

Supporting Information

In the text, the gas acidity ΔG_{acid} of superacid is defined as:

The deprotonation process of the composites could be described as shown in eqn (1):



Correspondingly, the Gibbs free energy change of this process in gas phase, i.e., ΔG_{acid} , is defined by eqn (2):

$$\Delta G_{\text{acid}} = \Delta G_{\text{H}^+} + \Delta G_{\text{A}^-} - \Delta G_{\text{HA}} \quad (2)$$

In principle, the lower the ΔG_{acid} value, the stronger would be the acidity. Generally, a compound could be theoretically characterized as a superacid in gas phase if its ΔG_{acid} is less than 300 kcal mol⁻¹.

Table S1. The gas ΔG_{acid} value of superacid HA (A= MgX₃, Mg₂X₅) and strong acid HX(X=F, Cl, Br) at the level of B3LYP-D3(BJ)/6-311++G(d,p).

	HF	HCl	HBr	HMgF ₃	HMgCl ₃	HMgBr ₃
ΔG_{acid}	362.61	326.53	318.33	288.18	266.73	263.42
	D-HMg ₂ F ₅	D-HMg ₂ Cl ₅	D-HMg ₂ Br ₅	T-HMg ₂ F ₅	T-HMg ₂ Cl ₅	T-HMg ₂ Br ₅
	285.77	261.63	258.93	266.61	246.66	245.12

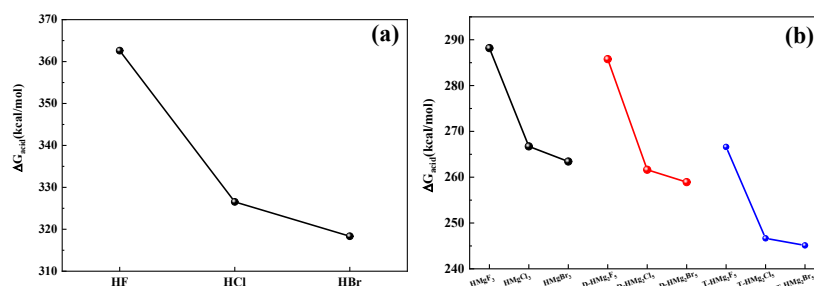


Figure S1. The trend of gas ΔG_{acid} value of superacid HA (A= MgX₃, Mg₂X₅) and strong acid HX(X=F, Cl, Br) with the order of F, Cl, Br.

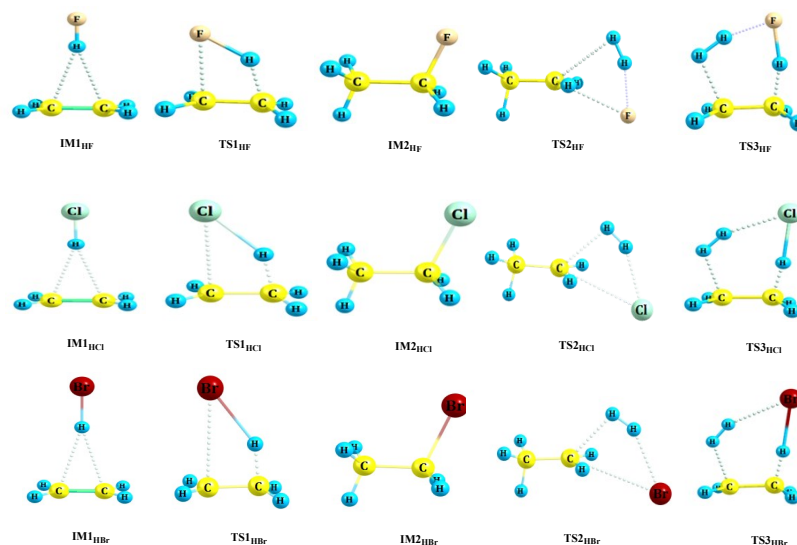


Figure S2. The 3D geometries of important intermediates and transition states in process of strong acid HX(X=F, Cl, Br) catalyzed hydrogenation of ethylene.

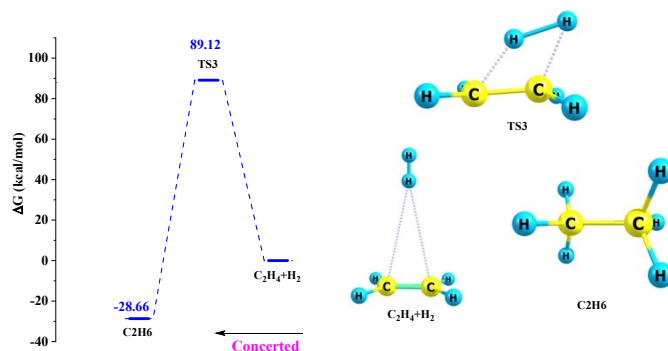
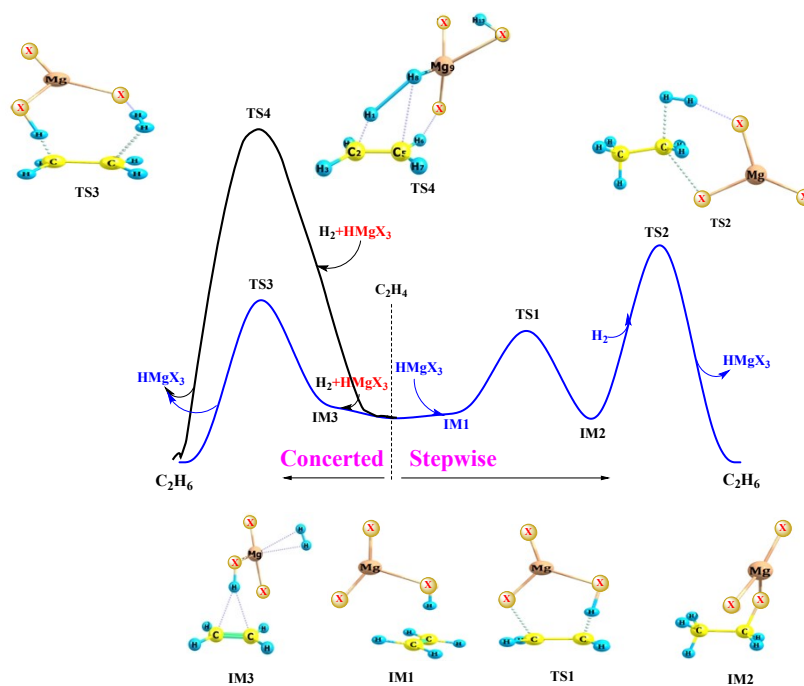


Figure S3. The free energy profile of direct hydrogenation of ethylene without any catalyst.



Scheme S1. The possible pathways of catalytic hydrogenation of ethene by superacid HA ($A = \text{MgX}_3, \text{Mg}_2\text{X}_5$; $X = \text{F}, \text{Cl}, \text{Br}$) including concerted process (left) and stepwise process (right).

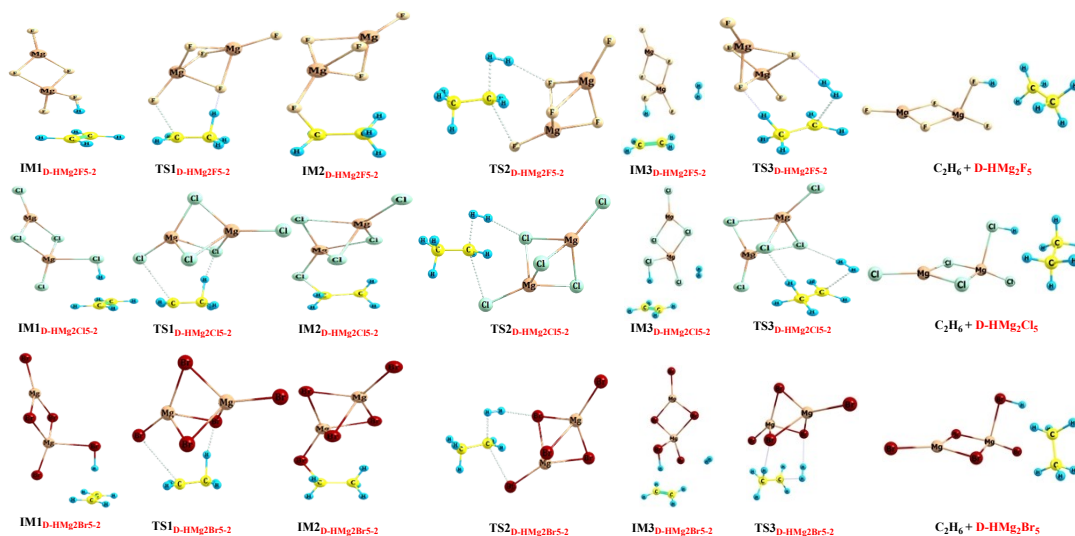


Figure S4. The 3D geometries of important intermediates and transition states in process of superacid $\text{D-HMg}_2\text{X}_5$ ($X = \text{F}, \text{Cl}, \text{Br}$) catalyzed hydrogenation of ethylene along path of $\text{D-HMg}_2\text{X}_5-2$.

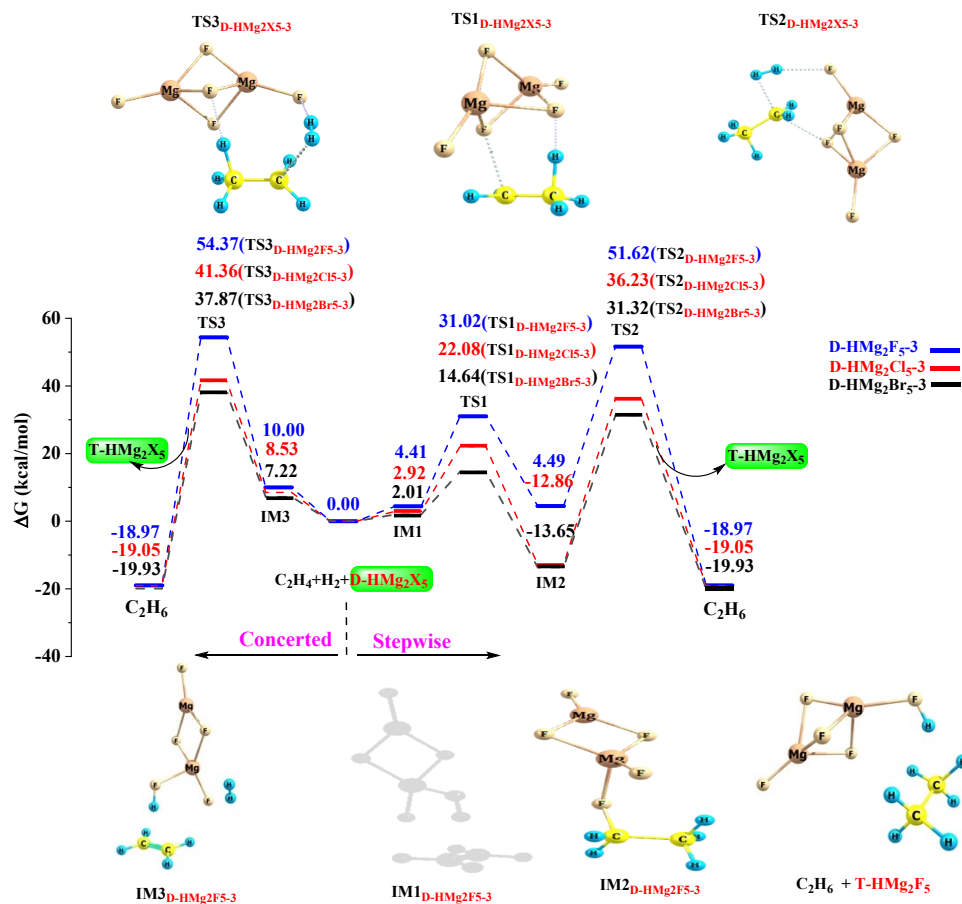


Figure S5. The free energy profile of hydrogenation of ethylene catalyzed by superacid $D\text{-HMg}_2X_5$ ($X=F, Cl, Br$) along path of $D\text{-HMg}_2X_5-3$.

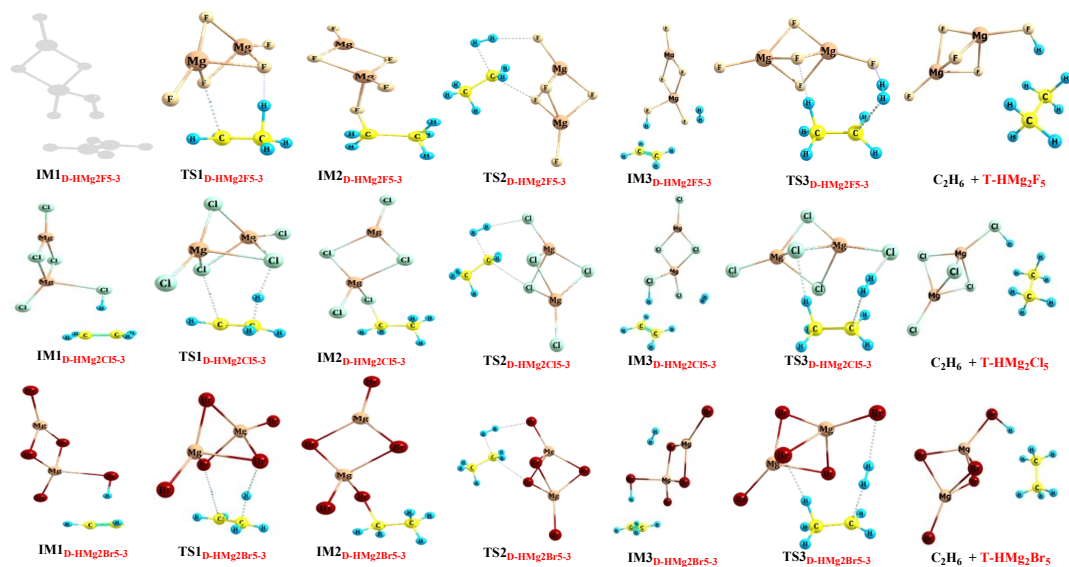


Figure S6. The 3D geometries of important intermediates and transition states in process of superacid $D\text{-HMg}_2X_5$ ($X=F, Cl, Br$) catalyzed hydrogenation of ethylene along path of $D\text{-HMg}_2X_5-3$.

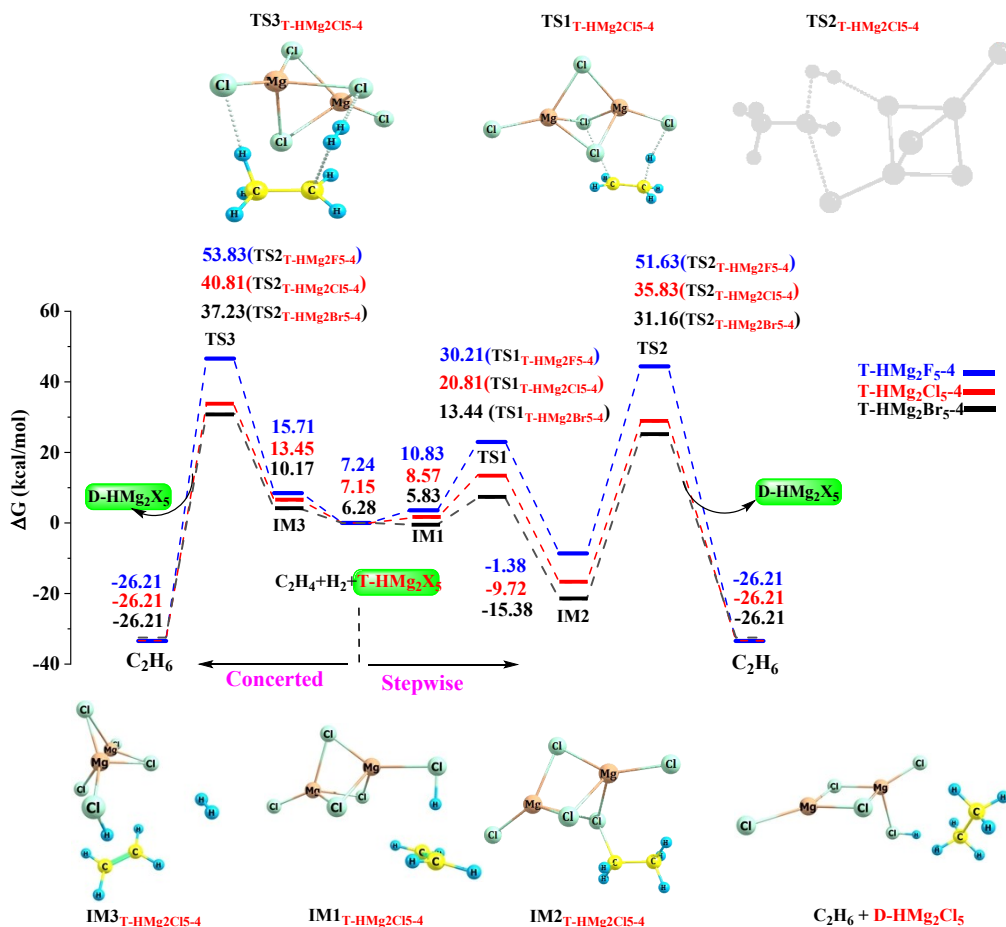


Figure S7. The free energy profile of hydrogenation of ethylene catalyzed by superacid D-HMg₂X₅ (X = F, Cl, Br) along path of T-HMg₂X₅-4.

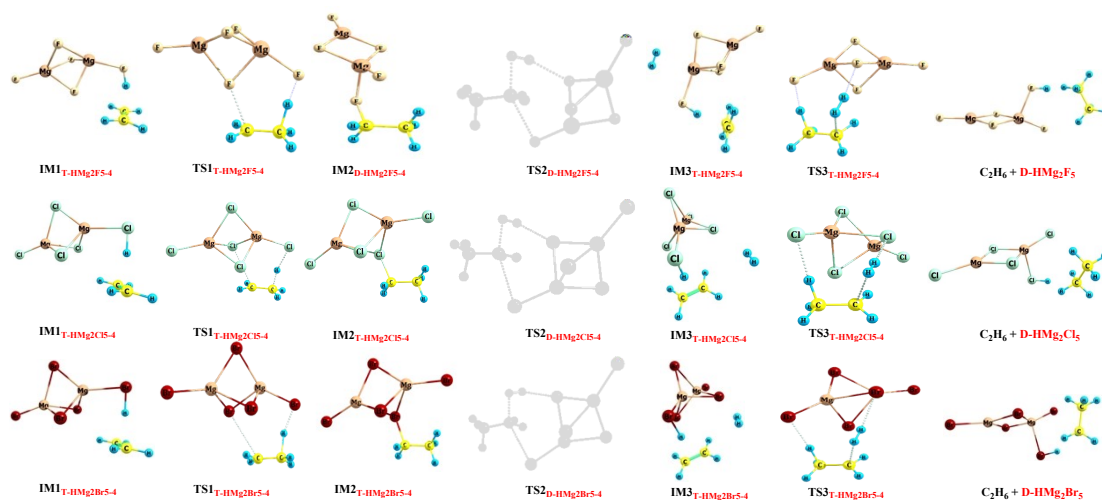


Figure S8. The 3D geometries of important intermediates and transition states in process of superacid HMg₂X₅ (X = F, Cl, Br) catalyzed hydrogenation of ethylene along path of T-HMg₂X₅-4.

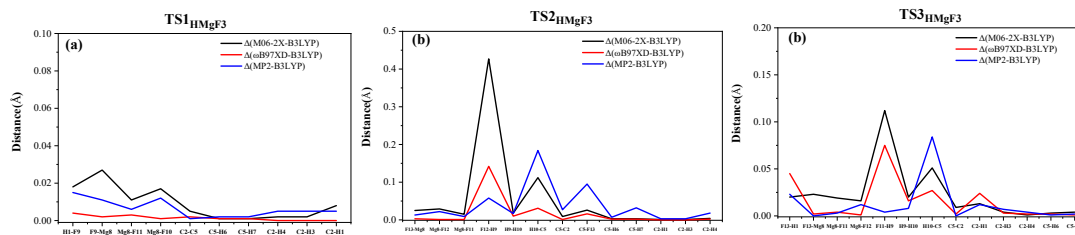


Figure S9. For the reaction catalyzed mono-nuclear superacid HMgF_3 , the distance difference of optimization geometry under various calculated levels including B3LYP/6-311++g(d,p), M06-2X/6-311++g(d,p), $\omega\text{B97XD}/6-311++g(d,p)$ and MP2/ aug-cc-pVTZ. (a) $\text{TS1}_{\text{HMgF}_3}$; (b) $\text{TS2}_{\text{HMgF}_3}$; (c) $\text{TS3}_{\text{HMgF}_3}$.

Table S2. The improved catalytic efficiency by superacid HA (A= MgX_3 , Mg_2X_5) and strong acid HX(X=F, Cl, Br) relative to that of no catalyst, HX and HMgX_3 .

Relative to	Paths	HX	HMgX_3	$\text{D-HMg}_2\text{X}_5-1$	$\text{D-HMg}_2\text{X}_5-2$	$\text{D-HMg}_2\text{X}_5-3$	$\text{T-HMg}_2\text{X}_5-4$
No catalyst	F	16.8%	42.8%	42.9%	38.8%	39.0%	39.6%
	Cl	34.1%	51.5%	52.0%	55.0%	53.6%	54.2%
	Br	41.9%	56.0%	55.4%	59.4%	57.5%	58.2%
HX	F		31.3%	31.5%	26.5%	26.7%	27.4%
	Cl		26.4%	27.2%	31.7%	29.6%	30.5%
	Br		24.3%	23.1%	30.0%	26.8%	28.1%
HMgX_3	F			0.2%	-6.9%	-6.7%	-5.6%
	Cl			1.1%	7.3%	4.4%	5.6%
	Br			-1.5%	7.6%	3.4%	5.0%

Table S3. The comparison of bond length for $\text{IM2}_{\text{HMgF}_3}$ under B3LYP/6-311++g(d,p), M06-2X/6-311++g(d,p), $\omega\text{B97XD}/6-311++g(d,p)$ and MP2/aug-cc-pVTZ levels (Å).

Bond(Å)	B3LYP	M06-2X	ωB97XD	MP2-aug-cc-pVTZ
F13-Mg8	2.027	2.001	2.046	2.036
Mg8-F12	1.807	1.792	1.808	1.797
Mg8-F11	1.79	1.773	1.789	1.778
C2-C5	1.499	1.5	1.498	1.497
C5-F13	1.478	1.454	1.462	1.454
C5-H6	1.088	1.088	1.088	1.084
C5-H7	1.087	1.087	1.088	1.085
C2-H4	1.094	1.092	1.091	1.087
C2-H3	1.091	1.091	1.094	1.088
C2-H1	1.092	1.091	1.092	1.09
H10-H9	0.748	0.745	0.749	0.741

Table S4. The comparison of bond length for $\text{TS1}_{\text{HMgF}_3}$ under B3LYP/6-311++g(d,p), M06-2X/6-311++g(d,p), $\omega\text{B97XD}/6-311++g(d,p)$ and MP2/aug-cc-pVTZ levels (Å).

Bond (Å)	B3LYP	M06-2X	ωB97XD	MP2-aug-cc-pVTZ
H1-F9	1.286	1.268	1.282	1.271
F9-Mg8	1.901	1.874	1.903	1.89
Mg8-F11	1.868	1.857	1.871	1.874
Mg8-F10	1.793	1.776	1.794	1.781
C2-C5	1.39	1.395	1.388	1.391

C5-H6	1.081	1.082	1.082	1.079
C5-H7	1.081	1.082	1.082	1.079
C2-H4	1.088	1.086	1.088	1.083
C2-H3	1.088	1.086	1.088	1.083
C2-H1	1.283	1.291	1.283	1.288

Table S5. The comparison of bond length for $\text{TS2}_{\text{HMgF3}}$ under B3LYP/6-311++g(d,p), M06-2X/6-311++g(d,p), ω B97XD/6-311++g(d,p) and MP2/aug-cc-pVTZ levels (Å).

Bond (Å)	B3LYP	M06-2X	ω B97XD	MP2-aug-cc-pVTZ
F13-Mg8	1.894	1.869	1.897	1.881
Mg8-F12	1.882	1.853	1.881	1.860
Mg8-F11	1.801	1.786	1.802	2.000
F12-H9	1.806	2.233	1.948	1.864
H9-H10	0.800	0.782	0.790	0.783
H10-C5	1.743	1.631	1.712	1.559
C5-C2	1.468	1.477	1.469	1.495
C5-F13	2.274	2.248	2.258	2.179
C5-H6	1.073	1.076	1.075	1.080
C5-H7	1.073	1.076	1.075	1.105
C2-H1	1.089	1.088	1.089	1.086
C2-H3	1.089	1.088	1.089	1.086
C2-H4	1.104	1.1	1.102	1.086

Table S6. The comparison of bond length for $\text{TS3}_{\text{HMgF3}}$ under B3LYP/6-311++g(d,p), M06-2X/6-311++g(d,p), ω B97XD/6-311++g(d,p) and MP2/aug-cc-pVTZ levels (Å).

Bond (Å)	B3LYP	M06-2X	ω B97XD	MP2-aug-cc-pVTZ
F13-H1	1.316	1.336	1.361	1.293
F13-Mg8	1.900	1.877	1.898	1.900
Mg8-F11	1.860	1.841	1.864	1.857
Mg8-F12	1.797	1.781	1.798	1.785
F11-H9	1.553	1.665	1.628	1.557
H9-H10	0.813	0.793	0.797	0.805
H10-C5	1.754	1.703	1.781	1.670
C5-C2	1.400	1.409	1.402	1.400
C2-H1	1.253	1.240	1.229	1.265
C2-H3	1.090	1.086	1.087	1.083
C2-H4	1.088	1.089	1.090	1.084
C5-H6	1.083	1.086	1.085	1.082
C5-H7	1.085	1.089	1.086	1.083

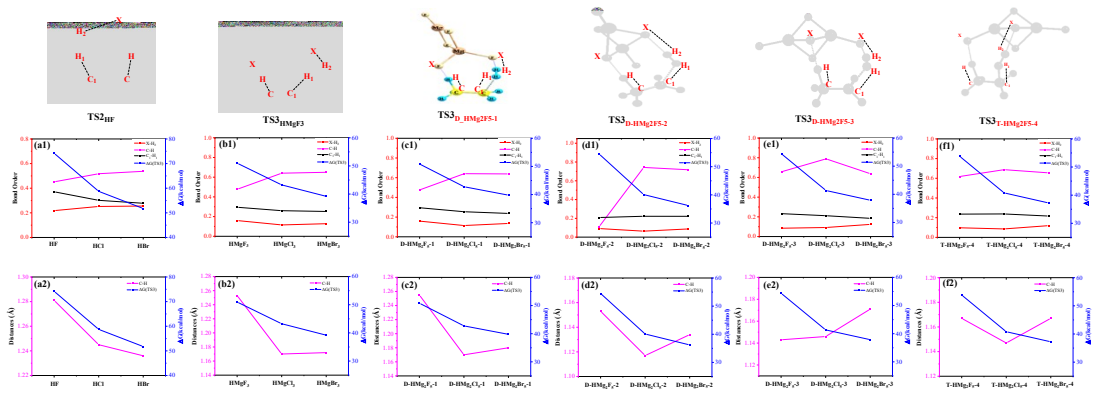


Figure S10. (a1 - f1) The relationship between bond order of partial bonds (X-H₂, C₁-H₁, C-H) and barrier energies for transition state (TS3) along the order of halogen ligands, F, Cl and Br under the same geometries. (a2 - f2) The relationship between distance of partial bond and barrier energies along the order of F, Cl and Br.

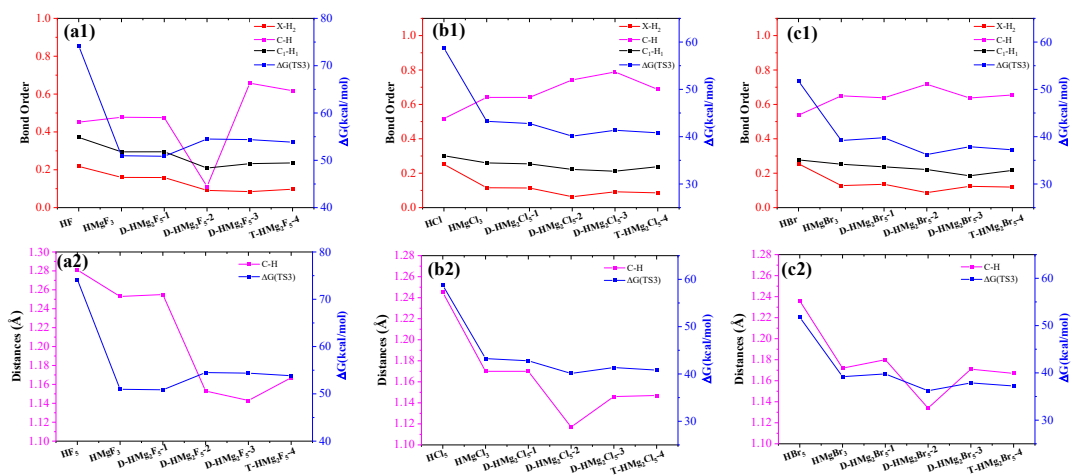


Figure S11. (a1 - c1) The relationship between Bond order of partial bonds (X-H₂, C₁-H₁, C-H) and barrier energies for TS3 with the increase of acid geometry size. (a2 - c2) The relationship between distance of partial bond and barrier energies.

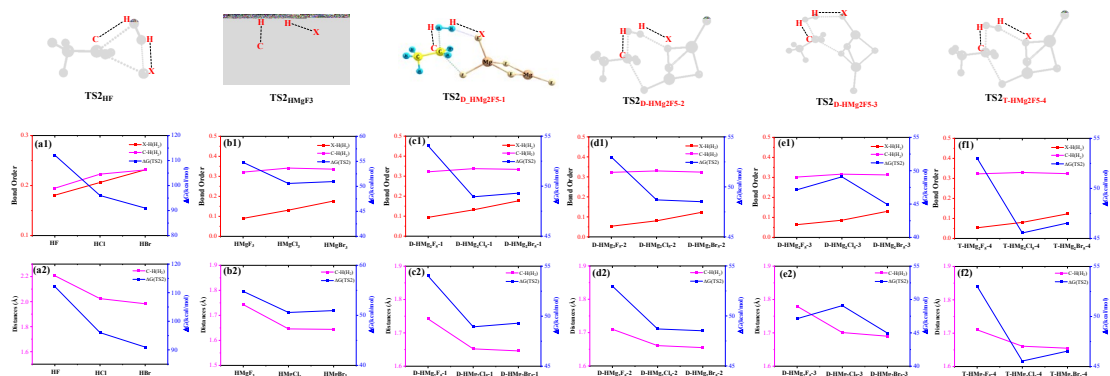


Figure S12. (a1 - f1) The relationship between bond order of partial bonds (X-H, C-H) and barrier energies for transition state (TS2) along the order of halogen ligands, F, Cl and Br under the same geometries. (a2 - f2) The relationship between distance of partial bond and barrier energy along the order of F, Cl and Br.

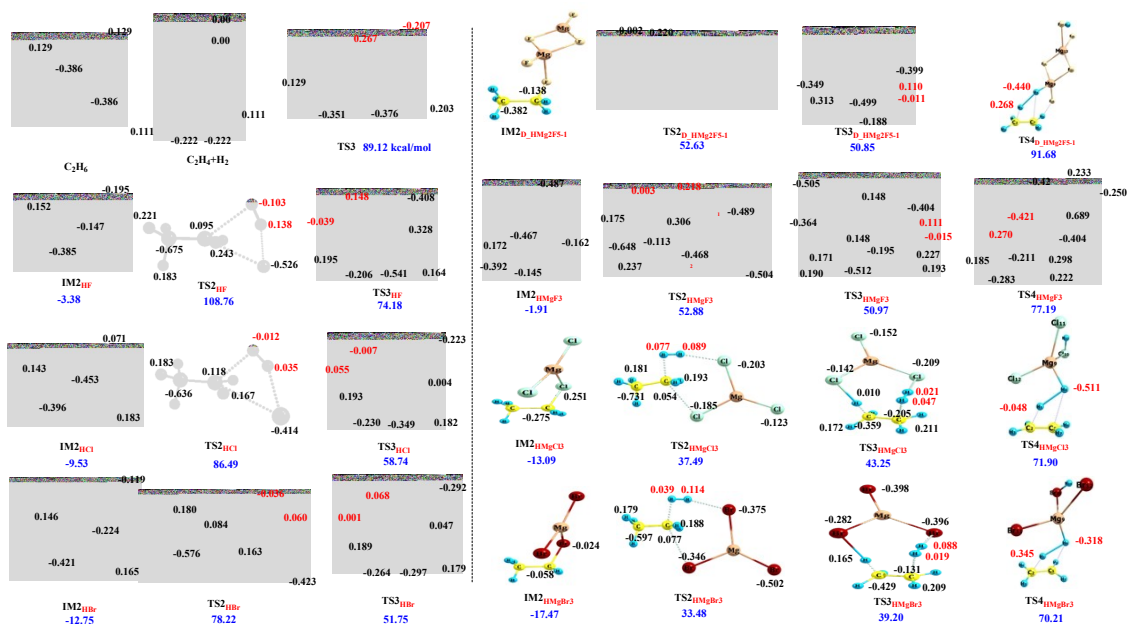


Figure S13. The Mulliken charge distribution in partial transition states and intermediates.

Cartesian Coordinates of the Stationary Points

C₂H₄

C	-0.66452200	0.00000000	0.00009600
H	-1.23480800	-0.92291000	-0.00038500
H	-1.23480400	0.92291300	-0.00038900
C	0.66448800	0.00000000	0.00023900
H	1.23490900	0.92284200	-0.00061600
H	1.23490800	-0.92284400	-0.00062000

C₂H₆

H	-1.16278800	-1.01107000	-0.12408200
C	-0.76507200	0.00000200	0.00000200
H	-1.16288700	0.61295100	-0.81355200
H	-1.16287100	0.39802100	0.93763700
C	0.76507600	0.00000700	0.00000100
H	1.16289300	-0.61336900	0.81323100
H	1.16278300	1.01102000	0.12456500
H	1.16285000	-0.39760900	-0.93781700

TS3

C	0.61319100	0.00006400	-0.18888200
H	1.09151100	0.91196300	-0.52319700
H	1.09184200	-0.91077900	-0.52552100
C	-0.82223400	0.00001200	-0.03324300
H	-1.34624700	-0.93227500	0.11559300
H	-1.34640500	0.93217100	0.11582700
H	0.27915400	-0.00092700	0.99912600
H	1.48440800	-0.00060900	1.15092400

HF

H	0.00000000	0.00000000	-0.83000700
F	0.00000000	0.00000000	0.09222300

HCl

H	0.00000000	0.00000000	-1.21482800
Cl	0.00000000	0.00000000	0.07146000

HBr

H	0.00000000	0.00000000	-1.38754500
Br	0.00000000	0.00000000	0.03964400

IM1_{HF}

H	-0.99364400	0.00058600	-0.00013000
C	1.14402600	-0.66648400	0.00005300
H	1.14986800	-1.23612700	-0.92324100
H	1.14929400	-1.23623400	0.92330700
C	1.14535000	0.66600400	0.00009900
H	1.15176500	1.23562800	0.92339700
H	1.15234500	1.23572400	-0.92316300
F	-1.92732000	0.00036700	-0.00012000

IM2_{HF}

H	1.26919700	-0.85780600	-0.88659700
C	1.19528600	-0.22457600	-0.00003100
H	2.04106000	0.46986700	-0.00135100
H	1.26982600	-0.85612000	0.88797100
C	-0.10278900	0.55027600	0.00001800
H	-0.20463800	1.17555300	0.89039600
H	-0.20508700	1.17589600	-0.89004100
F	-1.19170400	-0.34017700	-0.00003400

TS1_{HF}

H	0.12615300	-0.83064300	0.00063900
C	-1.10939100	-0.41904700	-0.00001300
H	-1.57717300	-0.74059000	0.92373200
H	-1.57599600	-0.74114700	-0.92415900
C	-0.35868400	0.76310200	-0.00005800
H	-0.11114600	1.27847800	-0.91881000

H	-0.11150600	1.27865000	0.91870000
F	1.33979100	-0.25656400	0.00003600

TS2_{HF}

H	-2.38344800	0.18594400	-0.90879200
C	-1.86214900	-0.11788900	-0.00009700
H	-1.86876900	-1.22966900	0.00269400
H	-2.38408400	0.18997700	0.90692800
C	-0.44368600	0.18951400	-0.00006500
H	0.13238900	0.21983400	0.90977900
H	0.13304000	0.21861200	-0.90957100
H	1.02611300	1.83630000	-0.00087400
H	1.51580100	1.17384700	0.00048200
F	1.96266300	-0.33606600	0.00003600

TS3_{HF}

H	0.52839100	0.54726700	0.00088200
C	-0.72781100	0.79963500	-0.00017900
H	-0.86167900	1.36495200	0.91891600
H	-0.86058800	1.36405200	-0.91996900
C	-1.21649800	-0.51964400	0.00019200
H	-1.55706500	-0.99228400	-0.91458200
H	-1.55715700	-0.99195900	0.91509900
H	0.04504700	-1.60299600	-0.00107900
H	0.76629200	-1.14192000	-0.00007800
F	1.68473500	-0.02522900	0.00008200

IM1_{HCl}

H	0.43874600	-0.00156800	-0.00183800
C	-1.87425400	-0.66525900	0.00030900
H	-1.87539200	-1.23507500	0.92343400
H	-1.88280700	-1.23533700	-0.92274600
C	-1.87069300	0.66634500	0.00024000
H	-1.87648200	1.23619400	-0.92285200
H	-1.86908900	1.23653000	0.92331100
Cl	1.73733600	-0.00042700	-0.00015300

IM2_{HCl}

H	1.56808000	-0.99508300	-0.88575900
C	1.61443300	-0.35905000	0.00000300
H	2.57702300	0.16256000	-0.00022700
H	1.56855500	-0.99472500	0.88605300
C	0.49291700	0.65954400	0.00003000
H	0.51033400	1.29015700	0.88694500
H	0.51017200	1.28947800	-0.88745900
Cl	-1.13989800	-0.15031500	0.00001500

IM3_{HCl}

H	0.39654400	-0.23178000	0.00001000
C	-1.95081000	-0.76436500	-0.00020100
H	-1.99845100	-1.33199100	-0.92352800
H	-1.99841900	-1.33261300	0.92274500
C	-1.84751100	0.56316700	0.00024400
H	-1.80531900	1.13192200	0.92298100
H	-1.80535100	1.13254100	-0.92211000
H	0.36345800	3.37789900	-0.00044100
H	0.80852500	2.78064800	-0.00036800
Cl	1.69582000	-0.25408500	0.00002600

TS1_{HCl}

H	-0.34996200	-0.77757700	0.00101100
C	-1.59209500	-0.55631400	-0.00007800
H	-1.96549600	-0.98307800	0.92460800
H	-1.96559800	-0.98280600	-0.92504700
C	-1.15962000	0.77039300	0.00004000
H	-0.97239300	1.30784000	-0.92065300
H	-0.97250500	1.30766300	0.92087300
Cl	1.33742600	-0.06803100	-0.00003300

TS2_{HCl}

H	-3.03787600	0.08677200	-0.90464800
C	-2.50199200	-0.20445900	-0.00002800
H	-2.47382000	-1.31295100	0.00096000
H	-3.03811100	0.08814400	0.90403500
C	-1.10141600	0.20167800	-0.00004200
H	-0.53526200	0.24456300	0.91616200
H	-0.53517800	0.24461700	-0.91619800
H	-0.05717200	1.93539600	0.00004000
H	0.65920100	1.56774900	0.00004800
Cl	1.80227500	-0.16691800	0.00000200

TS3_{HCl}

H	-0.06948600	0.53790700	-0.00040300
C	-1.28838800	0.79081600	0.00015100
H	-1.37505400	1.36909100	0.91754600
H	-1.37527200	1.37008600	-0.91659100
C	-1.88899100	-0.47720100	-0.00025000
H	-2.23374400	-0.93743100	-0.91917700
H	-2.23419900	-0.93746600	0.91847900
H	-0.61129600	-1.62766500	0.00111600
H	0.16119900	-1.36824800	0.00031700
Cl	1.57659600	-0.01693900	-0.00004100

IM1_{HBr}

H	0.24120200	-0.00012900	0.00024600
C	2.60361500	-0.66566500	-0.00001300
H	2.60634300	-1.23563000	-0.92306200
H	2.60669100	-1.23559700	0.92304400
C	2.60365900	0.66565700	-0.00002000
H	2.60677800	1.23562500	0.92303000
H	2.60643000	1.23559100	-0.92307500
Br	-1.19746000	0.00000500	0.00000000

IM2_{HBr}

H	1.99889900	-1.03672700	0.88297100
C	2.08637700	-0.40192400	0.00009100
H	2.00478200	-1.03134900	-0.88783700
H	3.08105800	0.05718000	0.00453000
C	1.03610600	0.68895600	-0.00017500
H	1.08051900	1.31343800	0.88911900
H	1.08160400	1.31504800	-0.88774300
Br	-0.79947900	-0.06685100	-0.00001500

IM3_{HBr}

C	-2.59270800	-0.82900700	-0.00007300
H	-2.60633800	-1.39867200	-0.92322100

H	-2.60632100	-1.39890100	0.92293300
C	-2.56699800	0.50210000	0.00009100
H	-2.55769400	1.07254800	0.92263000
H	-2.55771000	1.07277500	-0.92230800
H	-0.63672200	3.48025800	-0.00015800
H	-0.13368800	2.93101000	-0.00013700
Br	1.20819500	-0.10395700	0.00000400
H	-0.23010900	-0.15908800	0.00000100

TS1_{HBr}

H	-0.88563000	-0.79383300	0.00023300
C	-2.11814700	-0.59686000	-0.00001200
H	-2.47080000	-1.04567700	0.92378900
H	-2.47021700	-1.04582300	-0.92392800
C	-1.81508100	0.76708600	-0.00004200
H	-1.66495500	1.31588100	-0.92136800
H	-1.66560100	1.31604200	0.92130100
Br	0.93590200	-0.02194100	0.00000800

TS2_{HBr}

H	-3.72903300	0.04754900	-0.90256500
C	-3.18483200	-0.23521300	0.00001100
H	-3.13549400	-1.34180100	-0.00016100
H	-3.72894500	0.04730400	0.90271200
C	-1.79570000	0.21942900	-0.00000900
H	-1.23218400	0.27203100	0.91736600
H	-1.23223500	0.27206700	-0.91741200
H	-0.83610000	1.95462200	0.00005900
H	-0.08217700	1.66953700	-0.00002600
Br	1.25312500	-0.08076000	0.00000000

TS3_{HBr}

C	-1.90767500	0.78713800	0.00002700
H	-1.98405300	1.36972300	0.91584300
H	-1.98435900	1.36990200	-0.91565700
C	-2.54433000	-0.46335300	0.00000300
H	-2.88811200	-0.92185300	-0.91986600
H	-2.88815600	-0.92194900	0.91980700
H	-1.24636400	-1.64704700	-0.00022400
H	-0.46852200	-1.44005900	0.00026900
Br	1.11059400	-0.00800100	-0.00000100
H	-0.69919500	0.52860300	-0.00030600

HMgF₃

H	1.66610800	0.26318400	-0.00041000
Mg	-0.37261400	-0.12756100	0.00012300
F	1.24091100	1.16915500	0.00000100
F	-2.13641900	0.09616100	-0.00008300
F	1.20720300	-1.12447800	-0.00003500

HMgCl₃

Cl	-2.43989400	-0.34429800	-0.00008800
Cl	1.81102400	-1.34464700	-0.00019500
Cl	0.69276400	1.95712900	0.00032600
Mg	-0.24591100	-0.49628400	-0.00008300
H	1.86473600	1.39630100	0.00024900

HMgBr₃

Mg	0.15114800	-0.58658600	-0.00000300
H	-1.78614100	1.81178500	0.00001300
Br	2.49905600	-0.70598000	0.00000000
Br	-2.10939700	-1.29213100	0.00000000
Br	-0.39044900	2.14746100	0.00000000

IM1_{HMgF3}

H	1.01303100	-0.88509600	-0.11948500
C	2.77322200	-0.37530600	0.57389600
H	3.37687600	-1.27641400	0.61123200
H	2.39268900	0.00264100	1.51773700
C	2.54276700	0.27775500	-0.57031000
H	1.93653100	1.17840000	-0.58342800
H	2.94888500	-0.08023000	-1.51149700
Mg	-1.33749200	0.20614400	0.02264500
F	0.10065700	-1.22705900	-0.15355600
F	-3.00964200	-0.43084900	0.00618200
F	-0.14813100	1.56593900	0.12428300

IM2_{HMgF3}

H	1.79268700	0.86692400	1.12012200
C	2.37115400	0.02340400	0.74083800
H	2.41947600	-0.77597000	1.48278800
H	3.39049600	0.37217000	0.54810000
C	1.78970800	-0.46319000	-0.55313200
H	1.63686300	0.33439700	-1.27591700
H	2.30492700	-1.31743200	-0.98710000
Mg	-1.17652800	0.21546300	-0.01172300
F	-0.23320800	1.74353700	-0.20931100
F	-2.68845300	-0.69220000	0.29536500
F	0.43374000	-0.98766300	-0.29422700

IM3_{HMgF3}

H	1.06930000	-0.87231400	0.20723600
C	2.83366100	-0.45346000	-0.56300700
H	3.44326400	-1.34856000	-0.49264500
H	2.43938900	-0.20190500	-1.54269200
C	2.61027100	0.33820100	0.49133000
H	1.99583100	1.22853400	0.39709800
H	3.02982700	0.10499700	1.46529800
Mg	-1.28286800	0.19375000	-0.09045900
H	-1.49585100	0.74685700	2.16208600
H	-2.11594800	0.34541200	2.02869300
F	-0.08523200	1.53784100	-0.30703800
F	-2.92280800	-0.51162400	-0.28018500
F	0.15970700	-1.20804700	0.28616700

TS1_{HMgF3}

H	1.20325000	1.03330400	0.00001100
C	2.41058300	0.59843800	0.00001100
H	2.77431100	1.04781900	0.92174100
H	2.77431500	1.04783300	-0.92171100
C	2.22364700	-0.77930800	0.00000000
H	2.23981800	-1.35485000	-0.91520400
H	2.23981300	-1.35486300	0.91519600
Mg	-1.17809500	-0.01740300	-0.00000300
F	-0.00381000	1.47754300	0.00001200
F	-2.96915800	-0.10923100	-0.00001100

F 0.20632900 -1.27111000 -0.00000800

TS2_{HMGf3}

H 3.75224400 -0.20778800 0.90290500
C 3.17925100 -0.41507200 0.00000300
H 2.94143700 -1.49290400 -0.00002600
H 3.75225100 -0.20774200 -0.90288400
C 1.83829200 0.18169200 0.00001300
H 1.28843800 0.27550300 -0.91630900
H 1.28843100 0.27545500 0.91633500
Mg -1.34202600 -0.04280300 -0.00000700
H 1.38663900 1.95380700 0.00005300
H 2.18451800 1.88960800 0.00006000
F -3.11451200 -0.36003000 -0.00000500
F -0.37946800 1.57432900 0.00002100
F 0.09454600 -1.27785800 -0.00003200

TS3_{HMGf3}

H -1.28350400 -0.97839900 -0.02211800
C -2.47954600 -0.82665800 0.31921100
H -2.95879500 -1.63044100 -0.23638000
H -2.36726300 -0.99931600 1.38909400
C -2.85953900 0.47373200 -0.03422200
H -2.79554900 1.29006500 0.67484000
H -3.46627400 0.66627600 -0.91253700
Mg 1.37420000 0.04347300 -0.01464200
H -1.00177100 1.46162100 -0.64552000
H -1.68717500 1.29378700 -1.04847800
F 0.34440000 1.58699800 0.11869500
F 3.13098900 -0.31586600 0.10118500
F -0.01934000 -1.21643400 -0.30134000

IM1_{HMGCl3}

Cl -3.19073300 -0.47953400 -0.00015400
Cl 0.27729600 2.09959400 0.00028900
Cl 0.37624000 -1.60880200 -0.00018200
H 1.57095300 -1.01470800 -0.00008000
C 3.69418500 -0.89419500 0.00024200
H 3.89217200 -1.42912900 -0.92300600
H 3.89188700 -1.42860500 0.92385900
C 3.25962000 0.36803500 -0.00018000
H 3.07324900 0.91251900 0.91829600
H 3.07354000 0.91200100 -0.91902700
Mg -1.17435600 0.41779100 0.00003200

IM2_{HMGCl3}

Cl -2.94255000 -0.59990400 0.21990400
Cl 0.65612400 -1.45458000 -0.32061000
Cl 0.31725500 2.21220100 -0.14408400
H 2.26639300 0.40594600 1.42569900
C 2.88343200 -0.33258000 0.91330900
H 2.97534500 -1.22869100 1.52872800
H 3.88102200 0.09901000 0.78292300
C 2.33094100 -0.64665500 -0.45386700
H 2.15472300 0.24123300 -1.05398400
H 2.91249100 -1.38262600 -1.00329300
Mg -1.00002500 0.42161300 -0.02294200

IM3_{HMGCl3}

Cl 0.52716000 1.97311200 -0.06652000
Cl -3.16225800 -0.28983100 -0.20766600
Cl 0.31178500 -1.71594000 0.06387800
H 1.52377400 -1.15569500 0.01084600
C 3.30442800 -0.29358000 -0.76608600
H 3.77156100 -1.09415400 -1.33055200
H 2.79820600 0.48476000 -1.32686700
C 3.36119600 -0.24993900 0.56713100
H 2.90396000 0.56632600 1.11594500
H 3.87807800 -1.01223700 1.14121300
Mg -1.08172300 0.42808700 0.03810600
H -0.87912800 0.64532600 2.36852000
H -1.51321900 0.24495900 2.33258400

TS1_{HMGCl3}

Cl -3.22230500 0.00093700 -0.00000900
Cl 0.54245000 -1.80537700 -0.00000500
Cl 0.34510200 1.80794900 0.00000700
H 1.85219700 1.03677900 0.00000900
C 3.11168700 0.72925600 0.00001300
H 3.39047700 1.23188900 0.92334600
H 3.39048300 1.23189600 -0.92331500
C 3.06914300 -0.64835000 0.00000700
H 3.06857900 -1.21963100 -0.91879200
H 3.06857300 -1.21963700 0.91880200
Mg -1.01370800 -0.13386600 -0.00000400

TS2_{HMGCl3}

Cl -3.28823900 -0.35758400 -0.00003400
Cl 0.54161000 -1.70008100 0.00004500
Cl 0.01163900 2.03903200 0.00000900
H 4.41679200 -0.24215100 0.89968300
C 3.84216500 -0.46034500 -0.00009600
H 3.62680500 -1.53807200 -0.00011600
H 4.41663500 -0.24208900 -0.89996100
C 2.50901400 0.17902200 0.00004000
H 1.94838000 0.27180400 -0.91418500
H 1.94854500 0.27175000 0.91437700
Mg -1.09477200 -0.02082300 0.00000600
H 2.19545200 1.97488600 0.00009200
H 2.97240800 1.75844500 0.00004600

TS3_{HMGCl3}

Cl -0.35707100 1.86217000 -0.06302200
Cl 3.29690800 -0.03786400 0.16706300
Cl -0.30971900 -1.79772900 -0.27668600
H -1.95095400 -0.99826000 0.40770300
C -2.94400900 -0.54902500 0.83243000
H -3.56385700 -1.43535500 0.96589800
H -2.61082900 -0.07599500 1.75537800
C -3.41797000 0.36072000 -0.14386100
H -3.21563400 1.42194500 -0.06230600
H -4.16451100 0.06517800 -0.87482800
Mg 1.08976900 0.06918000 -0.04036800
H -1.77560600 0.66202700 -1.29803800
H -2.33597300 0.20830800 -1.60584700

IM1_{HMgBr3}

H	-1.93411200	-1.29458600	-0.00016100
C	-4.09191600	-1.32946100	0.00110200
H	-4.23887700	-1.87958100	0.92488400
H	-4.24007600	-1.88057100	-0.92192100
C	-3.77737700	-0.03223500	0.00025400
H	-3.64307800	0.52575100	-0.91920200
H	-3.64185500	0.52671200	0.91897300
Mg	0.79407800	0.52359700	-0.00000900
Br	-0.55906000	-1.82454500	-0.00041500
Br	3.04282400	-0.18693400	0.00027200
Br	-0.90134100	2.17974500	-0.00015900

IM2_{HMgBr3}

H	2.60146600	-0.05562100	1.58315500
C	3.14820500	-0.85772300	1.08714800
H	3.11863200	-1.75770300	1.70281100
H	4.19250700	-0.54012600	0.99406100
C	2.61477900	-1.10439900	-0.30112800
H	2.55660000	-0.20330800	-0.90438300
H	3.11890900	-1.90591100	-0.83456200
Mg	-0.67189600	0.52869900	-0.02816700
Br	1.01293000	2.20369600	-0.10608600
Br	-2.91919000	-0.16806700	0.14752000
Br	0.70331000	-1.75302800	-0.23912600

IM3_{HMgBr3}

H	1.84583900	-1.41404300	-0.01987900
C	3.71605200	-0.64672100	-0.78223100
H	4.12831000	-1.46563900	-1.36272400
H	3.26171100	0.17305400	-1.32820500
C	3.77702700	-0.63158500	0.55126100
H	3.37491100	0.20209500	1.11684000
H	4.24219100	-1.43690100	1.11042200
Mg	-0.73163100	0.52124900	0.09933200
H	-0.42706600	0.65400700	2.47154400
H	-1.10151700	0.32547500	2.45218900
Br	-3.03044300	0.00297000	-0.11333300
Br	1.10054800	2.03829200	-0.03563400
Br	0.45837200	-1.91621100	0.02764300

TS1_{HMgBr3}

H	-2.22750000	-1.17426600	0.00019900
C	-3.55394800	-0.93956400	0.00021200
H	-3.77879800	-1.46746100	0.92346100
H	-3.77885600	-1.46770100	-0.92288600
C	-3.59016900	0.43141600	0.00003400
H	-3.60455600	1.00184900	-0.91934500
H	-3.60450100	1.00208900	0.91926500
Mg	0.71320400	0.22737000	-0.00004800
Br	-0.62516600	-1.94180100	0.00026900
Br	3.06868700	0.05059800	-0.00007900
Br	-0.97779300	1.96051500	-0.00023600

TS2_{HMgBr3}

H	4.88441000	-0.23568500	0.89832600
C	4.31575300	-0.47643100	0.00005200
H	4.14682000	-1.56063200	-0.00000200

H	4.88444700	-0.23560100	-0.89817500
C	2.97128600	0.14583000	0.00005300
H	2.41447000	0.25187100	-0.91531700
H	2.41443400	0.25179800	0.91540900
Mg	-0.73054100	-0.02140700	-0.00001200
H	2.61664200	2.02253900	0.00010200
H	3.38068000	1.73763800	0.00014000
Br	-3.07426700	-0.35652700	-0.00004800
Br	0.97220500	-1.85443700	-0.00006800
Br	0.39641600	2.21120900	0.00008800

TS3_{HMgBr3}

H	-2.41564500	-1.05305500	0.54359600
C	-3.39978000	-0.58970600	0.97877500
H	-3.99955300	-1.47832900	1.17522400
H	-3.04727900	-0.07087600	1.86889400
C	-3.91877200	0.26203100	-0.02658700
H	-3.74370000	1.33057100	0.00050300
H	-4.66269300	-0.09015400	-0.73464700
Mg	0.75244400	0.09108300	-0.04032800
H	-2.24983000	0.56927400	-1.23322800
H	-2.81899700	0.08511000	-1.47218400
Br	3.11306400	-0.01681400	0.12851300
Br	-0.77274100	2.01617600	-0.08974300
Br	-0.68833200	-1.95420500	-0.19240800

D-HMg₂F₅

H	3.01765800	-0.00002800	0.40360000
Mg	-1.86682500	-0.00000100	0.00061700
Mg	1.04120400	0.00001300	-0.17831600
F	-3.64417200	-0.00000900	0.11921800
F	2.51620800	-0.00008600	1.27523100
F	-0.41279500	1.25034500	-0.09711900
F	-0.41279200	-1.25033100	-0.09726600
F	2.71908300	0.00006700	-1.00797700

D-HMg₂Cl₅

H	-3.32737200	0.02328000	-1.08904300
Cl	-2.34235200	0.04185200	-1.95780600
Cl	-3.23449200	-0.02783900	1.30294500
Mg	-1.18915100	-0.00823600	0.38571600
Mg	2.06795500	-0.00220900	0.10189700
Cl	4.24767400	0.00328200	-0.15258400
Cl	0.45228800	1.71029600	0.30024600
Cl	0.45227700	-1.72158600	0.22706100

D-HMg₂Br₅

H	-3.43484200	-0.00000100	0.89724900
Mg	-1.17620400	0.00000000	-0.37180200
Mg	2.19310200	0.00000000	-0.12288400
Br	4.52516800	0.00000000	0.11288900
Br	0.52186100	1.87616200	-0.26177000
Br	0.52186100	-1.87616200	-0.26177400
Br	-2.51096500	-0.00000200	2.04124200
Br	-3.30843700	0.00000100	-1.48661700

T-HMg₂F₅

H	1.03182500	1.53083200	-0.00001700
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Mg	-1.18726300	-0.00671500	-0.00000400
Mg	1.46138600	-0.81713200	0.00000900
F	0.08823100	-0.86160400	1.27522600
F	-2.97130800	0.14109200	0.00000100
F	0.08823000	-0.86163500	-1.27521500
F	0.04046500	1.67079900	-0.00000700
F	2.27423600	0.83972000	-0.00000900

T-HMg₂Cl₅

Cl	-3.69461600	0.47232100	-0.00046500
Cl	0.36485900	1.77528100	0.03104800
H	3.23012600	1.47677000	0.00977100
Mg	-1.52743800	0.06005000	-0.00084100
Mg	1.22343700	-0.41582000	0.00067700
Cl	3.64992000	0.24551900	-0.00102000
Cl	-0.14281500	-1.13819000	-1.73419500
Cl	-0.15276700	-1.19066800	1.70417500

T-HMg₂Br₅

H	3.52583600	1.54014900	-0.00097700
Mg	-1.59184300	0.03641900	0.00001000
Mg	1.25096600	-0.33128800	-0.00084700
Br	-3.92353900	0.37152900	0.00120200
Br	0.29937900	1.98285600	0.00461000
Br	-0.12101400	-1.22732900	1.86047300
Br	-0.12114700	-1.21801800	-1.86669300
Br	3.88245500	0.14805500	0.00072200

IM1_D-HMg₂F₅-1

H	-2.24177600	-0.97121700	0.29050600
C	-4.05499600	-0.91591700	-0.43320500
H	-4.48971900	-1.89918200	-0.28443600
H	-3.74278700	-0.66320000	-1.44186100
H	-3.51162900	0.95135700	0.39052100
H	-4.29091600	-0.26784100	1.56422000
Mg	-0.17529800	0.54254300	-0.10175800
Mg	2.65748900	-0.13102200	0.01165100
C	-3.95006300	-0.02773400	0.56162200
F	-1.27855800	-1.11244500	0.35426200
F	-1.57172600	1.66118300	-0.37146200
F	1.28985300	0.53476100	1.16727100
F	1.23561300	-0.10408200	-1.26373300
F	4.38269500	-0.58233400	0.09053200

IM2_D-HMg₂F₅-1

H	3.13737100	0.02053400	1.28165100
C	3.46741500	-0.84165800	0.70054800
H	3.18133400	-1.77160300	1.19547600
H	4.55961800	-0.80966800	0.63723200
H	3.10125200	0.18749200	-1.17461600
H	3.18629400	-1.60722200	-1.33076800
Mg	0.30817400	0.69259500	0.02645500
Mg	-2.47744500	-0.15980600	0.05452900
C	2.91584500	-0.76907200	-0.69221600
F	1.67217400	1.84640200	0.29286100
F	1.44331500	-0.86285800	-0.62259700
F	-0.97269500	-0.13092000	1.22913700
F	-1.24399000	0.68257000	-1.13551100

F	-4.16927000	-0.72948500	0.05491400
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IM3_D-HMg₂F₅-1

H	-2.20141600	-0.81812300	-0.65173400
C	-3.95712300	-1.21638100	0.11863700
H	-4.37448600	-2.04249900	-0.44813600
H	-3.57605200	-1.44354500	1.10959800
C	-3.95186400	0.03603500	-0.35113800
H	-3.52780200	0.84986600	0.23031100
H	-4.36051400	0.26774600	-1.33009400
H	-1.35620400	2.34746700	-1.27739000
H	-0.87023500	2.24072800	-1.83471900
Mg	-0.15624600	0.48597700	0.27098200
Mg	2.67309300	-0.17458000	-0.01170300
F	4.39420700	-0.60160800	-0.21904700
F	1.36855800	0.94940000	-0.83765500
F	1.19964100	-0.62554800	1.11091300
F	-1.24261500	-0.85328800	-0.82286300
F	-1.55107100	1.34700800	1.04485300

TS1_D-HMg₂F₅-1

H	2.63561500	1.02816100	-0.00030300
C	3.83109700	0.55644700	-0.00038100
H	4.20426900	0.99786100	0.92151900
H	4.20409300	0.99772600	-0.92241700
H	3.62746500	-1.39321800	-0.91557900
H	3.62764300	-1.39308500	0.91514100
Mg	0.26449000	0.01709800	-0.00001400
Mg	-2.64710800	-0.02235800	0.00022300
C	3.61976800	-0.81782700	-0.00026000
F	1.44530100	1.50750600	-0.00022500
F	1.59662000	-1.29061200	-0.00002700
F	-1.21597900	-0.00548700	1.26052500
F	-1.21618200	-0.00567700	-1.26031100
F	-4.43341000	-0.05084500	0.00036900

TS2_D-HMg₂F₅-1

H	5.12885200	-0.51729700	0.90270700
C	4.53853700	-0.66949400	-0.00001200
H	4.19853600	-1.71921000	0.00004000
H	5.12883700	-0.51738200	-0.90275600
C	3.26206700	0.05594600	-0.00003600
H	2.72833200	0.20614900	-0.91857300
H	2.72834700	0.20623600	0.91849600
H	2.97869700	1.87183900	-0.00011800
H	3.76763100	1.72317900	-0.00012000
Mg	0.12938900	0.14566900	-0.00001100
Mg	-2.76822600	-0.10464200	0.00003600
F	-4.55009200	-0.26330200	0.00006600
F	-1.35415100	0.01842400	1.26620600
F	-1.35418200	0.01830100	-1.26617900
F	1.20270100	1.69105700	-0.00010100
F	1.41163500	-1.24943000	0.00004200

TS3_D-HMg₂F₅-1

H	-2.59233800	-1.04832000	-0.25747900
C	-3.77675200	-1.10563100	0.15258000
H	-4.20833100	-1.81591900	-0.54997700

H	-3.58015500	-1.49477400	1.15115700	Mg	0.51994800	0.52280900	-0.14603000
C	-4.30492000	0.19049300	0.11569900	Mg	-2.71939600	-0.01345300	-0.04272700
H	-4.27430000	0.83382600	0.98658100	Cl	-4.87719900	-0.42062700	0.05937600
H	-4.98531300	0.50176100	-0.66961300	Cl	-1.09341700	-0.30434500	-1.71925000
H	-2.61100900	1.51183100	-0.32821600	Cl	-1.16661800	0.80990800	1.52841100
H	-3.28750700	1.33091600	-0.74192000				
Mg	-0.11156200	0.27176600	-0.04575400	TS1_{D-HMg2Cl5-1}			
Mg	2.77304200	-0.10509600	0.03453900	Cl	-2.16104500	-1.82322700	0.00023200
F	4.54287700	-0.35408500	0.07997000	Cl	-1.82101200	1.84344300	-0.00000600
F	1.45145900	0.53439100	-1.17867800	H	-3.34815900	1.12497000	-0.00039600
F	1.27091900	-0.35997900	1.17708800	C	-4.62382200	0.86584600	-0.00074600
F	-1.32935300	-1.07069500	-0.61870500	H	-4.87832400	1.38028800	-0.92454200
F	-1.25910000	1.65830800	0.42192000	H	-4.87885500	1.38047700	0.92279900
				C	-4.63495300	-0.51130000	-0.00060600
IM1_{D-HMg2Cl5-1}				H	-4.65272200	-1.08234300	0.91824100
Cl	-2.20980700	2.07111100	0.03054300	H	-4.65220200	-1.08253500	-0.91934400
Cl	-1.64446500	-1.64429800	-0.16762900	Mg	-0.58243400	-0.17816500	0.00015300
H	-2.92424000	-1.26010300	-0.06154000	Mg	2.69149700	-0.01860500	0.00008800
C	-4.99077500	-1.50313700	0.07983700	Cl	4.88832100	0.13047800	0.00003400
H	-5.03508700	-2.08276700	0.99630900	Cl	1.09549700	-0.11922300	-1.72348500
H	-5.15199800	-2.04458600	-0.84683100	Cl	1.09554300	-0.11893500	1.72372300
C	-4.78470200	-0.18367800	0.09420900				
H	-4.75280000	0.40393300	-0.81603400	TS2_{D-HMg2Cl5-1}			
H	-4.63660600	0.36590100	1.01649100	H	5.98721200	-0.59737900	0.90033900
Mg	-0.51223400	0.63521000	-0.02076200	C	5.39631300	-0.76409600	-0.00008400
Mg	2.69964800	-0.04571700	0.02581900	H	5.09068000	-1.82054400	-0.00016600
Cl	4.83906800	-0.54923000	0.04906800	H	5.98719200	-0.59723300	-0.90049300
Cl	1.08385800	0.21615800	1.71915000	C	4.12084400	-0.01692600	-0.00000900
Cl	1.16102900	0.35711700	-1.71309500	H	3.57098200	0.12462300	-0.91556000
				H	3.57100200	0.12447400	0.91557600
IM2_{D-HMg2Cl5-1}				H	3.98085000	1.81199700	0.00015000
Cl	-1.73536100	-0.96273200	1.41472800	H	4.72568400	1.52618000	0.00010700
Cl	-2.48319400	1.88602100	-0.86086600	Cl	1.76819100	2.09551700	0.00021700
H	-2.77219400	-1.25211000	-1.41941300	Cl	1.95698500	-1.72128500	-0.00012000
C	-3.31015400	-1.86924200	-0.69860400	Mg	0.49986800	0.12704400	0.00003100
H	-2.82553100	-2.84320800	-0.61961400	Mg	-2.79678600	-0.07446700	-0.00002700
H	-4.32430800	-2.01731000	-1.08341600	Cl	-4.99936400	-0.21400900	-0.00006500
C	-3.41966200	-1.18575700	0.64096600	Cl	-1.19975400	0.02248600	-1.72636100
H	-3.81128700	-0.17443800	0.57526900	Cl	-1.19979500	0.02217900	1.72636300
H	-3.95270600	-1.76823400	1.38792800				
Mg	-0.71198500	0.76808500	-0.10544900	TS3_{D-HMg2Cl5-1}			
Mg	2.46306400	-0.04306700	-0.11676400	Cl	1.91374900	1.84492700	-0.64938800
Cl	4.57476400	-0.64829800	-0.03790100	Cl	1.86165900	-1.51585800	1.01606900
Cl	0.66472200	-0.60259000	-1.52533900	H	3.53059000	-1.17026800	0.05785600
Cl	1.15859800	1.36789800	1.25476900	C	4.53875400	-1.05493100	-0.53479500
				H	5.11877900	-1.90903000	-0.18673900
IM3_{D-HMg2Cl5-1}				H	4.19299400	-1.12668700	-1.56637600
Cl	2.25970700	1.82400700	-0.65031700	C	5.07316200	0.20928600	-0.19203100
Cl	1.58726500	-1.65514600	0.60833000	H	4.86738000	1.08571400	-0.79580700
H	2.85730300	-1.28736600	0.36076000	H	5.85324500	0.31220000	0.55602700
C	4.63643600	-0.93125900	-0.65955800	H	3.48855900	1.19958900	0.78439300
H	4.96877800	-1.91752700	-0.96720200	H	4.07543600	0.89863200	1.20171700
H	4.20629900	-0.28737700	-1.41921000	Mg	0.50409700	0.17506500	0.09740500
C	4.76660800	-0.50821800	0.60084300	Mg	-2.79138900	-0.04632400	-0.06166400
H	4.44510700	0.48675900	0.88832300	Cl	-4.99082500	-0.19912500	-0.16580900
H	5.21075500	-1.13276200	1.36926500	Cl	-1.07399200	-0.68258400	-1.53932800
H	2.24525300	1.39709900	2.40040300	Cl	-1.31947100	0.80198300	1.56674900
H	1.97606800	0.95123000	2.93369900				

IM1_{D-HMg2Br5-1}			
H	-3.13600900	-1.60551000	-0.40413500
C	-4.92463800	-2.27201900	0.49002800
H	-4.51823000	-3.03104600	1.15054300
H	-5.40438600	-2.62304100	-0.41792300
H	-5.28728500	-0.21093200	0.14937700
H	-4.40889900	-0.61736300	1.71091100
Mg	-0.87899800	0.61389800	-0.01055500
Mg	2.46425100	0.03573200	0.14707200
Br	1.02450800	1.02607500	-1.65938200
Br	4.76417000	-0.43196700	0.19982300
Br	-1.86695900	-1.63347300	-1.16383300
Br	0.63372500	-0.36051400	1.81152800
Br	-2.76933500	1.96462400	0.48168100
C	-4.87235900	-0.97360600	0.79821600

IM2_{D-HMg2Br5-1}			
H	2.93666400	-1.51666300	1.55611800
C	3.50413000	-2.19353400	0.91655600
H	3.00530800	-3.16268900	0.88068900
H	4.48953900	-2.32978500	1.37519200
H	4.11953900	-0.60418900	-0.44473700
H	4.27076500	-2.25705700	-1.13241000
Mg	0.97626800	0.60053500	0.08064300
Mg	-2.37596900	0.06761900	0.13935000
Br	-0.91751800	1.36253600	-1.44694300
Br	-4.68240000	-0.36941800	0.09474000
Br	2.90779900	1.75262800	0.86138600
Br	-0.55998300	-0.65922300	1.70344700
Br	1.95684400	-1.38123500	-1.43049800
C	3.71397900	-1.61188100	-0.45812600

IM3_{D-HMg2Br5-1}			
H	-3.31730600	1.51571600	-0.05132900
C	-5.15950100	0.82048000	-0.80133500
H	-5.54019300	1.65535800	-1.38072100
H	-4.74481400	-0.01996200	-1.34751600
C	-5.21209200	0.81018300	0.53344100
H	-4.84176800	-0.03838500	1.09788900
H	-5.63797300	1.63588800	1.09417700
H	-2.69122100	-0.41425800	2.77493000
H	-2.50661600	0.19691800	3.15952100
Mg	-0.83972700	-0.45934100	-0.01162900
Mg	2.54042500	-0.08075900	-0.01035300
Br	4.86935000	0.21782600	-0.00568000
Br	0.88416800	-0.23048700	-1.88736600
Br	0.88289700	-0.26357400	1.86384500
Br	-1.91879800	2.01695800	-0.00297800
Br	-2.68615700	-1.96455300	-0.06713000

TS1_{D-HMg2Br5-1}			
H	-3.73104600	1.27330500	0.00011400
C	-5.07680300	1.07298300	0.00033500
H	-5.28235000	1.60786800	-0.92322100
H	-5.28205300	1.60784900	0.92396900
H	-5.16072800	-0.86582700	0.91953500
H	-5.16101800	-0.86580600	-0.91887800
Mg	-0.87509500	-0.22104700	-0.00007400

Mg	2.51648500	-0.04984900	0.00003300
Br	0.86527200	-0.14432200	1.88105200
Br	4.86247900	0.10774400	0.00010400
Br	-2.12613400	2.00675900	-0.00014100
Br	0.86538900	-0.14435300	-1.88108700
Br	-2.57506200	-1.94505900	-0.00007100
C	-5.13944500	-0.29523500	0.00033100

TS2_{D-HMg2Br5-1}			
H	6.35564500	-0.70587500	0.89840400
C	5.76581400	-0.88879200	0.00012000
H	5.48954300	-1.95050000	0.00004000
H	6.35574300	-0.70576500	-0.89807800
C	4.49124400	-0.13334300	0.00009600
H	3.95023500	0.03245500	-0.91604900
H	3.95014400	0.03235600	0.91620400
H	4.34024500	1.77966400	0.00017600
H	5.06629200	1.40946000	0.00021400
Mg	0.85196500	0.09074600	-0.00003300
Mg	-2.53639100	-0.05119900	0.00001300
Br	-4.88725500	-0.15777900	0.00004500
Br	-0.89253000	0.01884300	1.88563300
Br	-0.89258700	0.01898600	-1.88565000
Br	2.15817300	2.22277400	0.00003100
Br	2.31885400	-1.93806800	-0.00011600

TS3_{D-HMg2Br5-1}			
H	4.00443300	-1.30579700	-0.34494300
C	5.01079000	-1.07670400	-0.91786400
H	5.56623400	-2.00557800	-0.79251500
H	4.64842600	-0.89897900	-1.93033100
C	5.58588200	0.05467800	-0.29518500
H	5.39770400	1.05510300	-0.66665600
H	6.36408800	-0.04358200	0.45506200
H	3.97864200	0.86556300	0.94028900
H	4.56506700	0.42448900	1.20772900
Mg	0.84747700	0.15135500	0.10154300
Mg	-2.58222800	-0.01296700	-0.05584700
Br	-4.93572700	-0.13534600	-0.16311100
Br	-0.82923200	-0.27812000	-1.83369200
Br	-1.02817200	0.41133200	1.86950300
Br	2.24289700	-1.90268300	0.58469000
Br	2.34201700	2.08711100	-0.23278100

IM1_{D-HMg2F5-2}			
H	-2.24161000	-0.97222800	-0.28742700
C	-4.05618800	-0.91582000	0.43262100
H	-3.74589700	-0.66257900	1.44170900
H	-4.49090600	-1.89903000	0.28362300
C	-3.94910800	-0.02838900	-0.56261800
H	-4.28802400	-0.26906200	-1.56570800
H	-3.51064800	0.95065400	-0.39142100
Mg	-0.17524600	0.54298100	0.10176600
Mg	2.65742300	-0.13112900	-0.01189500
F	4.38249900	-0.58293900	-0.09087500
F	1.23628600	-0.10135400	1.26426200
F	-1.27832900	-1.11320700	-0.35041800
F	1.28922700	0.53258300	-1.16806000

F -1.57160000 1.66216900 0.36961800

IM2_{D-HMg2F5-2}

H 1.75394100 1.73575000 -0.06928300
C 2.76292700 1.45984300 0.24450000
H 2.81874500 1.39594400 1.33270000
H 3.44844000 2.24824100 -0.08337700
C 3.20122500 0.18315900 -0.40372100
H 3.09375700 0.17033800 -1.48585400
H 4.17630000 -0.18201400 -0.09257900
Mg 0.32555300 -0.81946400 0.13824500
Mg -1.97354200 0.22932000 -0.04174000
F -3.59185300 0.99897200 -0.18015500
F -0.72409200 -0.07156400 1.52808200
F -0.18769200 0.71398900 -0.88361600
F -1.26582300 -1.62305700 -0.48656300
F 2.29165600 -0.92328900 0.04399100

IM3_{D-HMg2F5-2}

H -2.20150100 -0.81892900 -0.65053100
C -3.95814300 -1.21556500 0.11856800
H -4.37553000 -2.04170100 -0.44815000
H -3.57817000 -1.44245800 1.11001200
C -3.95159400 0.03658900 -0.35188300
H -3.52752100 0.85046000 0.22949300
H -4.35914300 0.26804500 -1.33135700
H -0.87223600 2.23846900 -1.83662400
H -1.35754100 2.34566300 -1.27880500
Mg 2.67326900 -0.17434500 -0.01191200
Mg -0.15614500 0.48564500 0.27124100
F -1.55087200 1.34745200 1.04441900
F 1.20036400 -0.62469800 1.11169300
F -1.24261900 -0.85475500 -0.82108200
F 1.36809000 0.94846800 -0.83842400
F 4.39443300 -0.60105500 -0.21950500

TS1_{D-HMg2F5-2}

H -1.36146800 1.29748600 0.00073800
C -2.53947500 1.77224700 0.00007100
H -2.49880400 2.34490700 -0.92448100
H -2.49965300 2.34493400 0.92464800
C -3.29916600 0.61458600 -0.00024500
H -3.65488900 0.16344200 0.91611800
H -3.65419800 0.16347700 -0.91689300
Mg -0.29683100 -1.17248500 -0.00003300
Mg 1.90934200 0.24590200 -0.00009700
F 3.29684700 1.38466200 0.00000300
F 1.11038900 -1.01903800 -1.28855200
F -0.12320200 0.86374500 0.00150500
F 1.11176800 -1.02111100 1.28719300
F -2.13460900 -1.26561800 0.00012700

TS2_{D-HMg2F5-2}

H 4.18280600 -1.57117800 -0.64023100
C 3.58312200 -1.22713300 0.20124900
H 3.99734000 -0.25631100 0.52622200
H 3.63509400 -1.90679200 1.05048400
C 2.21721900 -0.82841400 -0.15999700

H 1.46836700 -0.71412500 0.61762600
H 2.03308700 -0.34863300 -1.10639100
H 1.02130800 -1.90963600 -0.85262400
H 1.62177200 -2.36205700 -0.62768700
Mg 0.13206300 1.28308600 -0.01710900
Mg -1.86386900 -0.36845100 0.04666800
F -1.73561600 1.60647500 -0.17590100
F -0.37015900 -0.03719800 1.33814700
F -0.26302700 -0.32292500 -1.17581100
F -3.14900300 -1.62867700 0.07167400
F 1.96445400 1.54081400 -0.01029000

TS3_{D-HMg2F5-2}

H 1.37636700 -1.27169700 -0.85160500
C 2.49235500 -1.53879200 -0.74186700
H 2.68009200 -2.58657700 -0.95464200
H 2.83195000 -0.83960400 -1.52258700
C 2.89665100 -1.04578300 0.51792300
H 2.84185700 0.03575900 0.68222200
H 3.37146800 -1.67367200 1.26610600
H 0.92106200 -0.93054400 1.73957600
H 1.49291600 -1.43856200 1.83762400
Mg -1.81366500 -0.31896500 0.01032100
Mg 0.24439200 1.28588900 -0.06385800
F 2.03926900 1.62446800 0.00974000
F -1.58189200 1.56622000 -0.54453200
F -0.04601600 -0.48953200 -0.97505400
F -0.50641000 0.24339800 1.42009000
F -3.12922600 -1.54352500 0.06635900

IM1_{D-HMg2Cl5-2}

Cl -2.29162000 1.93477700 -0.01680200
Cl -1.62600400 -1.75137300 0.02027400
H -2.90041700 -1.32002700 0.01256100
C -4.75524200 -0.64893500 0.66742100
H -4.37414800 0.20654200 1.21474600
H -5.15198500 -1.47791700 1.24473400
C -4.75150200 -0.66245700 -0.66852300
H -5.14502500 -1.50295700 -1.23117500
H -4.36735300 0.18181700 -1.23094400
Mg -0.54569800 0.55069300 -0.00534000
Mg 2.69017800 -0.00139400 0.00403400
Cl 4.84851900 -0.41661800 -0.00196500
Cl 1.09979900 0.28808900 1.71772500
Cl 1.10140200 0.25037800 -1.71850500

IM2_{D-HMg2Cl5-2}

Cl 3.11323300 0.87623700 0.02704700
Cl -0.30122600 -0.44435600 1.84640700
H 2.02470300 -1.90318300 0.64887100
C 3.09100200 -1.90153200 0.42007400
H 3.34071600 -2.88130200 -0.00080000
H 3.66046000 -1.76810600 1.34041900
C 3.44773100 -0.86965200 -0.61520300
H 4.50759800 -0.81772000 -0.84845900
H 2.84785900 -0.92789000 -1.51902800
Mg 0.68080700 0.80234100 0.11223000
Mg -1.95273500 -0.15572900 -0.01675800

Cl	-4.01814400	-0.93090600	-0.14662400
Cl	-0.02454300	-0.71500000	-1.55281600
Cl	-1.14288600	2.22378600	-0.15024300

IM3_D-HMg2Cl5-2

H	2.85766400	-1.29193800	0.34274400
C	4.64158300	-0.91952700	-0.66302300
H	4.97681000	-1.90112100	-0.98226500
H	4.21451200	-0.26595500	-1.41609700
C	4.76466700	-0.51346600	0.60365500
H	4.44038800	0.47711000	0.90293000
H	5.20559900	-1.14782000	1.36586900
H	1.97695100	0.90678700	2.94287900
H	2.24555800	1.36109900	2.41646700
Mg	-2.71977600	-0.01224800	-0.04121200
Mg	0.51970300	0.52388400	-0.14254500
Cl	-1.09664300	-0.28059200	-1.72433800
Cl	-1.16411000	0.78890300	1.53840400
Cl	1.58705300	-1.66529600	0.57874600
Cl	2.25977300	1.83147000	-0.62892500
Cl	-4.87749100	-0.42035800	0.05898100

TS1_D-HMg2Cl5-2

Cl	3.17531600	-0.94566500	-0.07970000
Cl	0.08589200	0.58086900	-1.59825100
H	1.11887700	1.67524300	-0.77801300
C	1.69743400	2.68947200	-0.21241000
H	0.87112400	2.97464500	0.43492500
H	1.86933800	3.30067100	-1.09513600
C	2.75830300	2.01892100	0.34561100
H	3.69418300	1.88310300	-0.18251400
H	2.68447600	1.56435800	1.32608600
Mg	0.94445700	-1.14025400	0.06283200
Mg	-1.79830700	-0.06334000	0.13586900
Cl	-3.73185200	0.98943800	-0.03095300
Cl	-0.04653500	0.24139300	1.78433100
Cl	-1.05495200	-2.34869800	-0.24536700

TS2_D-HMg2Cl5-2

H	4.43015000	-2.59395400	-0.57617900
C	3.87625400	-2.11728000	0.23165700
H	4.48152800	-1.27234800	0.59418000
H	3.72691300	-2.79163000	1.07427100
C	2.63001700	-1.46542200	-0.21468800
H	1.88561900	-1.18233200	0.52086900
H	2.58613500	-0.97732400	-1.17596500
H	1.27159300	-2.36563700	-0.92116800
H	1.83522900	-2.85427000	-0.65929400
Cl	2.90997700	1.34049100	0.01583500
Cl	-0.11411200	-0.30227800	1.73856600
Mg	0.62401700	1.21159900	-0.00978900
Mg	-1.91668500	-0.18753700	0.05166100
Cl	-3.79151300	-1.36670700	0.06695900
Cl	-0.09458000	-0.53639200	-1.63645600
Cl	-1.48287700	2.23223800	-0.15319800

TS3_D-HMg2Cl5-2

H	1.88795200	-1.59008600	-1.24997300
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C	2.81373800	-1.99524500	-0.77450100
H	3.28936300	-2.77513600	-1.36015700
H	3.36551600	-1.01823200	-0.75624800
C	2.58007400	-2.27271100	0.59368600
H	2.19689800	-1.48621300	1.23942000
H	2.94544800	-3.17166500	1.08312300
H	0.55500600	-2.65516500	0.83855300
H	0.88992100	-3.30498800	0.61037900
Mg	-1.84776500	-0.02973600	-0.01505300
Mg	0.79840100	1.17372300	0.01730700
Cl	-1.25292400	2.34198500	-0.07009300
Cl	-0.10035400	-0.34600500	1.72454400
Cl	-0.01372700	-0.41912900	-1.67230500
Cl	3.06122800	1.23346400	0.09058800
Cl	-3.74720000	-1.17023400	-0.03433700

IM1_D-HMg2Br5-2

H	3.33650200	1.51957600	0.00387700
C	5.20395700	0.82386100	0.68763600
H	4.80521600	-0.02089000	1.23900200
H	5.60445800	1.65287800	1.26207000
C	5.21509100	0.82521200	-0.64825100
H	5.62514400	1.65538400	-1.21422000
H	4.82556200	-0.01837200	-1.20792600
Mg	0.86106700	-0.47034000	-0.00409800
Mg	-2.51664200	-0.08251700	0.00208600
Br	-4.84423200	0.22438800	0.00583000
Br	-0.85738700	-0.25620400	1.87566400
Br	1.93464800	2.01333400	-0.00809200
Br	-0.86385900	-0.25507600	-1.87755200
Br	2.72099300	-1.95640600	-0.00427700

IM2_D-HMg2Br5-2

H	2.18989000	-2.20299700	0.69615400
C	3.24382100	-2.32497100	0.44421000
H	3.37287800	-3.33867900	0.04832900
H	3.84480400	-2.23269800	1.34927900
C	3.68821700	-1.36955700	-0.63002300
H	4.74173800	-1.43847100	-0.88637200
H	3.06367300	-1.37866800	-1.51858400
Mg	0.96775600	0.60979000	0.08844200
Mg	-1.83423400	-0.08025900	-0.00187400
Br	-4.11903300	-0.65832000	-0.11028000
Br	0.08699300	-0.96547200	-1.66886200
Br	-0.14552100	-0.55588000	2.01013600
Br	-0.76153100	2.36610800	-0.21838800
Br	3.55602100	0.56797300	-0.00154200

IM3_D-HMg2Br5-2

H	-3.31578000	-1.51726500	0.04820300
C	-5.15937800	-0.82516100	0.79695000
H	-5.53989500	-1.66162500	1.37416200
H	-4.74594700	0.01445700	1.34535400
C	-5.21076100	-0.81198000	-0.53784600
H	-4.84063900	0.03813600	-1.10008300
H	-5.63538700	-1.63682800	-1.10079300
H	-2.50718200	-0.19565700	-3.15841000
H	-2.69184900	0.41550500	-2.77390900

Mg	2.54026300	0.08141900	0.01162000
Mg	-0.83994600	0.46028100	0.01228100
Br	-2.68781200	1.96359700	0.07001200
Br	-1.91677000	-2.01716200	0.00102400
Br	0.88321300	0.26827800	-1.86279300
Br	0.88368300	0.22909900	1.88831900
Br	4.86893600	-0.21907700	0.00412500

TS1_{D-HMg2Br5-2}

H	-1.05815700	-2.04142700	-0.82322600
C	-1.51583100	-3.15744000	-0.21146800
H	-0.65481800	-3.30210200	0.43628800
H	-1.58168400	-3.78771600	-1.09457400
C	-2.65963400	-2.62949300	0.32081400
H	-3.59552600	-2.62138000	-0.22457400
H	-2.66118800	-2.15022800	1.29198200
Mg	-1.24763200	0.86897000	0.12747500
Mg	1.72647500	0.16435200	0.19057500
Br	3.92711800	-0.64027700	-0.05809200
Br	-0.02773200	-0.46570700	1.96535900
Br	-0.13328000	-0.81032500	-1.72547900
Br	0.65363400	2.47871600	-0.22965800
Br	-3.59522400	0.47258200	-0.06808800

TS2_{D-HMg2Br5-2}

H	4.28661000	-3.45247000	-0.63014400
C	3.84144800	-2.89216900	0.19151600
H	4.60473600	-2.19624900	0.56806800
H	3.56752900	-3.54552900	1.01979000
C	2.72702400	-2.02288900	-0.23764200
H	2.03886600	-1.63322400	0.50214300
H	2.74710000	-1.53950900	-1.20124300
H	1.13690200	-2.67794300	-0.99045700
H	1.66302500	-3.20444600	-0.69679000
Mg	1.03305800	0.94034200	0.00037900
Mg	-1.79884500	-0.04173900	0.07107400
Br	-0.96135900	2.43707600	-0.17154800
Br	0.03818300	-0.51862700	1.88538200
Br	0.00759300	-0.75721900	-1.78841100
Br	-3.99916200	-0.90331200	0.06814200
Br	3.47856900	0.79798200	0.03066300

TS3_{D-HMg2Br5-2}

H	-1.83792000	2.12012500	-1.20647700
C	-2.74112900	2.66336200	-0.78780400
H	-3.00904100	3.50601600	-1.41798300
H	-3.42831600	1.79143100	-0.83195400
C	-2.47662300	2.94800100	0.57217400
H	-2.36987200	2.12789600	1.27716700
H	-2.54659600	3.94640700	0.99344200
H	-0.38271800	2.70122600	0.86483200
H	-0.59670700	3.39013900	0.59533000
Mg	1.75240100	-0.10513600	0.03607000
Mg	-1.16336000	-0.86578100	-0.00275600
Br	-3.56405300	-0.65621800	0.06097200
Br	-0.06755200	0.79045500	-1.74706200
Br	0.01395700	0.42889500	1.94114900
Br	0.75412200	-2.48683600	-0.24133400

Br	3.96093200	0.73512100	0.00398000
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IM1_{D-HMg2F5-3}

H	-2.24162200	-0.97170000	-0.28946000
C	-4.05534300	-0.91639600	0.43288400
H	-3.74390400	-0.66409900	1.44190000
H	-4.49002900	-1.89958300	0.28339300
C	-3.94966300	-0.02789500	-0.56159100
H	-4.28973700	-0.26760000	-1.56456200
H	-3.51122100	0.95109200	-0.38986500
Mg	2.65740700	-0.13113800	-0.01167700
Mg	-0.17529200	0.54288500	0.10165600
F	-1.27836800	-1.11248600	-0.35349300
F	1.28978700	0.53441100	-1.16746800
F	1.23564300	-0.10336500	1.26381900
F	-1.57168400	1.66163200	0.37107500
F	4.38253100	-0.58278400	-0.09047800

IM2_{D-HMg2F5-3}

H	-3.13608700	0.01853300	1.28343300
C	-3.46766000	-0.84179000	0.70042500
H	-4.55992100	-0.80800500	0.63797600
H	-3.18249700	-1.77340600	1.19284300
C	-2.91702100	-0.76640400	-0.69263900
H	-3.18886900	-1.60264300	-1.33311400
H	-3.10164100	0.19165900	-1.17243100
Mg	2.47786900	-0.15976100	0.05439000
Mg	-0.30801600	0.69151000	0.02680100
F	0.97281200	-0.13332500	1.22861900
F	-1.44445200	-0.86224500	-0.62421400
F	1.24428500	0.68327700	-1.13501100
F	-1.67159800	1.84541600	0.29489800
F	4.16993600	-0.72845300	0.05462800

IM3_{D-HMg2F5-3}

H	-2.20131400	-0.81761100	-0.65264100
C	-3.95648800	-1.21589100	0.11890200
H	-4.37372200	-2.04276300	-0.44685800
H	-3.57487100	-1.44184500	1.10993100
C	-3.95197500	0.03605800	-0.35212400
H	-3.52807100	0.85055200	0.22849600
H	-4.36114700	0.26667500	-1.33112000
H	-1.35635500	2.34937800	-1.27450900
H	-0.87061700	2.24356100	-1.83221800
Mg	-0.15633100	0.48552900	0.27133100
Mg	2.67309400	-0.17444900	-0.01179900
F	4.39426600	-0.60110400	-0.21943700
F	1.19959000	-0.62673000	1.11023000
F	-1.24254200	-0.85264100	-0.82399900
F	1.36851800	0.95028000	-0.83667500
F	-1.55142000	1.34554000	1.04586500

TS1_{D-HMg2F5-3}

H	0.78977800	1.21456600	0.91517400
C	1.62858800	2.04812200	0.58082900
H	2.43317300	1.73256400	1.24469900
H	1.16290100	3.00731000	0.79114200
C	1.72186400	1.63562800	-0.74148000

H	1.18536400	2.12793600	-1.54251500
H	2.35862600	0.79330700	-1.00019900
Mg	-1.64443600	0.01136800	-0.03792300
Mg	0.67487400	-1.27599100	0.03884200
F	-0.08812000	0.15219300	1.30153000
F	-0.00280300	0.14715500	-1.18412600
F	-1.13533700	-1.87712700	0.02835000
F	2.48218600	-1.26712400	-0.01261700
F	-3.07790500	1.08904800	-0.07263000

TS2_{D-HMg2F5-3}

H	3.30837500	2.43518300	-0.78265600
C	2.44968700	2.27191300	-0.13310100
H	1.56186000	2.66975400	-0.65939900
H	2.52982900	2.81077300	0.80994300
C	2.06994700	0.86737400	0.01487400
H	1.41029900	0.57554300	0.82500400
H	2.20903600	0.17524600	-0.79810900
H	3.48746200	0.24230600	0.89081800
H	3.16770300	-0.44852100	0.70609400
Mg	-1.69273800	0.37512200	0.03615000
Mg	0.16357600	-1.45304900	-0.06846100
F	-0.39776500	-0.28967000	1.40119600
F	1.94815800	-1.89495600	0.00409300
F	-1.69182600	-1.53803900	-0.49391300
F	-2.83538100	1.76386000	0.10807600
F	0.03876800	0.36315100	-1.00774100

TS3_{D-HMg2F5-3}

H	0.95782400	1.36620600	-0.68421300
C	1.63581500	1.99529400	-0.01293500
H	1.76792400	2.99867200	-0.40528100
H	0.96721400	1.90660000	0.86426200
C	2.81096900	1.25513500	0.25072500
H	2.75397900	0.31047700	0.78740800
H	3.80438900	1.65773400	0.07578500
H	3.01394200	-0.30693200	-1.09389800
H	3.29955200	0.32220300	-1.44136600
Mg	0.34070200	-1.28882500	0.04615700
Mg	-1.78068100	0.20617000	0.00129500
F	-3.11212400	1.41467300	-0.04988700
F	-0.28016400	0.07104800	1.31733800
F	-0.13819600	0.19265000	-1.21064000
F	-1.50733400	-1.74602800	-0.10932600
F	2.15273300	-1.57297300	0.04153000

IM1_{D-HMg2Cl5-3}

Cl	-4.84666800	-0.42095100	0.00057000
Cl	1.62261500	-1.75140000	0.01456000
H	2.89767300	-1.32224000	0.00928700
C	4.74958000	-0.66632500	-0.66735600
H	4.36680600	0.17912400	-1.22888300
H	5.14214400	-1.50670300	-1.23080300
C	4.75292600	-0.65430900	0.66850100
H	5.14830100	-1.48448300	1.24496500
H	4.37274800	0.20102700	1.21663400
Mg	-2.68943700	0.00011200	0.00029400
Mg	0.54609200	0.55251700	-0.00316700

Cl	2.29402700	1.93408500	-0.01140700
Cl	-1.10101200	0.28625100	1.71689600
Cl	-1.09970200	0.25940000	-1.71965300

IM2_{D-HMg2Cl5-3}

Cl	-4.57464900	-0.64863000	-0.03794500
Cl	-0.66495200	-0.60093800	-1.52622300
H	2.82592000	-2.84350700	-0.62006500
C	3.31052300	-1.86954600	-0.69881200
H	2.77288300	-1.25232200	-1.41975300
H	4.32474600	-2.01759300	-1.08316100
C	3.41944000	-1.18623800	0.64070100
H	3.95228600	-1.76869400	1.38777800
H	3.81083100	-0.17488200	0.57517000
Mg	-2.46305200	-0.04289700	-0.11682200
Mg	0.71195500	0.76837100	-0.10522700
Cl	2.48347700	1.88641000	-0.85974600
Cl	1.73501800	-0.96364200	1.41381000
Cl	-1.15849900	1.36715400	1.25559200

IM3_{D-HMg2Cl5-3}

H	2.85884700	-1.29290900	0.33595200
C	4.64510900	-0.91316700	-0.66284400
H	4.98266600	-1.89272100	-0.98587200
H	4.21921300	-0.25657800	-1.41395600
C	4.76401300	-0.51307100	0.60612800
H	4.43745900	0.47557100	0.90927700
H	5.20368300	-1.15047600	1.36652300
H	2.24535700	1.34976900	2.42160000
H	1.97882000	0.89186500	2.94593600
Cl	2.25884600	1.83399800	-0.62208300
Cl	1.58817800	-1.66937300	0.56668300
Mg	0.51943100	0.52325000	-0.14190300
Mg	-2.72020200	-0.01202200	-0.04015500
Cl	-4.87823600	-0.41857200	0.05954400
Cl	-1.09858000	-0.27331200	-1.72591500
Cl	-1.16265100	0.78009400	1.54209700

TS1_{D-HMg2Cl5-3}

Cl	3.73662400	0.89379800	-0.01308000
Cl	-0.03868900	0.50935200	-1.65313600
H	-1.08768100	1.67944700	-0.87910000
C	-1.98514700	2.55386800	-0.61980200
H	-2.79174400	2.11385700	-1.20272300
H	-1.50623500	3.44454700	-1.01893300
C	-1.99059200	2.35072300	0.73984700
H	-1.34447500	2.91109900	1.40546000
H	-2.61589000	1.58076000	1.17935500
Mg	1.76785900	-0.10059800	0.09246300
Mg	-1.01907000	-1.13204500	0.04707100
Cl	-3.23948200	-0.92061200	-0.02311500
Cl	-0.00531500	0.35021200	1.71088500
Cl	0.97127400	-2.38366400	-0.13206900

TS2_{D-HMg2Cl5-3}

H	3.03688200	3.67760600	-0.70218200
C	2.19380900	3.27696600	-0.14061200
H	1.28352300	3.47504600	-0.72867600

H	2.06692200	3.77682200	0.81920400
C	2.20648200	1.80926400	-0.02984700
H	1.58201100	1.32434000	0.71222300
H	2.58555700	1.19859300	-0.83495400
H	3.60031000	1.66914000	0.93590200
H	3.56035000	0.89545300	0.79152000
Cl	-3.69912500	1.16228600	0.10808800
Cl	-1.25468300	-2.30799300	-0.52048700
Mg	-1.80464700	0.01612100	0.05719900
Mg	0.80720600	-1.27468000	-0.06503600
Cl	3.07959800	-1.33035500	0.03652900
Cl	-0.11249300	-0.07716300	1.83884000
Cl	0.09564400	0.70430300	-1.45569000

TS3_{D-HMg2Cl5-3}

H	0.80457600	2.09877100	-0.69804000
C	1.28279000	2.88136100	-0.01067600
H	1.17562900	3.87544400	-0.43375300
H	0.63466700	2.66009800	0.85392800
C	2.59688100	2.43466400	0.24548900
H	2.76295200	1.51797000	0.80710700
H	3.47580100	3.03227500	0.02486400
H	3.16876300	0.90816400	-1.17593000
H	3.14391300	1.61653300	-1.47546200
Cl	3.17852700	-1.14580100	0.04113400
Cl	0.00974600	0.42004500	-1.65913700
Mg	0.92141800	-1.16307100	0.03275700
Mg	-1.79462500	-0.11437700	0.03477200
Cl	-3.71427100	0.98977600	-0.00949400
Cl	-0.05015800	0.27147100	1.73905800
Cl	-1.06889500	-2.43408100	-0.11873300

IM1_{D-HMg2Br5-3}

H	-3.33669700	1.51939200	0.00055700
C	-5.21023800	0.82436900	-0.66618500
H	-4.81641100	-0.01963200	-1.22222100
H	-5.61602200	1.65406800	-1.23591900
C	-5.20926600	0.82405300	0.66976400
H	-5.61421800	1.65348100	1.24048500
H	-4.81463900	-0.02021700	1.22482200
Mg	2.51668400	-0.08245400	0.00016300
Mg	-0.86103900	-0.47026300	-0.00041600
Br	0.86091600	-0.25512000	-1.87673100
Br	-2.72084200	-1.95648500	-0.00064300
Br	-1.93483500	2.01332400	-0.00039300
Br	4.84430300	0.22427600	0.00052500
Br	0.86038000	-0.25585300	1.87649500

IM2_{D-HMg2Br5-3}

H	3.00030600	-3.16450000	-0.87819600
C	3.50062600	-2.19613600	-0.91500300
H	2.93393300	-1.51888300	-1.55487400
H	4.48564400	-2.33424500	-1.37395000
C	3.71195200	-1.61376900	0.45917200
H	4.26818100	-2.25922800	1.13364900
H	4.11891400	-0.60664500	0.44485600
Mg	-2.37560000	0.06799300	-0.13971300
Mg	0.97661400	0.60090600	-0.08105900

Br	-0.91740200	1.36484000	1.44526900
Br	2.90905700	1.75104100	-0.86239200
Br	-0.55951900	-0.65992000	-1.70319900
Br	-4.68188700	-0.36979900	-0.09442600
Br	1.95561900	-1.37998600	1.43225500

IM3_{D-HMg2Br5-3}

H	-2.76020600	-1.37859000	1.16893700
C	-4.53313900	-1.86785800	0.14862200
H	-5.08681500	-2.40544900	0.91166300
H	-4.82529600	-0.84285800	-0.05362700
C	-3.54443100	-2.44643800	-0.53804500
H	-3.01539600	-1.90565700	-1.31568100
H	-3.24661300	-3.47445500	-0.36015700
H	2.40644000	-1.41927600	1.85893700
H	1.65886500	-1.36039200	1.84071800
Mg	2.33070200	-0.08360900	-0.10652700
Mg	-0.97093800	0.64972900	-0.22977900
Br	-2.98501400	1.36975200	-1.26249100
Br	0.42534800	-1.21448600	-1.29668300
Br	-1.76252200	-0.68186000	2.01436200
Br	1.00744600	1.87528400	0.78361800
Br	4.65809200	-0.43786000	-0.17248000

TS1_{D-HMg2Br5-3}

H	1.07475300	-2.02632700	-0.90484800
C	1.96239400	-2.99924000	-0.64128000
H	2.78271700	-2.58410500	-1.22199800
H	1.41609600	-3.83345900	-1.07350100
C	1.97290700	-2.82920400	0.71541600
H	1.28116800	-3.35517600	1.36285200
H	2.64356300	-2.11258200	1.17659700
Mg	-1.71274300	0.16432800	0.16261800
Mg	1.28488900	0.86650200	0.10389500
Br	-0.62309000	2.48304800	-0.17234800
Br	3.62817200	0.47109100	-0.03535800
Br	0.08621500	-0.78249500	-1.75649000
Br	-3.93700700	-0.58949100	-0.03060000
Br	0.05497200	-0.53894300	1.90959400

TS2_{D-HMg2Br5-3}

H	2.69331300	4.38358500	-0.69379900
C	1.89499900	3.87371700	-0.15527100
H	0.97145700	4.00128400	-0.73892500
H	1.71640700	4.32375500	0.82131500
C	2.09014700	2.41404900	-0.07854600
H	1.53743200	1.83807700	0.65400100
H	2.56665600	1.87475000	-0.88194000
H	3.47542100	2.37800800	0.88862900
H	3.60496800	1.60032200	0.76702000
Mg	-1.72009300	-0.11623700	0.08001300
Mg	1.17586800	-0.92085100	-0.05425600
Br	-3.95138900	0.66171700	0.10714900
Br	0.03378400	0.15575700	2.00059700
Br	0.08532900	1.00247400	-1.59102600
Br	3.59879400	-0.66380900	0.03849000
Br	-0.73640000	-2.46132000	-0.54728100

TS3_{D-HMg2Br5-3}

H	-0.29617700	2.34005300	-0.90610100
C	-0.59473800	3.31499700	-0.33099200
H	-0.93368600	4.00139400	-1.10406800
H	-1.38457700	2.89530200	0.29894800
C	0.56699600	3.69287800	0.37158900
H	0.80237800	3.23431400	1.32569900
H	1.19238200	4.51805900	0.04702700
H	2.45427700	2.10890300	-0.28862200
H	1.98109200	2.72186100	-0.36036700
Mg	1.46116500	-0.64488300	0.07513500
Mg	-1.54780000	-0.57769700	0.07825400
Br	-3.78160700	0.21080200	-0.00978600
Br	0.01280600	0.49423700	1.88276600
Br	0.01296500	0.49147600	-1.85375100
Br	-0.06846300	-2.68407500	-0.01830500
Br	3.74973900	0.08195600	-0.03226000

IM1_{T-HMg2F5-4}

H	2.62350300	-0.50240400	-0.02463100
C	3.37760500	1.08090500	0.64768000
H	4.37508900	0.80673600	0.97614500
H	2.63701300	1.27171600	1.41866000
C	3.07586300	1.24067300	-0.64783100
H	2.07491700	1.53543300	-0.94941200
H	3.82165100	1.09123100	-1.42251100
Mg	-1.93034600	0.37665400	0.01892200
Mg	0.15221000	-1.07161600	-0.01860800
F	-1.03740800	-0.77780000	1.42509200
F	-3.37612100	1.44359600	0.03672700
F	-1.38140100	-1.21762000	-1.11258100
F	0.02688800	0.82060200	-0.31926200
F	2.11078100	-1.35684900	-0.03009900

IM2_{T-HMg2F5-4}

H	-3.14304200	0.03977200	1.27268300
C	-3.47155800	-0.83017000	0.70238100
H	-4.56349500	-0.79836500	0.63436700
H	-3.18806800	-1.75350400	1.21098600
C	-2.91474800	-0.77694500	-0.68913700
H	-3.18291600	-1.62379300	-1.31710000
H	-3.09846000	0.17274800	-1.18557600
Mg	2.47805200	-0.15870300	0.05500700
Mg	-0.30818800	0.69140200	0.02387200
F	0.97456600	-0.12240000	1.23109000
F	4.17017900	-0.72750300	0.05741600
F	1.24269800	0.67403500	-1.13980400
F	-1.44251000	-0.86982900	-0.61295600
F	-1.67210500	1.84719100	0.28187900

IM3_{T-HMg2F5-4}

H	-2.52296200	0.30733500	-0.00123700
C	-2.65565700	-1.47287100	-0.66876200
H	-3.58024600	-1.54183100	-1.23351900
H	-1.72591800	-1.42643800	-1.22955100
C	-2.65449800	-1.47111400	0.67135800
H	-1.72384500	-1.42321700	1.23052600
H	-3.57810100	-1.53855700	1.23790800

H	0.05705600	3.38915500	0.01116200
H	-0.69534400	3.40739000	0.01198900
Mg	1.75097900	-0.44951700	0.00005500
Mg	-0.19437200	1.20112900	-0.00132500
F	3.07890500	-1.66080400	0.00125900
F	1.67449700	1.56635100	-0.00369600
F	0.21909100	-0.15789900	1.28887800
F	0.21708800	-0.16265200	-1.28729700
F	-2.19502600	1.24508500	-0.00221200

TS1_{T-HMg2F5-4}

H	2.63886300	-0.14247800	0.00006100
C	3.15739900	1.00862200	0.00004900
H	3.73066600	0.94789200	-0.92339400
H	3.73050000	0.94797000	0.92360100
C	2.05756500	1.85613100	-0.00008300
H	1.64244900	2.25285400	0.91670500
H	1.64262300	2.25279800	-0.91697400
Mg	-1.80552700	0.26228400	-0.00004700
Mg	0.30038500	-1.23170700	0.00005200
F	-1.09954000	-1.07656900	1.29124300
F	-3.12991900	1.47688200	-0.00007300
F	-1.09969200	-1.07696500	-1.29100700
F	0.20397800	0.75209700	-0.00023700
F	2.16815400	-1.38816300	0.00009000

TS2_{T-HMg2F5-4}

H	4.18280600	-1.57117800	-0.64023100
C	3.58312200	-1.22713300	0.20124900
H	3.99734000	-0.25631100	0.52622200
H	3.63509400	-1.90679200	1.05048400
C	2.21721900	-0.82841400	-0.15999700
H	1.46836700	-0.71412500	0.61762600
H	2.03308700	-0.34863300	-1.10639100
H	1.02130800	-1.90963600	-0.85262400
H	1.62177200	-2.36205700	-0.62768700
Mg	0.13206300	1.28308600	-0.01710900
Mg	-1.86386900	-0.36845100	0.04666800
F	-1.73561600	1.60647500	-0.17590100
F	-0.37015900	-0.03719800	1.33814700
F	-0.26302700	-0.32292500	-1.17581100
F	-3.14900300	-1.62867700	0.07167400
F	1.96445400	1.54081400	-0.01029000

TS3_{T-HMg2F5-4}

H	2.77380900	-0.18187000	-0.08617100
C	3.12773800	0.88326300	-0.40542700
H	4.16570700	1.04034200	-0.12717300
H	2.96203900	0.71882500	-1.48021300
C	2.18838500	1.82381200	0.07382000
H	1.17875200	1.79674200	-0.33386100
H	2.46902700	2.66868500	0.69451800
H	0.97672700	0.92002900	1.70065100
H	1.66980400	1.26226100	1.79369600
Mg	-1.83168700	0.28355100	-0.05883500
Mg	0.25478900	-1.24635000	0.01310300
F	-3.16635700	1.48944500	-0.08422400
F	-0.49890000	-0.09061800	1.41466300

F	-0.08104300	0.38818900	-1.04325000
F	-1.56731200	-1.65656900	-0.37389000
F	2.07252100	-1.56532200	0.12858900

IM1_{T-HMg2Cl5-4}

Cl	3.87479800	-1.17910000	-0.00768800
Cl	-0.05259900	-0.70484000	-1.52128100
H	-3.16620100	-0.16810100	0.02269600
C	-3.37900300	-2.01945100	-0.62615200
H	-2.71166300	-1.97315400	-1.48022900
H	-4.44470100	-2.06292700	-0.82712900
C	-2.89777900	-2.06130900	0.62206200
H	-3.55467600	-2.13224800	1.48308400
H	-1.83099000	-2.04195200	0.81931600
Mg	1.89445700	-0.19917100	-0.00279500
Mg	-0.64144400	1.01111400	-0.00977800
Cl	-3.07281800	1.20363900	0.03858200
Cl	1.31260200	2.22657600	-0.34110600
Cl	0.19288600	-0.18629700	1.84076800

IM2_{T-HMg2Cl5-4}

Cl	3.76704400	0.59861800	-0.00968900
Cl	0.23146700	-0.41499900	1.92480800
H	-2.44511300	3.16885200	-1.06529500
C	-2.18406300	2.83787700	-0.05901200
H	-2.78614100	1.96393100	0.19495300
H	-2.43152300	3.64200600	0.64159900
C	-0.70754100	2.55807500	0.06736400
H	-0.06972000	3.38471500	-0.23447500
H	-0.41334200	2.18450700	1.04510000
Mg	1.82550200	-0.42617800	0.14951200
Mg	-1.17570600	-1.06265700	0.09661700
Cl	-3.38074700	-0.96984100	0.03494100
Cl	0.63268000	-2.10116300	-1.05643000
Cl	-0.20939100	1.19010800	-1.10454300

IM3_{T-HMg2Cl5-4}

H	-3.12749200	-0.16784000	-0.13541400
C	-3.31700000	-2.02610300	-0.77518900
H	-4.37490600	-2.07180200	-1.01337100
H	-2.62003300	-1.98662500	-1.60559700
C	-2.88062800	-2.05725900	0.48957600
H	-1.82137500	-2.03588400	0.72410400
H	-3.56657200	-2.12017900	1.32778800
H	-2.50286600	0.01517800	3.17090800
H	-3.22354400	0.18072800	3.26169400
Cl	3.92861700	-1.16443400	0.06923500
Cl	0.04435200	-0.72368200	-1.56121100
Mg	1.94354600	-0.19642900	0.00532600
Mg	-0.60040400	0.99972600	-0.08054300
Cl	-3.02862100	1.20322900	-0.13407400
Cl	1.35768200	2.22272500	-0.35928400
Cl	0.18649100	-0.18213000	1.80216800

TS1_{T-HMg2Cl5-4}

Cl	-3.74509700	-1.10444800	-0.00273100
Cl	-0.04293000	-0.29528200	1.76553000
H	2.92136200	-0.73403900	0.03588700

C	3.02202200	-1.99035600	0.30488700
H	3.04642900	-1.90863700	1.38944000
H	3.96882100	-2.17969000	-0.19637600
C	1.86623300	-2.45613100	-0.27821700
H	1.83361000	-2.76885000	-1.31515400
H	0.93690100	-2.49722100	0.27676000
Mg	-1.80281000	-0.04588400	0.03240700
Mg	0.81104000	1.10355600	0.01205600
Cl	3.13051800	0.98539700	-0.06234000
Cl	-1.17106000	2.34094400	-0.13722300
Cl	0.05589600	-0.51041800	-1.61524300

TS2_{T-HMg2Cl5-4}

H	3.03688200	3.67760600	-0.70218200
C	2.19380900	3.27696600	-0.14061200
H	1.28352300	3.47504600	-0.72867600
H	2.06692200	3.77682200	0.81920400
C	2.20648200	1.80926400	-0.02984700
H	1.58201100	1.32434000	0.71222300
H	2.58555700	1.19859300	-0.83495400
H	3.60031000	1.66914000	0.93590200
H	3.56035000	0.89545300	0.79152000
Cl	-3.69912500	1.16228600	0.10808800
Cl	-1.25468300	-2.30799300	-0.52048700
Mg	-1.80464700	0.01612100	0.05719900
Mg	0.80720600	-1.27468000	-0.06503600
Cl	3.07959800	-1.33035500	0.03652900
Cl	-0.11249300	-0.07716300	1.83884000
Cl	0.09564400	0.70430300	-1.45569000

TS3_{T-HMg2Cl5-4}

H	-3.14753500	-0.75337500	-0.42067300
C	-3.11268300	-1.87085500	-0.67543200
H	-4.12787500	-2.24494400	-0.77424700
H	-2.55380000	-1.78340800	-1.61771000
C	-2.30550500	-2.50451100	0.30313600
H	-1.23265700	-2.32891400	0.30435900
H	-2.67104900	-3.30486900	0.93888500
H	-1.97213300	-1.19894300	1.87475800
H	-2.67727300	-1.51080200	1.86927700
Cl	3.78822900	-1.19143800	-0.00739500
Cl	-0.03119200	-0.61425400	-1.54944700
Mg	1.87195800	-0.08052300	-0.03788400
Mg	-0.74533800	1.14177200	-0.01799200
Cl	-3.02673100	1.26899300	0.08201200
Cl	1.29282800	2.29306100	-0.28654300
Cl	0.17522100	-0.18915800	1.80429300

IM1_{T-HMg2Br5-4}

H	-3.45919600	-0.77376700	0.00976100
C	-3.43313900	-2.65854800	-0.62136800
H	-2.82155200	-2.52370300	-1.50719000
H	-4.49341400	-2.83548900	-0.77072300
C	-2.88722900	-2.64960300	0.60049500
H	-3.48476500	-2.80638200	1.49263400
H	-1.82294000	-2.49619200	0.74424200
Mg	1.80024700	-0.08267500	0.00290400
Mg	-0.97232100	0.73701500	-0.00969100

Br	0.84113900	2.39324000	-0.36478800
Br	-3.56737000	0.73847500	0.02371300
Br	-0.11982200	-0.97376800	-1.64944400
Br	0.04724000	-0.37915800	1.99885800
Br	4.05792600	-0.76643700	-0.00154000

IM2_{T-HMg2Br5-4}

H	-2.21181400	3.62288500	-1.02330800
C	-1.86865800	3.30090000	-0.03937300
H	-2.50502100	2.48427600	0.30419100
H	-1.98537100	4.14058700	0.65449900
C	-0.41063600	2.91732500	-0.05093300
H	0.25210000	3.68200700	-0.44648000
H	-0.04494800	2.54187000	0.90078900
Mg	1.72119100	-0.48938600	0.21245800
Mg	-1.42209800	-0.75656300	0.15802900
Br	0.30586200	-2.24920100	-0.95925300
Br	-3.74836100	-0.39641700	0.01922300
Br	0.07957800	-0.11891300	2.12310500
Br	-0.09350800	1.36500200	-1.30786200
Br	3.93019200	0.29011200	0.00210900

IM3_{T-HMg2Br5-4}

H	-3.44079900	-0.74238600	-0.11671300
C	-3.41289400	-2.59978500	-0.82561100
H	-4.46990800	-2.76454000	-1.00821800
H	-2.77946600	-2.43004500	-1.68976300
C	-2.89773500	-2.64615900	0.40856500
H	-1.83658900	-2.50441600	0.58471200
H	-3.51705200	-2.83711300	1.27830700
H	-2.85248500	-0.81036200	3.25876600
H	-3.58835100	-0.80817600	3.37438800
Mg	1.83172500	-0.08308500	0.00138600
Mg	-0.94070200	0.74347500	-0.03059800
Br	4.08628000	-0.77631200	0.02253500
Br	-0.06126900	-0.91880300	-1.70633000
Br	0.04243100	-0.43704100	1.96006200
Br	0.88443300	2.40380500	-0.30242600
Br	-3.53312800	0.76972300	-0.05465900

TS1_{T-HMg2Br5-4}

H	3.14600800	-1.19722900	0.04887600
C	3.12512400	-2.51697900	0.35829500
H	3.08540500	-2.40002100	1.43837700
H	4.09061200	-2.76455200	-0.07596900
C	1.98232200	-2.86745200	-0.30588200
H	1.99537500	-3.16288400	-1.34859200

H	1.01401700	-2.80799000	0.17584400
Mg	-1.73576700	0.00522400	0.02206500
Mg	1.07461400	0.83214000	0.02425900
Br	-0.79561300	2.47953400	-0.04523700
Br	3.55838500	0.54650900	-0.04722000
Br	0.06037400	-0.59003900	1.88613800
Br	0.11200200	-0.67525300	-1.80371400
Br	-3.96492600	-0.77243900	-0.02165100

TS2_{T-HMg2Br5-4}

H	4.28661000	-3.45247000	-0.63014400
C	3.84144800	-2.89216900	0.19151600
H	4.60473600	-2.19624900	0.56806800
H	3.56752900	-3.54552900	1.01979000
C	2.72702400	-2.02288900	-0.23764200
H	2.03886600	-1.63322400	0.50214300
H	2.74710000	-1.53950900	-1.20124300
H	1.13690200	-2.67794300	-0.99045700
H	1.66302500	-3.20444600	-0.69679000
Mg	1.03305800	0.94034200	0.00037900
Mg	-1.79884500	-0.04173900	0.07107400
Br	-0.96135900	2.43707600	-0.17154800
Br	0.03818300	-0.51862700	1.88538200
Br	0.00759300	-0.75721900	-1.78841100
Br	-3.99916200	-0.90331200	0.06814200
Br	3.47856900	0.79798200	0.03066300

TS3_{T-HMg2Br5-4}

H	-3.44613200	-1.30743500	-0.32109500
C	-3.44295400	-2.43161700	-0.63401600
H	-4.48823000	-2.73182500	-0.59166100
H	-3.02641800	-2.33265900	-1.63930100
C	-2.57726700	-3.10481800	0.25875000
H	-1.50907000	-3.12520100	0.06988400
H	-2.95248300	-3.73933700	1.05533600
H	-1.70248600	-1.55328900	1.75615100
H	-2.35635400	-1.96431900	1.67654500
Mg	1.78906000	-0.00962200	-0.04057100
Mg	-1.05840200	0.84214100	-0.05547500
Br	4.01121700	-0.81133900	0.03330400
Br	-0.14871300	-1.13381400	-1.46311400
Br	0.13570300	-0.04909400	2.06136500
Br	0.84798800	2.35573800	-0.67040800
Br	-3.50806400	0.78086500	0.07880300