

SUPPLEMENTARY MATERIAL

**A class of computationally designed tri-coordinate cyclic
silylenes: $\text{RSi}(\mu\text{-R})_2\text{AlR}_2$**

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Supporting Information Available (S1, S2 and S3).

S1. Optimized geometries (in angstrom) and total energies (in a.u.) for the ground state structure **1**. (2-9)

S2. Optimized geometries (in angstrom) and total energies (in a.u.) for the remaining structures. (9-31)

S3. Optimized geometries (in angstrom) and total energies (in a.u.) for the inserted intermediate of the ground state structure **1** toward HX. (31-65)

S1. Optimized geometries (in angstrom) and energies (in a.u.) for the ground state structure 1.

RSi(μ -R)₂AlR₂ R=OEt

Total Energy=-1304.668771

Al -0.718936 -0.053062 -0.171247

Si 1.533487 -1.187071 1.311139

O 2.841692 -0.308004 0.752966

O 0.222828 0.217533 1.381691

O 0.534535 -1.398925 -0.307630

O -2.255609 -0.818696 -0.087106

O -0.518234 1.361520 -1.131098

C -1.155652 1.940093 -2.247577

C -1.264135 3.450547 -2.087300

H -2.158273 1.512289 -2.395335

H -0.577140 1.708986 -3.153183

H -1.730991 3.902846 -2.968645

H -1.867546 3.707344 -1.211837

H -0.273611 3.894952 -1.958505

C -3.611752 -0.475538 -0.257769

C -4.499316 -1.345830 0.621523

H -3.894978 -0.609003 -1.311612

H -3.782000 0.584730 -0.018133

H -5.555778 -1.097020 0.475205

H -4.359113 -2.402930 0.380880

H -4.255853 -1.205647 1.678150

C 0.429408 -2.658886 -1.006639

C 1.121910 -2.596583 -2.356210

H -0.632565 -2.893438 -1.108154

H 0.879950 -3.425092 -0.368802

H 1.030856 -3.560155 -2.867116

H 0.674280 -1.832474 -2.997270

H 2.184986 -2.370618 -2.244481

C 0.279577 1.335947 2.286816

C -0.934061 1.372683 3.198769

H 0.358193 2.248251 1.689377

H 1.200363 1.239189 2.869093

H -0.858323 2.218863 3.888582

H -1.858719 1.489232 2.626982

H -1.009699 0.455793 3.787458

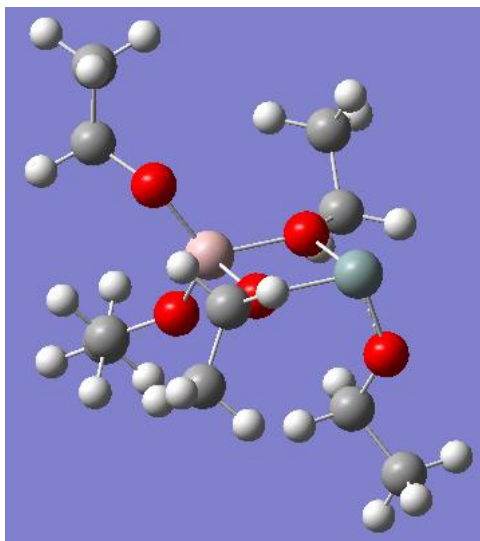
C 3.006372 0.716173 -0.231553

C 4.480930 1.049011 -0.374925

H 2.436798 1.602805 0.067003

H 2.590499 0.374988 -1.185270

H 4.623973 1.835989 -1.122400

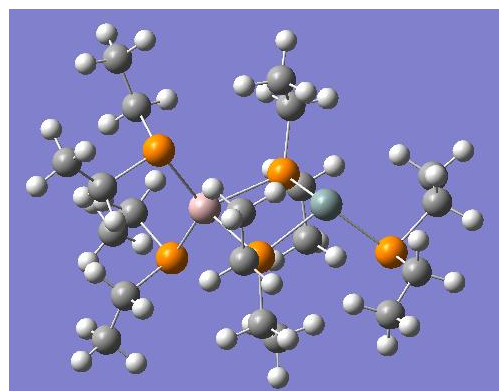


H 4.895389 1.398225 0.574135
H 5.049552 0.170111 -0.688999

RSi(μ -R)2AIR2 R=PEt

Total Energy=-3031.36141276

Al	1.14766300	0.00580500	0.00407700
Si	-2.24970300	-0.93451600	0.34900500
P	2.48798900	-1.84628100	0.72165800
P	2.00997600	2.09350000	-0.79885000
P	-0.70954100	-0.74293200	-1.44198600
P	-4.12522000	0.40452400	-0.15088700
P	-0.72946000	0.41729500	1.56216500
C	3.47242200	-2.25859100	-0.84438300
C	4.14473300	-3.63714000	-0.80439500
H	4.21659100	-1.47974900	-1.03973100
H	2.77503600	-2.23107600	-1.68869100
H	4.65405900	-3.85297300	-1.75035700
H	4.88990300	-3.70371000	-0.00823000
H	3.41257200	-4.42971100	-0.62889200
C	3.77409800	-0.96165000	1.78980800
C	4.72013000	-1.90028400	2.54886600
H	3.21537000	-0.35820900	2.51416800
H	4.35242600	-0.25556300	1.18523800
H	5.37827300	-1.33503700	3.21805200
H	4.16407000	-2.62081500	3.15464500
H	5.36022300	-2.46874600	1.86975700
C	-0.57231500	-2.42119000	-2.26235100
C	-0.36358700	-3.61803300	-1.33378700
H	0.24666000	-2.34917300	-2.98634300
H	-1.48754600	-2.55983400	-2.84873100
H	-0.29570800	-4.53849400	-1.92170200
H	0.55097600	-3.53034400	-0.74374800
H	-1.19208700	-3.72734000	-0.63180700
C	-1.00162300	0.30401400	-2.97204300
C	-1.38619700	1.76538400	-2.74618100
H	-1.77680800	-0.20503900	-3.55196200
H	-0.08186300	0.23799600	-3.56433900
H	-1.54955000	2.25638200	-3.71068400
H	-2.30837900	1.85351800	-2.16899700
H	-0.60017000	2.31544100	-2.22714100
C	-5.07504800	-0.82439500	-1.22819900
C	-4.66051800	-0.85584700	-2.69943400
H	-6.12221000	-0.50927300	-1.15593200
H	-5.02343700	-1.83016300	-0.79605100



H -5.33403500 -1.49372400 -3.28028000
H -4.68256800 0.14222300 -3.14594100
H -3.65133600 -1.25503000 -2.82671900
C -5.11722400 0.07212300 1.42293600
C -4.69827300 0.89650900 2.64058400
H -5.10059000 -0.99668500 1.66416300
H -6.15283700 0.31706000 1.16094200
H -5.39142800 0.74170500 3.47325900
H -3.70362700 0.61462100 2.99585400
H -4.68414500 1.96713300 2.41713400
C -1.10023000 2.20871700 1.97413400
C -1.38986200 3.14260800 0.79996400
H -0.24461000 2.57304500 2.55375400
H -1.95136000 2.19422000 2.66089700
H -1.58604700 4.15302800 1.17204100
H -0.54819500 3.20513200 0.10801800
H -2.26905600 2.81979200 0.23999200
C -0.59121300 -0.25751000 3.30387700
C -0.36474800 -1.76413900 3.43603600
H -1.50927300 0.03050200 3.82815300
H 0.22177700 0.29555600 3.78677000
H -0.29847100 -2.03835500 4.49342800
H -1.18539900 -2.33193000 2.99350500
H 0.55604200 -2.08781400 2.94663200
C 2.95685900 2.73151800 0.71245700
C 3.35608300 4.20975100 0.61959400
H 3.84057600 2.11149000 0.89372500
H 2.30606900 2.59535300 1.58327000
H 3.84189300 4.54314700 1.54347400
H 4.05441800 4.39275900 -0.20053500
H 2.48321500 4.84581600 0.45055000
C 3.40120200 1.50367900 -1.93754300
C 4.01306100 2.60969900 -2.80542200
H 2.97180900 0.73458800 -2.58925500
H 4.18304100 1.00665300 -1.35366200
H 4.75756900 2.19968600 -3.49684200
H 3.24752000 3.11759400 -3.39793000
H 4.51419100 3.36918000 -2.20062500

RSi(μ -R)₂AlR₂ R=SEt

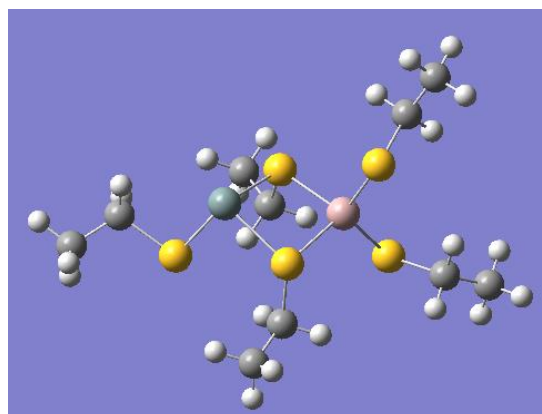
Total Energy=-2919.463215

Al 1.216066 -0.043095 -0.179520

Si -1.812827 -0.834660 -1.071688

S 2.128547 1.255350 1.380413

S -3.399590 0.280883 -0.021772
S -0.296582 -1.503242 0.839323
S -0.415615 1.047559 -1.527397
S 2.452314 -1.111577 -1.680524
C -4.693767 -1.051386 0.071408
C -6.087822 -0.465607 -0.119104
H -4.604003 -1.535065 1.045305
H -4.481062 -1.800696 -0.694917
H -6.841048 -1.255120 -0.029326
H -6.309236 0.294408 0.634218
H -6.192861 -0.004759 -1.103599
C -0.814996 -0.668435 2.420344
C -1.395126 -1.684714 3.395308
H -1.550938 0.096413 2.169128
H 0.067762 -0.181088 2.833995
H -1.690690 -1.180682 4.321095
H -2.280541 -2.175126 2.983639
H -0.668147 -2.459097 3.649581
C -0.883218 2.568756 -0.550458
C -1.765371 3.494632 -1.375255
H 0.060703 3.040266 -0.277511
H -1.374524 2.257313 0.370099
H -1.992836 4.393917 -0.793657
H -1.267945 3.805956 -2.296601
H -2.711365 3.018708 -1.638919
C 3.566267 2.031361 0.482290
C 4.633710 2.471451 1.476698
H 3.192965 2.886985 -0.083377
H 3.969112 1.311237 -0.230801
H 5.467083 2.945492 0.947442
H 4.238116 3.193455 2.195525
H 5.027563 1.621023 2.037952
C 3.369963 -2.335584 -0.616514
C 4.329997 -3.153351 -1.472589
H 2.643855 -2.986525 -0.126779
H 3.914106 -1.794359 0.159481
H 4.865603 -3.878293 -0.850743
H 3.796741 -3.704884 -2.250636
H 5.070091 -2.514765 -1.960994



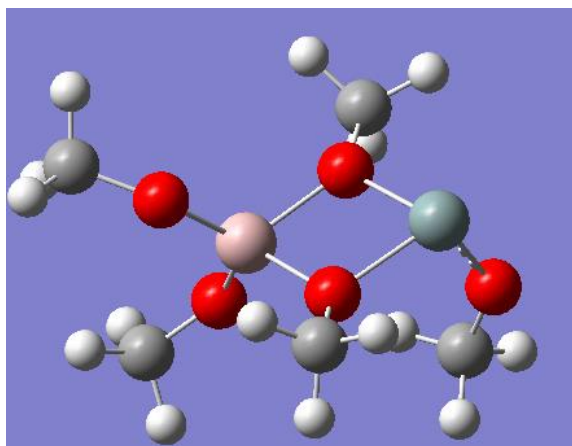
RSi(μ -R)₂AlR₂ R=OMe

Total Energy=-1108.033227

Al -1.195179 0.136007 0.045794

Si 1.609416 -0.713249 0.160431

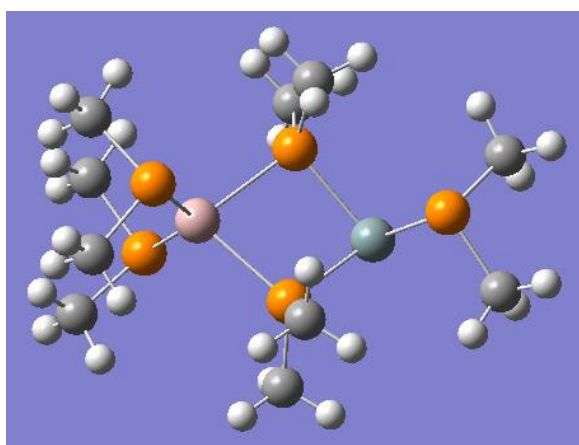
O 2.426370 0.649709 -0.347541
 O 0.227559 0.115394 1.207320
 O 0.090140 -0.658342 -1.008925
 O -2.449536 -1.012695 0.255074
 O -1.567139 1.786529 -0.255636
 C -2.614984 2.532303 -0.818778
 H -3.504141 1.923041 -1.029049
 H -2.912699 3.336735 -0.136528
 H -2.293912 2.993176 -1.760834
 C -3.771379 -1.076207 0.721008
 H -4.389474 -1.644066 0.016422
 H -3.813167 -1.587144 1.690528
 H -4.225996 -0.083903 0.843066
 C -0.078765 -1.544241 -2.123275
 H 0.772689 -2.226183 -2.172441
 H -0.994999 -2.122621 -1.997442
 H -0.126719 -0.963352 -3.046338
 C 0.461222 0.801474 2.439717
 H -0.354515 0.590422 3.133255
 H 1.396459 0.444809 2.876114
 H 0.527986 1.877197 2.266742
 C 2.034011 1.910326 -0.880706
 H 1.985330 1.853615 -1.972060
 H 1.059641 2.232242 -0.504239
 H 2.789882 2.648271 -0.603582



RSi(μ -R)₂AIR₂ R=PMe₂

Total Energy=-2638.171766

Al -1.398145 0.141709 0.005186
 Si 1.926200 -1.122890 0.011695
 P -2.716748 -1.845494 0.026549
 P -1.986873 2.454087 -0.005944
 P 0.443372 -0.171244 1.598689
 P 3.624924 0.499438 -0.012243
 P 0.435746 -0.207853 -1.589503
 C -3.970707 -1.513757 1.387489
 H -3.463683 -1.452786 2.353782
 H -4.550056 -0.597965 1.244533
 H -4.669829 -2.352846 1.442006
 C 0.207571 -1.383627 2.974527
 H -0.142957 -2.330228 2.561306
 H 1.150871 -1.563953 3.495952
 H -0.528599 -1.019523 3.695259
 C 0.982514 1.373530 2.467146

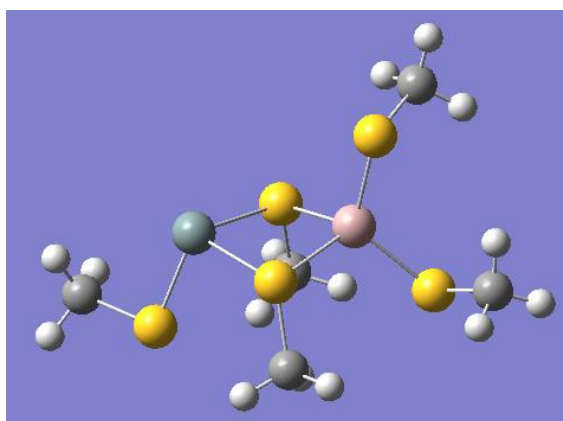


H 1.150825 2.165103 1.736973
H 0.213653 1.703700 3.169959
H 1.910610 1.208683 3.018577
C 4.640338 -0.181634 1.411418
H 5.616741 0.311097 1.419769
H 4.154907 0.046441 2.363597
H 4.796937 -1.262760 1.353280
C 4.630580 -0.214702 -1.426677
H 4.789135 -1.293908 -1.343391
H 4.137675 -0.010603 -2.380471
H 5.606157 0.278952 -1.454389
C 0.965091 1.317300 -2.497838
H 0.197213 1.619527 -3.214235
H 1.119798 2.131038 -1.789435
H 1.898187 1.146707 -3.038964
C 0.197768 -1.452508 -2.936199
H 1.138221 -1.636395 -3.461520
H -0.140421 -2.393252 -2.499932
H -0.547071 -1.110313 -3.658713
C -3.267025 2.552174 -1.378538
H -2.796588 2.336617 -2.341239
H -4.110247 1.869149 -1.248153
H -3.659517 3.571422 -1.431925
C -3.113682 2.597613 1.492329
H -2.539590 2.423239 2.406035
H -3.507175 3.616323 1.548596
H -3.959755 1.905991 1.480260
C -3.821539 -1.632097 -1.480022
H -3.218505 -1.672051 -2.390617
H -4.528793 -2.464935 -1.524848
H -4.392749 -0.700369 -1.485772

RSi(μ -R)₂AlR₂ R=SMe

Total Energy=-2722.845073

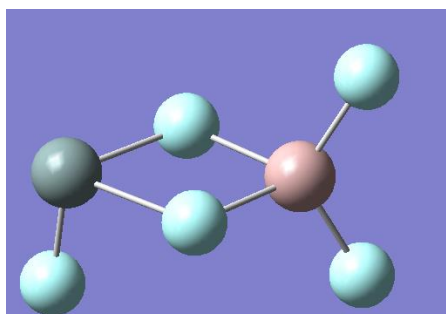
Al 1.220527 0.128906 -0.006258
Si -1.807095 -1.083213 0.084576
S 2.080087 2.173268 -0.166001
S -3.360941 0.439072 -0.279882
S -0.314038 0.108326 1.757574
S -0.377973 -0.393590 -1.696378
S 2.498765 -1.680684 0.031549
C 3.446420 1.924381 -1.389519
H 4.160833 2.732222 -1.236613
H 3.948635 0.969772 -1.238898



H 3.067058 1.978176 -2.409512
C 3.405493 -1.444154 1.628160
H 2.718008 -1.395053 2.472101
H 4.051604 -2.312189 1.753520
H 4.022351 -0.546301 1.606184
C -4.656970 -0.197114 0.869903
H -4.432215 0.072930 1.901157
H -5.595220 0.272320 0.576929
H -4.763245 -1.278707 0.787171
C -0.854328 1.861255 1.974814
H -1.184979 1.969150 3.006404
H -0.023487 2.538326 1.787701
H -1.682392 2.082164 1.300978
C -0.861448 1.257378 -2.368058
H -0.107374 1.537094 -3.101881
H -1.828924 1.153686 -2.854445
H -0.909428 2.014980 -1.590269

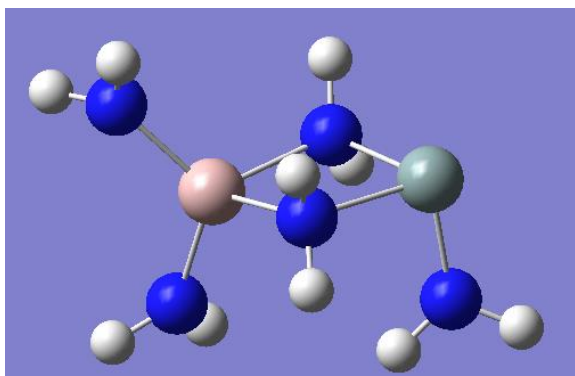
RSi(μ -R)2AIR2 R=F

Total Energy=-1031.701616
Al -0.025305 1.802410 0.474837
Si 0.050682 -0.957357 -0.510518
F -1.161695 2.869160 -0.096319
F 0.751468 0.832801 -0.839400
F 1.101719 2.246555 1.613837
F -0.721483 0.180931 0.871687
F -1.207821 -0.744500 -1.514124



RSi(μ -R)2AIR2 R=NH2

Total Energy=-812.028984
Al 1.070411 -0.242382 0.148689
Si -1.790336 0.025553 -0.495483
H -0.011764 -0.866667 -2.083491
H 0.054538 0.759235 -2.027965
N -1.754368 1.769445 -0.249609
N 1.877345 1.359395 0.401413
N 2.000704 -1.774958 0.365341
N -0.662819 -0.412986 1.066444
N -0.055209 -0.071702 -1.451588
H -0.997566 2.326878 0.130025
H -2.593010 2.314083 -0.377666
H -0.824222 0.259836 1.812237
H -0.887236 -1.325277 1.454172
H 2.602658 1.519334 1.087126

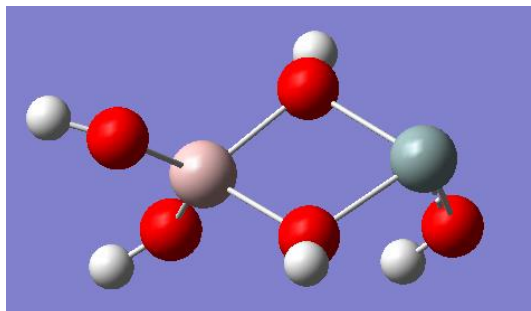


H 1.874900 2.126422 -0.256213
H 2.987002 -1.868138 0.166542
H 1.644830 -2.658874 0.700286

RSi(μ -R)₂AlR₂ R=OH

Total Energy=-911.495296

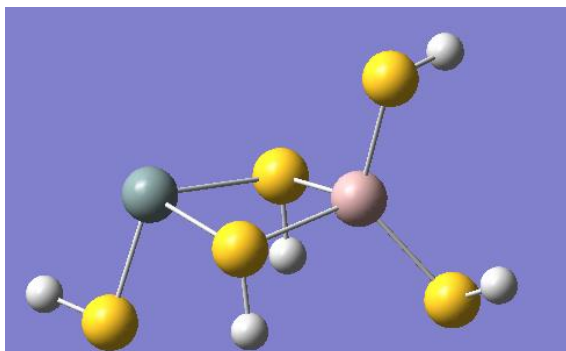
Al 1.145292 -0.142579 0.227306
Si -1.679059 -0.083392 -0.582313
O -1.744276 1.563975 -0.871515
O 0.105010 -0.372260 -1.279296
O -0.547120 -0.037935 0.967127
O 1.912587 -1.502367 0.939101
O 1.908510 1.383577 -0.028705
H 2.660575 1.770556 0.418441
H 2.831817 -1.762622 0.968897
H -0.825454 -0.459821 1.784312
H 0.324260 -0.051689 -2.159181
H -1.023639 2.172501 -0.663232



RSi(μ -R)₂AlR₂ R=SH

Total Energy=-2526.243960

Al 1.472803 0.092416 -0.011081
Si -1.707838 -0.944905 -0.151410
S 2.299198 2.140839 0.195860
H 3.344011 1.925860 -0.637676
S -3.010866 0.848329 -0.245448
H -4.049915 0.259120 0.390321
S -0.109819 -0.214963 1.694176
S -0.141823 -0.068665 -1.767094
S 2.717673 -1.711026 -0.335303
H 3.376961 -1.612454 0.843846
H -0.477455 1.082851 1.819453
H -0.440208 1.252910 -1.804200

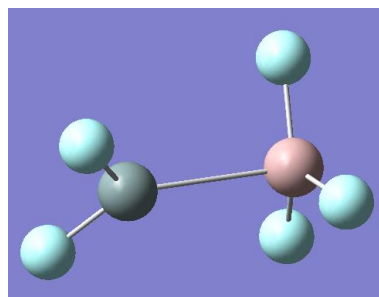


S2. Optimized geometries (in angstrom) and energies (in a.u.) for other structures.

R₃AlSiR₂ R=F

Total Energy=-1031.672282

Al -0.631272 1.122824 0.017289
Si 0.275432 -1.408635 0.002468
F 0.860111 1.843574 -0.214999
F 0.209049 -2.522289 1.152532
F 1.017554 -2.144565 -1.211803
F -1.294081 1.126220 1.551395



F -1.649230 0.932871 -1.296883

R3AlSiR2 R=Cl

Total Energy=-2833.386610

Al -0.827196 1.018111 -0.011818

Si 0.346712 -1.344293 0.009523

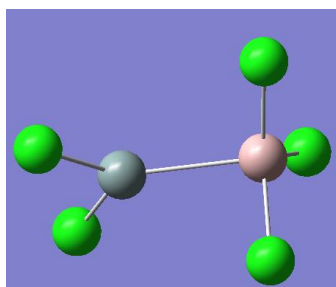
cl 1.028298 2.055920 0.004901

cl 1.010129 -2.350709 1.668218

cl 1.050670 -2.362234 -1.624676

cl -1.930735 0.972323 1.787182

cl -1.890313 0.960881 -1.833331



R2AlSiR3 R=OEt

Total Energy=-1304.647112

Al 1.303644 0.121554 0.361893

Si -1.108970 -0.004003 0.020485

O -1.550030 -1.255868 -0.986069

O -1.741698 -0.160822 1.543359

O -1.817131 1.334827 -0.649420

O 2.178390 -1.352201 0.334386

O 2.048893 1.638969 0.576439

C 3.487794 -1.854369 0.516425

C 3.886231 -2.763074 -0.637650

H 3.516987 -2.414876 1.459133

H 4.210603 -1.032103 0.610602

H 4.888195 -3.174285 -0.476987

H 3.185138 -3.596343 -0.730728

H 3.890079 -2.214790 -1.583857

C 3.249254 2.328151 0.848701

C 3.478956 3.438938 -0.166369

H 4.103155 1.636555 0.847107

H 3.184016 2.753804 1.857742

H 4.392939 3.994127 0.068819

H 3.577849 3.031058 -1.176328

H 2.640508 4.139752 -0.163097

C -3.120135 -0.045131 1.921304

C -3.232319 -0.152720 3.430742

H -3.698217 -0.839121 1.433618

H -3.510414 0.914642 1.568346

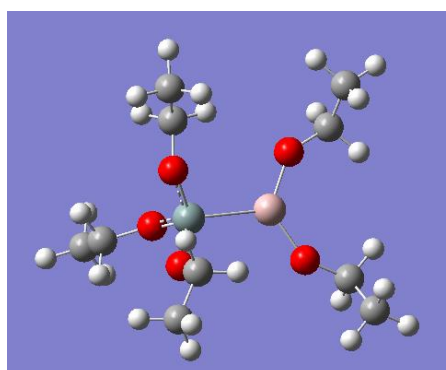
H -4.278254 -0.068970 3.742249

H -2.845641 -1.112268 3.783252

H -2.664747 0.643656 3.918367

C -1.765661 1.745123 -2.015570

C -2.647837 2.966047 -2.203331

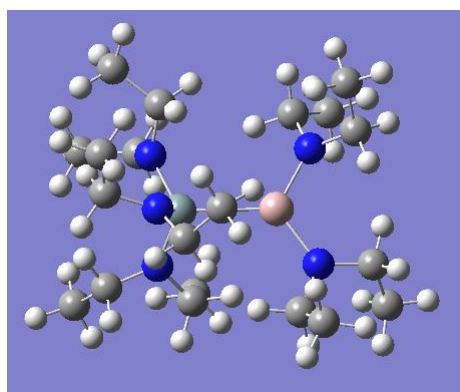


H -2.098076 0.922035 -2.657127
H -0.728584 1.983300 -2.288837
H -2.615486 3.304265 -3.243788
H -3.685616 2.735651 -1.949985
H -2.314224 3.786957 -1.564041
C -1.215111 -2.638034 -0.831318
C -1.485372 -3.368288 -2.134517
H -1.820426 -3.063756 -0.022127
H -0.161921 -2.740940 -0.543709
H -1.256573 -4.433503 -2.029778
H -2.534616 -3.269680 -2.423816
H -0.869733 -2.963768 -2.941927

R2AlSiR3 R=NEt2

Total Energy=-1598.32036493

Al	1.45908100	0.13493100	-0.08253400
Si	-1.01487400	-0.26527800	0.10571700
N	-1.40143500	-1.80775100	-0.65818400
N	-1.50102000	-0.18194100	1.80237300
N	-1.98739000	0.99981600	-0.65771800
N	2.06853000	1.77400900	-0.58402700
N	2.74977900	-1.09684500	0.27290700
C	3.20105500	2.43856500	0.06420200
C	2.82962100	3.68471500	0.88039000
H	3.97340700	2.71256700	-0.67017100
H	3.67970800	1.72120600	0.73828800
H	3.71970700	4.10331800	1.36186700
H	2.39617400	4.47332300	0.26005000
H	2.10455100	3.43742000	1.66122900
C	1.45796000	2.52047800	-1.68317200
C	2.31117000	2.60268800	-2.95713600
H	1.19234900	3.53984400	-1.36854900
H	0.50779000	2.03838100	-1.93856400
H	1.77634200	3.14902700	-3.74133400
H	3.25713400	3.12357600	-2.78704500
H	2.54497100	1.60379000	-3.33763900
C	4.12932600	-0.93564600	-0.20122000
C	4.59523500	-1.99116900	-1.21343100
H	4.83468000	-0.91821900	0.64293200
H	4.20754900	0.04440700	-0.67591000
H	5.60062000	-1.74715800	-1.57149200
H	4.64185300	-2.99589200	-0.78584800
H	3.92688400	-2.02483100	-2.07896500
C	2.50239200	-2.33629500	1.00953500



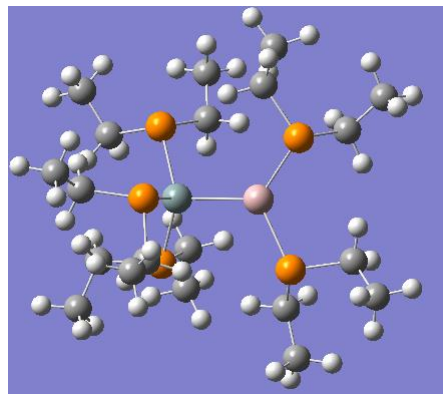
C	3.18927300	-2.42621100	2.37857600
H	2.79465400	-3.20928500	0.40940000
H	1.42260000	-2.44018700	1.15507200
H	2.91471800	-3.35851800	2.88307000
H	4.27897800	-2.41330200	2.29324300
H	2.89563400	-1.59161100	3.02135100
C	-0.65780500	-0.78666300	2.83766700
C	0.21955900	0.19928500	3.62084400
H	-0.00880600	-1.54762600	2.39061500
H	-1.29759800	-1.33966300	3.53828900
H	0.81474900	-0.32685600	4.37528500
H	0.91379500	0.72319600	2.95629800
H	-0.37671500	0.95831500	4.12973000
C	-2.88691300	0.06137700	2.21540500
C	-3.07765200	1.10735100	3.31998300
H	-3.34639100	-0.88275500	2.55335700
H	-3.44539700	0.37687000	1.33308400
H	-4.14606500	1.27608900	3.49175500
H	-2.64630500	0.78675200	4.27156000
H	-2.62350900	2.06365900	3.04836700
C	-2.61220700	-2.53256600	-0.25105600
C	-3.42765700	-3.16825300	-1.38228200
H	-3.25798900	-1.83941300	0.29174400
H	-2.34671400	-3.32537500	0.46834500
H	-4.33761400	-3.61937000	-0.97296300
H	-3.72282200	-2.43008800	-2.13160300
H	-2.87529100	-3.96255700	-1.88983800
C	-0.41108700	-2.61830900	-1.37163800
C	-0.45448000	-2.53400700	-2.90370800
H	-0.52307500	-3.66679900	-1.06197100
H	0.59618100	-2.32891500	-1.05398500
H	0.29755900	-3.20014200	-3.34146400
H	-1.42861900	-2.81411900	-3.30845700
H	-0.23508400	-1.51852500	-3.24647300
C	-2.37467400	0.91502400	-2.06935900
C	-3.87484900	0.71269400	-2.32169600
H	-1.84351500	0.08194200	-2.53634500
H	-2.03931100	1.82324400	-2.59205700
H	-4.06889900	0.61005200	-3.39552400
H	-4.23116300	-0.19420300	-1.82825500
H	-4.47519600	1.54588700	-1.95316500
C	-1.90557400	2.36568500	-0.12248700
C	-3.23493500	3.11982000	0.00340500
H	-1.22957800	2.97296600	-0.74290000

H	-1.44015200	2.31037100	0.86410100
H	-3.06901600	4.07633300	0.51034800
H	-3.67294100	3.34551400	-0.97145200
H	-3.97042700	2.55476400	0.58110000

R2AlSiR3 R=PEt2

Total Energy=-3031.34794279

Al	1.52518900	-0.03320900	0.04515500
Si	-0.96939100	0.06513000	0.07829800
P	-1.61138600	2.20274600	-0.52504900
P	-1.81624900	-1.80954500	-0.98396300
P	-1.28666000	0.02194700	2.36772900
P	2.98204300	1.72822300	0.62889100
P	2.53192200	-2.13463400	0.23592700
C	3.98274000	1.96164100	-0.96077500
C	5.18452300	2.89859600	-0.79381200
H	3.33708300	2.32582000	-1.76703500
H	4.33442800	0.97168500	-1.26799200
H	5.77513900	2.94267700	-1.71535400
H	4.87244500	3.91928800	-0.55914400
H	5.84148600	2.56143700	0.01219900
C	1.95548300	3.30779300	0.71785300
C	2.57687700	4.38673800	1.61402700
H	0.96744300	3.04614700	1.10472800
H	1.79535200	3.69893800	-0.29263500
H	1.93298600	5.27189900	1.65553600
H	2.70885200	4.02198400	2.63581200
H	3.55777000	4.70730200	1.25380900
C	4.37802200	-1.91941100	-0.07379700
C	5.24979200	-2.99109700	0.59311800
H	4.65562200	-0.93991400	0.32521200
H	4.56822500	-1.88599200	-1.15206200
H	6.31207300	-2.79139700	0.41514600
H	5.08984500	-3.01038100	1.67405000
H	5.03516100	-3.99240000	0.21315900
C	1.92839900	-3.21168000	-1.18505200
C	2.27349000	-4.69789700	-1.03515200
H	2.31375000	-2.83116700	-2.13698900
H	0.84071800	-3.09687800	-1.21089300
H	1.82186700	-5.28126100	-1.84466600
H	3.35127000	-4.87435000	-1.07056100
H	1.90300100	-5.09746000	-0.08767000
C	-1.12506200	-1.82085700	2.72307000
C	-1.10924100	-2.16031500	4.21840000



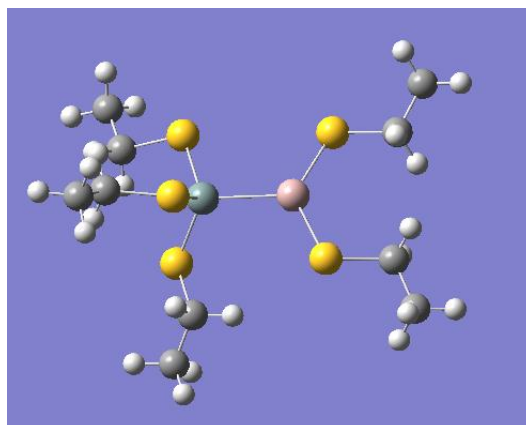
H	-0.18152100	-2.14408400	2.27223600
H	-1.91577900	-2.38101200	2.21420900
H	-0.90477200	-3.22548600	4.36637100
H	-0.33692000	-1.59641000	4.74822200
H	-2.06624300	-1.94505300	4.70049500
C	-3.13304800	0.33201100	2.62162200
C	-3.46883000	0.80384400	4.04230200
H	-3.70506500	-0.56776200	2.37132100
H	-3.43409400	1.10876200	1.91339200
H	-4.53874300	1.01782600	4.13675600
H	-3.21677600	0.05452300	4.79606500
H	-2.92144900	1.71603700	4.29298200
C	-3.69607600	-1.68416200	-0.83235600
C	-4.38947700	-3.05038100	-0.91398400
H	-4.08672200	-1.00823300	-1.59916300
H	-3.92326400	-1.22345200	0.13159400
H	-5.47325200	-2.94435200	-0.79724100
H	-4.20856500	-3.54639400	-1.87078300
H	-4.03314600	-3.72319600	-0.12959700
C	-1.54471000	-1.35705500	-2.79423800
C	-1.93700700	-2.47254800	-3.76993400
H	-0.47879700	-1.13274500	-2.90773500
H	-2.08513900	-0.43823800	-3.03998000
H	-1.69133700	-2.19223200	-4.79941300
H	-1.41388700	-3.40543700	-3.54349500
H	-3.00973500	-2.67943900	-3.73904600
C	-3.39295000	2.01690300	-1.12687000
C	-4.17738000	3.33504300	-1.08971500
H	-3.88838200	1.28829900	-0.48152500
H	-3.40324300	1.59115000	-2.13577200
H	-5.21135900	3.18173000	-1.41647000
H	-4.20450000	3.74899700	-0.07837300
H	-3.73713500	4.09593500	-1.73829000
C	-0.67446600	2.43388300	-2.14768000
C	-0.86501400	3.82057800	-2.77247100
H	-0.94096400	1.65735500	-2.87094000
H	0.38388600	2.28884000	-1.90717600
H	-0.21311900	3.94633600	-3.64298100
H	-1.89149900	3.97473300	-3.11381200
H	-0.63039700	4.61611100	-2.06006500

R2AISiR3 R=SEt

Total Energy=-2919.456379

Al -1.373790 -0.036527 0.006147

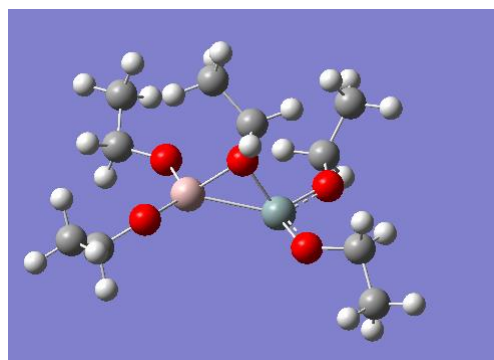
Si 1.088011 -0.073332 -0.070665
S -2.367149 1.917956 -0.160553
S 2.002454 -0.840407 1.753508
S 1.592099 -1.303774 -1.789086
S 1.713714 1.999720 -0.199137
S -2.326728 -1.999468 0.318795
C -4.185212 1.624542 -0.444691
C -4.853991 2.939794 -0.826190
H -4.622308 1.223184 0.469300
H -4.308031 0.887308 -1.238599
H -5.925479 2.782466 -0.987407
H -4.737826 3.687883 -0.038480
H -4.429677 3.350292 -1.745132
C -4.107179 -1.749313 0.805038
C -4.690637 -3.071029 1.290191
H -4.655782 -1.382113 -0.062011
H -4.158468 -0.995486 1.590977
H -5.741040 -2.937119 1.568473
H -4.643179 -3.836381 0.512022
H -4.153937 -3.445626 2.164669
C 1.471256 -2.620799 1.747836
C 2.097287 -3.345496 2.933847
H 1.781978 -3.067721 0.803234
H 0.382159 -2.660714 1.799920
H 1.781736 -4.393466 2.935108
H 3.188894 -3.322955 2.888072
H 1.789797 -2.902045 3.884037
C 3.433044 -1.125541 -1.946079
C 3.964772 -2.097683 -2.992994
H 3.882623 -1.316969 -0.970299
H 3.645613 -0.093878 -2.230822
H 5.048121 -1.980239 -3.096949
H 3.763057 -3.134563 -2.714010
H 3.513250 -1.917964 -3.971675
C 3.478611 2.056388 0.387274
C 3.935570 3.509663 0.440952
H 4.099229 1.479395 -0.299010
H 3.536583 1.593765 1.371812
H 4.974554 3.560304 0.781612
H 3.880403 3.985455 -0.541267
H 3.325294 4.093739 1.133704



R₂Si(μ -R)AIR₂ R=OEt

Total Energy=-1304.639563

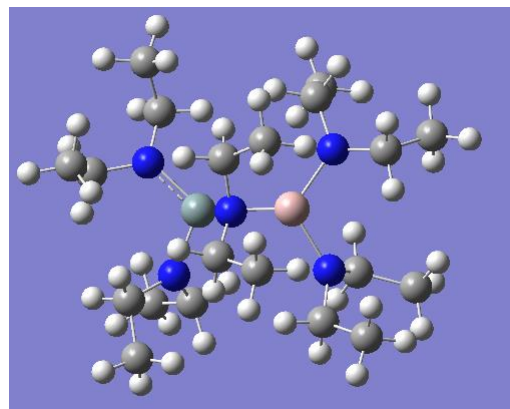
Al 0.784266 -0.398395 0.510593
Si -1.462289 -1.202610 0.755883
O 1.029133 1.306742 0.545642
O 2.115829 -1.481886 0.476166
O -0.499592 -0.951062 -0.787150
O -2.902775 -0.389264 0.574901
O -1.903618 -2.788143 0.825918
C -0.610048 -1.376363 -2.170268
C 0.301350 -0.553677 -3.059821
H -1.657439 -1.260186 -2.459980
H -0.355131 -2.438347 -2.211765
H 0.196250 -0.873358 -4.101060
H 0.053885 0.508810 -3.002523
H 1.348854 -0.682471 -2.775667
C -3.152870 -3.426538 0.530917
C -3.363245 -4.590447 1.482016
H -3.117792 -3.780770 -0.506003
H -3.966113 -2.699935 0.608724
H -4.296433 -5.111402 1.245018
H -2.541700 -5.306894 1.407173
H -3.418833 -4.242548 2.516531
C -3.069613 1.034991 0.575349
C -3.790902 1.479712 -0.685279
H -2.097864 1.534992 0.659299
H -3.654166 1.296234 1.463208
H -3.963989 2.560289 -0.662830
H -3.202025 1.249142 -1.576940
H -4.759030 0.980508 -0.774851
C 3.357150 -1.691437 1.108026
C 4.263586 -2.545112 0.231997
H 3.198216 -2.193920 2.072431
H 3.851461 -0.733154 1.326233
H 5.223237 -2.727415 0.727230
H 3.795708 -3.510630 0.022886
H 4.459616 -2.048836 -0.722629
C 2.130866 2.185875 0.617481
C 1.811558 3.501314 -0.079387
H 3.023024 1.733339 0.160372
H 2.377417 2.379145 1.670991
H 2.657207 4.193808 -0.009519
H 1.590275 3.336179 -1.137490
H 0.940447 3.977110 0.378795



R2Si(μ -R)AIR2 R=NEt2

Total Energy=-1205.09424561

Al	1.13762300	0.12812300	-0.03345500
Si	-1.22964600	0.08954600	-0.48262500
N	-2.49725000	1.29797400	-0.59600100
N	2.17750400	1.63194400	-0.05869800
N	2.07835700	-1.42117300	-0.32376600
N	-0.40628000	0.06315000	1.36817900
N	-1.84170300	-1.54150400	-0.72276800
C	-2.20396500	2.58457200	-1.24264900
C	-2.54777900	3.83494400	-0.42702500
H	-2.74282600	2.63601700	-2.20181900
H	-1.14183200	2.60284000	-1.49767800
H	-2.26528400	4.73386400	-0.98462000
H	-3.61904300	3.90639200	-0.22089400
H	-2.02119700	3.85245800	0.53061500
C	-3.92847100	1.03509400	-0.39915100
C	-4.43562500	1.22487700	1.03504300
H	-4.16255100	0.02108900	-0.73094700
H	-4.49227100	1.69707500	-1.06750900
H	-5.51092800	1.02364000	1.09276900
H	-3.93508900	0.54298900	1.72874100
H	-4.26136300	2.24182100	1.39293600
C	-2.98191400	-2.17430100	-0.04684700
C	-2.76924200	-3.63920500	0.35588200
H	-3.88767200	-2.12687300	-0.66920700
H	-3.21100000	-1.59649900	0.85137800
H	-3.62790500	-3.98788500	0.93793300
H	-2.68051900	-4.29812600	-0.51091900
H	-1.87217000	-3.77077900	0.96569600
C	-1.37638200	-2.23529200	-1.93574200
C	-2.38152200	-2.26732800	-3.09269000
H	-1.07840300	-3.26010600	-1.68398500
H	-0.46210500	-1.73924000	-2.27064700
H	-1.94413100	-2.77344100	-3.95933500
H	-3.29761900	-2.80551100	-2.83304300
H	-2.66307600	-1.25568500	-3.39919100
C	-0.73651400	-1.07771800	2.25458100
C	0.25882300	-1.41817400	3.36966200
H	-0.83888200	-1.94650100	1.60708400
H	-1.72627500	-0.90330700	2.70077200
H	0.05164600	-2.42583700	3.74407800
H	1.28854700	-1.40838600	3.00796200
H	0.19549500	-0.74069300	4.22075500
C	-0.58900600	1.38800600	2.02184500



C	0.45128100	1.81873500	3.06031600
H	-1.59324700	1.42265900	2.46287200
H	-0.59411500	2.13753000	1.22803000
H	0.30698300	2.87979900	3.28840300
H	0.36918100	1.27560500	4.00119000
H	1.46698300	1.70127700	2.67902600
C	1.74511900	2.94912000	-0.52028400
C	1.86648000	3.18079200	-2.03368100
H	2.31442900	3.72580600	0.01001800
H	0.69949800	3.12635100	-0.23719500
H	1.51148300	4.18189300	-2.30691800
H	2.89885400	3.08283400	-2.37625300
H	1.26725200	2.44952800	-2.58450000
C	3.51045200	1.61376700	0.54496200
C	4.67620000	1.98488600	-0.38209500
H	3.69257500	0.60806000	0.93714300
H	3.54216200	2.29149500	1.41736700
H	5.62866800	1.88945600	0.15115600
H	4.71010000	1.33142900	-1.25786600
H	4.60598500	3.01740600	-0.73488200
C	2.78062600	-1.46768200	-1.61064400
C	4.26683500	-1.85125000	-1.57562700
H	2.70223500	-0.47909600	-2.07815600
H	2.26545700	-2.16417300	-2.29652300
H	4.70937800	-1.72731000	-2.57039900
H	4.82297400	-1.22306600	-0.87504000
H	4.41476800	-2.89422900	-1.28611100
C	1.91949100	-2.71966100	0.31950900
C	3.02455300	-3.11209800	1.31547200
H	1.84218200	-3.50590100	-0.44897400
H	0.96454000	-2.75018900	0.85308500
H	2.78316300	-4.06530000	1.80085200
H	3.99713500	-3.22006700	0.83303100
H	3.13272600	-2.35561700	2.09773900

R2AlSiR3 R=OMe

Total Energy=-1108.010759

Al -1.309498 -0.080169 0.064177

Si 1.128738 -0.067869 0.020260

O 1.742071 1.213841 -0.846667

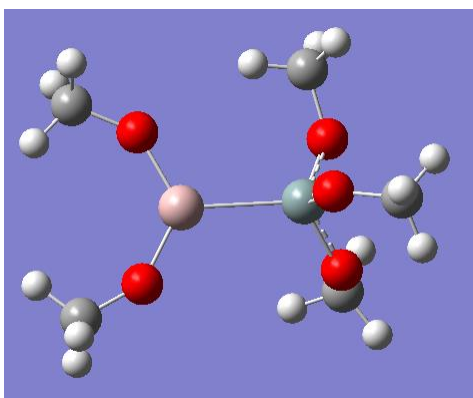
O 1.568654 -0.032414 1.614809

O 1.862134 -1.396722 -0.639177

O -2.085373 1.445224 0.006837

O -2.161234 -1.552705 0.116731

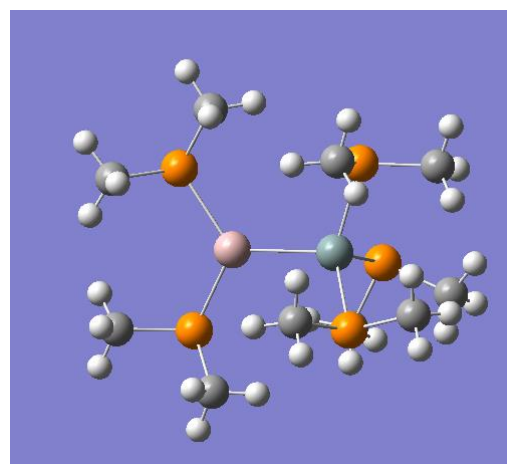
C -3.360555 2.038770 0.056383
 H -3.388393 2.793376 0.849174
 H -3.580877 2.535380 -0.894597
 H -4.154906 1.308137 0.252492
 C -3.416591 -2.177222 0.190189
 H -4.240749 -1.479108 -0.002281
 H -3.472283 -2.983115 -0.548644
 H -3.563527 -2.615643 1.183076
 C 2.866327 -0.266188 2.157895
 H 2.783280 -0.219540 3.244689
 H 3.238344 -1.251720 1.866908
 H 3.577525 0.496044 1.824121
 C 1.990811 -1.705387 -2.018833
 H 2.437074 -0.873550 -2.570803
 H 2.636091 -2.580933 -2.106407
 H 1.017627 -1.947943 -2.462020
 C 1.403855 2.587848 -0.693447
 H 1.734612 3.116121 -1.589349
 H 0.324520 2.729073 -0.575194
 H 1.913118 3.016831 0.175289



R2AISiR3 R=PMe2

Total Energy=-2638.152251

Al -1.501394 0.081162 -0.152553
 Si 1.001047 0.029388 -0.164413
 P 1.718364 2.222814 -0.276227
 P 1.633764 -1.392725 1.554540
 P 1.706823 -0.834162 -2.193543
 P -2.830816 1.910822 -0.791670
 P -2.583583 -1.995101 -0.320199
 C 1.562813 2.809512 1.495379
 H 2.138215 2.221305 2.212435
 H 1.907370 3.845779 1.549956
 H 0.513890 2.799504 1.800032
 C 3.580355 2.128422 -0.425272
 H 3.842991 1.757464 -1.417516
 H 3.980268 3.143203 -0.344145
 H 4.065350 1.505120 0.327555
 C 0.650446 -0.750694 3.015306
 H 0.946159 -1.312132 3.906157
 H 0.791566 0.312633 3.219093
 H -0.414105 -0.939075 2.856723
 C 3.346899 -0.845330 2.072507
 H 3.412249 0.207867 2.351229

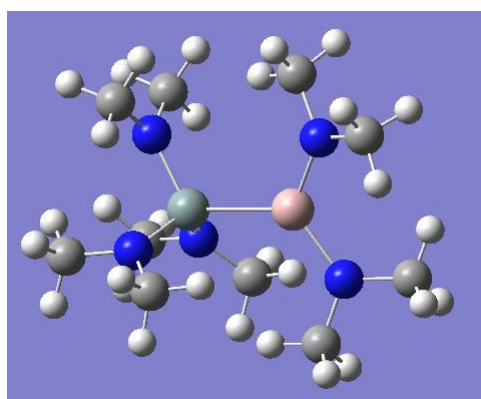


H 3.652791 -1.445878 2.933878
H 4.058713 -1.039379 1.268678
C 3.424287 -1.472828 -1.792672
H 4.100821 -0.647339 -1.565993
H 3.439047 -2.184405 -0.963280
H 3.812479 -1.979298 -2.680969
C 0.823141 -2.480307 -2.260533
H -0.246989 -2.338554 -2.418134
H 1.211730 -3.037358 -3.117871
H 0.967135 -3.085187 -1.361915
C -4.373687 -1.819151 0.193509
H -4.886288 -1.138320 -0.488583
H -4.858636 -2.794826 0.103380
H -4.510394 -1.464048 1.217725
C -1.924750 -3.111124 1.028453
H -0.839255 -3.196583 0.950503
H -2.174059 -2.766665 2.035169
H -2.346057 -4.111048 0.896826
C -4.207474 2.022566 0.478129
H -4.874601 2.841378 0.196149
H -4.797696 1.105284 0.480236
H -3.851415 2.209735 1.494188
C -1.906311 3.494338 -0.429125
H -1.692523 3.640851 0.632738
H -0.964240 3.512132 -0.978656
H -2.511713 4.337302 -0.773093

R2AlSiR3 R=NMe2

Total Energy=-1205.107390

Al -1.442520 0.018847 0.028537
Si 1.044100 -0.093030 0.032680
N 1.595821 -0.948422 1.464690
N 1.540452 -0.750154 -1.522039
N 1.907077 1.437014 0.125650
N -2.262198 1.610925 -0.225910
N -2.494428 -1.443337 0.234878
C -1.621450 2.886025 0.057754
H -2.153318 3.445111 0.843135
H -0.593219 2.740924 0.395223
H -1.590233 3.531048 -0.833591
C -3.611512 1.796741 -0.735988
H -4.055855 0.846121 -1.035920
H -4.278589 2.261390 0.007449
H -3.613040 2.451297 -1.620828

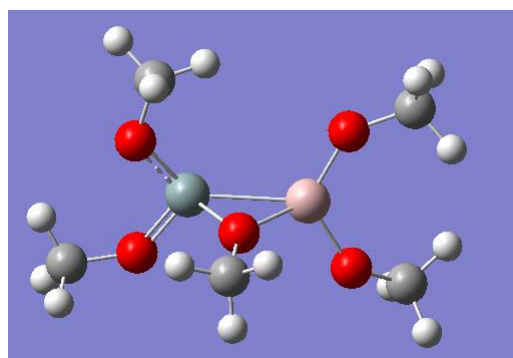


C -3.887389 -1.428587 0.656215
H -4.213131 -0.418531 0.910034
H -4.562842 -1.814567 -0.123576
H -4.037286 -2.054958 1.548699
C -2.025362 -2.801337 0.008643
H -2.571306 -3.292602 -0.811715
H -0.964156 -2.816065 -0.251788
H -2.153679 -3.429465 0.903465
C 0.771020 -1.852308 2.247172
H -0.289371 -1.697266 2.040909
H 0.998735 -2.911236 2.046206
H 0.924329 -1.686598 3.323039
C 3.010689 -1.101138 1.775348
H 3.195762 -0.938287 2.846705
H 3.382801 -2.107932 1.529864
H 3.610322 -0.375555 1.224329
C 2.942804 -0.877346 -1.892864
H 3.279497 -1.925177 -1.879151
H 3.120740 -0.490540 -2.906931
H 3.576951 -0.310148 -1.210460
C 2.160950 2.132443 1.377115
H 3.206542 2.468108 1.437013
H 1.530885 3.029348 1.487834
H 1.968528 1.478253 2.227064
C 2.120258 2.293638 -1.030040
H 1.495210 3.199261 -0.993929
H 3.166914 2.626754 -1.086493
H 1.886586 1.761078 -1.951533
C 0.669570 -1.429903 -2.460782
H 0.868169 -2.512029 -2.512183
H -0.383108 -1.305317 -2.191431
H 0.791232 -1.028548 -3.477493

R2Si(μ -R)AlR2 R=OMe

Total Energy=-1108.003382

Al 0.742851 -0.087648 0.247942
Si -1.628206 -0.458848 0.309846
O 1.394602 1.454884 -0.109025
O 1.746383 -1.391523 0.742824
O -0.489663 -0.588997 -1.121054
O -2.799030 0.639447 -0.052275
O -2.454510 -1.899202 0.409083
C -4.166913 0.456515 -0.408015
H -4.538491 -0.516501 -0.080775

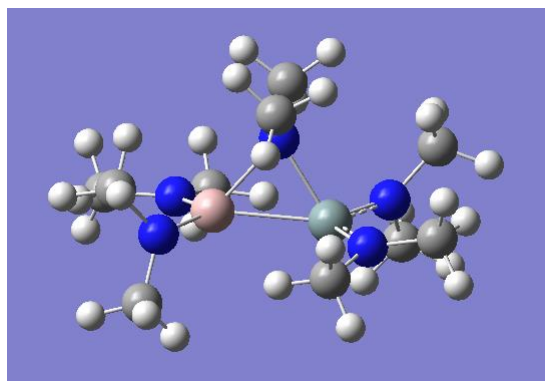


H -4.749491 1.248341 0.066121
H -4.280213 0.537719 -1.493065
C -1.883670 -3.166838 0.723810
H -2.568914 -3.697385 1.387521
H -1.753682 -3.750399 -0.191660
H -0.911171 -3.069304 1.216352
C -0.589499 -0.722499 -2.552828
H -1.481841 -1.299824 -2.797427
H -0.649961 0.266923 -3.008140
H 0.292903 -1.246627 -2.920774
C 2.334488 2.387181 0.351938
H 3.204435 1.909567 0.822432
H 2.695863 2.989950 -0.488277
H 1.884743 3.068015 1.085163
C 3.106426 -1.655019 0.973388
H 3.766950 -0.953230 0.447160
H 3.338023 -1.599731 2.044155
H 3.350085 -2.666363 0.629195

R2Si(μ -R)AlR2 R=NMe2

Total Energy=-1205.094246

Al 1.218286 0.011539 -0.196560
Si -1.177908 -0.065965 -0.315784
N -2.200960 1.344957 -0.383080
N 2.039123 1.640020 -0.265126
N 2.247479 -1.475248 -0.382806
N -0.135996 -0.045791 1.371277
N -2.145451 -1.514564 -0.235260
C -3.630846 1.375066 -0.120585
H -4.033327 0.366903 -0.038381
H -3.871858 1.918165 0.806421
H -4.163132 1.877431 -0.939863
C -1.662880 2.660037 -0.702309
H -0.594188 2.601235 -0.913469
H -2.163212 3.086059 -1.583294
H -1.799266 3.369733 0.127179
C -3.059254 -1.882304 0.835363
H -4.100329 -1.939927 0.483244
H -2.805551 -2.866200 1.255621
H -3.028498 -1.156674 1.649646
C -2.225111 -2.416110 -1.376401
H -2.007953 -3.452706 -1.081484
H -3.224421 -2.407017 -1.836396
H -1.503488 -2.130197 -2.144266

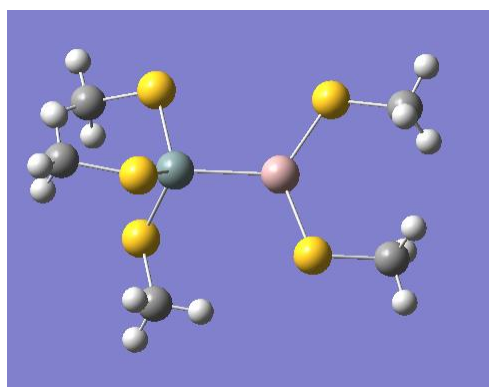


C -0.087280 -1.265458 2.198989
H 0.809427 -1.265479 2.828478
H -0.962266 -1.339231 2.855179
H -0.056917 -2.153631 1.569317
C -0.286110 1.144490 2.226843
H -1.247346 1.135890 2.755963
H 0.511248 1.182238 2.977136
H -0.230297 2.053726 1.630668
C 2.248304 2.344920 -1.516836
H 1.965861 3.408315 -1.440885
H 3.301053 2.319749 -1.846415
H 1.647869 1.907652 -2.321020
C 2.811408 2.224009 0.814687
H 3.895255 2.227467 0.605058
H 2.524829 3.271526 1.006775
H 2.668587 1.673445 1.749146
C 3.699068 -1.420732 -0.351251
H 4.119771 -2.013336 0.478407
H 4.143455 -1.813056 -1.280539
H 4.045831 -0.391467 -0.232121
C 1.765639 -2.823586 -0.605441
H 0.676345 -2.844061 -0.693300
H 2.173400 -3.254538 -1.534589
H 2.045267 -3.510373 0.211701

R2Si(μ -R)AlR2 R=SMe

Total Energy=-2722.838579

Al -1.369129 -0.047712 0.005414
Si 1.092579 -0.103029 -0.041389
S -2.347864 1.895298 -0.315367
S 1.990890 -0.765786 1.830788
S 1.613196 -1.433277 -1.678750
S 1.760337 1.947151 -0.299281
S -2.334030 -1.981789 0.438245
C -4.148916 1.577932 -0.589476
H -4.313764 0.812083 -1.345142
H -4.649364 1.303587 0.336914
H -4.567975 2.516536 -0.949457
C -4.112960 -1.686859 0.844438
H -4.227578 -0.924692 1.612894
H -4.680294 -1.412960 -0.042595
H -4.496592 -2.630849 1.228906
C 3.436129 -1.218238 -1.832856
H 3.936079 -1.433672 -0.888933

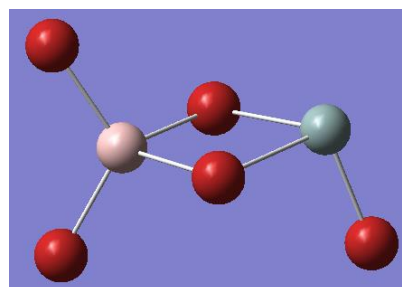


H 3.773565 -1.929380 -2.586134
H 3.672872 -0.208121 -2.165217
C 1.450537 -2.526154 1.907059
H 1.760420 -3.065746 1.013556
H 1.942847 -2.956830 2.778590
H 0.370865 -2.604218 2.030624
C 3.449153 2.023580 0.441330
H 4.132779 1.323363 -0.034806
H 3.799319 3.040183 0.263305
H 3.419508 1.839901 1.513245

RSi(μ -R)₂AlR₂ R=Br

Total Energy=-13402.991290

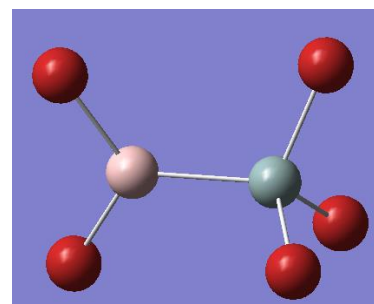
Al 1.393091 0.076436 -0.056895
Si -2.119326 -0.591327 0.134188
Br 2.247047 2.168071 -0.188378
Br 2.804395 -1.696451 -0.042410
Br -0.158142 -0.084943 1.817659
Br -0.321956 -0.242979 -1.760477
Br -3.141121 1.436617 0.092903



R₂AlSiR₃ R=Br

Total Energy=-13402.991223

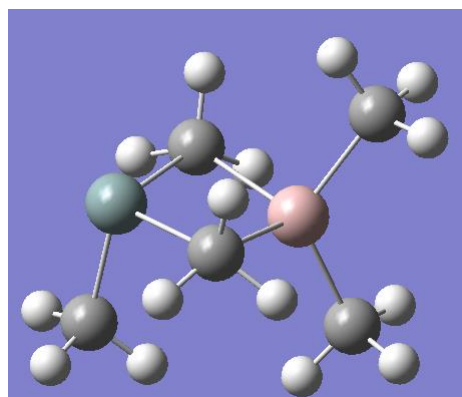
Al 1.461033 -0.005139 -0.051954
Si -0.991582 -0.004863 -0.010789
Br -1.656651 0.096492 2.139011
Br -1.837558 -1.864315 -0.938731
Br 2.592394 -1.948033 -0.192320
Br 2.571050 1.947958 0.117302
Br -1.815159 1.775314 -1.104226



RSi(μ -R)₂AlR₂ R=Me

Total Energy=-731.557831

Al 0.950755 0.176554 -0.001837
Si -1.480993 -0.867180 0.006756
C 1.191125 2.131044 -0.006866
C 2.494290 -1.043021 -0.001918
C -0.229989 -0.497505 1.684450
C -0.236522 -0.516463 -1.677615
C -2.391857 0.843047 -0.005724
H -1.783740 1.751075 -0.029661
H -3.062029 0.876445 -0.872752
H -3.038826 0.905740 0.877071
H 1.714424 2.466496 -0.910888

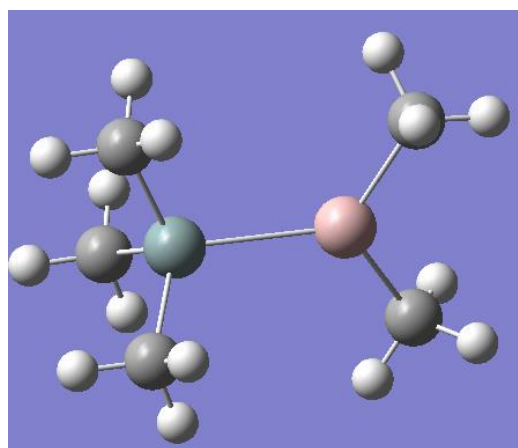


H 0.266899 2.713558 0.052795
H 1.817969 2.451782 0.834568
H 3.137879 -0.885541 0.871924
H 2.210216 -2.101026 0.002219
H 3.133287 -0.891290 -0.880147
H 0.422911 0.311604 2.076424
H -1.133116 -0.319609 2.275489
H 0.200383 -1.439985 2.023652
H 0.197048 -1.460609 -2.008017
H -1.141924 -0.349039 -2.268361
H 0.411421 0.291449 -2.079791

R2AlSiR3 R=Me

Total Energy=-731.626621

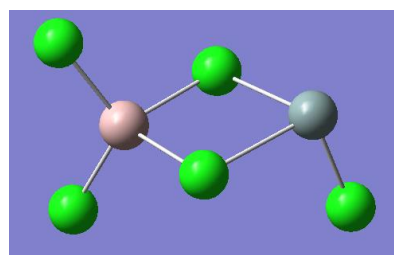
Al 1.424907 -0.006653 -0.023088
Si -1.065539 0.016113 0.017562
C -1.783112 -1.276279 -1.185049
H -1.439477 -2.288298 -0.949321
H -2.878192 -1.285352 -1.138279
H -1.505557 -1.072257 -2.224118
C -1.779293 1.714008 -0.458778
H -2.874581 1.707163 -0.419798
H -1.434052 2.503869 0.215608
H -1.491689 2.007891 -1.473134
C -1.711759 -0.415890 1.757939
H -1.368457 -1.401180 2.088200
H -1.389317 0.310933 2.510319
H -2.807672 -0.431606 1.772055
C 2.449096 1.643781 -0.400626
H 2.292816 2.397461 0.382720
H 3.529304 1.479209 -0.472595
H 2.129711 2.124297 -1.333739
C 2.436380 -1.669670 0.331766
H 2.980539 -1.994154 -0.565633
H 3.203971 -1.515927 1.100995
H 1.821375 -2.516313 0.651799



RSi(μ -R)2AlR2 R=Cl

Total Energy=-2833.395059

Al 1.341747 0.116788 -0.000252
Si -1.995362 -0.651391 0.000688
Cl 2.710243 -1.475879 0.002838
Cl 2.040740 2.093706 -0.003495
Cl -0.188666 -0.182360 1.640833

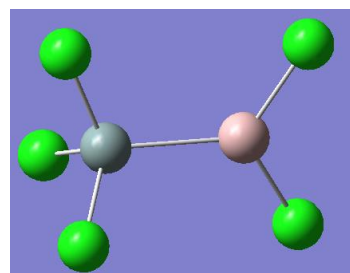


Cl -0.188033 -0.188184 -1.640743
Cl -2.894421 1.234519 -0.002887

R2AlSiR3 R=Cl

Total Energy=-2833.396054

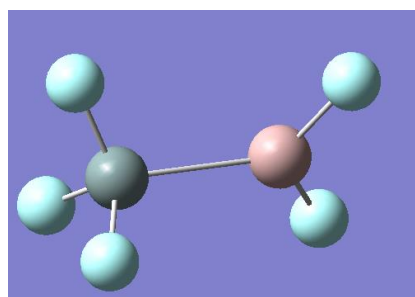
Al -1.436448 0.011806 -0.016543
Si 1.011387 0.009842 0.007397
Cl 1.714604 -0.465003 1.896673
Cl 1.787041 1.850590 -0.522521
Cl -2.505111 1.714340 -0.599008
Cl 1.738600 -1.402037 -1.322893
Cl -2.469609 -1.718858 0.548870



R2AlSiR3 R=F

Total Energy=-1031.692541

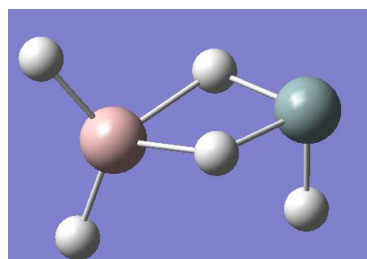
Al 0.007234 1.403427 0.000000
Si -0.014647 -1.033034 0.000000
F 0.002955 2.232029 -1.444266
F 0.002955 2.232029 1.444266
F -1.518467 -1.601805 0.000000
F 0.720974 -1.643648 1.290337
F 0.720974 -1.643648 -1.290337



RSi(μ -R)2AlR2 R=H

Total Energy=-534.924639

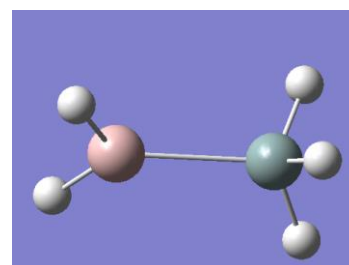
Al 0.901649 0.071063 -0.000017
Si -1.626816 -0.577324 0.000775
H -1.736334 0.940240 -0.001756
H -0.414377 -0.455017 1.080149
H 1.252762 1.607013 -0.002574
H 1.958530 -1.101013 0.002089
H -0.414116 -0.458621 -1.078717



R2AlSiR3 R=H

Total Energy=-534.949783

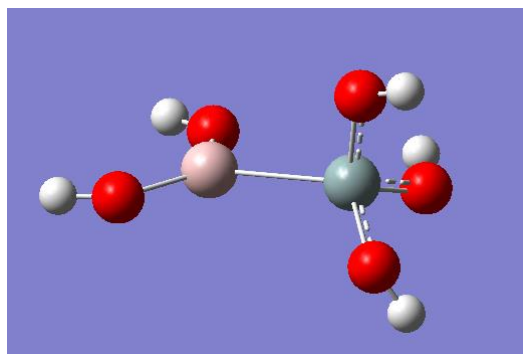
Al 0.276186 1.386495 0.000000
Si -0.182088 -1.035940 0.000000
H -1.655842 -1.276709 0.000000
H 0.368304 -1.723564 1.202050
H 0.411990 2.184520 1.365675
H 0.411990 2.184520 -1.365675
H 0.368304 -1.723564 -1.202050



R2AlSiR3 R=OH

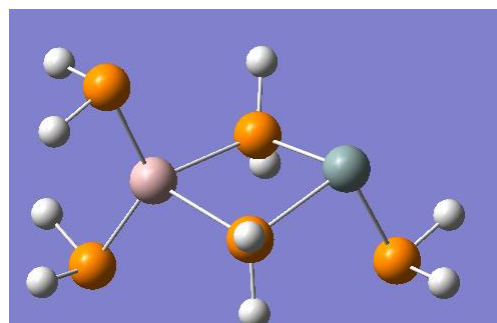
Total Energy=-911.470209

Al 0.552928 1.254478 -0.215652
Si -0.063805 -1.082008 0.056108
O 0.517518 -1.678274 1.502728
O -1.718345 -1.070232 -0.044485
O 0.488150 -2.188838 -1.050892
O 0.909744 1.999331 1.292068
O 0.634089 2.032141 -1.733518
H 1.237450 -2.745124 -0.818655
H -2.216567 -1.884314 -0.174269
H 0.509417 -1.134596 2.295964
H 1.145931 2.893405 1.541307
H 0.828357 2.919858 -2.031976



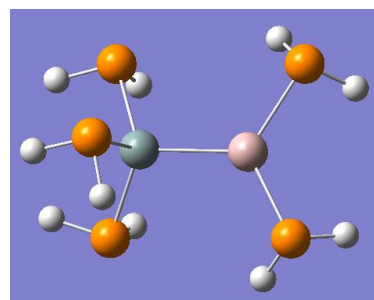
RSi(μ -R)2AIR2 R=OH

Total Energy=-2244.900463
Al 1.590958 0.158742 -0.000134
Si -1.945020 -0.734293 0.002297
P 2.754073 -1.908413 0.004191
H 3.645331 -1.509236 -1.037157
H 3.647639 -1.503751 1.041425
P 2.446877 2.369181 -0.004906
H 3.387750 2.102352 1.035206
H 3.388671 2.097586 -1.042946
P -0.290002 -0.004692 -1.582635
H -0.563559 1.188792 -2.291173
H -0.200046 -0.914053 -2.656964
P -3.174308 1.284960 -0.001748
H -4.056059 0.846243 -1.033992
H -4.052772 0.852057 1.035747
P -0.289693 0.002495 1.583481
H -0.199688 -0.901810 2.662065
H -0.563100 1.199309 2.286443



R2AlSiR3 R=PH2

Total Energy=-2244.905881
Al -0.044770 1.466180 -0.051042
Si -0.325811 -0.992136 -0.114977
P 0.448597 -1.786393 -2.130163
H 1.826649 -1.676127 -1.785584
H 0.380928 -3.167818 -1.785499
P 0.582783 -1.922888 1.784028
H 0.489332 -3.272010 1.335793
H 1.943252 -1.785084 1.379553

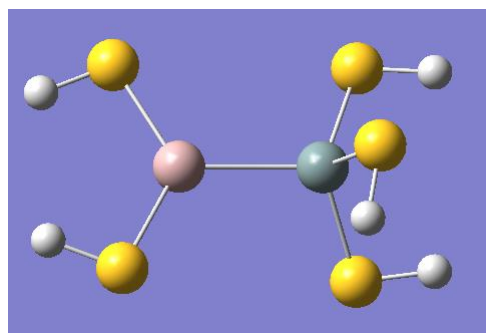


P -2.586887 -1.429998 -0.173470
H -2.472585 -2.825083 0.099589
H -2.817335 -1.090052 1.190225
P 0.124271 2.713732 -2.032929
H 1.131236 3.605322 -1.563790
H 1.026447 1.835171 -2.696211
P -0.436736 2.613346 1.960301
H 0.329055 1.742294 2.785371
H 0.593736 3.582792 1.799728

R2AlSiR3 R=SH

Total Energy=-2526.241920

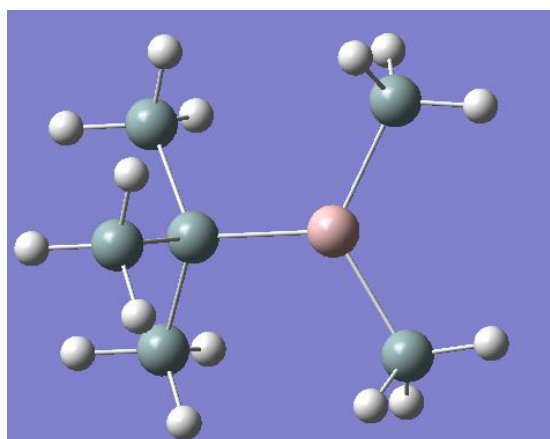
Al 0.287200 1.249617 0.047510
Si -0.060825 -1.181790 0.142247
S 0.931286 2.328881 1.853217
H 0.950465 3.560645 1.291306
S -2.164075 -1.761496 0.181841
H -2.390806 -1.543086 -1.134653
S 0.894653 -2.012870 -1.623257
H 0.500298 -3.294498 -1.430860
S 0.718424 -1.879134 2.040790
H 0.205530 -3.130900 1.968627
S -0.145510 2.261069 -1.860451
H 0.078876 3.522906 -1.424296



R2AlSiR3 R=SiH3

Total Energy=-1988.573187

Al 0.258380 1.391838 -0.000446
Si -0.135795 -1.045002 -0.001695
Si 0.412557 2.578883 2.166149
H 1.530152 2.032123 2.989298
H 0.641934 4.043240 2.018545
H -0.839038 2.399237 2.957603
Si 0.439896 2.579832 -2.164394
H 0.696514 4.039318 -2.013293
H 1.546567 2.014039 -2.989242
H -0.815273 2.425772 -2.955758
Si 0.746316 -2.090569 -1.925116
H 0.144563 -1.511514 -3.155985
H 2.219795 -1.894493 -1.995220
H 0.475151 -3.553384 -1.917178
Si -2.468471 -1.436354 0.008293
H -2.763430 -2.894137 0.007302
H -3.097167 -0.834646 1.215308

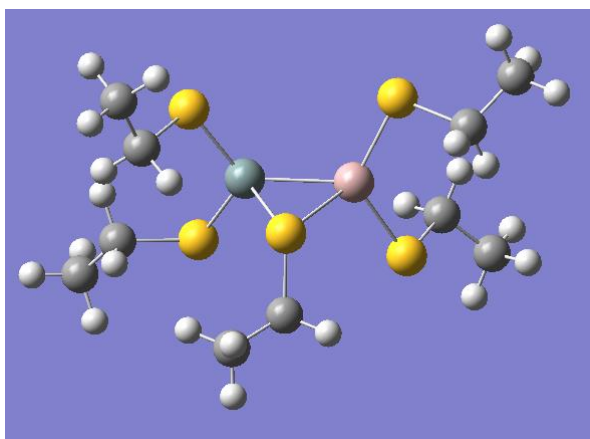


H -3.108253 -0.831021 -1.191100
Si 0.760664 -2.091542 1.914700
H 2.234619 -1.895371 1.974154
H 0.167980 -1.513230 3.150287
H 0.489594 -3.554373 1.907790

R2Si(μ -R)AlR2 R=SEt

Total Energy=-2919.452582

Al 1.191020 -0.391037 0.405429
Si -1.176447 -0.794126 0.698297
S -0.137083 -1.589290 -1.294831
S -2.623231 0.733322 0.219498
S -1.967232 -2.573452 1.631137
S 1.890901 1.475849 -0.577149
S 2.540764 -1.649742 1.620343
C -0.526982 -0.353530 -2.627685
C -1.648717 -0.842659 -3.532767
H 0.403423 -0.219977 -3.180680
H -0.779878 0.596728 -2.158745
H -1.825007 -0.111676 -4.328387
H -1.403308 -1.798184 -4.002117
H -2.583157 -0.964220 -2.980137
C -4.256026 -0.126847 0.011118
C -5.368922 0.911286 -0.078591
H -4.401550 -0.783038 0.869570
H -4.218852 -0.736504 -0.892913
H -6.335169 0.411198 -0.197368
H -5.415563 1.523382 0.824892
H -5.229529 1.578713 -0.932340
C -2.871748 -3.518195 0.307268
C -3.020013 -4.972904 0.738816
H -2.298125 -3.442869 -0.616959
H -3.847432 -3.057650 0.149970
H -3.560896 -5.533972 -0.029917
H -2.046133 -5.445643 0.881738
H -3.580104 -5.062229 1.672895
C 2.510512 2.461622 0.879405
C 3.339573 3.644223 0.392856
H 3.105605 1.812093 1.523404
H 1.648265 2.807069 1.451989
H 3.689935 4.234611 1.245940
H 4.214017 3.310848 -0.171012
H 2.753399 4.302135 -0.253496
C 4.107985 -1.665799 0.609853

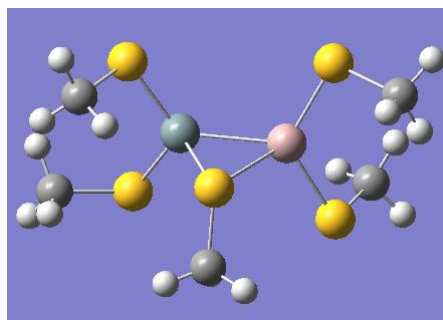


C 5.300503 -2.009645 1.494335
H 4.242144 -0.691190 0.138356
H 3.989298 -2.407759 -0.181614
H 6.216796 -2.043665 0.895324
H 5.437630 -1.265986 2.282970
H 5.175336 -2.984763 1.971672

R2Si(μ -R)AlR2 R=SMe

Total Energy=-2722.834167

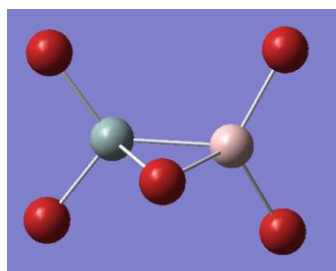
Al 1.133655 -0.271070 0.290649
Si -1.213628 -0.683149 0.707213
C -4.278608 -0.022594 0.076837
H -4.494844 -0.680099 0.917309
H -5.043725 0.751557 0.025881
H -4.277938 -0.583369 -0.856952
C -2.891159 -3.394825 0.334208
H -3.049611 -4.397979 0.729332
H -3.856859 -2.936806 0.128974
H -2.303714 -3.462992 -0.580200
C -0.768984 -0.196744 -2.620174
H -1.677579 -0.538786 -3.113119
H -0.936598 0.780637 -2.173361
H 0.041175 -0.136417 -3.344870
C 2.402546 2.583088 0.743221
H 3.114457 2.008681 1.335011
H 2.907736 3.458477 0.336837
H 1.581265 2.914719 1.377587
C 4.043099 -1.528292 0.306814
H 3.917408 -2.218502 -0.526703
H 4.249535 -0.529428 -0.075448
H 4.885696 -1.857573 0.913914
S -0.293043 -1.445586 -1.350139
S -2.679532 0.853835 0.336471
S -1.963735 -2.482124 1.642305
S 1.775608 1.610569 -0.702619
S 2.550183 -1.549506 1.402685



R2Si(μ -R)AlR2 R=Br

Total Energy=-13402.985207

Al 1.038569 -0.082725 -0.122746
Si -1.269864 -0.656678 0.448097
Br -3.012635 0.730611 0.347208
Br -1.999364 -2.689305 1.003903
Br -0.420966 -0.872135 -1.982077

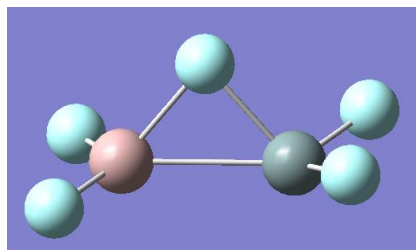


Br 1.521327 2.121022 -0.269280
Br 2.621773 -1.593191 0.444780

R2Si(μ -R)AlR2 R=F

Total Energy=-1031.672580

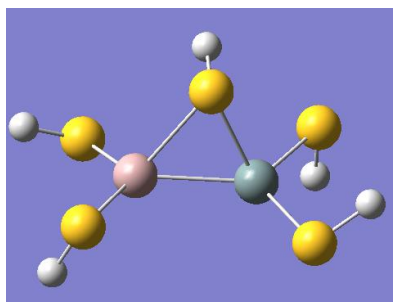
Al 0.971593 -0.086651 -0.090099
Si -1.293624 -0.677745 0.455011
F -0.411040 -0.697876 -1.200924
F -2.581742 0.229536 0.151868
F -1.853685 -2.176916 0.569834
F 1.317897 1.518199 -0.354433
F 2.155408 -1.235828 0.118056



R2Si(μ -R)AlR2 R=SH

Total Energy=-2526.234982

Al 0.960567 -0.247404 -0.074712
Si -1.326563 -0.905676 0.339485
S 1.293459 1.934093 -0.241135
H 2.524082 1.819470 -0.795156
S -3.103683 0.283553 -0.053636
H -3.104886 0.873291 1.164937
S -0.491620 -1.229508 -1.856797
S 2.606927 -1.701472 0.204218
H 3.141944 -1.045957 1.262441
H -0.867543 -0.025692 -2.349533
S -1.793844 -2.850877 1.137258
H -2.993634 -2.989271 0.523983

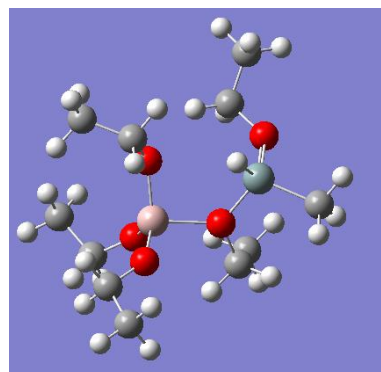


S3. Optimized geometries (in angstrom) and energies (in a.u.) for the ground state structure **1** with HX.

R=OEt + HCH3

Total Energy=-1345.209527

Al -0.783212 0.002949 -0.095699
Si 1.838238 -1.637822 0.784243
O 3.135883 -0.788901 0.256710
O 0.147249 1.026472 0.966770
O 0.486356 -1.445547 -0.288064
O -2.147290 -0.796024 0.607925
O -0.894476 0.484286 -1.757266
C -1.818914 1.201978 -2.537606
C -1.489125 2.690340 -2.598288
H -2.844234 1.066918 -2.160114
H -1.808104 0.786175 -3.554736
H -2.202187 3.221636 -3.238411

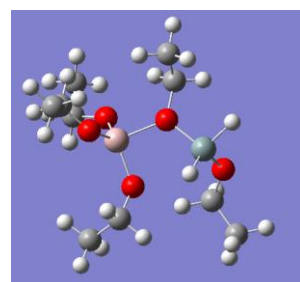


H -1.521822 3.141731 -1.602369
H -0.484871 2.844430 -3.002332
C -3.506807 -0.575715 0.874407
C -4.180115 -1.862336 1.335598
H -4.023198 -0.196789 -0.021436
H -3.624019 0.194473 1.652634
H -5.239864 -1.692593 1.554546
H -4.108881 -2.633052 0.562841
H -3.699212 -2.244778 2.240164
C 0.276676 -2.333356 -1.447624
C 1.166639 -1.951358 -2.611733
H -0.776622 -2.232767 -1.701373
H 0.448428 -3.354703 -1.106547
H 0.959180 -2.614613 -3.457530
H 0.959582 -0.925332 -2.916668
H 2.226771 -2.044183 -2.362899
C -0.093661 1.448686 2.292265
C -0.583874 2.891583 2.344865
H 0.843239 1.362697 2.860720
H -0.821626 0.790730 2.787988
H -0.718752 3.219707 3.381305
H 0.134770 3.560527 1.863734
H -1.542555 3.000154 1.828449
C 3.324671 0.630958 0.076035
C 4.573017 1.078682 0.813178
H 2.436611 1.167504 0.416325
H 3.430759 0.801684 -0.999235
H 4.750838 2.144206 0.636996
H 4.471475 0.926408 1.890995
H 5.451025 0.525151 0.470560
H 1.336032 -1.201443 2.096299
C 2.337574 -3.432268 0.787558
H 3.142751 -3.572251 1.514869
H 1.510568 -4.081964 1.088930
H 2.715532 -3.777828 -0.177410

R=OEt + HH

Total Energy=-1305.871855

Al -0.607599 0.078845 -0.301418
Si 1.743520 -0.246130 1.808051
O 3.090615 0.375351 1.124161
O 0.294254 0.569476 1.336264
O 0.741573 -0.879064 -0.861451
O -1.993774 -0.887427 0.055784



O -0.856919 1.679358 -0.927119
C -1.546499 2.178546 -2.050443
C -1.835811 3.664692 -1.885194
H -2.493307 1.637999 -2.203390
H -0.944104 2.023789 -2.957783
H -2.347543 4.063672 -2.767376
H -2.472073 3.842239 -1.013162
H -0.905844 4.223296 -1.747408
C -3.388055 -0.724684 0.123141
C -4.036340 -1.936262 0.780184
H -3.805483 -0.590560 -0.886126
H -3.650952 0.182943 0.689567
H -5.124492 -1.820073 0.827284
H -3.811734 -2.844737 0.214993
H -3.660199 -2.071589 1.798118
C 0.778332 -2.177299 -1.419841
C 0.636944 -2.154060 -2.938449
H -0.008903 -2.806165 -0.983928
H 1.739266 -2.637407 -1.151277
H 0.715573 -3.165891 -3.350490
H -0.333249 -1.745204 -3.237217
H 1.417508 -1.537616 -3.393189
C -0.114455 1.801799 2.039648
C -1.170804 1.499605 3.081681
H -0.473592 2.469339 1.259178
H 0.781717 2.237299 2.485414
H -1.481025 2.431483 3.564175
H -2.053219 1.042112 2.629575
H -0.792765 0.827793 3.856056
C 3.655254 0.268032 -0.201570
C 4.889553 -0.615206 -0.172048
H 3.915204 1.286639 -0.500950
H 2.895685 -0.107610 -0.887402
H 5.355124 -0.644663 -1.162323
H 5.626074 -0.235267 0.540126
H 4.635874 -1.640658 0.110962
H 1.866276 0.118823 3.233382
H 1.515227 -1.685332 1.619589

R=OEt + HOH

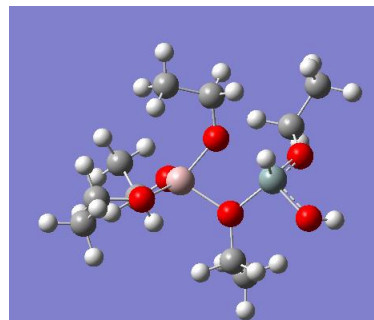
Total Energy=-1381.173524

Al -0.682605 -0.013573 -0.060584

Si 1.766452 -1.432085 0.910902

O 3.047111 -0.554747 0.357323

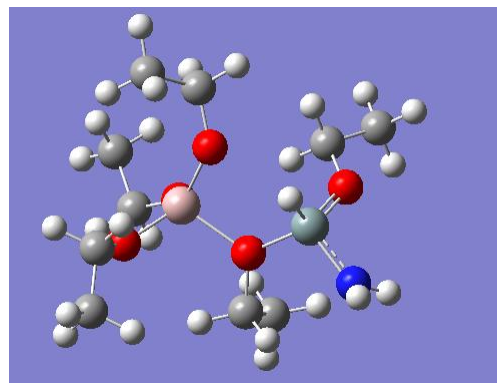
O 0.567556 0.400806 1.140273
O 0.405395 -1.547154 -0.204551
O -2.214710 -0.590121 0.472439
O -0.593024 0.992720 -1.455494
C -1.399528 1.307326 -2.564974
C -1.422580 2.809874 -2.814615
H -2.428082 0.941645 -2.426999
H -1.003354 0.797440 -3.455556
H -2.021247 3.048827 -3.700147
H -1.850693 3.340010 -1.959046
H -0.408835 3.187004 -2.973314
C -3.554499 -0.160344 0.507161
C -4.442402 -1.236430 1.116944
H -3.909989 0.077869 -0.506205
H -3.643949 0.764626 1.096591
H -5.486093 -0.906505 1.152321
H -4.393336 -2.156782 0.528597
H -4.120381 -1.469797 2.135251
C 0.116012 -2.684696 -1.076940
C 0.716889 -2.485841 -2.454885
H -0.972506 -2.756221 -1.111149
H 0.515132 -3.569890 -0.588042
H 0.441991 -3.327534 -3.098154
H 0.354469 -1.567225 -2.921487
H 1.807224 -2.440043 -2.407168
C 0.657849 1.252965 2.271592
C -0.695566 1.770116 2.737864
H 1.317399 2.094584 2.026789
H 1.138483 0.687845 3.079771
H -0.570689 2.407814 3.618409
H -1.180026 2.372501 1.962643
H -1.362737 0.947206 3.004709
C 3.287716 0.790733 -0.055927
C 4.345144 1.434936 0.825490
H 2.356859 1.358957 -0.044157
H 3.634590 0.746906 -1.093268
H 4.567102 2.447090 0.472418
H 4.007970 1.502856 1.863254
H 5.272395 0.856721 0.807916
H 1.420111 -1.502871 2.334210
O 2.388336 -2.977649 0.680692
H 3.250148 -3.042556 0.260555



R=OEt + HNH₂

Total Energy=-1361.283795

Al -0.755591 0.181079 -0.007526
Si 1.605305 -1.681054 1.142605
O 2.897278 -0.776129 0.709184
O -0.029950 0.775574 1.458212
O 0.332986 -1.418511 -0.014412
O -2.401755 -0.355220 -0.021838
O -0.309928 0.967833 -1.488070
C -1.069410 1.518214 -2.541125
C -0.977599 3.040225 -2.564313
H -2.121503 1.210156 -2.466490
H -0.689483 1.119286 -3.493105
H -1.532416 3.451923 -3.414628
H -1.392994 3.471357 -1.648259
H 0.064357 3.362101 -2.646718
C -3.338072 -0.721806 0.962738
C -3.960083 -2.079312 0.654493
H -4.131090 0.038451 1.003628
H -2.876487 -0.746026 1.961370
H -4.720665 -2.338700 1.398986
H -4.435144 -2.068371 -0.330369
H -3.201133 -2.867857 0.655714
C 0.078886 -2.346482 -1.132245
C 1.010158 -2.088298 -2.299542
H -0.965286 -2.187070 -1.401179
H 0.191541 -3.354884 -0.736798
H 0.739570 -2.750291 -3.128299
H 0.926347 -1.054813 -2.637606
H 2.051761 -2.290734 -2.037526
C 0.055566 2.034400 2.083605
C -1.204030 2.384241 2.870147
H 0.259683 2.821255 1.342264
H 0.914108 2.017702 2.768883
H -1.089768 3.349373 3.375504
H -2.076027 2.449330 2.212255
H -1.409063 1.623488 3.628245
C 3.013657 0.594017 0.287567
C 4.437077 0.841763 -0.173100
H 2.755749 1.242714 1.128046
H 2.299848 0.791070 -0.516505
H 4.553233 1.883349 -0.487485
H 5.149431 0.645778 0.632190
H 4.692847 0.200196 -1.020240
H 1.006008 -1.459311 2.459936



N 2.112076 -3.312640 1.010982

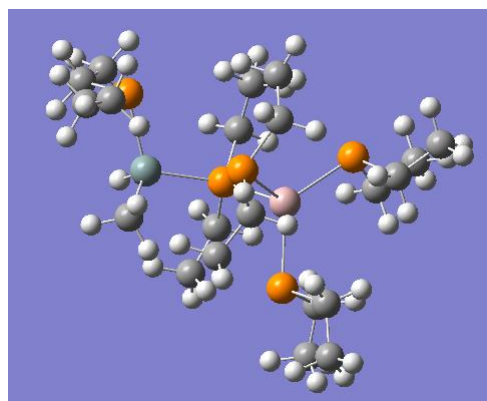
H 2.964316 -3.556664 0.528536

H 1.879633 -3.988140 1.723326

R=PEt₂+HCH₃

Total Energy=-3071.89217028

Al	0.98528800	0.18763700	0.39862500
Si	-2.74088200	-1.51999100	-0.45622300
P	2.25392900	-1.78402500	0.97558200
P	1.91361300	2.06836500	-0.77924900
P	-0.70853300	-0.78008700	-1.29382600
P	-4.38335300	0.09005400	-0.37503200
P	-0.59003800	0.78168500	2.13551400
C	3.40585300	-2.06317500	-0.50450300
C	3.98399300	-3.48163100	-0.59179800
H	4.21622100	-1.32759100	-0.47156400
H	2.84761500	-1.84917700	-1.42030000
H	4.62159000	-3.59279500	-1.47653700
H	4.58940100	-3.72998700	0.28278800
H	3.19096600	-4.23141900	-0.65557000
C	3.46681900	-1.08977400	2.25025700
C	4.36070000	-2.14831600	2.90738400
H	2.86788700	-0.60163100	3.02362300
H	4.08560100	-0.30629400	1.79976500
H	4.97023700	-1.70528700	3.70285900
H	3.76427700	-2.95152900	3.34840100
H	5.04779100	-2.60425000	2.19012200
C	-0.10632200	-2.27990700	-2.25018400
C	-0.02328700	-3.60481900	-1.48847700
H	0.87767300	-2.00800300	-2.64446800
H	-0.76835300	-2.38630500	-3.11535600
H	0.44147300	-4.36606900	-2.12149500
H	0.57066600	-3.52251900	-0.57604800
H	-1.01411900	-3.97413100	-1.21528300
C	-1.11905300	0.32496900	-2.75246900
C	-1.54850000	1.76041800	-2.44166400
H	-1.88403300	-0.19202900	-3.34084400
H	-0.21430300	0.33466700	-3.36975900
H	-1.81080900	2.27107200	-3.37336600
H	-2.41971100	1.79976100	-1.78629500
H	-0.74043900	2.32345000	-1.97320200
C	-5.60016100	-0.68769100	-1.59351000
C	-5.22458600	-0.48590100	-3.06256700
H	-6.55414300	-0.18778800	-1.39262000

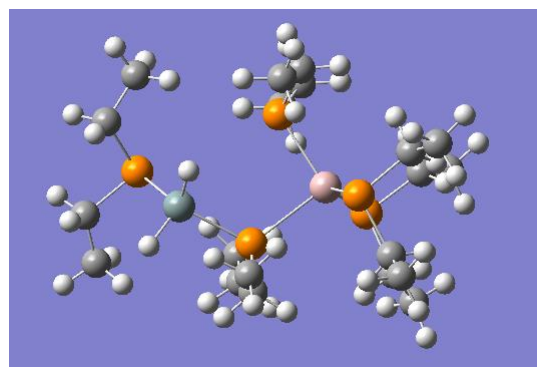


H	-5.75493600	-1.75039100	-1.38014400
H	-6.01868600	-0.85383700	-3.71920000
H	-5.06692300	0.57125200	-3.29341200
H	-4.31221800	-1.02631100	-3.32913900
C	-5.26293900	-0.35644700	1.23833900
C	-4.78869500	0.46936000	2.43673500
H	-5.20119800	-1.42647900	1.45712100
H	-6.32068300	-0.14871600	1.04246100
H	-5.33808500	0.18564900	3.34018800
H	-3.72223000	0.33599100	2.63102200
H	-4.95410500	1.53678300	2.26728100
C	-0.54219400	2.66143000	2.31708400
C	-1.23983600	3.42302700	1.18877300
H	0.48520600	3.02096900	2.43691000
H	-1.05096100	2.86952800	3.26541600
H	-1.29270000	4.49247300	1.41821700
H	-0.70241400	3.32120400	0.24395900
H	-2.26178500	3.06449400	1.03629400
C	0.20866800	0.33407500	3.78978000
C	0.07823000	-1.14310300	4.17035800
H	-0.31226500	0.94462600	4.53609700
H	1.25622400	0.64856500	3.82647500
H	0.53978300	-1.33763100	5.14424800
H	-0.97176400	-1.44161400	4.23908100
H	0.55797400	-1.80265700	3.44273800
C	3.17962000	2.66556300	0.49505200
C	3.70765000	4.08371000	0.24377200
H	4.01283900	1.95704700	0.55635100
H	2.68573100	2.64068700	1.47235300
H	4.37952800	4.40052600	1.04951400
H	4.26638000	4.15188700	-0.69294500
H	2.88808100	4.80483000	0.18676800
C	3.00902600	1.29116000	-2.11105000
C	3.54304300	2.28890600	-3.14645000
H	2.39800800	0.53948300	-2.62367400
H	3.83844200	0.74535400	-1.65119500
H	4.10575700	1.77617500	-3.93493000
H	2.72883100	2.84414000	-3.62007300
H	4.21448800	3.02214800	-2.69312300
H	-3.15807400	-2.47979400	-1.52845900
C	-2.46356600	-2.47203500	1.14775300
H	-1.48920200	-2.96521000	1.16246100
H	-2.50100500	-1.80207400	2.00677000
H	-3.23168300	-3.24167100	1.26749900

R=PEt2 +HH

Total Energy= -3032.55845413

Al	1.02630200	0.15590000	0.32424300
Si	-2.69670900	-1.44604700	-0.48836100
P	2.35909400	-1.75537100	0.93032800
P	1.89151900	2.06856500	-0.85301800
P	-0.64581000	-0.85487200	-1.36965200
P	-4.30761500	0.17560800	-0.28456400
P	-0.65449500	0.70818100	1.96741400
C	3.53775600	-2.01658100	-0.53017300
C	4.16027700	-3.41797100	-0.58133300
H	4.32379000	-1.25467200	-0.50607500
H	2.98029300	-1.84075700	-1.45524700
H	4.80857600	-3.53003300	-1.45809900
H	4.76522500	-3.62735800	0.30388100
H	3.39012500	-4.19237400	-0.63315100
C	3.50756800	-0.97093800	2.21216100
C	4.42409900	-1.96807700	2.93164300
H	2.86502400	-0.48118200	2.95014400
H	4.10784600	-0.17779400	1.75376000
H	4.98867800	-1.47392000	3.73020700
H	3.84895600	-2.78241900	3.38019500
H	5.15285300	-2.41575000	2.25089900
C	-0.11583600	-2.44918000	-2.20378000
C	-0.04889100	-3.68263800	-1.29893800
H	0.86439400	-2.25046200	-2.64827200
H	-0.80586900	-2.62440000	-3.03549100
H	0.34657700	-4.53383700	-1.86042400
H	0.59640200	-3.52421600	-0.43263600
H	-1.03742500	-3.96900800	-0.93199000
C	-1.01255800	0.19197900	-2.87797700
C	-1.47906400	1.62545400	-2.61191700
H	-1.74545300	-0.35111400	-3.48334100
H	-0.08396700	0.20194900	-3.45864000
H	-1.70184900	2.12006400	-3.56206600
H	-2.38292200	1.66128400	-2.00081900
H	-0.70737500	2.20906600	-2.10811500
C	-5.50025800	-0.44099500	-1.61419000
C	-5.07671600	-0.10514200	-3.04505600
H	-6.44916400	0.05908400	-1.39029600
H	-5.68359400	-1.51552800	-1.51168400
H	-5.85285600	-0.39881500	-3.75791900
H	-4.89885400	0.96600200	-3.17136200
H	-4.16200400	-0.63065400	-3.33429400



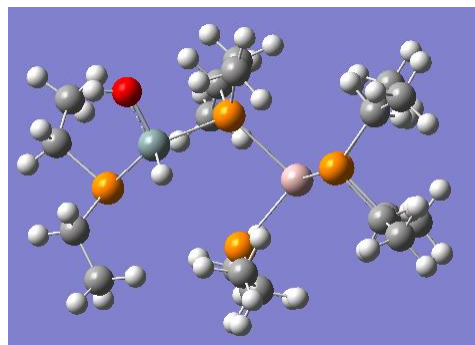
C	-5.22385900	-0.51513900	1.21723600
C	-4.65748500	-0.05551000	2.56153700
H	-5.28706700	-1.60773100	1.17591400
H	-6.24978200	-0.14681400	1.10348100
H	-5.26051400	-0.45178700	3.38455600
H	-3.62729500	-0.38565200	2.70544000
H	-4.65840600	1.03460600	2.63931900
C	-0.50758000	2.55331100	2.33859200
C	-1.13163500	3.45367100	1.26921400
H	0.53182700	2.84435400	2.52168400
H	-1.03573900	2.69886600	3.28793200
H	-1.10212400	4.50321100	1.58064600
H	-0.59913100	3.38255200	0.31794800
H	-2.17684200	3.18792300	1.08838800
C	-0.07787200	0.02791400	3.63225800
C	-0.26364400	-1.48386100	3.78633200
H	-0.68799200	0.54484000	4.38191800
H	0.95893900	0.30836200	3.84416100
H	0.02998200	-1.81201900	4.78899900
H	-1.30878800	-1.77105800	3.63854200
H	0.33742200	-2.04810300	3.06883500
C	3.14421500	2.70776500	0.41397500
C	3.62633100	4.14066100	0.15426700
H	3.99918500	2.02543100	0.47168900
H	2.65781600	2.67124000	1.39433800
H	4.29348200	4.48094600	0.95432100
H	4.17651500	4.22272900	-0.78634900
H	2.78440700	4.83580300	0.10054200
C	3.00813400	1.32873600	-2.18929700
C	3.48684100	2.34007400	-3.23840200
H	2.42975800	0.54433400	-2.69054100
H	3.86523700	0.82573200	-1.73122900
H	4.06431800	1.84576000	-4.02798500
H	2.64386600	2.85365100	-3.70880100
H	4.12866700	3.10740800	-2.79893400
H	-2.42106200	-2.11703800	0.80369800
H	-3.19177300	-2.48475900	-1.44553500

R=PEt2 +HOH

Total Energy= -3107.84903868

Al	1.05040900	-0.07352300	-0.25819000
Si	-2.65548900	-0.79945600	1.29035900
P	2.39680400	-1.92167400	0.48694200
P	1.90362100	2.14402600	-0.63524600
P	-0.63500200	-0.78661300	-1.83084900

P	-4.20759500	0.19621100	-0.08714700
P	-0.63779500	0.26698300	1.63737200
C	3.54924500	-2.12237300	-1.00600300
C	4.16470300	-3.52168000	-1.13464600
H	4.33807700	-1.36339200	-0.96170900
H	2.97286300	-1.90569600	-1.91041500
H	4.79132400	-3.59446600	-2.03099800
H	4.78979600	-3.77358100	-0.27443000
H	3.38853100	-4.28805800	-1.20548200
C	3.56764600	-1.18478700	1.77524300
C	4.49320400	-2.21448100	2.43454600
H	2.94121500	-0.72286200	2.54581300
H	4.16056900	-0.37515200	1.33940200
H	5.08405000	-1.75671900	3.23592300
H	3.92346300	-3.04212200	2.86578100
H	5.19819300	-2.64214400	1.71706500
C	-0.06071400	-2.39767200	-2.62998000
C	-0.26036700	-3.63529000	-1.75087000
H	0.98030000	-2.33031100	-2.96092600
H	-0.66107000	-2.49955700	-3.54146800
H	0.03638100	-4.54354300	-2.28596700
H	0.33258100	-3.58723300	-0.83424400
H	-1.30873800	-3.75038700	-1.46066600
C	-0.56843200	0.33826800	-3.34395800
C	-1.14505500	1.73649300	-3.10990000
H	-1.15903700	-0.17468900	-4.11180300
H	0.45032700	0.40763000	-3.74019100
H	-1.16462100	2.30836500	-4.04362300
H	-2.16830000	1.68376500	-2.72871100
H	-0.54974900	2.30646700	-2.39250700
C	-5.05067600	-1.36022400	-0.76154800
C	-4.48033300	-1.85496500	-2.09169100
H	-6.09803300	-1.06814600	-0.89702000
H	-5.05510100	-2.16963900	-0.02326000
H	-5.04320200	-2.72310200	-2.44924100
H	-4.53872500	-1.07784600	-2.85825600
H	-3.43136400	-2.14024100	-2.00116900
C	-5.52492100	0.66049700	1.18765600
C	-5.18943300	1.89041100	2.03381500
H	-5.78753700	-0.18789600	1.83022600
H	-6.41831500	0.86502300	0.58722700
H	-6.03834300	2.16801900	2.66607000
H	-4.33874800	1.70705700	2.69396500
H	-4.95046200	2.75293600	1.40630600

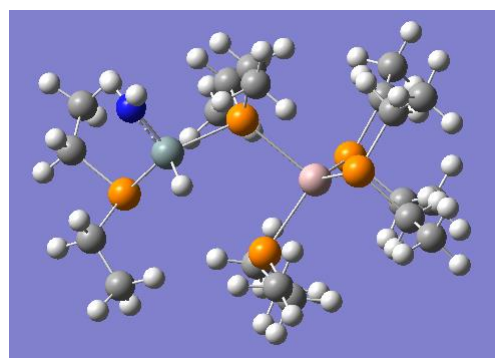


C	-1.06324500	2.03835900	2.06539500
C	-1.53741300	2.92456200	0.91116200
H	-0.15504900	2.45710200	2.51161900
H	-1.81006800	2.00166800	2.86430100
H	-1.80969200	3.91194000	1.29592900
H	-0.75422400	3.06422600	0.16499400
H	-2.41420500	2.51388800	0.40712400
C	-0.13275200	-0.36236900	3.32860500
C	-0.00845200	-1.88124500	3.47615700
H	-0.86613800	0.02353000	4.04087400
H	0.82177400	0.12543100	3.55275100
H	0.38903600	-2.12240000	4.46644200
H	-0.98269800	-2.36572000	3.39093200
H	0.65912200	-2.32380500	2.73422900
C	3.07854300	2.45557000	0.81715600
C	3.36723600	3.94121400	1.06845700
H	4.01398900	1.90909600	0.65817200
H	2.62860500	2.02341700	1.71713200
H	4.03592700	4.07462800	1.92670100
H	3.83975100	4.41524800	0.20486100
H	2.44601300	4.49409600	1.27234700
C	3.10478000	1.80441400	-2.05499800
C	3.76553200	3.06131600	-2.63353700
H	2.52044700	1.31304400	-2.84027400
H	3.87365600	1.08684800	-1.74850100
H	4.36645800	2.81713300	-3.51665000
H	3.01761900	3.80192500	-2.92935500
H	4.43314100	3.53824000	-1.91104000
H	-2.34789600	-2.17312000	0.81856900
O	-3.20526900	-0.86492100	2.88439800
H	-4.07327100	-1.21926300	3.09649100

R=PEt2 +HNH2

Total Energy=-3087.95822329

Al	1.19555800	-0.06630500	-0.22281800
Si	-2.74055300	-0.51900800	1.11899100
P	2.50028300	-1.57346000	1.12983200
P	2.04743700	2.03900300	-1.02914600
P	-0.21496000	-1.25411900	-1.78249600
P	-4.03007800	0.09880100	-0.68531100
P	-0.72978600	0.65139500	1.33335600
C	3.84630600	-2.08181300	-0.10489700
C	4.49917900	-3.43408500	0.20914000
H	4.60785800	-1.29595000	-0.15726800



H	3.39448600	-2.13021400	-1.09979800
H	5.24474600	-3.69643600	-0.55031100
H	5.00375300	-3.42874700	1.17851200
H	3.75418700	-4.23340400	0.23728200
C	3.47127400	-0.45882900	2.30865800
C	4.33645400	-1.22332800	3.31821100
H	2.73736000	0.14513500	2.85302700
H	4.09011600	0.24833700	1.74864700
H	4.80379700	-0.53844400	4.03487500
H	3.74320000	-1.94858300	3.88203200
H	5.14200000	-1.77368700	2.82533900
C	0.55291300	-2.95430000	-2.08000900
C	0.27249700	-3.96398100	-0.96387700
H	1.62853300	-2.88686600	-2.27062400
H	0.10343600	-3.31313500	-3.01312200
H	0.68389400	-4.94734800	-1.21534500
H	0.71521000	-3.65790400	-0.01265900
H	-0.80264200	-4.08653900	-0.80402800
C	0.05946300	-0.50467600	-3.49338500
C	-0.60767000	0.85895500	-3.68896200
H	-0.37359800	-1.22533600	-4.19683300
H	1.12541300	-0.44540300	-3.73796100
H	-0.50381300	1.19683700	-4.72557200
H	-1.67509500	0.81427600	-3.45658200
H	-0.15899000	1.62492100	-3.05165200
C	-4.89531400	-1.56034200	-0.95795500
C	-4.12279400	-2.53545300	-1.84752500
H	-5.84502000	-1.29846500	-1.43809000
H	-5.15485100	-2.02512600	-0.00122100
H	-4.70451800	-3.44927400	-2.00526500
H	-3.91111100	-2.09799800	-2.82623000
H	-3.16366400	-2.81666800	-1.40969300
C	-5.46196600	0.95706800	0.20205700
C	-5.18388400	2.39310100	0.65350700
H	-5.82430900	0.34729300	1.03526300
H	-6.26786700	0.96868100	-0.54019200
H	-6.08136200	2.84281400	1.08895400
H	-4.39511200	2.45031900	1.41052400
H	-4.87183600	3.02337200	-0.18258400
C	-1.16779400	2.47101100	1.27089800
C	-1.51465800	3.03262900	-0.11051400
H	-0.30495000	3.00238400	1.68553400
H	-1.99042300	2.63290100	1.97613000
H	-1.83609200	4.07421200	-0.01570100

H	-0.65151700	3.01143400	-0.77693200
H	-2.32221200	2.47861300	-0.59222000
C	-0.39320800	0.47778200	3.17006500
C	-0.19384500	-0.94971700	3.68752600
H	-1.22739100	0.95647000	3.69270900
H	0.49481100	1.08281600	3.37941000
H	0.03502900	-0.93001700	4.75707400
H	-1.09048500	-1.56105700	3.55877300
H	0.62186500	-1.46773600	3.18016200
C	2.99837100	2.77312600	0.43586500
C	3.18399200	4.29355100	0.34784700
H	3.97070100	2.27788400	0.52696000
H	2.45390100	2.53270400	1.35476700
H	3.72610200	4.67781500	1.21977400
H	3.74488900	4.58290700	-0.54410600
H	2.21994400	4.80763600	0.29928200
C	3.45083500	1.43063000	-2.13988100
C	4.16917400	2.54590100	-2.90888600
H	2.99906400	0.73576700	-2.85555500
H	4.17708100	0.84881000	-1.56197700
H	4.90140300	2.13007700	-3.61003700
H	3.46119200	3.15159900	-3.48100100
H	4.71084900	3.21823300	-2.23805400
H	-2.30975200	-1.93295300	1.02883900
N	-3.67186300	-0.40286100	2.58337700
H	-4.22669100	0.40423500	2.82479400
H	-3.46239300	-0.96077600	3.39825400

R=SEt +HCH3

Total Energy=-2960.008619

Al 1.248375 0.129702 -0.609377

Si -1.905039 -1.804301 -0.991666

S 2.230792 0.883896 1.261446

S -3.442458 -0.305672 -0.878278

S -0.294858 -1.490942 0.528911

S 0.030276 1.548155 -1.829679

S 2.321681 -1.278417 -1.966877

C -4.764288 -1.118161 0.149983

C -5.958844 -0.176435 0.252975

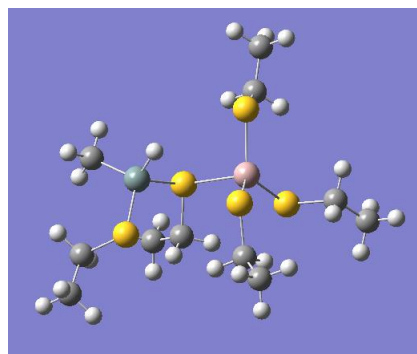
H -4.366394 -1.342416 1.140716

H -5.054912 -2.055798 -0.324423

H -6.749329 -0.641569 0.849448

H -5.686213 0.766720 0.732126

H -6.371164 0.052648 -0.732270

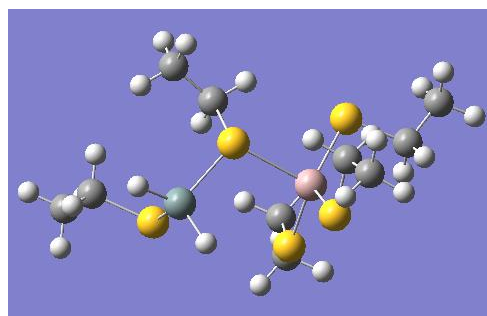


C -1.108759 -0.645037 1.971588
C -1.666385 -1.632313 2.987564
H -1.873273 0.025771 1.578982
H -0.316997 -0.033213 2.403835
H -2.101108 -1.084511 3.829636
H -2.449987 -2.264542 2.562415
H -0.885278 -2.285928 3.380629
C -0.695325 2.716754 -0.577067
C -0.982981 4.070101 -1.217349
H -0.002681 2.821225 0.259395
H -1.617390 2.272619 -0.197148
H -1.435583 4.747716 -0.484959
H -0.067713 4.535350 -1.590896
H -1.674774 3.973639 -2.057964
C 3.409313 2.147700 0.566348
C 4.141186 2.863167 1.695405
H 2.846916 2.858820 -0.040917
H 4.117459 1.637084 -0.088251
H 4.840084 3.599653 1.284966
H 3.443092 3.388836 2.351713
H 4.712401 2.160371 2.307004
C 3.324959 -2.302916 -0.780214
C 4.282276 -3.207550 -1.547511
H 2.646409 -2.898756 -0.166490
H 3.872254 -1.635470 -0.113654
H 4.871016 -3.813416 -0.850250
H 3.742810 -3.887223 -2.212241
H 4.975938 -2.624382 -2.158024
H -1.182815 -1.643463 -2.264150
C -2.556174 -3.548342 -0.762426
H -3.020089 -3.711176 0.212567
H -3.291652 -3.788359 -1.535788
H -1.728781 -4.256985 -0.857694

R=SEt +HH

Total Energy=-2920.670502

Al 1.242398 0.101698 -0.565458
Si -1.889157 -1.865897 -0.780285
S 2.180423 0.973220 1.273033
S -3.365951 -0.315624 -0.743178
S -0.204227 -1.576439 0.634214
S -0.117574 1.350997 -1.822228
S 2.393254 -1.263739 -1.896616
C -4.743364 -1.130071 0.214882

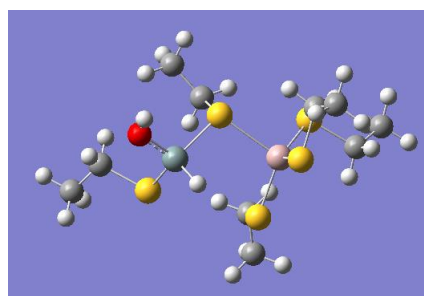


C -5.961614 -0.214311 0.202025
H -4.409837 -1.313567 1.237167
H -4.974561 -2.089003 -0.249559
H -6.780554 -0.677599 0.760296
H -5.743541 0.750794 0.665455
H -6.310305 -0.029221 -0.816426
C -0.973299 -0.782044 2.129666
C -1.593425 -1.801479 3.074816
H -1.694779 -0.041673 1.783256
H -0.147882 -0.248265 2.600564
H -2.002548 -1.286732 3.949746
H -2.408462 -2.357531 2.605010
H -0.853675 -2.523641 3.425536
C -0.780781 2.634827 -0.650173
C -1.242816 3.864869 -1.422866
H -0.005996 2.894726 0.071910
H -1.615412 2.194412 -0.101889
H -1.651300 4.612923 -0.734556
H -0.416462 4.323088 -1.971397
H -2.022989 3.611160 -2.144963
C 3.424862 2.146337 0.534613
C 4.206739 2.845312 1.640216
H 2.897537 2.875131 -0.083226
H 4.095724 1.580941 -0.114092
H 4.938393 3.535089 1.206589
H 3.544848 3.420634 2.292288
H 4.746945 2.125867 2.260462
C 3.372226 -2.291202 -0.692590
C 4.345665 -3.192002 -1.444146
H 2.681961 -2.890717 -0.095957
H 3.905936 -1.626078 -0.012558
H 4.921424 -3.799582 -0.737723
H 3.819411 -3.869709 -2.121166
H 5.050383 -2.606088 -2.039192
H -1.212210 -1.986438 -2.081220
H -2.551595 -3.127605 -0.372860

R=SEt +HOH

Total Energy=-2995.966579

Al 1.237985 0.114126 -0.582430
Si -1.926201 -1.737203 -0.893224
S 2.213387 0.916877 1.267491
S -3.403714 -0.209902 -0.728658
S -0.254832 -1.549208 0.564643



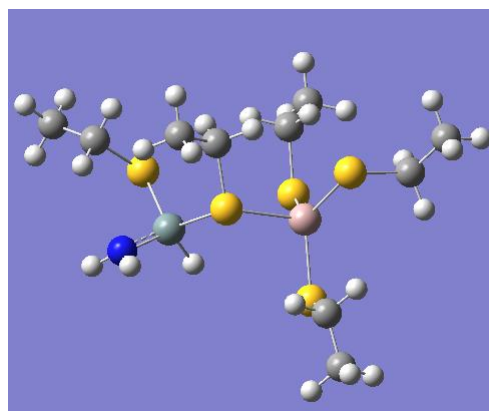
S -0.085207 1.443551 -1.797644
S 2.342528 -1.254117 -1.953320
C -4.758620 -1.048478 0.244465
C -6.060597 -0.285507 0.034325
H -4.473085 -1.051507 1.296964
H -4.836285 -2.079261 -0.094073
H -6.859249 -0.753725 0.617856
H -5.978773 0.755417 0.357082
H -6.361052 -0.291665 -1.015639
C -1.018226 -0.782299 2.078122
C -1.661829 -1.818496 2.988751
H -1.727027 -0.024135 1.744720
H -0.188129 -0.273704 2.568249
H -2.074001 -1.320911 3.872291
H -2.476265 -2.350477 2.492047
H -0.934324 -2.557807 3.330104
C -0.727124 2.693200 -0.577084
C -1.072210 3.997722 -1.286065
H 0.024112 2.855605 0.196836
H -1.613965 2.272414 -0.099997
H -1.473960 4.722729 -0.569666
H -0.191179 4.438725 -1.758289
H -1.824430 3.841705 -2.063434
C 3.429327 2.128466 0.543349
C 4.199468 2.828062 1.656752
H 2.885196 2.854607 -0.062962
H 4.110428 1.586987 -0.115067
H 4.916562 3.537775 1.231017
H 3.527694 3.381511 2.317572
H 4.755136 2.111418 2.266513
C 3.336111 -2.297067 -0.774994
C 4.291426 -3.197995 -1.549211
H 2.652459 -2.896120 -0.169999
H 3.885019 -1.639977 -0.099395
H 4.875520 -3.813982 -0.857047
H 3.750637 -3.867754 -2.222842
H 4.989451 -2.611591 -2.151560
H -1.230156 -1.738262 -2.188133
O -2.703300 -3.169467 -0.575936
H -2.250430 -4.014575 -0.650434

R=SEt +HNH2

Total Energy=-2976.076952

Al 1.273635 0.127479 -0.644797

Si -1.938102 -1.742556 -0.974718
S 2.298181 0.814946 1.229200
S -3.531429 -0.313155 -0.919821
S -0.317948 -1.441469 0.515637
S 0.107150 1.611510 -1.832478
S 2.268585 -1.314114 -2.025185
C -4.689970 -0.955889 0.389465
C -6.135817 -0.713409 -0.027547
H -4.462855 -0.433462 1.319757
H -4.491010 -2.016936 0.534967
H -6.812132 -1.058013 0.761236
H -6.335503 0.347456 -0.196631
H -6.381517 -1.251086 -0.945877
C -1.122057 -0.571799 1.951489
C -1.737547 -1.543315 2.948187
H -1.851101 0.131746 1.549457
H -0.311807 0.005256 2.397228
H -2.171233 -0.983737 3.783146
H -2.530509 -2.143804 2.497579
H -0.987227 -2.223557 3.356416
C -0.654573 2.715796 -0.543676
C -0.843401 4.126384 -1.090491
H -0.017544 2.726334 0.342464
H -1.617920 2.285285 -0.263050
H -1.320551 4.764264 -0.338197
H 0.113488 4.578356 -1.362053
H -1.476763 4.126771 -1.981194
C 3.452492 2.111905 0.554978
C 4.179829 2.815098 1.694637
H 2.875381 2.825724 -0.034901
H 4.165014 1.625898 -0.113497
H 4.866256 3.569320 1.295513
H 3.477818 3.317831 2.364600
H 4.764161 2.108686 2.289491
C 3.309881 -2.337968 -0.871198
C 4.254530 -3.229611 -1.668745
H 2.650967 -2.943311 -0.245396
H 3.867963 -1.670996 -0.213273
H 4.863377 -3.837637 -0.990911
H 3.704065 -3.907121 -2.326684
H 4.929763 -2.636516 -2.290218
H -1.267356 -1.553234 -2.271993
N -2.528866 -3.316701 -0.587667
H -3.219209 -3.765242 -1.175016



H -1.912898 -3.996892 -0.164926

R=OEt +HCH3

Total Energy=-1148.573288

Al -1.015424 0.080680 0.123118

Si 1.850023 -0.593772 0.227330

O 2.747865 0.823379 0.237049

O 0.449153 0.455518 1.119577

O 0.317522 -0.869199 -0.750886

O -2.125477 -1.082621 0.725101

O -1.592937 1.482882 -0.675642

C -2.767257 1.943037 -1.288351

H -3.577469 1.201434 -1.267094

H -3.127857 2.848907 -0.786694

H -2.572961 2.197170 -2.337277

C -3.411205 -1.133067 1.282118

H -3.967137 -1.979341 0.862554

H -3.357814 -1.274172 2.368918

H -3.993374 -0.221405 1.090115

C 0.172489 -1.818851 -1.814592

H 1.161004 -2.143225 -2.138158

H -0.404296 -2.675079 -1.461455

H -0.343840 -1.340139 -2.648142

C 0.695167 1.523514 2.033822

H -0.234969 1.774619 2.548909

H 1.434185 1.207385 2.771759

H 1.072427 2.396123 1.501663

C 3.975205 1.034219 -0.436426

H 4.152550 0.281871 -1.213071

H 3.954381 2.022983 -0.901952

H 4.806087 1.001143 0.275771

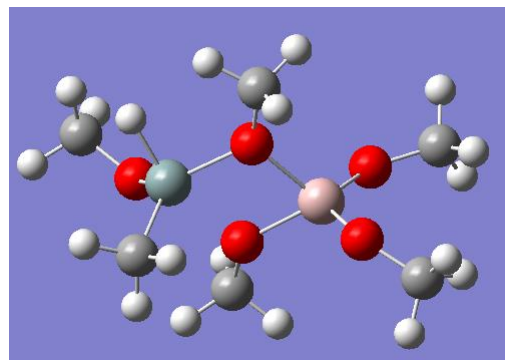
H 2.627060 -1.304899 -0.857346

C 2.016020 -1.754547 1.695307

H 2.964252 -2.298197 1.647917

H 1.964758 -1.237575 2.656416

H 1.211699 -2.497780 1.688797



R=OEt +HH

Total Energy=-1109.236284

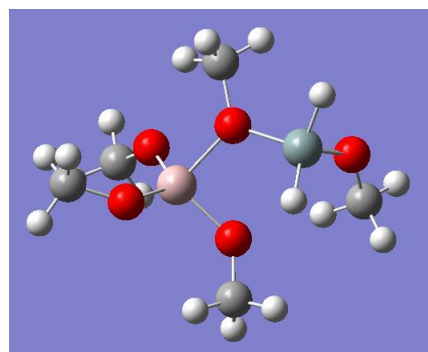
Al -0.902929 0.031632 -0.126526

Si 1.972013 -0.659944 1.001082

O 3.045188 0.260330 0.184733

O 0.453788 0.139192 1.247078

O 0.261985 -0.518088 -1.303742

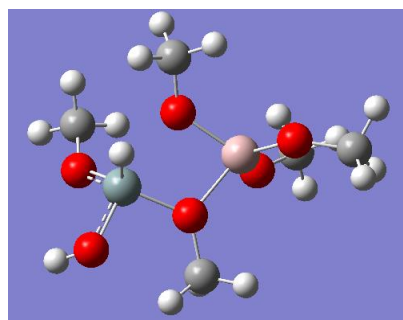


O -2.047375 -1.195198 0.271308
O -1.425677 1.680897 -0.088299
C -2.207749 2.516472 -0.899321
H -3.227047 2.128681 -1.033309
H -2.287404 3.506692 -0.436830
H -1.764392 2.649020 -1.895503
C -3.307796 -1.242922 0.882713
H -3.999516 -1.839599 0.275783
H -3.241970 -1.716381 1.871281
H -3.752917 -0.247049 1.016993
C 0.175694 -1.551216 -2.258768
H 1.073957 -2.179957 -2.214057
H -0.693701 -2.197506 -2.092363
H 0.108663 -1.135010 -3.271427
C 0.287891 1.058938 2.367519
H 0.029485 0.488312 3.259361
H 1.214117 1.610363 2.526941
H -0.507004 1.748338 2.096078
C 3.222729 0.530071 -1.207796
H 3.590028 -0.362708 -1.721343
H 2.286104 0.845422 -1.665092
H 3.970931 1.319108 -1.287592
H 2.511364 -0.719970 2.373560
H 1.697903 -1.989761 0.440082

R=OEt +HOH

Total Energy=-1184.540423

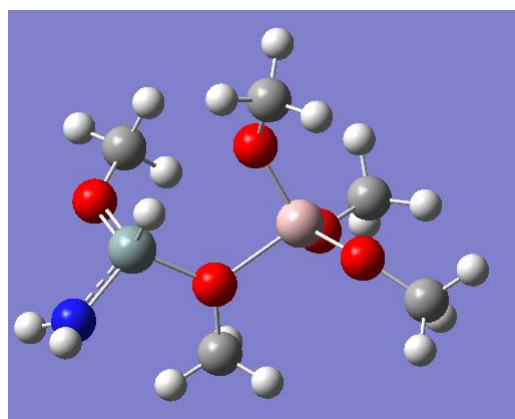
Al -0.849702 -0.011913 -0.002713
Si 1.933797 -0.815299 0.736100
O 2.921691 0.159502 -0.154938
O 0.461172 -0.066992 1.352398
O 0.459837 -0.796277 -0.922493
O -2.167897 -1.089930 0.210553
O -1.133950 1.673284 -0.193610
C -2.053255 2.518680 -0.831569
H -3.058426 2.079929 -0.892652
H -2.133254 3.461522 -0.279119
H -1.728732 2.756628 -1.852885
C -3.517138 -1.040350 0.590372
H -4.145991 -1.490610 -0.186726
H -3.673632 -1.606674 1.516431
H -3.874158 -0.015135 0.759135
C 0.389738 -1.809431 -1.910790
H 1.135727 -2.582809 -1.699578



H -0.596346 -2.281788 -1.920975
H 0.596230 -1.388109 -2.900034
C 0.359449 0.677066 2.594054
H -0.627423 0.484529 3.014188
H 1.134886 0.330715 3.270250
H 0.472346 1.739103 2.378842
C 2.852436 0.700533 -1.466350
H 2.831213 -0.088269 -2.222452
H 1.971219 1.332151 -1.588269
H 3.751289 1.302336 -1.611391
H 1.813005 -2.251178 0.466316
O 2.795612 -0.803105 2.176154
H 3.643220 -0.350548 2.174711

R=OEt +HNH2

Total Energy=-1164.648395
Al -0.793861 -0.145604 -0.194845
Si 2.130944 -0.819140 0.860813
O 3.018497 0.268390 0.025143
O 0.558086 -0.149731 1.185879
O 0.234055 -0.853786 -1.407657
O -2.087007 -1.169241 0.312378
O -1.069553 1.566710 -0.245384
C -1.827673 2.416590 -1.064045
H -2.888783 2.131074 -1.092285
H -1.771579 3.442079 -0.681081
H -1.456634 2.426754 -2.098398
C -3.365772 -1.003365 0.859281
H -4.127028 -1.427214 0.192197
H -3.442182 -1.526314 1.821589
H -3.621470 0.052030 1.030385
C 0.085952 -2.007384 -2.199909
H 0.903170 -2.713644 -2.001320
H -0.859762 -2.527062 -2.005856
H 0.122450 -1.745066 -3.264237
C 0.282500 0.670944 2.359209
H -0.686607 0.366821 2.752563
H 1.058207 0.493755 3.100602
H 0.249323 1.714103 2.052443
C 2.699479 1.097242 -1.095886
H 2.377031 0.494467 -1.944091
H 1.901044 1.797936 -0.841363
H 3.603745 1.651817 -1.348422
H 1.867608 -2.128355 0.259316



N 2.951902 -0.992253 2.353090

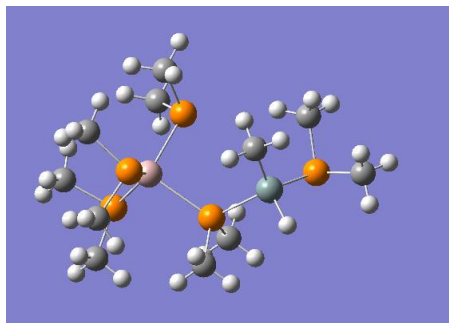
H 2.981628 -1.871660 2.846288

H 3.742188 -0.405701 2.576270

R=PMe₂+HCH₃

Total Energy=-2678.70531754

Al	-1.35904900	0.18566900	-0.03903000
Si	2.58728500	-0.89571300	0.67116400
P	-1.87005300	-0.32849700	2.25372800
P	-2.67921500	-0.30267000	-1.98666400
P	-0.10356600	2.21256300	-0.35325500
P	4.08400600	-0.02044400	-0.81857200
P	0.58065800	-1.39055600	-0.36953900
C	-3.11788600	0.98763300	2.74206800
H	-2.63183100	1.96359000	2.78779900
H	-3.97160800	1.05843000	2.06244000
H	-3.49824400	0.76504100	3.74310500
C	-0.53229300	3.32406900	1.09553800
H	-0.20959000	2.86241000	2.03160900
H	0.00182000	4.27317000	0.99553500
H	-1.60063800	3.54329900	1.17110000
C	-0.98743000	3.12468800	-1.73200100
H	-0.96980000	2.52429500	-2.64388100
H	-2.02937800	3.36110900	-1.49838000
H	-0.46604500	4.06309100	-1.94084300
C	3.97444500	1.80695600	-0.44759000
H	4.70030000	2.33051100	-1.07510800
H	2.97728400	2.17636200	-0.69566700
H	4.18455900	2.04774500	0.59764600
C	5.65571200	-0.45336200	0.10932100
H	5.67928400	-0.08881200	1.13976500
H	5.79979500	-1.53553700	0.11600900
H	6.50094800	-0.01266600	-0.42566800
C	0.99776300	-1.60530700	-2.15935600
H	0.11349900	-1.95103700	-2.69780900
H	1.29762600	-0.64635400	-2.58258300
H	1.81336300	-2.31662300	-2.30202000
C	0.24324800	-3.12262700	0.20255100
H	1.08277500	-3.78382400	-0.02036500
H	0.07138400	-3.12682700	1.28028100
H	-0.65201800	-3.50847500	-0.28852400
C	-3.36294100	-2.03676100	-1.73516400
H	-2.56048700	-2.77374300	-1.82875900
H	-3.86036800	-2.19133200	-0.77517000

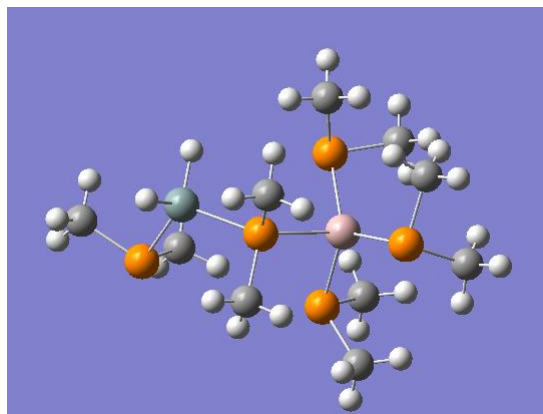


H	-4.08359700	-2.25102100	-2.52984800
C	-4.23900800	0.68721600	-1.63974600
H	-4.01100800	1.75535300	-1.66156600
H	-4.97001100	0.49537000	-2.43039800
H	-4.70779200	0.45415800	-0.67967700
C	-3.02942100	-1.80514500	2.16372800
H	-2.51487900	-2.66884800	1.73625000
H	-3.34107000	-2.08001600	3.17558700
H	-3.92878300	-1.61662600	1.57221000
H	3.11356400	-2.25586500	0.99654800
C	2.27885500	0.07254400	2.25681800
H	1.47538300	-0.37283800	2.84940900
H	3.18364400	0.09374300	2.87166300
H	1.99387000	1.10372100	2.03792300

R=PMe₂+HH

Total Energy=-2639.370165

Al	-0.894642	0.361380	0.315519
Si	2.393735	-1.881669	-0.986998
P	-1.037261	0.687505	-2.057454
P	-2.622653	-0.469693	1.765697
P	0.671414	-1.615114	0.502759
P	4.163069	-0.495361	-0.637305
P	0.593655	2.008181	1.218987
C	-1.773005	-0.904542	-2.735600
H	-1.029644	-1.704720	-2.685942
H	-2.678238	-1.238977	-2.223372
H	-2.014217	-0.762078	-3.793085
C	-0.217253	-3.238836	0.399036
H	-0.691825	-3.347187	-0.577443
H	0.463232	-4.077929	0.556529
H	-0.995002	-3.262818	1.165183
C	1.479514	-1.689427	2.165565
H	2.110410	-0.811174	2.307195
H	0.703843	-1.693011	2.933939
H	2.092719	-2.586660	2.272828
C	5.233300	-1.161782	-2.026833
H	6.128466	-0.538002	-2.093710
H	5.560491	-2.177933	-1.796720
H	4.742902	-1.159681	-3.003651
C	3.551725	1.087639	-1.412173
H	3.100932	0.952594	-2.397700
H	2.824116	1.554972	-0.746075
H	4.403168	1.767213	-1.505350

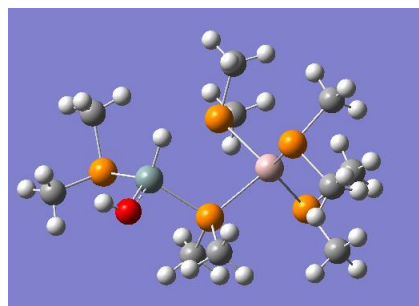


C 0.145186 2.183077 3.032152
H -0.897189 2.463775 3.201324
H 0.331697 1.243409 3.557481
H 0.780720 2.946156 3.490303
C -0.086484 3.626539 0.555315
H 0.504215 4.456509 0.953146
H 0.014285 3.646829 -0.532229
H -1.135050 3.803758 0.811168
C -3.618701 1.077482 2.144335
H -3.034667 1.750045 2.775140
H -3.936646 1.627442 1.254585
H -4.512867 0.797058 2.708357
C -3.843801 -1.329671 0.623338
H -3.400873 -2.239444 0.210513
H -4.722091 -1.631576 1.201422
H -4.182857 -0.706534 -0.208047
C -2.545609 1.802348 -2.194503
H -2.330689 2.772272 -1.739639
H -2.768028 1.980972 -3.250400
H -3.443351 1.393200 -1.722920
H 1.784211 -1.801767 -2.342479
H 2.871399 -3.277610 -0.769156

R=PMe₂+HOH

Total Energy=-2714.659097

Al -1.158270 0.229976 0.156772
Si 2.370477 -0.783180 -1.324076
P -2.126439 0.410389 -2.028729
P -2.161848 -0.433489 2.228238
P 0.499549 -1.603517 -0.268523
P 4.039625 -0.214641 0.142702
P 0.614928 1.821842 0.476839
C -3.486080 -0.887778 -2.070685
H -3.059134 -1.889813 -1.983304
H -4.232084 -0.764687 -1.281672
H -4.000772 -0.836848 -3.034501
C -0.042818 -3.020617 -1.326708
H -0.442262 -2.639132 -2.267384
H 0.794600 -3.681699 -1.549021
H -0.829098 -3.579821 -0.814754
C 1.138189 -2.410826 1.268505
H 1.605422 -1.662619 1.908885
H 0.307160 -2.857010 1.817424
H 1.871837 -3.185229 1.035184

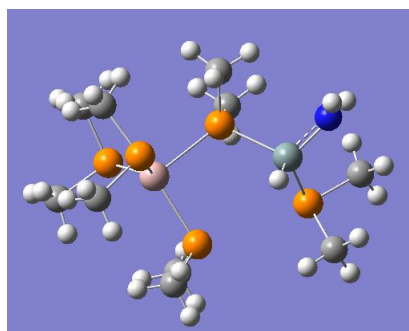


C 5.445852 -1.182130 -0.640654
 H 6.360266 -0.965645 -0.082344
 H 5.257328 -2.253930 -0.558245
 H 5.631064 -0.935579 -1.690774
 C 4.456944 1.498428 -0.478325
 H 4.661635 1.541283 -1.551307
 H 3.624808 2.163963 -0.247946
 H 5.340516 1.855209 0.057207
 C 0.418969 2.496747 2.211297
 H -0.537715 3.003464 2.365714
 H 0.494317 1.682828 2.935102
 H 1.220477 3.209274 2.425199
 C 0.190331 3.339036 -0.535281
 H 0.969279 4.096391 -0.408378
 H 0.153923 3.076866 -1.594891
 H -0.766487 3.788762 -0.256265
 C -3.436234 0.922977 2.491224
 H -2.928758 1.871860 2.681163
 H -4.119012 1.059825 1.648233
 H -4.032939 0.691744 3.378197
 C -3.306795 -1.854086 1.775061
 H -2.718699 -2.721223 1.461542
 H -3.873559 -2.155199 2.660902
 H -4.017551 -1.619032 0.979574
 C -3.197434 1.949165 -1.901080
 H -2.568367 2.831596 -1.770781
 H -3.750670 2.078453 -2.835687
 H -3.920341 1.916614 -1.081191
 H 1.964787 0.323491 -2.227910
 O 2.802580 -2.129973 -2.237674
 H 3.505878 -2.089782 -2.891482

R=PMe₂+HNH₂

Total Energy= -2694.76958929

Al	-1.10288800	0.31515500	0.05891700
Si	2.47268600	-0.76550200	-1.44158900
P	-2.24356100	0.38430600	-2.05809900
P	-1.96758000	-0.36497700	2.19200000
P	0.52042300	-1.54578600	-0.46684400
P	3.80236300	0.02312900	0.25295100
P	0.57643200	2.03419900	0.21326600
C	-3.59055200	-0.92086500	-1.93129900
H	-3.15230200	-1.91723900	-1.83805100
H	-4.26872700	-0.76621800	-1.08875100

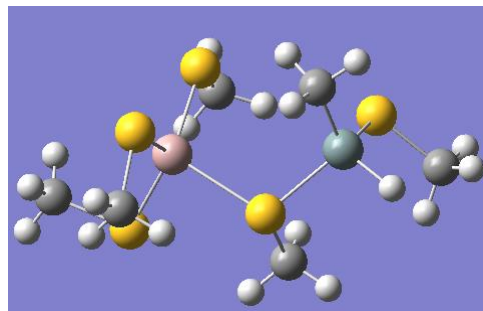


H	-4.18447400	-0.91181400	-2.84995300
C	-0.10889700	-2.82092400	-1.65245500
H	-0.48106400	-2.32853100	-2.55244000
H	0.68141200	-3.52079900	-1.93170200
H	-0.93254400	-3.37789000	-1.20065200
C	1.07444400	-2.55314900	0.98588300
H	1.53853300	-1.90200300	1.72718800
H	0.21353700	-3.03328800	1.45410200
H	1.78774500	-3.32658100	0.68978000
C	5.23075200	-1.18908100	0.11660500
H	6.04074200	-0.82923700	0.75647800
H	4.93440000	-2.16893400	0.50088200
H	5.61962000	-1.30502600	-0.89773800
C	4.55216600	1.48360300	-0.64322900
H	4.98617800	1.22935900	-1.61332700
H	3.77878000	2.24035100	-0.78050800
H	5.33700700	1.91050700	-0.01316900
C	0.61868200	2.51017400	2.02472000
H	-0.34206200	2.87303400	2.40018000
H	0.91817900	1.65062200	2.62719000
H	1.36277700	3.29724600	2.17730000
C	-0.17781300	3.59016100	-0.51167600
H	0.51909500	4.42178200	-0.37275900
H	-0.32539800	3.46535400	-1.58648300
H	-1.13283100	3.87003500	-0.05824500
C	-3.25168600	0.96593500	2.52967300
H	-2.75518600	1.92798100	2.67649000
H	-3.99162000	1.07889100	1.73244100
H	-3.78325400	0.73088700	3.45626100
C	-3.11650600	-1.80650300	1.81888700
H	-2.53841100	-2.66544000	1.46634800
H	-3.61807700	-2.11461800	2.74096900
H	-3.88197000	-1.58304400	1.07285900
C	-3.32470000	1.91557600	-1.93008200
H	-2.70350600	2.81223600	-1.90575000
H	-3.95775400	1.98063500	-2.81970700
H	-3.97457300	1.92308300	-1.05044700
H	2.02620100	0.25141900	-2.41939700
N	3.27157400	-1.99437800	-2.36922700
H	3.86000900	-2.71275400	-1.97649200
H	3.04169500	-2.17973700	-3.33421900

R=SMc+HCH3

Total Energy=-2763.393796

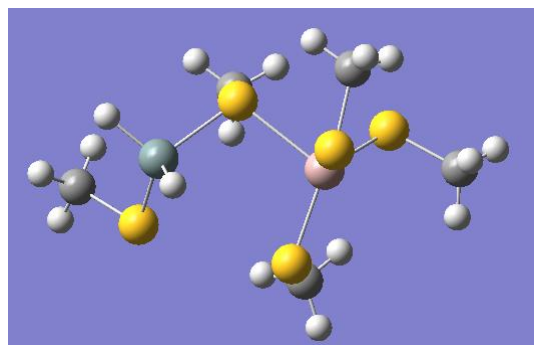
Al 1.190015 0.242607 -0.578547
 Si -2.196552 -1.612297 -0.593292
 S 2.034951 1.235398 1.244219
 S -3.495193 0.096814 -0.704752
 S -0.392508 -1.270096 0.668395
 S 0.032535 1.457259 -2.049735
 S 2.397987 -1.267988 -1.688252
 C 3.459751 2.153245 0.501262
 H 3.991325 2.632314 1.322722
 H 4.140719 1.477180 -0.014608
 H 3.116786 2.920542 -0.192028
 C 3.171456 -2.243140 -0.320640
 H 2.428160 -2.829157 0.219911
 H 3.886443 -2.923359 -0.782752
 H 3.698551 -1.597658 0.380756
 C -4.748445 -0.300815 0.592900
 H -4.330978 -0.217744 1.595324
 H -5.539471 0.439644 0.479961
 H -5.172309 -1.293027 0.447177
 C -1.067393 -0.353087 2.114509
 H -1.738036 -1.007527 2.669784
 H -0.218871 -0.084575 2.740217
 H -1.583985 0.548063 1.791302
 C -0.669517 2.836697 -1.038522
 H 0.008599 3.128817 -0.237821
 H -0.817348 3.683129 -1.708491
 H -1.631199 2.545836 -0.616808
 H -2.937533 -2.659258 0.153889
 C -1.590955 -2.165475 -2.265768
 H -2.418614 -2.619717 -2.817809
 H -1.215663 -1.319124 -2.843593
 H -0.785626 -2.898808 -2.180698



R=SMc+HH

Total Energy=-2724.052658

Al 1.226675 0.119282 -0.462457
 Si -2.021216 -1.667406 -0.413010
 S 2.125202 1.278959 1.228757
 S -3.380148 -0.027203 -0.629383
 S -0.308509 -1.297325 0.947909
 S -0.058570 1.158581 -1.963501
 S 2.384438 -1.481043 -1.488604
 C 3.489154 2.172640 0.353370
 H 4.059407 2.704016 1.114409

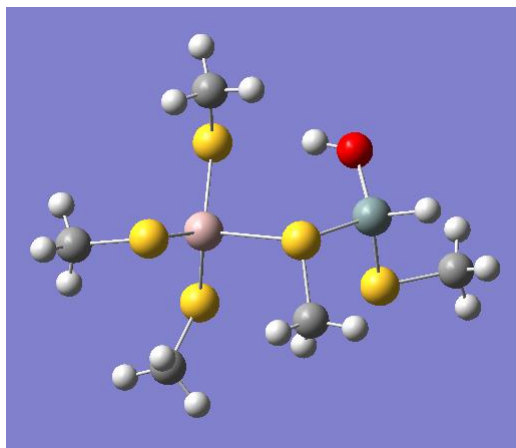


H 4.150440 1.477959 -0.163246
H 3.093504 2.895416 -0.359475
C 3.210760 -2.341683 -0.075286
H 2.492480 -2.903916 0.521335
H 3.929564 -3.037994 -0.506260
H 3.739291 -1.638066 0.566577
C -4.734430 -0.539601 0.520490
H -4.414975 -0.508560 1.561235
H -5.533762 0.186698 0.377670
H -5.112430 -1.530583 0.274930
C -1.034142 -0.257654 2.284077
H -1.720924 -0.862427 2.874537
H -0.204709 0.067007 2.908948
H -1.541564 0.610328 1.868622
C -0.606933 2.702860 -1.106148
H 0.071818 2.977671 -0.299857
H -0.624862 3.500762 -1.847722
H -1.611256 2.568236 -0.705455
H -1.372038 -2.049182 -1.676861
H -2.769757 -2.787563 0.205361

R=SMe+HOH

Total Energy=-2799.356364

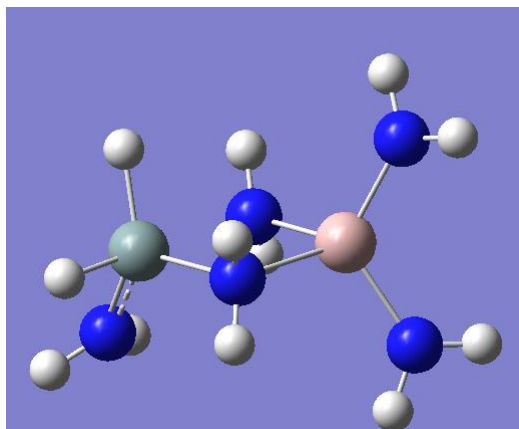
Al 0.991206 0.311309 -0.318739
Si -2.063323 -1.857159 0.478601
S 2.649677 0.888264 1.061959
S -3.443278 -0.447119 -0.343461
S -0.432187 -0.731200 1.478639
S -0.222202 1.895370 -1.304044
S 1.288860 -1.410253 -1.741537
C 3.704596 1.930082 -0.045790
H 4.541361 2.282590 0.556255
H 4.094096 1.350072 -0.881688
H 3.157615 2.792160 -0.426230
C 2.399980 -2.538397 -0.781358
H 1.846725 -3.079269 -0.014220
H 2.813801 -3.254035 -1.490542
H 3.210863 -1.979608 -0.317678
C -4.919861 -1.553242 -0.480432
H -5.153646 -2.028990 0.471604
H -5.751282 -0.910302 -0.765753
H -4.773535 -2.307007 -1.252048
C -1.268086 0.683628 2.310030
H -2.010159 0.300535 3.007876



R=NH₂+HH

Total Energy=-813.228652

Al -1.151294 0.147411 -0.027939
Si 1.735347 -0.673758 0.256171
H 0.050370 -0.894047 1.991131
H 0.537282 0.647191 1.894950
N 2.690954 0.571423 -0.468494
N -1.656170 1.879727 0.112867
N -2.439247 -1.121900 0.005767
N 0.242732 -0.275365 -1.286257
N 0.278552 -0.156594 1.326154
H 2.557826 0.947960 -1.393037
H 3.608904 0.766823 -0.097163
H 0.418733 0.483216 -1.939956
H 0.138153 -1.113292 -1.850848
H -2.534481 2.235980 -0.236740
H -1.099732 2.649336 0.456845
H -3.318127 -1.032457 0.495822
H -2.455333 -1.961743 -0.554717
H 1.533749 -2.089313 -0.166037
H 2.691710 -0.897656 1.416165



R=NH₂+HNH₂

Total Energy=-868.641064

Al -1.374732 0.011325 0.095940
Si 1.398252 -1.015476 0.434637
H -0.393622 -1.257251 2.071313
H 0.217699 0.245392 2.157228
N 2.124417 0.361962 -0.335288
N -1.430114 1.811791 -0.039387
N -2.950913 -0.875445 0.171714
N -0.102066 -0.935598 -1.027443
N -0.070049 -0.477001 1.502153
H 1.887578 0.756538 -1.232019
H 3.009675 0.703066 0.007807
H 0.163296 -0.473997 -1.892060
H -0.416665 -1.862654 -1.300656
H -2.209647 2.327623 -0.421475
H -0.672973 2.446151 0.171176
H -3.788787 -0.512445 0.603951
H -3.164196 -1.755678 -0.274623
H 2.392296 -1.034553 1.585695
N 1.477300 -2.736011 0.179462
H 2.195548 -3.252426 0.666602

H 1.175088 -3.220385 -0.651815

R=NH₂+HOH

Total Energy=-888.527878

Al 1.210793 0.093001 0.054261

Si -1.655474 -0.655788 -0.103035

H -0.058952 -1.020027 -1.909104

H -0.486780 0.541576 -1.862346

N 1.807076 1.779036 -0.208558

N 2.437872 -1.234010 0.114884

N -0.223841 -0.230856 1.312022

N -0.242850 -0.250214 -1.270122

H -0.506763 0.582522 1.851883

H -0.109730 -0.994844 1.971093

H 2.706073 2.103503 0.119241

H 1.251221 2.574856 -0.488628

H 3.328658 -1.207845 -0.360937

H 2.407363 -2.044182 0.716825

H -1.578952 -2.053227 0.418310

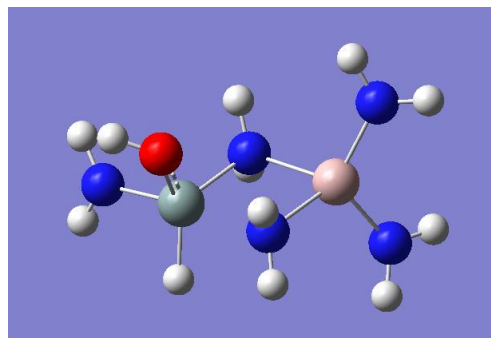
N -2.962713 -1.087923 -1.231518

H -3.186782 -2.058322 -1.396758

H -3.342221 -0.502184 -1.963704

O -2.321592 0.821574 0.396583

H -3.235228 0.941081 0.118302



R=F+HCH₃

Total Energy=-1072.264581

Al 1.062576 0.012416 0.384669

Si -2.105245 -0.723210 -0.314319

F 1.646111 1.315657 -0.479007

F -0.844765 0.256490 0.292584

F 0.957205 -1.469121 -0.419968

F 1.314932 -0.060834 2.034678

F -3.390514 0.191690 -0.007493

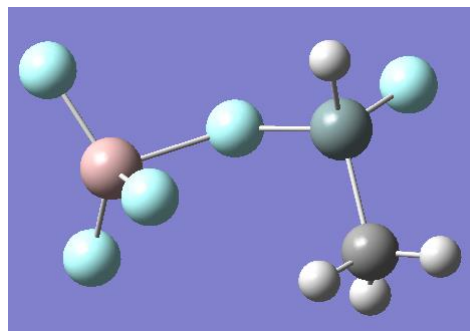
H -1.876946 -0.752421 -1.759900

C -2.108797 -2.279744 0.658413

H -2.947177 -2.916337 0.361125

H -1.181208 -2.831967 0.490530

H -2.203447 -2.077099 1.728389

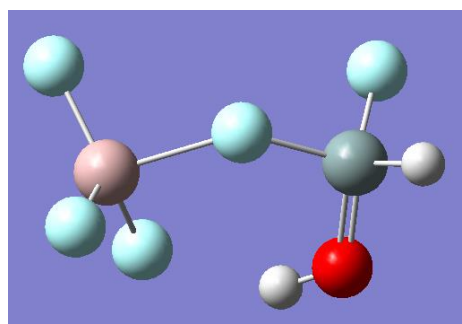


R=F+HOH

Total Energy=-1108.226635

Al 0.879821 -0.004559 0.543051

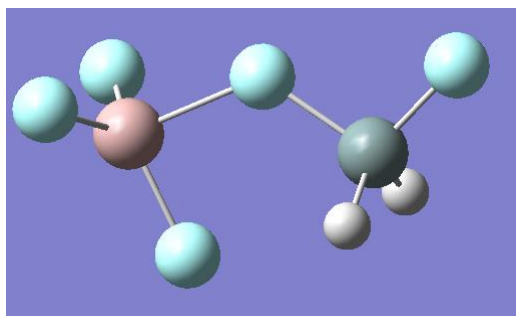
Si -2.286409 -0.641641 -0.414571



F 1.807648 0.352589 -0.795949
 F -0.907529 0.316386 -0.132082
 F 0.561089 -1.652576 0.804585
 F 0.935937 0.970151 1.892831
 F -3.186637 -0.294855 0.856448
 H -2.901234 -0.146342 -1.633654
 O -1.776372 -2.157669 -0.505461
 H -1.006190 -2.476480 -0.006548

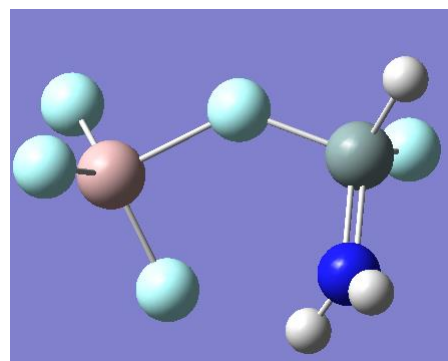
R=F+HH

Total Energy=-1032.916634
 13 1.066274 0.088268 0.399097
 14 -1.956340 -0.698497 -0.345311
 9 1.675127 1.352358 -0.500543
 9 -0.848669 0.390298 0.352409
 9 0.782173 -1.369321 -0.418520
 9 1.393710 -0.013823 2.030166
 9 -3.352719 0.050678 -0.097786
 1 -1.902979 -1.914239 0.461666
 1 -1.662351 -0.727230 -1.775162



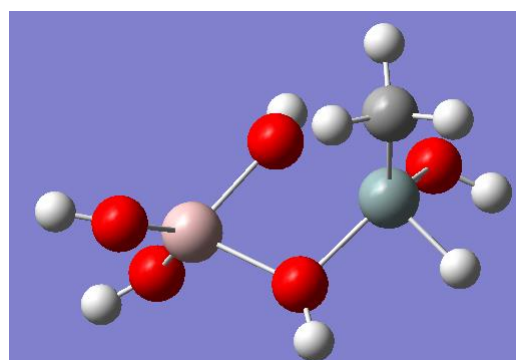
R=F+HNH2

Total Energy=-1088.337918
 Al 0.975763 -0.107776 0.400093
 Si -2.202416 -0.659713 -0.472649
 F 1.523356 1.464046 0.283923
 F -0.605220 -0.096798 -0.695495
 F 1.860759 -1.329378 -0.322447
 F 0.126041 -0.544367 1.795599
 F -2.857965 0.671146 0.126826
 H -2.705722 -0.943966 -1.811582
 N -2.173247 -1.970235 0.561946
 H -1.711153 -1.937830 1.462139
 H -2.463345 -2.896346 0.287595



R=OH+HCH3

Total Energy=-952.038198
 Al -1.061970 0.055625 0.185871
 Si 1.860289 -0.387798 0.061432
 O 2.571453 1.135700 0.174272
 O 0.424754 0.465182 1.147487
 O 0.307327 -0.704527 -0.833685
 O -2.029440 -1.263512 0.721060
 O -1.741187 1.499205 -0.463046

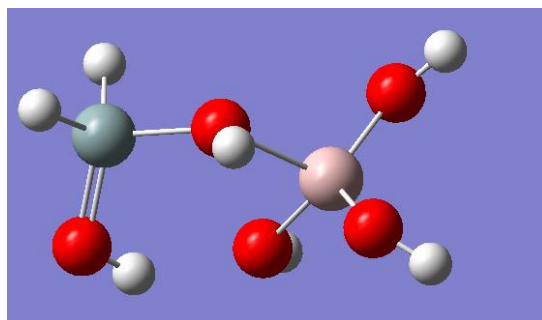


H -2.640554 1.670202 -0.739827
 H -2.901792 -1.259769 1.112512
 H 0.322688 -1.242906 -1.628404
 H 0.662023 1.363559 1.395549
 H 3.294218 1.316109 -0.432965
 H 2.640124 -0.900245 -1.131456
 C 2.197242 -1.632758 1.415712
 H 1.352530 -2.318382 1.533995
 H 3.085995 -2.229435 1.192872
 H 2.342295 -1.136077 2.377940

R=OH+HH

Total Energy=-912.708684

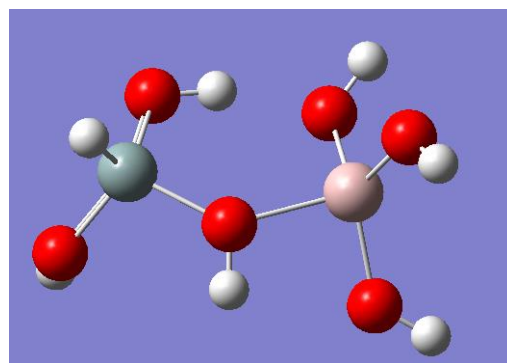
Al -1.027483 0.104884 -0.290584
 Si 1.958104 -0.600198 0.721865
 O 2.539966 0.312424 -0.499377
 O 0.337058 -0.092398 1.086299
 O 0.093612 0.076234 -1.652062
 O -2.118735 -1.225786 -0.408056
 O -1.488834 1.608242 0.451258
 H -2.183484 2.227462 0.233251
 H -2.900649 -1.391130 0.118484
 H -0.140856 -0.393547 -2.455647
 H 0.202786 0.681299 1.654633
 H 1.906716 0.396986 -1.243116
 H 2.754334 -0.349566 1.934958
 H 1.777280 -2.027214 0.408626



R=OH+HOH

Total Energy=-988.014724

Al -0.949239 0.218553 -0.317719
 Si 1.966340 -1.133966 0.657870
 O 2.339789 -0.731356 -0.861718
 O 0.367425 -0.501488 0.910945
 O 0.143694 0.487971 -1.678313
 O -2.166426 -0.910208 -0.792392
 O -1.294404 1.470504 0.839835
 H -1.997663 2.118210 0.852027
 H -2.963909 -1.147657 -0.319457
 H -0.181781 0.372309 -2.574151
 H 0.202744 -0.050825 1.753047
 H 1.664881 -0.218400 -1.379803
 H 1.923074 -2.568139 0.935284
 O 2.904541 -0.456900 1.822476



H 3.371684 0.372348 1.686809

R=OH+H2

Total Energy=-968.125707

Al -1.001571 0.210951 -0.325439

Si 1.935457 -1.140231 0.525837

O 2.392112 -0.423674 -0.856573

O 0.354436 -0.473612 0.864508

O 0.042586 0.477490 -1.724143

O -2.210796 -0.950829 -0.748832

O -1.346332 1.485292 0.807606

H -2.019683 2.163535 0.784933

H -2.993750 -1.179741 -0.247979

H -0.290069 0.292839 -2.605372

H 0.273158 0.024098 1.691237

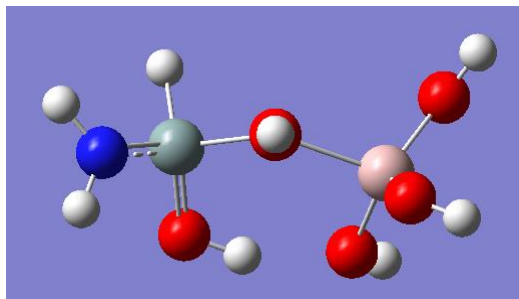
H 1.674700 -0.002351 -1.393269

H 1.715099 -2.593137 0.474565

N 2.954320 -0.749158 1.832849

H 3.259067 -1.434084 2.507424

H 3.552000 0.064317 1.815572



R=SH+HCH3

Total Energy=-2566.796719

Al 1.116227 -0.113933 -0.488211

Si -2.398994 -1.021093 1.135644

S 1.729763 2.027531 -0.295257

H 3.054789 1.766830 -0.373007

S -3.480173 0.197975 -0.271262

H -4.269394 0.755806 0.676419

S -0.382230 -0.187058 1.606141

S -0.216934 -0.703786 -2.178696

S 2.539884 -1.761970 -0.029812

H 2.948619 -1.260126 1.159627

H -0.744465 1.108960 1.727056

H -0.516207 0.559520 -2.557841

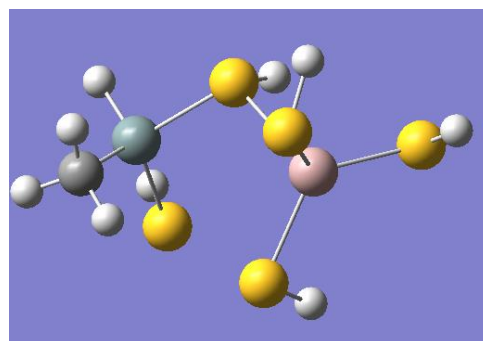
C -2.101016 -2.759425 0.542213

H -3.052505 -3.295817 0.492246

H -1.656473 -2.766417 -0.454175

H -1.438710 -3.303416 1.220993

H -3.118459 -0.949764 2.426862

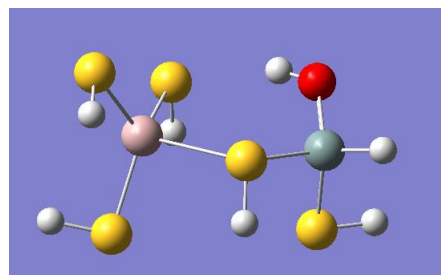


R=SH+HOH

Total Energy=-2602.757320

Al 1.132375 -0.296499 -0.395295

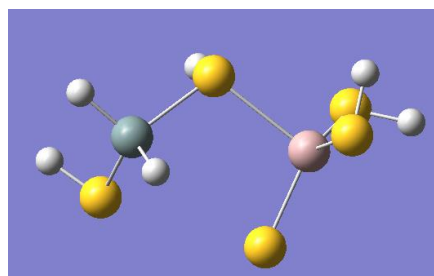
Si -2.467991 -0.898616 1.121363
 S 1.333169 1.922428 -0.266406
 H 2.594326 1.944365 -0.756375
 S -3.143524 1.021643 0.433522
 H -4.454004 0.680057 0.459747
 S -0.350388 -0.564150 1.718862
 S -0.129010 -1.177579 -2.038602
 S 2.858869 -1.625599 0.008632
 H 3.279683 -0.959213 1.109750
 H -0.460172 0.717755 2.134028
 H -0.672286 0.000401 -2.421394
 O -2.460445 -2.125816 0.051347
 H -1.930289 -2.065120 -0.765836
 H -3.225537 -1.353670 2.294707



R=SH+HH

Total Energy=-2527.454852

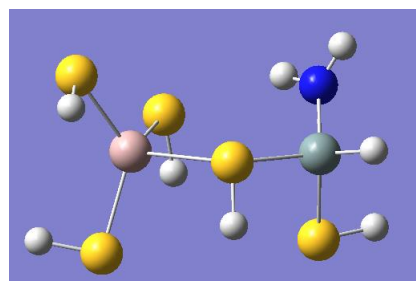
Al 1.225026 0.086243 -0.496634
 Si -2.152759 -1.156836 0.766289
 S 1.924207 2.143641 0.021998
 H 3.145105 1.991001 -0.541646
 S -3.376893 0.151061 -0.410126
 H -4.284505 0.333943 0.579272
 S -0.306423 -0.189818 1.546770
 S -0.144960 -0.211866 -2.237206
 S 2.544127 -1.686410 -0.259099
 H 3.074228 -1.293029 0.923169
 H -0.817695 1.049999 1.723767
 H -0.398937 1.105422 -2.411731
 H -1.628195 -2.301240 0.007142
 H -2.915139 -1.567411 1.963860



R=SH+HNH2

Total Energy=-2582.867322

Al 1.230952 -0.240521 -0.356738
 Si -2.365116 -0.907562 1.218476
 S 1.478631 1.980944 -0.301235
 H 2.730129 1.963545 -0.815343
 S -3.074757 0.843464 0.194922
 H -4.328221 0.359267 0.026342
 S -0.261940 -0.370453 1.750532
 S 0.021267 -1.174784 -1.992864
 S 2.932694 -1.574471 0.154637
 H 3.330457 -0.867583 1.238730



H -0.441620 0.938205 2.042122
H -0.574001 -0.024527 -2.381722
N -2.398104 -2.341852 0.317722
H -2.613321 -3.235566 0.734885
H -1.937683 -2.415222 -0.582049
H -3.062216 -1.155125 2.494518