

Table S7: Atomic Coordinates (Angstroms).

AlH ₃	Atom Number	Atomic Number	x	y	z
	1	1	0.000000	0.000000	-1.588819
	2	13	0.000000	0.000000	0.000000
	3	1	1.375958	0.000000	0.794410
	4	1	-1.375958	0.000000	0.794410
AlH ₂	1	1	-0.070825	0.000000	-1.545572
	2	13	-0.094790	0.000000	0.054727
	3	1	1.303093	0.000000	0.834122
AlH	1	13	0.000000	0.000000	-0.118488
	2	1	0.000000	0.000000	1.540338
AlCl ₃	1	17	0.000000	2.069244	0.000000
	2	13	0.000000	0.000000	0.000000
	3	17	-1.792018	-1.034622	0.000000
	4	17	1.792018	-1.034622	0.000000
AlCl ₂ ² A ₁	1	17	0.000000	1.804187	-0.295438
	2	13	0.000000	0.000000	0.772684
	3	17	0.000000	-1.804187	-0.295438
AlCl ¹ Σ	1	13	0.000000	0.000000	-1.209794
	2	17	0.000000	0.000000	0.925136
AlF ₃	1	13	0.000000	0.000000	0.000000
	2	9	0.000000	0.000000	1.644717
	3	9	1.424367	0.000000	-0.822359
	4	9	-1.424367	0.000000	-0.822359
AlF ₂ ² A'	1	9	0.000000	1.412270	-0.409309
	2	13	0.000000	0.018769	0.491318
	3	9	0.000000	-1.439381	-0.300372
AlF ¹ Σ	1	13	0.000000	0.000000	-0.683459
	2	9	0.000000	0.000000	0.987218
Al(OH) ₃ C ₃ axis	1	13	0.000000	0.000000	0.000000
	2	8	-0.008305	0.000000	1.712172
	3	8	1.486937	0.000000	-0.848894
	4	8	-1.478632	0.000000	-0.863278
	5	1	0.828950	0.000000	2.196196
	6	1	1.487487	0.000000	-1.815990
	7	1	-2.316437	0.000000	-0.380207
Al(OH) ₂ ² A ₁ planar, trans, trans	1	13	0.000000	0.000000	0.494187

	2	8	0.000000	1.464544	-0.409032
	3	8	0.000000	-1.464544	-0.409032
	4	1	0.000000	2.310929	0.060046
	5	1	0.000000	-2.310929	0.060046
AlOH ¹ A' linear	1	13	-0.244275	0.000000	-0.692842
	2	8	0.316342	0.000000	0.900642
	3	1	0.644840	0.000000	1.801804
Al(CH ₃) ₃	1	6	-0.721883	1.832006	-0.006156
	2	13	-0.000001	0.000002	0.000000
	3	6	-1.225624	-1.541180	0.000931
	4	6	1.947507	-0.290828	0.005227
	5	1	-1.358324	2.003446	-0.882131
	6	1	-1.359412	2.008818	0.867975
	7	1	0.053165	2.603545	-0.008005
	8	1	-1.058471	-2.178978	0.876746
	9	1	-1.057380	-2.180799	-0.873368
	10	1	-2.281322	-1.255747	-0.000070
	11	1	2.414736	0.175699	0.880355
	12	1	2.418860	0.171809	-0.869752
	13	1	2.228153	-1.347805	0.008243
Al(CH ₃) ₂ ² A'	1	13	-0.497897	-0.257224	-0.287461
	2	6	-0.549253	0.155507	1.646484
	3	6	1.151270	0.155507	-1.298909
	4	1	-0.372699	1.224763	1.812687
	5	1	0.249589	-0.381041	2.171909
	6	1	-1.496283	-0.104810	2.123359
	7	1	1.383483	1.224763	-1.229110
	8	1	1.090741	-0.104810	-2.357499
	9	1	2.005723	-0.381041	-0.869805
AlCH ₃ ¹ A ₁	1	13	0.000000	0.000000	-0.871689
	2	6	0.000000	0.000000	1.122112
	3	1	1.018285	0.000000	1.533093
	4	1	-0.509142	0.881861	1.533093
	5	1	-0.509142	-0.881861	1.533093
AlH ₂ Cl	1	1	1.828389	0.856941	-1.055621
	2	13	0.462560	0.925120	-0.267059
	3	1	-0.271489	2.256859	0.156744
	4	17	-0.445305	-0.890609	0.257097
AlHCl ₂	1	1	0.000000	0.000000	2.289292
	2	13	0.000000	0.000000	0.721237
	3	17	0.000000	1.788778	-0.343099
	4	17	0.000000	-1.788778	-0.343099
HAICI ² A'	1	1	-1.391012	1.835776	0.000000
	2	13	0.046644	1.133795	0.000000
	3	17	0.046155	-0.975006	0.000000

AlH ₂ F	1	13	0.000000	0.000000	-0.562981
	2	9	0.000000	0.000000	1.099735
	3	1	1.403103	0.000000	-1.289432
	4	1	-1.403103	0.000000	-1.289432
AlHF ₂	1	13	0.000000	0.000000	0.433285
	2	1	0.000000	0.000000	1.998117
	3	9	1.413303	0.000000	-0.423935
	4	9	-1.413303	0.000000	-0.423935
HAlF	1	13	-0.080479	0.000000	-0.619190
	2	9	-0.032209	0.000000	1.047292
	3	1	1.336112	0.000000	-1.376163
H ₂ AlOH	1	8	0.046017	0.000000	-1.116225
	2	13	-0.075415	0.000000	0.599883
	3	1	0.913398	0.000000	-1.545040
	4	1	-1.542667	0.000000	1.186535
	5	1	1.241528	0.000000	1.489818
HAl(OH) ₂ OAlOH cis, trans	1	13	0.017135	0.000000	0.463113
	2	1	0.061011	0.000000	2.039308
	3	8	1.503055	0.000000	-0.388645
	4	8	-1.439645	0.000000	-0.447574
	5	1	1.512500	0.000000	-1.356200
	6	1	-2.303551	0.000000	-0.013826
HAlOH ² A' trans	1	13	-0.040286	0.000000	-0.666215
	2	8	-0.004594	0.000000	1.059733
	3	1	1.397835	0.000000	-1.370510
	4	1	-0.837368	0.000000	1.553438
AlH ₂ (CH ₃) HCAIH planar	1	13	0.003174	0.000000	-0.718084
	2	6	0.003585	0.000000	1.242945
	3	1	1.361082	0.000000	-1.552463
	4	1	-1.378878	0.000000	-1.512486
	5	1	1.007888	0.000000	1.672604
	6	1	-0.526432	0.875031	1.634882
	7	1	-0.526432	-0.875031	1.634882
AlH(CH ₃) ₂	1	1	0.000000	0.483176	-2.048823
	2	13	0.000000	0.116033	-0.492011
	3	6	1.730696	-0.097331	0.412714
	4	6	-1.730696	-0.097331	0.412714
	5	1	2.326393	0.819400	0.337465
	6	1	2.326357	-0.883897	-0.064167
	7	1	1.642066	-0.347319	1.472903
	8	1	-2.326393	0.819400	0.337465
	9	1	-1.642066	-0.347319	1.472903

	10	1	-2.326357	-0.883897	-0.064167
HAl(CH ₃) ² A'					
HAICH trans					
	1	13	0.365350	-0.350440	0.611196
	2	1	0.325463	-1.956178	0.544469
	3	6	-0.503472	0.662592	-0.842261
	4	1	-0.434187	1.745444	-0.726354
	5	1	-1.564708	0.395449	-0.903911
	6	1	-0.055286	0.395449	-1.806187
AlFCl ₂					
	1	13	0.000000	0.000000	0.350858
	2	9	0.000000	0.000000	1.998363
	3	17	1.799331	0.000000	-0.663130
	4	17	-1.799331	0.000000	-0.663130
AlF ₂ Cl					
	1	13	0.000000	0.000000	-0.415425
	2	17	0.000000	0.000000	1.646789
	3	9	1.415890	0.000000	-1.255271
	4	9	-1.415890	0.000000	-1.255271
ClAlF					
	1	13	-0.798777	0.000000	0.069247
	2	9	-0.779176	0.000000	1.728533
	3	17	1.023335	0.000000	-0.968059
Al(OH)Cl ₂					
	1	8	-0.127190	2.044509	-0.008033
	2	13	-0.025316	0.347011	-0.001599
	3	1	-0.974061	2.510356	-0.061517
	4	17	1.852555	-0.515395	0.116999
	5	17	-1.716044	-0.859756	-0.108378
AlCl(OH) ₂ OAlOH cis, trans					
	1	13	0.000226	0.000000	-0.407029
	2	17	0.035008	0.000000	1.674885
	3	8	1.491903	0.000000	-1.231211
	4	8	-1.464083	0.000000	-1.285504
	5	1	1.506342	0.000000	-2.199096
	6	1	-2.326982	0.000000	-0.848842
ClAlOH ² A', trans					
	1	13	-0.793530	0.000000	0.047046
	2	8	-0.703024	0.000000	1.761798
	3	17	1.026604	0.000000	-1.000021
	4	1	-1.512190	0.000000	2.294362
AlCl ₂ (CH ₃) HCAICI planar					
	1	13	0.007122	0.000000	0.334418
	2	6	0.003877	0.000000	2.272864
	3	17	1.775467	0.000000	-0.779530
	4	17	-1.780642	0.000000	-0.748899
	5	1	1.015990	0.000000	2.682821
	6	1	-0.521932	0.878804	2.657932
	7	1	-0.521932	-0.878804	2.657932
AlCl(CH ₃) ₂					

	1	17	-1.677844	0.066598	-0.330975
	2	13	0.395303	-0.015690	0.077978
	3	6	1.245083	-1.764539	-0.099501
	4	6	1.245083	1.665698	0.590717
	5	1	1.126547	-2.156404	-1.114852
	6	1	0.780678	-2.495477	0.570276
	7	1	2.314477	-1.736417	0.125648
	8	1	1.126547	2.419776	-0.194051
	9	1	2.314477	1.552684	0.787468
	10	1	0.780678	2.080700	1.491077
AlCl(CH ₃) trans					
	1	13	-0.610727	-0.549583	0.097588
	2	17	0.409370	1.162676	0.813633
	3	6	0.060786	-1.353420	-1.568088
	4	1	1.106388	-1.653110	-1.442767
	5	1	0.025235	-0.617789	-2.378266
	6	1	-0.516178	-2.229493	-1.870847
AlF ₂ (OH)					
	1	8	0.019418	1.682944	0.000000
	2	13	0.011302	-0.016125	0.000000
	3	1	-0.803116	2.190985	0.000000
	4	9	1.446880	-0.825393	0.000000
	5	9	-1.391231	-0.890708	0.000000
AlF(OH) ₂ FAIOH cis, cis					
	1	9	-0.000001	-1.657324	0.000000
	2	13	0.000000	0.004428	0.000000
	3	8	0.000001	0.876326	1.463539
	4	8	0.000001	0.876326	-1.463539
	5	1	0.000000	0.418568	2.314745
	6	1	0.000000	0.418568	-2.314745
FAIOH trans					
	1	13	-0.304861	0.388598	0.000000
	2	8	1.411720	0.453625	0.000000
	3	9	-1.020389	-1.110703	0.000000
	4	1	1.852931	1.315556	0.000000
Al(OH) ₂ CH ₃ OAlOH cis, trans					
	1	13	-0.000070	-0.000135	-0.043144
	2	6	0.036858	-0.001432	1.904590
	3	8	1.478648	-0.160920	-0.903329
	4	8	-1.420331	0.152114	-1.007944
	5	1	1.466179	-0.160604	-1.871116
	6	1	-2.298025	0.247327	-0.614809
	7	1	-0.358621	0.929867	2.320798
	8	1	1.061985	-0.117746	2.264725
	9	1	-0.558294	-0.818045	2.323918
Al(OH)(CH ₃) ₂					
	1	8	-0.222706	0.547845	0.535121
	2	13	-0.073754	0.040921	2.181475
	3	6	1.687395	-0.277925	2.988507
	4	6	-1.761082	-0.183696	3.142719

	5	1	2.524560	0.071113	2.377449
	6	1	1.840181	-1.348481	3.165868
	7	1	1.764798	0.212025	3.964837
	8	1	-2.614733	-0.158002	2.460700
	9	1	-1.905779	0.614583	3.878821
	10	1	-1.797926	-1.127961	3.695144
	11	1	0.559046	0.700593	-0.013734
CH ₃ AlOH HOAlC cis					
	1	6	-0.447374	0.012178	-1.616326
	2	13	-0.452855	-0.054840	0.360382
	3	8	1.011373	0.051468	1.275705
	4	1	1.869912	0.137167	0.833779
	5	1	0.558688	-0.054363	-2.041626
	6	1	-1.048856	-0.804017	-2.027170
	7	1	-0.899367	0.949316	-1.957624
HAl(OH)Cl ClAlOH cis					
	1	8	-0.750592	0.000000	-1.779584
	2	13	-0.755119	0.000000	-0.072173
	3	1	0.063084	0.000000	-2.303298
	4	1	-2.130126	0.000000	0.681497
	5	17	1.052254	0.000000	0.988042
HAl(CH ₃)Cl HCAICI trans					
	1	13	-0.755956	0.000000	-0.003709
	2	6	-0.714297	0.000000	1.943977
	3	17	1.074101	0.000000	-1.043919
	4	1	-2.060411	0.000000	-0.900420
	5	1	-1.718807	0.000000	2.375189
	6	1	-0.183644	-0.876894	2.328105
	7	1	-0.183644	0.876894	2.328105
HAl(OH)CH ₃ ClAlOH trans, HCAIO cis					
	1	13	-0.380269	0.083460	-0.302596
	2	6	-0.391041	0.020768	1.645965
	3	8	1.124550	-0.180424	-1.102570
	4	1	-1.674414	0.362822	-1.191300
	5	1	1.174089	-0.157865	-2.068597
	6	1	-0.737828	0.968062	2.071861
	7	1	0.602326	-0.184756	2.051936
	8	1	-1.070833	-0.754468	2.014614
Al(OH)CH ₃ Cl					
	1	13	0.094228	0.036285	-0.055494
	2	6	0.059233	0.004107	1.882496
	3	8	1.568365	-0.179934	-0.899868
	4	17	-1.661756	0.335230	-1.177205
	5	1	1.615989	-0.168648	-1.866402
	6	1	-0.321751	0.946516	2.286302
	7	1	1.059559	-0.161662	2.289038
	8	1	-0.595768	-0.789867	2.252523
AlO ² Σ					
	1	13	0.000000	0.000000	-0.627735

HAIO $^1\Sigma$	2	8	0.000000	0.000000	1.020070
	1	8	0.000000	0.000000	-1.108153
	2	13	0.000000	0.000000	0.520868
H ₂ AlO 2B_2	3	1	0.000000	0.000000	2.093938
	1	8	0.000000	0.000000	-1.206275
	2	13	0.000000	0.000000	0.551180
	3	1	1.420081	0.000000	1.242427
	4	1	-1.420081	0.000000	1.242427
AlC $^4\Sigma^-$	1	13	0.000000	0.000000	-0.620877
	2	6	0.000000	0.000000	1.345233
AlCH singlet linear	1	13	-0.270680	0.000000	-0.274469
	2	6	0.412127	0.000000	1.547509
	3	1	0.793861	0.000000	2.566960
HAICH HAICH trans $^2A''$	1	13	-0.082743	-0.092090	-0.619087
	2	6	0.057174	0.185732	1.237010
	3	1	1.198948	-0.253011	-1.550185
	4	1	-0.466329	0.335794	2.176256
HAICH ₂ singlet linear C_{2v}	1	13	0.000000	0.634320	0.000000
	2	1	0.000000	2.208762	0.000000
	3	6	0.000000	-1.160675	0.000000
	4	1	-0.916517	-1.745439	0.000000
	5	1	0.916517	-1.745439	0.000000
H ₂ AlCH $^3A''$	1	13	0.053764	0.000000	-0.577885
	2	6	-0.091933	0.000000	1.312216
	3	1	1.496400	0.000000	-1.237502
	4	1	-1.256560	0.000000	-1.474689
	5	1	-0.387168	0.000000	2.351400
AlH ₂ OCH ₃ HCOAl cis	1	13	-0.465070	0.000000	-1.097101
	2	8	-0.261576	0.000000	0.604408
	3	6	0.925787	0.000000	1.379392
	4	1	0.822127	0.000000	-2.029049
	5	1	-1.956404	0.000000	-1.620246
	6	1	1.831733	0.000000	0.761038
	7	1	0.943171	0.886846	2.019480
	8	1	0.943171	-0.886846	2.019480

Table S8. Moments of Inertia (amu Bohr²).

Species	I_1	I_2	I_3
AlH ₃	13.628	13.628	27.255
AlH ₂	4.513	13.587	18.101
AlH	0.000	9.547	9.547
AlCl ₃	802.036	802.036	1604.071
AlCl ₂ ² A ₁	79.324	812.965	892.290
AlCl ¹ Σ	0.000	247.896	247.896
AlF ₃	275.289	275.289	550.578
AlF ₂ ² A'	40.400	276.256	316.655
AlF ¹ Σ	0.000	111.122	111.122
Al(OH) ₃ C ₃ axis	280.923	280.923	561.846
Al(OH) ₂ ² A ₁ planar, trans, trans	42.662	283.468	326.130
AlOH ¹ A' linear	0.000	116.671	116.671
Al(CH ₃) ₃	365.770	365.771	698.471
Al(CH ₃) ₂ ² A'	76.512	351.553	405.788
AlCH ₃ ¹ A ₁	11.195	155.649	155.649
AlH ₂ Cl	14.106	264.591	278.697
AlHCl ₂	98.202	799.139	897.341
HAICl ² A'	6.946	254.917	261.863
AlH ₂ F	14.171	123.842	138.013
AlHF ₂	56.531	271.029	327.560
HAIF	6.825	118.061	124.886
H ₂ AlOH	16.379	128.835	145.214
HA(OH) ₂ OAlOH cis, trans	62.288	274.798	337.086
HAIOH ² A' trans	8.921	123.065	131.986
AlH ₂ (CH ₃) HCAIH planar	24.673	167.080	180.730
AlH(CH ₃) ₂	83.532	365.057	426.544
HA(CH ₃) ² A' HAICH trans	17.901	160.393	167.164
AlFCl ₂	392.587	808.595	1201.183
AlF ₂ Cl	272.022	569.025	841.047
ClAlF	52.176	501.412	553.588
Al(OH)Cl ₂	394.091	807.907	1201.998
AlCl(OH) ₂ OAlOH cis, trans	277.266	566.653	843.919
ClAlOH ² A', trans	55.058	494.418	549.476
AlCl ₂ (CH ₃) HCAICl planar	457.648	800.928	1247.457
AlCl(CH ₃) ₂	372.061	580.760	930.693
AlCl(CH ₃) trans	77.924	521.787	588.496
AlF ₂ (OH)	275.164	278.963	554.126
AlF(OH) ₂ FAIOH cis, cis	275.065	283.259	558.323
FAIOH trans	41.475	279.738	321.214
Al(OH) ₂ CH ₃ OAlOH cis, trans	280.801	336.577	606.238
Al(OH)(CH ₃) ₂	309.072	364.945	651.855
CH ₃ AlOH HOAlC cis	60.401	320.239	369.476
HA(OH)Cl ClAlOH cis	73.187	492.088	565.275
HA(CH ₃)Cl HCAICl trans	91.393	523.893	604.216
HA(OH)CH ₃ CAIOH trans, HCAIO cis	73.641	315.104	377.655
Al(OH)CH ₃ Cl	315.736	586.512	891.122

AlO $^2\Sigma$	0.000	97.370	97.370
HAIO $^1\Sigma$	0.000	111.865	111.865
H ₂ AlO 2B_2	14.516	123.205	137.720
AlC $^4\Sigma^-$	0.000	114.657	114.657
AlCH singlet linear	0.000	133.099	133.099
HAICH HAICH trans $^2A''$	6.650	131.042	137.692
HAICH ₂ singlet linear C _{2v}	6.046	135.681	141.727
H ₂ AlCH $^3A''$	13.876	140.242	154.118
AlH ₂ OCH ₃ HCOAl cis	42.045	338.687	369.409

Table S9. Scaled Vibrational Frequencies (cm⁻¹).

Species	ν	ν	ν	ν	ν
AlH ₃	678.5	755.6	755.6	1811.3	1811.3
	1815.5				
AlH ₂	732.3	1743.0	1762.9		
AlH	1580.9				
AlCl ₃	139.8	139.8	190.7	356.7	573.4
	573.4				
AlCl ₂ ² A ₁	145.2	428.8	524.7		
AlCl ¹ Σ	424.7				
AlF ₃	242.3	242.3	282.2	665.6	923.8
	923.8				
AlF ₂ ² A'	245.1	738.0	868.5		
AlF ¹ Σ	771.2				
Al(OH) ₃	216.2	216.2	255.7	327.7	327.7
C ₃ axis	334.3	603.2	621.6	621.6	657.7
	884.8	884.8	3729.1	3729.1	3731.1
Al(OH) ₂ ² A ₁	232.8	265.3	291.4	540.8	612.0
planar,trans, trans	711.8	856.5	3730.4	3730.7	
AlOH ¹ A' linear	148.5	781.5	3780.6		
Al(CH ₃) ₃	22.7	22.8	38.8	157.3	157.3
	175.1	473.1	553.9	553.9	575.9
	596.1	596.1	708.0	736.6	736.6
	1246.6	1246.6	1250.6	1428.4	1428.4
	1429.1	1431.3	1431.3	1432.5	2822.7
	2822.7	2824.7	2868.4	2868.4	2869.0
	2893.5	2894.4	2894.4		
Al(CH ₃) ₂ ² A'	27.0	44.0	157.2	512.5	536.1
	553.0	559.5	630.2	732.5	1228.7
	1236.8	1419.6	1424.6	1426.8	1435.4
	2820.3	2822.7	2869.7	2871.7	2907.1
	2907.3				
AlCH ₃ ¹ A ₁	482.8	482.8	530.8	1228.9	1414.9
	1414.9	2797.6	2854.9	2854.9	
AlH ₂ Cl	479.1	490.3	579.7	746.7	1853.5
	1861.3				
AlHCl ₂	154.4	433.3	443.6	539.4	634.4
	1899.6				
HAICl ² A'	461.2	551.6	1750.6		
AlH ₂ F	547.7	607.5	747.9	816.9	1851.6
	1851.6				
AlHF ₂	261.3	481.1	654.6	751.4	893.6
	1908.8				
HAIF	584.3	789.2	1717.4		
H ₂ AlOH	399.3	470.7	602.7	653.9	741.8
	812.8	1812.7	1843.6	3727.1	
HAl(OH) ₂	228.6	309.8	359.8	495.8	543.6
OAlOH cis, trans	613.6	679.6	745.9	870.6	1857.7
	3724.7	3734.8			
HAlOH ² A' trans	396.0	526.0	646.9	776.8	1733.7

	3727.3				
AlH ₂ (CH ₃)	14.0	391.0	465.7	576.5	698.5
HCAIH planar	736.5	768.7	1248.7	1427.4	1430.6
	1788.7	1795.9	2829.9	2877.4	2906.1
AlH(CH ₃) ₂	19.9	29.8	167.5	367.0	498.0
	516.5	549.6	619.3	705.7	730.6
	759.3	1246.6	1249.5	1424.7	1429.0
	1431.0	1432.3	1771.1	2826.2	2827.1
	2872.8	2873.6	2899.0	2900.5	
HAl(CH ₃)	85.7	444.9	547.9	568.4	739.7
² A' HAICH trans	1232.8	1421.5	1430.3	1724.7	2825.5
	2875.9	2913.2			
AlFCl ₂	144.4	196.1	220.3	405.5	581.7
	854.1				
AlF ₂ Cl	178.0	229.9	251.3	471.8	792.9
	914.9				
ClAlF	189.9	468.4	812.8		
Al(OH)Cl ₂	145.1	185.6	216.2	326.4	403.9
	534.4	607.1	852.2	3730.4	
AlCl(OH) ₂	174.2	207.1	238.7	321.6	330.4
OAlOH cis, trans	450.6	590.9	608.4	777.2	896.6
	3725.7	3735.7			
ClAlOH ² A' trans	186.6	296.7	453.9	566.0	803.5
	3727.0				
AlCl ₂ (CH ₃)	9.5	145.2	148.5	181.1	386.8
HCAICl planar	525.2	638.2	662.5	711.0	1253.9
	1423.4	1425.1	2846.2	2902.8	2924.4
AlCl(CH ₃) ₂	26.6	33.7	152.8	153.2	178.0
	413.1	551.6	574.1	622.6	673.6
	692.0	737.4	1250.7	1254.0	1422.9
	1425.7	1429.3	1429.3	2836.1	2837.7
	2891.0	2891.6	2903.6	2905.1	
AlCl(CH ₃) trans	47.6	151.9	432.9	574.8	574.9
	681.8	1225.0	1418.1	1424.9	2837.0
	2896.6	2918.2			
AlF ₂ (OH)	225.1	246.4	277.0	323.4	575.0
	665.6	899.9	921.7	3738.6	
AlF(OH) ₂	226.0	227.5	269.6	279.9	333.1
FAIOH cis, cis	567.6	598.2	666.6	875.5	915.0
	3738.5	3739.6			
FAIOH trans	239.7	299.7	572.1	724.6	864.9
	3728.2				
Al(OH) ₂ CH ₃	8.9	174.3	221.1	224.1	304.6
OAlOH cis, trans	367.1	536.0	574.8	625.9	661.5
	684.0	779.4	861.7	1251.4	1432.7
	1434.6	2838.6	2889.9	2911.6	3722.4
	3736.7				
Al(OH)(CH ₃) ₂	16.5	24.8	156.3	194.6	201.9
	351.1	500.8	568.3	580.8	596.6
	683.9	694.9	700.7	814.8	1247.9
	1250.7	1429.3	1430.0	1432.7	1433.8

	2825.6	2831.2	2878.1	2880.4	2894.2
	2905.9	3730.0			
CH ₃ AlOH	10.0	172.7	321.4	515.2	559.7
HOAlCl cis	575.9	676.2	760.1	1222.4	1423.4
	1431.5	2806.5	2881.6	2908.1	3683.3
HA(OH)Cl	191.3	356.8	463.2	464.5	578.8
ClAlOH cis	657.1	824.6	1893.9	3730.8	
HA(CH ₃)Cl	17.9	158.3	378.8	449.9	574.7
HCAICl trans	619.7	669.8	738.5	1252.6	1425.0
	1426.4	1841.6	2838.8	2894.5	2907.3
HA(OH)CH ₃	32.0	192.3	327.6	449.4	522.3
CAIOH trans, HCAIO	565.0	670.8	678.5	720.4	820.2
cis	1248.4	1428.8	1430.6	1793.2	2833.5
	2882.1	2910.7	3727.8		
Al(OH)CH ₃ Cl	30.8	148.6	190.9	199.1	360.3
	424.6	583.0	619.4	666.4	706.8
	833.1	1252.2	1427.6	1428.1	2845.8
	2902.1	2919.1	3729.8		
AlO ² Σ	722.1				
HAIO ¹ Σ	432.6	432.6	1069.2	1914.6	
H ₂ AlO ² B ₂	461.2	586.5	691.9	775.4	1849.2
	1855.3				
AlC ⁴ Σ ⁻	595.3				
AlCH singlet linear	499.4	640.0	3023.5		
HAICH	365.3	441.3	566.7	676.3	1768.8
² A'' HAICH trans	3006.3				
HAICH ₂	120.5	358.1	605.1	655.8	841.5
singlet linear C _{2v}	1338.1	1884.3	2945.0	3014.2	
H ₂ AlCH ³ A''	123.7	299.2	490.7	576.2	680.8
	767.3	1811.5	1819.6	3041.6	
AlH ₂ OCH ₃	83.2	147.6	174.2	539.7	599.9
HCOAl cis	661.6	766.4	1139.6	1167.8	1189.4
	1469.6	1478.0	1484.7	1811.4	1840.6
	2840.7	2892.2	2907.0		

TABLE S10: Calculated Electronic Energies for Al-H-C-O-F-Cl Compounds at G2 Level of Theory (hartrees).

species	G2
AlH ₃	-243.753958
AlH ₂	-243.118964
AlH	-242.546190
AlCl ₃	-1621.448747
AlCl ₂ ² A ₁	-1161.585244
AlCl ¹ Σ	-701.800168
AlF ₃	-541.499452
AlF ₂ ² A'	-441.618733
AlF ¹ Σ	-341.821260
Al(OH) ₃ C ₃ axis	-469.400344
Al(OH) ₂ ² A ₁ planar,trans,trans	-393.548819
AlOH ¹ A' linear	-317.784010
Al(CH ₃) ₃	-361.476928
Al(CH ₃) ₂ ² A'	-321.599290
AlCH ₃ ¹ A ₁	-281.789132
AlH ₂ Cl	-702.987801
AlHCl ₂	-1162.220232
HAICl ² A'	-702.353344
AlH ₂ F	-343.005223
AlHF ₂	-442.256099
HAIF	-342.369944
H ₂ AlOH	-318.970018
HAl(OH) ₂ OAlOH cis,trans	-394.186773
HAIOH ² A' trans	-318.334669
AlH ₂ (CH ₃) HCAIH planar	-282.994635
AlH(CH ₃) ₂	-322.235711
HAl(CH ₃) ² A' HAlCH trans	-282.358735
AlFCl ₂	-1261.465704
AlF ₂ Cl	-901.482694
ClAlF	-801.601716
Al(OH)Cl ₂	-1237.433798
AlCl(OH) ₂ OAlOH cis, trans	-853.417789
ClAlOH ² A',trans	-777.567650
AlCl ₂ (CH ₃) HCAICl planar	-1201.464929
AlCl(CH ₃) ₂	-781.473995
AlCl(CH ₃) trans	-741.595938
AlF ₂ (OH)	-517.467592
AlF(OH) ₂ FAIOH cis, cis	-493.434284
FAIOH trans	-417.584276
Al(OH) ₂ CH ₃ OAlOH cis, trans	-433.429104
Al(OH)(CH ₃) ₂	-397.454003
CH ₃ AlOH HAOLC cis	-357.574221
HAl(OH)Cl ClAlOH cis	-778.204910
HAl(CH ₃)Cl HCAICl trans	-742.231008
HAl(OH)CH ₃ CAIOH trans,hcalo cis	-358.212373
Al(OH)CH ₃ Cl	-817.448704
AlO ² Σ	-317.102389

HAIO $^1\Sigma$	-317.717402
H ₂ AlO 2B_2	-318.278195
AlC $^4\Sigma^-$	-279.837286
AlCH singlet linear	-280.443388
HAICH HAICH trans $^2A''$	-281.076878
HAICH ₂ singlet linear C _{2v}	-281.730266
H ₂ AlCH $^3A''$	-281.681210
AlH ₂ OCH ₃ HCOAl cis	-358.173936
Al	-241.930950
H	-0.500000
Cl	-459.676627
F	-99.632814
O	-74.982030
C	-37.784301

Table S11. Polynomial Coefficients for Thermochemical Data in CHEMKIN^a format.

ALH3	H	3Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.36136173E+01	0.86060067E-02	-0.49030616E-05	0.13093924E-08	-0.13426153E-12					2	
0.14005457E+05	0.17496452E+01	0.25175901E+01	0.10497049E-01	-0.51033191E-05					3	
0.42088884E-09	0.15948427E-12	0.14386092E+05	0.77525506E+01						4	
ALH2	H	2Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.32629111E+01	0.50466104E-02	-0.28814143E-05	0.77111851E-09	-0.79223387E-13					2	
0.31055749E+05	0.56251145E+01	0.37869097E+01	0.72466810E-03	0.66452812E-05					3	
-0.74124397E-08	0.23755831E-11	0.31072085E+05	0.36782064E+01						4	
ALH	H	1Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.29913047E+01	0.20894600E-02	-0.12165514E-05	0.33063586E-09	-0.34391629E-13					2	
0.28827046E+05	0.49311859E+01	0.36951400E+01	-0.23219920E-02	0.79194099E-05					3	
-0.75222719E-08	0.23901715E-11	0.28761931E+05	0.19242302E+01						4	
AlCl3	Al	1Cl	3	0	OG	300.000	3000.000	1000.00	0	1
0.93315504E+01	0.94087032E-03	-0.54168101E-06	0.14379077E-09	-0.14532189E-13					2	
-0.74135693E+05	-0.15788797E+02	0.53258550E+01	0.19081379E-01	-0.32420784E-04					3	
0.25503251E-07	-0.76297036E-11	-0.73390715E+05	0.31312484E+01						4	
AlCl2 2Al	Al	1Cl	2	0	OG	300.000	3000.000	1000.00	0	1
0.66317414E+01	0.51378823E-03	-0.29294840E-06	0.77014564E-10	-0.77103876E-14					2	
-0.28423278E+05	-0.31849167E+01	0.42237259E+01	0.11497745E-01	-0.19714373E-04					3	
0.15600056E-07	-0.46852682E-11	-0.27978681E+05	0.81708628E+01						4	
AlCl 1sigma	Al	1Cl	1	0	OG	300.000	3000.000	1000.00	0	1
0.43650488E+01	0.18564461E-03	-0.10411274E-06	0.26913038E-10	-0.26495484E-14					2	
-0.73226583E+04	0.24702735E+01	0.33720458E+01	0.47578656E-02	-0.82539209E-05					3	
0.65818785E-08	-0.19870248E-11	-0.71410293E+04	0.71434838E+01						4	
AlF3	F	3Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.80899255E+01	0.28084728E-02	-0.16933344E-05	0.46998815E-09	-0.49519149E-13					2	
-0.14721820E+06	-0.13832194E+02	0.31369899E+01	0.23030198E-01	-0.34000791E-04					3	
0.24231467E-07	-0.67723314E-11	-0.14620279E+06	0.10073686E+02						4	
AlF2 2A'	111601F	2Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.58773701E+01	0.16568770E-02	-0.10016144E-05	0.27854896E-09	-0.29393794E-13					2	
-0.76890498E+05	-0.23171139E+01	0.28563439E+01	0.13990770E-01	-0.20675507E-04					3	
0.14708760E-07	-0.40985789E-11	-0.76272170E+05	0.12261675E+02						4	
AlF 1sigma	F	1Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.40033527E+01	0.73539741E-03	-0.44555701E-06	0.12412623E-09	-0.13116773E-13					2	
-0.32882780E+05	0.27481167E+01	0.26458597E+01	0.62664647E-02	-0.92398742E-05					3	
0.65495308E-08	-0.18177784E-11	-0.32604800E+05	0.93008017E+01						4	
Al(OH)3 C3 axis	72401H	3O	3Al	1	OG	300.000	3000.000	1000.00	0	1
0.14727820E+02	-0.66992604E-03	0.18330674E-05	-0.72963835E-09	0.91011438E-13					2	
-0.12225153E+06	-0.47178942E+02	-0.29820043E-02	0.68547616E-01	-0.12026094E-03					3	
0.94728953E-07	-0.27760315E-10	-0.11972588E+06	0.21550595E+02						4	
Al(OH)2 2Al planar	H	2O	2Al	1	OG	300.000	3000.000	1000.00	0	1
0.96518823E+01	-0.68692424E-04	0.11357681E-05	-0.49010375E-09	0.63207907E-13					2	
-0.58997622E+05	-0.20709573E+02	0.26094049E+01	0.35533525E-01	-0.65323792E-04					3	
0.53792274E-07	-0.16319350E-10	-0.57897149E+05	0.11567214E+02						4	
ALOH 1A' linear	H	1O	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.52817396E+01	0.75726795E-03	0.75329534E-07	-0.10248966E-09	0.15947418E-13					2	
-0.23157811E+05	-0.54226919E+01	0.39478484E+01	0.71903061E-02	-0.11186529E-04					3	
0.84576790E-08	-0.23815091E-11	-0.22947036E+05	0.73536832E+00						4	
Al(CH3)3	H	9C	3Al	1	OG	300.000	3000.000	1000.00	0	1
0.54565587E+01	0.33630084E-01	-0.16636859E-04	0.39870175E-08	-0.37587108E-12					2	
-0.95254466E+04	0.92997488E+01	0.22248582E+01	0.48643936E-01	-0.43865122E-04					3	
0.26328789E-07	-0.72715314E-11	-0.89308953E+04	0.24500482E+02						4	

Al(CH ₃) ₂ 2A'	H	6C	2Al	1	OG	300.000	3000.000	1000.00	0	1
0.42476118E+01	0.21997354E-01	-0.10831479E-04	0.25851225E-08	-0.24284556E-12					2	
0.16024834E+05	0.11422025E+02	0.23584282E+01	0.31114834E-01	-0.27823370E-04					3	
0.16773201E-07	-0.46673284E-11	0.16357119E+05	0.20227270E+02						4	
AlCH ₃ 1A1	H	3C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.33858389E+01	0.10689312E-01	-0.52493455E-05	0.12489087E-08	-0.11693916E-12					2	
0.20496741E+05	0.65398826E+01	0.28518820E+01	0.13815289E-01	-0.11937265E-04					3	
0.73826468E-08	-0.21547769E-11	0.20571149E+05	0.89111900E+01						4	
AlH ₂ Cl	H	2Al	1Cl	1	OG	300.000	3000.000	1000.00	0	1
0.54797946E+01	0.60291321E-02	-0.34011143E-05	0.90006488E-09	-0.91540392E-13					2	
-0.16142639E+05	-0.26502271E+01	0.25710559E+01	0.17828258E-01	-0.23054177E-04					3	
0.16443768E-07	-0.48725681E-11	-0.15512163E+05	0.11484056E+02						4	
AlHCl ₂	H	1Al	1Cl	2	OG	300.000	3000.000	1000.00	0	1
0.74012122E+01	0.34526363E-02	-0.19350664E-05	0.50829419E-09	-0.51304481E-13					2	
-0.45787457E+05	-0.85762363E+01	0.35817709E+01	0.20395813E-01	-0.31659475E-04					3	
0.24405345E-07	-0.73476829E-11	-0.45046455E+05	0.95849675E+01						4	
HALCl 2A'	H	1Al	1Cl	1	OG	300.000	3000.000	1000.00	0	1
0.49516450E+01	0.27647135E-02	-0.15722649E-05	0.41848253E-09	-0.42741595E-13					2	
0.87852967E+03	0.19588845E+01	0.35225653E+01	0.84786291E-02	-0.10970102E-04					3	
0.77887282E-08	-0.22999863E-11	0.11921514E+04	0.89231827E+01						4	
AlH ₂ F	H	2F	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.50227364E+01	0.67336170E-02	-0.38428006E-05	0.10266715E-08	-0.10524188E-12					2	
-0.40621323E+05	-0.18200974E+01	0.17967045E+01	0.19003779E-01	-0.22880150E-04					3	
0.15195011E-07	-0.42803625E-11	-0.39891650E+05	0.14034054E+02						4	
AlHF ₂	H	1F	2Al	1	OG	300.000	3000.000	1000.00	0	1
0.65502286E+01	0.47346363E-02	-0.27271025E-05	0.73304033E-09	-0.75449238E-13					2	
-0.95116571E+05	-0.71806890E+01	0.20887755E+01	0.23020337E-01	-0.32488675E-04					3	
0.23244895E-07	-0.66499794E-11	-0.94190502E+05	0.14372703E+02						4	
HALF	H	1F	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.45841938E+01	0.33458489E-02	-0.19421706E-05	0.52554425E-09	-0.54404340E-13					2	
-0.23293111E+05	0.23191574E+01	0.28234906E+01	0.96781098E-02	-0.11097421E-04					3	
0.68820748E-08	-0.18272424E-11	-0.22881353E+05	0.11051394E+02						4	
H ₂ AlOH	H	3O	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.72973364E+01	0.57965725E-02	-0.29222352E-05	0.72069375E-09	-0.70071173E-13					2	
-0.31766945E+05	-0.13155804E+02	0.65214085E+00	0.33292168E-01	-0.47346473E-04					3	
0.33663165E-07	-0.94387043E-11	-0.30423359E+05	0.18825438E+02						4	
HAL(OH) ₂ OAlOcis	72401H	3O	2Al	1	OG	300.000	3000.000	1000.00	0	1
0.10901080E+02	0.26022129E-02	-0.51732323E-06	-0.22184311E-10	0.13144113E-13					2	
-0.77484649E+05	-0.28833360E+02	0.23691655E+00	0.51669211E-01	-0.86322567E-04					3	
0.67043964E-07	-0.19650595E-10	-0.75586026E+05	0.21228249E+02						4	
HALOH 2A' trans	H	2O	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.67873102E+01	0.22995619E-02	-0.87374109E-06	0.16290839E-09	-0.12069563E-13					2	
-0.14486646E+05	-0.91455541E+01	0.15271630E+01	0.25369749E-01	-0.39663157E-04					3	
0.29571767E-07	-0.84415525E-11	-0.13498105E+05	0.15819194E+02						4	
AlH ₂ (CH ₃)	H	5C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.42179887E+01	0.16955440E-01	-0.88170886E-05	0.22022709E-08	-0.21479437E-12					2	
0.61598754E+04	0.64439127E+01	0.18131674E+01	0.25898396E-01	-0.22676393E-04					3	
0.12711296E-07	-0.34026497E-11	0.67233015E+04	0.18336481E+02						4	
AlH(CH ₃) ₂	H	7C	2Al	1	OG	300.000	3000.000	1000.00	0	1
0.48344201E+01	0.25295015E-01	-0.12727832E-04	0.30947810E-08	-0.29533678E-12					2	
-0.17097813E+04	0.76702702E+01	0.17170905E+01	0.38606215E-01	-0.35570086E-04					3	
0.21315009E-07	-0.58671805E-11	-0.10746550E+04	0.22633500E+02						4	
HAL(CH ₃) 2A'	H	4C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.37577924E+01	0.13516201E-01	-0.68522145E-05	0.16767532E-08	-0.16086964E-12					2	
0.23598588E+05	0.83572824E+01	0.26797709E+01	0.17698182E-01	-0.13696261E-04					3	

0.71309904E-08-0.18750193E-11	0.23846239E+05	0.13654492E+02							4
AlFC12	F	1A1	1Cl	2	OG	300.000	3000.000	1000.00	0 1
0.89262287E+01	0.15524876E-02	-0.91972793E-06	0.25106400E-09	-0.26054340E-13					2
-0.98521501E+05	-0.14053594E+02	0.46178514E+01	0.20320970E-01	-0.32810708E-04					3
0.24961084E-07	-0.73052004E-11	-0.97688714E+05	0.64677418E+01						4
AlF2Cl	F	2A1	1Cl	1	OG	300.000	3000.000	1000.00	0 1
0.85115282E+01	0.21763672E-02	-0.13044819E-05	0.36005015E-09	-0.37744416E-13					2
-0.12290861E+06	-0.13402724E+02	0.38839107E+01	0.21652207E-01	-0.33358457E-04					3
0.24550952E-07	-0.70228933E-11	-0.12198495E+06	0.87975267E+01						4
ClAlF	F	1A1	1Cl	1	OG	300.000	3000.000	1000.00	0 1
0.62560909E+01	0.10839329E-02	-0.64689117E-06	0.17778268E-09	-0.18562111E-13					2
-0.52568646E+05	-0.20390869E+01	0.35686777E+01	0.12609478E-01	-0.19943411E-04					3
0.14943838E-07	-0.43262304E-11	-0.52041813E+05	0.10802518E+02						4
Al(OH)Cl2	H	1O	1A1	1Cl	2G	300.000	3000.000	1000.00	0 1
0.11101832E+02	0.38975596E-03	0.28080833E-06	-0.16032953E-09	0.22361318E-13					2
-0.90513162E+05	-0.24411276E+02	0.37619375E+01	0.34843285E-01	-0.61019978E-04					3
0.48440238E-07	-0.14391053E-10	-0.89233895E+05	0.98909513E+01						4
AlCl(OH)2	H	2O	2A1	1Cl	1G	300.000	3000.000	1000.00	0 1
0.12876039E+02	-0.12843833E-03	0.10679187E-05	-0.45156395E-09	0.57656193E-13					2
-0.10657716E+06	-0.34945130E+02	0.20324909E+01	0.51127126E-01	-0.90080563E-04					3
0.71452898E-07	-0.21110341E-10	-0.10472108E+06	0.15601968E+02						4
ClAlOH 2A' trans	H	1O	1A1	1Cl	1G	300.000	3000.000	1000.00	0 1
0.82931046E+01	0.33528713E-04	0.52337010E-06	-0.23269608E-09	0.30349940E-13					2
-0.43961397E+05	-0.12163385E+02	0.31102225E+01	0.25388843E-01	-0.45915563E-04					3
0.37310757E-07	-0.11246602E-10	-0.43107001E+05	0.11807602E+02						4
AlCl2(CH3)	H	3C	1A1	1Cl	2G	300.000	3000.000	1000.00	0 1
0.79959189E+01	0.11836732E-01	-0.58893733E-05	0.14179411E-08	-0.13415412E-12					2
-0.54670727E+05	-0.49497326E+01	0.41325946E+01	0.29268026E-01	-0.36438190E-04					3
0.25674991E-07	-0.74103561E-11	-0.53949133E+05	0.13313648E+02						4
AlCl(CH3)2	H	6C	2A1	1Cl	1G	300.000	3000.000	1000.00	0 1
0.67056443E+01	0.22725936E-01	-0.11248437E-04	0.26970825E-08	-0.25437851E-12					2
-0.33021213E+05	0.15490120E+01	0.30899976E+01	0.39168878E-01	-0.40347095E-04					3
0.26028160E-07	-0.73140929E-11	-0.32348311E+05	0.18619304E+02						4
AlCl(CH3) trans	H	3C	1A1	1Cl	1G	300.000	3000.000	1000.00	0 1
0.54510255E+01	0.11201286E-01	-0.55194094E-05	0.13178760E-08	-0.12382189E-12					2
-0.73352980E+04	0.40951419E+01	0.31640747E+01	0.21819724E-01	-0.24576238E-04					3
0.16724021E-07	-0.48046262E-11	-0.69206656E+04	0.14837634E+02						4
AlF2(OH)	H	1O	1F	2A1	1G	300.000	3000.000	1000.00	0 1
0.99407738E+01	0.19817299E-02	-0.64026033E-06	0.88872252E-10	-0.34709244E-14					2
-0.13908290E+06	-0.21118661E+02	0.29380683E+01	0.34075412E-01	-0.56877057E-04					3
0.44292240E-07	-0.13061019E-10	-0.13782077E+06	0.11808961E+02						4
AlF(OH)2	H	2O	2F	1A1	1G	300.000	3000.000	1000.00	0 1
0.11781703E+02	0.11709285E-02	0.40195107E-06	-0.28886310E-09	0.42184533E-13					2
-0.13047757E+06	-0.30019926E+02	0.28883542E+01	0.44357703E-01	-0.78315915E-04					3
0.63159939E-07	-0.18982178E-10	-0.12899565E+06	0.11191796E+02						4
FAlOH trans	H	1O	1F	1A1	1G	300.000	3000.000	1000.00	0 1
0.79345609E+01	0.58673254E-03	0.17648460E-06	-0.13330165E-09	0.19600191E-13					2
-0.68172164E+05	-0.11905604E+02	0.22834929E+01	0.27305536E-01	-0.47509085E-04					3
0.37685698E-07	-0.11181566E-10	-0.67199825E+05	0.14448530E+02						4
Al(OH)2CH3	H	5C	1O	2A1	1G	300.000	3000.000	1000.00	0 1
0.11510041E+02	0.11043443E-01	-0.45304542E-05	0.90758819E-09	-0.72064926E-13					2
-0.85671590E+05	-0.25943886E+02	0.94307635E+00	0.59904551E-01	-0.90019409E-04					3
0.67570036E-07	-0.19539700E-10	-0.83810945E+05	0.23579586E+02						4
Al(OH)(CH3)2	H	7C	2O	1A1	1G	300.000	3000.000	1000.00	0 1

0.77848007E+01	0.23077537E-01	-0.10923370E-04	0.25217553E-08	-0.23033693E-12	2					
-0.47642496E+05	-0.41475331E+01	0.25035151E+01	0.48491102E-01	-0.57325386E-04	3					
0.40210237E-07	-0.11649081E-10	-0.46739026E+05	0.20413597E+02		4					
CH3ALOH	H	4C	1O	1Al	1G	300.000	3000.000	1000.00	0	1
0.72604034E+01	0.10645100E-01	-0.47012993E-05	0.10146979E-08	-0.86914594E-13	2					
-0.21673058E+05	-0.48976921E+01	0.17160942E+01	0.37612495E-01	-0.53860994E-04	3					
0.40609138E-07	-0.11944746E-10	-0.20752925E+05	0.20779802E+02		4					
HAL(OH)Cl	H	2O	1Al	1Cl	1G	300.000	3000.000	1000.00	0	1
0.88443737E+01	0.44691215E-02	-0.24271392E-05	0.63278685E-09	-0.64069683E-13	2					
-0.62125180E+05	-0.17267019E+02	0.23962186E+01	0.31284011E-01	-0.46476984E-04	3					
0.34080428E-07	-0.98286007E-11	-0.60810192E+05	0.13777210E+02		4					
HAL(CH3)Cl	H	4C	1Al	1Cl	1G	300.000	3000.000	1000.00	0	1
0.60914428E+01	0.14379672E-01	-0.73260448E-05	0.17988693E-08	-0.17298125E-12	2					
-0.24662685E+05	0.37355737E+00	0.25859658E+01	0.29597696E-01	-0.33617630E-04	3					
0.22749876E-07	-0.65449492E-11	-0.23965716E+05	0.17125626E+02		4					
HAL(OH)CH3	H	5C	1O	1Al	1G	300.000	3000.000	1000.00	0	1
0.75567870E+01	0.15380269E-01	-0.78164726E-05	0.19246222E-08	-0.18602149E-12	2					
-0.40007574E+05	-0.98202745E+01	0.12694315E+01	0.40984307E-01	-0.49053346E-04	3					
0.32735676E-07	-0.90768846E-11	-0.38701204E+05	0.20578001E+02		4					
Al(OH)CH3Cl	H	4C	1O	1Al	1G	300.000	3000.000	1000.00	Cl	1
0.98597746E+01	0.11351939E-01	-0.51867901E-05	0.11626264E-08	-0.10360901E-12	2					
-0.70741000E+05	-0.17327961E+02	0.22921161E+01	0.45515312E-01	-0.63999014E-04	3					
0.46567589E-07	-0.13292062E-10	-0.69364503E+05	0.18352437E+02		4					
AlO 2sigma	O	1Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.40662791E+01	0.63893725E-03	-0.38505490E-06	0.10673806E-09	-0.11228753E-13	2					
0.87438698E+04	0.29044572E+01	0.26721244E+01	0.64790440E-02	-0.99318572E-05	3					
0.72566413E-08	-0.20602817E-11	0.90225734E+04	0.95971936E+01		4					
HALO 1sigma	H	1O	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.45685048E+01	0.39645995E-02	-0.22629498E-05	0.60485141E-09	-0.62035510E-13	2					
-0.21550435E+04	-0.73397689E+00	0.29472935E+01	0.98448109E-02	-0.11003115E-04	3					
0.69293921E-08	-0.19054115E-11	-0.17730095E+04	0.73074891E+01		4					
H2AlO 2B2	H	2O	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.52456704E+01	0.63937942E-02	-0.36311701E-05	0.96627379E-09	-0.98725268E-13	2					
0.40225551E+04	-0.21875809E+01	0.21553868E+01	0.18494659E-01	-0.23033540E-04	3					
0.15829554E-07	-0.45702163E-11	0.47083412E+04	0.12923108E+02		4					
AlC 4sigma-	C	1Al	1	0	OG	300.000	3000.000	1000.00	0	1
0.42135758E+01	0.41316068E-03	-0.24373056E-06	0.66227503E-10	-0.68416101E-14	2					
0.85701877E+05	0.29441290E+01	0.28623424E+01	0.63756295E-02	-0.10479462E-04	3					
0.80552179E-08	-0.23713357E-11	0.85959438E+05	0.93616420E+01		4					
AlCH singlet	H	1C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.48168916E+01	0.19396844E-02	-0.73132567E-06	0.12662612E-09	-0.79274019E-14	2					
0.78297243E+05	-0.76572484E+01	0.29485705E+01	0.11952876E-01	-0.20228611E-04	3					
0.16554905E-07	-0.50837923E-11	0.78566166E+05	0.77698065E+00		4					
HALCH 2A"	H	2C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.58748077E+01	0.37969863E-02	-0.17453199E-05	0.38717610E-09	-0.33744342E-13	2					
0.61151832E+05	-0.36825933E+01	0.34607270E+01	0.16619048E-01	-0.27167299E-04	3					
0.22421270E-07	-0.70538411E-11	0.61524370E+05	0.72925391E+01		4					
HALCH2 singlet	H	3C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.53234231E+01	0.84935526E-02	-0.41564760E-05	0.98616020E-09	-0.92117379E-13	2					
0.38511733E+05	-0.17499040E+01	0.30905463E+01	0.19159666E-01	-0.23760341E-04	3					
0.17127057E-07	-0.50623861E-11	0.38905004E+05	0.86723492E+01		4					
H2ALCH 3A"	H	3C	1Al	1	OG	300.000	3000.000	1000.00	0	1
0.65830172E+01	0.76056399E-02	-0.39414956E-05	0.97999518E-09	-0.95092792E-13	2					
0.53263093E+05	-0.67423369E+01	0.33418400E+01	0.22106474E-01	-0.29717300E-04	3					
0.21993811E-07	-0.65927605E-11	0.53891868E+05	0.86538021E+01		4					

AlH2OCH3	H	5C	1O	1Al	1G	300.000	3000.000	1000.00	0	1
0.51035642E+01	0.19634583E-01	-0.10568041E-04	0.27173620E-08	-0.27151701E-12						2
-0.26909281E+05	0.20288455E+01	0.29057191E+01	0.22896474E-01	-0.77082618E-05						3
-0.39964891E-08	0.25185090E-11	-0.26175184E+05	0.14059685E+02							4

* Thermodynamic data are presented in the form of polynomial coefficients for the heat capacity (C_p), enthalpy (H) and entropy (S) as a function of temperature. These fits can be used with the CHEMKIN software package (Ref. 17) and are defined by:

$$C_p/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{H^\circ}{RT} = a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T}$$

$$\frac{S^\circ}{R} = a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7$$

Note that $H^\circ = H^\circ(T) - H^\circ(298) + \Delta H_f^\circ(298)$, where $\Delta H_f^\circ(298)$ is the species heat of formation at 298 K, $H^\circ(T)$ is the standard enthalpy at temperature T , and $H^\circ(298)$ is the standard enthalpy at 298 K. Fits were carried out over two separate temperature ranges. The low, high, and break temperatures for these two fits are given at the end of the first line of the thermo data. For example, for the species AlH₃, the data were fit over the ranges 300 - 1000 K and 1000 - 3000 K. The subsequent three lines of numbers in the data record are the fitting parameters $a_1 - a_7$ for each fit. The parameters for the high-temperature range are given first, followed by those for the low-temperature range. More information concerning this format can be found in the CHEMKIN documentation (Ref. 17).