

Allyl-MgH

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.343800
C	1.204393	0.000000	2.239589
Mg	1.634516	2.034801	2.811251
H	-0.915971	0.026347	-0.562649
H	0.914538	-0.046953	-0.568391
H	-0.958214	0.037462	1.843000
H	1.034759	-0.633839	3.106717
H	2.070552	-0.401704	1.716038
X	0.855065	2.351429	2.270694
H	1.952555	3.685308	3.198493

Allyl-MgCl

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.342800
C	1.210529	0.000000	2.230956
Mg	1.623453	1.986363	2.929137
H	-0.916625	0.018458	-0.561514
H	0.914584	-0.034531	-0.568639
H	-0.955200	0.026099	1.846959
H	1.065444	-0.665431	3.078268
H	2.085973	-0.354419	1.691038
X	0.834905	2.329633	2.418885
Cl	2.030478	4.061973	3.600388

MgH-Comp

C	0.037148	0.005096	-0.008127
C	0.014115	0.005443	1.335915
C	1.194331	-0.002409	2.257656
Mg	1.602267	1.952514	3.104232
H	1.877250	3.219893	4.256100
H	0.961359	-0.050284	-0.560239
H	-0.868724	0.030011	-0.588015
H	-0.955446	0.040110	1.813998
H	1.025580	-0.708572	3.069820
H	2.084024	-0.343344	1.727862
C	1.233971	3.699728	0.747535
C	2.516632	3.313313	0.635048
H	0.441918	3.146903	0.274828
H	2.790932	2.445353	0.061946
H	0.962838	4.589141	1.288417
H	3.316187	3.882899	1.075576

MgCl-Comp

C	0.188189	-0.030926	-0.050306
C	0.044355	0.056559	1.283094
C	1.134648	-0.000578	2.308835
Mg	1.685613	1.954943	3.023208
Cl	2.214771	3.505100	4.555799
H	1.148555	-0.204917	-0.507867
H	-0.655906	0.035093	-0.713818
H	-0.954989	0.208906	1.666720
H	0.824760	-0.612741	3.153507
H	2.025048	-0.469687	1.891003
C	1.260302	3.706280	0.869175
C	2.541492	3.316860	0.730743
H	0.463551	3.183118	0.370784
H	2.804999	2.477613	0.110894
H	1.001068	4.574813	1.448551
H	3.346101	3.864764	1.189078

MgH-TS1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.439800
C	1.244037	0.000000	2.251273
Mg	2.109289	1.995207	2.456435
H	-0.972549	-0.175802	-0.434733
H	0.738613	-0.654042	-0.442840
H	-0.888231	0.383754	1.921816
H	1.041569	-0.345717	3.263252
H	1.993598	-0.666120	1.827607
X	1.569061	2.144323	3.284637
H	2.758405	3.576232	2.704502
C	0.482161	1.613610	-0.650302
C	0.363995	1.682743	-2.077551
H	-0.157910	2.310929	-0.127141
H	-0.585598	1.911819	-2.528264
X	1.453847	1.395565	-0.741312
H	1.507133	1.690122	-0.303047
H	1.068925	1.161955	-2.701927

MgCl-TS1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.438800
C	1.241578	0.000000	2.248002
Mg	2.110942	1.989006	2.438013
H	-0.970223	-0.186562	-0.434206
H	0.747797	-0.641451	-0.445103
H	-0.889592	0.373625	1.924012
H	1.048006	-0.332035	3.264573
H	2.000591	-0.653678	1.825382
X	1.571664	2.145671	3.265440
Cl	2.945879	4.026155	2.747797
C	0.457845	1.626285	-0.648530
C	0.332183	1.693611	-2.073617
H	-0.190259	2.312667	-0.120816
H	-0.619478	1.918972	-2.520873
X	1.429753	1.411327	-0.744386
H	1.484058	1.716376	-0.306678
H	1.044365	1.189448	-2.702872

MgH-Int

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.484500
C	1.260843	0.000000	2.270552
Mg	2.178890	1.979495	2.378722
H	-0.990141	-0.220844	-0.382543
H	0.681586	-0.749684	-0.390352
H	-0.866344	0.440486	1.957538
H	1.071823	-0.304676	3.298199
H	1.983604	-0.701168	1.856206
X	1.660020	2.174656	3.211000
H	2.853229	3.563910	2.520820
C	0.455147	1.423726	-0.641112
C	0.350622	1.455505	-2.114868
H	-0.158163	2.200826	-0.195098
H	-0.595109	1.684097	-2.573871
X	1.425072	1.191779	-0.714904
H	1.488087	1.589804	-0.338832
H	1.025266	0.857150	-2.702629

MgCl-Int

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.484500
C	1.253399	0.000000	2.270762
Mg	2.175523	1.979066	2.369910
H	-0.984712	-0.246046	-0.380035
H	0.699519	-0.732363	-0.390956
H	-0.872108	0.422760	1.961277
H	1.073249	-0.288138	3.302647
H	1.991062	-0.684049	1.858531
X	1.654964	2.180042	3.199745
Cl	3.026165	4.027995	2.537348
C	0.415389	1.435554	-0.637915
C	0.310620	1.465316	-2.111596
H	-0.218717	2.195483	-0.191638
H	-0.637519	1.679360	-2.571942
X	1.388698	1.218175	-0.711501
H	1.444086	1.631838	-0.337113
H	1.002022	0.888305	-2.700674

MgH-TS2

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.479600
C	1.273113	0.000000	2.241147
Mg	2.377876	1.884258	2.052232
H	-0.895896	-0.466195	-0.393538
H	0.848077	-0.557916	-0.380199
H	-0.855654	0.457714	1.955274
H	1.097822	-0.155156	3.303358
H	1.933312	-0.796650	1.903036
X	1.899135	2.245191	2.852566
H	3.217093	3.393318	1.967367
C	0.049386	1.520747	-0.651087
C	1.126549	1.700922	-1.644275
H	-0.922275	1.687648	-1.101004
H	1.106179	1.124800	-2.552933
X	0.480097	2.202911	-0.060206
H	0.143295	2.242398	0.155822
H	2.094756	2.064915	-1.343891

MgCl-TS2

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.480700
C	1.266048	0.000000	2.239059
Mg	2.383329	1.876506	1.995309
H	-0.869546	-0.512742	-0.394196
H	0.875917	-0.514148	-0.379070
H	-0.860676	0.441437	1.960636
H	1.106308	-0.125054	3.305332
H	1.939931	-0.783990	1.904485
X	1.909116	2.261691	2.786988
Cl	3.456716	3.817184	1.799180
C	-0.029995	1.519610	-0.638308
C	0.993339	1.740333	-1.680795
H	-1.027859	1.658092	-1.037947
H	0.967325	1.151359	-2.580552
X	0.388861	2.232736	-0.076158
H	0.080643	2.242893	0.165687
H	1.938277	2.195524	-1.439310

MgH-TS

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.388400
C	1.144778	0.000000	2.203995
Mg	2.003913	2.150537	2.201075
H	2.993747	3.044808	3.326809
H	0.876977	-0.359970	-0.512400
H	-0.928808	-0.165105	-0.518149
H	-0.945001	0.187820	1.877237
H	0.999608	-0.159517	3.263565
H	2.026259	-0.494871	1.815429
C	0.246356	2.124029	-0.538771
C	1.179427	2.890403	0.180200
H	0.504183	1.766834	-1.517828
H	2.127720	3.092172	-0.299265
H	-0.799932	2.326329	-0.406039
H	0.781542	3.743325	0.719245

MgCl-TS

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.388000
C	1.146748	0.000000	2.204621
Mg	1.939286	2.145219	2.125644
Cl	3.210743	3.301942	3.574400
H	0.880930	-0.347969	-0.513699
H	-0.927336	-0.171461	-0.517889
H	-0.945496	0.181499	1.877602
H	1.002691	-0.156246	3.264015
H	2.028329	-0.493776	1.815727
C	0.202892	2.132354	-0.553329
C	1.127435	2.931173	0.144553
H	0.459855	1.765026	-1.528418
H	2.064793	3.145288	-0.349707
H	-0.845975	2.312031	-0.410415
H	0.715746	3.784071	0.671730

MgH-Products

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.505600
C	1.089751	0.000000	2.295126
Mg	0.615498	2.820613	1.780124
H	1.045705	3.439233	3.343515
H	1.019487	-0.064437	-0.370689
H	-0.524119	-0.887728	-0.346885
H	-0.972387	-0.007130	1.977571
H	1.012674	-0.028835	3.367172
H	2.084254	-0.035594	1.881184
C	-0.689114	1.273220	-0.600384
C	0.071470	2.573829	-0.300653
H	-0.795652	1.108460	-1.672071
H	0.991432	2.586578	-0.890885
H	-1.702160	1.325814	-0.202913
H	-0.511128	3.420981	-0.661101

MgCl-Products

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.506000
C	1.091479	0.000000	2.295527
Mg	0.660200	2.709934	1.785140
Cl	1.195861	3.496330	3.812346
H	1.017719	-0.086306	-0.370809
H	-0.543905	-0.875416	-0.346148
H	-0.971705	-0.002605	1.979650
H	1.015784	-0.028196	3.367588
H	2.084942	-0.048878	1.879405
C	-0.662659	1.289462	-0.599420
C	0.118448	2.575574	-0.290567
H	-0.763088	1.132352	-1.672033
H	1.033299	2.590786	-0.886071
H	-1.676798	1.359338	-0.208552
H	-0.457028	3.439821	-0.615936