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

Supporting Information

Radical Attached Aluminum Nanoclusters : An Alternative Way for Cluster Stabilization

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1. Cartesian Coordinates and Normal Modes of Vibrations of Pristine Aluminum Clusters

M06-2X/TZVP

Al_3(-727.155327)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.592829	-0.269131	-0.830979
2	13	0	3.916194	0.683313	-0.613071
3	13	0	2.855662	-0.510630	1.335723

Frequencies -- 65.1946 62.8617 347.5374

Al_4 Planner(-969.561357)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.292355	-0.505770	0.092632
2	13	0	1.273223	0.531013	-0.142758
3	13	0	0.613602	-1.903380	0.800922
4	13	0	-0.633711	1.927456	-0.849918

Frequencies -- 80.7943 193.7879 217.5976 220.7152 331.8263 349.3781

Al_4 Tetrahedral(-969.558755)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.181180	-0.739081	-0.829498
2	13	0	1.246940	-0.118477	-0.998864
3	13	0	0.337169	-1.003923	1.159589
4	13	0	-0.442172	1.910800	0.569651

Frequencies -- 52.3896 58.2176 148.2644 158.5426 197.6659 371.5468

Al_6(-1454.451846)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.356374	-0.144623	1.253363
2	13	0	-0.489263	-0.162946	3.679846

3	13	0	2.263681	0.372155	2.894664
4	13	0	2.466811	-2.018070	1.973219
5	13	0	1.621177	-2.036392	4.399704
6	13	0	-0.286128	-2.553170	2.758401

Frequencies -- 101.5801 104.6636 156.7363 195.6805 197.0970 218.2145

Al_7(-1696.913890)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.565405	-0.824268	1.427535
2	13	0	1.439984	0.782518	1.351599
3	13	0	1.443478	-1.558815	0.000899
4	13	0	-0.567808	1.648511	-0.000989
5	13	0	1.439938	0.781036	-1.352510
6	13	0	-0.565255	-0.825960	-1.426701
7	13	0	-2.624832	-0.003022	0.000068

Frequencies -- 63.7099 65.0425 183.2799 203.1327 205.3922 226.3671

Al_{12}(-2909.116980)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.601895	-0.476080	-0.767791
2	13	0	-1.017531	1.188980	-2.007724
3	13	0	1.538546	0.302029	-2.005199
4	13	0	1.748193	-1.986275	-0.763731
5	13	0	-0.828537	-2.382231	0.818445
6	13	0	-0.550562	-1.589939	-1.734478
7	13	0	0.022940	0.067525	0.285840
8	13	0	1.562898	-1.553218	1.804635
9	13	0	-2.192704	-0.248338	1.800800
10	13	0	-1.754046	2.024654	0.513010
11	13	0	0.888037	2.556413	-0.496066
12	13	0	2.629989	0.501680	0.517684

Frequencies -- 48.2971 82.5760 102.3879 108.2080 125.8132 126.9787

Al_{13}(-3151.604815)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.005675	-1.701688	0.546421
2	13	0	1.591747	0.568192	2.033203

3	13	0	-1.290386	1.092551	2.032775
4	13	0	-2.476902	-0.885816	0.545902
5	13	0	-0.470139	-2.587666	-0.549972
6	13	0	-0.303401	-1.665778	2.030638
7	13	0	-0.000009	0.000010	-0.000016
8	13	0	-1.591845	-0.568373	-2.033126
9	13	0	1.290273	-1.092365	-2.032928
10	13	0	2.476959	0.885760	-0.545773
11	13	0	0.470247	2.587651	0.550053
12	13	0	-2.005681	1.701627	-0.546598
13	13	0	0.303462	1.665899	-2.030579

Frequencies -- 68.4897 70.2036 82.5406 100.9306 102.9135 123.9017

Al_{13}^-(-3151.729520)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.556849	-0.486153	-0.500652
2	13	0	-1.048607	1.221583	-2.105966
3	13	0	1.582732	0.303122	-2.104385
4	13	0	1.701128	-1.970893	-0.497063
5	13	0	-0.857729	-2.458841	0.493366
6	13	0	-0.527571	-1.517097	-2.108418
7	13	0	0.000013	-0.000012	-0.000191
8	13	0	1.048432	-1.220924	2.106006
9	13	0	-1.582627	-0.303142	2.104182
10	13	0	-1.701095	1.970815	0.497257
11	13	0	0.857704	2.458885	-0.493029
12	13	0	2.556989	0.486316	0.500301
13	13	0	0.527481	1.516340	2.108594

Frequencies -- 90.7159 91.6244 92.7096 93.3573 94.7662 186.6391

Al_{20}(-4848.718453)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.507921	0.711679	2.392897
2	13	0	2.527725	-2.044223	1.390959
3	13	0	2.545692	-1.923436	-1.482604
4	13	0	2.553821	0.792130	-2.284490
5	13	0	2.537523	2.456530	0.049443
6	13	0	3.834386	0.007177	0.068081
7	13	0	1.357434	0.001846	0.023914

8	13	0	0.208706	1.984578	1.438834
9	13	0	0.206127	-0.867205	2.296738
10	13	0	0.231591	-2.446626	-0.132734
11	13	0	0.244848	-0.691511	-2.342706
12	13	0	0.245162	1.974765	-1.443587
13	13	0	-2.334309	2.516106	-0.658863
14	13	0	-2.490372	1.841993	1.822107
15	13	0	-2.502106	-0.630985	2.510730
16	13	0	-2.374039	-2.482791	0.727950
17	13	0	-2.263513	-1.870026	-1.806162
18	13	0	-2.248527	0.671208	-2.513816
19	13	0	-1.157577	0.007502	0.036169
20	13	0	-3.630494	-0.008713	-0.092860

Frequencies -- 2.6197 73.5673 80.7288 87.8530 101.0933 105.6185

B3LYP/TZVP

Al_3(-727.269870)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.270123	-0.733212	0.000000
2	13	0	-1.270102	-0.733257	0.000000
3	13	0	-0.000022	1.466469	0.000000

Frequencies -- 229.0489 229.1836 342.6061

Al_4 Planner(-969.710838)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.057215	-0.667168	0.102853
2	13	0	2.037620	0.691826	-0.152428
3	13	0	0.431699	-1.215694	0.507534
4	13	0	-0.451346	1.240356	-0.557080

Frequencies -- 66.7588 166.1262 257.3732 294.4008 316.8767

Al_4 Tetrahedral(-969.706000)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-1.172385	-0.706604	-0.810903
2	13	0	1.331156	-0.205910	-1.073498
3	13	0	0.325637	-0.979292	1.158632
4	13	0	-0.523650	1.941126	0.626649

Frequencies -- -5.0784 38.4665 182.0240 185.3189 197.9254 355.9211

Al_6(-1454.651360)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.958738	1.433533	-0.964648
2	13	0	-1.722990	-0.114956	0.961173
3	13	0	0.760194	1.548191	0.964527
4	13	0	1.722990	0.114955	-0.961173
5	13	0	0.958738	-1.433533	0.964649
6	13	0	-0.760194	-1.548190	-0.964527

Frequencies -- 77.6070 78.0517 104.2260 188.7274 189.3076 205.6981

Al_7(-1697.139613)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.567634	-0.866222	-1.475699
2	13	0	-1.439645	0.782643	-1.375979
3	13	0	-1.443385	-1.581206	0.009759
4	13	0	0.567356	1.712672	-0.010172
5	13	0	-1.440376	0.799010	1.366153
6	13	0	0.567708	-0.847612	1.485982
7	13	0	2.620708	0.000715	-0.000045

Frequencies -- 168.7864 193.2875 193.8656 194.0514 212.8390 213.3911

Al_{12}(-2909.468378)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.701519	0.081816	-1.247601
2	13	0	-0.606163	1.463885	-2.003744
3	13	0	1.916231	-0.483601	-1.669466
4	13	0	0.972385	-2.754775	-0.762807
5	13	0	-0.261816	-2.272496	1.735224
6	13	0	-0.756925	-1.371589	-2.026986
7	13	0	-0.015878	-0.018014	0.269347

8	13	0	2.160994	-1.337763	1.219012
9	13	0	-2.354430	-0.658065	1.459926
10	13	0	-1.955722	1.839240	0.676258
11	13	0	0.504183	2.745647	0.022737
12	13	0	2.543987	1.170914	0.293524

Frequencies -- 54.6643 55.3174 72.7504 80.0116 99.5115 110.8817

Al_{13}(-3151.945645)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.613556	-0.496636	-0.580875
2	13	0	-1.128213	1.313384	-2.043027
3	13	0	1.703187	0.326554	-2.040583
4	13	0	1.738100	-2.014306	-0.578223
5	13	0	-0.876720	-2.513249	0.573729
6	13	0	-0.567871	-1.632324	-2.045312
7	13	0	0.000042	0.000005	0.000003
8	13	0	1.128216	-1.313755	2.042860
9	13	0	-1.702705	-0.326439	2.040887
10	13	0	-1.738234	2.014244	0.577971
11	13	0	0.876553	2.513272	-0.573936
12	13	0	2.613480	0.496625	0.581333
13	13	0	0.567720	1.632624	2.045175

Frequencies -- 38.5009 70.3693 71.4412 77.5508 127.8895 128.2919

Al_{13}^-(-3152.062632)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.588019	-0.491684	-0.505162
2	13	0	-1.061430	1.233748	-2.131673
3	13	0	1.603420	0.307053	-2.128080
4	13	0	1.721168	-1.993986	-0.503664
5	13	0	-0.868382	-2.488012	0.498333
6	13	0	-0.533906	-1.534272	-2.134328
7	13	0	-0.000057	-0.000096	-0.000150
8	13	0	1.061342	-1.236122	2.130358
9	13	0	-1.600422	-0.306593	2.129978
10	13	0	-1.721041	1.994225	0.503167
11	13	0	0.866702	2.487852	-0.500760
12	13	0	2.586928	0.493010	0.508290
13	13	0	0.533698	1.534875	2.133691

Frequencies --	46.1848	46.9250	47.2340	47.7681	48.2196	154.7055

Al_{20} (-4849.221431)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.513103	0.325492	2.567384
2	13	0	2.533390	-2.297367	1.068604
3	13	0	2.623392	-1.663773	-1.739101
4	13	0	2.634877	1.166119	-2.092117
5	13	0	2.543882	2.474486	0.466367
6	13	0	3.838597	0.007388	0.171785
7	13	0	1.348278	0.004700	0.074843
8	13	0	0.241756	1.775025	1.840204
9	13	0	0.244681	-1.258209	2.235298
10	13	0	0.232969	-2.430297	-0.518178
11	13	0	0.288874	-0.307154	-2.439463
12	13	0	0.243280	2.218580	-1.106676
13	13	0	-2.434200	2.609604	-0.374181
14	13	0	-2.524701	1.566458	2.038094
15	13	0	-2.525208	-1.050393	2.341631
16	13	0	-2.459226	-2.612073	0.224817
17	13	0	-2.273967	-1.577430	-2.180939
18	13	0	-2.260865	1.050699	-2.481288
19	13	0	-1.163688	0.002866	0.040357
20	13	0	-3.645223	-0.004721	-0.137441

Frequencies --	6.8967	51.8782	56.5187	61.9101	68.6043	75.3720

2. Cartesian Coordinates and Normal Modes of Vibrations of mono radical/ligand attached Aluminum Clusters

M062X

Al_3

CH_3•(-767.049470)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.837937	-0.064145	-0.003467
2	13	0	4.143036	0.444770	-1.002331
3	13	0	4.051815	-0.895922	0.985890
4	6	0	-0.123777	0.080788	-0.013040
5	1	0	-0.489478	0.662145	0.835276
6	1	0	-0.595774	-0.903323	0.015748
7	1	0	-0.459076	0.579240	-0.926402

Frequencies -- 45.8270 105.3050 117.6215 295.7523 296.6028 379.1774

CH_3CH_2•(-806.319683)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.851536	-0.085481	-0.035464
2	13	0	4.177585	0.619104	-0.852798
3	13	0	4.045900	-1.104367	0.814090
4	6	0	-0.116047	0.097402	-0.001873
5	1	0	-0.545657	-0.889510	0.199305
6	1	0	-0.450042	0.361058	-1.010802
7	6	0	-0.633851	1.123319	1.017427
8	1	0	-0.238985	2.120939	0.815891
9	1	0	-1.723931	1.193760	1.004294
10	1	0	-0.335059	0.861850	2.034351

Frequencies -- 46.2468 76.2690 98.8349 223.8303 227.4251 296.1142

$(CH_3)_2CH$•(-845.595186)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.840606	-0.043444	-0.064135
2	13	0	4.223852	0.884784	-0.270734
3	13	0	3.964537	-1.436156	0.292688
4	6	0	-0.141260	0.074753	-0.021128
5	1	0	-0.491126	0.308499	-1.031922
6	6	0	-0.632022	1.165355	0.937213
7	1	0	-0.281994	2.159511	0.650695
8	1	0	-1.726569	1.197816	0.965590
9	1	0	-0.287013	0.978633	1.958025
10	6	0	-0.704410	-1.295639	0.381417
11	1	0	-1.798609	-1.272659	0.418357
12	1	0	-0.417977	-2.085920	-0.316935
13	1	0	-0.358803	-1.590909	1.377013

Frequencies -- 9.9277 52.2254 71.1975 186.4033 211.6201 225.6922

$(CH_3)_3C•$(-884.874622)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.689262	-1.782728	-2.027506
2	13	0	3.484199	-0.189912	-2.161125
3	13	0	3.734883	-2.144825	-0.518438
4	6	0	4.818065	-3.109169	0.850451
5	6	0	6.163465	-2.380291	0.954996
6	1	0	6.708477	-2.384132	0.006390
7	1	0	6.045712	-1.340073	1.273277
8	1	0	6.801883	-2.875933	1.698242
9	6	0	5.060391	-4.559139	0.421870
10	1	0	4.128281	-5.125414	0.343108
11	1	0	5.569651	-4.621893	-0.543311
12	1	0	5.690480	-5.070316	1.162042
13	6	0	4.122319	-3.086115	2.214181
14	1	0	3.944848	-2.066735	2.566625
15	1	0	3.158824	-3.602303	2.192598
16	1	0	4.746453	-3.590807	2.963688

Frequencies -- 47.2741 58.8696 178.8661 203.6932 218.2278 229.9027

$H_2C=CH•$(-805.116374)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.917972	-0.039715	-0.073065
2	13	0	4.309098	0.755659	-0.534424
3	13	0	4.016594	-1.299863	0.682490
4	6	0	-0.024341	0.211754	-0.115103
5	1	0	-0.651377	-0.174439	-0.916848
6	6	0	-0.639131	0.879996	0.864372
7	1	0	-1.714730	1.041356	0.878414
8	1	0	-0.096487	1.302127	1.706597

Frequencies -- 76.1838 96.0094 238.0834 285.5237 315.3319 374.1838

HC≡C•(-803.913418)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.421136	0.017460	-0.115439
2	13	0	1.816442	-1.203625	0.060523
3	13	0	1.817963	1.200462	0.225733
4	6	0	-2.329238	0.029574	-0.338155
5	6	0	-3.530740	0.036212	-0.480289
6	1	0	-4.589219	0.041305	-0.603422

Frequencies -- 69.5951 83.3762 221.4798 244.9036 272.8534 312.8223

Ph•(-958.712134)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.835900	-0.057554	-0.010389
2	13	0	4.157706	0.659613	-0.821200
3	13	0	4.026451	-1.065805	0.854138
4	6	0	-0.122424	0.069428	-0.033249
5	6	0	-0.891652	-0.714329	-0.904613
6	6	0	-0.803639	0.947472	0.821301
7	6	0	-2.277914	-0.626971	-0.923565
8	1	0	-0.404841	-1.407789	-1.583453
9	6	0	-2.189613	1.040301	0.808119
10	1	0	-0.246988	1.573095	1.512265
11	6	0	-2.927363	0.251747	-0.065758
12	1	0	-2.851616	-1.242599	-1.605650

13	1	0	-2.694420	1.726047	1.477667
14	1	0	-4.008038	0.321997	-0.078288

Frequencies -- 23.4167 49.3619 50.7230 159.8353 203.0220 209.7726

$PhCH_2$•(-997.996601)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.116927	0.018717	-0.091527
2	13	0	1.422826	0.285917	0.214924
3	13	0	0.623261	-1.108216	-1.593325
4	6	0	-3.089108	0.165842	0.131544
5	1	0	-3.432599	-0.227461	1.087854
6	1	0	-3.449218	1.186680	0.007399
7	6	0	-3.479133	-0.714694	-1.014868
8	6	0	-3.591777	-2.100701	-0.852001
9	6	0	-3.615426	-0.195034	-2.307763
10	6	0	-3.864118	-2.928890	-1.931528
11	1	0	-3.473400	-2.527784	0.138236
12	6	0	-3.887806	-1.023035	-3.387408
13	1	0	-3.515574	0.874360	-2.460706
14	6	0	-4.012946	-2.394866	-3.205608
15	1	0	-3.958437	-3.996657	-1.776566
16	1	0	-4.000718	-0.594351	-4.375596
17	1	0	-4.223517	-3.040963	-4.047979

Frequencies -- 16.5735 24.7702 42.0694 98.3448 107.0057 195.7779

Ph_2CH•(-1228.942328)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.131208	-0.176341	-0.061596
2	13	0	1.405643	0.096408	0.282609
3	13	0	0.624999	-1.646228	-1.210132
4	6	0	-3.110168	0.162247	-0.005119
5	1	0	-3.505443	-0.261995	0.920375
6	6	0	-3.485758	-0.746695	-1.148680
7	6	0	-3.378953	-2.133106	-0.958870
8	6	0	-3.850212	-0.288600	-2.417494
9	6	0	-3.626198	-3.023589	-1.993332
10	1	0	-3.113378	-2.514674	0.022812
11	6	0	-4.103274	-1.182234	-3.449816

12	1	0	-3.955936	0.773966	-2.593116
13	6	0	-3.985811	-2.551447	-3.249037
14	1	0	-3.542887	-4.088526	-1.814883
15	1	0	-4.395666	-0.802288	-4.420969
16	1	0	-4.179471	-3.242556	-4.059054
17	6	0	-3.483687	1.611107	-0.100394
18	6	0	-2.866108	2.474639	-1.011599
19	6	0	-4.449830	2.146650	0.752729
20	6	0	-3.213266	3.816453	-1.076971
21	1	0	-2.097189	2.092265	-1.677382
22	6	0	-4.792439	3.491147	0.697423
23	1	0	-4.941845	1.495692	1.466511
24	6	0	-4.177982	4.331768	-0.220627
25	1	0	-2.719750	4.463284	-1.791684
26	1	0	-5.545370	3.880492	1.371575
27	1	0	-4.444726	5.379822	-0.266707

Frequencies -- 18.6400 29.7137 38.9422 45.2318 59.6825 91.9005

$Ph_3C•$(-1459.887461)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.110959	-0.291325	-0.113086
2	13	0	1.426225	0.058919	0.203949
3	13	0	0.682080	-1.596478	-1.401883
4	6	0	-3.105893	0.017486	0.083248
5	6	0	-3.496070	-0.797722	-1.134715
6	6	0	-3.174290	-2.166864	-1.159220
7	6	0	-4.099109	-0.256818	-2.273084
8	6	0	-3.431047	-2.951244	-2.273555
9	1	0	-2.747911	-2.629548	-0.273259
10	6	0	-4.361917	-1.046039	-3.386037
11	1	0	-4.375298	0.789139	-2.287771
12	6	0	-4.023420	-2.392070	-3.398801
13	1	0	-3.175055	-4.003518	-2.257117
14	1	0	-4.837936	-0.600712	-4.250955
15	1	0	-4.225529	-3.000221	-4.270997
16	6	0	-3.413430	1.499346	-0.018221
17	6	0	-2.770767	2.297158	-0.974142
18	6	0	-4.337400	2.119655	0.824287
19	6	0	-3.040107	3.652261	-1.085210
20	1	0	-2.051801	1.848747	-1.654997
21	6	0	-4.605936	3.479648	0.717509
22	1	0	-4.854359	1.535004	1.574446

23	6	0	-3.960341	4.253562	-0.234600
24	1	0	-2.523570	4.240100	-1.833856
25	1	0	-5.327413	3.933027	1.386197
26	1	0	-4.167200	5.313230	-0.313025
27	6	0	-3.583843	-0.585866	1.390097
28	6	0	-4.716201	-1.396601	1.462823
29	6	0	-2.924133	-0.276829	2.582955
30	6	0	-5.165848	-1.889066	2.682298
31	1	0	-5.254255	-1.642426	0.555509
32	6	0	-3.371918	-0.760936	3.802519
33	1	0	-2.053174	0.372776	2.557900
34	6	0	-4.496210	-1.575537	3.856513
35	1	0	-6.047647	-2.517259	2.711963
36	1	0	-2.839665	-0.506605	4.710507
37	1	0	-4.844585	-1.962434	4.805633

Frequencies -- 13.9171 20.9808 33.8941 44.7626 52.5177 62.4807

Cl•(-1187.445057)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.404232	-0.000110	0.000257
2	13	0	-1.853821	1.209629	-0.000062
3	13	0	-1.853925	-1.209546	-0.000062
4	17	0	2.526217	0.000022	-0.000102

Frequencies -- 79.7888 103.6297 247.2188 300.1902 367.9603 556.9070

$(CF_3)_3C$•(-1778.247331)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.507139	-1.121657	-0.722752
2	13	0	-2.620882	0.813889	0.736528
3	13	0	-0.331900	-0.035303	0.013148
4	6	0	1.754711	0.044975	-0.000632
5	6	0	2.213692	1.484366	-0.208915
6	6	0	2.222780	-0.845277	-1.147005
7	6	0	2.257219	-0.493334	1.336361
8	9	0	2.046690	2.190937	0.916061
9	9	0	3.493299	1.593019	-0.568149
10	9	0	1.485310	2.088601	-1.157697
11	9	0	2.114883	-0.214263	-2.317887

12	9	0	3.478544	-1.270231	-1.029643
13	9	0	1.441113	-1.943063	-1.226568
14	9	0	3.535075	-0.208609	1.586733
15	9	0	1.536667	0.012227	2.350372
16	9	0	2.120838	-1.822198	1.384937

Frequencies -- 36.8354 39.6147 67.5274 73.6444 79.1164 111.5368

Cp(-920.624919)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.094530	0.000965	0.001241
2	13	0	2.428155	1.171521	-0.302656
3	13	0	2.430431	-1.163369	0.309962
4	6	0	-1.841417	1.162657	0.306255
5	1	0	-1.821321	2.206078	0.578138
6	6	0	-1.843848	0.643969	-1.016282
7	1	0	-1.816887	1.224981	-1.924372
8	6	0	-1.845180	-0.764619	-0.932230
9	1	0	-1.809076	-1.448700	-1.764924
10	6	0	-1.847326	0.071719	1.203526
11	1	0	-1.810635	0.135847	2.279144
12	6	0	-1.834241	-1.121229	0.440574
13	1	0	-1.815582	-2.124945	0.834932

Frequencies -- 70.2424 90.9241 197.9499 224.0657 244.6814 299.4775

Cp*(-1117.039359)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.079535	-0.000226	0.014929
2	13	0	2.429865	-1.154942	0.189969
3	13	0	2.388259	1.237366	-0.142764
4	6	0	-1.794463	-1.059081	-0.598716
5	6	0	-1.808356	-0.895951	0.822509
6	6	0	-1.820791	0.497086	1.101416
7	6	0	-1.803162	0.232394	-1.190456
8	6	0	-1.800548	1.197770	-0.141249
9	6	0	-1.812308	2.687775	-0.299516
10	1	0	-1.203358	3.006416	-1.146408
11	1	0	-2.828860	3.054141	-0.461665
12	1	0	-1.421828	3.176407	0.593635

13	6	0	-1.821534	1.131501	2.458518
14	1	0	-1.036331	1.885041	2.550512
15	1	0	-2.778966	1.617795	2.658567
16	1	0	-1.654468	0.387987	3.236827
17	6	0	-1.811916	-1.992458	1.844518
18	1	0	-1.102789	-1.789838	2.648711
19	1	0	-2.803056	-2.104707	2.289717
20	1	0	-1.539155	-2.947386	1.396602
21	6	0	-1.790467	-2.351107	-1.356616
22	1	0	-1.289247	-3.143640	-0.800720
23	1	0	-2.810952	-2.682489	-1.564473
24	1	0	-1.274220	-2.239562	-2.310782
25	6	0	-1.775391	0.509002	-2.662625
26	1	0	-0.935295	0.006173	-3.147685
27	1	0	-2.694981	0.161557	-3.138442
28	1	0	-1.680498	1.576293	-2.858923

Frequencies -- 16.7842 43.8682 51.2642 68.5432 105.2764 127.3188

Al_6

CH_3•(-1494.327658)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.731200	1.091686	-1.652898
2	13	0	-1.972727	0.653842	0.567915
3	13	0	0.619806	1.233319	0.761265
4	13	0	1.446779	-0.158531	-1.486569
5	13	0	1.434350	-1.301694	0.828201
6	13	0	-0.861415	-1.472317	-0.177584
7	6	0	1.265315	2.535321	2.094967
8	1	0	0.815977	3.514621	1.927993
9	1	0	2.350043	2.633951	2.045240
10	1	0	0.998653	2.204823	3.100799

Frequencies -- 60.0078 72.6759 79.0644 84.1359 111.2422 165.9571

CH_3CH_2•(-1533.599232)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.118867	0.587868	-1.236288
2	13	0	-1.596535	0.673610	1.300936
3	13	0	0.568495	1.983510	0.449756

4	13	0	1.350299	0.143649	-1.459162
5	13	0	2.260729	-0.019546	0.952899
6	13	0	0.035722	-1.176674	0.836756
7	6	0	0.958983	3.791048	1.169789
8	1	0	1.875779	4.151231	0.696646
9	1	0	0.156519	4.460881	0.851324
10	6	0	1.100692	3.815853	2.696158
11	1	0	1.314980	4.822555	3.063490
12	1	0	0.186882	3.474367	3.187206
13	1	0	1.910007	3.164071	3.032283

Frequencies -- 50.0574 64.4660 71.1765 76.6045 111.6693 164.0866

$(CH_3)_2CH$•(-1572.876318)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.423368	0.914194	-1.886457
2	13	0	-2.013235	1.108441	0.143881
3	13	0	0.580860	1.047639	0.707075
4	13	0	1.313888	-0.791221	-1.243876
5	13	0	0.695161	-1.567268	1.143859
6	13	0	-1.414719	-1.308094	-0.196326
7	6	0	1.432506	2.377618	1.921115
8	1	0	0.922784	2.289108	2.885856
9	6	0	1.239205	3.800317	1.387028
10	1	0	1.684389	3.912914	0.393732
11	1	0	0.184497	4.068673	1.305478
12	1	0	1.724232	4.531334	2.043362
13	6	0	2.920070	2.069256	2.115952
14	1	0	3.389760	2.814062	2.767945
15	1	0	3.080624	1.084967	2.559066
16	1	0	3.455944	2.090792	1.162109

Frequencies -- 6.7709 44.9821 52.6987 73.8865 102.7715 153.5908

$(CH_3)_3C$•(-1612.156666)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.046668	0.645627	-2.157243
2	13	0	-1.915301	0.999416	-0.406026
3	13	0	0.575333	0.986066	0.529037
4	13	0	1.555506	-1.006170	-1.130714

5	13	0	0.578299	-1.587201	1.190975
6	13	0	-1.310105	-1.439653	-0.462223
7	6	0	1.212872	2.403790	1.791644
8	6	0	1.206878	3.751259	1.063379
9	1	0	0.200510	4.038092	0.749069
10	1	0	1.587601	4.537639	1.728756
11	1	0	1.843354	3.738342	0.173888
12	6	0	2.641213	2.079505	2.238768
13	1	0	3.016547	2.875929	2.895171
14	1	0	2.688700	1.139658	2.793840
15	1	0	3.327666	2.001248	1.391070
16	6	0	0.297836	2.478220	3.014621
17	1	0	0.274778	1.534491	3.565765
18	1	0	0.656722	3.254774	3.703545
19	1	0	-0.729249	2.731005	2.739178

Frequencies -- 5.8982 44.1981 53.6406 68.2637 98.9587 147.1733

$H_2C=CH•$(-1532.400058)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.550883	1.300015	-1.332579
2	13	0	-0.756112	0.894582	1.363766
3	13	0	1.612023	1.513389	0.323762
4	13	0	1.598802	-0.303195	-1.439597
5	13	0	1.126429	-1.147918	1.036148
6	13	0	-1.223963	-1.038322	-0.202666
7	6	0	0.308248	3.652926	2.032915
8	1	0	-0.184885	4.069944	1.158527
9	6	0	0.671980	2.356767	2.086903
10	1	0	0.487337	4.342909	2.853472
11	1	0	1.159526	2.050776	3.014503

Frequencies -- 69.4355 87.3602 109.2993 116.2416 144.2097 182.0815

HC≡C•(-1531.190863)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.700794	0.772185	-1.842379
2	13	0	-2.212533	0.110924	0.145916
3	13	0	0.089834	1.257054	0.757832

4	13	0	1.643247	0.092466	-1.208141
5	13	0	1.484290	-0.955662	1.148207
6	13	0	-0.508020	-1.707190	-0.188800
7	6	0	0.185083	3.563920	2.867174
8	1	0	0.221717	4.360001	3.574003
9	6	0	0.141875	2.658713	2.066026

Frequencies -- 42.1334 56.5436 80.1973 100.5994 166.5173 177.4327

Ph•(-1685.996648)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.239160	1.264418	-0.512883
2	13	0	-0.211213	0.449510	1.923401
3	13	0	1.299668	1.958966	0.341127
4	13	0	1.018242	0.537752	-1.738494
5	13	0	1.801578	-0.759410	0.459412
6	13	0	-0.800484	-1.279650	0.166615
7	6	0	0.242507	4.262941	3.762945
8	6	0	1.330480	4.053797	4.602594
9	6	0	2.178269	2.974362	4.382375
10	6	0	1.937408	2.108948	3.326479
11	6	0	0.843335	2.288631	2.452951
12	6	0	0.005074	3.395222	2.708169
13	1	0	-0.419730	5.102833	3.931791
14	1	0	1.517270	4.730625	5.426833
15	1	0	3.026578	2.808691	5.034608
16	1	0	2.609932	1.271349	3.169594
17	1	0	-0.849251	3.574015	2.062692

Frequencies -- 50.5839 54.9798 60.1759 115.8751 120.7483 122.9298

$PhCH_2$•(-1725.275279)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.634077	2.053399	-1.415776
2	13	0	-1.499787	1.759497	0.018553
3	13	0	0.757641	1.190898	1.272008
4	13	0	2.107239	0.088802	-0.886713
5	13	0	0.790527	-1.381959	0.776652
6	13	0	-0.842437	-0.474781	-0.921026
7	6	0	1.150393	2.140800	2.983896

8	1	0	1.969073	1.623816	3.485936
9	1	0	0.275243	2.115943	3.633535
10	6	0	1.527773	3.539402	2.612971
11	6	0	0.589513	4.574023	2.642485
12	6	0	2.814522	3.834428	2.153145
13	6	0	0.928095	5.858947	2.244412
14	1	0	-0.417117	4.363631	2.987562
15	6	0	3.155406	5.119324	1.753602
16	1	0	3.557254	3.043839	2.115386
17	6	0	2.213727	6.139265	1.796750
18	1	0	0.185386	6.646354	2.285281
19	1	0	4.160862	5.323859	1.406833
20	1	0	2.478757	7.141994	1.487433

Frequencies -- 19.9079 27.7567 36.3438 75.9436 81.4786 106.1894

Ph_2CH•(-1956.223064)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.460349	-0.644942	-0.974672
2	13	0	-1.801939	-0.836167	1.576737
3	13	0	-0.107233	1.043288	0.457029
4	13	0	1.125586	-0.656301	-1.133710
5	13	0	1.886038	-0.787600	1.332765
6	13	0	0.012902	-2.468572	0.853013
7	6	0	0.211696	2.667275	1.630605
8	1	0	-0.756961	2.904143	2.076718
9	6	0	0.665820	3.837508	0.803068
10	6	0	0.044191	5.078904	0.949100
11	6	0	1.690464	3.728624	-0.142193
12	6	0	0.433508	6.172503	0.187696
13	1	0	-0.753662	5.186416	1.675037
14	6	0	2.089848	4.821886	-0.898014
15	1	0	2.180212	2.771153	-0.291969
16	6	0	1.461647	6.049952	-0.737021
17	1	0	-0.066902	7.123637	0.320984
18	1	0	2.886864	4.710201	-1.622623
19	1	0	1.767482	6.901712	-1.331077
20	6	0	1.129005	2.186838	2.720532
21	6	0	0.601635	1.388902	3.745456
22	6	0	2.507521	2.421623	2.723996
23	6	0	1.421093	0.808960	4.703616
24	1	0	-0.470028	1.221687	3.785041
25	6	0	3.326230	1.847707	3.688053

26	1	0	2.943908	3.060084	1.967271
27	6	0	2.793606	1.023926	4.672504
28	1	0	0.984949	0.188331	5.476511
29	1	0	4.390885	2.046041	3.667438
30	1	0	3.436163	0.570544	5.415870

Frequencies -- 19.4202 24.9245 43.4057 47.4611 51.9081 61.7502

$Ph_3C•$(-2187.168614)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.479628	1.405310	-2.315027
2	13	0	2.641943	-1.234400	-1.947250
3	13	0	0.698456	0.311878	-0.904590
4	13	0	2.866214	1.757057	0.227657
5	13	0	3.040237	-1.137423	0.644115
6	13	0	4.859733	0.153646	-0.617868
7	6	0	-1.059438	-0.015128	0.058821
8	6	0	-1.763660	1.330383	0.142885
9	6	0	-1.960044	2.061941	-1.031783
10	6	0	-2.297192	1.841446	1.326790
11	6	0	-2.651935	3.262990	-1.027152
12	1	0	-1.571502	1.673510	-1.969577
13	6	0	-2.989121	3.046371	1.336172
14	1	0	-2.176931	1.290184	2.251699
15	6	0	-3.166717	3.764238	0.161839
16	1	0	-2.787559	3.808127	-1.952744
17	1	0	-3.395193	3.421789	2.267585
18	1	0	-3.704566	4.703506	0.171460
19	6	0	-0.428364	-0.497463	1.342385
20	6	0	-0.405869	-1.855699	1.691572
21	6	0	0.303369	0.390281	2.154093
22	6	0	0.302603	-2.302184	2.798292
23	1	0	-0.948714	-2.568289	1.083984
24	6	0	1.028753	-0.064123	3.249595
25	1	0	0.278367	1.453308	1.938763
26	6	0	1.033235	-1.414103	3.579419
27	1	0	0.293692	-3.357045	3.043631
28	1	0	1.587994	0.644811	3.847889
29	1	0	1.593230	-1.766013	4.436049
30	6	0	-1.997155	-1.034427	-0.570366
31	6	0	-3.221091	-1.292759	0.055150
32	6	0	-1.697019	-1.736081	-1.733854
33	6	0	-4.105577	-2.226706	-0.457600

34	1	0	-3.475507	-0.747485	0.957379
35	6	0	-2.584100	-2.674425	-2.256113
36	1	0	-0.759257	-1.562200	-2.251806
37	6	0	-3.788117	-2.924916	-1.618915
38	1	0	-5.046972	-2.410157	0.045379
39	1	0	-2.326769	-3.207050	-3.163092
40	1	0	-4.479366	-3.653349	-2.023633

Frequencies -- 13.8417 21.5879 40.5737 46.2281 56.6373 60.7742

Cl•(-1914.718885)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.830241	1.189279	-1.334996
2	13	0	-1.840426	0.079613	0.805545
3	13	0	0.695373	1.748476	0.846467
4	13	0	1.636662	0.342392	-1.020702
5	13	0	0.945522	-0.998750	1.133557
6	13	0	-0.824895	-1.703670	-0.674845
7	17	0	0.301593	2.757735	2.688248

Frequencies -- 38.6341 69.3401 83.7616 108.4501 109.9319 156.8429

$(CF_3)_3C•$ (-2505.530100)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.239377	1.090397	-1.866439
2	13	0	-1.912071	1.172564	0.110104
3	13	0	0.609510	1.200585	0.773463
4	13	0	1.609412	-0.490008	-1.186268
5	13	0	1.022859	-1.337692	1.190574
6	13	0	-1.136168	-1.210193	-0.094169
7	6	0	1.322930	2.640236	2.098040
8	6	0	1.427798	3.982689	1.371327
9	6	0	2.707236	2.218574	2.598012
10	6	0	0.359842	2.754981	3.280707
11	9	0	2.456851	3.966708	0.515127
12	9	0	1.605231	5.020965	2.192523
13	9	0	0.328494	4.245039	0.652495
14	9	0	3.394230	3.212528	3.166219
15	9	0	3.467777	1.749930	1.597878
16	9	0	2.603906	1.238742	3.503383

17	9	0	-0.060030	1.544025	3.678308
18	9	0	0.895759	3.347444	4.350514
19	9	0	-0.729587	3.454335	2.944504

Frequencies -- 14.0887 40.4221 42.9867 70.6965 74.4494 81.8399

Cp(-1647.901992)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.141707	1.263378	1.036662
2	13	0	0.418985	1.429072	-1.463433
3	13	0	-1.231736	-0.130642	0.733149
4	13	0	1.034254	-1.319877	1.168892
5	13	0	0.305062	-1.460109	-1.328338
6	13	0	2.521058	-0.027115	-1.459855
7	6	0	-2.965451	1.292248	0.382426
8	1	0	-2.780921	2.319530	0.110824
9	6	0	-3.089681	0.203301	-0.518183
10	1	0	-3.039755	0.260257	-1.595096
11	6	0	-3.287175	-0.974594	0.247776
12	1	0	-3.386500	-1.973628	-0.145857
13	6	0	-3.072848	0.786213	1.698220
14	1	0	-2.986773	1.361190	2.606524
15	6	0	-3.273067	-0.616261	1.614640
16	1	0	-3.362432	-1.293876	2.448777

Frequencies -- 34.9224 49.5606 62.4775 79.9795 89.6163 104.3353

Cp*(-1844.319946)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.258674	0.354318	1.818560
2	13	0	1.505439	1.607849	-0.458879
3	13	0	-0.889961	-0.267668	0.205893
4	13	0	0.975272	-1.999357	0.769787
5	13	0	1.199601	-1.015683	-1.626424
6	13	0	3.413098	-0.103629	-0.480865
7	6	0	-2.422511	1.372374	0.197306
8	6	0	-2.265264	0.884863	-1.135948
9	6	0	-2.661071	-0.488421	-1.148550
10	6	0	-2.893817	0.298440	1.004754
11	6	0	-3.044497	-0.849898	0.171680

12	6	0	-2.164493	2.765060	0.683222
13	1	0	-1.594480	2.762509	1.614023
14	1	0	-1.593789	3.341227	-0.044018
15	1	0	-3.107194	3.286966	0.863800
16	6	0	-3.191266	0.369780	2.470201
17	1	0	-2.603033	1.150551	2.952794
18	1	0	-4.247709	0.592339	2.639110
19	1	0	-2.964337	-0.573337	2.968453
20	6	0	-1.853928	1.683204	-2.336882
21	1	0	-2.733435	2.017496	-2.892638
22	1	0	-1.282914	2.566581	-2.052852
23	1	0	-1.232220	1.098063	-3.016422
24	6	0	-3.510776	-2.202630	0.611552
25	1	0	-3.198125	-2.417339	1.634153
26	1	0	-4.600842	-2.268295	0.574347
27	1	0	-3.106250	-2.985032	-0.031139
28	6	0	-2.685367	-1.389777	-2.343311
29	1	0	-2.065083	-0.993876	-3.147370
30	1	0	-2.309664	-2.384847	-2.099835
31	1	0	-3.703979	-1.495326	-2.724559

Frequencies -- 14.5804 30.2216 46.2684 63.5702 69.9658 78.6354

Al_7

CH_3•(-1736.817427)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.504120	-0.804589	-1.483911
2	13	0	-1.522863	0.765661	-1.306009
3	13	0	-1.430684	-1.561605	0.028076
4	13	0	0.524788	1.672960	-0.045972
5	13	0	-1.412058	0.759723	1.375265
6	13	0	0.622150	-0.810177	1.378023
7	13	0	2.563541	0.050251	-0.133196
8	6	0	4.523069	0.079119	-0.210795
9	1	0	4.930088	-0.933627	-0.180284
10	1	0	4.938387	0.634146	0.632982
11	1	0	4.870422	0.553932	-1.130217

67.0392 69.1949 74.5149 124.3688 127.4960 184.6663

CH_3CH_2•(-1776.087606)

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.509737	-0.346546	-1.638080
2	13	0	-1.434962	1.210273	-1.011760
3	13	0	-1.545233	-1.429390	-0.536433
4	13	0	0.583494	1.503711	0.552742
5	13	0	-1.472807	0.296956	1.514027
6	13	0	0.473493	-1.315417	1.053043
7	13	0	2.536601	-0.133202	-0.014470
8	6	0	4.507147	-0.139475	0.025732
9	1	0	4.842352	-1.074783	0.483486
10	1	0	4.876476	-0.156602	-1.003807
11	6	0	5.091192	1.063487	0.781765
12	1	0	4.790733	2.008604	0.324524
13	1	0	4.753786	1.087150	1.820097
14	1	0	6.183040	1.040903	0.794710

Frequencies -- 50.3340 54.6015 77.2571 95.7454 123.9659 181.0850

$(CH_3)_2CH$•(-1815.363819)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.480158	-0.938987	-1.431773
2	13	0	-1.533913	0.656015	-1.386147
3	13	0	-1.460999	-1.548183	0.141570
4	13	0	0.522319	1.653891	-0.210078
5	13	0	-1.417897	0.878748	1.286032
6	13	0	0.601770	-0.702384	1.421078
7	13	0	2.548224	0.009805	-0.159092
8	6	0	4.523674	0.106942	-0.235483
9	1	0	4.896016	-0.921981	-0.288140
10	6	0	5.084926	0.765565	1.030548
11	1	0	4.720714	1.791602	1.137050
12	1	0	4.810019	0.224753	1.938766
13	1	0	6.178247	0.814857	0.993031
14	6	0	4.984888	0.858332	-1.490131
15	1	0	4.635891	0.385983	-2.410981
16	1	0	4.617979	1.888939	-1.490773
17	1	0	6.077921	0.906448	-1.536540

Frequencies -- 41.2963 42.6684 89.7690 93.0287 166.6923 186.4622

$(CH_3)_3C$•(-1854.643390)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.767136	0.746666	1.478816
2	13	0	2.774061	1.547093	0.087148
3	13	0	2.773822	-0.848686	1.296345
4	13	0	0.766149	0.908109	-1.384261
5	13	0	2.772976	-0.698236	-1.383662
6	13	0	0.765664	-1.652764	-0.092227
7	13	0	-1.248036	0.001607	0.000187
8	6	0	-3.235553	0.000551	-0.000847
9	6	0	-3.743186	-0.751022	-1.235453
10	1	0	-3.410505	-0.283631	-2.166345
11	1	0	-3.410147	-1.792476	-1.247582
12	1	0	-4.841050	-0.758069	-1.246006
13	6	0	-3.749067	1.443328	-0.034309
14	1	0	-3.420014	2.017129	0.836513
15	1	0	-3.418033	1.976644	-0.930054
16	1	0	-4.847078	1.450746	-0.035603
17	6	0	-3.745934	-0.694194	1.265557
18	1	0	-3.408005	-1.732277	1.329309
19	1	0	-3.420280	-0.180829	2.174463
20	1	0	-4.843806	-0.705856	1.271276

Frequencies -- 41.7969 43.9387 88.1791 89.7944 155.2216 182.0632

$H_2C=CH\bullet$(-1774.883442)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.556110	-1.086509	-1.329014
2	13	0	-1.437226	0.528358	-1.445689
3	13	0	-1.420825	-1.576197	0.234004
4	13	0	0.591721	1.588134	-0.277225
5	13	0	-1.399806	0.921346	1.206132
6	13	0	0.608750	-0.652903	1.511576
7	13	0	2.592704	-0.067039	-0.070218
8	6	0	4.542561	-0.145524	-0.164775
9	6	0	5.155052	-0.962304	-1.023640
10	1	0	5.177678	0.465476	0.474254
11	1	0	6.237675	-1.029123	-1.097412
12	1	0	4.605326	-1.610653	-1.701729

Frequencies -- 54.6355 61.2562 97.1062 117.7125 186.0448 187.9923

HC≡C•(-1773.680422)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.074707	1.486609	-0.750764
2	13	0	-2.075717	1.301223	0.848062
3	13	0	-2.076222	0.089612	-1.550108
4	13	0	-0.078278	-0.092880	1.662955
5	13	0	-2.080436	-1.381462	0.698884
6	13	0	-0.079273	-1.393741	-0.912037
7	13	0	1.911020	-0.004838	0.000218
8	6	0	3.828791	-0.002905	0.002532
9	6	0	5.037753	0.002113	0.008542
10	1	0	6.103426	0.006324	0.013196

Frequencies -- 52.0593 53.8004 99.1892 100.8719 187.7736 197.5016

Ph•(-1928.479112)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.688972	-1.274674	-1.134964
2	13	0	-1.298410	0.307844	-1.509129
3	13	0	-1.275932	-1.469881	0.508330
4	13	0	0.745380	1.539869	-0.560862
5	13	0	-1.223382	1.151660	1.043019
6	13	0	0.779966	-0.365640	1.588729
7	13	0	2.742529	-0.060742	-0.099241
8	6	0	5.400969	-1.269917	-0.428273
9	6	0	6.789068	-1.291607	-0.477957
10	6	0	7.507629	-0.122318	-0.264074
11	6	0	6.836021	1.064750	-0.001153
12	6	0	5.447766	1.078595	0.046939
13	6	0	4.699541	-0.086326	-0.165423
14	1	0	4.861152	-2.196507	-0.599020
15	1	0	7.310542	-2.218467	-0.683301
16	1	0	8.589799	-0.136118	-0.302440
17	1	0	7.394157	1.977864	0.165817
18	1	0	4.945144	2.018629	0.253895

Frequencies -- 19.0471 29.4066 39.0683 82.8887 88.6386 149.2375

$PhCH_2$•(-1967.763209)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.347265	-0.337189	-1.257307
2	13	0	-1.006650	1.252291	0.239341
3	13	0	-0.906471	-1.385229	0.724944
4	13	0	1.529881	1.510610	0.604049
5	13	0	0.199959	0.342077	2.460398
6	13	0	1.636830	-1.309704	1.123700
7	13	0	2.911643	-0.162071	-0.834756
8	6	0	6.174862	-1.058885	0.187325
9	6	0	7.044981	-0.825726	1.242924
10	6	0	7.441830	0.469009	1.551675
11	6	0	6.959863	1.526794	0.791514
12	6	0	6.089691	1.292044	-0.263753
13	1	0	5.872756	-2.074494	-0.046472
14	1	0	7.415249	-1.659864	1.826230
15	1	0	8.119376	0.651562	2.375610
16	1	0	7.263442	2.541089	1.019978
17	1	0	5.720818	2.125532	-0.852441
18	6	0	5.687594	-0.005599	-0.590999
19	6	0	4.697908	-0.252604	-1.688940
20	1	0	4.773210	0.500913	-2.475072
21	1	0	4.841320	-1.233592	-2.145741

Frequencies -- 6.7571 11.2277 21.5230 63.4115 68.0409 114.8831

Ph_2CH•(-2198.708417)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.887645	-1.043865	-1.032994
2	13	0	-1.137067	0.480843	-1.480249
3	13	0	-0.866768	-0.859412	0.835033
4	13	0	1.007181	1.826821	-1.041363
5	13	0	-0.766570	1.823330	0.822524
6	13	0	1.288153	0.403908	1.439076
7	13	0	3.043308	0.308137	-0.482404
8	6	0	5.023710	0.127100	-0.711978
9	1	0	5.374533	1.054931	-1.173098
10	6	0	5.281591	-1.009812	-1.674464
11	6	0	6.013930	-2.148497	-1.341952
12	6	0	4.762676	-0.921998	-2.972662

13	6	0	6.216377	-3.161958	-2.272553
14	1	0	6.446892	-2.240211	-0.354455
15	6	0	4.967255	-1.929254	-3.901732
16	1	0	4.195340	-0.040562	-3.260057
17	6	0	5.693732	-3.061884	-3.553178
18	1	0	6.793895	-4.033964	-1.990582
19	1	0	4.555899	-1.831202	-4.898803
20	1	0	5.851912	-3.854137	-4.273618
21	6	0	5.591704	0.019870	0.673647
22	6	0	6.453387	0.997597	1.172410
23	6	0	5.215207	-1.019960	1.533253
24	6	0	6.926930	0.939672	2.477091
25	1	0	6.757718	1.813363	0.526495
26	6	0	5.692887	-1.085036	2.833494
27	1	0	4.541666	-1.792581	1.173066
28	6	0	6.551238	-0.102468	3.312962
29	1	0	7.594456	1.711967	2.838975
30	1	0	5.387965	-1.901650	3.476044
31	1	0	6.921670	-0.149122	4.328922

Frequencies -- 10.6757 15.6570 27.1051 39.4599 46.0516 68.4778

$Ph_3C•$(-2429.654304)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.554252	1.651168	-0.323679
2	13	0	4.559225	0.531788	-1.483497
3	13	0	4.567754	1.047904	1.155025
4	13	0	2.562996	-1.071336	-1.263115
5	13	0	4.573424	-1.496407	0.283810
6	13	0	2.571284	-0.521389	1.565931
7	13	0	0.555430	0.009814	0.000459
8	6	0	-1.466954	-0.003425	0.005568
9	6	0	-1.870702	-0.125014	1.465708
10	6	0	-2.778605	-1.079882	1.922203
11	6	0	-1.332502	0.763001	2.407110
12	6	0	-3.127939	-1.149744	3.266647
13	1	0	-3.223364	-1.774795	1.221649
14	6	0	-1.679598	0.696400	3.746567
15	1	0	-0.644956	1.538428	2.079056
16	6	0	-2.579984	-0.267719	4.185368
17	1	0	-3.837712	-1.899970	3.592968
18	1	0	-1.244273	1.396521	4.448668
19	1	0	-2.850457	-0.327686	5.231815

20	6	0	-1.869610	-1.210147	-0.826044
21	6	0	-2.789401	-1.134008	-1.871430
22	6	0	-1.317554	-2.464980	-0.535556
23	6	0	-3.136726	-2.265021	-2.602539
24	1	0	-3.245010	-0.183217	-2.116224
25	6	0	-1.662751	-3.593517	-1.261351
26	1	0	-0.620324	-2.564262	0.292380
27	6	0	-2.574914	-3.497537	-2.306079
28	1	0	-3.855653	-2.176857	-3.407761
29	1	0	-1.216287	-4.548003	-1.011835
30	1	0	-2.843874	-4.375113	-2.879788
31	6	0	-1.883656	1.317351	-0.620650
32	6	0	-2.795013	2.185510	-0.020617
33	6	0	-1.352272	1.689715	-1.863018
34	6	0	-3.153793	3.381781	-0.633151
35	1	0	-3.234615	1.925921	0.933733
36	6	0	-1.708817	2.879827	-2.475810
37	1	0	-0.661741	1.021909	-2.371721
38	6	0	-2.612291	3.737706	-1.858776
39	1	0	-3.866095	4.035608	-0.145013
40	1	0	-1.278768	3.138139	-3.435533
41	1	0	-2.890549	4.670996	-2.331320

Frequencies -- 18.1348 20.9131 42.6625 45.0975 48.7894 70.0313

Cl•(-2157.211229)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.102368	1.498803	-0.757706
2	13	0	-2.092498	1.304927	0.851222
3	13	0	-2.095975	0.090634	-1.552526
4	13	0	-0.104639	-0.093875	1.676061
5	13	0	-2.098222	-1.383972	0.701454
6	13	0	-0.108747	-1.405928	-0.920136
7	13	0	1.872661	-0.005708	-0.002440
8	17	0	3.992631	-0.008999	-0.002760

Frequencies -- 57.3042 58.0857 111.7624 114.8366 181.1561 189.8045

$(CF_3)_3C$•(-2748.015458)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-2.188057	-0.215586	-1.672216
2	13	0	-4.176190	1.232051	-0.939985
3	13	0	-4.171623	-1.440403	-0.601400
4	13	0	-2.192246	1.552229	0.654464
5	13	0	-4.177795	0.188642	1.541845
6	13	0	-2.187830	-1.344456	1.022853
7	13	0	-0.241692	0.001134	0.002569
8	6	0	1.836796	0.001811	-0.000126
9	6	0	2.319149	-0.308344	1.414424
10	6	0	2.318120	1.383056	-0.438607
11	6	0	2.317698	-1.067723	-0.977560
12	9	0	3.594363	0.013713	1.631722
13	9	0	1.586076	0.357495	2.321473
14	9	0	2.179160	-1.610820	1.682437
15	9	0	1.583373	-2.185434	-0.856293
16	9	0	3.592472	-1.418025	-0.808020
17	9	0	2.177842	-0.647111	-2.239085
18	9	0	1.586137	1.835555	-1.469631
19	9	0	3.593737	1.410434	-0.823755
20	9	0	2.175717	2.266788	0.555096

Frequencies -- 11.8695 31.9652 32.4312 66.6260 67.3115 79.0700

Cp(-1890.386005)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.080439	-1.206692	-1.098542
2	13	0	-1.828166	0.465232	-1.529837
3	13	0	-2.020862	-1.446378	0.367401
4	13	0	0.181442	1.552809	-0.345601
5	13	0	-1.926704	1.157530	1.077183
6	13	0	-0.024561	-0.471875	1.666928
7	13	0	2.169784	-0.148851	0.181943
8	6	0	4.155410	0.957748	0.223448
9	1	0	4.183045	2.034463	0.168849
10	6	0	4.169069	0.068136	-0.878214
11	1	0	4.206931	0.348326	-1.918882
12	6	0	4.076797	-1.252414	-0.374682
13	1	0	4.033546	-2.154051	-0.964703
14	6	0	4.054607	0.187639	1.407215
15	1	0	3.990161	0.575532	2.411426
16	6	0	4.006085	-1.178603	1.037753
17	1	0	3.898259	-2.014108	1.711059

Frequencies -- 53.0617 55.1752 109.7498 110.8682 157.7135 166.0696

Cp^*(-2086.804071)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.471618	-0.306899	1.633393
2	13	0	-3.492394	-1.473258	0.538582
3	13	0	-3.486603	1.177407	1.021430
4	13	0	-1.482362	-1.273202	-1.061284
5	13	0	-3.497939	0.266229	-1.517373
6	13	0	-1.482158	1.547709	-0.552195
7	13	0	0.609132	-0.010223	-0.005861
8	6	0	2.491365	-0.984929	-0.699911
9	6	0	2.491175	-0.961147	0.725728
10	6	0	2.477478	0.401631	1.143181
11	6	0	2.481154	0.362861	-1.163637
12	6	0	2.471248	1.219515	-0.024177
13	6	0	2.447702	2.716779	-0.046771
14	1	0	2.184009	3.086917	-1.037474
15	1	0	1.718995	3.117038	0.661099
16	1	0	3.427065	3.124806	0.213192
17	6	0	2.461653	0.897607	2.556074
18	1	0	2.057338	1.908583	2.609473
19	1	0	1.846013	0.263919	3.196146
20	1	0	3.471252	0.917308	2.973344
21	6	0	2.494063	-2.163108	1.619131
22	1	0	3.479917	-2.633527	1.633304
23	1	0	2.240740	-1.889614	2.643112
24	1	0	1.770505	-2.910920	1.288518
25	6	0	2.509380	-2.214846	-1.553578
26	1	0	3.525904	-2.442582	-1.883675
27	1	0	2.136189	-3.078450	-1.003007
28	1	0	1.888231	-2.097910	-2.443178
29	6	0	2.462426	0.804777	-2.594635
30	1	0	2.193714	-0.020149	-3.253757
31	1	0	1.737419	1.604631	-2.758026
32	1	0	3.443595	1.173961	-2.901004

Frequencies – 23.3672 40.0853 48.0229 81.3601 85.0106 85.9553

Al_{13}

CH_3•(-3191.485711)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-2.584092	-0.767635	-0.442833
2	13	0	-1.140625	1.643650	-1.788946
3	13	0	1.612271	0.227371	-2.150101
4	13	0	1.630889	-2.084935	-0.708639
5	13	0	-0.738571	-2.646788	0.255364
6	13	0	-0.758703	-0.957222	-2.367627
7	13	0	-0.008993	-0.077894	-0.012025
8	13	0	1.133359	-1.459712	1.990399
9	13	0	-1.453225	-0.757896	2.132405
10	13	0	-1.957657	1.576965	0.766689
11	13	0	1.108216	2.304021	-0.481286
12	13	0	2.603236	0.203899	0.481791
13	13	0	0.573563	1.182941	2.153505
14	6	0	0.662866	2.786263	3.308824
15	1	0	0.099988	2.602255	4.224299
16	1	0	1.702773	2.985321	3.569001
17	1	0	0.251557	3.666744	2.817249

Frequencies -- 46.6491 52.3500 76.4636 85.7581 105.7253 115.5511

CH_3CH_2•(-3230.758029)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.440089	2.303798	0.745291
2	13	0	0.788984	-0.028869	2.680090
3	13	0	1.370753	-2.338319	0.678790
4	13	0	1.656702	-1.294869	-1.829418
5	13	0	1.690424	1.330205	-1.794432
6	13	0	2.706039	-0.039977	0.803232
7	13	0	0.214671	0.012025	0.016889
8	13	0	-0.717350	0.059608	-2.497625
9	13	0	-0.768497	2.284219	-0.989425
10	13	0	-1.026634	1.683224	1.689894
11	13	0	-1.074969	-1.663547	1.645666
12	13	0	-0.836764	-2.199497	-1.051855
13	13	0	-2.334331	0.069127	-0.318238
14	6	0	-4.242500	-0.002060	0.245138
15	1	0	-4.719940	0.871148	-0.207316
16	1	0	-4.308724	0.130753	1.325964
17	6	0	-4.944161	-1.292093	-0.190566
18	1	0	-4.507854	-2.164014	0.300156
19	1	0	-6.008213	-1.268143	0.058325
20	1	0	-4.862215	-1.452913	-1.267499

Frequencies -- 41.0751 45.1662 68.0347 80.3187 106.1313 117.5458

$(CH_3)_2CH•$(-3270.034496)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.495008	2.305312	0.665057
2	13	0	0.889098	-0.028318	2.664990
3	13	0	1.447876	-2.342055	0.636098
4	13	0	1.646199	-1.312137	-1.880661
5	13	0	1.665308	1.306438	-1.868344
6	13	0	2.766002	-0.030190	0.752190
7	13	0	0.262413	-0.001749	0.007756
8	13	0	-0.776470	0.022226	-2.464433
9	13	0	-0.777926	2.253640	-0.986602
10	13	0	-0.929993	1.687543	1.704247
11	13	0	-0.967811	-1.689206	1.677213
12	13	0	-0.818843	-2.222739	-1.018275
13	13	0	-2.300064	0.033344	-0.201731
14	6	0	-4.224078	-0.030915	0.350379
15	1	0	-4.648133	0.857542	-0.130477
16	6	0	-4.891607	-1.273892	-0.246338
17	1	0	-4.483480	-2.186601	0.195954
18	1	0	-5.968165	-1.262763	-0.043758
19	1	0	-4.757106	-1.343384	-1.327715
20	6	0	-4.487542	0.057967	1.853006
21	1	0	-4.073700	0.965811	2.295193
22	1	0	-5.564996	0.049961	2.051656
23	1	0	-4.052936	-0.794357	2.382047

Frequencies -- 36.6149 42.7027 65.5927 69.4391 105.7053 119.1905

$(CH_3)_3C•$(-3309.314338)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.271054	-1.702301	2.009961
2	13	0	-1.944398	1.354521	2.027126
3	13	0	-2.261276	2.224065	-0.539764
4	13	0	-2.276670	0.238446	-2.245931
5	13	0	-1.970866	-2.169112	-0.999316
6	13	0	-3.244132	-0.510491	0.647016
7	13	0	-0.781534	0.046856	-0.026303

8	13	0	0.213090	-0.963835	-2.295130
9	13	0	0.506147	-2.294411	0.095585
10	13	0	0.521945	0.265883	2.298653
11	13	0	0.237105	2.434118	0.625177
12	13	0	0.133175	1.685801	-1.941875
13	13	0	1.768799	0.257464	-0.287278
14	6	0	3.742465	-0.029720	0.013859
15	6	0	4.376768	1.350015	0.223043
16	1	0	4.003341	1.836060	1.127485
17	1	0	5.464326	1.240070	0.326541
18	1	0	4.192358	2.021495	-0.619548
19	6	0	4.059839	-0.917879	1.216574
20	1	0	5.148115	-1.030782	1.310185
21	1	0	3.691470	-0.488357	2.151069
22	1	0	3.630972	-1.917408	1.114413
23	6	0	4.324025	-0.665643	-1.253417
24	1	0	3.919698	-1.665173	-1.429724
25	1	0	4.129278	-0.063537	-2.144631
26	1	0	5.412971	-0.758423	-1.148744

Frequencies -- 14.0770 37.1025 39.1351 60.0011 67.5294 105.0499

$H_2C=CH•$(-3229.552447)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.096817	2.376474	0.674212
2	13	0	0.103375	0.114940	2.544702
3	13	0	1.240984	-2.255297	0.901184
4	13	0	2.061355	-1.350944	-1.540354
5	13	0	1.978693	1.287618	-1.669077
6	13	0	2.425446	0.118608	1.189864
7	13	0	0.182011	-0.018130	-0.170227
8	13	0	-0.116346	-0.161012	-2.841616
9	13	0	-0.643022	2.134580	-1.524005
10	13	0	-1.502804	1.655803	1.049310
11	13	0	-1.397487	-1.664330	1.213073
12	13	0	-0.501310	-2.341590	-1.301895
13	13	0	-2.202023	-0.147859	-1.148682
14	6	0	-4.896289	0.937475	-0.814161
15	6	0	-4.142562	-0.161966	-0.821990
16	1	0	-4.475407	1.929512	-0.951488
17	1	0	-5.973590	0.897441	-0.673111
18	1	0	-4.648099	-1.115423	-0.682092

Frequencies -- 32.8345 45.9432 54.7062 69.7744 97.3766 104.5446

HC≡C•(-3228.347673)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.463090	2.245666	0.842023
2	13	0	0.075228	0.048673	2.561877
3	13	0	0.962571	-2.367604	0.806076
4	13	0	1.938107	-1.452400	-1.575666
5	13	0	2.223589	1.179358	-1.555179
6	13	0	2.438618	-0.197578	1.286601
7	13	0	0.242513	0.051883	-0.144374
8	13	0	-0.026666	0.101993	-2.836189
9	13	0	-0.254370	2.372546	-1.389603
10	13	0	-1.222686	1.897599	1.124698
11	13	0	-1.586590	-1.456268	1.098287
12	13	0	-0.738258	-2.088928	-1.424548
13	13	0	-2.102456	0.314107	-1.172527
14	6	0	-5.145641	0.638683	-0.512368
15	6	0	-3.964243	0.513338	-0.739702
16	1	0	-6.186430	0.750757	-0.313477

Frequencies -- 43.2472 44.2484 55.5192 69.9599 103.0175 114.5723

Ph•(-3383.149175)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.270795	2.316264	0.840956
2	13	0	0.305982	-0.013655	2.645118
3	13	0	1.292115	-2.324922	0.828549
4	13	0	2.017803	-1.317247	-1.605682
5	13	0	2.005659	1.328316	-1.598585
6	13	0	2.558120	0.000627	1.178970
7	13	0	0.250235	-0.006641	-0.075691
8	13	0	-0.183375	-0.001539	-2.732261
9	13	0	-0.580720	2.233180	-1.273397
10	13	0	-1.326444	1.641339	1.310589
11	13	0	-1.311209	-1.676395	1.301719
12	13	0	-0.560148	-2.247580	-1.285350
13	13	0	-2.183431	-0.015525	-0.942081
14	6	0	-6.190076	-1.236541	-0.168822

15	6	0	-4.822389	-1.227274	-0.413665
16	6	0	-4.113900	-0.025292	-0.537294
17	6	0	-4.833265	1.169607	-0.407940
18	6	0	-6.200975	1.165295	-0.163091
19	6	0	-6.881368	-0.039037	-0.039716
20	1	0	-6.715295	-2.179518	-0.077955
21	1	0	-4.305066	-2.175751	-0.514929
22	1	0	-4.324568	2.123210	-0.504655
23	1	0	-6.734728	2.103022	-0.067739
24	1	0	-7.947114	-0.044331	0.152508

Frequencies -- 10.9021 27.9154 38.8832 52.7665 68.5926 102.9817

$PhCH_2$•(-3422.435197)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.266522	1.517042	1.083901
2	13	0	1.054418	0.738394	-2.002639
3	13	0	-1.983869	0.294075	-2.014856
4	13	0	-2.969959	0.210574	0.517411
5	13	0	-1.121554	0.913399	2.263594
6	13	0	-0.705781	2.170986	-0.564271
7	13	0	-0.375453	-0.367355	0.033986
8	13	0	-1.614530	-1.823257	1.930469
9	13	0	0.914580	-0.980050	2.290897
10	13	0	2.284928	-0.697973	-0.112175
11	13	0	-0.109886	-1.656843	-2.293137
12	13	0	-2.233862	-2.169568	-0.655220
13	13	0	0.275207	-2.851543	0.300172
14	6	0	1.487603	-4.410065	-0.060422
15	1	0	1.531182	-4.981998	0.868915
16	1	0	1.013467	-5.034496	-0.818881
17	6	0	2.849281	-3.965257	-0.488193
18	6	0	3.146957	-3.754470	-1.837193
19	6	0	3.840372	-3.675441	0.454901
20	6	0	4.375338	-3.239878	-2.228069
21	1	0	2.395922	-3.984240	-2.585854
22	6	0	5.071700	-3.164964	0.066445
23	1	0	3.631461	-3.836892	1.507130
24	6	0	5.341607	-2.932518	-1.277343
25	1	0	4.578167	-3.076393	-3.279242
26	1	0	5.820793	-2.942744	0.816348
27	1	0	6.297864	-2.527397	-1.581825

Frequencies -- 34.5652 39.6837 52.2894 69.8517 81.9826 88.1073

$Ph_2CH•$(-3653.379005)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.101842	2.182181	1.466366
2	13	0	0.836467	-0.925093	2.381238
3	13	0	1.622619	-2.069960	-0.363098
4	13	0	1.544122	-0.162903	-2.298879
5	13	0	1.251815	2.226286	-1.252975
6	13	0	2.655165	0.169336	0.726570
7	13	0	0.129595	0.131040	-0.017711
8	13	0	-1.047287	0.987093	-2.292438
9	13	0	-1.249828	2.423794	-0.044261
10	13	0	-1.141017	0.864442	2.239042
11	13	0	-0.832948	-2.252315	0.771645
12	13	0	-0.739620	-1.625907	-1.864028
13	13	0	-2.423425	-0.142067	-0.239189
14	6	0	-4.335583	-0.345260	0.404883
15	1	0	-4.812279	0.506104	-0.092814
16	6	0	-4.980191	-1.602124	-0.131766
17	6	0	-5.682171	-2.505910	0.664889
18	6	0	-4.924501	-1.855165	-1.507556
19	6	0	-6.288478	-3.627552	0.108517
20	1	0	-5.780780	-2.326541	1.727003
21	6	0	-5.531670	-2.968281	-2.064085
22	1	0	-4.399951	-1.159542	-2.156279
23	6	0	-6.213682	-3.869363	-1.254092
24	1	0	-6.830453	-4.310766	0.750955
25	1	0	-5.472164	-3.133461	-3.132766
26	1	0	-6.685532	-4.743708	-1.683521
27	6	0	-4.367171	-0.095756	1.884516
28	6	0	-3.901088	-1.037707	2.809847
29	6	0	-4.771667	1.149417	2.371913
30	6	0	-3.827539	-0.738833	4.162437
31	1	0	-3.568293	-2.008133	2.458173
32	6	0	-4.687441	1.456552	3.723864
33	1	0	-5.134922	1.896061	1.674470
34	6	0	-4.210311	0.515084	4.626458
35	1	0	-3.452474	-1.482772	4.854369
36	1	0	-4.996005	2.434568	4.071705
37	1	0	-4.140876	0.752262	5.680217

Frequencies -- 9.5367 25.4377 29.1902 42.6055 45.9221 53.7723

$Ph_3C^{\bullet}$ (-3884.317981)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.719071	1.353594	1.410911
2	13	0	0.752113	-1.659322	1.934420
3	13	0	1.128300	-2.513755	-1.069980
4	13	0	1.320194	-0.318505	-2.675798
5	13	0	1.646278	1.856539	-1.256570
6	13	0	2.691802	-0.817635	0.251761
7	13	0	0.176836	-0.142016	-0.234463
8	13	0	-0.962574	1.316042	-2.210228
9	13	0	-0.624669	2.374371	0.218076
10	13	0	-0.738542	0.534226	2.204778
11	13	0	-1.211853	-2.394148	0.271929
12	13	0	-1.186059	-1.335797	-2.214225
13	13	0	-2.398327	0.202791	-0.182463
14	6	0	-4.367905	0.075287	0.458888
15	6	0	-4.881661	-1.292166	0.017247
16	6	0	-5.498400	-2.197656	0.878521
17	6	0	-4.791069	-1.649217	-1.335243
18	6	0	-5.961674	-3.427763	0.417252
19	1	0	-5.633306	-1.946734	1.921595
20	6	0	-5.254138	-2.867737	-1.798664
21	1	0	-4.366142	-0.941855	-2.040527
22	6	0	-5.834573	-3.775139	-0.917225
23	1	0	-6.431729	-4.111465	1.113462
24	1	0	-5.161567	-3.111420	-2.849991
25	1	0	-6.191587	-4.733179	-1.272604
26	6	0	-4.374072	0.263844	1.971817
27	6	0	-3.702376	-0.652662	2.794100
28	6	0	-5.018344	1.328053	2.601969
29	6	0	-3.652078	-0.501426	4.169862
30	1	0	-3.219970	-1.513814	2.344568
31	6	0	-4.963660	1.488550	3.984662
32	1	0	-5.572037	2.048608	2.016252
33	6	0	-4.276866	0.583838	4.776674
34	1	0	-3.117431	-1.230324	4.766979
35	1	0	-5.469161	2.332184	4.438344
36	1	0	-4.233387	0.712400	5.850441
37	6	0	-5.121165	1.195494	-0.259289
38	6	0	-6.365056	0.981640	-0.856200
39	6	0	-4.615694	2.499603	-0.275966
40	6	0	-7.061346	2.022771	-1.459740

41	1	0	-6.804146	-0.006975	-0.846277
42	6	0	-5.306175	3.540950	-0.875663
43	1	0	-3.672829	2.711136	0.216391
44	6	0	-6.535064	3.305151	-1.479714
45	1	0	-8.024065	1.824357	-1.914483
46	1	0	-4.881675	4.537184	-0.871412
47	1	0	-7.075636	4.113269	-1.955645

Frequencies -- 17.6939 24.7367 37.2940 48.6916 52.3819 62.5924

Cl•(-3611.872838)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.421203	2.304857	0.732175
2	13	0	0.445784	0.014576	2.634255
3	13	0	1.212338	-2.324842	0.696391
4	13	0	1.668433	-1.335474	-1.797254
5	13	0	1.788030	1.317071	-1.776758
6	13	0	2.605499	-0.070412	1.006531
7	13	0	0.174534	0.047538	-0.057425
8	13	0	-0.561185	0.100920	-2.678664
9	13	0	-0.684866	2.342024	-1.163246
10	13	0	-1.147989	1.816051	1.464176
11	13	0	-1.302826	-1.618005	1.437738
12	13	0	-0.887053	-2.143076	-1.197846
13	13	0	-2.331078	0.165400	-0.693338
14	17	0	-4.374778	0.252862	-0.075914

Frequencies -- 50.9132 51.0117 62.3353 72.3007 97.4056 104.8072

$(CF_3)_3C$•(-4202.682686)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.299209	2.366446	0.382893
2	13	0	0.031894	0.318856	2.591224
3	13	0	1.263588	-2.250269	0.975194
4	13	0	1.863868	-1.558523	-1.580326
5	13	0	1.882374	1.042130	-1.917673
6	13	0	2.403504	0.136271	1.351278
7	13	0	0.224242	-0.034252	-0.108366
8	13	0	-0.449143	-0.368022	-2.729391

9	13	0	-0.671798	2.024423	-1.631238
10	13	0	-1.299032	1.938429	0.976110
11	13	0	-1.329448	-1.637888	1.441828
12	13	0	-0.709915	-2.396661	-1.054891
13	13	0	-2.259291	-0.088555	-0.728024
14	6	0	-4.350024	-0.072895	-0.659403
15	6	0	-4.887125	0.445826	0.678347
16	6	0	-4.861156	-1.500954	-0.890620
17	6	0	-4.852519	0.832732	-1.792512
18	9	0	-6.179254	0.169560	0.867001
19	9	0	-4.227630	-0.082360	1.718932
20	9	0	-4.749097	1.774645	0.762654
21	9	0	-6.146729	-1.552948	-1.244393
22	9	0	-4.723741	-2.236008	0.219347
23	9	0	-4.170763	-2.118022	-1.858823
24	9	0	-4.669175	0.241744	-2.977735
25	9	0	-6.147787	1.137439	-1.691817
26	9	0	-4.186734	1.994702	-1.826153

Frequencies -- 19.7388 28.4789 35.9512 40.7721 52.1746 72.7758

Cp(-3345.039329)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.513719	-0.917795	-0.323473
2	13	0	-1.413935	1.504263	-1.740132
3	13	0	1.301959	0.367349	-2.378650
4	13	0	1.734990	-1.794803	-0.823298
5	13	0	-0.464963	-2.536714	0.362744
6	13	0	-0.801825	-1.172491	-2.275563
7	13	0	0.011746	0.103091	0.032410
8	13	0	1.475262	-1.284323	1.878903
9	13	0	-1.237715	-0.715502	2.234308
10	13	0	-2.136581	1.466559	0.859704
11	13	0	0.904867	2.491588	-0.777983
12	13	0	2.625480	0.587738	0.155535
13	13	0	0.885990	1.235423	2.373192
14	6	0	2.162132	2.432776	3.910218
15	1	0	3.162330	2.120157	4.164527
16	6	0	1.806955	3.258336	2.821632
17	1	0	2.484302	3.706674	2.112662
18	6	0	0.388127	3.361040	2.791414
19	1	0	-0.195530	3.932401	2.084721
20	6	0	0.973915	2.026450	4.561741

21	1	0	0.910668	1.349499	5.398937
22	6	0	-0.121095	2.598901	3.879234
23	1	0	-1.163973	2.457688	4.113536

Frequencies -- 38.7458 53.3083 64.2835 73.2907 83.8892 91.0003

Cp*(-3541.457104)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.274032	2.156102	-0.532405
2	13	0	-1.933241	-0.313371	-2.297903
3	13	0	-2.173668	-2.368149	-0.052257
4	13	0	-1.823513	-1.128803	2.318261
5	13	0	-1.883738	1.464521	2.040597
6	13	0	-3.501812	-0.106134	-0.022028
7	13	0	-0.755181	-0.030335	0.100766
8	13	0	0.583438	0.254877	2.458116
9	13	0	0.317187	2.343403	0.678262
10	13	0	-0.044736	1.568322	-1.918887
11	13	0	0.033117	-1.988514	-1.536699
12	13	0	0.413730	-2.183007	1.167598
13	13	0	1.963408	0.012751	0.168105
14	6	0	4.080379	-0.742450	0.580459
15	6	0	3.682170	-1.126560	-0.728621
16	6	0	3.445743	0.065993	-1.487842
17	6	0	4.103160	0.677813	0.637141
18	6	0	3.722526	1.180808	-0.635012
19	6	0	3.164503	0.119145	-2.959487
20	1	0	2.856662	1.118334	-3.266245
21	1	0	4.064108	-0.139798	-3.523901
22	1	0	2.373558	-0.573920	-3.252697
23	6	0	3.688543	2.625704	-1.016644
24	1	0	4.665470	2.945434	-1.388601
25	1	0	2.948184	2.822555	-1.792856
26	1	0	3.435118	3.250853	-0.158666
27	6	0	4.430971	1.510847	1.836005
28	1	0	5.394277	2.011164	1.712657
29	1	0	3.672147	2.279701	2.004104
30	1	0	4.483258	0.896743	2.734940
31	6	0	4.386278	-1.671671	1.712951
32	1	0	5.456054	-1.679569	1.934244
33	1	0	3.855495	-1.379445	2.622254
34	1	0	4.085308	-2.691158	1.471186
35	6	0	3.639837	-2.524607	-1.260286

36	1	0	4.654655	-2.904150	-1.404017
37	1	0	3.117177	-3.202910	-0.583402
38	1	0	3.128591	-2.563141	-2.222718

Frequencies -- 22.8711 45.6328 58.8047 68.2947 72.6847 86.8126

Al_{20}

CH_3•(-4888.585420)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.399906	0.310763	2.527097
2	13	0	2.430175	-2.267880	1.116664
3	13	0	2.510402	-1.704839	-1.726184
4	13	0	2.537475	1.130238	-2.099514
5	13	0	2.479010	2.411951	0.484901
6	13	0	3.843903	-0.033932	0.115972
7	13	0	1.358323	-0.017734	0.048294
8	13	0	0.135377	1.702750	1.706819
9	13	0	0.103707	-1.199232	2.104074
10	13	0	0.188858	-2.384039	-0.501883
11	13	0	0.255088	-0.325523	-2.404380
12	13	0	0.234943	2.149907	-1.101537
13	13	0	-2.334594	2.590498	-0.277534
14	13	0	-2.554828	1.527046	2.056748
15	13	0	-2.597838	-1.023966	2.333715
16	13	0	-2.414564	-2.564759	0.283854
17	13	0	-2.247083	-1.555539	-2.115036
18	13	0	-2.211354	1.069496	-2.406827
19	13	0	-1.192259	-0.002620	0.000607
20	13	0	-3.638759	0.017422	-0.157540
21	6	0	5.808520	-0.049493	0.204523
22	1	0	6.147600	0.552980	1.047697
23	1	0	6.168075	-1.070818	0.332678
24	1	0	6.227775	0.360209	-0.714981

Frequencies -- 3.0717 60.9265 75.2870 76.0228 77.8458 83.2287

CH_3CH_2•(-4927.855768)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.163055	-0.709317	-2.349404
2	13	0	-2.306928	-2.261843	0.123335
3	13	0	-2.204818	-0.429659	2.297912
4	13	0	-2.037951	2.165573	1.307554
5	13	0	-2.025466	2.089448	-1.532904
6	13	0	-3.545138	0.251682	-0.074728
7	13	0	-0.995491	0.095746	-0.033151
8	13	0	0.293138	0.740814	-2.287685
9	13	0	0.116526	-2.013953	-1.239697
10	13	0	0.066551	-1.774415	1.588809
11	13	0	0.207464	0.897711	2.257913
12	13	0	0.329028	2.441995	-0.021794
13	13	0	2.871331	2.232780	-0.957949
14	13	0	2.959235	0.234799	-2.512082
15	13	0	2.811025	-2.112753	-1.594501
16	13	0	2.593984	-2.502184	0.897446
17	13	0	2.587997	-0.518419	2.529899
18	13	0	2.731346	1.890261	1.588675
19	13	0	1.633443	-0.067016	-0.025049
20	13	0	4.225571	-0.157751	0.129737
21	6	0	-5.521594	0.307898	-0.061776
22	1	0	-5.840167	0.909981	-0.917429
23	1	0	-5.833298	0.851618	0.834611
24	6	0	-6.170274	-1.079493	-0.105740
25	1	0	-5.881000	-1.627368	-1.005551
26	1	0	-5.871419	-1.688217	0.750808
27	1	0	-7.261049	-1.015429	-0.097561

Frequencies -- 6.8443 20.9613 54.5537 62.6272 81.4788 86.3259

$(CH_3)_2CH$•(-4967.135480)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.483164	0.233220	2.497931
2	13	0	2.533648	-2.268028	0.975926
3	13	0	2.569194	-1.584890	-1.829983
4	13	0	2.543275	1.265762	-2.087449
5	13	0	2.494404	2.433313	0.556438
6	13	0	3.893885	0.035155	0.045898
7	13	0	1.404383	0.007254	0.023525

8	13	0	0.178389	1.622302	1.778669
9	13	0	0.200413	-1.292398	2.035859
10	13	0	0.271279	-2.356121	-0.613017
11	13	0	0.284775	-0.224044	-2.429118
12	13	0	0.234230	2.199703	-1.019684
13	13	0	-2.351591	2.558200	-0.222749
14	13	0	-2.517945	1.459925	2.098276
15	13	0	-2.497362	-1.096707	2.335622
16	13	0	-2.305401	-2.604482	0.258766
17	13	0	-2.188504	-1.545374	-2.126497
18	13	0	-2.205963	1.083848	-2.371106
19	13	0	-1.143311	-0.013850	0.004202
20	13	0	-3.593533	-0.046736	-0.127493
21	6	0	5.883172	0.042276	0.199185
22	1	0	6.233211	0.314543	-0.801991
23	6	0	6.416311	-1.345837	0.555437
24	1	0	6.049844	-1.668560	1.534004
25	1	0	6.122286	-2.104077	-0.173405
26	1	0	7.510498	-1.333887	0.603524
27	6	0	6.360880	1.095039	1.199516
28	1	0	6.025013	2.100064	0.936334
29	1	0	5.991855	0.878067	2.205773
30	1	0	7.455033	1.108305	1.247113

Frequencies -- 10.4339 40.0771 46.4539 75.6442 77.2495 93.5017

$(CH_3)_3C•$(-5006.415780)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.338775	0.388798	2.529322
2	13	0	2.371722	-2.227938	1.217959
3	13	0	2.471009	-1.779432	-1.634215
4	13	0	2.503184	1.034069	-2.127861
5	13	0	2.435886	2.417931	0.408811
6	13	0	3.790816	-0.036783	0.144560
7	13	0	1.302970	-0.020686	0.058351
8	13	0	0.082678	1.760382	1.649342
9	13	0	0.037485	-1.128857	2.146731
10	13	0	0.138202	-2.406953	-0.403609
11	13	0	0.218227	-0.432796	-2.384877
12	13	0	0.196911	2.101034	-1.183331
13	13	0	-2.394299	2.568071	-0.464252
14	13	0	-2.619457	1.669224	1.935281
15	13	0	-2.657494	-0.857062	2.382118
16	13	0	-2.454079	-2.536619	0.445877

17	13	0	-2.284148	-1.681710	-2.019674
18	13	0	-2.250562	0.917768	-2.483675
19	13	0	-1.242353	0.004726	-0.004113
20	13	0	-3.688793	0.000688	-0.177969
21	6	0	5.798077	-0.049606	0.228551
22	6	0	6.286749	-1.496858	0.302923
23	1	0	5.913275	-2.008564	1.193507
24	1	0	5.980572	-2.078759	-0.570262
25	1	0	7.383583	-1.512750	0.345130
26	6	0	6.258163	0.716516	1.469100
27	1	0	5.930986	1.759133	1.451346
28	1	0	5.883441	0.263950	2.390535
29	1	0	7.354849	0.711944	1.517387
30	6	0	6.353035	0.620156	-1.029695
31	1	0	6.052109	0.094947	-1.939987
32	1	0	6.027238	1.659887	-1.117458
33	1	0	7.450232	0.617628	-0.992627

Frequencies -- 3.7598 21.7212 44.7538 47.3624 77.1634 78.9499

$H_2C=CH•$(-4926.651553)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.325974	0.319849	2.589254
2	13	0	2.438622	-2.223994	1.138188
3	13	0	2.565338	-1.613773	-1.683900
4	13	0	2.548537	1.227745	-2.015959
5	13	0	2.409073	2.468349	0.592416
6	13	0	3.818067	0.051667	0.200718
7	13	0	1.337080	0.025134	0.087261
8	13	0	0.049634	1.681291	1.752644
9	13	0	0.069354	-1.230998	2.088255
10	13	0	0.233275	-2.357651	-0.522169
11	13	0	0.301832	-0.272221	-2.393496
12	13	0	0.201593	2.187230	-1.054839
13	13	0	-2.412375	2.559986	-0.363312
14	13	0	-2.658930	1.533005	1.983769
15	13	0	-2.633943	-1.015958	2.304688
16	13	0	-2.367255	-2.588479	0.283019
17	13	0	-2.172352	-1.604047	-2.129670
18	13	0	-2.197042	1.017562	-2.457492
19	13	0	-1.207140	-0.003069	-0.017354
20	13	0	-3.649254	-0.051649	-0.227194

21	6	0	6.369112	0.587567	1.476238
22	6	0	5.764578	0.105147	0.392886
23	1	0	5.813966	0.981297	2.323559
24	1	0	7.451704	0.612299	1.571535
25	1	0	6.388346	-0.272833	-0.414896

Frequencies -- 13.5225 50.1345 54.4467 74.1060 76.7387 95.0115

HC≡C•(-4925.445043)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.119961	0.557375	2.749550
2	13	0	2.443550	-2.020530	1.374781
3	13	0	2.700476	-1.468770	-1.458612
4	13	0	2.555684	1.359656	-1.857431
5	13	0	2.205495	2.647271	0.700827
6	13	0	3.738619	0.296276	0.459773
7	13	0	1.283780	0.140739	0.203200
8	13	0	-0.170435	1.775774	1.745681
9	13	0	-0.021494	-1.120105	2.170478
10	13	0	0.347669	-2.307831	-0.405692
11	13	0	0.410691	-0.259655	-2.321450
12	13	0	0.113165	2.215713	-1.051118
13	13	0	-2.539575	2.475322	-0.436528
14	13	0	-2.865256	1.422261	1.892637
15	13	0	-2.741919	-1.125563	2.208717
16	13	0	-2.285971	-2.670773	0.201103
17	13	0	-2.011868	-1.675755	-2.196569
18	13	0	-2.145368	0.943923	-2.525243
19	13	0	-1.239331	-0.028938	-0.036684
20	13	0	-3.658457	-0.188284	-0.367794
21	6	0	6.827449	0.523766	0.816690
22	6	0	5.629915	0.437816	0.680387
23	1	0	7.883276	0.599487	0.936773

Frequencies -- 6.1107 38.2460 40.5713 72.0914 74.1353 94.7502

Ph•(-5080.259623)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	1.489370	-1.287744	-2.132103
2	13	0	1.503177	1.785706	-1.719946
3	13	0	1.551667	2.195079	1.070912
4	13	0	1.633361	-0.315950	2.297751
5	13	0	1.534128	-2.416374	0.452595
6	13	0	2.950268	0.005407	-0.163776
7	13	0	0.380946	0.001462	-0.040473
8	13	0	-0.816187	-2.218796	-0.968315
9	13	0	-0.820340	0.326297	-2.392272
10	13	0	-0.795603	2.397034	-0.348971
11	13	0	-0.740085	1.125265	2.136062
12	13	0	-0.747206	-1.644761	1.767519
13	13	0	-3.281798	-2.412985	0.954051
14	13	0	-3.459184	-2.076693	-1.581323
15	13	0	-3.592188	0.322846	-2.443392
16	13	0	-3.431767	2.425024	-1.003632
17	13	0	-3.269253	2.104738	1.537481
18	13	0	-3.144929	-0.320549	2.520259
19	13	0	-2.222972	0.009254	-0.041571
20	13	0	-4.841311	-0.012850	0.196436
21	6	0	7.020539	1.213061	-0.099789
22	6	0	5.631880	1.204658	-0.149011
23	6	0	4.910865	0.006474	-0.097589
24	6	0	5.634281	-1.186895	0.004121
25	6	0	7.022942	-1.186190	0.053701
26	6	0	7.717614	0.015716	0.001738
27	1	0	7.558720	2.152192	-0.141329
28	1	0	5.106369	2.151745	-0.229527
29	1	0	5.110982	-2.137721	0.045530
30	1	0	7.563010	-2.121865	0.132291
31	1	0	8.799897	0.019227	0.040131

Frequencies -- 13.3549 17.1187 24.8785 31.2654 61.8618 82.4572

$PhCH_2$•(-5119.546507)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.753174	-1.559294	-1.778007
2	13	0	0.830635	0.758599	-3.112706
3	13	0	0.644305	2.964509	-0.934917
4	13	0	1.476150	1.735556	1.473829
5	13	0	2.177670	-0.905657	0.902110
6	13	0	2.651403	1.088937	-1.075847
7	13	0	0.258205	0.330976	-0.513873
8	13	0	-0.129588	-2.260733	0.090062

9	13	0	-0.915062	-1.215732	-2.372324
10	13	0	-1.606875	1.586435	-1.946045
11	13	0	-1.193768	2.097160	0.899005
12	13	0	-0.294557	-0.281462	2.045560
13	13	0	-2.333722	-2.243870	1.869094
14	13	0	-2.710951	-3.042027	-0.595400
15	13	0	-3.624836	-1.385168	-2.332862
16	13	0	-4.266250	0.940801	-1.506965
17	13	0	-3.894645	1.828975	0.854816
18	13	0	-2.979434	0.184204	2.601694
19	13	0	-2.226920	-0.312474	-0.071824
20	13	0	-4.656018	-1.113545	0.532929
21	6	0	5.948926	-0.129482	2.017158
22	6	0	5.459982	0.785292	1.094299
23	6	0	5.269100	0.429794	-0.244484
24	6	0	5.590072	-0.876670	-0.625600
25	6	0	6.078954	-1.793331	0.295302
26	6	0	6.255418	-1.426909	1.624288
27	1	0	6.087160	0.171951	3.048117
28	1	0	5.214090	1.792431	1.413672
29	1	0	5.446856	-1.175959	-1.658424
30	1	0	6.319271	-2.799112	-0.026381
31	1	0	6.634103	-2.141524	2.343379
32	6	0	4.626277	1.373651	-1.204890
33	1	0	4.937365	1.184909	-2.233627
34	1	0	4.842768	2.415053	-0.961296

Frequencies – 16.0755 29.9251 52.8348 59.4518 64.1018 77.0958

$Ph_2CH•$(-5350.479065)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.505974	-0.039792	2.567343
2	13	0	2.628450	-2.369435	0.773971
3	13	0	2.620632	-1.348712	-1.967413
4	13	0	2.476254	1.538151	-1.813094
5	13	0	2.394704	2.319345	0.941184
6	13	0	3.879480	0.062214	0.082120
7	13	0	1.396292	-0.058375	0.093040
8	13	0	0.127137	1.293097	2.043764
9	13	0	0.279223	-1.551606	2.008377
10	13	0	0.340971	-2.350605	-0.814760
11	13	0	0.280573	0.053770	-2.354353
12	13	0	0.135772	2.228220	-0.595298

13	13	0	-2.382534	2.241264	0.670370
14	13	0	-2.419791	0.417518	2.535855
15	13	0	-2.392193	-2.079754	1.901742
16	13	0	-2.331096	-2.807877	-0.560949
17	13	0	-2.216269	-1.050628	-2.434849
18	13	0	-2.283143	1.499247	-1.862273
19	13	0	-1.139205	-0.217925	0.057588
20	13	0	-3.590329	-0.274653	-0.012414
21	6	0	5.885737	0.168841	0.306329
22	1	0	6.085653	-0.629618	1.025844
23	6	0	6.566018	-0.188551	-0.990624
24	6	0	6.456850	-1.505418	-1.456396
25	6	0	7.307645	0.711756	-1.754099
26	6	0	7.050613	-1.903076	-2.642190
27	1	0	5.898959	-2.229052	-0.869663
28	6	0	7.902082	0.313250	-2.947117
29	1	0	7.451127	1.726167	-1.408998
30	6	0	7.772676	-0.989290	-3.402319
31	1	0	6.949741	-2.928999	-2.974114
32	1	0	8.475603	1.032337	-3.519021
33	1	0	8.234446	-1.294250	-4.332573
34	6	0	6.186313	1.487630	0.953607
35	6	0	5.939854	2.706974	0.311462
36	6	0	6.646171	1.527610	2.270827
37	6	0	6.169049	3.915632	0.952788
38	1	0	5.548125	2.707197	-0.700240
39	6	0	6.863777	2.735899	2.920550
40	1	0	6.833634	0.596196	2.793252
41	6	0	6.631023	3.935797	2.263304
42	1	0	5.972465	4.844149	0.430922
43	1	0	7.220149	2.737421	3.943206
44	1	0	6.803226	4.877918	2.767473

Frequencies --	4.6261	13.7331	14.6958	26.6143	44.0174	46.9844

$Ph_3C•$(-5581.430907)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.267122	1.880114	1.584493
2	13	0	0.299371	-1.225395	2.119076
3	13	0	0.247558	-2.435782	-0.409420
4	13	0	0.337501	-0.403898	-2.305836
5	13	0	0.239818	2.171804	-1.185925
6	13	0	1.723447	0.025544	0.097179

7	13	0	-0.875535	0.004911	0.031475
8	13	0	-2.095236	2.395926	0.283835
9	13	0	-1.989984	0.409866	2.407827
10	13	0	-2.071623	-2.173380	1.072366
11	13	0	-2.048593	-1.703237	-1.694370
12	13	0	-2.049322	1.037776	-2.161459
13	13	0	-4.562719	2.044082	-1.542550
14	13	0	-4.737993	2.436558	0.983565
15	13	0	-4.745730	0.401128	2.530525
16	13	0	-4.723255	-2.024699	1.718782
17	13	0	-4.556464	-2.460715	-0.797686
18	13	0	-4.466257	-0.416978	-2.429115
19	13	0	-3.479793	0.003833	0.097483
20	13	0	-6.090585	-0.031903	-0.081639
21	6	0	3.795751	0.014988	0.006396
22	6	0	4.184446	1.432057	-0.391070
23	6	0	3.702085	1.988228	-1.585801
24	6	0	5.003081	2.240896	0.399935
25	6	0	4.010875	3.284068	-1.966361
26	1	0	3.090635	1.381962	-2.244429
27	6	0	5.311514	3.544079	0.022479
28	1	0	5.415485	1.853801	1.321328
29	6	0	4.815688	4.076893	-1.156544
30	1	0	3.618103	3.674871	-2.897196
31	1	0	5.950134	4.141931	0.660922
32	1	0	5.055339	5.091946	-1.445791
33	6	0	4.345524	-0.367905	1.377368
34	6	0	3.850263	0.234269	2.538905
35	6	0	5.403469	-1.267056	1.523900
36	6	0	4.366336	-0.062441	3.791070
37	1	0	3.062547	0.975224	2.461191
38	6	0	5.923727	-1.569582	2.777125
39	1	0	5.833579	-1.736538	0.649095
40	6	0	5.404584	-0.976601	3.918228
41	1	0	3.954229	0.422154	4.667509
42	1	0	6.743975	-2.272306	2.856069
43	1	0	5.807036	-1.217137	4.893886
44	6	0	4.122545	-1.040576	-1.041812
45	6	0	4.806017	-0.779499	-2.229033
46	6	0	3.737853	-2.368833	-0.802781
47	6	0	5.058004	-1.791451	-3.152141
48	1	0	5.165428	0.218058	-2.438690
49	6	0	3.989634	-3.377637	-1.716209
50	1	0	3.260215	-2.615443	0.139871
51	6	0	4.644470	-3.091009	-2.909563
52	1	0	5.591658	-1.553627	-4.064070
53	1	0	3.674879	-4.390258	-1.495343

54	1	0	4.839071	-3.874206	-3.630774

Frequencies -- 10.7381 15.1448 17.7592 22.9780 41.4239 44.8696

Cl•(-5308.985899)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.439966	0.252755	2.559764
2	13	0	2.552376	-2.214051	0.990065
3	13	0	2.694874	-1.445476	-1.703181
4	13	0	2.667003	1.485119	-1.740628
5	13	0	2.431504	2.489277	0.868135
6	13	0	3.947648	0.120807	0.271562
7	13	0	1.376837	0.071209	0.118226
8	13	0	0.053149	1.492271	1.975543
9	13	0	0.159710	-1.380784	2.008621
10	13	0	0.338077	-2.303527	-0.611181
11	13	0	0.386438	-0.134562	-2.356227
12	13	0	0.198932	2.293294	-0.821978
13	13	0	-2.506020	2.524861	-0.713093
14	13	0	-2.631246	1.832500	1.733601
15	13	0	-2.436338	-0.647751	2.346266
16	13	0	-2.239935	-2.535137	0.552249
17	13	0	-2.111348	-1.826243	-1.955279
18	13	0	-2.188115	0.724160	-2.506477
19	13	0	-1.198709	0.034402	-0.023359
20	13	0	-3.796016	-0.128448	-0.202825
21	17	0	6.073384	0.164132	0.402238

Frequencies --55.7454 58.2398 62.0154 85.1854 88.8527 93.7631

$(CF_3)_3C$•(-5899.794583)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.642065	1.580516	-1.857259
2	13	0	0.634907	2.309380	0.862223
3	13	0	0.702731	-0.042712	2.362034
4	13	0	0.640008	-2.343318	0.769540
5	13	0	0.625958	-1.520675	-1.913186
6	13	0	2.018144	0.000097	-0.082041
7	13	0	-0.540376	-0.000932	-0.008677
8	13	0	-1.662307	0.061425	-2.412129

9	13	0	-1.688532	2.346922	-0.614187
10	13	0	-1.669078	1.365016	2.009285
11	13	0	-1.663361	-1.435229	1.964372
12	13	0	-1.707860	-2.316649	-0.696429
13	13	0	-4.354077	-2.261999	-1.348625
14	13	0	-4.431023	0.017164	-2.512036
15	13	0	-4.321452	2.280503	-1.325273
16	13	0	-4.190068	2.273565	1.245571
17	13	0	-4.074178	-0.021180	2.511901
18	13	0	-4.195409	-2.290834	1.211276
19	13	0	-3.116278	0.000601	-0.060520
20	13	0	-5.715431	0.007985	0.142428
21	6	0	4.120384	-0.001144	-0.040146
22	6	0	4.641263	-1.002761	-1.073568
23	6	0	4.605990	-0.402629	1.354236
24	6	0	4.631957	1.401316	-0.378903
25	9	0	4.450166	-2.256486	-0.648033
26	9	0	5.942184	-0.866263	-1.342773
27	9	0	3.994670	-0.883187	-2.241635
28	9	0	3.937154	-1.467291	1.820490
29	9	0	5.902301	-0.717593	1.399703
30	9	0	4.407137	0.593576	2.226075
31	9	0	3.948562	2.345126	0.286078
32	9	0	4.480987	1.656315	-1.682914
33	9	0	5.920780	1.585350	-0.083346

Frequencies -- 10.7477 21.4659 35.7075 38.3057 63.1593 65.9010

Cp(-5042.148559)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.224759	0.317546	-2.560861
2	13	0	-2.343641	-2.156518	-1.200909
3	13	0	-2.442618	-1.469520	1.835730
4	13	0	-2.373309	1.349901	2.005476
5	13	0	-2.355819	2.345359	-0.620900
6	13	0	-3.920408	-0.039853	-0.133915
7	13	0	-1.243553	0.005491	-0.056223
8	13	0	0.068556	1.615134	-1.808985
9	13	0	0.061933	-1.161736	-2.129946
10	13	0	-0.099370	-2.343545	0.511556
11	13	0	-0.084856	-0.138969	2.393914
12	13	0	-0.019638	2.230518	0.911602
13	13	0	2.457152	2.422248	-0.484160

14	13	0	2.610336	0.669563	-2.409983
15	13	0	2.711428	-1.819071	-1.832204
16	13	0	2.667381	-2.472229	0.633285
17	13	0	2.569454	-0.819104	2.573573
18	13	0	2.467410	1.673287	2.014146
19	13	0	1.386830	-0.067813	0.045980
20	13	0	3.985629	0.070376	0.098560
21	6	0	-5.856618	1.114075	0.268980
22	1	0	-5.813620	2.102890	0.697401
23	6	0	-5.811889	0.802221	-1.111790
24	1	0	-5.728864	1.511770	-1.919753
25	6	0	-5.854855	-0.606514	-1.242986
26	1	0	-5.801424	-1.158281	-2.168054
27	6	0	-5.927160	-0.102283	0.989435
28	1	0	-5.938469	-0.202549	2.063140
29	6	0	-5.925734	-1.164658	0.055133
30	1	0	-5.930530	-2.216502	0.292561

Frequencies -- 18.4723 21.7368 46.0573 48.5559 57.6133 91.2859

Cp*(-3541.457104)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.274032	2.156102	-0.532405
2	13	0	-1.933241	-0.313371	-2.297903
3	13	0	-2.173668	-2.368149	-0.052257
4	13	0	-1.823513	-1.128803	2.318261
5	13	0	-1.883738	1.464521	2.040597
6	13	0	-3.501812	-0.106134	-0.022028
7	13	0	-0.755181	-0.030335	0.100766
8	13	0	0.583438	0.254877	2.458116
9	13	0	0.317187	2.343403	0.678262
10	13	0	-0.044736	1.568322	-1.918887
11	13	0	0.033117	-1.988514	-1.536699
12	13	0	0.413730	-2.183007	1.167598
13	13	0	1.963408	0.012751	0.168105
14	6	0	4.080379	-0.742450	0.580459
15	6	0	3.682170	-1.126560	-0.728621
16	6	0	3.445743	0.065993	-1.487842
17	6	0	4.103160	0.677813	0.637141
18	6	0	3.722526	1.180808	-0.635012
19	6	0	3.164503	0.119145	-2.959487
20	1	0	2.856662	1.118334	-3.266245
21	1	0	4.064108	-0.139798	-3.523901

22	1	0	2.373558	-0.573920	-3.252697
23	6	0	3.688543	2.625704	-1.016644
24	1	0	4.665470	2.945434	-1.388601
25	1	0	2.948184	2.822555	-1.792856
26	1	0	3.435118	3.250853	-0.158666
27	6	0	4.430971	1.510847	1.836005
28	1	0	5.394277	2.011164	1.712657
29	1	0	3.672147	2.279701	2.004104
30	1	0	4.483258	0.896743	2.734940
31	6	0	4.386278	-1.671671	1.712951
32	1	0	5.456054	-1.679569	1.934244
33	1	0	3.855495	-1.379445	2.622254
34	1	0	4.085308	-2.691158	1.471186
35	6	0	3.639837	-2.524607	-1.260286
36	1	0	4.654655	-2.904150	-1.404017
37	1	0	3.117177	-3.202910	-0.583402
38	1	0	3.128591	-2.563141	-2.222718

Frequencies -- 22.8711 45.6328 58.8047 68.2947 72.6847 86.8126

B3LYP

Al_3

CH_3•(-767.188668)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.828572	-0.009356	-0.000074
2	13	0	1.441320	1.210722	-0.063457
3	13	0	1.455752	-1.203415	0.064072
4	6	0	-2.809483	-0.002848	-0.001862
5	1	0	-3.214892	-0.441360	0.913421
6	1	0	-3.213053	-0.555014	-0.854342
7	1	0	-3.181420	1.024518	-0.068507

Frequencies -- 28.2972 102.5984 105.3507

CH_3CH_2•(-806.480600)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.257228	-0.000068	-0.276474

2	13	0	1.995095	1.209207	0.071657
3	13	0	1.995129	-1.209078	0.072357
4	6	0	-2.226162	-0.000198	-0.583207
5	1	0	-2.454528	-0.871137	-1.209589
6	1	0	-2.454568	0.870353	-1.210113
7	6	0	-3.115576	0.000159	0.672597
8	1	0	-2.934055	0.878497	1.296513
9	1	0	-4.178962	0.000050	0.414420
10	1	0	-2.934004	-0.877788	1.297049

Frequencies -- 21.8501 71.6872 84.0782

$(CH_3)_2CH•$(-845.775718)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.081092	-0.061961	-0.199226
2	13	0	-2.362302	-1.208734	0.184019
3	13	0	-2.334487	1.193163	-0.095166
4	6	0	1.919212	-0.090354	-0.373154
5	1	0	2.126547	-0.335113	-1.422114
6	6	0	2.557298	-1.178570	0.506256
7	1	0	2.183249	-2.178561	0.269394
8	1	0	3.645651	-1.202367	0.373328
9	1	0	2.367595	-1.001930	1.569047
10	6	0	2.524561	1.293083	-0.079664
11	1	0	3.612583	1.281653	-0.215561
12	1	0	2.127494	2.070619	-0.738422
13	1	0	2.334709	1.607738	0.950875

Frequencies -- -4.9980 58.4716 71.7716 187.3233 200.8187 228.1236

$(CH_3)_3C•$(-885.073308)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.611362	-1.241926	0.065384
2	13	0	-2.604838	1.174032	-0.045060
3	13	0	-0.325398	-0.038455	0.005668
4	6	0	1.696196	0.001233	-0.002436
5	6	0	2.140831	1.471482	-0.103056
6	1	0	1.786716	1.950176	-1.021009
7	1	0	1.789625	2.070282	0.742758
8	1	0	3.237570	1.538268	-0.109232
9	6	0	2.235709	-0.782184	-1.210988

10	1	0	1.948821	-1.837421	-1.181402
11	1	0	1.882228	-0.371846	-2.160666
12	1	0	3.334061	-0.748354	-1.229195
13	6	0	2.244053	-0.612518	1.297010
14	1	0	1.896452	-0.077738	2.184938
15	1	0	1.957497	-1.661894	1.412009
16	1	0	3.342468	-0.576336	1.303151

Frequencies -- -5.6333 56.4017 61.1915 179.7470 191.8502 216.2581

$H_2C=CH•$(-805.270204)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.374685	-0.000205	-0.239462
2	13	0	1.880012	1.211865	0.055884
3	13	0	1.880191	-1.211685	0.056941
4	6	0	-2.332149	-0.000422	-0.460917
5	1	0	-2.779380	-0.001169	-1.455083
6	6	0	-3.177388	0.000357	0.576829
7	1	0	-4.258489	0.000264	0.452618
8	1	0	-2.832890	0.001130	1.607541

Frequencies -- 12.0687 73.5514 101.2860 227.4126 275.6975 303.4589

HC≡C•(-804.057309)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.346770	-0.223623	-0.245707
2	13	0	-1.587228	1.202495	0.666949
3	13	0	-2.115638	-0.958353	-0.306825
4	6	0	2.211348	-0.518862	-0.606748
5	6	0	3.388251	-0.706450	-0.835703
6	1	0	4.420882	-0.870392	-1.035942

Frequencies -- 70.0940 75.1065 217.6550 241.9178 254.3170 298.0242

Ph•(-958.926466)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.040128	-0.000263	-0.000017

2	13	0	-3.313990	-0.008559	1.212107
3	13	0	-3.313986	0.007736	-1.212152
4	6	0	0.933813	-0.000020	-0.000005
5	6	0	1.665007	-1.200819	-0.006618
6	6	0	1.664693	1.200970	0.006621
7	6	0	3.056450	-1.204147	-0.006611
8	1	0	1.144295	-2.153117	-0.011910
9	6	0	3.056135	1.204660	0.006639
10	1	0	1.143734	2.153132	0.011903
11	6	0	3.753672	0.000347	0.000020
12	1	0	3.596681	-2.143688	-0.011802
13	1	0	3.596122	2.144341	0.011840
14	1	0	4.837228	0.000489	0.000030

Frequencies -- 23.1378 48.6748 49.4938 156.2612 191.8315 204.6650

$PhCH_2$• (-998.229427)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.572454	0.752287	-0.000035
2	13	0	-4.129333	0.397667	-0.000541
3	13	0	-2.704408	-1.564956	0.001563
4	6	0	0.116581	1.837795	-0.000697
5	1	0	0.142100	2.479552	-0.884036
6	1	0	0.142180	2.480376	0.882041
7	6	0	1.253588	0.857453	-0.000309
8	6	0	1.783789	0.362187	-1.200189
9	6	0	1.783837	0.363220	1.199977
10	6	0	2.812697	-0.572751	-1.200176
11	1	0	1.392641	0.726024	-2.144160
12	6	0	2.812744	-0.571730	1.200729
13	1	0	1.392756	0.727897	2.143653
14	6	0	3.333460	-1.046053	0.000472
15	1	0	3.210871	-0.930061	-2.142500
16	1	0	3.210956	-0.928225	2.143345
17	1	0	4.136433	-1.772595	0.000765

Frequencies -- 18.1628 27.9647 28.8327 102.8865 105.3822 185.2646

Ph_2CH• (-1229.267073)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-0.890251	1.467656	-0.363917
2	13	0	-1.445942	3.964247	0.008370
3	13	0	-3.203081	2.329919	0.388919
4	6	0	0.299169	-0.104020	-0.838255
5	1	0	0.312165	-0.129237	-1.931483
6	6	0	-0.492231	-1.304033	-0.365145
7	6	0	-1.585608	-1.737121	-1.134386
8	6	0	-0.227705	-1.987592	0.827927
9	6	0	-2.377523	-2.804607	-0.730227
10	1	0	-1.805297	-1.238747	-2.073130
11	6	0	-1.018321	-3.059686	1.229359
12	1	0	0.614867	-1.693658	1.439192
13	6	0	-2.099280	-3.473288	0.458099
14	1	0	-3.208248	-3.119881	-1.350451
15	1	0	-0.782933	-3.576461	2.152325
16	1	0	-2.712370	-4.307771	0.774899
17	6	0	1.714988	0.062617	-0.351091
18	6	0	2.018995	0.470356	0.955296
19	6	0	2.785929	-0.160790	-1.225712
20	6	0	3.335783	0.630815	1.373645
21	1	0	1.215695	0.676900	1.654936
22	6	0	4.103388	0.007811	-0.814220
23	1	0	2.580312	-0.476143	-2.242529
24	6	0	4.385330	0.400647	0.490259
25	1	0	3.540016	0.946716	2.389740
26	1	0	4.911038	-0.172647	-1.513680
27	1	0	5.410771	0.531560	0.813153

Frequencies -- 16.5397 25.5698 27.2288 38.7966 48.1966 79.7417

$Ph_3C^{\bullet}$ (-1460.298495)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.207200	0.144931	-1.318966
2	13	0	-2.185712	0.802599	-3.633104
3	13	0	-3.709365	-0.056104	-1.944433
4	6	0	0.264601	-0.014276	0.104783
5	6	0	-0.659890	-0.214070	1.300130
6	6	0	-1.542674	-1.312610	1.309464
7	6	0	-0.727783	0.670481	2.384222
8	6	0	-2.448120	-1.510041	2.345031
9	1	0	-1.492141	-2.046749	0.511613
10	6	0	-1.631482	0.469526	3.422727
11	1	0	-0.063002	1.522165	2.421110

12	6	0	-2.500463	-0.616272	3.409628
13	1	0	-3.108041	-2.369095	2.321084
14	1	0	-1.652115	1.168979	4.250121
15	1	0	-3.204233	-0.766671	4.218747
16	6	0	1.082542	1.273007	0.151149
17	6	0	0.463426	2.525066	0.014773
18	6	0	2.469529	1.262184	0.339650
19	6	0	1.190593	3.707741	0.064859
20	1	0	-0.611910	2.581698	-0.126574
21	6	0	3.202439	2.444890	0.387089
22	1	0	2.986765	0.318748	0.448963
23	6	0	2.569570	3.674372	0.249270
24	1	0	0.677867	4.655563	-0.047764
25	1	0	4.275262	2.400058	0.533266
26	1	0	3.141112	4.593784	0.281838
27	6	0	1.123787	-1.235161	-0.210443
28	6	0	1.472930	-2.179432	0.760881
29	6	0	1.641018	-1.415412	-1.500352
30	6	0	2.292477	-3.262071	0.452937
31	1	0	1.101815	-2.068332	1.771235
32	6	0	2.463016	-2.490437	-1.812077
33	1	0	1.407264	-0.692676	-2.275937
34	6	0	2.790642	-3.425408	-0.834343
35	1	0	2.544226	-3.977369	1.227057
36	1	0	2.841710	-2.601731	-2.821000
37	1	0	3.424788	-4.269842	-1.074600

Frequencies -- 16.1580 22.2028 31.0819 46.6426 50.4306 58.5149

Cl•(-1187.584691)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.575409	-0.000749	0.001287
2	13	0	-1.696160	1.219321	-0.002280
3	13	0	-1.698327	-1.216779	-0.002873
4	17	0	2.714532	-0.002582	0.004830

Frequencies -- 81.6954 93.9859 229.0968 281.2858 353.4035 534.0760

$(CF_3)_3C$•(-1778.686773)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	3.794288	1.170513	0.050479
2	13	0	3.779332	-1.266788	-0.078001
3	13	0	1.535061	-0.029668	-0.010184
4	6	0	-0.583770	-0.007982	-0.005404
5	6	0	-1.102613	-1.034965	-1.022021
6	6	0	-1.000597	1.418439	-0.391700
7	6	0	-1.053456	-0.350251	1.417561
8	9	0	-0.948907	-2.290890	-0.552343
9	9	0	-2.399769	-0.880163	-1.338926
10	9	0	-0.402872	-0.967971	-2.177175
11	9	0	-0.913052	1.615800	-1.718459
12	9	0	-2.243513	1.754622	-0.014847
13	9	0	-0.156182	2.318603	0.187937
14	9	0	-2.358097	-0.661596	1.503445
15	9	0	-0.364347	-1.408168	1.907357
16	9	0	-0.828390	0.680933	2.255490

Frequencies -- 5.3646 37.6482 39.9601 60.8057 65.5715 72.0220

Cp(-920.807694)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.199845	-0.092920	0.132497
2	13	0	3.657452	0.606275	-0.566289
3	13	0	3.400054	-1.465457	0.672736
4	6	0	-0.575864	1.386463	0.175083
5	1	0	-0.410219	2.452079	0.149275
6	6	0	-0.743761	0.538687	-0.955558
7	1	0	-0.718919	0.847984	-1.988578
8	6	0	-0.924557	-0.783320	-0.487640
9	1	0	-1.051587	-1.661248	-1.100970
10	6	0	-0.659764	0.585846	1.339147
11	1	0	-0.547218	0.929923	2.354986
12	6	0	-0.859081	-0.758661	0.931749
13	1	0	-0.954726	-1.611338	1.585717

Frequencies -- 9.1047 74.4712 89.9562 181.1574 185.1480 193.6754

Cp*(-1117.321303)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.797486	-0.018107	-0.006492

2	13	0	-3.135666	-1.266695	-0.025543
3	13	0	-3.172993	1.157820	-0.010763
4	6	0	1.144621	-0.969468	0.714774
5	6	0	1.151580	-0.960892	-0.720189
6	6	0	1.134130	0.396710	-1.152695
7	6	0	1.122889	0.382865	1.163286
8	6	0	1.101215	1.230404	0.010186
9	6	0	1.145198	2.730329	0.019362
10	1	0	0.652960	3.145325	0.899684
11	1	0	2.179760	3.088051	0.026503
12	1	0	0.661472	3.155844	-0.860656
13	6	0	1.175744	0.869016	-2.575508
14	1	0	0.670806	1.827814	-2.699084
15	1	0	2.208959	0.996839	-2.913832
16	1	0	0.695349	0.159878	-3.250556
17	6	0	1.239429	-2.165690	-1.609883
18	1	0	0.721094	-2.008326	-2.556489
19	1	0	2.282682	-2.401667	-1.842760
20	1	0	0.804360	-3.049116	-1.141256
21	6	0	1.223884	-2.184822	1.590812
22	1	0	0.793368	-3.062538	1.107481
23	1	0	2.264840	-2.423677	1.830919
24	1	0	0.696425	-2.038728	2.534178
25	6	0	1.150672	0.838128	2.591980
26	1	0	0.663779	0.121008	3.253809
27	1	0	2.180550	0.961821	2.941818
28	1	0	0.644521	1.795419	2.722102

Frequencies --	6.3757	49.6800	53.6828	76.6621	81.2769	90.8304

Al_6

CH_3•(-1494.559982)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.830978	1.268836	1.504662
2	13	0	0.218006	1.972214	-0.900491
3	13	0	-1.320532	0.000013	-0.017877
4	13	0	0.830989	-1.268885	1.504626
5	13	0	0.217978	-1.972200	-0.900537
6	13	0	1.797649	-0.000001	-1.243506
7	6	0	-3.306039	0.000005	0.011063
8	1	0	-3.691431	0.886488	0.518524
9	1	0	-3.691426	-0.886493	0.518503
10	1	0	-3.695046	0.000016	-1.010543

Frequencies --	45.4356	72.8286	82.2442	99.8375	102.6955	128.8121

CH_3CH_2•(-1533.852439)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.549191	-1.267971	1.356353
2	13	0	-0.433770	-1.973040	-0.861982
3	13	0	0.885229	0.000036	0.317936
4	13	0	-1.549294	1.268231	1.356079
5	13	0	-0.433794	1.972908	-0.862345
6	13	0	-1.903952	-0.000133	-1.531780
7	6	0	2.831795	0.000154	0.779293
8	1	0	3.019042	0.876310	1.407690
9	1	0	3.019093	-0.875846	1.407895
10	6	0	3.783995	0.000040	-0.426983
11	1	0	4.831589	0.000106	-0.109543
12	1	0	3.636962	-0.879495	-1.058391
13	1	0	3.636912	0.879419	-1.058597

Frequencies --	45.9763	57.8938	87.9711	92.2523	126.8929	139.1844

$(CH_3)_2CH$•(-1573.148257)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.284765	-1.251368	1.585017
2	13	0	-0.991156	-1.972248	-0.875866
3	13	0	0.657970	-0.001352	-0.220724
4	13	0	-1.276760	1.286249	1.564643
5	13	0	-0.982060	1.965692	-0.907768
6	13	0	-2.601648	-0.000676	-1.023402
7	6	0	2.659593	-0.009405	-0.454016
8	1	0	2.796757	-0.020615	-1.542708
9	6	0	3.313560	-1.273638	0.123654
10	1	0	3.167007	-1.346949	1.205528
11	1	0	2.912086	-2.185920	-0.322366
12	1	0	4.396377	-1.267456	-0.052408
13	6	0	3.320764	1.262323	0.098446
14	1	0	4.403493	1.246587	-0.077567
15	1	0	2.924326	2.167835	-0.365515
16	1	0	3.174840	1.357868	1.178667

Frequencies -- 6.7070 46.1077 55.7095 74.7777 87.8336 124.4435

$(CH_3)_3C•$(-1612.445895)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.686254	-1.168637	1.621360
2	13	0	-1.114354	-2.016523	-0.747265
3	13	0	0.448615	-0.000881	-0.023938
4	13	0	-1.684182	1.364639	1.463330
5	13	0	-1.112154	1.910701	-0.992441
6	13	0	-2.703252	-0.072055	-1.190468
7	6	0	2.480823	-0.002174	-0.020299
8	6	0	2.992785	-1.209307	0.782167
9	1	0	2.672209	-2.157858	0.345035
10	1	0	4.091596	-1.210888	0.804661
11	1	0	2.649882	-1.190916	1.820529
12	6	0	2.994574	1.294752	0.625673
13	1	0	4.093388	1.297562	0.647883
14	1	0	2.675299	2.181960	0.073832
15	1	0	2.651749	1.406257	1.658221
16	6	0	2.988391	-0.093012	-1.467958
17	1	0	2.657407	0.753638	-2.075151
18	1	0	4.087419	-0.094768	-1.483845
19	1	0	2.656181	-1.008219	-1.965029

Frequencies -- 15.0498 47.4008 54.5051 74.5867 86.5049 123.5730

$H_2C=CH•$(-1532.638332)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.536598	0.001121	1.930414
2	13	0	-0.756917	1.334697	-0.121518
3	13	0	-0.755983	-1.335186	-0.120245
4	13	0	1.757899	-1.661250	0.159380
5	13	0	1.128412	-0.000247	-1.848578
6	13	0	1.756684	1.662863	0.158061
7	6	0	-3.482891	-0.000983	0.283700
8	1	0	-3.370174	-0.000408	1.363958
9	6	0	-2.415719	-0.000993	-0.548713
10	1	0	-4.506634	-0.001548	-0.081982

11	1	0	-2.667505	-0.001607	-1.611804

Frequencies -- 57.3143 67.9302 104.7756 111.1876 142.2179 156.6379

HC≡C•(-1531.428330)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.035614	1.272216	1.505440
2	13	0	0.429828	1.986084	-0.901143
3	13	0	-1.075525	0.000097	-0.044844
4	13	0	1.036618	-1.270162	1.506571
5	13	0	0.430259	-1.986650	-0.899117
6	13	0	1.988388	-0.000339	-1.285203
7	6	0	-4.207414	-0.000977	0.054625
8	1	0	-5.270683	-0.001315	0.097625
9	6	0	-2.995370	-0.000593	0.002373

Frequencies -- 37.2715 60.0707 76.1731 93.1453 127.8084 146.4675

Ph•(-1686.292703)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.833021	1.903868	0.000177
2	13	0	-0.230524	-0.000076	1.332177
3	13	0	-0.230562	0.000042	-1.332133
4	13	0	-2.758826	0.000109	-1.677733
5	13	0	-1.832993	-1.903894	-0.000073
6	13	0	-2.758779	-0.000140	1.677857
7	6	0	3.652947	1.205033	0.000013
8	6	0	4.351766	0.000068	-0.000056
9	6	0	3.652991	-1.204922	-0.000098
10	6	0	2.264830	-1.203712	-0.000071
11	6	0	1.517290	0.000017	-0.000003
12	6	0	2.264786	1.203772	0.000039
13	1	0	4.191866	2.144925	0.000047
14	1	0	5.434920	0.000088	-0.000077
15	1	0	4.191944	-2.144795	-0.000153
16	1	0	1.742335	-2.154214	-0.000104
17	1	0	1.742257	2.154255	0.000094

Frequencies -- 45.2184 50.1809 55.4508 104.0406 107.0356 117.7591

$PhCH_2$•(-1725.601028)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.377339	1.921319	1.070508
2	13	0	2.188410	1.816797	-1.375462
3	13	0	0.594929	-0.206452	-0.800459
4	13	0	1.571772	-0.447325	1.961882
5	13	0	2.489031	-1.857205	0.006761
6	13	0	3.853850	0.297803	-0.168511
7	6	0	-1.117888	-0.702447	-1.744998
8	1	0	-1.059106	-1.752755	-2.034104
9	1	0	-1.193949	-0.105071	-2.654695
10	6	0	-2.275367	-0.451750	-0.827878
11	6	0	-2.916007	0.794717	-0.792455
12	6	0	-2.732810	-1.443858	0.050655
13	6	0	-3.980411	1.033030	0.069187
14	1	0	-2.581966	1.581226	-1.460454
15	6	0	-3.797088	-1.207115	0.912889
16	1	0	-2.254730	-2.417415	0.045545
17	6	0	-4.427727	0.033464	0.928114
18	1	0	-4.464406	2.002650	0.067169
19	1	0	-4.137153	-1.996220	1.573258
20	1	0	-5.258473	0.217745	1.597914

Frequencies -- 4.4673 26.2124 26.6044 54.4368 77.2152 93.0459

Ph_2CH•(-1956.637345)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.391173	-3.557128	0.479364
2	13	0	2.360682	-1.780643	2.077486
3	13	0	0.692589	-0.700349	0.334447
4	13	0	1.507220	-2.505379	-1.832729
5	13	0	2.500281	-0.149993	-1.501268
6	13	0	3.925848	-1.586612	0.066969
7	6	0	-0.945065	0.413023	0.838517
8	1	0	-0.923186	0.391461	1.930774
9	6	0	-2.160897	-0.351882	0.386737
10	6	0	-3.099737	-0.794252	1.328202
11	6	0	-2.383889	-0.689496	-0.956994
12	6	0	-4.215731	-1.530484	0.947400

13	1	0	-2.952230	-0.550700	2.374364
14	6	0	-3.504659	-1.416862	-1.342555
15	1	0	-1.668750	-0.380470	-1.710959
16	6	0	-4.427047	-1.841930	-0.392039
17	1	0	-4.925050	-1.856232	1.699018
18	1	0	-3.652549	-1.658706	-2.388363
19	1	0	-5.297226	-2.413249	-0.690804
20	6	0	-0.792777	1.854743	0.413584
21	6	0	0.113905	2.667862	1.112512
22	6	0	-1.506102	2.439960	-0.637424
23	6	0	0.307712	3.998880	0.770940
24	1	0	0.672127	2.246841	1.942492
25	6	0	-1.312087	3.775374	-0.981656
26	1	0	-2.235526	1.858267	-1.183776
27	6	0	-0.403096	4.562744	-0.285735
28	1	0	1.013318	4.598996	1.333385
29	1	0	-1.884235	4.201418	-1.797642
30	1	0	-0.254386	5.600928	-0.555722

Frequencies -- 7.4521 20.6576 30.0674 34.7270 46.2844 63.8510

Ph_3C•(-2187.664528)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.909059	-3.353137	0.797315
2	13	0	2.918642	-1.229015	1.843351
3	13	0	0.709179	-0.740896	0.454338
4	13	0	1.416052	-2.735635	-1.625692
5	13	0	2.026667	-0.239644	-1.821649
6	13	0	3.979392	-1.188713	-0.480903
7	6	0	-0.989565	0.283391	1.093872
8	6	0	-2.179943	-0.435970	0.451613
9	6	0	-3.296444	-0.853699	1.185971
10	6	0	-2.201889	-0.677220	-0.931999
11	6	0	-4.371540	-1.491951	0.571891
12	1	0	-3.335471	-0.675497	2.251007
13	6	0	-3.273228	-1.309516	-1.548388
14	1	0	-1.371689	-0.342040	-1.542058
15	6	0	-4.366973	-1.728864	-0.796574
16	1	0	-5.218851	-1.799764	1.173297
17	1	0	-3.251280	-1.476927	-2.618776
18	1	0	-5.201800	-2.228985	-1.271879
19	6	0	-0.812136	1.712169	0.578651
20	6	0	0.379092	2.407112	0.841391

21	6	0	-1.806922	2.393223	-0.129993
22	6	0	0.573682	3.711661	0.408750
23	1	0	1.163810	1.923303	1.414196
24	6	0	-1.614906	3.701464	-0.568641
25	1	0	-2.745874	1.901104	-0.341887
26	6	0	-0.424697	4.368054	-0.306105
27	1	0	1.507857	4.214858	0.628041
28	1	0	-2.406620	4.199884	-1.115632
29	1	0	-0.275684	5.384171	-0.650106
30	6	0	-1.033857	0.222696	2.622666
31	6	0	-1.225247	1.359538	3.414397
32	6	0	-0.924043	-1.008108	3.287763
33	6	0	-1.286901	1.273519	4.804154
34	1	0	-1.330166	2.327901	2.945832
35	6	0	-0.992363	-1.100640	4.670407
36	1	0	-0.796731	-1.916189	2.709192
37	6	0	-1.167964	0.046145	5.441689
38	1	0	-1.433338	2.176003	5.385904
39	1	0	-0.903492	-2.069413	5.147743
40	1	0	-1.213710	-0.020327	6.521780

Frequencies -- 10.0341 19.9476 22.3188 37.9779 48.7425 52.8542

Cl• (-1914.952020)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.180832	0.080251	1.899948
2	13	0	-0.368562	-1.989639	0.630146
3	13	0	1.154141	0.311034	0.038864
4	13	0	-0.631511	2.133837	0.423254
5	13	0	-0.788274	0.867454	-1.832096
6	13	0	-2.309157	-0.955684	-0.759073
7	17	0	3.166387	-0.346852	-0.348730

Frequencies -- 23.0536 65.1147 70.3833 77.9502 106.7973 117.3557

$(CF_3)_3C$•(-2506.059324)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.908395	-1.290379	-1.558951
2	13	0	2.315061	-1.981496	0.861213

3	13	0	0.840704	0.013496	0.055654
4	13	0	2.908169	1.257907	-1.587050
5	13	0	2.339309	1.999544	0.824481
6	13	0	3.864487	0.002921	1.294060
7	6	0	-1.280482	-0.002055	0.012165
8	6	0	-1.763952	-0.962776	-1.089586
9	6	0	-1.781854	1.426779	-0.274599
10	6	0	-1.772898	-0.469927	1.393904
11	9	0	-1.547647	-0.433116	-2.312464
12	9	0	-3.074167	-1.262612	-1.011164
13	9	0	-1.097425	-2.137277	-1.055920
14	9	0	-3.080324	1.487256	-0.625881
15	9	0	-1.084605	1.998972	-1.283361
16	9	0	-1.626552	2.219594	0.804398
17	9	0	-1.036855	0.096887	2.380791
18	9	0	-3.058908	-0.165475	1.647978
19	9	0	-1.646626	-1.803622	1.534698

Frequencies -- 13.5790 40.3345 41.7183 61.5225 64.4480 73.0101

Cp(-1648.175676)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.097580	1.451489	0.975801
2	13	0	0.706278	1.379287	-1.600213
3	13	0	-1.244540	-0.071405	0.665590
4	13	0	1.090093	-1.152866	1.274073
5	13	0	0.475683	-1.513310	-1.256797
6	13	0	2.726776	-0.233256	-1.609754
7	6	0	-3.083347	1.302563	0.460034
8	1	0	-2.962415	2.350208	0.235243
9	6	0	-3.195604	0.253508	-0.491861
10	1	0	-3.198121	0.367478	-1.564617
11	6	0	-3.316578	-0.970190	0.219203
12	1	0	-3.404629	-1.951124	-0.219904
13	6	0	-3.124639	0.726394	1.753179
14	1	0	-3.041599	1.259422	2.687188
15	6	0	-3.267162	-0.679076	1.604528
16	1	0	-3.313049	-1.400034	2.405436

Frequencies -- 19.1921 34.1111 50.7898 58.6998 69.3822 89.6985

Cp*(-1844.689277)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.208736	0.170915	2.059523
2	13	0	1.822290	1.507613	-0.086593
3	13	0	-0.824842	-0.230294	0.210776
4	13	0	1.004217	-2.113416	0.785845
5	13	0	1.482512	-0.980915	-1.516895
6	13	0	3.745049	-0.198618	-0.465500
7	6	0	-2.431220	1.381831	0.174478
8	6	0	-2.247646	0.880795	-1.155438
9	6	0	-2.622206	-0.501632	-1.159977
10	6	0	-2.900843	0.308452	0.989226
11	6	0	-3.015911	-0.856560	0.164927
12	6	0	-2.248187	2.805524	0.607602
13	1	0	-1.444118	3.297087	0.059152
14	1	0	-3.164423	3.379709	0.435835
15	1	0	-2.009626	2.878731	1.668731
16	6	0	-3.277643	0.400119	2.437832
17	1	0	-2.695567	1.159782	2.960166
18	1	0	-4.334221	0.665118	2.545859
19	1	0	-3.124473	-0.545930	2.958036
20	6	0	-1.877963	1.699696	-2.357821
21	1	0	-2.774118	2.124966	-2.821112
22	1	0	-1.220303	2.529191	-2.097207
23	1	0	-1.369736	1.104435	-3.116543
24	6	0	-3.528110	-2.196239	0.603993
25	1	0	-3.262298	-2.412987	1.639316
26	1	0	-4.619512	-2.236612	0.531117
27	1	0	-3.130089	-3.002754	-0.012264
28	6	0	-2.665181	-1.398189	-2.360656
29	1	0	-1.947885	-1.089855	-3.121358
30	1	0	-2.440978	-2.433674	-2.103022
31	1	0	-3.659624	-1.379785	-2.818089

Frequencies -- 3.4788 23.0245 41.6282 51.2681 54.8084 85.2755

Al_7

CH_3•(-1737.070065)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.155637	-1.331204	-1.100636
2	13	0	-1.850773	0.261284	-1.541199
3	13	0	-1.852888	-1.464685	0.543892
4	13	0	0.155050	1.619990	-0.599860

5	13	0	-1.853397	1.202651	0.996624
6	13	0	0.154642	-0.288918	1.703829
7	13	0	2.147179	0.000145	0.001250
8	6	0	4.124101	0.000320	0.000510
9	1	0	4.518384	-0.956679	0.352525
10	1	0	4.518453	0.783911	0.652963
11	1	0	4.517660	0.173844	-1.004608

Frequencies -- 38.4172 51.2273 52.6402 113.9420 114.9796 167.4221

CH_3CH_2•(-1776.361775)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.453478	-1.547130	-0.937587
2	13	0	-2.318117	0.171282	-1.507922
3	13	0	-2.339102	-1.214222	0.820273
4	13	0	-0.124271	1.427687	-0.903414
5	13	0	-2.046053	1.474135	0.847268
6	13	0	-0.146027	-0.101854	1.663181
7	13	0	1.737899	-0.293386	-0.174040
8	6	0	3.711929	-0.509298	-0.287461
9	1	0	3.972341	-1.444187	0.221858
10	1	0	3.967582	-0.667978	-1.341352
11	6	0	4.541632	0.652839	0.286978
12	1	0	4.330526	1.594285	-0.226359
13	1	0	4.335403	0.812753	1.348244
14	1	0	5.615695	0.467749	0.191782

Frequencies -- 36.6367 45.5876 51.9734 80.5089 99.7810 164.8281

$(CH_3)_2CH$•(-1815.657156)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.604504	-1.448211	-0.983317
2	13	0	2.480211	-1.388194	0.815066
3	13	0	2.660046	0.070903	-1.457809
4	13	0	0.404750	-0.072470	1.663653
5	13	0	2.480432	1.315197	0.939022
6	13	0	0.604117	1.539563	-0.845799
7	13	0	-1.452823	0.013014	-0.209075
8	6	0	-3.449318	0.019632	-0.364092

9	1	0	-3.648760	0.068661	-1.442727
10	6	0	-4.080116	1.260705	0.289451
11	1	0	-3.898751	1.285497	1.368212
12	1	0	-3.691485	2.193460	-0.127406
13	1	0	-5.167514	1.269455	0.148238
14	6	0	-4.079690	-1.275835	0.174111
15	1	0	-3.690678	-2.166786	-0.325604
16	1	0	-3.898387	-1.398314	1.246187
17	1	0	-5.167068	-1.272142	0.032571

Frequencies -- 4.4549 41.5162 42.0447 74.3370 80.1240 152.2261

$(CH_3)_3C\bullet$(-1854.954557)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.775005	0.824727	1.516668
2	13	0	2.785469	1.562425	0.043433
3	13	0	2.781677	-0.817236	1.334942
4	13	0	0.778773	0.903427	-1.471904
5	13	0	2.787339	-0.743915	-1.371422
6	13	0	0.776788	-1.725220	-0.047745
7	13	0	-1.221245	0.000663	-0.002957
8	6	0	-3.237922	0.000191	-0.000898
9	6	0	-3.754288	-0.692179	-1.274235
10	1	0	-3.426538	-0.182274	-2.184632
11	1	0	-3.425140	-1.733022	-1.342026
12	1	0	-4.852946	-0.699584	-1.285907
13	6	0	-3.752181	1.449838	0.037074
14	1	0	-3.422155	1.982546	0.933409
15	1	0	-3.423601	2.028877	-0.830626
16	1	0	-4.850846	1.464910	0.037954
17	6	0	-3.750517	-0.756825	1.236525
18	1	0	-3.422034	-1.799950	1.248866
19	1	0	-3.418833	-0.295348	2.171004
20	1	0	-4.849186	-0.763685	1.251904

Frequencies -- 21.2055 40.7713 42.5838 73.7189 77.1378 142.1999

$H_2C{=}CH\bullet$(-1775.150953)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-0.018194	1.650544	-0.114708
2	13	0	2.065365	0.806606	-1.415567
3	13	0	2.061893	0.998929	1.297312
4	13	0	0.240334	-1.045091	-1.421832
5	13	0	2.314243	-1.410360	0.105068
6	13	0	0.236881	-0.834158	1.560666
7	13	0	-1.821797	-0.262309	0.018901
8	6	0	-3.780424	-0.443487	0.029940
9	6	0	-4.626338	0.590280	-0.029798
10	1	0	-4.229543	-1.435716	0.087756
11	1	0	-5.706817	0.464798	-0.022094
12	1	0	-4.285386	1.620601	-0.089785

Frequencies -- 43.6819 51.5052 80.8235 110.2127 168.2980 168.4889

HC≡C•(-1773.938340)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.068993	-1.296451	-1.166937
2	13	0	-2.073564	0.318388	-1.527639
3	13	0	-2.061747	-1.489397	0.489903
4	13	0	-0.073504	1.658578	-0.546823
5	13	0	-2.070374	1.163219	1.042581
6	13	0	-0.066358	-0.352685	1.705991
7	13	0	1.890420	0.005406	-0.004795
8	6	0	3.813394	0.002842	-0.003552
9	6	0	5.026207	-0.001703	-0.000773
10	1	0	6.090718	-0.005894	0.001845

Frequencies -- 45.6413 46.3223 84.4179 84.9083 169.8081 170.7730

Ph• (-1928.806959)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.294372	-1.502059	-0.860257
2	13	0	-3.289067	0.001041	-1.573762
3	13	0	-3.305345	-1.348628	0.779724
4	13	0	-1.294388	1.503191	-0.858217
5	13	0	-3.305373	1.347529	0.781535
6	13	0	-1.295706	-0.001175	1.735967
7	13	0	0.689430	0.000001	-0.001067

8	6	0	3.394186	-1.199404	-0.002696
9	6	0	4.785858	-1.203493	-0.001610
10	6	0	5.484366	0.000039	-0.000435
11	6	0	4.785837	1.203559	-0.000236
12	6	0	3.394165	1.199446	-0.001327
13	6	0	2.662829	0.000015	-0.002776
14	1	0	2.875785	-2.153337	-0.003793
15	1	0	5.324991	-2.143732	-0.001888
16	1	0	6.567871	0.000048	0.000233
17	1	0	5.324953	2.143807	0.000558
18	1	0	2.875747	2.153371	-0.001336

Frequencies -- 6.6438 33.5871 35.3919 64.1421 70.1952 136.9900

$PhCH_2$• (-1968.110063)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.325805	1.842064	-0.006340
2	13	0	-3.793617	0.192374	1.360848
3	13	0	-3.795501	0.178977	-1.355141
4	13	0	-1.305730	-0.555106	1.498399
5	13	0	-2.898013	-1.973029	0.012883
6	13	0	-1.307803	-0.569850	-1.488768
7	13	0	0.180982	1.014314	-0.003996
8	6	0	3.582394	0.206520	-1.201719
9	6	0	4.543067	-0.798556	-1.198799
10	6	0	5.029827	-1.303056	0.003188
11	6	0	4.544958	-0.787136	1.201086
12	6	0	3.584281	0.217927	1.195955
13	1	0	3.219239	0.594165	-2.147585
14	1	0	4.915163	-1.186070	-2.139931
15	1	0	5.779234	-2.084720	0.006318
16	1	0	4.918535	-1.165683	2.145275
17	1	0	3.222607	0.614551	2.138661
18	6	0	3.084940	0.738647	-0.004995
19	6	0	2.024241	1.800231	-0.009211
20	1	0	2.112335	2.449361	0.866474
21	1	0	2.110931	2.440976	-0.891189

Frequencies -- 12.1639 25.4004 29.4860 51.1718 55.5183 107.8093

Ph_2CH• (-2199.146523)

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.955391	1.141368	1.369138
2	13	0	4.230791	1.691566	0.238740
3	13	0	3.947002	-0.453134	1.869744
4	13	0	2.581753	0.738572	-1.527068
5	13	0	4.523721	-0.810987	-0.753660
6	13	0	2.287214	-1.650930	0.267445
7	13	0	0.332179	0.005110	-0.365262
8	6	0	-1.640060	-0.041138	-0.824149
9	1	0	-1.638413	-0.043088	-1.919278
10	6	0	-2.274630	1.262570	-0.384665
11	6	0	-3.047786	1.393476	0.774167
12	6	0	-2.064801	2.414814	-1.158275
13	6	0	-3.585211	2.623526	1.143160
14	1	0	-3.250684	0.525379	1.386651
15	6	0	-2.599390	3.642338	-0.790164
16	1	0	-1.480200	2.343326	-2.069806
17	6	0	-3.363650	3.755657	0.367905
18	1	0	-4.186901	2.691957	2.041922
19	1	0	-2.423616	4.511445	-1.413052
20	1	0	-3.783756	4.710953	0.657043
21	6	0	-2.283498	-1.325552	-0.362368
22	6	0	-3.017599	-2.106742	-1.263383
23	6	0	-2.158604	-1.798148	0.951325
24	6	0	-3.607952	-3.302813	-0.870470
25	1	0	-3.131274	-1.766518	-2.286575
26	6	0	-2.755297	-2.989096	1.351529
27	1	0	-1.581184	-1.231885	1.674340
28	6	0	-3.483382	-3.748302	0.441590
29	1	0	-4.170741	-3.885053	-1.590428
30	1	0	-2.641998	-3.327968	2.374417
31	1	0	-3.943873	-4.678702	0.750119

Frequencies -- 7.2330 17.6322 22.3036 31.1259 42.7017 51.8101

$Ph_3C•$(-2430.177033)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.600385	-1.376057	1.052134
2	13	0	4.580684	0.212954	1.611972
3	13	0	4.620681	-1.387124	-0.577517
4	13	0	2.576013	1.609180	0.733783
5	13	0	4.599297	1.305640	-0.869603

6	13	0	2.615521	-0.157444	-1.686682
7	13	0	0.597266	0.007268	0.014579
8	6	0	-1.460777	-0.007869	-0.005011
9	6	0	-1.869738	-0.762053	-1.270647
10	6	0	-2.825482	-0.273407	-2.168039
11	6	0	-1.296801	-2.010573	-1.560014
12	6	0	-3.183466	-0.993239	-3.305274
13	1	0	-3.300479	0.679151	-1.977769
14	6	0	-1.651652	-2.732164	-2.692051
15	1	0	-0.569748	-2.438432	-0.877279
16	6	0	-2.597818	-2.223578	-3.577297
17	1	0	-3.928235	-0.586289	-3.979062
18	1	0	-1.184695	-3.690767	-2.884178
19	1	0	-2.873581	-2.779667	-4.464759
20	6	0	-1.881914	1.461510	-0.030793
21	6	0	-2.816587	1.999828	0.860178
22	6	0	-1.336837	2.329514	-0.991102
23	6	0	-3.183585	3.342122	0.798894
24	1	0	-3.268413	1.366098	1.610644
25	6	0	-1.701849	3.667394	-1.056964
26	1	0	-0.628568	1.946754	-1.718784
27	6	0	-2.628479	4.184814	-0.156035
28	1	0	-3.911726	3.726183	1.503616
29	1	0	-1.258574	4.306663	-1.811113
30	1	0	-2.912591	5.228952	-0.200024
31	6	0	-1.889793	-0.726938	1.273551
32	6	0	-2.835457	-1.758035	1.280125
33	6	0	-1.343873	-0.348435	2.510544
34	6	0	-3.211420	-2.385953	2.465034
35	1	0	-3.287219	-2.075556	0.350564
36	6	0	-1.718068	-0.969839	3.694569
37	1	0	-0.626386	0.464855	2.552701
38	6	0	-2.654996	-1.999198	3.678056
39	1	0	-3.947769	-3.180436	2.434894
40	1	0	-1.274736	-0.651092	4.630354
41	1	0	-2.946198	-2.490721	4.598118

Frequencies -- 10.4722 19.8240 20.3981 40.0739 41.3193 50.6662

Cl•(-2157.465432)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.098780	1.572767	-0.793911
2	13	0	-2.086375	1.314224	0.857187

3	13	0	-2.088017	0.091229	-1.564538
4	13	0	-0.101609	-0.097930	1.759046
5	13	0	-2.091204	-1.394391	0.706250
6	13	0	-0.105495	-1.475536	-0.964926
7	13	0	1.845952	-0.004716	-0.001438
8	17	0	3.988369	-0.009765	-0.004501

Frequencies -- 46.5245 47.9721 100.5167 100.9592 157.8271 173.2364

$(CF_3)_3C\bullet$ (-2748.569073)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.190857	0.335422	1.736982
2	13	0	4.176174	1.477813	0.513981
3	13	0	4.171495	-1.185602	1.027381
4	13	0	2.194568	1.337196	-1.157942
5	13	0	4.177837	-0.296364	-1.534949
6	13	0	2.192072	-1.670591	-0.581209
7	13	0	0.272776	0.001495	-0.002470
8	6	0	-1.845448	0.000336	-0.000802
9	6	0	-2.324378	-0.763480	-1.245569
10	6	0	-2.324179	1.460313	-0.039444
11	6	0	-2.320760	-0.696242	1.284130
12	9	0	-3.615174	-0.551568	-1.556217
13	9	0	-1.597157	-0.411521	-2.333545
14	9	0	-2.162615	-2.092546	-1.088666
15	9	0	-1.589197	-1.811446	1.524650
16	9	0	-3.610024	-1.076206	1.257144
17	9	0	-2.161049	0.106312	2.355416
18	9	0	-1.591724	2.228362	0.803309
19	9	0	-3.612785	1.623981	0.307005
20	9	0	-2.169726	1.986228	-1.270951

Frequencies -- 12.1357 30.1744 32.4201 55.8576 56.8065 66.1747

Cp(-1890.680529)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.057176	-1.232487	-1.167993
2	13	0	-1.846553	0.495177	-1.541454
3	13	0	-2.045945	-1.464322	0.338804
4	13	0	0.153184	1.631962	-0.334149

5	13	0	-1.958013	1.147367	1.100257
6	13	0	-0.062511	-0.516847	1.723617
7	13	0	2.133328	-0.140584	0.184869
8	6	0	4.171836	0.957397	0.213535
9	1	0	4.214877	2.033198	0.149843
10	6	0	4.181028	0.056028	-0.881727
11	1	0	4.230757	0.326238	-1.924734
12	6	0	4.087154	-1.261365	-0.365099
13	1	0	4.052180	-2.169025	-0.946544
14	6	0	4.071080	0.197212	1.406462
15	1	0	4.023279	0.593855	2.408321
16	6	0	4.018755	-1.174555	1.048431
17	1	0	3.923669	-2.004805	1.730303

Frequencies -- 46.9687 47.2846 94.1329 95.2449 142.9050 147.3215

Cp*(-2087.194833)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.525772	-1.450487	-0.920406
2	13	0	-3.538609	0.060625	-1.570261
3	13	0	-3.537565	-1.400645	0.724996
4	13	0	-1.533576	1.520378	-0.790646
5	13	0	-3.548202	1.316075	0.840421
6	13	0	-1.532474	-0.074564	1.714951
7	13	0	0.569425	0.005252	0.004284
8	6	0	2.501202	1.132247	-0.447368
9	6	0	2.494861	-0.073273	-1.215577
10	6	0	2.495655	-1.175691	-0.305828
11	6	0	2.503825	0.774677	0.937073
12	6	0	2.501605	-0.652499	1.024077
13	6	0	2.561502	-1.461279	2.285614
14	1	0	2.152982	-0.914297	3.135687
15	1	0	2.002723	-2.394159	2.197968
16	1	0	3.595924	-1.721148	2.531815
17	6	0	2.553245	-2.625835	-0.682628
18	1	0	3.589678	-2.950034	-0.820645
19	1	0	2.112671	-3.261506	0.086094
20	1	0	2.023679	-2.824550	-1.615516
21	6	0	2.541433	-0.168306	-2.711494
22	1	0	3.575487	-0.226452	-3.066056
23	1	0	2.021583	-1.054751	-3.077616
24	1	0	2.082366	0.699210	-3.186882
25	6	0	2.567993	2.526108	-0.996113

26	1	0	3.607868	2.842429	-1.126349
27	1	0	2.080777	2.603242	-1.968871
28	1	0	2.089666	3.247289	-0.332374
29	6	0	2.564643	1.729704	2.091940
30	1	0	3.602587	1.953444	2.358120
31	1	0	2.076207	2.677003	1.860687
32	1	0	2.081271	1.322683	2.980824

Frequencies -- 8.5356 35.5622 40.4862 49.6689 66.6890 73.8811

Al_{13}

CH_3• (-3191.866826)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.687704	2.287059	0.464867
2	13	0	-0.101237	0.002119	2.739801
3	13	0	1.688008	-2.284944	0.474392
4	13	0	1.648867	-1.302808	-2.015553
5	13	0	1.646222	1.296209	-2.021196
6	13	0	2.513993	0.003899	1.644872
7	13	0	0.363458	-0.000222	-0.002317
8	13	0	-0.951854	-0.002977	-2.499388
9	13	0	-0.851657	2.206411	-1.190092
10	13	0	-0.831880	2.140108	1.407080
11	13	0	-0.833475	-2.137593	1.410912
12	13	0	-0.850069	-2.210010	-1.186065
13	13	0	-2.217010	-0.000274	0.160918
14	6	0	-4.184584	0.000885	0.435035
15	1	0	-4.633743	0.884766	-0.021627
16	1	0	-4.634158	-0.885524	-0.016279
17	1	0	-4.426700	0.004189	1.499369

Frequencies -- 25.7088 44.6075 51.9921 66.3393 82.1618 94.9568

CH_3CH_2•(-3231.159667)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.270388	-2.006674	0.353731
2	13	0	-0.203909	-0.125099	2.740346
3	13	0	-1.524318	2.506563	0.529271
4	13	0	-1.595665	1.615359	-1.996025
5	13	0	-2.024834	-0.944904	-2.092476

6	13	0	-2.750021	0.346942	1.588131
7	13	0	-0.584361	0.051024	-0.011592
8	13	0	0.768268	-0.071222	-2.483409
9	13	0	0.275111	-2.281283	-1.266146
10	13	0	0.225969	-2.298215	1.332298
11	13	0	0.913121	1.906304	1.507056
12	13	0	0.994187	2.077379	-1.087791
13	13	0	1.962974	-0.366012	0.189611
14	6	0	3.906309	-0.737077	0.492448
15	1	0	4.124272	-1.681990	-0.014575
16	1	0	4.033454	-0.930581	1.561663
17	6	0	4.882085	0.352360	0.027675
18	1	0	4.712425	1.296901	0.549883
19	1	0	5.921612	0.061602	0.210690
20	1	0	4.785724	0.553951	-1.041983

Frequencies -- 17.5469 23.4333 44.8303 51.6937 61.5568 79.1497

$(CH_3)_2CH$•(-3270.455139)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.267237	1.635716	-1.477957
2	13	0	0.085873	2.261221	1.462450
3	13	0	1.821009	-0.803268	2.371732
4	13	0	2.152183	-2.366606	0.216244
5	13	0	2.342811	-0.991573	-1.979231
6	13	0	2.778236	1.417033	1.157498
7	13	0	0.781087	-0.021721	0.026046
8	13	0	-0.290305	-2.147305	-1.482967
9	13	0	-0.118002	0.162556	-2.601034
10	13	0	-0.323308	2.300955	-1.131896
11	13	0	-0.761570	-0.042981	2.398809
12	13	0	-0.494233	-2.264422	1.075514
13	13	0	-1.799647	0.048911	-0.211933
14	6	0	-3.806262	0.207583	-0.381943
15	1	0	-3.957659	0.382313	-1.453503
16	6	0	-4.527218	-1.094409	-0.006431
17	1	0	-4.394161	-1.337814	1.051496
18	1	0	-5.605998	-1.004858	-0.184163
19	1	0	-4.170357	-1.949165	-0.585750
20	6	0	-4.385630	1.405229	0.382007
21	1	0	-3.932014	2.350777	0.076589
22	1	0	-5.466081	1.487898	0.211191
23	1	0	-4.237120	1.305670	1.460969

Frequencies --	22.3673	25.3155	45.0764	52.3838	57.7803	59.4695

$(CH_3)_3C•$(-3309.751918)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.361264	-0.110790	2.696780
2	13	0	2.223395	-2.314191	0.427804
3	13	0	2.333274	-1.227718	-2.019550
4	13	0	2.334409	1.366233	-1.921997
5	13	0	2.232476	2.262606	0.600453
6	13	0	3.016928	-0.071867	1.701632
7	13	0	0.933718	-0.002905	-0.029398
8	13	0	-0.197214	2.260307	-1.188055
9	13	0	-0.334533	2.066667	1.401940
10	13	0	-0.345730	-2.174151	1.232511
11	13	0	-0.203453	-2.164095	-1.364410
12	13	0	-0.243574	0.100071	-2.584191
13	13	0	-1.666475	0.001445	-0.007942
14	6	0	-3.704503	0.000815	0.131374
15	6	0	-4.267251	-1.240176	-0.580579
16	1	0	-3.922247	-2.170056	-0.122409
17	1	0	-5.364815	-1.236601	-0.528125
18	1	0	-3.993293	-1.270264	-1.638220
19	6	0	-4.135412	-0.020973	1.605985
20	1	0	-5.231979	-0.022808	1.676874
21	1	0	-3.774122	-0.910084	2.128584
22	1	0	-3.775473	0.853300	2.153955
23	6	0	-4.263927	1.264086	-0.543042
24	1	0	-3.915316	2.179082	-0.058373
25	1	0	-3.991078	1.324024	-1.599727
26	1	0	-5.361463	1.262716	-0.489657

Frequencies --	3.3554	22.1105	42.9967	52.5483	56.4551	59.2465

$H_2C=CH•$(-3229.947854)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.519084	2.554292	-0.012073

2	13	0	-0.221822	0.618157	2.613948
3	13	0	2.121573	-1.833902	1.100390
4	13	0	2.187470	-1.475097	-1.550467
5	13	0	1.840627	1.024630	-2.189697
6	13	0	2.480766	0.758553	1.772916
7	13	0	0.563684	0.050558	0.000576
8	13	0	-0.500944	-0.737992	-2.497201
9	13	0	-0.824942	1.703361	-1.771373
10	13	0	-1.043118	2.268068	0.753470
11	13	0	-0.478938	-1.859736	1.816375
12	13	0	-0.247193	-2.525567	-0.676918
13	13	0	-2.000451	-0.268930	0.011602
14	6	0	-4.879500	0.322606	0.376633
15	6	0	-3.942221	-0.594176	0.126682
16	1	0	-4.642241	1.368504	0.548516
17	1	0	-5.937433	0.073610	0.423313
18	1	0	-4.287078	-1.616368	-0.030268

Frequencies -- 25.2639 33.5971 44.5884 49.6122 64.6148 83.6588

HC≡C•(-3228.734410)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.810102	2.281952	0.645596
2	13	0	-0.273143	0.001870	2.728165
3	13	0	1.809725	-2.281266	0.648560
4	13	0	1.954350	-1.307934	-1.845620
5	13	0	1.954626	1.305267	-1.847323
6	13	0	2.452279	0.001166	1.970382
7	13	0	0.546037	0.000048	0.062590
8	13	0	-0.587840	-0.001771	-2.540563
9	13	0	-0.610163	2.200771	-1.227089
10	13	0	-0.790891	2.159668	1.353605
11	13	0	-0.791355	-2.157426	1.356682
12	13	0	-0.610555	-2.202395	-1.223805
13	13	0	-2.029845	0.000227	0.014206
14	6	0	-5.158577	0.000276	0.163544
15	6	0	-3.947493	0.000230	0.108932
16	1	0	-6.221449	0.000307	0.212553

Frequencies -- 25.7014 41.5703 49.6598 54.7850 55.8744 86.3716

Ph• (-3383.603637)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.591051	-2.283551	0.639646
2	13	0	-0.545068	0.004396	2.723051
3	13	0	-2.592044	2.284130	0.635419
4	13	0	-2.776109	1.299852	-1.846510
5	13	0	-2.774810	-1.304411	-1.844186
6	13	0	-3.261179	0.001093	1.929105
7	13	0	-1.320321	0.000067	0.044190
8	13	0	-0.233637	-0.003261	-2.567669
9	13	0	-0.207370	-2.205359	-1.249921
10	13	0	0.009029	-2.141598	1.334210
11	13	0	0.008731	2.146077	1.327487
12	13	0	-0.208741	2.202582	-1.256411
13	13	0	1.266746	0.000468	-0.031182
14	6	0	5.373823	1.201748	0.052183
15	6	0	3.981866	1.198027	0.030773
16	6	0	3.250191	0.000289	0.016426
17	6	0	3.981514	-1.197736	0.023676
18	6	0	5.373468	-1.202002	0.045043
19	6	0	6.074136	-0.000264	0.060145
20	1	0	5.911039	2.143208	0.063126
21	1	0	3.462936	2.150499	0.024299
22	1	0	3.462294	-2.149999	0.011594
23	1	0	5.910403	-2.143670	0.050385
24	1	0	7.157512	-0.000475	0.077236

Frequencies -- 24.6805 31.1444 41.3692 41.5043 50.7262 83.8876

$PhCH_2$•(-3422.907240)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.100713	1.864673	2.075342
2	13	0	0.070690	2.094359	-0.879003
3	13	0	-3.046525	0.440306	-2.153095
4	13	0	-3.899748	-1.328524	-0.336390
5	13	0	-3.401786	-0.482400	2.076611
6	13	0	-2.702157	2.531087	-0.480422
7	13	0	-1.637069	0.112243	0.103204
8	13	0	-1.599685	-2.574916	0.958340
9	13	0	-0.672966	-0.794536	2.552644
10	13	0	0.487089	1.307306	1.578737

11	13	0	-0.397365	0.050205	-2.444818
12	13	0	-1.518611	-2.117060	-1.562144
13	13	0	0.705389	-0.973203	-0.047509
14	6	0	2.541810	-1.802650	-0.167030
15	1	0	2.613823	-2.493998	0.675593
16	1	0	2.549355	-2.403228	-1.078900
17	6	0	3.675628	-0.824266	-0.157916
18	6	0	4.162464	-0.266795	-1.346933
19	6	0	4.278459	-0.424388	1.041787
20	6	0	5.209338	0.648176	-1.338935
21	1	0	3.719871	-0.562393	-2.291791
22	6	0	5.325472	0.490535	1.052911
23	1	0	3.929729	-0.847497	1.977586
24	6	0	5.796338	1.035034	-0.138082
25	1	0	5.569843	1.057633	-2.275360
26	1	0	5.778406	0.775111	1.995487
27	1	0	6.613619	1.745529	-0.131150

Frequencies -- 10.9630 20.8132 25.8619 37.1260 44.9164 48.3165

$Ph_2CH•$(-3653.942007)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	3.934401	1.331605	-0.354079
2	13	0	1.288805	1.170698	2.273744
3	13	0	2.628377	-2.201171	2.259628
4	13	0	3.225492	-2.975903	-0.244626
5	13	0	3.917157	-0.956808	-1.740922
6	13	0	3.927910	0.176222	2.085780
7	13	0	2.099693	-0.543324	0.230777
8	13	0	1.169915	-1.844773	-2.084008
9	13	0	1.702882	0.665177	-2.255411
10	13	0	1.368113	2.161697	-0.156041
11	13	0	0.131859	-1.183153	2.166693
12	13	0	0.479978	-2.819627	0.187311
13	13	0	-0.386366	-0.053077	-0.349240
14	6	0	-2.345681	0.333033	-0.806305
15	1	0	-2.296191	0.290939	-1.898355
16	6	0	-3.237880	-0.808665	-0.371028
17	6	0	-3.943583	-0.821211	0.837409
18	6	0	-3.365568	-1.928710	-1.205517
19	6	0	-4.732812	-1.909124	1.198309
20	1	0	-3.893861	0.032143	1.499415
21	6	0	-4.150789	-3.017022	-0.846030

22	1	0	-2.844511	-1.942254	-2.156748
23	6	0	-4.838756	-3.016120	0.363767
24	1	0	-5.272647	-1.885699	2.137814
25	1	0	-4.232056	-3.863870	-1.517398
26	1	0	-5.454991	-3.860750	0.646070
27	6	0	-2.787565	1.729574	-0.437397
28	6	0	-2.688987	2.247400	0.860111
29	6	0	-3.317682	2.566623	-1.427409
30	6	0	-3.119678	3.535606	1.159340
31	1	0	-2.254717	1.642909	1.647024
32	6	0	-3.739168	3.859523	-1.135965
33	1	0	-3.406751	2.193924	-2.441741
34	6	0	-3.646871	4.349806	0.162303
35	1	0	-3.031914	3.907070	2.173530
36	1	0	-4.144945	4.482040	-1.924645
37	1	0	-3.976652	5.355204	0.393604

Frequencies -- 7.7172 21.0533 26.8376 31.6979 35.4992 43.9389

$Ph_3C•$(-3884.962995)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	3.872113	-2.044185	0.965480
2	13	0	2.405887	-0.918131	-2.217671
3	13	0	3.824035	2.109940	-1.003932
4	13	0	3.688423	2.254091	1.687800
5	13	0	3.650235	-0.092821	2.798149
6	13	0	4.834345	-0.390733	-0.927211
7	13	0	2.513729	0.191997	0.337315
8	13	0	1.040701	1.149657	2.517759
9	13	0	1.281470	-1.414353	2.242436
10	13	0	1.429646	-2.320536	-0.201986
11	13	0	1.330229	1.465269	-1.857726
12	13	0	1.259951	2.677717	0.441398
13	13	0	-0.123517	0.056004	0.128539
14	6	0	-2.222749	-0.065813	-0.168482
15	6	0	-2.635395	1.322078	-0.671630
16	6	0	-3.240813	1.521545	-1.917661
17	6	0	-2.410750	2.466664	0.112793
18	6	0	-3.591592	2.795269	-2.361553
19	1	0	-3.448666	0.675842	-2.556462
20	6	0	-2.766736	3.735643	-0.321813
21	1	0	-1.960961	2.361398	1.091476
22	6	0	-3.357326	3.911252	-1.570410

23	1	0	-4.058300	2.906489	-3.333239
24	1	0	-2.580116	4.590479	0.317693
25	1	0	-3.632443	4.900339	-1.915264
26	6	0	-2.567791	-1.160004	-1.189216
27	6	0	-1.800791	-1.356216	-2.343031
28	6	0	-3.715384	-1.950432	-1.046613
29	6	0	-2.145635	-2.301667	-3.301799
30	1	0	-0.919862	-0.748188	-2.506372
31	6	0	-4.065439	-2.901011	-2.001035
32	1	0	-4.349559	-1.823340	-0.180296
33	6	0	-3.280911	-3.087041	-3.133108
34	1	0	-1.521041	-2.425739	-4.178574
35	1	0	-4.959117	-3.496303	-1.855218
36	1	0	-3.550287	-3.830337	-3.873468
37	6	0	-2.817185	-0.417027	1.203646
38	6	0	-3.792187	0.353512	1.845712
39	6	0	-2.435912	-1.611687	1.835793
40	6	0	-4.334876	-0.033353	3.070366
41	1	0	-4.152632	1.261646	1.385719
42	6	0	-2.976525	-2.003954	3.051490
43	1	0	-1.719403	-2.261018	1.348782
44	6	0	-3.927938	-1.208782	3.685563
45	1	0	-5.088745	0.590785	3.535692
46	1	0	-2.655594	-2.934765	3.504197
47	1	0	-4.349143	-1.507713	4.637510

Frequencies --	3.4692	13.0407	18.7347	25.0180	41.6896	50.0792

Cl•(-3612.256679)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.744736	2.261287	0.492179
2	13	0	-0.425223	0.068519	2.606302
3	13	0	1.543369	-2.298149	0.479444
4	13	0	1.654027	-1.325279	-2.026420
5	13	0	1.770918	1.295878	-2.019031
6	13	0	2.287401	-0.050810	1.833096
7	13	0	0.382956	0.038715	-0.070270
8	13	0	-0.840618	0.099105	-2.637676
9	13	0	-0.731049	2.294392	-1.322996
10	13	0	-0.845061	2.255619	1.253673
11	13	0	-1.035635	-2.066370	1.243452
12	13	0	-0.926421	-2.102746	-1.333171
13	13	0	-2.201230	0.155006	-0.046240

14	17	0	-4.352125	0.244324	0.078481

Frequencies --	24.9951	40.4462	48.7898	69.7731	74.2840	89.3945

$(CF_3)_3C$•(-4203.362455)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-3.436399	-2.263661	0.570521
2	13	0	-1.387606	0.106434	2.659115
3	13	0	-3.424455	2.302785	0.450657
4	13	0	-3.511261	1.247806	-2.032442
5	13	0	-3.478431	-1.368589	-1.970190
6	13	0	-4.081154	0.051490	1.849831
7	13	0	-2.177361	0.002593	-0.041241
8	13	0	-0.919706	-0.088557	-2.581249
9	13	0	-0.962812	-2.251792	-1.207718
10	13	0	-0.848949	-2.089350	1.363636
11	13	0	-0.821740	2.186407	1.195041
12	13	0	-0.979929	2.171299	-1.378040
13	13	0	0.425541	-0.001635	-0.011990
14	6	0	2.569577	-0.002603	0.077416
15	6	0	3.019473	-0.421220	1.494108
16	6	0	3.096758	1.416510	-0.232117
17	6	0	3.133039	-0.996571	-0.961852
18	9	0	4.317229	-0.167081	1.748581
19	9	0	2.310164	0.221140	2.448105
20	9	0	2.831688	-1.742041	1.693538
21	9	0	4.420461	1.462286	-0.474827
22	9	0	2.856959	2.257368	0.795507
23	9	0	2.493427	1.946725	-1.318723
24	9	0	2.975021	-0.524690	-2.215373
25	9	0	4.444562	-1.259376	-0.801679
26	9	0	2.499137	-2.188178	-0.911873

Frequencies --	13.4347	21.9448	41.2529	46.9115	50.0841	52.3969

Cp(-3345.460346)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.444706	2.275343	-0.586154
2	13	0	-1.684594	-0.114754	-2.625625

3	13	0	-2.415580	-2.358064	-0.397906
4	13	0	-1.979200	-1.226575	1.993426
5	13	0	-1.999031	1.345350	1.889520
6	13	0	-3.563001	-0.041560	-0.305650
7	13	0	-0.711914	-0.018000	-0.194435
8	13	0	0.451600	0.094212	2.448992
9	13	0	0.308557	2.274230	0.642802
10	13	0	-0.204261	2.032547	-1.998064
11	13	0	-0.185176	-2.194605	-1.836519
12	13	0	0.336914	-2.226150	0.815624
13	13	0	2.171043	0.023339	0.460817
14	6	0	4.381294	-0.780107	0.598768
15	1	0	4.679025	-1.489874	1.354413
16	6	0	3.814709	-1.098283	-0.660018
17	1	0	3.626232	-2.088500	-1.042006
18	6	0	3.519970	0.122543	-1.330938
19	1	0	3.091805	0.219965	-2.316353
20	6	0	4.443777	0.629825	0.710317
21	1	0	4.795611	1.182388	1.567288
22	6	0	3.916321	1.190327	-0.477458
23	1	0	3.812100	2.241138	-0.694192

Frequencies -- 21.2420 28.8271 38.1380 54.3933 60.7435 79.9905

Cp*(-3541.972261)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.727729	2.420145	0.086037
2	13	0	-2.217394	0.341701	-2.429485
3	13	0	-2.806071	-2.255724	-0.472029
4	13	0	-2.035447	-1.493241	1.960939
5	13	0	-1.992737	1.077377	2.269886
6	13	0	-3.820188	0.066240	0.090747
7	13	0	-1.003331	0.047235	-0.143905
8	13	0	0.430245	-0.282247	2.383073
9	13	0	0.252352	2.103383	0.893987
10	13	0	-0.718798	2.403798	-1.617528
11	13	0	-0.793949	-1.902821	-2.134603
12	13	0	0.180967	-2.236287	0.367561
13	13	0	2.111365	-0.062391	0.346890
14	6	0	4.301685	-0.693472	0.668190
15	6	0	3.860086	-1.179671	-0.599776
16	6	0	3.522868	-0.051150	-1.415680
17	6	0	4.248860	0.732077	0.638853

18	6	0	3.774170	1.132630	-0.647989
19	6	0	3.129496	-0.100070	-2.863211
20	1	0	2.553642	0.776656	-3.158336
21	1	0	4.018662	-0.138364	-3.500822
22	1	0	2.525890	-0.978718	-3.091473
23	6	0	3.681271	2.544444	-1.141640
24	1	0	4.658101	2.888627	-1.496832
25	1	0	2.977948	2.641870	-1.968224
26	1	0	3.358282	3.230291	-0.357312
27	6	0	4.662269	1.660928	1.740812
28	1	0	5.702071	1.978357	1.613582
29	1	0	4.047178	2.562050	1.761409
30	1	0	4.583215	1.188082	2.719971
31	6	0	4.786329	-1.540150	1.807195
32	1	0	5.856010	-1.749594	1.707258
33	1	0	4.639612	-1.049009	2.769570
34	1	0	4.269739	-2.500091	1.847547
35	6	0	3.854637	-2.613101	-1.036083
36	1	0	3.595978	-3.287961	-0.218791
37	1	0	3.143080	-2.788861	-1.842674
38	1	0	4.844767	-2.905589	-1.400643

Frequencies -- 17.4235 25.5748 32.2146 50.8091 53.8374 64.3523

Al_{20}

CH_3•(-4889.126691)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.426730	-0.080319	2.602664
2	13	0	2.446800	-2.382037	0.956418
3	13	0	2.643728	-1.561774	-1.707909
4	13	0	2.570967	1.203804	-2.104455
5	13	0	2.514790	2.470143	0.425609
6	13	0	3.933125	0.092177	0.281798
7	13	0	1.334951	0.007455	0.077206
8	13	0	0.246360	1.617435	1.919039
9	13	0	0.074997	-1.386937	2.058658
10	13	0	0.159438	-2.379763	-0.605619
11	13	0	0.233360	-0.246586	-2.426559
12	13	0	0.200041	2.230953	-1.029945
13	13	0	-2.505912	2.609011	-0.551534
14	13	0	-2.502584	1.695211	1.899653
15	13	0	-2.626176	-0.866648	2.414130
16	13	0	-2.453355	-2.569960	0.465935
17	13	0	-2.253253	-1.627494	-1.984414

18	13	0	-2.331266	0.946334	-2.534232
19	13	0	-1.296500	0.060057	0.032298
20	13	0	-3.971191	-0.026057	-0.177283
21	6	0	5.909387	-0.029092	0.219287
22	1	0	6.353154	0.622836	0.975468
23	1	0	6.242806	-1.051415	0.411170
24	1	0	6.287463	0.275552	-0.759154

Frequencies -- 23.2350 28.9158 40.7947 57.8190 59.6896 70.2254

CH_3CH_2•(-4928.419182)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.100770	-2.260387	1.248161
2	13	0	2.255880	-1.855903	-1.548274
3	13	0	2.262183	1.481501	-1.883309
4	13	0	2.109638	2.434344	0.776865
5	13	0	2.136307	0.236585	2.503387
6	13	0	3.604948	-0.014447	0.030406
7	13	0	0.996520	-0.007169	0.053827
8	13	0	-0.287111	-1.202858	2.168804
9	13	0	-0.161957	-2.440735	-0.389244
10	13	0	0.078210	-0.256708	-2.449205
11	13	0	-0.153014	2.294084	-0.864563
12	13	0	-0.281836	1.589855	1.888449
13	13	0	-2.764273	0.237124	2.416525
14	13	0	-2.825926	-2.187661	1.392833
15	13	0	-2.815573	-2.422169	-1.190504
16	13	0	-2.663678	-0.274268	-2.675711
17	13	0	-2.806980	2.126545	-1.647144
18	13	0	-2.817238	2.410255	0.931254
19	13	0	-1.629528	-0.020612	-0.129507
20	13	0	-4.314761	-0.012406	-0.098300
21	6	0	5.583257	0.008161	0.292833
22	1	0	5.825721	-0.801415	0.988953
23	1	0	5.829008	0.939045	0.814223
24	6	0	6.418442	-0.122161	-0.989574
25	1	0	6.211869	-1.058044	-1.514550
26	1	0	6.215172	0.691456	-1.690188
27	1	0	7.491002	-0.102404	-0.772605

Frequencies -- 14.1519 25.0502 42.1126 52.8357 59.0740 61.5926

$(CH_3)_2CH$•(-4967.714563)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.413250	0.446800	2.570341
2	13	0	2.472134	-2.417640	0.856751
3	13	0	2.566644	-1.593171	-1.849645
4	13	0	2.669837	1.200937	-1.920523
5	13	0	2.470396	2.452998	0.569393
6	13	0	3.934321	-0.109390	0.318737
7	13	0	1.332192	-0.036403	0.089618
8	13	0	0.086248	1.684571	1.805608
9	13	0	0.198572	-1.301314	2.159639
10	13	0	0.173176	-2.397083	-0.644029
11	13	0	0.251223	-0.188302	-2.432230
12	13	0	0.192629	2.220651	-0.987845
13	13	0	-2.428253	2.618420	0.000039
14	13	0	-2.622773	1.277756	2.213474
15	13	0	-2.555452	-1.336091	2.128755
16	13	0	-2.537621	-2.658932	-0.128154
17	13	0	-2.329913	-1.351143	-2.357079
18	13	0	-2.214535	1.279075	-2.254147
19	13	0	-1.298218	-0.058611	0.029262
20	13	0	-3.970818	0.028590	-0.217337
21	6	0	5.946934	-0.051023	0.246932
22	1	0	6.178136	0.041963	-0.820927
23	6	0	6.574180	-1.355183	0.760785
24	1	0	6.348305	-1.523003	1.817974
25	1	0	6.223119	-2.230832	0.209541
26	1	0	7.666399	-1.325204	0.666128
27	6	0	6.528519	1.171114	0.971006
28	1	0	6.142331	2.113028	0.573841
29	1	0	6.304152	1.151476	2.041435
30	1	0	7.620422	1.197935	0.872166

Frequencies -- 24.2435 41.8364 46.6755 49.1023 61.6095 67.2341

$(CH_3)_3C•$(-5007.011418)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.340252	0.121623	2.581837
2	13	0	2.389505	-2.487998	0.518714
3	13	0	2.456131	-1.331616	-2.057357
4	13	0	2.561161	1.452148	-1.767578

5	13	0	2.376837	2.371306	0.868656
6	13	0	3.850215	-0.120902	0.253834
7	13	0	1.236529	-0.034279	0.073487
8	13	0	-0.000692	1.441656	2.008546
9	13	0	0.126378	-1.565290	1.970374
10	13	0	0.072510	-2.282579	-0.948858
11	13	0	0.144113	0.139545	-2.442073
12	13	0	0.095011	2.343699	-0.695863
13	13	0	-2.518913	2.607024	0.350545
14	13	0	-2.711016	0.990644	2.370678
15	13	0	-2.627063	-1.591857	1.959610
16	13	0	-2.638057	-2.609828	-0.451373
17	13	0	-2.433537	-1.032326	-2.499176
18	13	0	-2.321762	1.564052	-2.058166
19	13	0	-1.390817	-0.052097	0.029324
20	13	0	-4.060994	0.066706	-0.197412
21	6	0	5.886374	-0.077190	0.252811
22	6	0	6.398588	-1.209532	1.158481
23	1	0	6.050426	-1.104177	2.189523
24	1	0	6.087657	-2.196003	0.804235
25	1	0	7.497008	-1.204413	1.183511
26	6	0	6.378944	1.272052	0.797929
27	1	0	6.053262	2.112152	0.178928
28	1	0	6.032829	1.458003	1.818149
29	1	0	7.477293	1.290932	0.819424
30	6	0	6.424955	-0.280594	-1.171134
31	1	0	6.108291	-1.234339	-1.601967
32	1	0	6.103844	0.512212	-1.851884
33	1	0	7.523726	-0.277253	-1.162529

Frequencies -- 23.6080 28.1130 40.5870 47.3316 48.6008 67.0513

$H_2C=CH\bullet$ (-4927.207565)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.290194	0.722937	2.617770
2	13	0	2.442329	-2.295896	1.111452
3	13	0	2.618053	-1.649986	-1.632465
4	13	0	2.685743	1.126760	-1.904320
5	13	0	2.386413	2.561770	0.462535
6	13	0	3.873475	-0.008892	0.484569
7	13	0	1.292238	0.022772	0.147308
8	13	0	-0.027895	1.847748	1.687280
9	13	0	0.133260	-1.107610	2.277048

10	13	0	0.189371	-2.404045	-0.450345
11	13	0	0.300790	-0.334359	-2.388401
12	13	0	0.150070	2.166881	-1.134056
13	13	0	-2.509694	2.593462	-0.257255
14	13	0	-2.743650	1.416120	2.044554
15	13	0	-2.614195	-1.193153	2.176726
16	13	0	-2.536182	-2.673539	0.019934
17	13	0	-2.254360	-1.550629	-2.299189
18	13	0	-2.202315	1.081088	-2.389373
19	13	0	-1.331344	-0.054029	0.015242
20	13	0	-3.992596	-0.043147	-0.313776
21	6	0	6.592814	0.537145	1.456323
22	6	0	5.839343	0.109989	0.440091
23	1	0	6.167263	0.862569	2.401763
24	1	0	7.678006	0.585163	1.398099
25	1	0	6.360664	-0.195665	-0.467365

Frequencies -- 21.3433 26.0926 41.9277 53.8052 56.8844 66.0969

HC≡C•(-4925.993672)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.383683	0.004837	-2.323420
2	13	0	2.260189	2.351526	-0.830601
3	13	0	2.226365	1.676188	1.918149
4	13	0	2.225394	-1.693005	1.907543
5	13	0	2.258787	-2.351088	-0.845371
6	13	0	3.647804	-0.003617	0.271154
7	13	0	1.059766	-0.002227	0.053841
8	13	0	-0.071938	-1.397809	-2.013666
9	13	0	-0.071070	1.406991	-2.004875
10	13	0	-0.110186	2.381109	0.664984
11	13	0	0.011543	-0.009641	2.512348
12	13	0	-0.111619	-2.388640	0.650025
13	13	0	-2.814981	-2.292329	1.287994
14	13	0	-2.662589	-2.310317	-1.303193
15	13	0	-2.529097	0.007059	-2.546998
16	13	0	-2.661132	2.316647	-1.288631
17	13	0	-2.813583	2.282435	1.302389
18	13	0	-2.740187	-0.008972	2.567360
19	13	0	-1.554760	-0.001503	0.076528
20	13	0	-4.219224	-0.000060	-0.112325
21	6	0	6.770857	-0.003953	-0.002133

22	6	0	5.562442	-0.003724	0.096732
23	1	0	7.831532	-0.004133	-0.089221

Frequencies -- 24.8831 40.7422 51.2026 53.0439 56.7481 63.7628

Ph•(-5080.863519)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.916110	0.439586	3.033948
2	13	0	2.076129	-2.532532	1.485442
3	13	0	2.670337	-1.871286	-1.206766
4	13	0	2.980094	0.887325	-1.392255
5	13	0	2.458240	2.296275	0.960767
6	13	0	3.737912	-0.355864	1.112572
7	13	0	1.234316	-0.136998	0.421340
8	13	0	-0.151907	1.758679	1.810860
9	13	0	-0.298404	-1.210113	2.336535
10	13	0	0.068167	-2.468038	-0.380956
11	13	0	0.569796	-0.369311	-2.233482
12	13	0	0.454933	2.115211	-0.941781
13	13	0	-2.252284	2.731281	-0.391186
14	13	0	-2.917829	1.513494	1.799208
15	13	0	-3.005836	-1.101798	1.840040
16	13	0	-2.702109	-2.534499	-0.326854
17	13	0	-2.063026	-1.356267	-2.548299
18	13	0	-1.791762	1.262663	-2.528094
19	13	0	-1.340737	-0.010206	-0.073339
20	13	0	-3.922845	0.224709	-0.755055
21	6	0	7.792404	-1.670883	1.356145
22	6	0	6.413872	-1.610874	1.171737
23	6	0	5.700625	-0.417420	1.361380
24	6	0	6.431115	0.716651	1.747230
25	6	0	7.809550	0.664344	1.933971
26	6	0	8.493561	-0.531443	1.738077
27	1	0	8.318304	-2.606241	1.203066
28	1	0	5.891887	-2.515236	0.875636
29	1	0	5.923479	1.662495	1.907835
30	1	0	8.349066	1.555849	2.232358
31	1	0	9.566441	-0.575230	1.883095

Frequencies -- 17.1429 24.8467 27.9809 32.0144 40.5841 56.3698

$PhCH_2$•(-5120.167174)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.644722	0.994913	2.462161
2	13	0	2.808562	-2.099749	1.184737
3	13	0	2.800988	-1.685301	-1.615906
4	13	0	2.780234	1.060260	-2.097468
5	13	0	2.572463	2.665227	0.175451
6	13	0	4.135143	0.154567	0.298670
7	13	0	1.533189	0.090103	0.104201
8	13	0	0.246944	1.995190	1.576523
9	13	0	0.526534	-0.901178	2.380433
10	13	0	0.476670	-2.404231	-0.234380
11	13	0	0.405532	-0.483993	-2.332830
12	13	0	0.272181	2.108337	-1.268231
13	13	0	-2.338061	2.540461	-0.258066
14	13	0	-2.428434	1.524987	2.128526
15	13	0	-2.218519	-1.064956	2.439078
16	13	0	-2.209254	-2.696143	0.393355
17	13	0	-2.120098	-1.731721	-2.014375
18	13	0	-2.124405	0.884984	-2.294864
19	13	0	-1.087142	-0.057519	0.130518
20	13	0	-3.761368	-0.123247	-0.038106
21	6	0	7.760695	1.067945	3.488499
22	6	0	7.111220	1.231860	2.270245
23	6	0	6.854655	0.139122	1.431471
24	6	0	7.270957	-1.126301	1.865743
25	6	0	7.920002	-1.292548	3.083883
26	6	0	8.168059	-0.196069	3.904111
27	1	0	7.952416	1.932226	4.113567
28	1	0	6.805687	2.224542	1.957948
29	1	0	7.091282	-1.990069	1.234943
30	1	0	8.236339	-2.282412	3.391304
31	1	0	8.675423	-0.324212	4.852260
32	6	0	6.135054	0.314242	0.130184
33	1	0	6.446101	-0.437170	-0.599783
34	1	0	6.338001	1.294963	-0.306603

Frequencies -- 9.0453 19.7342 24.6150 28.6145 41.0853 52.9092

$Ph_2CH•$(-5351.201922)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.449221	2.199270	1.454149

2	13	0	0.546145	-0.906462	2.566239
3	13	0	0.877346	-2.482955	0.253152
4	13	0	1.069594	-0.766513	-1.944937
5	13	0	0.714965	1.958073	-1.347042
6	13	0	2.112432	0.179468	0.509702
7	13	0	-0.475234	-0.047905	0.169202
8	13	0	-1.785834	2.320251	-0.148866
9	13	0	-1.793999	0.692073	2.376990
10	13	0	-1.637665	-2.159455	1.439146
11	13	0	-1.332287	-2.139767	-1.386615
12	13	0	-1.422713	0.516819	-2.339535
13	13	0	-4.102000	1.421241	-2.229075
14	13	0	-4.541023	2.266004	0.183794
15	13	0	-4.543148	0.545720	2.158396
16	13	0	-4.397100	-2.037929	1.753996
17	13	0	-3.955802	-2.921554	-0.643028
18	13	0	-3.749448	-1.163381	-2.597008
19	13	0	-3.075238	-0.212753	-0.052491
20	13	0	-5.697368	-0.459240	-0.502723
21	6	0	4.142663	0.239906	0.761950
22	1	0	4.193868	0.244642	1.855028
23	6	0	4.784616	-1.048387	0.301853
24	6	0	4.751685	-2.162975	1.154777
25	6	0	5.407308	-1.208389	-0.941507
26	6	0	5.307771	-3.380426	0.782612
27	1	0	4.293854	-2.067686	2.133404
28	6	0	5.967003	-2.426948	-1.314576
29	1	0	5.481880	-0.370651	-1.620540
30	6	0	5.917795	-3.522243	-0.460115
31	1	0	5.271168	-4.217583	1.469757
32	1	0	6.449497	-2.515366	-2.280974
33	1	0	6.355612	-4.468488	-0.752783
34	6	0	4.734583	1.540759	0.280540
35	6	0	4.634972	1.984378	-1.045526
36	6	0	5.401531	2.372824	1.189291
37	6	0	5.195971	3.191776	-1.448405
38	1	0	4.102888	1.385848	-1.774500
39	6	0	5.955127	3.585161	0.793153
40	1	0	5.494580	2.058163	2.222706
41	6	0	5.859539	3.999528	-0.531231
42	1	0	5.104329	3.505496	-2.481550
43	1	0	6.466650	4.204062	1.520752
44	1	0	6.292172	4.941915	-0.843711

Frequencies -- 10.1478 18.9360 24.6509 29.9034 35.2638 39.8115

$Ph_3C•$(-5582.224078)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.287512	-1.556710	1.920106
2	13	0	0.166597	-2.450058	-0.722620
3	13	0	0.297409	-0.242989	-2.395428
4	13	0	0.172444	2.248438	-1.165230
5	13	0	0.296095	1.855002	1.600652
6	13	0	1.738824	0.005592	0.104868
7	13	0	-0.924697	-0.011689	0.000772
8	13	0	-1.857115	0.221875	2.495377
9	13	0	-2.143625	-2.304570	0.867023
10	13	0	-2.173489	-1.586610	-1.891349
11	13	0	-2.171808	1.184667	-2.144417
12	13	0	-2.122910	2.411653	0.433485
13	13	0	-4.814418	2.380465	1.166741
14	13	0	-4.601064	0.247843	2.667348
15	13	0	-4.835713	-2.129205	1.587464
16	13	0	-4.723803	-2.432323	-0.983039
17	13	0	-4.656283	-0.231876	-2.439561
18	13	0	-4.720631	2.197704	-1.422593
19	13	0	-3.547914	0.006620	0.125062
20	13	0	-6.203631	0.007395	0.023962
21	6	0	3.859214	0.010015	0.025474
22	6	0	4.271232	1.484745	0.003926
23	6	0	3.807613	2.337169	-1.011775
24	6	0	5.131471	2.046873	0.954617
25	6	0	4.169200	3.676220	-1.069445
26	1	0	3.171903	1.937443	-1.792016
27	6	0	5.494000	3.390950	0.903325
28	1	0	5.534371	1.431817	1.745999
29	6	0	5.013629	4.216742	-0.104226
30	1	0	3.788271	4.298201	-1.870845
31	1	0	6.162622	3.787628	1.658269
32	1	0	5.294588	5.261985	-0.141860
33	6	0	4.344837	-0.701466	1.294192
34	6	0	3.838326	-0.343229	2.553300
35	6	0	5.342746	-1.682957	1.269205
36	6	0	4.291400	-0.939364	3.723140
37	1	0	3.090420	0.437266	2.625909
38	6	0	5.797832	-2.286735	2.438763
39	1	0	5.780829	-1.979405	0.327025
40	6	0	5.272971	-1.924208	3.672660
41	1	0	3.873055	-0.634164	4.674919

42	1	0	6.572470	-3.042131	2.378701
43	1	0	5.625287	-2.396465	4.581443
44	6	0	4.277167	-0.741714	-1.241271
45	6	0	5.128293	-0.198437	-2.210177
46	6	0	3.844131	-2.061417	-1.446927
47	6	0	5.506705	-0.926929	-3.336182
48	1	0	5.513514	0.803323	-2.087722
49	6	0	4.220828	-2.792943	-2.564245
50	1	0	3.221037	-2.537455	-0.699452
51	6	0	5.053477	-2.225614	-3.524964
52	1	0	6.168078	-0.471248	-4.063728
53	1	0	3.862711	-3.808595	-2.683896
54	1	0	5.347233	-2.790341	-4.401179

Frequencies -- 6.7271 13.6402 17.9270 28.3792 32.1197 38.7221

Cl•(-5309.519475)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.409204	0.761522	2.615128
2	13	0	2.578196	-2.236104	1.121479
3	13	0	2.715364	-1.606822	-1.631082
4	13	0	2.764492	1.156969	-1.900687
5	13	0	2.477973	2.589963	0.461193
6	13	0	3.955709	0.047187	0.457574
7	13	0	1.368530	0.053747	0.154027
8	13	0	0.068360	1.880596	1.706629
9	13	0	0.266599	-1.083301	2.310674
10	13	0	0.310527	-2.392748	-0.424037
11	13	0	0.371228	-0.314967	-2.373200
12	13	0	0.228864	2.197284	-1.120335
13	13	0	-2.431598	2.602678	-0.199307
14	13	0	-2.652103	1.415630	2.099214
15	13	0	-2.489677	-1.196311	2.219584
16	13	0	-2.420600	-2.673768	0.057335
17	13	0	-2.197806	-1.529665	-2.262458
18	13	0	-2.138726	1.100466	-2.340739
19	13	0	-1.221893	-0.042498	0.052435
20	13	0	-3.854579	-0.045248	-0.240594
21	17	0	6.104107	0.184198	0.429211

Frequencies -- 24.2891 40.6100 51.8480 53.0107 68.8305 72.1572

$(CF_3)_3C•$(-5900.621853)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.666160	0.167536	2.549098
2	13	0	2.656431	-2.278243	1.164154
3	13	0	2.847567	-1.731052	-1.553195
4	13	0	2.766791	0.960188	-2.255761
5	13	0	2.735894	2.479635	0.112605
6	13	0	4.111440	0.097680	0.204117
7	13	0	1.501867	0.007458	0.047214
8	13	0	0.502497	1.820651	1.736607
9	13	0	0.287700	-1.168941	2.175849
10	13	0	0.361402	-2.443574	-0.378173
11	13	0	0.429642	-0.513022	-2.415490
12	13	0	0.396889	2.106986	-1.281039
13	13	0	-2.318106	2.542629	-0.814705
14	13	0	-2.253543	1.903292	1.728184
15	13	0	-2.424117	-0.600152	2.491396
16	13	0	-2.254360	-2.511078	0.737260
17	13	0	-2.060757	-1.815355	-1.801717
18	13	0	-2.140897	0.689752	-2.629330
19	13	0	-1.082330	0.072196	0.025663
20	13	0	-3.714052	-0.034583	-0.165699
21	6	0	6.266414	0.052072	0.237752
22	6	0	6.764476	1.372220	0.861210
23	6	0	6.811126	-0.088567	-1.196015
24	6	0	6.734752	-1.139620	1.095971
25	9	0	6.613941	2.400035	0.001481
26	9	0	8.061430	1.346866	1.223330
27	9	0	6.062090	1.688205	1.971981
28	9	0	6.181592	0.750993	-2.049486
29	9	0	8.127223	0.173709	-1.307133
30	9	0	6.616072	-1.337184	-1.667535
31	9	0	6.063473	-2.271252	0.779336
32	9	0	6.510290	-0.910879	2.405289
33	9	0	8.043777	-1.425467	0.963065

Frequencies -- 7.9629 25.3418 32.9579 33.8088 45.9021 50.6536

Cp(-5042.728072)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-2.352938	1.392459	-1.840109
2	13	0	-2.429330	-2.206709	0.146702
3	13	0	-2.036535	-1.156905	2.626370
4	13	0	-1.890172	1.566491	2.751545
5	13	0	-1.953888	2.915804	0.379033
6	13	0	-4.126617	-0.299013	-0.719619
7	13	0	-1.353842	0.286960	0.452172
8	13	0	0.214692	1.906401	-1.427240
9	13	0	-0.605131	-0.967698	-1.776941
10	13	0	0.127390	-2.213851	0.863707
11	13	0	0.474306	-0.084562	2.666671
12	13	0	0.524044	2.306742	1.337776
13	13	0	2.872255	2.560758	-0.171785
14	13	0	2.793075	1.097822	-2.326259
15	13	0	1.940110	-1.383835	-2.430673
16	13	0	2.712989	-2.631858	-0.252518
17	13	0	2.787445	-1.572815	2.127978
18	13	0	2.971729	1.069310	2.016802
19	13	0	1.473285	-0.038107	-0.024917
20	13	0	4.177754	-0.254124	-0.313176
21	6	0	-6.030021	0.997243	-0.507456
22	1	0	-5.939485	2.065288	-0.389636
23	6	0	-6.153192	0.301363	-1.732788
24	1	0	-6.166781	0.746790	-2.714818
25	6	0	-6.213119	-1.087172	-1.446656
26	1	0	-6.297943	-1.881092	-2.172182
27	6	0	-6.012145	0.037608	0.542210
28	1	0	-5.928723	0.251306	1.596108
29	6	0	-6.143619	-1.247801	-0.041156
30	1	0	-6.146616	-2.185571	0.490655

Frequencies -- 5.6467 18.9281 33.4946 42.1782 48.0744 52.3114

Cp*(-5239.244079)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.103236	-2.128049	0.653907
2	13	0	2.149938	1.882921	0.926682
3	13	0	0.596973	2.006109	3.072629
4	13	0	-0.390366	-0.340973	3.961554
5	13	0	0.345308	-2.556024	2.598868
6	13	0	3.793322	-0.023369	0.018454
7	13	0	0.463645	-0.122881	1.421362
8	13	0	-0.528760	-2.442802	-0.083385

9	13	0	1.049967	-0.256462	-1.201894
10	13	0	-0.166161	2.254554	-0.293705
11	13	0	-1.803223	1.500524	1.933382
12	13	0	-2.103892	-1.263852	1.969934
13	13	0	-3.629047	-2.133479	-0.136709
14	13	0	-2.193126	-2.094815	-2.302562
15	13	0	-0.746401	-0.072579	-3.187192
16	13	0	-2.013601	2.109521	-2.473185
17	13	0	-3.114658	2.601662	-0.207590
18	13	0	-4.150446	0.340624	0.740063
19	13	0	-1.698927	0.035475	-0.512087
20	13	0	-3.943540	0.143333	-2.159138
21	6	0	5.882761	-0.930093	0.127062
22	6	0	5.409795	-1.028410	-1.217862
23	6	0	5.240559	0.300675	-1.724507
24	6	0	6.015805	0.458831	0.446977
25	6	0	5.632997	1.213892	-0.698732
26	6	0	5.669660	2.707297	-0.809342
27	1	0	5.003203	3.072563	-1.590939
28	1	0	5.375744	3.191141	0.124115
29	1	0	6.679079	3.054862	-1.051827
30	6	0	4.840841	0.664730	-3.124441
31	1	0	4.328876	1.626714	-3.163902
32	1	0	5.720725	0.735862	-3.771578
33	1	0	4.173639	-0.077941	-3.562726
34	6	0	5.207411	-2.303435	-1.978212
35	1	0	4.542353	-2.165564	-2.830753
36	1	0	6.160192	-2.680983	-2.362891
37	1	0	4.777074	-3.085868	-1.350089
38	6	0	6.257791	-2.088051	1.001780
39	1	0	5.589522	-2.938539	0.855487
40	1	0	7.273765	-2.428992	0.778464
41	1	0	6.226226	-1.825588	2.059379
42	6	0	6.538579	1.029294	1.731807
43	1	0	6.415758	0.335996	2.564118
44	1	0	7.606613	1.254630	1.650280
45	1	0	6.031594	1.957808	2.000307

Frequencies --	14.1237	16.7231	20.2592	34.2843	54.2326	56.5251

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3. Cartesian Coordinates and Normal Modes of Vibrations of radical/ligand attached Al4X4 complexes

M062X

Al_4Cp_4(-1743.441680)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.572439	1.363658	0.767102
2	13	0	0.442187	-1.145085	1.127437
3	13	0	1.332626	0.401597	-0.938072
4	13	0	-1.201708	-0.623314	-0.990443
5	6	0	-0.146788	3.370458	1.931637
6	1	0	0.871607	3.669824	2.122498
7	6	0	-0.909736	3.698213	0.787938
8	1	0	-0.576458	4.292285	-0.048493
9	6	0	-2.177037	3.086330	0.918929
10	1	0	-2.980303	3.131160	0.199957
11	6	0	-0.942314	2.555531	2.768781
12	1	0	-0.636286	2.126015	3.709908
13	6	0	-2.197323	2.379783	2.142999
14	1	0	-3.018214	1.790500	2.519973
15	6	0	3.142877	1.854936	-1.354679
16	1	0	3.292050	2.714496	-0.720192
17	6	0	2.351754	1.814034	-2.525358
18	1	0	1.792366	2.636758	-2.941849
19	6	0	2.397275	0.497429	-3.037318
20	1	0	1.880446	0.140128	-3.914200
21	6	0	3.677315	0.563878	-1.143397
22	1	0	4.306559	0.265907	-0.319208
23	6	0	3.216294	-0.275481	-2.183188
24	6	0	-3.488928	-0.748172	-1.557481
25	1	0	-4.206719	-0.164548	-1.002557
26	6	0	-2.787959	-0.325627	-2.709850
27	1	0	-2.878418	0.635881	-3.190681
28	6	0	-1.925535	-1.373722	-3.104260
29	1	0	-1.242779	-1.353071	-3.939250
30	6	0	-3.059726	-2.056396	-1.239760
31	1	0	-3.391593	-2.646928	-0.400300
32	6	0	-2.093384	-2.443285	-2.195806
33	6	0	2.081497	-2.587901	2.018457
34	1	0	3.056548	-2.634389	1.559335
35	6	0	1.689632	-1.704981	3.050298
36	1	0	2.312421	-0.957645	3.516311
37	6	0	0.328342	-1.950329	3.341077
38	1	0	-0.268803	-1.424035	4.069401
39	6	0	0.962657	-3.378968	1.672092
40	1	0	0.934576	-4.135544	0.903581
41	6	0	-0.121054	-2.984775	2.489777
42	1	0	-1.560041	-3.380684	-2.214697
43	1	0	-1.120696	-3.388165	2.455021

44	1	0	3.432678	-1.326470	-2.292397

Frequencies -- 17.8333 21.7345 25.0343 28.1703 32.9805 36.7872

$Al_4(C_2H)_4$(-1276.618547)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.218996	-0.628201	-0.765537
2	13	0	1.266961	0.019775	-0.931620
3	13	0	0.307050	-0.851238	1.291447
4	13	0	-0.354604	1.480588	0.430791
5	6	0	-3.634761	-1.923166	-2.281921
6	1	0	-4.456716	-2.370121	-2.793909
7	6	0	-2.702265	-1.417975	-1.700060
8	6	0	3.825974	0.042613	-2.737958
9	1	0	4.705561	0.048795	-3.340813
10	6	0	2.830507	0.033795	-2.050757
11	6	0	-1.056713	4.405707	1.303471
12	1	0	-1.291977	5.400942	1.605243
13	6	0	-0.788285	3.276782	0.961410
14	6	0	0.929645	-2.580469	3.827088
15	1	0	1.143722	-3.173565	4.686649
16	6	0	0.686948	-1.908275	2.851098

Frequencies -- 48.0435 51.6385 57.0083 58.5002 59.9887 93.6596

Al_4Ph_4(-1895.810527)

1	13	0	1.001531	-0.914450	-0.886351
2	13	0	0.114189	-0.411875	1.486709
3	13	0	-1.480858	-0.316162	-0.543410
4	13	0	0.327042	1.495677	-0.248109
5	6	0	3.663870	-1.922466	-1.621673
6	6	0	2.292059	-2.001160	-1.894163
7	6	0	1.884377	-2.880932	-2.904913
8	6	0	2.801489	-3.648248	-3.612046
9	6	0	4.156372	-3.550402	-3.321117
10	6	0	4.588497	-2.685759	-2.323614
11	1	0	4.026788	-1.253917	-0.846148
12	1	0	0.830775	-2.975805	-3.151482
13	1	0	2.461075	-4.321750	-4.389226
14	1	0	4.873887	-4.147137	-3.870724
15	1	0	5.644278	-2.607183	-2.094159

16	6	0	-3.887414	-1.899020	-1.198551
17	6	0	-3.330946	-0.615123	-1.135924
18	6	0	-4.147146	0.460840	-1.508278
19	6	0	-5.458309	0.267884	-1.924650
20	6	0	-5.985191	-1.016377	-1.976835
21	6	0	-5.197929	-2.101765	-1.613292
22	1	0	-3.292862	-2.764037	-0.919181
23	1	0	-3.758772	1.474849	-1.475415
24	1	0	-6.068714	1.116922	-2.207697
25	1	0	-7.006963	-1.171365	-2.300883
26	1	0	-5.605853	-3.104526	-1.653727
27	6	0	0.194710	4.354067	0.419809
28	6	0	0.758911	3.403020	-0.440440
29	6	0	1.630573	3.867329	-1.433759
30	6	0	1.927008	5.218256	-1.564476
31	6	0	1.352954	6.140114	-0.697807
32	6	0	0.485462	5.707069	0.296632
33	1	0	-0.486175	4.040152	1.205868
34	1	0	2.090838	3.166794	-2.124658
35	1	0	2.603861	5.553410	-2.341049
36	1	0	1.581579	7.194051	-0.797621
37	1	0	0.037795	6.423117	0.975209
38	6	0	1.530159	-0.875435	4.023007
39	6	0	0.279849	-0.861445	3.391999
40	6	0	-0.840561	-1.177870	4.171167
41	6	0	-0.720536	-1.494743	5.518458
42	6	0	0.532046	-1.501281	6.118973
43	6	0	1.659910	-1.191103	5.369824
44	1	0	2.426674	-0.635155	3.458760
45	1	0	-1.831167	-1.179465	3.725408
46	1	0	-1.601791	-1.737319	6.099958
47	1	0	0.629108	-1.747905	7.169108
48	1	0	2.638095	-1.195321	5.835230

Frequencies --	12.5674	16.1089	17.4675	19.2208	22.4462	24.2948

Al_4Cl_4(-2810.746140)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.290572	-0.812420	0.458971
2	13	0	-0.869248	0.382594	1.278277

3	13	0	-0.871509	-0.899107	-0.983956
4	13	0	0.450371	1.328805	-0.753332
5	17	0	1.055151	3.088486	-1.751492
6	17	0	-2.028212	0.886214	2.969942
7	17	0	-2.033135	-2.091164	-2.283256
8	17	0	3.006383	-1.883664	1.064767

Frequencies -- 46.4402 47.4687 53.0790 53.0790 55.2816 109.3335

B3LYP

Al_4Cp_4(-1743.876125)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.560596	0.186721	1.585891
2	13	0	-1.359502	-1.024083	-0.002417
3	13	0	1.217981	-0.685206	-0.957032
4	13	0	-0.436350	1.510945	-0.630506
5	6	0	1.580412	-0.730778	3.551236
6	1	0	1.871359	-1.769610	3.568009
7	6	0	2.387932	0.353381	3.129712
8	1	0	3.402311	0.285397	2.768493
9	6	0	1.626873	1.540449	3.254149
10	1	0	1.959585	2.535911	3.004027
11	6	0	0.320127	-0.212924	3.936677
12	1	0	-0.517733	-0.788219	4.298814
13	6	0	0.348419	1.190671	3.752878
14	1	0	-0.464109	1.872856	3.949794
15	6	0	3.093612	-2.162254	-1.174674
16	1	0	3.421541	-2.739567	-0.323917
17	6	0	3.541039	-0.864493	-1.523079
18	1	0	4.269387	-0.278377	-0.984422
19	6	0	2.855072	-0.465568	-2.695470
20	1	0	2.969523	0.477408	-3.207228
21	6	0	2.131045	-2.564510	-2.131757
22	1	0	1.598338	-3.502724	-2.138978
23	6	0	1.982962	-1.515730	-3.071627
24	6	0	-1.340215	3.707878	-0.305433
25	1	0	-1.679180	4.007043	0.674207
26	6	0	-0.029491	3.867050	-0.817483
27	1	0	0.805664	4.309870	-0.297316
28	6	0	-0.004226	3.333192	-2.128322
29	1	0	0.853542	3.297940	-2.781648

30	6	0	-2.124454	3.075465	-1.300085
31	1	0	-3.166336	2.809204	-1.211750
32	6	0	-1.298619	2.842980	-2.426905
33	6	0	-2.422176	-3.052996	-0.714735
34	1	0	-1.887274	-3.743320	-1.348456
35	6	0	-2.424033	-3.053454	0.701198
36	1	0	-1.892000	-3.744932	1.336064
37	6	0	-3.238380	-1.980039	1.137495
38	1	0	-3.435621	-1.709425	2.163147
39	6	0	-3.234441	-1.979611	-1.153537
40	1	0	-3.428259	-1.709220	-2.179915
41	6	0	-3.739162	-1.316811	-0.008523
42	1	0	-1.600388	2.368633	-3.347946
43	1	0	-4.385471	-0.453000	-0.009230
44	1	0	1.316716	-1.513750	-3.920281

Frequencies -- 2.3755 19.2009 24.5598 27.0704 34.7805 37.8849

$Al_4(C_2H)_4$(-1276.891504)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.309442	-0.724370	-0.532806
2	13	0	1.247307	-0.420297	-0.892075
3	13	0	0.265227	-0.431797	1.514771
4	13	0	-0.196138	1.578333	-0.067826
5	6	0	-3.894806	-2.153139	-1.593535
6	1	0	-4.771885	-2.637812	-1.953349
7	6	0	-2.895587	-1.600990	-1.183589
8	6	0	3.703985	-1.249384	-2.661123
9	1	0	4.537579	-1.530676	-3.261096
10	6	0	2.754394	-0.928977	-1.977500
11	6	0	-0.585675	4.689294	-0.211607
12	1	0	-0.717854	5.744637	-0.260301
13	6	0	-0.435158	3.486983	-0.156147
14	6	0	0.785706	-1.283724	4.490265
15	1	0	0.962317	-1.572716	5.499637
16	6	0	0.584455	-0.954489	3.340339

Frequencies -- 46.0107 46.0478 49.8825 50.3323 50.3808 93.7882

Al_4Ph_4(-1896.365402)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-1.473713	-0.538706	-0.295928
2	13	0	0.146873	0.369703	1.538578
3	13	0	0.284405	1.291803	-0.901148
4	13	0	1.060396	-1.143200	-0.381738
5	6	0	-3.540508	-2.490389	-1.142673
6	6	0	-3.307258	-1.202706	-0.631783
7	6	0	-4.432374	-0.405615	-0.362501
8	6	0	-5.725308	-0.867911	-0.590452
9	6	0	-5.925546	-2.148544	-1.096874
10	6	0	-4.829830	-2.960881	-1.373420
11	1	0	-2.704722	-3.146481	-1.367506
12	1	0	-4.306221	0.597520	0.034340
13	1	0	-6.575394	-0.231385	-0.373421
14	1	0	-6.930682	-2.511866	-1.275144
15	1	0	-4.980553	-3.959117	-1.767967
16	6	0	-0.400918	3.767448	-2.384764
17	6	0	0.634000	2.897339	-2.003632
18	6	0	1.931751	3.214210	-2.438477
19	6	0	2.186259	4.340976	-3.214837
20	6	0	1.140586	5.184676	-3.577515
21	6	0	-0.155637	4.896260	-3.161113
22	1	0	-1.422167	3.567724	-2.073937
23	1	0	2.766953	2.573678	-2.170412
24	1	0	3.197568	4.561095	-3.536796
25	1	0	1.334803	6.062856	-4.181810
26	1	0	-0.973290	5.550421	-3.441123
27	6	0	3.069841	-3.254581	0.175529
28	6	0	2.383317	-2.546670	-0.825000
29	6	0	2.673894	-2.877410	-2.159230
30	6	0	3.601771	-3.863785	-2.480911
31	6	0	4.266608	-4.548466	-1.468134
32	6	0	3.999269	-4.242246	-0.137044
33	1	0	2.881706	-3.037237	1.222861
34	1	0	2.170519	-2.359673	-2.970542
35	1	0	3.806237	-4.098419	-3.519210
36	1	0	4.989389	-5.317096	-1.714849
37	1	0	4.514411	-4.772656	0.655531
38	6	0	-0.435440	0.171596	4.436496
39	6	0	0.303570	0.848790	3.452054
40	6	0	1.157597	1.876928	3.884660
41	6	0	1.269781	2.213933	5.230381
42	6	0	0.525112	1.525394	6.183356
43	6	0	-0.329291	0.501925	5.784377
44	1	0	-1.110144	-0.631502	4.154635
45	1	0	1.750793	2.431579	3.163589
46	1	0	1.936478	3.012075	5.535915

47	1	0	0.610339	1.785111	7.231857
48	1	0	-0.911487	-0.037526	6.522563

Frequencies -- 8.3236 10.9344 14.1314 16.4243 18.4043 19.5682

Al_4Cl_4(-2811.004155)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.254649	-0.639963	-0.804094
2	13	0	1.287040	0.025280	-0.971691
3	13	0	0.310467	-0.881032	1.298962
4	13	0	-0.372318	1.509709	0.433288
5	17	0	-0.854752	3.498943	1.020779
6	17	0	2.997373	0.054330	-2.240415
7	17	0	0.729896	-2.050447	3.028592
8	17	0	-2.902243	-1.490457	-1.851686

Frequencies -- 47.7854 47.8180 57.7099 57.8697 57.9213 114.4228

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4. Additional Information

A. Cartesian Coordinates and normal modes of vibrations of Al_4X_4 Cations

M062X

$Al_4Cp_4^+$(-1743.234267)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.263386	-1.070019	-0.676088
2	13	0	1.263514	1.069558	-0.676044
3	13	0	1.065399	-1.251950	0.676479
4	13	0	-1.066025	1.252409	0.675951
5	6	0	-1.777883	-3.079409	-1.606028
6	1	0	-1.048114	-3.869437	-1.689104
7	6	0	-2.661549	-2.870798	-0.520285
8	1	0	-2.725603	-3.475110	0.371280
9	6	0	-3.445185	-1.727250	-0.806722
10	1	0	-4.208668	-1.307794	-0.169981
11	6	0	-2.010976	-2.060926	-2.562849
12	1	0	-1.496882	-1.943976	-3.503940
13	6	0	-3.044762	-1.225728	-2.067934

14	1	0	-3.450194	-0.358731	-2.565361
15	6	0	2.144120	-3.264787	0.529515
16	1	0	2.095159	-3.880794	-0.354730
17	6	0	1.251581	-3.311221	1.626300
18	1	0	0.401110	-3.967692	1.726272
19	6	0	1.663186	-2.335139	2.567784
20	1	0	1.187780	-2.123907	3.512736
21	6	0	3.111063	-2.265546	0.793156
22	1	0	3.926160	-1.986405	0.143680
23	6	0	2.816362	-1.690099	2.052139
24	6	0	-3.111845	2.265604	0.792712
25	1	0	-3.927249	1.985724	0.143938
26	6	0	-2.816298	1.691348	2.052057
27	1	0	-3.366404	0.899299	2.535806
28	6	0	-1.663098	2.337153	2.566542
29	1	0	-1.187203	2.126953	3.511481
30	6	0	-2.145314	3.264875	0.527728
31	1	0	-2.097059	3.880057	-0.357130
32	6	0	-1.252275	3.312457	1.624034
33	6	0	3.445714	1.725835	-0.806968
34	1	0	4.209192	1.305969	-0.170469
35	6	0	3.044856	1.224731	-2.068201
36	1	0	3.449869	0.357643	-2.565800
37	6	0	2.011289	2.060417	-2.562778
38	1	0	1.496989	1.943840	-3.503797
39	6	0	2.662572	2.869629	-0.520150
40	1	0	2.727127	3.473773	0.371491
41	6	0	1.778832	3.078846	-1.605742
42	1	0	-0.401970	3.969311	1.723034
43	1	0	1.049336	3.869164	-1.688553
44	1	0	3.366886	-0.897746	2.534930

Frequencies -- 6.9160 28.3702 29.6147 31.7683 36.6266 44.7991

$Al_4(C_2H)_4^+$ (-1276.337557)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.797045	1.177011	-0.836969
2	13	0	-0.820128	-1.162573	0.823310
3	13	0	0.806722	0.828198	1.172620
4	13	0	0.811277	-0.832116	-1.167060
5	6	0	-3.011812	2.934792	-2.073265
6	1	0	-3.775460	3.546922	-2.501811
7	6	0	-2.144755	2.245297	-1.589100
8	6	0	-3.070391	-2.893798	2.032265

9	1	0	-3.846534	-3.496627	2.451309
10	6	0	-2.189204	-2.215074	1.558693
11	6	0	3.048170	-2.067242	-2.897123
12	1	0	3.819698	-2.495345	-3.499515
13	6	0	2.172163	-1.583399	-2.218930
14	6	0	3.035111	2.038392	2.931339
15	1	0	3.803471	2.457826	3.543944
16	6	0	2.162709	1.564244	2.241616

Frequencies -- 39.7951 40.1524 40.3268 40.7844 50.3996 78.5091

$Al_4Ph_4^+$(-1895.556989)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.855746	-0.346762	-1.347907
2	13	0	0.854899	0.341315	1.347671
3	13	0	-0.857881	-1.348043	0.342507
4	13	0	-0.854356	1.347264	-0.346268
5	6	0	2.828727	0.362027	-3.368342
6	6	0	2.282575	-0.679902	-2.604995
7	6	0	2.793726	-1.974241	-2.778265
8	6	0	3.809716	-2.220223	-3.690547
9	6	0	4.334024	-1.174414	-4.440652
10	6	0	3.844548	0.116373	-4.280849
11	1	0	2.463993	1.378445	-3.258989
12	1	0	2.401345	-2.806277	-2.202074
13	1	0	4.194185	-3.224220	-3.816160
14	1	0	5.127529	-1.365861	-5.151670
15	1	0	4.256205	0.929101	-4.865328
16	6	0	-2.799047	-2.773071	1.970366
17	6	0	-2.284249	-2.605313	0.676758
18	6	0	-2.826314	-3.374360	-0.363144
19	6	0	-3.841903	-4.286723	-0.116177
20	6	0	-4.334905	-4.441100	1.173849
21	6	0	-3.814683	-3.685349	2.217646
22	1	0	-2.410052	-2.192224	2.800801
23	1	0	-2.458816	-3.269332	-1.379005
24	1	0	-4.250475	-4.875540	-0.927354
25	1	0	-5.128039	-5.152241	1.366312
26	1	0	-4.201962	-3.806672	3.221091
27	6	0	-2.819659	3.376154	0.360174
28	6	0	-2.277632	2.608038	-0.680415
29	6	0	-2.790601	2.778936	-1.974323
30	6	0	-3.804573	3.693209	-2.221182

31	6	0	-4.324831	4.447939	-1.176696
32	6	0	-3.833444	4.290651	0.113632
33	1	0	-2.453450	3.268816	1.376269
34	1	0	-2.401335	2.199167	-2.805355
35	1	0	-4.190509	3.816884	-3.224853
36	1	0	-5.116746	5.160553	-1.368823
37	1	0	-4.241912	4.878805	0.925324
38	6	0	2.791026	1.969765	2.778863
39	6	0	2.279029	0.675547	2.607417
40	6	0	2.822318	-0.365108	3.374646
41	6	0	3.836494	-0.118322	4.288619
42	6	0	4.326943	1.172263	4.446376
43	6	0	3.805404	2.216821	3.692585
44	1	0	2.400916	2.800837	2.199664
45	1	0	2.456941	-1.381440	3.266813
46	1	0	4.245984	-0.930061	4.876027
47	1	0	5.119148	1.364572	5.158605
48	1	0	4.190645	3.220712	3.816628

Frequencies -- -0.8471 6.3825 7.6167 9.7484 14.6266 14.6615

$Al_4Cl_4^+$(-2810.429003)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.229337	-0.997540	0.567963
2	13	0	-0.749697	0.511698	1.415895
3	13	0	-0.750001	-0.956697	-1.162331
4	13	0	0.270549	1.442412	-0.821566
5	17	0	1.118892	3.072918	-1.750458
6	17	0	-2.083205	0.859375	2.946240
7	17	0	-2.083727	-2.095649	-2.241703
8	17	0	3.048227	-1.836773	1.045882

Frequencies -- 35.1470 44.6015 51.8978 52.5737 52.5737 88.3919

B3LYP

$Al_4Cp_4^+$(-1743.669745)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.298689	0.988336	-0.729333
2	13	0	-0.988221	-1.297936	0.727745
3	13	0	0.988751	1.300988	0.725741

4	13	0	1.299104	-0.983524	-0.728676
5	6	0	-2.800100	2.754781	-0.774936
6	1	0	-2.932668	3.424610	0.060492
7	6	0	-1.879978	2.922219	-1.840075
8	1	0	-1.186590	3.739942	-1.958716
9	6	0	-2.031457	1.824553	-2.727857
10	1	0	-1.483488	1.668281	-3.643805
11	6	0	-3.527602	1.559637	-1.006764
12	1	0	-4.307936	1.161667	-0.377106
13	6	0	-3.055453	0.983954	-2.212765
14	1	0	-3.412367	0.072077	-2.665296
15	6	0	1.059902	3.376462	1.731364
16	1	0	0.202234	4.030316	1.750533
17	6	0	2.069333	3.352217	0.736574
18	1	0	2.117555	3.986940	-0.134457
19	6	0	3.015437	2.358527	1.095411
20	1	0	3.906651	2.104542	0.543401
21	6	0	1.375145	2.389650	2.701435
22	1	0	0.806944	2.169929	3.591681
23	6	0	2.589019	1.762575	2.308448
24	6	0	2.139111	-1.640768	-2.750553
25	1	0	1.695936	-1.319467	-3.680015
26	6	0	3.184261	-0.980797	-2.050214
27	1	0	3.665291	-0.063435	-2.351282
28	6	0	3.484582	-1.741784	-0.892979
29	1	0	4.236227	-1.506210	-0.155814
30	6	0	1.803032	-2.816195	-2.026970
31	1	0	1.051046	-3.537420	-2.306329
32	6	0	2.631883	-2.875110	-0.878711
33	6	0	-1.500750	-2.252464	2.741059
34	1	0	-1.053283	-1.911934	3.661597
35	6	0	-2.712031	-1.771787	2.173265
36	1	0	-3.338531	-0.995415	2.583558
37	6	0	-2.953074	-2.498888	0.980163
38	1	0	-3.796106	-2.371758	0.319321
39	6	0	-1.001497	-3.282131	1.899013
40	1	0	-0.100582	-3.851954	2.063437
41	6	0	-1.896251	-3.429553	0.810331
42	1	0	2.622632	-3.650973	-0.129221
43	1	0	-1.797637	-4.134194	-0.000618
44	1	0	3.097965	0.977740	2.845562

Frequencies -- 19.8307 31.8273 38.4434 43.2131 43.7162 48.7120

$Al_4(C_2H)_4^+$ (-1276.618491)

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.794726	1.199596	-0.846518
2	13	0	-0.818952	-1.183861	0.832423
3	13	0	0.804839	0.838126	1.194743
4	13	0	0.810007	-0.840893	-1.188799
5	6	0	-2.977592	2.990130	-2.112604
6	1	0	-3.727626	3.609809	-2.550822
7	6	0	-2.121945	2.288499	-1.616376
8	6	0	-3.036962	-2.949870	2.071587
9	1	0	-3.799100	-3.561186	2.500574
10	6	0	-2.167608	-2.257784	1.585889
11	6	0	3.014243	-2.106559	-2.953255
12	1	0	3.771642	-2.544641	-3.564008
13	6	0	2.150259	-1.610482	-2.261809
14	6	0	3.001247	2.077447	2.987454
15	1	0	3.755922	2.506399	3.607988
16	6	0	2.140342	1.591779	2.284859

Frequencies -- 34.8594 38.8563 38.8604 38.9225 45.9335 80.5850

$Al_4Ph_4^+$(-1896.121507)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.865292	-0.979956	-1.009233
2	13	0	-0.864343	1.003040	-0.988495
3	13	0	0.860753	0.984613	0.999222
4	13	0	-0.861408	-1.006411	0.976047
5	6	0	2.783023	-3.138866	-1.484218
6	6	0	2.269164	-1.922802	-1.969361
7	6	0	2.787201	-1.416903	-3.175463
8	6	0	3.771740	-2.105416	-3.873857
9	6	0	4.262499	-3.309725	-3.376857
10	6	0	3.767903	-3.826954	-2.182540
11	1	0	2.416644	-3.562996	-0.554897
12	1	0	2.425127	-0.478156	-3.582266
13	1	0	4.157572	-1.703927	-4.802687
14	1	0	5.031686	-3.844721	-3.919691
15	1	0	4.150376	-4.763950	-1.797151
16	6	0	2.760216	3.157324	1.484817
17	6	0	2.253355	1.936759	1.966307
18	6	0	2.770897	1.432730	3.173469
19	6	0	3.748293	2.126709	3.876362

20	6	0	4.232275	3.335191	3.382704
21	6	0	3.738085	3.850899	2.187524
22	1	0	2.393690	3.580560	0.555117
23	1	0	2.413832	0.490998	3.577789
24	1	0	4.134097	1.726331	4.805656
25	1	0	4.996071	3.874721	3.928732
26	1	0	4.115699	4.790975	1.804879
27	6	0	-2.769878	-3.181514	1.418549
28	6	0	-2.254692	-1.974659	1.925442
29	6	0	-2.761723	-1.497480	3.147489
30	6	0	-3.736755	-2.204858	3.840413
31	6	0	-4.228267	-3.400070	3.322214
32	6	0	-3.744770	-3.888831	2.111604
33	1	0	-2.412793	-3.582166	0.475239
34	1	0	-2.397678	-0.567612	3.572553
35	1	0	-4.114163	-1.825759	4.782027
36	1	0	-4.989583	-3.949835	3.861404
37	1	0	-4.128743	-4.817913	1.708944
38	6	0	-2.779084	1.483118	-3.149197
39	6	0	-2.269400	1.962848	-1.929282
40	6	0	-2.791857	3.164436	-1.417276
41	6	0	-3.777341	3.863968	-2.103193
42	6	0	-4.263910	3.372501	-3.311531
43	6	0	-3.764684	2.182772	-3.834923
44	1	0	-2.408481	0.557700	-3.578186
45	1	0	-2.432077	3.567171	-0.475905
46	1	0	-4.167000	4.789071	-1.696886
47	1	0	-5.033658	3.916054	-3.845054
48	1	0	-4.144475	1.801994	-4.774885

Frequencies -- 15.4690 16.8169 20.6941 22.4709 23.3162 23.3437

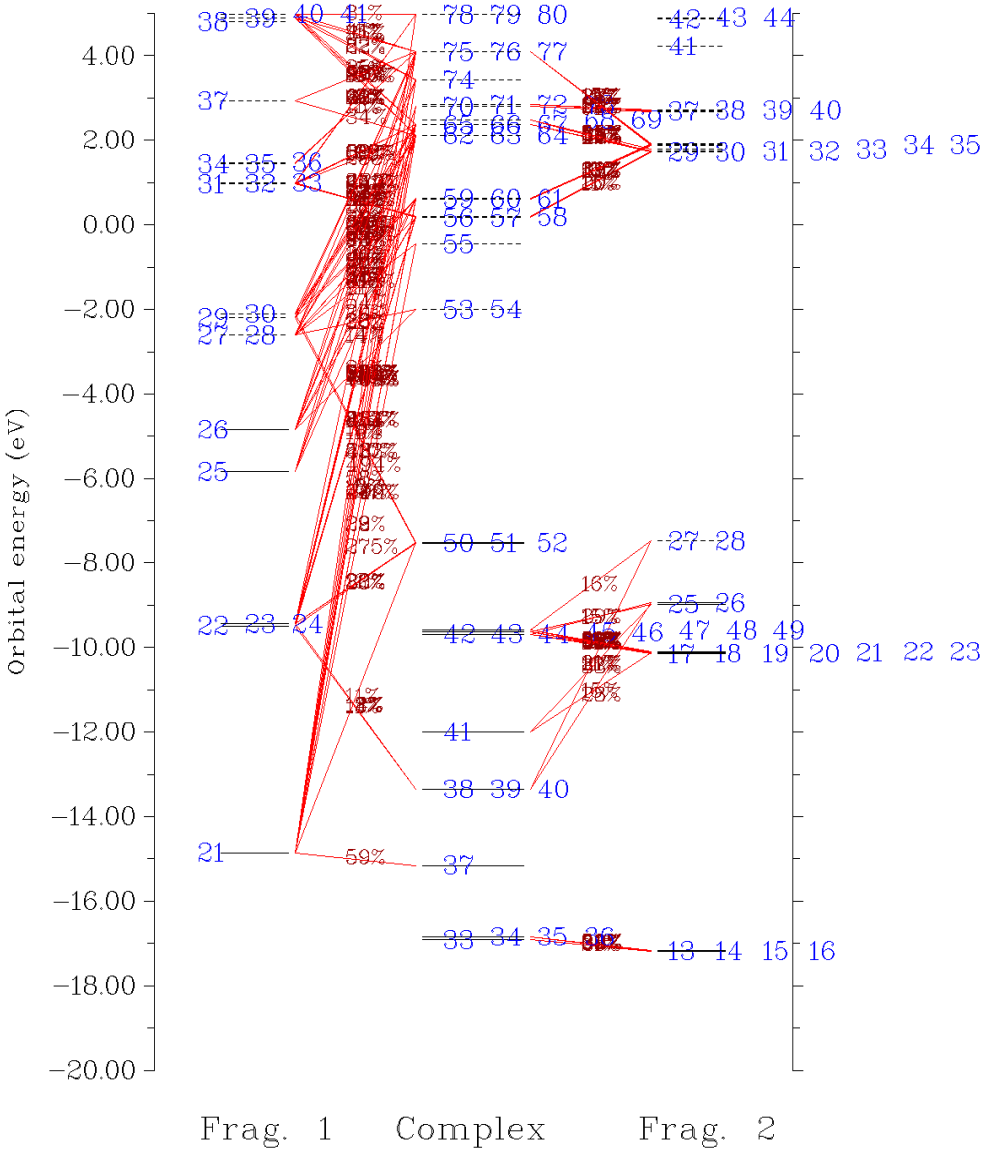
$Al_4Cl_4^+$(-2810.695058)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.297303	-0.515554	-0.991658
2	13	0	1.337252	-0.195568	-1.033137
3	13	0	0.494055	-0.779400	1.415173
4	13	0	-0.564184	1.503037	0.567977
5	17	0	-0.846652	3.515430	0.996489
6	17	0	3.004454	0.075106	-2.241549
7	17	0	0.718285	-2.055415	3.038317
8	17	0	-2.905092	-1.521273	-1.837878

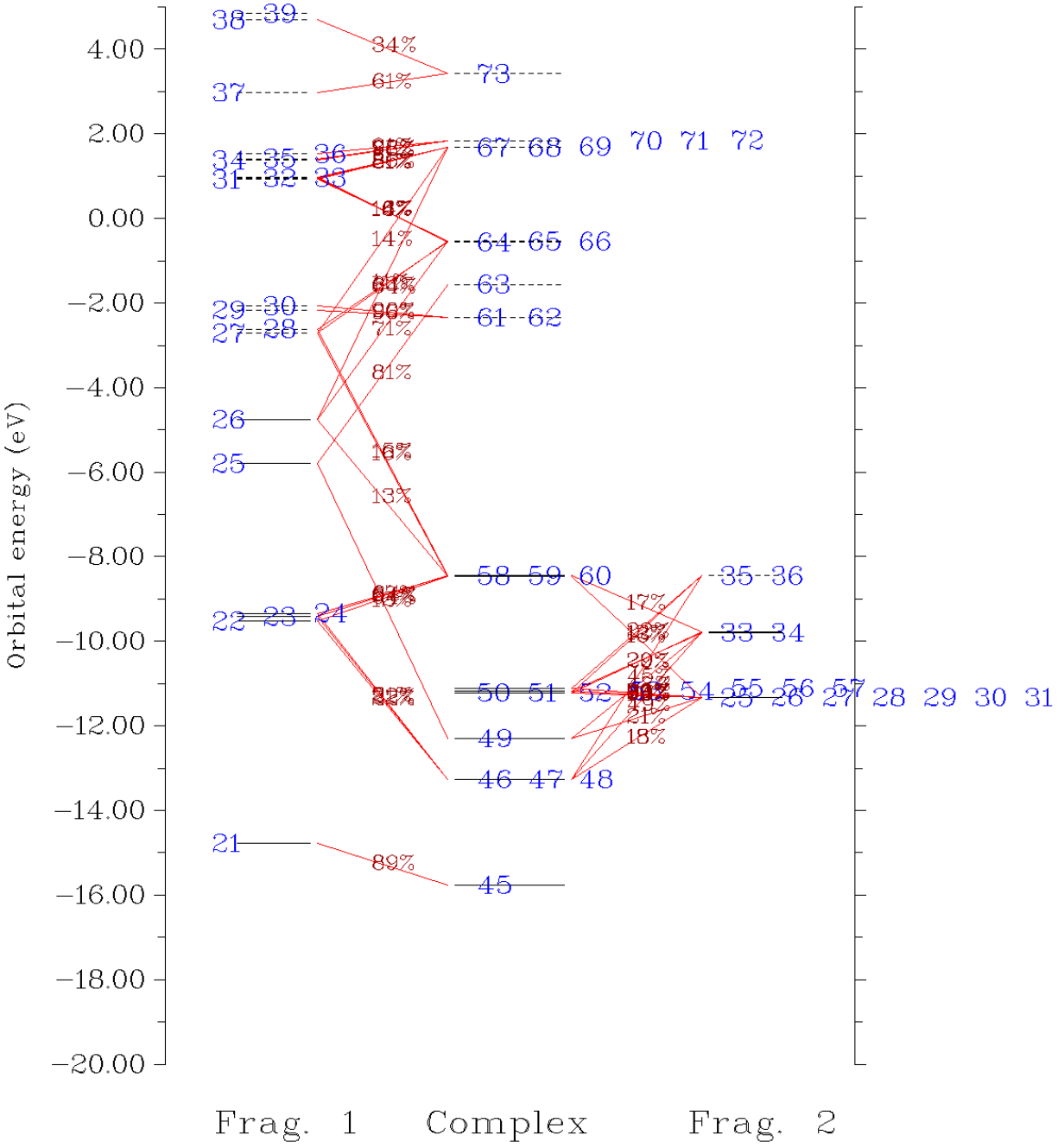
Frequencies -- 29.3958 38.8465 46.4063 46.4254 47.8225 89.2631

A. KS Orbital Correlation Diagram of Radical Attached Al_4 Complexes

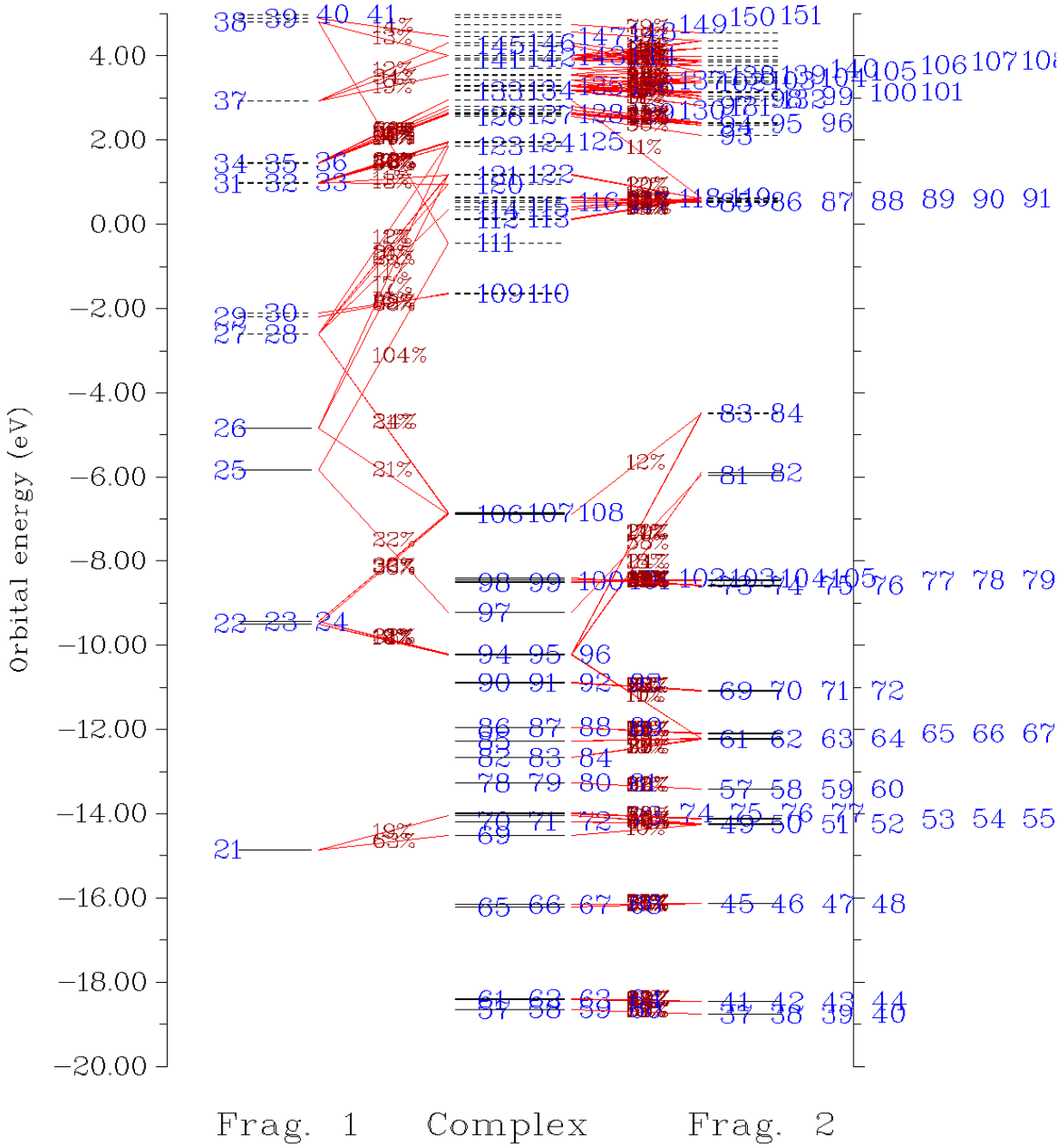
1.$Al_4(C_2H)_4$



2. Al_4Cl_4

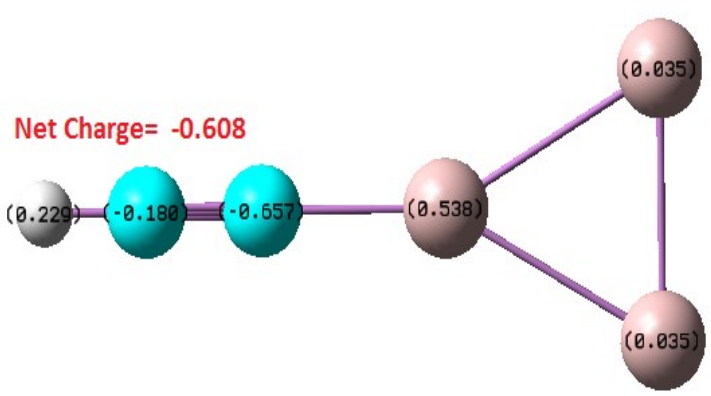

Orbital energy (eV)
4.00
2.00
0.00
−2.00
−4.00
−6.00
−8.00
−10.00
−12.00
−14.00
−16.00
−18.00
−20.00
Frag. 1
Complex
Frag. 2

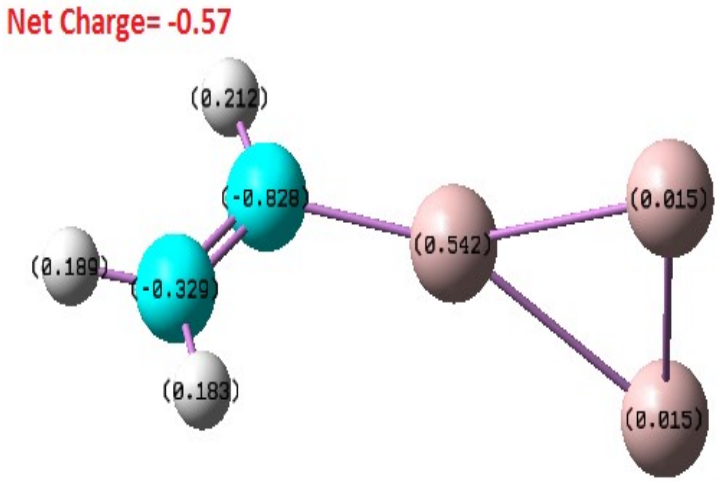
3.Al_4Ph_4


Orbital energy (eV)
4.00
2.00
0.00
−2.00
−4.00
−6.00
−8.00
−10.00
−12.00
−14.00
−16.00
−18.00
−20.00
Frag. 1
Complex
Frag. 2

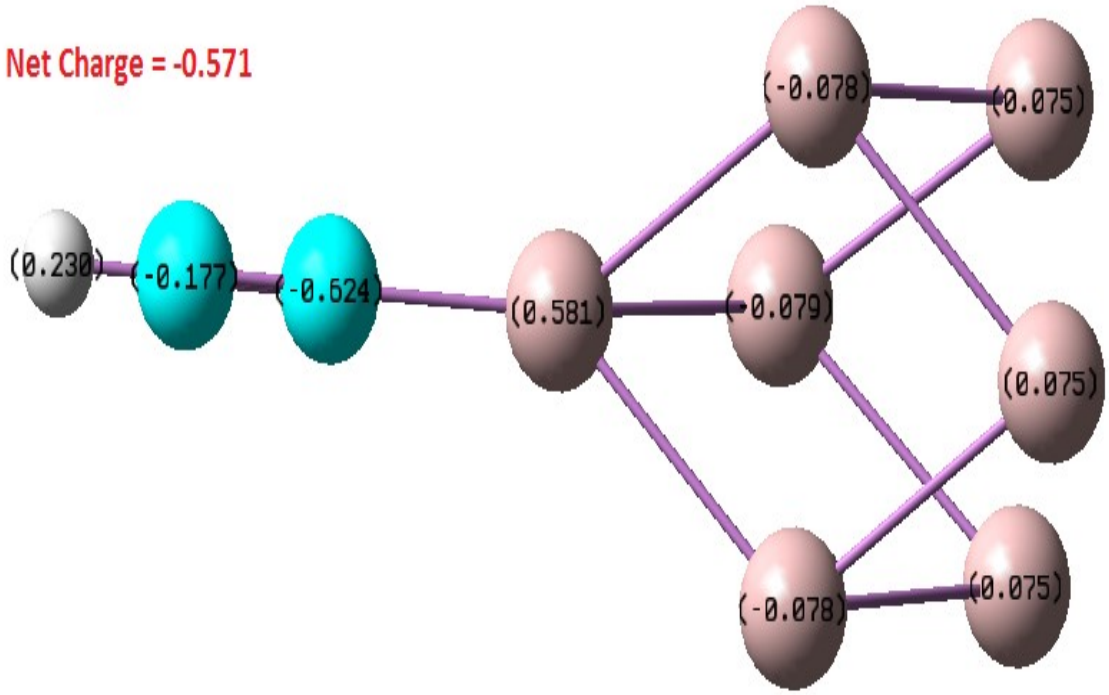
NBO Charge Calculation

Al_3 complex

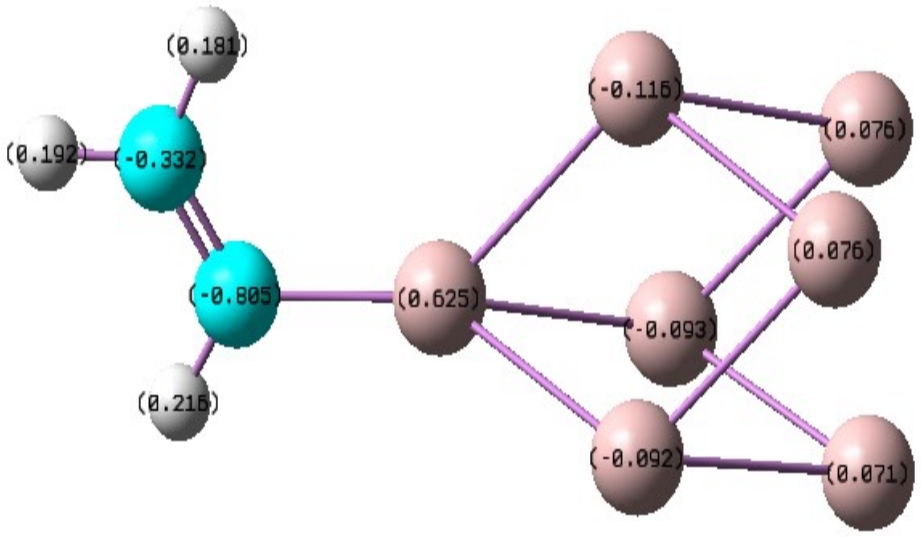




Al_7 complex



Net Charge = -0.548



Tetramerization Energies

			m062x							b3lyp			
		Ecomplex	Emono	4*Emono	delta(in a.u)	delta(in kcal)		Ecomplex	Emono	4*Emono	delta(in a.u)	delta(in kcal)
	U	-1743.44168	-435.84913	-1743.39652	-0.04516	-28.3383516		-1743.876125	-435.963791	-1743.855164	-0.020961	-13.15323711
al4cp4	U+Thermal	-1743.417803	-435.844152	-1743.376608	-0.041195	-25.85027445		-1743.850229	-435.958602	-1743.834408	-0.015821	-9.92783571
	H	-1743.416859	-435.843208	-1743.372832	-0.044027	-27.62738277		-1743.849285	-435.957658	-1743.830632	-0.018653	-11.70494403
	G	-1743.499798	-435.877471	-1743.509884	0.010086	6.32906586		-1743.939457	-435.992368	-1743.969472	0.030015	18.83471265
					0	0				0	0	0
	U	-1276.618547	-319.117462	-1276.469848	-0.148699	-93.31010949		-1276.891504	-319.190103	-1276.760412	-0.131092	-82.26154092
al4ace4	U+Thermal	-1276.601491	-319.113614	-1276.454456	-0.147035	-92.26593285		-1276.873976	-319.186212	-1276.744848	-0.129128	-81.02911128
	H	-1276.600547	-319.11267	-1276.45068	-0.149867	-94.04304117		-1276.873032	-319.185268	-1276.741072	-0.13196	-82.8062196
	G	-1276.664978	-319.136296	-1276.545184	-0.119794	-75.17193294		-1276.938914	-319.208173	-1276.832692	-0.106222	-66.65536722
				0	0	0				0	0	0
	U	-1895.810527	-473.910218	-1895.640872	-0.169655	-106.4602091		-1896.365402	-474.05423	-1896.21692	-0.148482	-93.17393982
al4ph4	U+Thermal	-1895.78262	-473.904144	-1895.616576	-0.166044	-104.1942704		-1896.337209	-474.048162	-1896.192648	-0.144561	-90.71347311
	H	-1895.781676	-473.9032	-1895.6128	-0.168876	-105.9713788		-1896.336265	-474.047218	-1896.188872	-0.147393	-92.49058143
	G	-1895.878583	-473.941081	-1895.764324	-0.114259	-71.69866509		-1896.435574	-474.084971	-1896.339884	-0.09569	-60.0464319
				0	0	0				0	0	0
	U	-2810.74614	-702.6621	-2810.6484	-0.09774	-61.3328274		-2811.004155	-702.731024	-2810.924096	-0.080059	-50.23782309
al4cl4	U+Thermal	-2810.733401	-702.659488	-2810.637952	-0.095449	-59.89520199		-2810.991287	-702.728401	-2810.913604	-0.077683	-48.74685933
	H	-2810.732456	-702.658544	-2810.634176	-0.09828	-61.6716828		-2810.990343	-702.727457	-2810.909828	-0.080515	-50.52396765
	G	-2810.789627	-702.684435	-2810.73774	-0.051887	-32.55961137		-2811.048237	-702.753379	-2811.013516	-0.034721	-21.78777471

Energies of optimized Pristine aluminum clusters with different spin Multiplicities (M062X/TZVP)

(Lowest energy conformer is highlighted in 'red')

Only few clusters are included as these are well known

Multiplicities	1	2	3	4	5	6	7	8	9
Al3		-727.155327		-727.147407		-727.06506		-726.929482	
Al6	-1454.451845		-1454.447703		-1454.421817		-1454.402776		-1454.326979
Al13		-3151.604796		-3151.553395		-3151.507915		-3151.466674	

All the ground state clusters follow rule of minimum spin multiplicities

Calculated Fukui functions of pristine aluminum clusters B3PW91/DGTZVP

Al3

Atom ID	f+
1	0.325452
2	0.339561
3	0.339513

two Sets of equivalent sites

Al6

Atom ID	f+
1	0.1668
2	0.1668
3	0.1668
4	0.1668
5	0.1668
6	0.1668

All sites are equivalent

Al7

Atom ID	f+
1	0.0799
2	0.1445
3	0.1456
4	0.0801
5	0.1445
6	0.0799
7	0.3263

three Sets of equivalent sites

Al13

Atom ID	f+
1	0.065712
2	0.101506
3	0.101677
4	0.065705
5	0.065674
6	0.101541
7	-0.003186
8	0.101744
9	0.10145
10	0.065709
11	0.06569
12	0.065728
13	0.101503

three Sets of equivalent site, Site No 7 is endohedral hence inaccessible

Al20

Atom ID	f+
1	0.053829
2	0.052541
3	0.050473
4	0.049924
5	0.051507
6	0.156296
7	-0.005097
8	0.032626
9	0.032999
10	0.031477
11	0.030127
12	0.030646
13	0.047991
14	0.048252
15	0.04808
16	0.048339
17	0.04705
18	0.046644
19	0.002107
20	0.144551

four Sets of equivalent site, Site No 7 and 19 are endohedral hence inaccessible

Energies,coordinates and normal modes of vibrations of optimized radical attached aluminum clusters (M062X/TZVP)

The data calculated for methyl radicals are included

Al3Me

Conf1(E=-767.049470)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.837937	-0.064145	-0.003467
2	13	0	4.143036	0.444770	-1.002331
3	13	0	4.051815	-0.895922	0.985890
4	6	0	-0.123777	0.080788	-0.013040
5	1	0	-0.489478	0.662145	0.835276
6	1	0	-0.595774	-0.903323	0.015748
7	1	0	-0.459076	0.579240	-0.926402

Frequencies --	45.8270	105.3050	117.6215	295.7523	296.6028	379.1774

Conf2(E=-767.049475)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.717580	-0.219696	0.486691
2	13	0	1.412010	1.116077	-0.014280
3	13	0	1.136396	-1.387328	-0.492219
4	6	0	2.451952	2.785667	-0.007119
5	1	0	2.027848	3.491196	0.712030
6	1	0	2.458472	3.267436	-0.986182
7	1	0	3.486473	2.600476	0.290330

Frequencies --	109.0569	121.1900	296.2085	296.5868	379.1469	619.2972

both conformers are equivalent in energy.

Al6Me

Conf1(E=-1494.327658)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.731200	1.091686	-1.652898

2	13	0	-1.972727	0.653842	0.567915
3	13	0	0.619806	1.233319	0.761265
4	13	0	1.446779	-0.158531	-1.486569
5	13	0	1.434350	-1.301694	0.828201
6	13	0	-0.861415	-1.472317	-0.177584
7	6	0	1.265315	2.535321	2.094967
8	1	0	0.815977	3.514621	1.927993
9	1	0	2.350043	2.633951	2.045240
10	1	0	0.998653	2.204823	3.100799

Frequencies -- 60.0078 72.6759 79.0644 84.1359 111.2422 165.9571

All sites are chemically equivalent

Al7Me

Conf1(E=-1736.817427)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.504120	-0.804589	-1.483911
2	13	0	-1.522863	0.765661	-1.306009
3	13	0	-1.430684	-1.561605	0.028076
4	13	0	0.524788	1.672960	-0.045972
5	13	0	-1.412058	0.759723	1.375265
6	13	0	0.622150	-0.810177	1.378023
7	13	0	2.563541	0.050251	-0.133196
8	6	0	4.523069	0.079119	-0.210795
9	1	0	4.930088	-0.933627	-0.180284
10	1	0	4.938387	0.634146	0.632982
11	1	0	4.870422	0.553932	-1.130217

Frequencies -- 67.0392 69.1949 74.5149 124.3688 127.4960 184.6663

Conf2(E=-1736.817441)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.166971	-0.010237	-0.000900
2	13	0	0.146687	-1.508342	-0.689341
3	13	0	0.153005	0.148366	1.646384
4	13	0	-1.855061	-0.140612	-1.543039
5	13	0	-1.860726	-1.260839	0.896396
6	13	0	-1.850717	1.409979	0.648003
7	13	0	0.156207	1.345553	-0.954252
8	6	0	4.128320	-0.014363	-0.002591
9	1	0	4.516887	-0.883221	0.532459
10	1	0	4.520771	0.882435	0.480518
11	1	0	4.517512	-0.045253	-1.022070

Frequencies -- 62.5342 69.4725 72.0831 124.2962 127.7203 185.3394

Conf3(E=-1736.810696)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.167899	-1.354151	-0.979402
2	13	0	-1.412244	0.480266	-1.580142
3	13	0	-2.007608	-1.183955	0.510580
4	13	0	0.452440	2.024098	-0.719274
5	13	0	-1.307985	1.407312	1.047511
6	13	0	0.272292	-0.436777	1.617900
7	13	0	2.059963	0.195873	-0.139967
8	6	0	-3.610752	-2.231472	0.941020
9	1	0	-3.675939	-2.430727	2.012279
10	1	0	-3.602641	-3.188802	0.416138
11	1	0	-4.515197	-1.695748	0.643652

Frequencies -- 50.1357 53.3481 75.4555 88.9494 102.7760 140.6329

Conf 1 and Conf 2 are energetically degenerate.

Al13Me

Conf1(E=-3191.485711)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.584092	-0.767635	-0.442833
2	13	0	-1.140625	1.643650	-1.788946
3	13	0	1.612271	0.227371	-2.150101
4	13	0	1.630889	-2.084935	-0.708639
5	13	0	-0.738571	-2.646788	0.255364
6	13	0	-0.758703	-0.957222	-2.367627
7	13	0	-0.008993	-0.077894	-0.012025
8	13	0	1.133359	-1.459712	1.990399
9	13	0	-1.453225	-0.757896	2.132405
10	13	0	-1.957657	1.576965	0.766689
11	13	0	1.108216	2.304021	-0.481286
12	13	0	2.603236	0.203899	0.481791
13	13	0	0.573563	1.182941	2.153505
14	6	0	0.662866	2.786263	3.308824
15	1	0	0.099988	2.602255	4.224299
16	1	0	1.702773	2.985321	3.569001
17	1	0	0.251557	3.666744	2.817249

Frequencies -- 46.6491 52.3500 76.4636 85.7581 105.7253 115.5511

Conf2(E=-3191.485709)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-1.050482	1.683079	1.673781
2	13	0	-1.051366	-1.705704	1.650940
3	13	0	1.406618	-2.324820	0.688122
4	13	0	2.703780	-0.006856	0.818828
5	13	0	1.408065	2.313545	0.719642
6	13	0	0.762769	-0.018675	2.683510
7	13	0	0.204379	-0.000592	0.020792
8	13	0	1.661280	1.320804	-1.805254
9	13	0	-0.809678	2.248701	-1.008480
10	13	0	-2.345341	0.002848	-0.322044
11	13	0	-0.811362	-2.234975	-1.038743
12	13	0	1.660334	-1.298134	-1.823026
13	13	0	-0.735400	0.016790	-2.497257
14	6	0	-4.223518	-0.001244	0.299232
15	1	0	-4.727389	0.892421	-0.069821
16	1	0	-4.731589	-0.880816	-0.096987
17	1	0	-4.293632	-0.017808	1.385924

Frequencies -- 46.6566 52.2998 76.4567 85.8660 105.7237 115.5642

Conf3(E=-3191.485710)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.240136	2.155002	0.813947
2	13	0	1.095232	-0.108167	2.466625
3	13	0	1.309511	-2.315541	0.828518
4	13	0	1.752465	-1.549395	-1.636435
5	13	0	1.853338	1.203411	-1.753441
6	13	0	2.846159	0.009974	0.436003
7	13	0	0.203508	-0.034397	-0.052537
8	13	0	-0.385920	-0.222631	-2.681246
9	13	0	-0.710932	2.116290	-1.348647
10	13	0	-1.283661	1.125072	1.841054
11	13	0	-1.170392	-1.579598	1.684399
12	13	0	-1.249176	-2.033153	-0.935060
13	13	0	-2.469310	0.311197	-0.425004
14	6	0	1.177197	4.046445	1.390123
15	1	0	1.826335	4.640980	0.746778
16	1	0	0.168639	4.454464	1.340907
17	1	0	1.534797	4.122020	2.417328

Frequencies -- 46.6757 52.3122 76.4692 85.8246 105.7152 115.5652 120.7991 133.9480

all conformers are equivalent in energy.

Al20Me

Conf1(E=-4888.585420)

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.399906	0.310763	2.527097
2	13	0	2.430175	-2.267880	1.116664
3	13	0	2.510402	-1.704839	-1.726184
4	13	0	2.537475	1.130238	-2.099514
5	13	0	2.479010	2.411951	0.484901
6	13	0	3.843903	-0.033932	0.115972
7	13	0	1.358323	-0.017734	0.048294
8	13	0	0.135377	1.702750	1.706819
9	13	0	0.103707	-1.199232	2.104074
10	13	0	0.188858	-2.384039	-0.501883
11	13	0	0.255088	-0.325523	-2.404380
12	13	0	0.234943	2.149907	-1.101537
13	13	0	-2.334594	2.590498	-0.277534
14	13	0	-2.554828	1.527046	2.056748
15	13	0	-2.597838	-1.023966	2.333715
16	13	0	-2.414564	-2.564759	0.283854
17	13	0	-2.247083	-1.555539	-2.115036
18	13	0	-2.211354	1.069496	-2.406827
19	13	0	-1.192259	-0.002620	0.000607
20	13	0	-3.638759	0.017422	-0.157540
21	6	0	5.808520	-0.049493	0.204523
22	1	0	6.147600	0.552980	1.047697
23	1	0	6.168075	-1.070818	0.332678
24	1	0	6.227775	0.360209	-0.714981

Frequencies --	3.0717	60.9265	75.2870	76.0228	77.8458	83.2287

Conf2(E=-4888.586182)[g]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.210053	0.301474	-2.513695
2	13	0	-2.287091	-2.238129	-1.055276
3	13	0	-2.365273	-1.622028	1.759835
4	13	0	-2.351118	1.203594	2.076100
5	13	0	-2.264458	2.431204	-0.517178
6	13	0	-3.628719	0.025759	-0.135824
7	13	0	-1.146013	0.004293	-0.033176
8	13	0	0.075148	1.681615	-1.725265
9	13	0	0.061736	-1.242622	-2.070166
10	13	0	-0.041314	-2.368963	0.567498
11	13	0	-0.077380	-0.271525	2.423592
12	13	0	-0.020118	2.175660	1.079139
13	13	0	2.541935	2.562985	0.241803
14	13	0	2.735361	1.444463	-2.070204
15	13	0	2.740831	-1.110254	-2.294250
16	13	0	2.544432	-2.604111	-0.211242
17	13	0	2.395465	-1.544379	2.171427
18	13	0	2.398753	1.089065	2.408604
19	13	0	1.399769	-0.018662	0.010601
20	13	0	3.847249	-0.034335	0.185479
21	6	0	5.810710	-0.034219	0.305340

22	1	0	6.143808	0.788777	0.938602
23	1	0	6.160164	-0.973751	0.734853
24	1	0	6.248362	0.084490	-0.686523

Frequencies -- -7.0332 65.0570 76.4439 77.5473 79.6920 87.6396

Conf3(E=-4888.583193)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.322119	0.082580	-2.651663
2	13	0	-2.377569	-2.231403	-1.013246
3	13	0	-2.556199	-1.402185	1.694870
4	13	0	-2.446825	1.424033	1.923662
5	13	0	-2.369055	2.527072	-0.687696
6	13	0	-3.718575	0.140455	-0.252625
7	13	0	-1.232561	0.104863	-0.149868
8	13	0	-0.074604	1.653934	-2.050724
9	13	0	0.026014	-1.319511	-2.087500
10	13	0	-0.171710	-2.273343	0.587884
11	13	0	-0.213548	-0.078665	2.350858
12	13	0	-0.043572	2.332380	0.846189
13	13	0	2.632748	2.599769	0.392667
14	13	0	2.637072	1.663776	-2.001431
15	13	0	2.699371	-0.875524	-2.395936
16	13	0	2.345346	-2.495526	-0.442459
17	13	0	2.166603	-1.619017	2.082716
18	13	0	2.278979	1.035964	2.391069
19	13	0	1.266144	0.112704	-0.101330
20	13	0	3.715653	-0.135952	0.267378
21	6	0	2.539254	-2.841988	3.590192
22	1	0	2.181699	-2.417124	4.529366
23	1	0	2.047723	-3.803678	3.433848
24	1	0	3.613445	-3.016004	3.678070

Frequencies -- 45.0584 62.7520 76.0488 81.6174 89.0080 93.0412

Conf4(E=-4888.571768)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.161222	0.471458	-2.509605
2	13	0	-2.330894	-2.187770	-1.347278
3	13	0	-2.516980	-1.799744	1.421656
4	13	0	-2.465328	1.011891	2.002314
5	13	0	-2.245569	2.457858	-0.387908
6	13	0	-3.638887	0.052063	-0.345404
7	13	0	-1.146002	-0.050234	-0.072034
8	13	0	0.094955	1.832518	-1.613231
9	13	0	0.039169	-1.211261	-2.241706
10	13	0	-0.090576	-2.480483	0.334179
11	13	0	-0.142068	-0.593293	2.470183
12	13	0	-0.008727	1.981768	1.255725
13	13	0	2.561705	2.440870	0.313649
14	13	0	2.741226	1.593463	-2.123018

15	13	0	2.695843	-0.882955	-2.634115
16	13	0	2.468896	-2.619236	-0.731171
17	13	0	2.410368	-1.851341	1.762522
18	13	0	2.458211	0.750927	2.299880
19	13	0	1.356970	-0.083441	-0.133418
20	13	0	3.819151	-0.143764	-0.060212
21	6	0	-0.271116	-0.996284	4.408836
22	1	0	-1.298427	-1.040906	4.770085
23	1	0	0.215125	-1.956201	4.600994
24	1	0	0.268763	-0.226120	4.965677

Frequencies -- 6.0787 44.0879 73.9607 81.0705 82.0192 107.0178

Conf5(E=-4888.582642)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.341214	0.529284	-2.295773
2	13	0	-2.386193	-2.112722	-0.887180
3	13	0	-2.251537	-1.571832	1.893981
4	13	0	-2.189867	1.250063	2.239084
5	13	0	-2.179429	2.533581	-0.295441
6	13	0	-3.587676	0.151216	0.137614
7	13	0	-1.099680	0.064886	0.055850
8	13	0	0.064277	1.776191	-1.667887
9	13	0	-0.100087	-1.121918	-2.138524
10	13	0	-0.006976	-2.350322	0.534142
11	13	0	0.100515	-0.257676	2.465615
12	13	0	0.145103	2.213126	1.145609
13	13	0	2.652407	2.559640	0.004520
14	13	0	2.715840	1.296558	-2.249675
15	13	0	2.507550	-1.275552	-2.329256
16	13	0	2.649479	-2.640077	-0.142510
17	13	0	2.580723	-1.463647	2.157252
18	13	0	2.650455	1.157540	2.221479
19	13	0	1.415852	-0.020158	-0.020154
20	13	0	3.920831	-0.067089	-0.025832
21	6	0	-3.035639	2.101065	3.805606
22	1	0	-3.775233	2.834247	3.480145
23	1	0	-3.535141	1.350450	4.419756
24	1	0	-2.289790	2.609958	4.417479

Frequencies -- 17.8159 57.1034 65.1100 79.9438 82.2196 85.9580

conf 2 is the global minima, however, conf 1 lies very close ~0.47 kcal/mol in energy which is well within DFT error range.

Energies of optimized ground state radical attached aluminum clusters with different spin Multiplicities (M062X/TZVP)

(Lowest energy conformer is highlighted in 'red')

The data calculated for methyl radicals are included

Multiplicities	1	2	3	4	5	6	7	8	9
Al3Me	-767.049472		-767.043032		-766.996556		-766.887700		No Binding
Al6Me		-1494.327658		-1494.310428		-1494.292907		-1494.248367	
Al13Me	-3191.485711		-3191.467981		-3191.420296		-3191.368259		-3191.323180

Energies,Coordinates and normal modes of vibrartions of optimized ground state radical attached aluminum clusters Anions. (M062X/TZVP)

$Al_4Cp_4^-$ (E=-1743.444411)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.066997	1.423750	0.369503
2	13	0	0.642853	-1.292787	0.916337
3	13	0	1.670027	-0.197226	-1.320038
4	13	0	-0.937270	-0.836294	-1.150593
5	6	0	-0.874179	3.410494	2.329650
6	1	0	-0.212414	4.129940	2.788648
7	6	0	-1.720646	3.648433	1.243451
8	1	0	-1.828348	4.583878	0.714761
9	6	0	-2.339754	2.431354	0.887560
10	1	0	-3.066738	2.290137	0.101238
11	6	0	-0.955154	2.042301	2.664746
12	1	0	-0.437315	1.551317	3.475648
13	6	0	-1.898877	1.435113	1.796380
14	1	0	-2.240657	0.411179	1.838254
15	6	0	3.716848	1.069141	-1.488668
16	1	0	4.024229	1.608676	-0.606245
17	6	0	2.839802	1.552089	-2.486225
18	1	0	2.361756	2.519504	-2.490460
19	6	0	2.651422	0.522918	-3.434512
20	1	0	2.004837	0.567663	-4.297117
21	6	0	4.068411	-0.256950	-1.821883
22	1	0	4.693813	-0.912252	-1.235663

23	6	0	3.407911	-0.595667	-3.022364
24	6	0	-3.365222	-0.460668	-1.116817
25	1	0	-3.802339	-0.044285	-0.221743
26	6	0	-2.865532	0.274607	-2.213398
27	1	0	-2.839905	1.350556	-2.293989
28	6	0	-2.336285	-0.640059	-3.147997
29	1	0	-1.846903	-0.386840	-4.075818
30	6	0	-3.147102	-1.831230	-1.374182
31	1	0	-3.391054	-2.647850	-0.712445
32	6	0	-2.508488	-1.943727	-2.630144
33	6	0	2.125432	-2.002311	2.727233
34	1	0	3.188492	-1.952058	2.549466
35	6	0	1.324495	-0.971809	3.263340
36	1	0	1.664966	0.010369	3.553678
37	6	0	-0.012948	-1.423420	3.283123
38	1	0	-0.869553	-0.851215	3.606748
39	6	0	1.283362	-3.093144	2.414293
40	1	0	1.589614	-4.023307	1.961810
41	6	0	-0.039069	-2.734088	2.760119
42	1	0	-2.182323	-2.860631	-3.095462
43	1	0	-0.918736	-3.341844	2.614836
44	1	0	3.443002	-1.554469	-3.515985

Frequencies -- 14.8167 23.9931 28.0096 37.0418 51.9622 55.7571

$Al4(C_2H)_4^-$ (E= -1276.677254)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.835812	-1.083952	0.805098
2	13	0	-1.093744	-0.837173	-0.772109
3	13	0	1.089558	0.822546	-0.799843
4	13	0	-0.823027	1.099958	0.792901
5	6	0	2.437804	-3.163732	2.583916
6	1	0	2.973292	-3.858731	3.186858
7	6	0	1.828764	-2.372806	1.895448
8	6	0	-3.201677	-2.444573	-2.512506
9	1	0	-3.906216	-2.981817	-3.102640
10	6	0	-2.399859	-1.833439	-1.838607
11	6	0	-2.406258	3.211894	2.550564
12	1	0	-2.935276	3.917493	3.146793
13	6	0	-1.804531	2.408690	1.869821

14	6	0	3.179421	2.394518	-2.593601
15	1	0	3.877882	2.919649	-3.201608
16	6	0	2.384573	1.797193	-1.899391

Frequencies -- 30.2441 43.1978 49.8626 49.9521 51.5688 91.7241

$Al_4Ph_4^-$ (E=-1895.863780)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.031569	-0.772833	-0.895770
2	13	0	-0.005226	-0.488404	1.555631
3	13	0	-1.508399	-0.336167	-0.362421
4	13	0	0.450348	1.474662	-0.136320
5	6	0	3.456979	-1.560052	-2.443606
6	6	0	2.194398	-1.972438	-1.997461
7	6	0	1.785375	-3.259046	-2.371505
8	6	0	2.584629	-4.089020	-3.151157
9	6	0	3.832882	-3.650577	-3.576117
10	6	0	4.269899	-2.381125	-3.217847
11	1	0	3.814358	-0.567810	-2.182304
12	1	0	0.815651	-3.625703	-2.046660
13	1	0	2.235544	-5.077923	-3.426885
14	1	0	4.460254	-4.293310	-4.183102
15	1	0	5.242297	-2.030622	-3.545797
16	6	0	-4.434454	-0.966515	-0.475038
17	6	0	-3.303149	-0.589655	-1.210603
18	6	0	-3.484173	-0.393191	-2.585874
19	6	0	-4.721385	-0.562403	-3.198563
20	6	0	-5.824634	-0.935459	-2.440517
21	6	0	-5.678480	-1.137852	-1.073519
22	1	0	-4.341173	-1.132111	0.594813
23	1	0	-2.635750	-0.099894	-3.197950
24	1	0	-4.826508	-0.402494	-4.265957
25	1	0	-6.791938	-1.067876	-2.911596
26	1	0	-6.534698	-1.428917	-0.474832
27	6	0	0.183187	4.315025	0.749115
28	6	0	0.784780	3.447027	-0.171360
29	6	0	1.634463	4.028803	-1.121503
30	6	0	1.872765	5.398546	-1.156660
31	6	0	1.262454	6.232430	-0.227778
32	6	0	0.415407	5.686325	0.729071
33	1	0	-0.487062	3.911469	1.502917
34	1	0	2.125640	3.393580	-1.853541

35	1	0	2.536269	5.816047	-1.906006
36	1	0	1.445863	7.300483	-0.248718
37	1	0	-0.064735	6.330182	1.457687
38	6	0	1.523788	-0.620444	4.110588
39	6	0	0.321301	-0.954112	3.473830
40	6	0	-0.638310	-1.616015	4.250534
41	6	0	-0.416756	-1.928131	5.587745
42	6	0	0.786115	-1.581141	6.190868
43	6	0	1.759121	-0.924539	5.447254
44	1	0	2.299657	-0.106463	3.549898
45	1	0	-1.586957	-1.893611	3.799027
46	1	0	-1.181844	-2.441299	6.159916
47	1	0	0.964468	-1.820330	7.232972
48	1	0	2.700744	-0.650046	5.909844

Frequencies -- 7.6072 14.1414 16.4572 22.4776 23.7874 27.4370

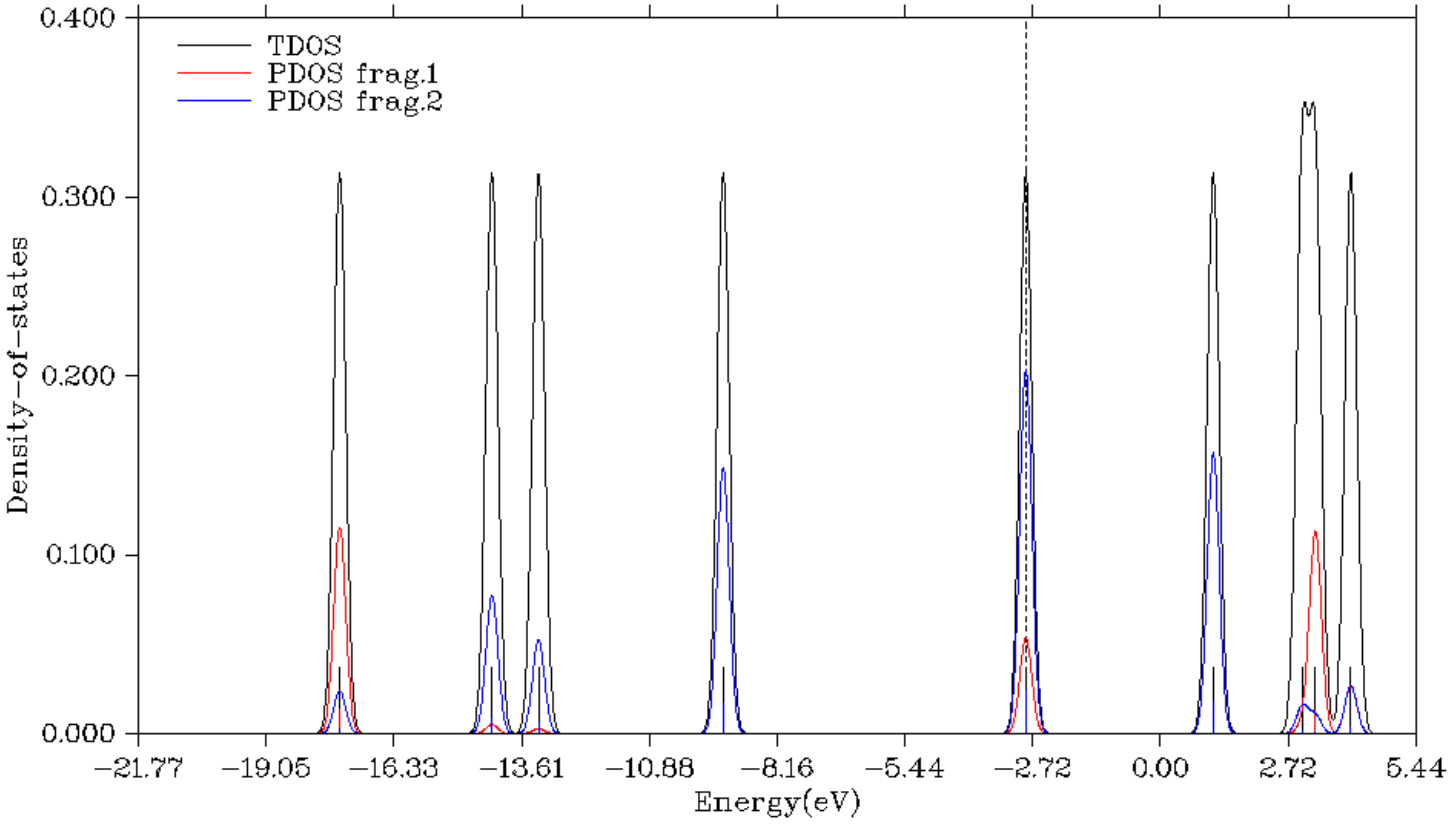
$Al_4Cl_4^-$ (E=-2810.818030)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.247049	-0.903255	0.391414
2	13	0	-0.851055	0.497322	1.246939
3	13	0	-0.786662	-0.983266	-0.970039
4	13	0	0.388130	1.388264	-0.667892
5	17	0	1.129124	3.036138	-1.885616
6	17	0	-2.052898	0.745184	3.047274
7	17	0	-2.151025	-1.992432	-2.336482
8	17	0	3.077710	-1.788210	1.174325

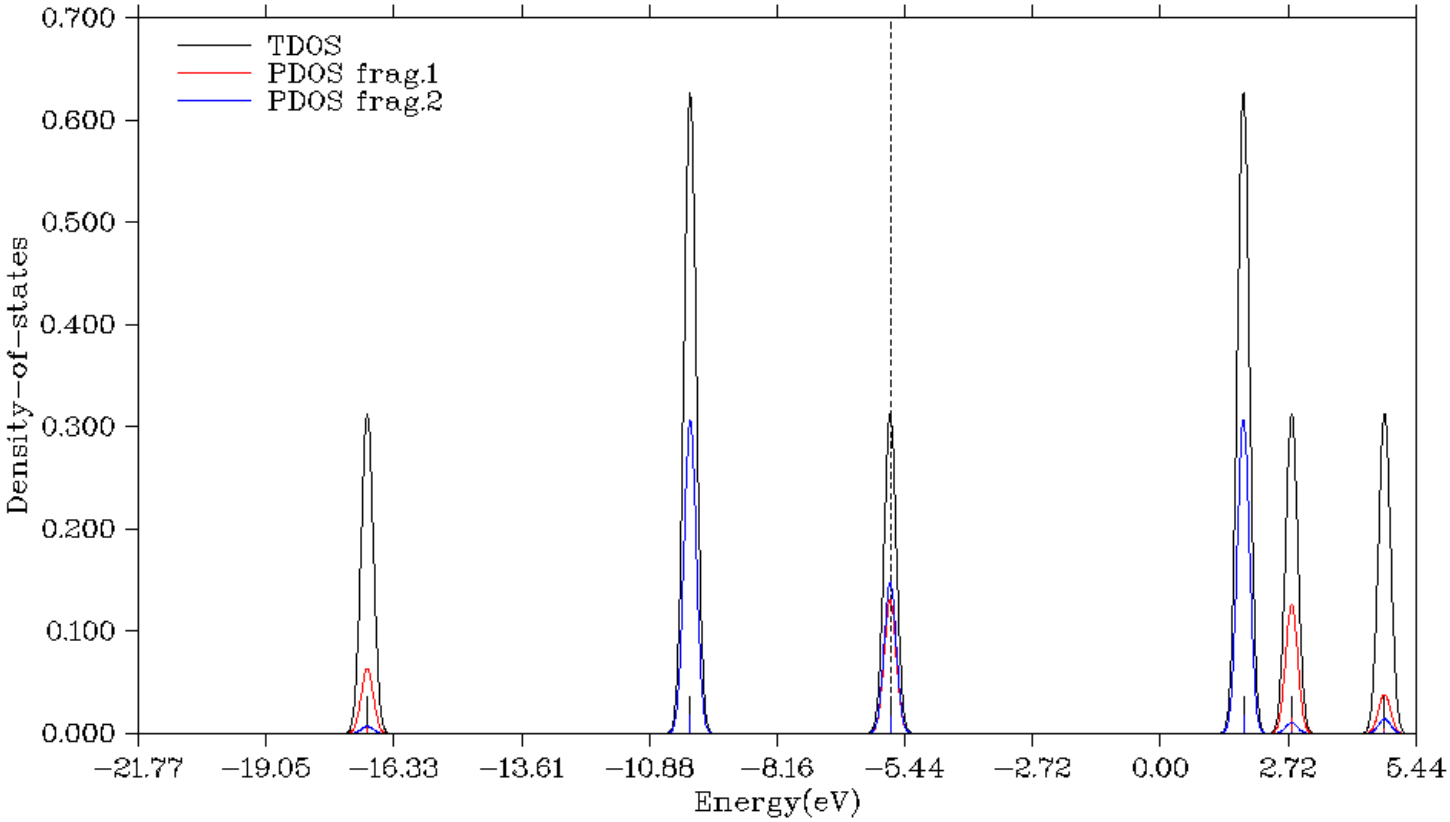
Frequencies -- 30.6101 47.5035 49.4810 51.8670 75.2695 103.9739

DOS Plots

C2H3 radical



C2H radical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PDOS frag.2
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0.000
-21.77
-19.05
-16.33
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-8.16
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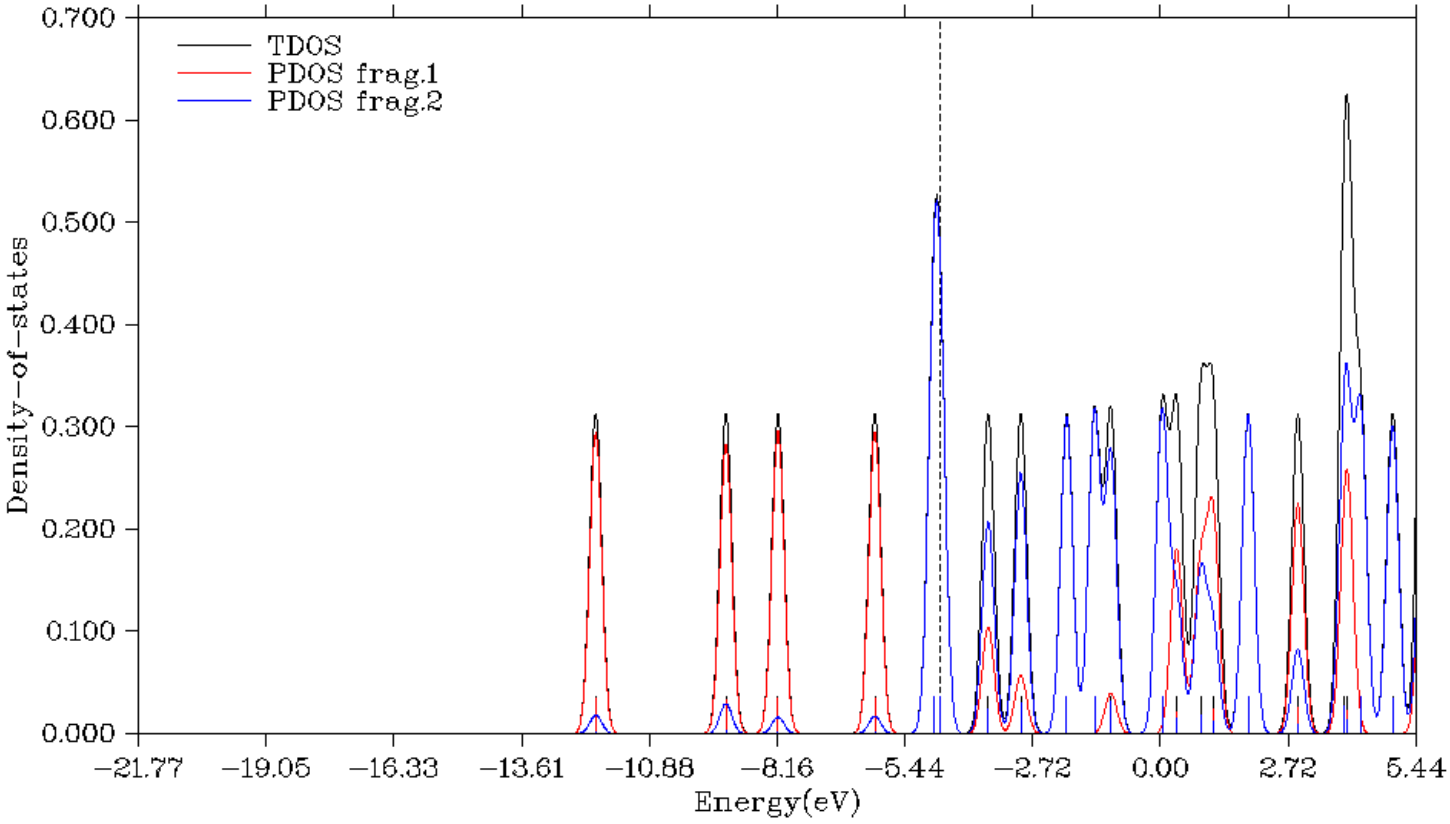
2.72
5.44
Energy(eV)

Al4 Planar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PDOS frag.1
PDOS frag.2
Density-of-states
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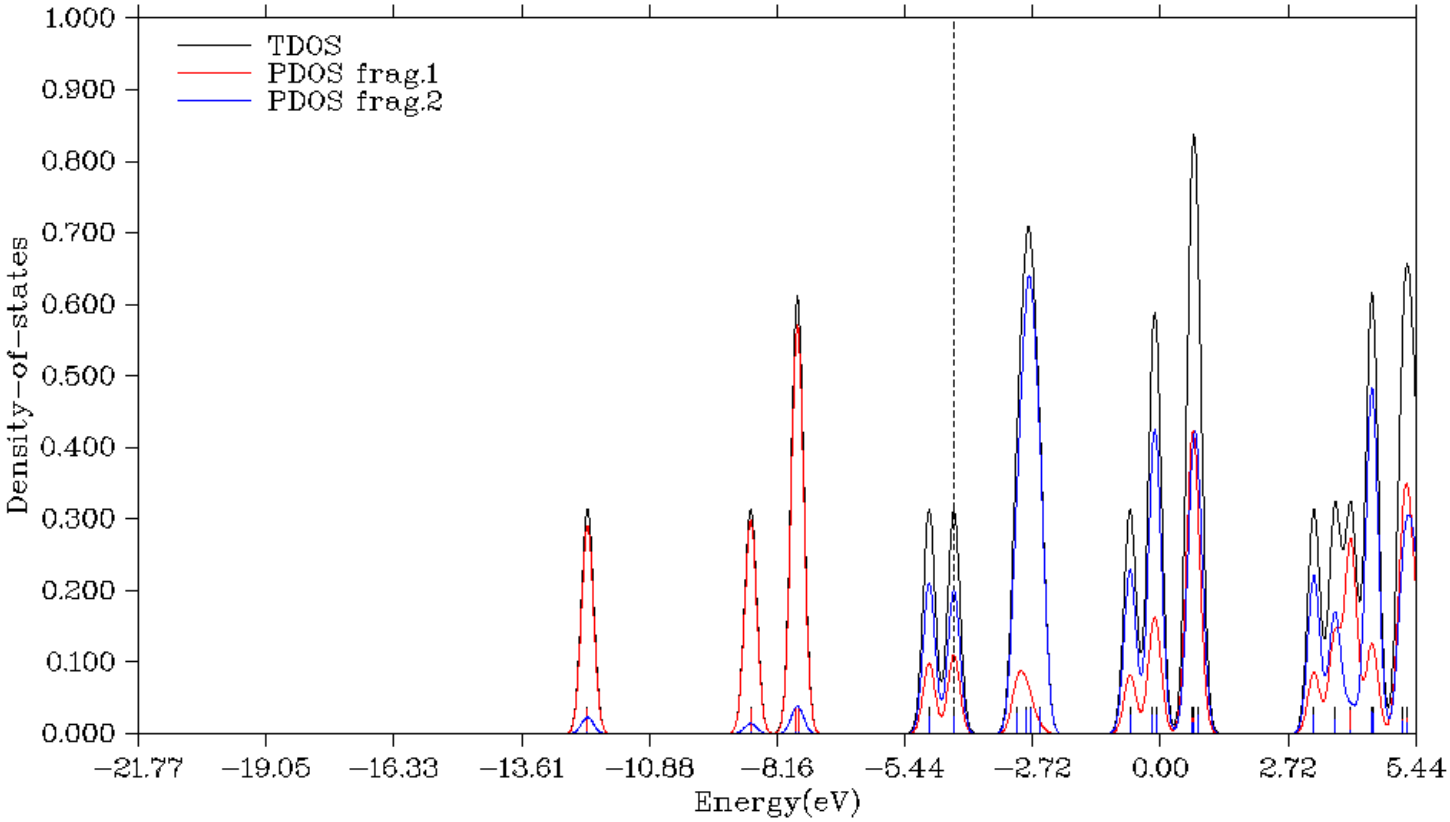
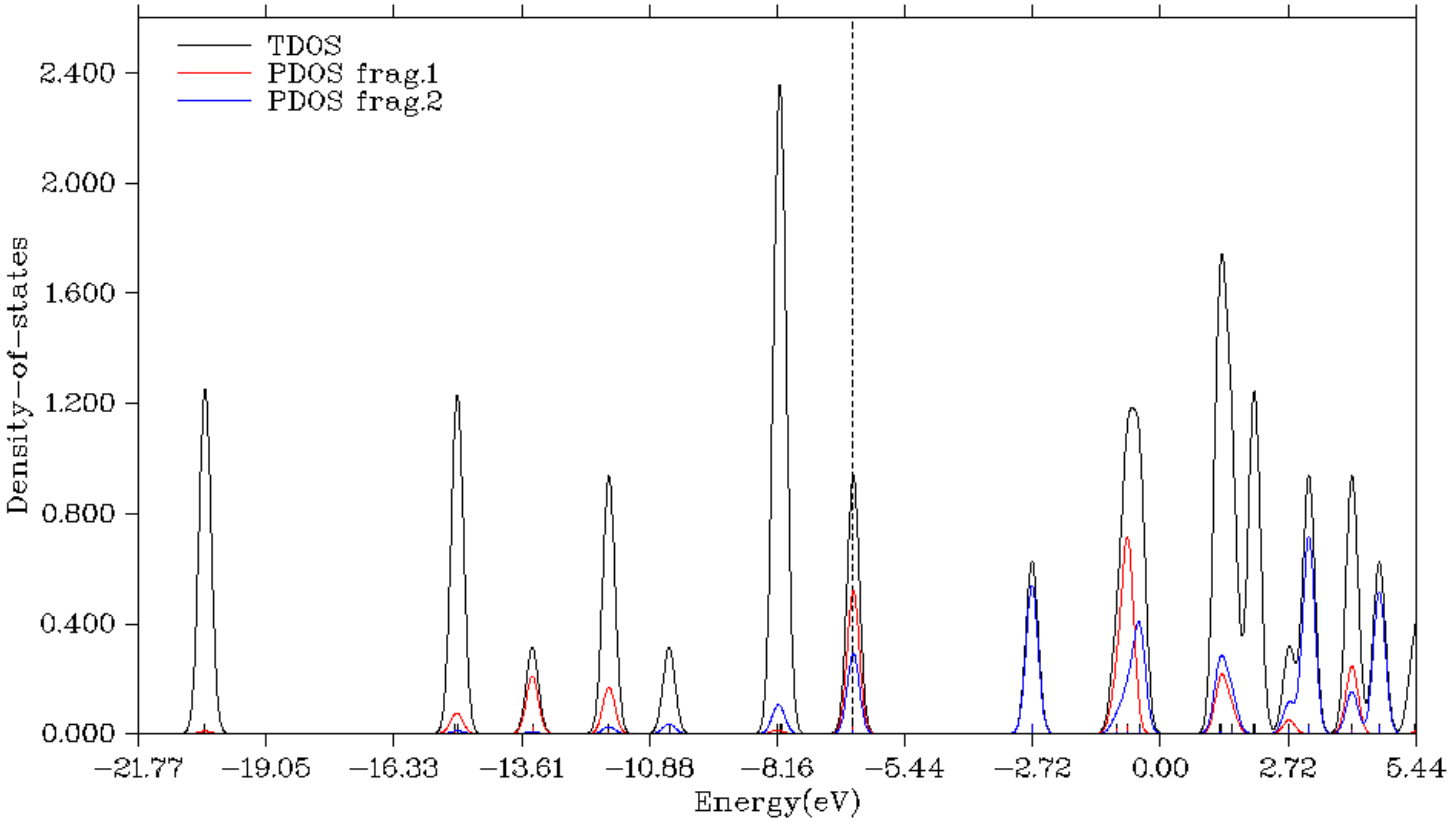
0.000
-21.77
-19.05
-16.33
-13.61
-10.88
-8.16
-5.44
-2.72
0.00
2.72
5.44
Energy(eV)

Al4 Tetrahedral



Al4(C2H4)


TDOS
PDOS frag.1
PDOS frag.2
Density-of-states
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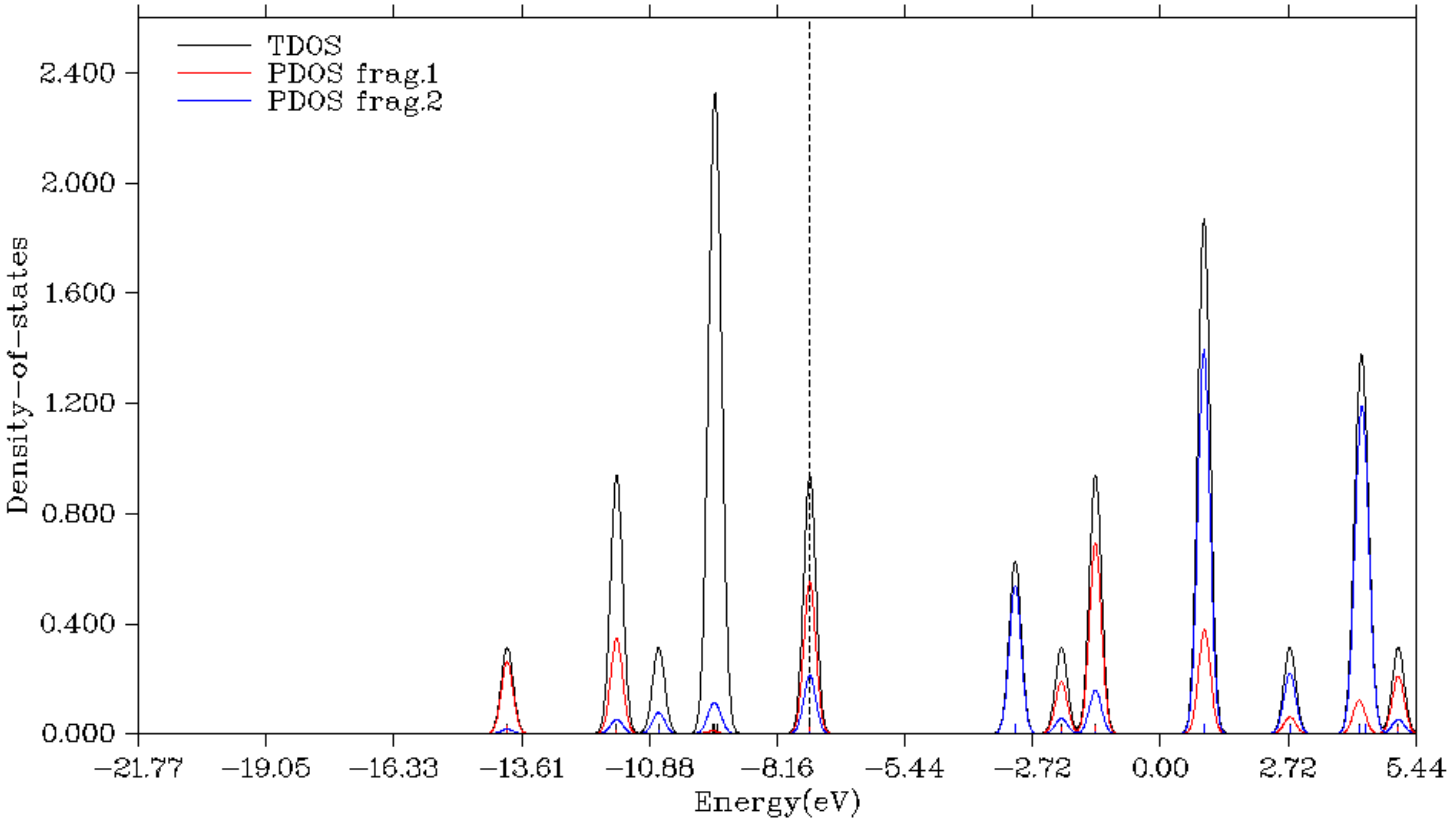
1.600
1.200
0.800
0.400
0.000
−21.77
−19.05
−16.33
−13.61
−10.88
−8.16
−5.44
−2.72
0.00
2.72
5.44
Energy(eV)

Al4Cl4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PDOS frag.1
PDOS frag.2
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2.000
1.600
1.200
0.800
0.400
0.000
Density-of-states
−21.77
−19.05
−16.33
−13.61
−10.88
−8.16
−5.44
−2.72
0.00
2.72
5.44
Energy(eV)