B3LYP_ccpVDZ	-200.378316	-200.375953	-200.375009	-200.396164
6A_B3LYP_ccpVQZ	-200.389773	-200.387411	-200.386467	-200.407609
6A_B3LYP_ccpVTZ	-200.387773	-200.385411	-200.384466	-200.405613
6A_M11	-200.361876	-200.359514	-200.358569	-200.379709
6A_MP2	-199.931982	-199.929619	-199.928675	-199.949819

6A_wb97xd	-200.361665	-200.359303	-200.358359	-200.379495

Table S19. Absolute energies of the structures in Table S6, regarding the binding energy of formate to neutrally charged earth alkali dichloride species. B3LYP/LANL2DZ energies in Hartree at 298 K.

	Sum(E + ZPE)	**Sum(E + therm. energies)**	**Sum(E + therm. enthalpies)**	**Sum(E + therm. free energies)**
BeCl2	-44,7791860	-44.7755220	-44.7745780	-44.8036880
MgCl2	-30.8732820	-30.8688560	-30.8679120	-30.8991190
CaCl2	-66.5955470	-66.5907360	-66.5897910	-66.6229720
SrCl2	-60.4717760	-60.4667460	-60.4658020	-60.5006490
BaCl2	-55.2593140	-55.2541610	-55.2532160	-55.2892290
HCO2-	-189.150175	-189.147173	-189.146229	-189.174061

XYZ geometries

Structures in Figure 1:

H-
H -0.026580 -0.320250 0.000000

Mg2+
Mg -0.067930 0.417290 0.000000

MgCl+
Mg -0.339354 0.417290 0.000000
Cl 1.782494 0.417290 0.000000

MgCl2
Mg -0.067930 0.417290 -0.000000
Cl 2.108265 0.417290 0.000000
Cl -2.244125 0.417290 0.000000

HCO2-
C -0.298966 0.809482 -0.027293
H 0.382757 0.173258 0.653761
O -0.625498 1.913462 0.455366
O -0.582153 0.274528 -1.119074

CH3O-
C -1.118216 -0.280734 0.047104
H 0.030400 -0.390362 -0.084977
H -1.421273 -1.400811 0.095775
H -1.422743 -0.038994 -1.047241
O -1.551048 0.509650 0.989339

Structures in Figure 4:
CO2
C -0.576664 -2.234195 -0.260501
O 0.586215 -2.234195 -0.260501
O -1.739543 -2.234195 -0.260501

1A
Mg -0.679146 -0.544815 -0.125424
C -0.850943 1.669811 0.074143
O 0.296363 1.127856 -0.058362
O -1.899889 0.943886 0.092426
H -0.935316 2.757356 0.172118

1B
Mg -4.578002 1.801678 0.327872
C -4.267907 3.484380 1.865250
O -3.813148 3.621068 0.690503
O -4.890858 2.434956 2.206101
H -4.119872 4.287786 2.599271
Cl -4.872515 0.202194 -1.133679

1C
Mg -4.081510 1.038862 -4.695733
C -3.596739 3.087898 -3.597222
O -3.342659 2.991134 -4.827347
O -4.096073 2.148323 -2.922704
H -3.370683 4.043080 -3.085132
Cl -6.150942 0.747009 -5.643579
Cl -2.466430 -0.589276 -4.777060

2A
Mg -3.187797 3.790073 -0.679357
C -4.721735 1.288951 0.564698
O -4.151108 2.219965 0.102027
O -5.269817 0.394746 1.009101
H -2.390570 5.088237 -1.325652

2B
Mg -2.689158 3.594592 -1.274456
C -4.326321 1.507870 0.347052
O -3.983101 2.628056 0.247971
O -4.684684 0.423329 0.480507
H -2.530326 5.239409 -0.923350
Cl -2.388763 1.679530 -2.382074

2C
Mg -2.287723 3.806009 -1.555677
C -4.073151 1.875408 0.141434
O -3.399755 1.573181 -0.764536
O -4.771304 2.065832 1.048949
H -3.282851 4.331131 -0.195343
Cl -3.111235 3.939332 -3.706978
Cl -0.060744 3.298724 -1.228269

3A
H 1.381369 0.117148 0.000000
Mg -0.278277 0.158638 0.000000

3B
H 1.346269 0.118020 0.000000
Mg -0.334860 0.160061 0.000000
Cl -2.529967 0.214927 0.000000

3C
Mg -0.276920 0.158578 -0.009459
Cl -2.325741 0.209826 -1.071326
H -0.157554 0.155646 1.733321
Cl 1.608037 0.111481 -1.340922

TS1primeA
Mg -2.731705 1.850077 -1.462211
C -4.202709 2.195083 0.391647
O -3.916701 1.101247 -0.275290
O -4.926401 2.376133 1.306945
H -3.610693 3.140710 -0.030581

TS1A

Mg	-2.787853	3.257283	-1.050152
C	-4.234087	2.236535	0.448095
O	-3.603883	1.647830	-0.472718
O	-4.982967	2.111840	1.328799
H	-3.846214	3.656127	0.342986

TS1B

Mg	-2.749886	2.903994	-1.422254
C	-4.240046	1.988287	0.386387
O	-3.736301	1.347991	-0.510346
O	-4.875398	2.187427	1.334548
H	-3.559078	3.671528	-0.059854
Cl	-1.475645	2.914557	-3.203830

TS1C

Mg	-2.334962	3.669393	-1.533576
C	-4.001487	2.015789	0.090471
O	-3.347545	1.633433	-0.812858
O	-4.714465	2.140468	0.999939
H	-3.358287	4.148425	-0.150537
Cl	-3.151585	3.941250	-3.670174
Cl	-0.088932	3.298859	-1.181584

TS1primeA

Mg	-2.731705	1.850077	-1.462211
C	-4.202709	2.195083	0.391647
O	-3.916701	1.101247	-0.275290
O	-4.926401	2.376133	1.306945
H	-3.610693	3.140710	-0.030581

Structures in Figure 6:

CH2O

C	0.469637	0.531595	0.753747
H	0.948798	1.054063	1.608997
H	-0.640788	0.562042	0.746580
O	1.104539	-0.024512	-0.099222

4A

C	-4.210402	-1.714394	-0.943236
H	-3.701844	-2.639139	-0.644858
H	-3.824527	-1.401613	-1.918025
H	-5.282877	-1.915191	-1.023516
O	-3.941155	-0.743251	0.052945
Mg	-4.116137	0.861885	0.695359

4B

C	0.016949	-0.125454	0.469948
H	0.386806	-1.158042	0.379917
H	0.289526	0.234116	1.473715
H	-1.081845	-0.165488	0.423177
O	0.539452	0.690902	-0.522645
Mg	1.199443	1.722638	-1.776860
Cl	2.022196	3.008237	-3.340212

4C

Mg	-1.976616	0.534139	-2.018654
Cl	-0.625410	-1.240663	-2.540136
Cl	-1.814090	2.454406	-3.269807
O	-3.157805	0.403018	-0.626245
C	-4.135557	0.955971	0.156934
H	-5.083574	0.378853	0.125272
H	-3.849081	0.998910	1.228798
H	-4.401785	1.994270	-0.128651

5A

C	-3.898946	-1.919708	-0.867107
H	-4.334633	-2.881422	-0.563701
H	-3.214240	-1.889018	-1.725601
H	-4.977862	2.125731	1.541450
O	-4.172706	-0.896092	-0.256725
Mg	-4.607916	0.737570	0.715489

5B

C	-3.783556	-1.718311	-0.620815
H	-3.821700	-2.778169	-0.917725
H	-2.895773	-1.117562	-0.870871
H	-6.353016	1.096288	1.456436
O	-4.720540	-1.225158	-0.021517
Mg	-4.892395	0.772968	0.656196
Cl	-2.895297	1.499414	-0.090136

5C

C	-3.957472	-1.603475	-0.709242
H	-3.860554	-2.628259	-1.118011
H	-3.379882	-0.799780	-1.186664
H	-5.784578	0.924620	2.253933
O	-4.681453	-1.392972	0.236918
Mg	-4.723826	0.762618	0.866560
Cl	-2.368536	0.794229	1.076364
Cl	-5.379632	1.427880	-1.304527

6A

H	1.381369	0.117148	0.000000
Mg	-0.278277	0.158638	0.000000

6B

H	1.346269	0.118020	0.000000
Mg	-0.334860	0.160061	0.000000
Cl	-2.529967	0.214927	0.000000

6C

Mg	-0.276920	0.158578	-0.009459
Cl	-2.325741	0.209826	-1.071326
H	-0.157554	0.155646	1.733321
Cl	1.608037	0.111481	-1.340922

TS2A

C	-4.191257	-1.470804	-0.804469
H	-5.059971	-2.137006	-0.757024
H	-3.571649	-1.560148	-1.703825
H	-5.123845	-0.143299	-1.461640

O	-3.695601	-0.973881	0.277449
Mg	-4.523379	0.668289	-0.022953

TS2B

C	-4.104839	-1.689522	-0.724750
H	-4.930040	-2.417662	-0.678221
H	-3.532971	-1.654654	-1.663259
H	-5.287698	0.219293	-1.667048
O	-3.786525	-1.024175	0.257118
Mg	-4.590915	0.839878	-0.195692
Cl	-4.277997	2.506088	1.215961

TS2C

C	-3.911743	-1.658608	-0.640682
H	-4.135760	-2.712298	-0.899134
H	-3.411187	-1.055170	-1.410917
H	-5.594533	-0.016655	-1.676068
O	-4.155307	-1.225471	0.470524
Mg	-4.923414	0.818149	-0.226198
Cl	-2.842170	1.795135	-0.627995
Cl	-6.307086	1.556928	1.465888

Structures in Table 1 (B3LYP/LANL2DZ):

CH2O

C	0.461100	0.539070	0.765214
H	0.948078	1.056638	1.613057
H	-0.644788	0.563602	0.748862
O	1.117795	-0.036122	-0.117031

CO2

C	-0.576664	-2.234195	-0.260501
O	0.616604	-2.234195	-0.260501
O	-1.769932	-2.234195	-0.260501

HCO2MgBr2

Mg	-4.082227	1.036145	-4.697162
C	-3.579405	3.161058	-3.557998
O	-3.330039	3.026613	-4.826551
O	-4.094974	2.170751	-2.892444
H	-3.355386	4.107536	-3.050567
Br	-6.357113	0.717074	-5.738467
Br	-2.305894	-0.752148	-4.785589

HCO2MgBr

Mg	-4.579436	1.793403	0.320275
C	-4.255880	3.549729	1.924944
O	-3.801107	3.655632	0.704988
O	-4.893010	2.453900	2.240455
H	-4.108857	4.347853	2.654150
Br	-4.904011	0.031546	-1.289493

HCO2MgCl2

Mg	-4.088088	1.011480	-4.710389
C	-3.584575	3.139176	-3.569726
O	-3.334363	3.007235	-4.837989
O	-4.100016	2.150638	-2.902180
H	-3.360401	4.086182	-3.062003
Cl	-6.193313	0.715922	-5.674152
Cl	-2.444282	-0.643604	-4.792339

HCO2MgCl

Mg	-4.582832	1.775046	0.303505
C	-4.259736	3.528785	1.905808
O	-3.805003	3.634555	0.685761
O	-4.896880	2.432857	2.221201
H	-4.112712	4.326871	2.634977
Cl	-4.885139	0.133948	-1.195933

HCO2MgF2

Mg	-4.107719	0.931882	-4.753369
C	-3.598534	3.076297	-3.603084
O	-3.345694	2.953438	-4.870208
O	-4.113779	2.094296	-2.928672
H	-3.373099	4.025468	-3.093877
F	-5.751917	0.726469	-5.494804
F	-2.814295	-0.340823	-4.804763

HCO2MgF

Mg	-4.593702	1.716213	0.249848
C	-4.270480	3.470445	1.852494
O	-3.815307	3.577441	0.632908
O	-4.907744	2.375170	2.169198
H	-4.123408	4.268672	2.581753
F	-4.831661	0.424121	-0.930884

HCO2MgI2

Mg	-4.075227	1.065679	-4.681340
C	-3.573297	3.186950	-3.544122
O	-3.324753	3.050330	-4.813028
O	-4.088930	2.195002	-2.880258
H	-3.349417	4.132903	-3.036979
I	-6.543251	0.714689	-5.813244
I	-2.150161	-0.878525	-4.779806

HCO2MgI

Mg	-4.575403	1.815318	0.340305
C	-4.251470	3.573679	1.946828
O	-3.796701	3.679698	0.727043
O	-4.888549	2.478029	2.262438
H	-4.104429	4.371874	2.676099
I	-4.925750	-0.086536	-1.397395

HMgBr2

H	0.615160	1.142620	1.172854
Mg	0.615160	-0.092803	-0.062569
Br	2.783358	-1.033013	-1.002779
Br	-1.553038	-1.033013	-1.002779

HMgBr

H	1.425853	0.116035	0.000000
Mg	-0.261155	0.158210	0.000000
Br	-2.683256	0.218763	0.000000

HMgCl2
H 0.615160 1.220063 1.250298
Cl -1.391803 -0.888031 -0.857796
Cl 2.622123 -0.888031 -0.857796
Mg 0.615160 -0.021805 0.008429

HMgCl
H 1.369342 0.117448 0.000000
Mg -0.317588 0.159621 0.000000
Cl -2.570312 0.215939 0.000000

HMgF2
H 0.615160 1.123492 1.153726
Mg 0.615160 -0.140383 -0.110149
F 2.180457 -0.801669 -0.771435
F -0.950138 -0.801669 -0.771435

HMgF
H 1.213777 0.121338 0.000000
Mg -0.481432 0.163713 0.000000
F -2.250904 0.207957 0.000000

HMgI2
H 0.615160 1.145832 1.176066
Mg 0.615160 -0.084727 -0.054493
I 2.972321 -1.105832 -1.075598
I -1.742001 -1.105832 -1.075598

HMgI
H 1.490545 0.114410 0.000000
Mg -0.195678 0.156587 0.000000
I -2.813425 0.222011 0.000000

MeOMgBr2
Mg -1.997419 0.657175 -2.064722
Br -0.652176 -1.462551 -2.402403
Br -1.510640 2.567483 -3.656921
O -3.228601 0.799019 -0.768446
C -4.196453 0.947251 0.230083
H -5.003287 0.189880 0.146252
H -3.767328 0.838882 1.247791
H -4.688015 1.941764 0.195877

MeOMgBr
C -0.000696 -0.153014 0.503472
H 0.374955 -1.184207 0.405434
H 0.277197 0.214589 1.504336
H -1.100673 -0.187000 0.448881
O 0.532635 0.680338 -0.509862
Mg 1.190532 1.708578 -1.759946
Br 2.098576 3.127625 -3.485275

MeOMgCl2
Mg -1.974816 0.648260 -2.083451
Cl -0.751333 -1.326502 -2.391395
Cl -1.505258 2.415512 -3.549766
O -3.212501 0.800312 -0.786693
C -4.180874 0.951971 0.208711
H -4.980644 0.184489 0.138778
H -3.752472 0.864807 1.229707
H -4.686020 1.940055 0.161619

MeOMgCl
C 0.008487 -0.138664 0.486024
H 0.384007 -1.169974 0.388192
H 0.286254 0.228757 1.487042
H -1.091542 -0.172807 0.431629
O 0.541637 0.694383 -0.526937
Mg 1.198745 1.721395 -1.775522
Cl 2.044938 3.043819 -3.383389

MeOMgF2
Mg -1.908810 0.603182 -2.134349
F -0.971269 -0.944158 -2.350807
F -1.549704 1.981035 -3.271952
O -3.163381 0.766994 -0.824086
C -4.136525 0.971777 0.149878
H -4.968884 0.234069 0.088421
H -3.733487 0.888604 1.184992
H -4.611856 1.977400 0.085414

MeOMgF
C 0.034595 -0.097861 0.436414
H 0.409214 -1.130137 0.340144
H 0.311533 0.268314 1.438625
H -1.065932 -0.133173 0.383510
O 0.567275 0.734336 -0.575667
Mg 1.224533 1.761598 -1.824539
F 1.891308 2.803832 -3.091446

MeOMgI2
Mg -2.021257 0.669893 -2.045086
I -0.541361 -1.618149 -2.420814
I -1.515589 2.751507 -3.772667
O -3.246761 0.799470 -0.748180
C -4.214349 0.939039 0.254715
H -5.024410 0.188114 0.157557
H -3.783129 0.811877 1.268324
H -4.697062 1.937153 0.233663

MeOMgI
C -0.011177 -0.169399 0.523391
H 0.364552 -1.200545 0.425213
H 0.266769 0.198287 1.524205
H -1.111146 -0.203297 0.468670
O 0.522264 0.664132 -0.490094
Mg 1.180849 1.693447 -1.741480
I 2.160415 3.224285 -3.602865

TS_HCO2MgBr2
Mg -2.221061 3.847593 -1.637985

C	-4.190165	1.821506	0.296259
O	-3.620925	1.277841	-0.607374
O	-4.821495	2.209964	1.233021
H	-3.268809	3.996736	-0.234538
Br	-3.138153	4.247163	-3.966081
Br	0.263343	3.446816	-1.341618

TS_HCO2MgBr

Mg	-2.742572	2.928484	-1.416980
C	-4.299398	1.948858	0.445322
O	-3.772988	1.355968	-0.505458
O	-4.942484	2.143984	1.422941
H	-3.528963	3.714240	-0.031160
Br	-1.349949	2.922251	-3.390014

TS_HCO2MgCl2

Mg	-2.077653	3.879657	-1.785090
C	-4.322116	1.774033	0.402984
O	-3.863542	0.930339	-0.314317
O	-4.894476	2.441767	1.216534
H	-3.232852	3.540589	-0.500904
Cl	-2.826529	4.416235	-3.936182
Cl	0.219905	3.864999	-1.341344

TS_HCO2MgCl

Mg	-2.729336	2.927369	-1.439456
C	-4.278102	1.955973	0.423242
O	-3.738333	1.355630	-0.516049
O	-4.930371	2.152086	1.394674
H	-3.535313	3.720354	-0.068739
Cl	-1.424899	2.902373	-3.269022

TS_HCO2MgF2

Mg	-1.895445	3.732068	-1.498541
C	-4.357222	2.054412	-0.100147
O	-3.779359	1.004638	-0.028445
O	-5.164805	2.941372	-0.147269
H	-2.521831	3.382229	0.143221
F	-2.847899	2.966929	-2.842918
F	-0.430702	4.765971	-1.784218

TS_HCO2MgF

Mg	-2.678858	2.923178	-1.508583
C	-4.233600	1.965183	0.363849
O	-3.685666	1.356201	-0.563504
O	-4.891178	2.174426	1.329319
H	-3.496499	3.737079	-0.151306
F	-1.650553	2.857716	-2.945125

TS_HCO2MgI2

Mg	-2.233114	3.875843	-1.600585
C	-4.238890	1.781081	0.308860
O	-3.602050	1.282934	-0.573494
O	-4.917384	2.162574	1.213473
H	-3.323475	4.069747	-0.245351
I	-3.143489	4.193878	-4.181629
I	0.461139	3.481560	-1.179592

TS_HCO2MgI

Mg	-2.766552	2.935520	-1.395234
C	-4.311565	1.938265	0.477824
O	-3.774538	1.350091	-0.468897
O	-4.957046	2.133237	1.453785
H	-3.564858	3.719377	-0.016464
I	-1.261794	2.937294	-3.526364

TS_MeOMgBr2

C	-3.919643	-1.696798	-0.686443
H	-4.190549	-2.748731	-0.871988
H	-3.404067	-1.157279	-1.490358
H	-5.543838	-0.062166	-1.674486
O	-4.124634	-1.176791	0.444708
Mg	-4.913750	0.788160	-0.193230
Br	-2.665558	1.950980	-0.672726
Br	-6.519160	1.604635	1.599941

TS_MeOMgBr

C	-4.101648	-1.725849	-0.786242
H	-5.003103	-2.350636	-0.728177
H	-3.482220	-1.820578	-1.688291
H	-5.290536	0.155541	-1.629177
O	-3.723037	-1.022418	0.201818
Mg	-4.582989	0.810297	-0.146747
Br	-4.327453	2.732890	1.320925

TS_MeOMgCl2

C	-3.901863	-1.663994	-0.677217
H	-4.119967	-2.719234	-0.909966
H	-3.393764	-1.068141	-1.445438
H	-5.593722	-0.049897	-1.657094
O	-4.160486	-1.197609	0.464847
Mg	-4.933801	0.802177	-0.181021
Cl	-2.811188	1.776655	-0.629950
Cl	-6.366407	1.622052	1.491259

TS_MeOMgCl

C	-4.101921	-1.702966	-0.775029
H	-5.003786	-2.327285	-0.718384
H	-3.482819	-1.796312	-1.677441
H	-5.287353	0.175666	-1.614076
O	-3.721443	-1.003965	0.215352
Mg	-4.579105	0.827155	-0.130091
Cl	-4.334560	2.606955	1.243779

TS_MeOMgF2

C	-6.745820	-2.217614	-0.168275
O	-7.554395	-1.325808	0.235456
Mg	-4.830038	-0.156460	-0.589800
F	-4.329036	1.335153	0.311175
F	-5.136163	-0.218765	-2.379318
H	-6.435775	-2.277445	-1.224438
H	-6.501127	-3.096459	0.451894

H -4.769437 -1.787502 0.200455

TS_MeOMgF
C -4.097062 -1.653439 -0.742495
H -5.001604 -2.274751 -0.689911
H -3.479621 -1.743148 -1.646776
H -5.287408 0.256273 -1.570860
O -3.716196 -0.959613 0.248681
Mg -4.569172 0.888342 -0.077197
F -4.359922 2.265584 1.022669

TS_MeOMgI2
C -3.938684 -1.731425 -0.692811
H -4.260461 -2.775534 -0.832949
H -3.415314 -1.247806 -1.526620
H -5.500845 -0.075313 -1.699123
O -4.094215 -1.161902 0.423713
Mg -4.892569 0.771526 -0.214641
I -2.497805 2.134110 -0.726201
I -6.681306 1.588353 1.724052

TS_MeOMgI
C -4.100699 -1.750758 -0.797780
H -5.000494 -2.377685 -0.737075
H -3.480326 -1.847850 -1.698929
H -5.297509 0.131624 -1.650841
O -3.726448 -1.038937 0.185782
Mg -4.591886 0.792194 -0.171623
I -4.313624 2.870659 1.414576

Structures in Table 2 (B3LYP/LANL2DZ):
HBaCl2
H 0.267963 1.682375 1.782663
Cl -1.801812 -1.294383 -1.401112
Cl 3.396520 -0.911399 -0.818931
Ba 0.597968 -0.054396 -0.019485

HBaCl
H 1.931483 -0.258814 0.000000
Ba -0.296256 0.787603 0.000000
Cl -3.153785 -0.035782 0.000000

HBa
H 0.615160 1.239631 1.269865
Ba 0.615160 -0.443124 -0.412889

HBeCl2
Be 0.615160 -0.021046 0.009188
H 0.615160 0.950042 0.980276
Cl -1.100942 -0.753399 -0.723165
Cl 2.331261 -0.753399 -0.723165

HBeCl
H 0.985145 0.127054 0.000000
Be -0.330256 0.159936 0.000000
Cl -2.173446 0.206018 0.000000

HBe
Be 0.615160 -0.074460 -0.044226
H 0.615160 0.870968 0.901202

HCaCl2
H 0.615160 1.484263 1.514497
Cl -1.704394 -1.014186 -0.983952
Cl 2.934714 -1.014186 -0.983952
Ca 0.615160 -0.033693 -0.003459

HCaCl
H 1.778452 0.107308 0.000000
Ca -0.325210 0.159656 0.000000
Cl -2.971800 0.226044 0.000000

HCa
H 0.615160 1.124405 1.154639
Ca 0.615160 -0.327897 -0.297663

HCO2BaCl2
Ba -4.181166 0.774283 -4.855884
C -3.461606 3.448584 -3.380445
O -3.212510 3.367998 -4.651872
O -3.990153 2.490455 -2.682109
H -3.208430 4.389580 -2.861304
Cl -6.922109 0.437829 -6.090864
Cl -2.129062 -1.441701 -5.026298

HCO2BaCl
Ba -4.579240 1.489898 0.085349
C -4.266925 3.802715 2.109371
O -3.733020 3.929462 0.929351
O -4.927353 2.741342 2.471094
H -4.155618 4.624587 2.828946
Cl -4.880147 -0.755942 -1.868794

HCO2Ba
Ba -0.630726 -1.168897 -0.181472
C -0.863201 1.827654 0.088316
O 0.315181 1.285261 -0.046687
O -1.942756 1.096079 0.108332
H -0.947429 2.913997 0.186412

HCO2BeCl2
Be -4.021347 0.969643 -5.055489
C -3.670970 3.063934 -3.319616
O -3.681926 2.321022 -4.409842
O -4.060404 2.737407 -2.174802
H -3.259523 4.073102 -3.512410
Cl -5.782897 0.723560 -5.907781
Cl -2.627972 -0.421639 -5.168837

HCO2BeCl
Be -4.555931 1.909198 0.419495
C -4.284550 3.406494 1.800982

O	-3.847700	3.465701	0.566611
O	-4.913879	2.285244	2.055428
H	-4.140889	4.199195	2.532396
Cl	-4.799353	0.566229	-0.819594

HCO2Be

Be	-0.694109	-0.288116	-0.102653
C	-0.852324	1.667049	0.074012
O	0.297447	1.008072	-0.068546
O	-1.880097	0.818412	0.080345
H	-0.939849	2.748677	0.171742

HCO2CaCl2

Ca	-4.115731	0.893262	-4.773732
C	-3.545061	3.306703	-3.479957
O	-3.284256	3.201427	-4.748174
O	-4.060453	2.334774	-2.789151
H	-3.320691	4.256038	-2.971117
Cl	-6.528296	0.513326	-5.895904
Cl	-2.250548	-1.038502	-4.890742

HCO2CaCl

Ca	-4.606142	1.644570	0.184898
C	-4.236862	3.653508	2.019705
O	-3.768933	3.793220	0.811272
O	-4.877569	2.573773	2.369654
H	-4.089740	4.453846	2.750584
Cl	-4.963056	-0.286856	-1.580794

HCO2Ca

Ca	-0.651030	-0.907919	-0.158108
C	-0.858816	1.771471	0.083294
O	0.315015	1.212034	-0.052709
O	-1.931215	1.023806	0.101504
H	-0.942885	2.854702	0.180920

HCO2Mg

Mg	-0.673913	-0.612174	-0.131478
C	-0.854558	1.716369	0.078334
O	0.308216	1.118927	-0.060025
O	-1.910221	0.933106	0.092286
H	-0.938455	2.797867	0.175784

HCO2SrCl2

Sr	-4.147317	0.840901	-4.811003
C	-3.504235	3.371222	-3.432985
O	-3.248808	3.278708	-4.702841
O	-4.028102	2.406914	-2.738703
H	-3.264303	4.315847	-2.918514
Cl	-6.708674	0.480103	-5.987316
Cl	-2.203598	-1.226666	-4.957415

HCO2SrCl

Sr	-4.601464	1.573859	0.139097
C	-4.242410	3.720500	2.062010
O	-3.670928	3.814026	0.895508
O	-4.970308	2.691799	2.390681
H	-4.106936	4.530401	2.787635
Cl	-4.950256	-0.498524	-1.719614

HCO2Sr

Sr	-0.641600	-1.028802	-0.168975
C	-0.860789	1.796594	0.085552
O	0.315556	1.246872	-0.049901
O	-1.937201	1.058126	0.104763
H	-0.944897	2.881304	0.183462

HMg

H	0.615160	0.984543	1.014777
Mg	0.615160	-0.188036	-0.157802

HSrCl2

H	0.462897	1.618198	1.595876
Cl	-1.760553	-1.218898	-1.091981
Cl	3.151882	-0.936495	-0.947387
Sr	0.606414	-0.040608	-0.013374

HSrCl

H	1.811193	0.395430	0.000000
Sr	-0.323500	-0.346178	0.000000
Cl	-3.006251	0.443756	0.000000

HSr

H	0.615160	1.175008	1.205242
Sr	0.615160	-0.378501	-0.348266

TS_HCO2BaCl2

C	-4.613115	1.821367	-0.227185
O	-3.470418	1.533959	-0.454937
O	-5.757393	2.014288	0.023853
Ba	-1.808011	3.582870	-1.624032
Cl	-3.840193	2.727942	-3.724094
Cl	1.215847	3.574265	-1.941535
H	-3.133658	4.513690	0.333771

TS_HCO2Ba

C	-4.277065	2.107862	0.474414
O	-3.538024	1.781449	-0.444304
O	-5.037389	2.180311	1.373864
H	-3.647357	4.312317	0.119926
Ba	-2.170792	3.706100	-1.709594

TS_HCO2BeCl2

O	-4.121066	0.740017	-0.092323
Be	-2.260829	3.475771	-1.673512
Cl	-0.356662	3.673852	-1.192831
Cl	-3.002287	4.227980	-3.341003
H	-3.109475	2.782121	-0.807255
C	-4.237615	1.863070	0.340306
O	-4.619706	2.769729	1.043136

TS_HCO2BeCl

Be	-2.866667	2.808658	-1.284040
C	-4.161528	2.023671	0.283162
O	-3.613724	1.399674	-0.652270
O	-4.816904	2.226799	1.247392
H	-3.411157	3.652041	-0.290586
Cl	-1.766375	2.902943	-2.779007

TS_HCO2Be

C	-4.233530	2.373841	0.483025
O	-3.569706	1.678418	-0.506335
O	-5.005131	2.083665	1.348404
H	-3.877275	3.553874	0.354480
Be	-2.917800	2.927051	-0.977526

TS_HCO2CaCl2

C	-5.302717	4.115750	-0.543412
O	-4.331484	3.427099	-0.670656
Ca	-2.049352	4.494215	-1.287205
O	-6.300247	4.744783	-0.405641
Cl	-3.227929	4.645681	-3.734165
Cl	0.139659	2.974100	-0.862129
H	-2.837794	5.906225	0.159564

TS_HCO2CaCl

Ca	-2.538832	3.124333	-1.553489
C	-4.475085	1.801789	0.550694
O	-3.929346	1.425938	-0.470363
O	-5.091189	1.954994	1.548314
H	-3.436981	3.925454	0.232124
Cl	-1.164921	2.781277	-3.782629

TS_HCO2Ca

C	-4.280960	2.083376	0.477235
O	-3.558437	1.718883	-0.471819
O	-5.047075	1.985505	1.374850
H	-3.834390	3.937105	0.358270
Ca	-2.516484	3.614033	-1.295544

TS_HCO2Mg

Mg	-2.747807	3.275288	-1.094440
C	-4.261612	2.207438	0.474133
O	-3.594251	1.655009	-0.482495
O	-5.027429	2.076976	1.373846
H	-3.823905	3.694903	0.325965

TS_HCO2SrCl2

C	-4.436188	1.859627	0.051696
O	-5.565010	1.932439	0.411944
O	-3.298424	1.710012	-0.294471
Sr	-1.961462	3.812398	-1.393490
Cl	-3.765215	3.065940	-3.496452
Cl	0.879691	3.779946	-1.660228
H	-3.117243	4.672343	0.446447

TS_HCO2SrCl

Sr	-2.820809	3.071819	-1.646373
C	-4.639597	1.816226	1.075175
O	-3.745157	1.564462	0.307136
O	-5.504359	1.997099	1.858734
H	-4.539024	4.203362	-0.595258
Cl	-0.704784	2.162352	-3.259874

TS_HCO2Sr

C	-4.330475	2.196216	0.561306
O	-3.598764	1.927230	-0.398293
O	-5.091827	2.085292	1.459675
H	-3.867869	4.191585	0.509493
Sr	-2.465595	3.959439	-1.255776

Structures in Table 4 (B3LYP/LANL2DZ):

MeOBaCl2

Ba	-1.791215	0.617369	-2.345454
Cl	-0.228179	-1.970231	-2.672336
Cl	-1.281780	2.912067	-4.274341
O	-3.417650	0.850166	-0.572411
C	-4.360148	0.985726	0.456734
H	-5.344247	0.516961	0.215509
H	-4.032761	0.516944	1.415383
H	-4.587938	2.049902	0.704428

MeOBaCl

C	-0.097339	-0.291843	0.686894
H	0.451767	-1.251630	0.784855
H	-0.065635	0.189158	1.686886
H	-1.159230	-0.557413	0.502020
O	0.436511	0.534157	-0.326331
Ba	1.333567	1.922785	-2.028652
Cl	2.472882	3.661694	-4.198632

MeOBa

C	-4.222116	-1.785366	-1.013067
H	-3.715003	-2.659540	-0.566760
H	-3.761358	-1.612349	-2.002160
H	-5.273387	-2.075213	-1.190577
O	-4.125839	-0.638925	-0.179791
Ba	-3.979237	1.219689	1.171025

MeOBeCl2

Be	-2.128642	0.447934	-1.801673
Cl	-0.843933	-0.910794	-2.477511
Cl	-2.205362	2.239125	-2.719408
O	-3.024651	0.159791	-0.637963
C	-4.003112	0.971303	0.001438
H	-4.997414	0.490197	-0.043878
H	-3.754186	1.111997	1.069323
H	-4.086618	1.969350	-0.462817

MeOBeCl

C	0.073913	-0.050401	0.383045
H	0.431184	-1.079495	0.248381
H	0.396682	0.310821	1.368006
H	-1.023127	-0.048469	0.346840

O	0.595618	0.782754	-0.635464
Be	1.108913	1.602494	-1.637584
Cl	1.789342	2.689206	-2.966184

MeOBe

C	-4.220250	-1.693756	-0.949233
H	-3.652230	-2.505901	-0.490009
H	-3.808131	-1.437280	-1.927747
H	-5.277121	-1.957411	-1.030598
O	-4.110715	-0.524213	-0.091827
Be	-4.008494	0.566859	0.708083

MeOCaCl2

Ca	-1.826069	0.675916	-2.186124
Cl	-0.958825	-1.723641	-3.060511
Cl	-0.717129	2.871713	-3.291975
O	-3.324891	0.829270	-0.682207
C	-4.309841	0.932443	0.309249
H	-4.406114	0.005171	0.917543
H	-4.108890	1.756080	1.030785
H	-5.322160	1.131950	-0.109249

MeOCaCl

C	-0.044480	-0.216576	0.599757
H	0.471920	-1.193412	0.649814
H	0.051751	0.252559	1.596753
H	-1.119103	-0.425585	0.442072
O	0.485853	0.606164	-0.421165
Ca	1.268558	1.818840	-1.927773
Cl	2.258026	3.364918	-3.832418

MeOCa

C	-4.227526	-1.758488	-0.995854
H	-3.668722	-2.607479	-0.573686
H	-3.824140	-1.550073	-1.998413
H	-5.278592	-2.064727	-1.108487
O	-4.119608	-0.609044	-0.154515
Ca	-3.958352	1.038107	1.049625

MeOMg

C	-4.224184	-1.725939	-0.972098
H	-3.662019	-2.558672	-0.533935
H	-3.818043	-1.497405	-1.964207
H	-5.277794	-2.012092	-1.069490
O	-4.113136	-0.567144	-0.124376
Mg	-3.981765	0.809548	0.882774

MeOSrCl2

Sr	-1.805435	0.674159	-2.259382
Cl	0.287879	-1.256879	-2.089711
Cl	-1.869079	2.392770	-4.535770
O	-3.375232	0.835273	-0.630448
C	-4.345299	0.934974	0.376729
H	-5.368468	1.124067	-0.023311
H	-4.425308	0.010827	0.994775
H	-4.142976	1.763712	1.094630

MeOSrCl

C	-0.077869	-0.260536	0.630680
H	0.308769	-1.297140	0.568416
H	0.160909	0.107384	1.648281
H	-1.182105	-0.328657	0.568076
O	0.462409	0.570818	-0.376642
Sr	1.313719	1.879740	-1.963927
Cl	2.386692	3.535298	-3.967843

MeOSr

C	-4.225458	-1.775382	-0.999505
H	-3.704907	-2.636939	-0.549408
H	-3.779706	-1.598750	-1.992457
H	-5.277883	-2.065853	-1.153937
O	-4.123392	-0.619254	-0.173008
Sr	-3.965595	1.144476	1.086984

TS_MeOBaCl2

C	-3.666823	-1.830778	-0.770793
H	-3.664905	-2.862916	-1.155382
H	-3.123366	-1.056092	-1.336207
H	-6.132323	-0.159399	-2.082255
O	-4.239765	-1.561095	0.314322
Ba	-5.267191	1.037392	0.000702
Cl	-2.301653	1.449792	-0.655657
Cl	-6.885173	2.485106	2.140690

TS_MeOBaCl

C	-4.132816	-2.100720	-0.794818
H	-4.482742	-3.103599	-0.507841
H	-4.003525	-1.878639	-1.861751
H	-5.406274	0.219078	-2.199007
O	-3.894972	-1.237377	0.087083
Ba	-4.580863	1.379023	-0.110493
Cl	-4.009794	3.501482	1.930938

TS_MeOBa

C	-4.036128	-1.831508	-0.779200
H	-4.907943	-2.495995	-0.730780
H	-3.388669	-1.907951	-1.661764
H	-5.451913	0.297570	-1.748592
O	-3.749590	-1.056889	0.177701
Ba	-4.631459	1.377925	0.270172

TS_MeOBeCl2

C	-4.088681	-1.516339	-0.647664
H	-5.030248	-2.053248	-0.868633
H	-3.378257	-1.461340	-1.493503
H	-4.872897	-0.079841	-1.350937
O	-3.694225	-1.345404	0.557227
Be	-4.717529	0.811570	-0.261412
Cl	-3.195402	2.071532	-0.369684
Cl	-6.303960	1.075079	0.890025

TS_MeOBeCl

C	-5.131911	-1.154194	-0.684709
O	-4.703758	-0.595349	0.386100
Be	-4.676873	1.004492	-0.169104
Cl	-4.048350	2.377077	0.964641
H	-4.469137	-1.808808	-1.267529
H	-6.186361	-1.103030	-0.979042
H	-5.099950	0.943292	-1.495810

TS_MeOBe

C	-4.213078	-1.451110	-0.826752
H	-5.061478	-2.133812	-0.729903
H	-3.550607	-1.548157	-1.691020
H	-5.111559	-0.026547	-1.371103
O	-3.738676	-0.829474	0.297798
Be	-4.490305	0.372252	-0.151484

TS_MeOCaCl2

C	-3.780852	-1.753003	-0.722259
H	-3.835840	-2.814042	-1.011955
H	-3.295661	-1.051861	-1.416216
H	-5.885552	-0.136980	-1.859995
O	-4.213392	-1.379020	0.397104
Ca	-5.107994	0.914929	-0.093983
Cl	-2.533242	1.645704	-0.651432
Cl	-6.628666	2.076282	1.814154

TS_MeOCaCl

C	-4.088910	-1.915874	-0.790134
H	-4.817590	-2.727481	-0.654291
H	-3.551380	-1.872661	-1.746128
H	-5.401392	0.218390	-1.915453
O	-3.844337	-1.107523	0.143047
Ca	-4.618372	1.117812	-0.116449
Cl	-4.189005	3.066584	1.623517

TS_MeOCa

C	-4.132467	-1.637117	-0.813479
H	-5.019300	-2.278475	-0.768160
H	-3.521803	-1.698376	-1.720779
H	-5.243403	-0.016711	-1.572577
O	-3.696559	-1.033915	0.239065
Ca	-4.552170	1.047747	0.163467

TS_MeOMg

C	-4.195596	-1.495783	-0.826496
H	-5.054121	-2.172245	-0.763525
H	-3.561063	-1.593493	-1.713317
H	-5.132344	-0.120986	-1.461335
O	-3.699422	-0.953281	0.284062
Mg	-4.523156	0.718942	0.008149

TS_MeOSrCl2

C	-3.730439	-1.787483	-0.742054
H	-3.756532	-2.837149	-1.073939
H	-3.222944	-1.050811	-1.383340
H	-5.998867	-0.160534	-1.952084
O	-4.224602	-1.461029	0.366085
Sr	-5.178381	0.971725	-0.054622
Cl	-2.421548	1.565716	-0.664142
Cl	-6.747886	2.261575	1.959516

TS_MeOSrCl

C	-4.095404	-2.005205	-0.794033
H	-4.693415	-2.907870	-0.602465
H	-3.662106	-1.884534	-1.794935
H	-5.410345	0.241397	-2.056473
O	-3.894604	-1.165987	0.119564
Sr	-4.622162	1.239596	-0.110453
Cl	-4.132949	3.261850	1.782905

TS_MeOSr

C	-4.097923	-1.709543	-0.803256
H	-4.987955	-2.347701	-0.758092
H	-3.488136	-1.766541	-1.712290
H	-5.312859	0.070162	-1.628944
O	-3.702009	-1.053991	0.218345
Sr	-4.576820	1.190766	0.211774

Structures in Figure 9 (G4):

7A

C	-4.099756	-1.992151	-1.217781
H	-3.868846	-2.863708	-0.595573
H	-3.344821	-1.919000	-2.008222
H	-5.078550	-2.147321	-1.684639
O	-4.108418	-0.821436	-0.438120
Mg	-4.118802	0.605485	0.512790
C	-4.138416	3.231144	2.260486
O	-4.145543	4.178916	2.891117
O	-4.130989	2.243915	1.603590

7B

C	0.766586	-1.510563	2.061310
H	0.927988	-2.506859	1.643470
H	1.716323	-1.085740	2.394142
H	0.060313	-1.557372	2.891638
O	0.201705	-0.664438	1.052573
Mg	0.237856	0.249339	-0.716460
Cl	1.576732	0.414503	-2.436377
C	-1.153571	-0.042043	1.299927
O	-1.391979	0.642714	0.253371
O	-1.713455	-0.271599	2.324208

7C

Mg	-2.118155	0.299635	-1.436548
Cl	-0.047962	-0.628807	-1.818891
Cl	-3.216421	1.205345	-3.288379
O	-3.026963	0.008622	0.125903
C	-4.154501	0.044808	0.897936
H	-5.048037	0.431283	0.364594
H	-4.441951	-0.956371	1.283706
H	-4.038212	0.686643	1.797415

C	-1.414463	3.388940	-1.932633
O	-1.300253	2.587282	-1.091696
O	-1.481835	4.239871	-2.716933

7Cprime

Mg	-1.925682	0.719207	-1.629557
Cl	0.191276	-0.152653	-1.629033
Cl	-3.269976	0.617774	-3.480032
O	-2.976717	0.191082	0.116127
C	-3.627359	-0.762685	0.936193
H	-4.465255	-1.204832	0.386778
H	-2.918227	-1.550302	1.212231
H	-3.991768	-0.254160	1.831895
C	-2.904551	1.591708	0.564896
O	-2.283190	2.219995	-0.335718
O	-3.403001	1.891367	1.622361

8A

C	-4.196964	-0.169472	-2.327354
H	-3.277184	-0.736895	-2.523891
H	-5.074253	-0.331529	-2.968207
O	-4.243691	0.632687	-1.406599
Mg	-4.317164	1.900886	0.050085
C	-4.403922	3.377339	1.746857
O	-4.033140	3.758648	0.589743
O	-4.725611	2.161097	1.944467
H	-4.446159	4.095642	2.572315

8B

C	1.040943	-0.031730	0.075150
H	1.574105	-0.984296	0.217353
H	0.895654	0.628190	0.944450
H	-2.761213	2.198740	0.859339
O	0.620831	0.273024	-1.022397
Mg	-0.354044	2.032230	-1.586119
Cl	0.749832	2.965047	-3.263199
C	-1.981904	2.142076	0.084452
O	-0.806827	2.524958	0.359095
O	-2.281572	1.693150	-1.058565

8C

Mg	-2.583467	0.351692	-1.849364
Cl	-1.438317	-1.635402	-1.631189
Cl	-4.821906	0.473625	-2.380553
H	-0.455096	3.140558	-3.614870
C	-0.861161	2.843508	-2.620088
O	-1.530081	1.759611	-2.643156
O	-0.624034	3.570388	-1.654075
C	-2.070030	2.050782	0.602816
O	-2.598956	1.045649	0.170347
H	-2.165861	2.281594	1.682468
H	-1.498802	2.735020	-0.055345

TS3A

C	-3.876856	-1.325329	-2.506983
H	-2.935202	-1.736761	-2.887412
H	-3.517721	0.117475	-2.963803
H	-4.748057	-1.374984	-3.169740
O	-4.060997	-1.261025	-1.242408
Mg	-3.912015	0.274053	-0.221098
C	-3.311692	1.320113	-2.741932
O	-3.035554	1.966042	-3.689790
O	-3.459204	1.555515	-1.487285

TS3B

C	0.411501	0.466119	0.457143
H	-0.039907	-0.526755	0.594590
H	0.772538	0.953604	1.373910
H	-0.924200	1.166833	0.518514
O	0.923232	0.771722	-0.656810
Mg	0.299269	1.873123	-2.102383
Cl	1.135530	2.437239	-4.048798
C	-1.766555	1.911773	-0.020113
O	-1.335801	2.267725	-1.147293
O	-2.739903	2.097606	0.642197

TS3C

Mg	-1.893513	0.007204	-1.822734
Cl	0.154754	-1.016706	-1.792026
Cl	-3.320404	-0.047678	-3.633510
O	-2.930876	-0.216846	-0.146382
C	-3.754051	0.638000	0.312662
H	-4.700652	0.825093	-0.226406
H	-3.847121	0.744330	1.409408
H	-3.244185	1.896419	0.100711
C	-2.408952	2.703711	-0.547745
O	-1.722571	1.997220	-1.278703
O	-2.575684	3.844407	-0.220900

Structures in Figure 10 (G4):

H2O

O	-3.195900	2.218261	-0.012667
H	-2.234996	2.253641	0.020216
H	-3.470654	2.893648	0.615051

10A

C	-0.227519	-2.213623	0.755934
H	-1.223369	-2.630302	0.959752
H	0.652014	-2.867600	0.830881
H	-0.064317	0.621303	-2.064588
O	-0.099884	-1.037966	0.448388
Mg	0.112691	0.851500	0.069732
O	0.339575	2.578004	0.200564
H	0.474573	3.334281	0.766046
H	0.036236	1.364402	-1.966707

10B

C	-0.115336	-2.404259	-1.212651
H	-0.353197	-3.478018	-1.274171
H	0.412427	-1.901494	-2.036580
H	-0.387183	-0.002063	-4.740885

O	-0.443127	-1.773853	-0.221835
Mg	-0.014162	0.259263	-0.082717
O	0.730455	0.320930	-1.751861
H	1.171219	1.039469	-2.202186
H	-0.162692	0.074884	-4.033455
Cl	-0.619554	1.200489	1.822357

10C

C	-0.111205	-2.417083	-1.125702
H	-0.265292	-1.737669	-1.983054
H	-0.076023	-3.516519	-1.263356
H	0.733888	0.285321	-4.656540
O	0.022006	-1.946932	-0.015032
Mg	-0.058376	0.260636	0.052223
O	-0.223942	0.350132	-1.848223
H	-1.025894	0.788637	-2.140537
H	0.541831	0.312551	-3.928054
Cl	-2.057598	0.634777	1.185823
Cl	1.984826	0.694443	1.050122

11A

C	-3.637686	-2.072896	-0.221385
H	-4.283598	-2.846192	0.215972
H	-2.837174	-2.368619	-0.912800
O	-3.806866	-0.894095	0.057711
Mg	-4.136823	0.938181	0.546102
O	-4.552309	2.529747	1.071984
H	-4.486727	3.477907	1.135163

11B

C	-0.482579	-2.065857	-1.609185
H	-0.863736	-3.072742	-1.842958
H	-0.027494	-1.442629	-2.393700
O	-0.568316	-1.643042	-0.468829
Mg	0.149766	0.261279	-0.015760
O	0.690407	0.574711	-1.727097
H	1.113081	1.334827	-2.121809
Cl	-0.097864	0.846258	2.101419

11C

C	0.107727	-2.088566	-1.610567
H	0.039479	-1.250918	-2.329641
H	0.197388	-3.140093	-1.952454
O	0.083249	-1.845873	-0.421621
Mg	-0.071474	0.320319	0.029110
O	-0.014830	0.742010	-1.819605
H	-0.775524	1.239283	-2.126001
Cl	-2.196331	0.474131	0.978129
Cl	1.828989	0.564868	1.336323

9A

C	-4.213345	-1.879604	-1.040172
H	-3.277191	-2.422721	-0.869464
H	-4.297081	-1.660808	-2.110522
H	-5.048379	-2.528051	-0.752525
O	-4.234815	-0.689458	-0.292388
Mg	-4.260271	0.763245	0.623482
O	-4.290198	2.431650	1.673884
H	-4.291056	2.505268	2.640726
H	-4.306932	3.335086	1.322135

9B

C	-0.173194	-2.417131	-1.850794
H	-0.064192	-3.147466	-1.034390
H	0.590802	-2.660366	-2.605768
H	-1.156497	-2.593220	-2.314525
O	-0.047027	-1.101524	-1.407127
Mg	0.141981	0.107338	-0.044611
O	-0.138869	1.407776	-1.595286
H	0.434088	2.080332	-1.974259
H	-0.126254	0.591380	-2.155136
Cl	0.566360	0.734986	2.026566

9C

C	-0.060667	-2.483352	-1.770452
H	0.259030	-3.181103	-0.972617
H	0.563138	-2.726157	-2.654176
H	-1.096677	-2.773167	-2.039257
O	0.047422	-1.162077	-1.403716
Mg	-0.111777	0.134037	-0.014112
O	0.558747	1.275518	-1.730908
H	-0.299388	1.705962	-1.857416
H	0.440205	0.347207	-2.079739
Cl	-2.152941	1.291931	0.028933
Cl	1.165101	-0.016491	1.891702

TS4A

C	-4.956992	-1.350564	-0.379886
H	-5.959288	-1.652957	-0.700673
H	-4.114501	-1.886943	-0.828721
H	-4.900621	-0.276655	-1.530329
O	-4.809578	-0.817205	0.769104
Mg	-4.555477	0.967023	1.178433
O	-4.567415	1.759101	-0.438148
H	-4.501745	2.561237	-0.957603
H	-4.780855	0.529789	-1.273848

TS4B

C	-4.974734	-1.404007	-0.395920
H	-5.921372	-1.711992	-0.858082
H	-4.071629	-1.920051	-0.746165
H	-4.768979	-0.294060	-1.732679
O	-4.970657	-0.787749	0.683877
Mg	-4.803826	1.063830	1.266294
O	-4.632740	1.651095	-0.489443
H	-4.512421	2.458223	-0.986613
H	-4.706267	0.477753	-1.378691
Cl	-4.851166	1.789378	3.350903

TS4C

C	-4.889795	-1.339472	-0.264164
H	-5.972119	-1.165244	-0.326677

H	-4.478860	-2.139754	-0.899507
H	-4.762344	-0.199279	-1.734711
O	-4.217777	-0.870359	0.659232
Mg	-4.639722	1.046227	1.314066
O	-4.460260	1.718992	-0.515951
H	-5.215514	2.252005	-0.781450
H	-4.635855	0.577892	-1.328506
Cl	-6.933090	0.951246	1.779865
Cl	-3.102515	1.678158	2.908531

Structures in Figure S6:

H2

H	0.658739	-1.588608	0.000000
H	-0.084056	-1.588608	0.000000

12A

Mg	-4.201360	3.037718	0.290551
C	-4.748543	3.211103	2.463269
O	-3.805811	3.922414	1.985216
O	-5.381131	2.401524	1.709838
H	-5.015155	3.295574	3.521902
O	-3.720159	2.885361	-1.618328
H	-4.136119	2.303338	-2.272604
H	-3.023371	3.378453	-2.077892

12B

Mg	-4.533271	3.196897	0.069324
C	-4.550603	3.115412	2.388918
O	-3.685034	3.831881	1.805311
O	-5.402305	2.446144	1.735857
H	-4.561922	3.073123	3.488010
O	-3.077848	1.970209	-0.717929
H	-3.055285	2.167941	-1.665791
H	-2.170525	1.923230	-0.396786
Cl	-5.188186	3.986397	-1.919896

12C

Mg	-2.226909	4.950508	1.194298
C	-4.124967	3.620385	3.154169
O	-3.661281	3.977132	2.011286
O	-5.083835	2.914591	3.395084
H	-3.538888	4.039660	4.029606
O	-1.379899	5.705106	3.030569
H	-0.605164	5.131859	2.851205
H	-1.886727	5.250066	3.717198
Cl	-0.186196	3.758092	1.072583
Cl	-2.722421	6.578037	-0.324731

13A

Mg	-2.290637	4.826130	2.857313
C	-4.872086	3.103222	2.232499
O	-3.919717	3.732636	2.550474
O	-5.788827	2.496886	1.932881
H	-2.337029	4.641091	4.984948
O	-0.877463	5.812287	2.597334
H	-0.304617	6.249333	1.971394
H	-1.726045	5.068761	4.853362

13B

Mg	-1.867397	4.887062	1.036656
C	-4.357778	3.985464	2.204331
O	-3.733065	3.831077	1.215305
O	-5.036917	4.074367	3.126838
H	-1.772889	3.896926	5.547725
O	-2.237631	5.477179	2.714312
H	-1.835262	6.100405	3.315538
H	-1.903865	4.210922	4.884805
Cl	-0.813685	4.596260	-0.869786

13C

Mg	-2.000823	4.668712	0.353132
C	-3.250348	3.974873	2.472847
O	-3.423488	3.587719	1.283959
O	-3.775646	3.716476	3.533532
H	-2.911988	5.001369	6.204952
O	-2.163390	4.937919	2.460344
H	-1.993328	5.263455	3.348713
H	-3.156520	4.663816	5.583981
Cl	-0.075994	3.565157	-0.193738
Cl	-2.706764	6.526340	-0.775059

14A

Mg	1.694651	-0.691042	-1.454305
O	2.800699	-1.466346	-2.530770
H	3.436386	-2.141151	-2.754113
C	-0.387668	0.963732	0.239977
O	-1.140357	1.567054	0.844110
O	0.396963	0.334063	-0.388524

14B

Mg	-1.871656	4.892779	1.030770
C	-4.346571	3.992894	2.207112
O	-3.745515	3.847136	1.201984
O	-5.008087	4.067490	3.143901
O	-2.262268	5.498386	2.692086
H	-1.846729	6.073045	3.330745
Cl	-0.800910	4.580085	-0.863404

14C

Mg	0.550402	0.107967	-2.030065
C	-0.723515	-0.660010	0.046771
O	-0.964167	-0.902316	-1.169775
O	-1.239460	-0.958052	1.097713
O	0.470834	0.179597	0.087093
H	0.691602	0.390063	0.998316
Cl	2.328316	-1.134441	-2.756466
Cl	0.034520	2.136006	-2.953719

15A

Mg	-0.678981	0.665789	1.046856
O	-0.348521	2.358697	0.751125

H 0.267931 2.803935 0.164121

15B
O -5.224571 1.622300 0.459988
H -6.149719 1.830752 0.548267
Mg -4.114357 0.367106 -0.116921
Cl -2.682404 -1.133607 -0.805134

15C
O -5.456636 0.971902 0.200239
H -6.008463 0.268595 -0.146522
Mg -3.630812 0.696861 0.064486
Cl -2.126472 2.250770 0.830350
Cl -2.851975 -1.251490 -0.895553

TS5A
Mg -2.028499 4.800440 1.379446
C -4.065023 3.625236 2.955905
O -3.572308 3.807364 1.829784
O -4.909261 3.133671 3.579915
H -3.182305 4.365211 3.947509
O -1.444249 5.419644 2.974187
H -0.797410 5.929661 3.468634
H -2.444956 4.839098 3.727416

TS5B
Mg -1.869638 4.894720 1.275266
C -4.057624 3.622593 2.900595
O -3.487744 3.868879 1.860701
O -4.916096 3.119394 3.508278
H -3.182582 4.382298 4.071168
O -1.478085 5.402917 3.020772
H -0.837140 5.909413 3.519110
H -2.473713 4.826969 3.782390
Cl -1.234867 5.040177 -0.822756

TS5C
Mg -1.869195 5.050083 1.219916
C -4.113725 3.587000 2.884385
O -3.558445 3.868820 1.871026
O -4.923472 3.074873 3.560064
H -3.143630 4.451296 4.124817
O -1.535304 5.623737 3.048229
H -0.697741 5.284473 3.379457
H -2.482099 4.940883 3.766338
Cl -0.278271 3.500333 0.586740
Cl -2.835406 6.534139 -0.239006

Structures in Table S5:

4A_CCSD(T)_augccpVTZ
C 0.00000000 0.00000000 -1.64830149
H 0.72585757 0.72585757 -2.01883800
H -0.99153988 0.26568231 -2.01883800
H 0.26568231 -0.99153988 -2.01883800
O 0.00000000 0.00000000 -0.23068994
Mg 0.00000000 0.00000000 1.48265353

4A_B3LYP_augccpVDZ
C -4.208089 -1.712563 -0.938285
H -3.708923 -2.655726 -0.665944
H -3.821721 -1.381819 -1.911875
H -5.288140 -1.898391 -1.012613
O -3.907768 -0.775667 0.089343
Mg -4.142300 0.872463 0.658044

4A_B3LYP_augccpVQZ
C -4.209909 -1.714796 -0.942494
H -3.705283 -2.637382 -0.649501
H -3.826447 -1.400933 -1.912647
H -5.278245 -1.912393 -1.022347
O -3.938031 -0.745869 0.057251
Mg -4.119026 0.859669 0.688408

4A_B3LYP_augccpVTZ
C -4.209368 -1.714999 -0.941729
H -3.707551 -2.642269 -0.655907
H -3.825861 -1.395122 -1.910527
H -5.279447 -1.907135 -1.019165
O -3.927513 -0.756466 0.068263
Mg -4.127201 0.864288 0.677734

4A_B3LYP_ccpVDZ
C -4.208813 -1.711038 -0.938414
H -3.706528 -2.656305 -0.662665
H -3.820329 -1.385271 -1.917029
H -5.291239 -1.903859 -1.015312
O -3.911859 -0.772675 0.085595
Mg -4.138173 0.877444 0.666494

4A_B3LYP_ccpVQZ
C -4.209333 -1.714422 -0.941217
H -3.707372 -2.640587 -0.654327
H -3.826234 -1.397151 -1.910453
H -5.278464 -1.908457 -1.019768
O -3.930447 -0.753525 0.064842
Mg -4.125090 0.862438 0.679592

4A_B3LYP_ccpVTZ
C -4.208679 -1.713774 -0.939922
H -3.709685 -2.645321 -0.661516
H -3.825677 -1.391060 -1.908271
H -5.279478 -1.903508 -1.016975
O -3.920550 -0.764418 0.075723
Mg -4.132872 0.866379 0.669631

4A_M11
C -4.223560 -1.717504 -0.966086
H -3.664931 -2.550991 -0.533798
H -3.819915 -1.495340 -1.956713
H -5.272207 -2.007080 -1.066695
O -4.114382 -0.579003 -0.133362

Mg -3.981947 0.798215 0.875324

4A_MP2
C -4.223810 -1.721899 -0.969146
H -3.666230 -2.548777 -0.535138
H -3.820994 -1.496082 -1.953895
H -5.268988 -2.006709 -1.066450
O -4.114564 -0.580363 -0.134055
Mg -3.982355 0.802127 0.877353

4A_wb97xd
C -4.210326 -1.726457 -0.949058
H -3.647933 -2.547911 -0.504541
H -3.805818 -1.521121 -1.940449
H -5.252224 -2.030609 -1.051967
O -4.116990 -0.580981 -0.140280
Mg -4.004182 0.802915 0.841620

5A_CCSD(T)_augccpVTZ
Mg 0.00000000 0.00000000 1.40429945
C 0.00000000 0.00000000 -1.79105657
H 0.00000000 0.94568889 -2.34074911
H 0.00000000 -0.94568889 -2.34074911
O 0.00000000 0.00000000 -0.56217775
H 0.00000000 0.00000000 3.07366635

5A_B3LYP_augccpVDZ
C -3.897411 -1.925370 -0.870497
H -4.335538 -2.890462 -0.564817
H -3.209676 -1.893420 -1.732357
H -4.981116 2.138437 1.549266
O -4.172279 -0.897675 -0.257868
Mg -4.610283 0.745551 0.720078

5A_B3LYP_augccpVQZ
C -3.899473 -1.917824 -0.865973
H -4.333497 -2.876067 -0.563760
H -3.217327 -1.887262 -1.721362
H -4.976240 2.119159 1.537291
O -4.172700 -0.896190 -0.256690
Mg -4.607066 0.735245 0.714299

5A_B3LYP_augccpVTZ
C -3.898623 -1.921052 -0.867876
H -4.332917 -2.879475 -0.565247
H -3.216220 -1.890045 -1.723527
H -4.978149 2.126149 1.541181
O -4.172319 -0.898149 -0.257896
Mg -4.608075 0.739633 0.717170

5A_B3LYP_ccpVDZ
C -3.896841 -1.927454 -0.871744
H -4.336475 -2.895776 -0.564987
H -3.206746 -1.895424 -1.736484
H -4.982237 2.142850 1.552088
O -4.171998 -0.898787 -0.258637
Mg -4.612006 0.751652 0.723570

5A_B3LYP_ccpVQZ
C -3.898991 -1.919635 -0.867059
H -4.333008 -2.877888 -0.564832
H -3.216836 -1.889123 -1.722455
H -4.977475 2.123765 1.540047
O -4.172186 -0.898069 -0.257845
Mg -4.607807 0.738011 0.715948

5A_B3LYP_ccpVTZ
C -3.898456 -1.921447 -0.868118
H -4.332996 -2.879814 -0.565457
H -3.216068 -1.890570 -1.723860
H -4.978472 2.127248 1.542238
O -4.171902 -0.898556 -0.258177
Mg -4.608409 0.740201 0.717179

5A_M11
C -3.898418 -1.921228 -0.868085
H -4.336843 -2.880632 -0.561113
H -3.213916 -1.887814 -1.726712
H -4.980213 2.129567 1.543446
O -4.169873 -0.899674 -0.259545
Mg -4.607039 0.736842 0.715815

5A_MP2
C -3.896056 -1.930543 -0.873514
H -4.331055 -2.883261 -0.568507
H -3.215912 -1.895071 -1.725616
H -4.981799 2.140179 1.549654
O -4.170728 -0.902930 -0.260557
Mg -4.610754 0.748688 0.722346

5A_wb97xd
C -3.898365 -1.920880 -0.868115
H -4.334345 -2.877429 -0.562654
H -3.215980 -1.891391 -1.723593
H -4.979428 2.126497 1.544322
O -4.169784 -0.899902 -0.262442
Mg -4.608401 0.740166 0.716286

6A_CCSD(T)_ccpVTZ
H 0.00000000 0.00000000 1.53793063
Mg 0.00000000 0.00000000 -0.13317603

6A_B3LYP_augccpVDZ
H 1.383057 0.117105 0.000000
Mg -0.279965 0.158681 0.000000

6A_B3LYP_augccpVQZ
H 1.377860 0.117235 0.000000
Mg -0.274768 0.158551 0.000000

6A_B3LYP_augccpVTZ
H 1.379350 0.117198 0.000000

Mg -0.276258 0.158588 0.000000

6A_B3LYP_ccpVDZ
H 1.383819 0.117086 0.000000
Mg -0.280727 0.158700 0.000000

6A_B3LYP_ccpVQZ
H 1.378703 0.117214 0.000000
Mg -0.275611 0.158572 0.000000

6A_B3LYP_ccpVTZ
H 1.380386 0.117172 0.000000
Mg -0.277294 0.158614 0.000000

6A_M11
H 1.377578 0.117242 0.000000
Mg -0.274486 0.158544 0.000000

6A_MP2
H 1.379350 0.117198 0.000000
Mg -0.276258 0.158588 0.000000

6A_wb97xd
H 1.376141 0.117278 0.000000
Mg -0.273049 0.158508 0.000000

TS2A_CCSD(T)_augccpVTZ
C -0.37759394 1.14380148 0.00000000
H -0.80385767 1.53573667 -0.92644938
H -0.80385767 1.53573667 0.92644938
H -1.56151791 -0.26900965 0.00000000
O 0.75925510 0.54925782 0.00000000
Mg -0.04620868 -1.14632746 0.00000000

TS2A_B3LYP_augccpVDZ
C -4.188377 -1.477496 -0.804022
H -5.062630 -2.144122 -0.754609
H -3.565355 -1.563814 -1.707094
H -5.131753 -0.129738 -1.465806
O -3.691159 -0.978160 0.281806
Mg -4.526428 0.676481 -0.022738

TS2A_B3LYP_augccpVQZ
C -4.187316 -1.475905 -0.801378
H -5.055911 -2.135463 -0.755669
H -3.572465 -1.560480 -1.699357
H -5.129522 -0.130481 -1.462726
O -3.695337 -0.977844 0.275468
Mg -4.525151 0.663326 -0.028801

TS2A_B3LYP_augccpVTZ
C -4.188257 -1.474762 -0.802147
H -5.056991 -2.134801 -0.756060
H -3.572827 -1.559475 -1.700222
H -5.128511 -0.134305 -1.463464
O -3.693377 -0.979630 0.277511
Mg -4.525739 0.666125 -0.028081

TS2A_B3LYP_ccpVDZ
C -4.196108 -1.465047 -0.808604
H -5.068260 -2.141358 -0.760236
H -3.569726 -1.560610 -1.713532
H -5.112737 -0.162143 -1.455698
O -3.692647 -0.973436 0.282298
Mg -4.526224 0.685747 -0.016692

TS2A_B3LYP_ccpVQZ
C -4.187924 -1.474937 -0.801744
H -5.056203 -2.134878 -0.756033
H -3.572971 -1.559983 -1.699584
H -5.128468 -0.133329 -1.462811
O -3.695224 -0.977835 0.275646
Mg -4.524913 0.664114 -0.027937

TS2A_B3LYP_ccpVTZ
C -4.189672 -1.472523 -0.803036
H -5.057286 -2.134176 -0.756801
H -3.573636 -1.559178 -1.700623
H -5.126184 -0.138883 -1.462644
O -3.693859 -0.978283 0.277461
Mg -4.525065 0.666195 -0.026819

TS2A_M11
C -4.165438 -1.508339 -0.786929
H -5.053657 -2.149157 -0.743240
H -3.556175 -1.569425 -1.696072
H -5.167557 -0.063052 -1.482120
O -3.689665 -0.996229 0.272488
Mg -4.533210 0.669354 -0.036590

TS2A_MP2
C -4.169897 -1.502917 -0.790442
H -5.053359 -2.140328 -0.749605
H -3.565801 -1.563704 -1.695891
H -5.155916 -0.086155 -1.477155
O -3.684762 -1.000846 0.278130
Mg -4.535967 0.677103 -0.037500

TS2A_wb97xd
C -4.172669 -1.495947 -0.790412
H -5.052680 -2.141768 -0.748704
H -3.564767 -1.564462 -1.695403
H -5.154510 -0.088805 -1.476662
O -3.691318 -0.991975 0.273536
Mg -4.529757 0.666109 -0.034817

Structures in Table S6 (B3LYP/LANDL2DZ):

BeCl2
Cl -1.155486 -0.858876 -0.759320
Cl 2.487315 -0.605124 -0.609175
Be 0.665914 -0.732001 -0.684248

MgCl2
Cl -1.559553 -0.859940 -0.749755
Cl 2.891382 -0.604062 -0.618740
Mg 0.665914 -0.731999 -0.684246

CaCl2
Cl -1.954661 -0.882644 -0.761376
Cl 3.286490 -0.581356 -0.607118
Ca 0.665914 -0.732000 -0.684247

SrCl2
Cl -2.117703 -0.892037 -0.766194
Cl 3.449532 -0.571964 -0.602300
Sr 0.665914 -0.732000 -0.684247

BaCl2
Cl -2.300405 -0.902543 -0.771573
Cl 3.632233 -0.561458 -0.596921
Ba 0.665914 -0.732000 -0.684247

HCO2-
C -0.287064 0.798371 -0.015416
H 0.382337 0.174227 0.654671
O -0.632619 1.943272 0.471103
O -0.586513 0.254860 -1.147598