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Computational Studies on the Reactivity of Alkyl Halide over $(Al_2O_3)_n$ nanoclusters: An Approach towards Room Temperature Dehydrohalogenation

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Supplementary Information:

- **Procedure for VASP calculation.**
- **IRC Plots for the elimination and the dissociative addition reactions.**
- **Comparison between the structural parameters of the bulk Al_2O_3 and the $(Al_2O_3)_n$ nanoclusters.**
- **Reaction profile for the elimination reactions of the propyl and iso-propyl halides on the dehydrated and hydrated Al_8O_{12} nanocluster.**
- **Cartesian co-ordinates for the optimized geometries of reactant, TS and product along with the lowest harmonic frequency in absence and presence of H_2O (using B3PW91/TZVP, LANL2DZ level of theory).**

Procedure for VASP calculation:

For comparing the geometry and relative energy of the alumina nanoclusters with that of bulk we reoptimized the cluster geometries obtained from Gaussian outputs using VASP software package[1-4] with a very large supercell. Electron-ion interactions were described by the projector-augmented wave (PAW) method,[5] and the exchange-correlation was treated within the generalized gradient approximation (GGA) proposed by Perdew, Burke, and Ernzerhof (PBE).[6,7] The bulk alumina was also optimized using same level of calculation within the periodic model using 8X8X8 k-grid.

1. G. Kresse and J. Hafner. Ab initio molecular dynamics for liquid metals. Phys. Rev. B, 47:558, 1993.
2. G. Kresse and J. Hafner. Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium. Phys. Rev. B, 49:14251, 1994.
3. G. Kresse and J. Furthmüller. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput. Mat. Sci., 6:15, 1996.
4. G. Kresse and J. Furthmüller. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B, 54:11169, 1996.
5. G. Kresse and D. Joubert. From ultrasoft pseudopotentials to the projector augmented-wave method. Phys. Rev. B, 59:1758, 1999.
6. J. P. Perdew, K. Burke, and M. Ernzerhof. Generalized gradient approximation made simple. Phys. Rev. Lett., 77:3865, 1996.
7. J. P. Perdew, K. Burke, and M. Ernzerhof. Erratum: Generalized gradient approximation made simple. Phys. Rev. Lett., 78:1396, 1997.

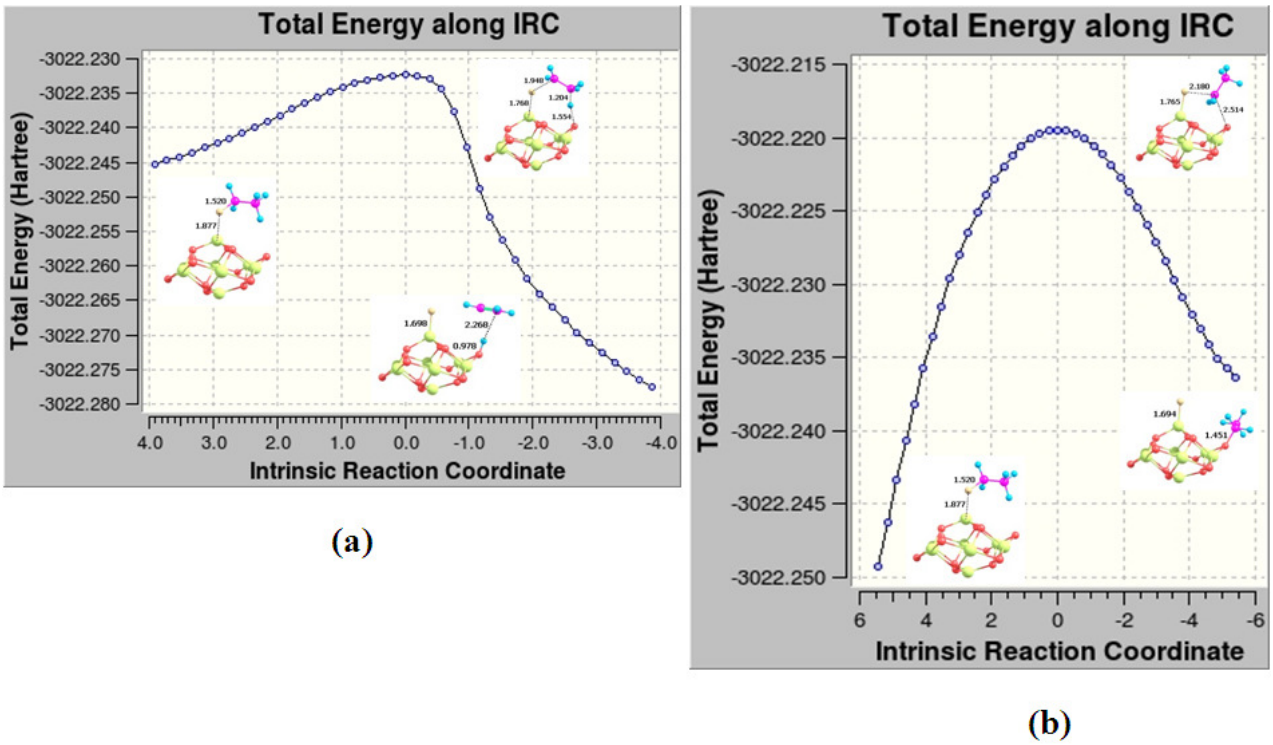

Figure S1: IRC plots for (a) elimination and (b) dissociative addition reaction of C_2H_5F over Al_8O_{12} nanocluster.

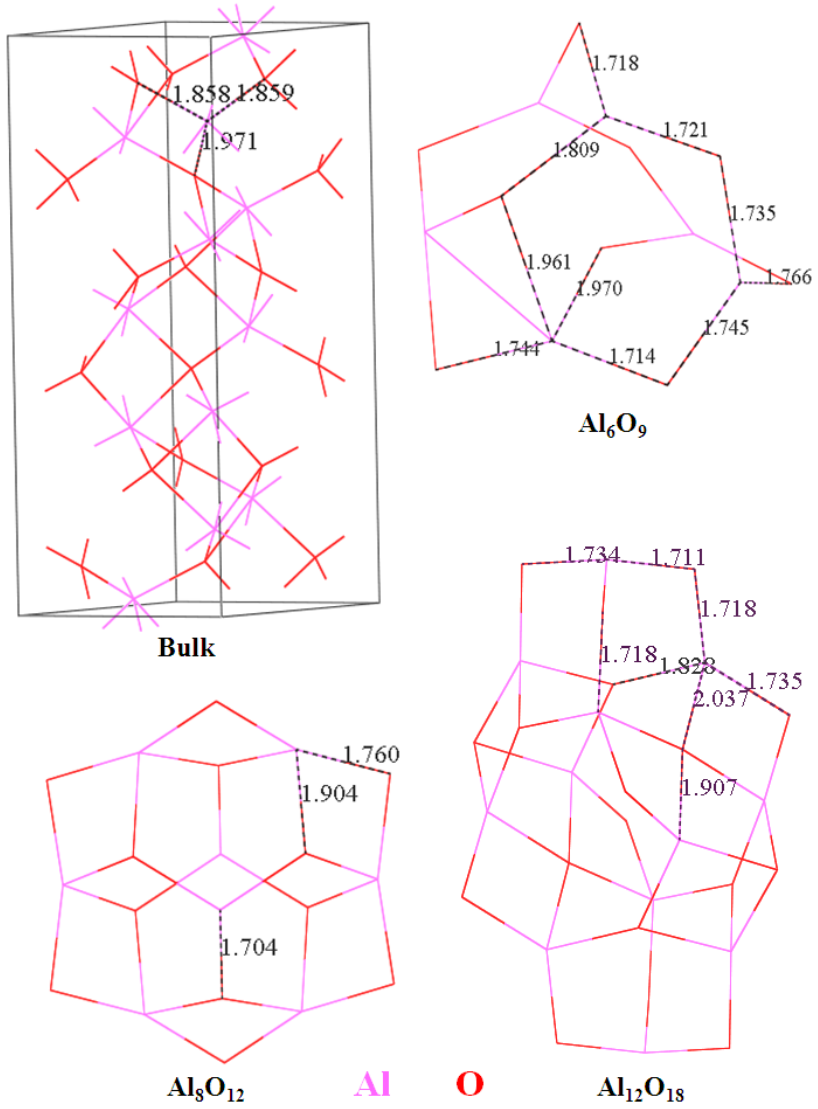

Figure S2: Comparison between the structural parameters (Al-O bond lengths in Å) of the bulk α-Al_2O_3 and the Al_2O_3 nanoclusters.

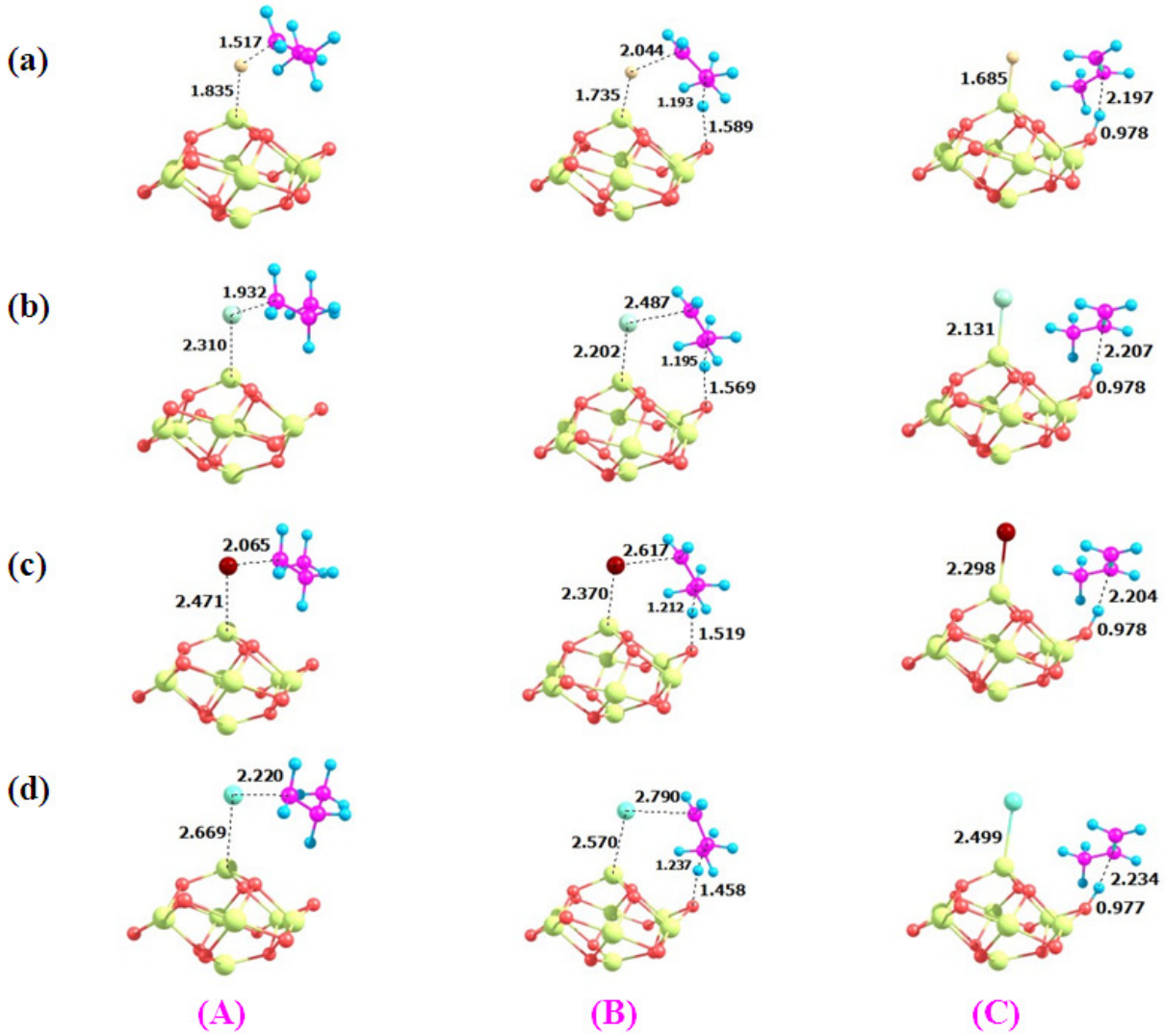

Figure S3: Reaction profile for the elimination reactions of the propyl halides, $CH_3CH_2CH_2X$ (X = F, Cl, Br, I, from top to bottom) on the Al_8O_{12} nanocluster. The interatomic distances are shown in Å.

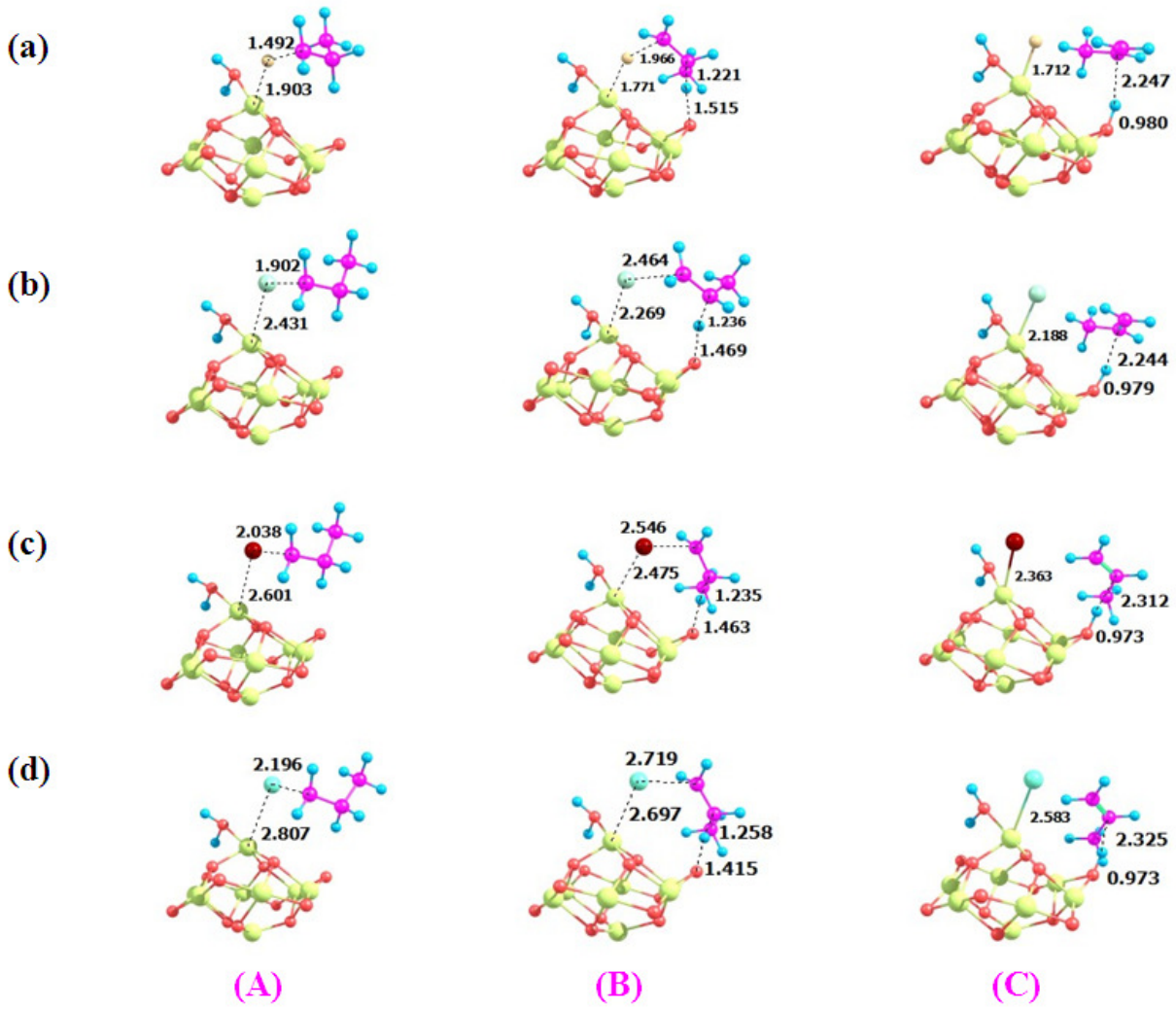

Figure S4: Reaction profile for the elimination reactions of the propyl halides, $CH_3CH_2CH_2X$ (X = F, Cl, Br, I, from top to bottom) on the Al_8O_{12} nanocluster in presence of H_2O. The interatomic distances are shown in Å.

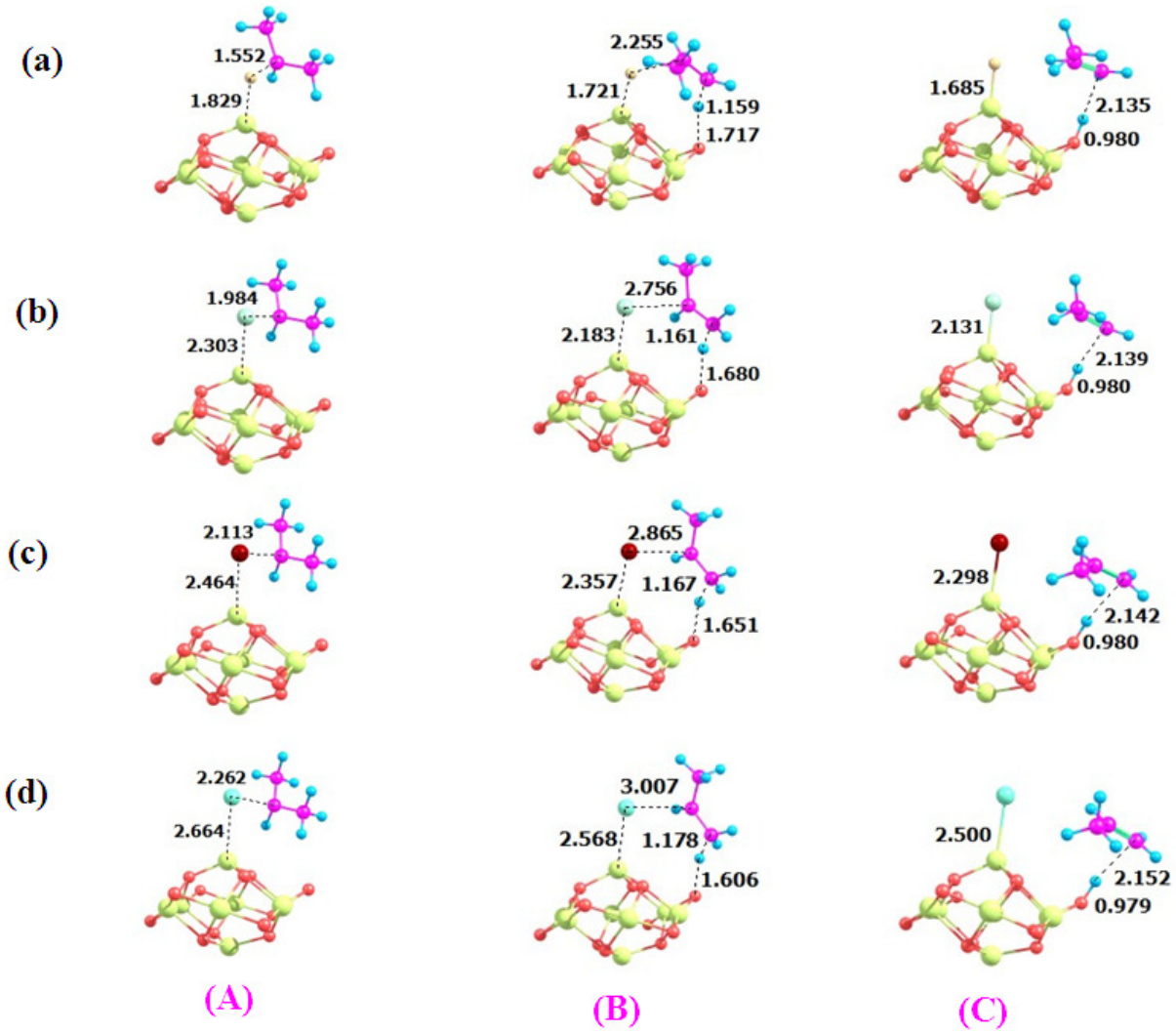

Figure S5: Reaction profile for the elimination reactions of the iso-propyl halides, CH_3CHXCH_3 (X = F, Cl, Br, I, from top to bottom) on the Al_8O_{12} nanocluster. The interatomic distances are shown in Å.

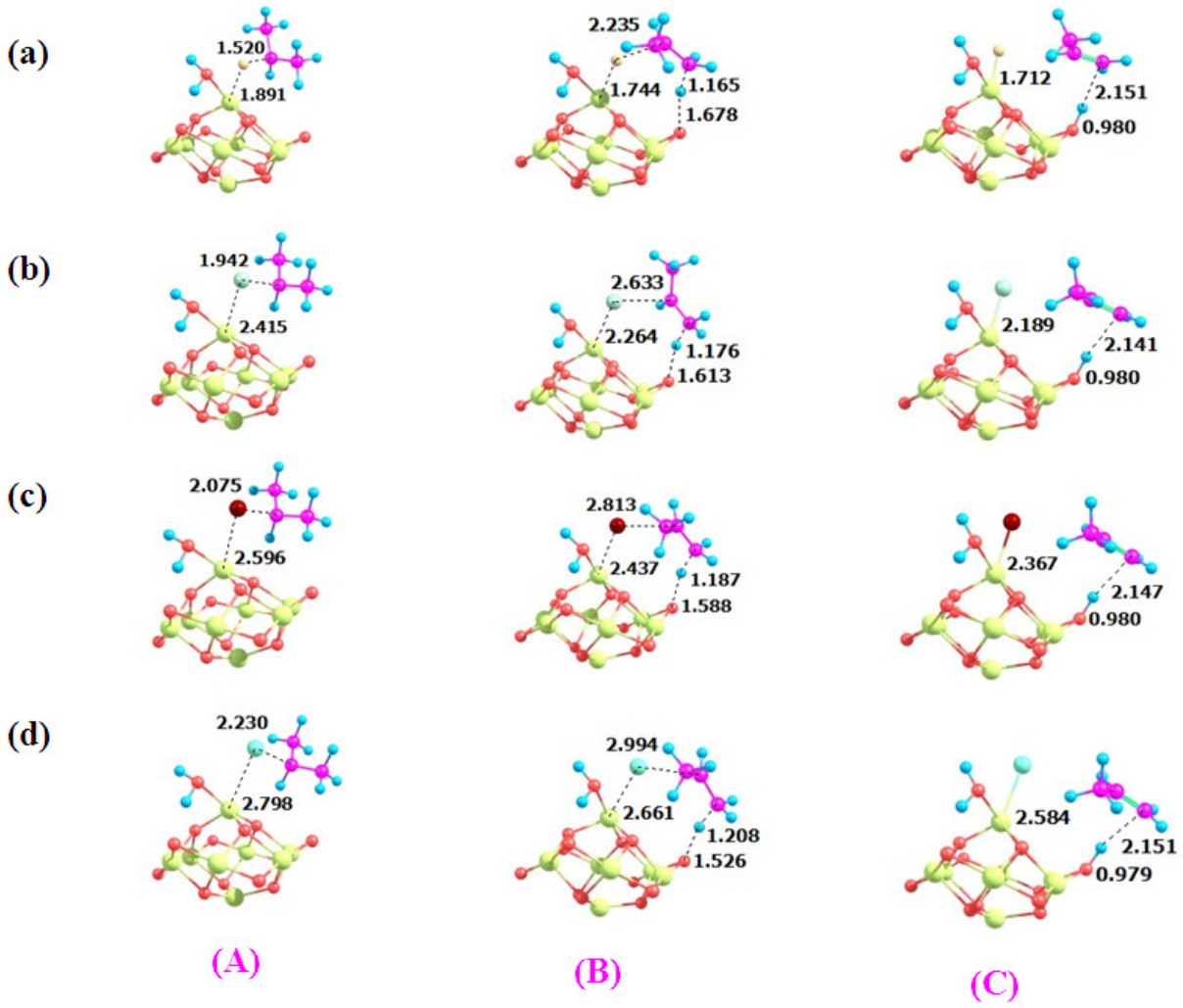

Figure S6: Reaction profile for the elimination reactions of the iso-propyl halides, CH_3CHXCH_3 (X = F, Cl, Br, I, from top to bottom) on the Al_8O_{12} nanocluster in presence of H_2O. The interatomic distances are shown in Å.

Completely dehydrated alumina clusters-

Al_8O_{12}---C_2H_5F reactant geometry:
v1=31.52 cm^{-1}

0 1

O	1.00160700	-0.34380400	1.63070200
O	0.99726300	-3.10980500	0.70556300
Al	-0.63468900	-0.05186100	1.18541800
Al	2.38433700	0.85093300	1.16156900
O	-0.19040600	0.38683100	-2.26079600
O	-0.17794600	3.15217200	-1.29526500
Al	-1.55301500	-0.82197400	-1.73716100
O	1.60483900	-1.49677200	-1.05675500
O	-0.95713200	-2.43788500	-2.10460000
Al	0.76784500	2.55971300	0.07326800
O	3.38686600	-0.59622500	1.07702000
O	2.00469200	1.31277500	-0.65199100
Al	1.37289100	0.08386000	-1.64472400
Al	2.02918900	-1.68269100	0.79540200
O	-2.56681800	0.62286200	-1.62446100
O	-1.14242700	-1.25361600	0.04585300
Al	-1.20239900	1.72141500	-1.36510100
Al	0.05890000	-2.52262000	-0.66350400
O	-0.74382800	1.49863800	0.43532900
O	1.77760300	2.46701700	1.51292800
C	-4.10489100	0.38292800	1.63449800
H	-4.09595000	1.36507300	2.10779700
H	-5.14446200	0.04043300	1.58853000
H	-3.73300600	0.45404000	0.60829000
C	-3.35863600	-0.62027800	2.43932600
H	-3.26347300	-1.59982600	1.97763800
H	-3.63912400	-0.68436100	3.48651700
F	-1.91078700	-0.17187200	2.55698800

Al_8O_{12}---C_2H_5F TS1 geometry:
v1=-380.86 cm^{-1}

0 1

O	1.19295500	-0.06793500	1.59285100
O	1.47916500	-2.92124900	0.97219900
Al	-0.53033700	-0.00916900	1.35950500
Al	2.38298000	1.20091900	0.88534200
O	-0.43343700	0.07604000	-2.20440300

O	-0.61686700	2.93705800	-1.54024500
Al	-1.51526100	-1.22637400	-1.39079900
O	1.70611000	-1.45745300	-1.00524300
O	-0.79196100	-2.79843500	-1.68083900
Al	0.51858000	2.60730700	-0.21513800
O	3.54392000	-0.12226500	0.84767600
O	1.79863700	1.41512200	-0.93726500
Al	1.21152400	0.01374900	-1.69694700
Al	2.30282100	-1.37069800	0.82363700
O	-2.71132300	0.12048800	-1.24169900
O	-0.89179500	-1.37586400	0.32411100
Al	-1.43734000	1.40108300	-1.32446600
Al	0.35691300	-2.60399700	-0.34111000
O	-0.79765800	1.42208200	0.38888900
O	1.65625600	2.78976800	1.11057200
C	-4.19752300	0.12058300	1.06218700
H	-4.66887700	1.09669600	0.95772200
H	-4.82690000	-0.70225300	0.70906900
H	-3.42360900	0.09587400	0.13956100
C	-3.71387400	-0.14359700	2.36632500
H	-3.63654100	-1.16409500	2.71886900
H	-3.75380300	0.61269200	3.13843200
F	-1.78470600	-0.01181800	2.60579100

Al_8O_{12}---C_2H_5F product-1 geometry:
v1=26.56 cm^{-1}

0 1

O	1.38410900	0.00298600	1.47633100
O	1.76426600	-2.83757500	0.93907600
Al	-0.36828500	-0.02225500	1.53542700
Al	2.45889400	1.30752800	0.71123900
O	-0.59683400	0.01128500	-2.08660800
O	-0.80260000	2.90745400	-1.45177400
Al	-1.46280900	-1.36607100	-1.19381100
O	1.72209700	-1.41652700	-1.09025600
O	-0.72069800	-2.90218800	-1.51014600
Al	0.43918200	2.62153900	-0.20248100
O	3.67561600	0.04479900	0.56070600
O	1.68159000	1.48372800	-1.06130900
Al	1.10889700	0.03164400	-1.72017900
Al	2.49529200	-1.25473200	0.68542100
O	-2.78924100	-0.02942900	-1.10514600
O	-0.75514700	-1.38823300	0.45189200
Al	-1.50087900	1.34501500	-1.16714200

Al	0.51337700	-2.60645800	-0.25531500
O	-0.79418000	1.35321100	0.47907200
O	1.68313500	2.86341100	0.99694700
C	-5.14363300	0.42532400	1.05716200
H	-4.91151700	1.47246800	1.22723300
H	-6.00361800	0.21326800	0.42917700
H	-3.49352700	-0.04454600	-0.42608200
C	-4.44229300	-0.54307600	1.64189800
H	-4.70604200	-1.58802100	1.50618500
H	-3.60383200	-0.33399500	2.30052700
F	-1.25227800	-0.05408600	2.98524900

$A_{l8}O_{12}$---C_2H_5Cl reactant geometry:
v1=31.98 cm^{-1}

0 1

O	0.46127900	-1.56277100	0.50659800
O	-1.99231700	-1.95941700	2.02266400
Al	0.67668300	0.07390100	1.01288200
Al	0.61330000	-2.09388400	-1.28231000
O	-1.64839200	1.54504100	-1.13711500
O	0.84191800	1.91420100	-2.62295500
Al	-1.76895100	2.04079500	0.70411700
O	-2.36732600	-1.08996100	-0.25150600
O	-3.20919400	1.23213900	1.31632700
Al	1.25027100	0.28586300	-2.09145900
O	-0.58031600	-3.31852900	-0.86527500
O	-0.32529300	-0.74618800	-2.24195500
Al	-1.72408600	-0.11898600	-1.49123300
Al	-1.22252400	-2.40676900	0.50390800
O	-0.57049000	3.25922500	0.26813300
O	-0.82845100	0.67735300	1.59451600
Al	0.06516500	2.35252400	-1.09964600
Al	-2.41719500	-0.33208400	1.49860000
O	1.17441000	1.01420800	-0.35658700
O	2.06173200	-1.27155600	-1.88611400
C	4.43183900	-0.53492500	0.60454300
H	4.74304700	-1.33769600	1.27317100
H	5.30921500	-0.22634900	0.02287700
H	3.68470900	-0.89876900	-0.10585700
C	3.97914300	0.67356000	1.35046300
H	3.55423100	1.45916900	0.73367800
H	4.67910400	1.06076100	2.08398800
Cl	2.48698300	0.24373200	2.51030100

Al_8O_{12}---C_2H_5Cl TS1 geometry:
v1=-317.38 cm^{-1}

0 1

O	0.66741400	1.45058500	-0.25268400
O	-1.74662700	2.67356600	-1.32003900
Al	0.56912700	-0.01450200	-1.20088700
Al	1.08470500	1.52326700	1.52901000
O	-1.86230800	-1.49707400	0.93130600
O	0.59544600	-2.68650500	1.94810700
Al	-2.24009000	-1.49939500	-0.95598200
O	-2.08313700	1.36547900	0.74739700
O	-3.52557800	-0.31590100	-1.17160500
Al	1.26983500	-1.08666600	1.70036600
O	0.17381600	3.02132700	1.57658500
O	0.03087600	0.17875100	2.32156300
Al	-1.53699000	0.01894400	1.62758900
Al	-0.77140500	2.59039500	0.13764500
O	-1.32628700	-3.00618700	-0.94938100
O	-1.10722900	-0.16744200	-1.63121000
Al	-0.38625100	-2.58992200	0.47318100
Al	-2.43089300	1.06275800	-1.12175800
O	0.88869200	-1.32324700	-0.08180600
O	2.41292900	0.30935900	1.68537800
C	4.43840800	0.23576000	-0.17606400
H	4.87146400	1.23171700	-0.11591100
H	4.96786600	-0.49628500	0.44920200
H	3.46431500	0.24953700	0.51000900
C	4.33260200	-0.28142600	-1.49019000
H	4.20829100	-1.34652800	-1.64466700
H	4.69725300	0.27431700	-2.34357200
Cl	2.23330600	0.01624300	-2.69091600

Al_8O_{12}---C_2H_5Cl product-1 geometry:
v1=20.73 cm^{-1}

0 1

O	0.72323900	-1.35364400	0.36323700
O	-1.74349200	-2.84224700	1.00184300
Al	0.34679000	0.03614800	1.42034500
Al	1.35810500	-1.37286600	-1.31313800
O	-1.84367800	1.41220000	-1.13757300
O	0.58970000	2.87408300	-1.67477100
Al	-2.54538200	1.27716000	0.66854600

O	-1.81979100	-1.49174400	-1.07367600
O	-3.73709700	-0.01705500	0.61046700
Al	1.33533700	1.33749500	-1.37242900
O	0.63949800	-2.93427800	-1.54490400
O	0.42048800	-0.04498600	-2.20565600
Al	-1.26850900	-0.04967600	-1.77110700
Al	-0.54825300	-2.62404500	-0.24990800
O	-1.79250800	2.85673800	0.87418900
O	-1.40753600	0.02126100	1.42132500
Al	-0.59246200	2.60283600	-0.36620000
Al	-2.52349500	-1.28675800	0.72596900
O	0.70207300	1.38489300	0.30425900
O	2.65481300	-0.00675300	-1.34211700
C	5.34787700	-0.51251600	0.35515100
H	5.06381900	-1.49587000	0.71750200
H	6.05600200	-0.48119300	-0.46715100
H	3.44252800	0.01168300	-0.76300400
C	4.88982400	0.59609700	0.93091600
H	5.20847000	1.57935200	0.59762900
H	4.20861100	0.56204700	1.77578500
Cl	1.48241100	0.08770100	3.23546200

Al_8O_{12}---C_2H_5Br reactant geometry:
v1=27.54 cm^{-1}

0 1

O	-0.29572700	0.75251400	1.40907600
O	1.63237400	-0.77558700	2.96246100
Al	-0.69814100	-0.55430600	0.35221800
Al	0.07514000	2.48069200	0.79561100
O	2.10224600	-0.33245000	-1.72010300
O	0.12847400	1.19740000	-3.23600400
Al	1.68761700	-2.07110900	-1.05047100
O	2.61844600	0.36921800	1.01578500
O	2.91751100	-2.41407100	0.16351300
Al	-0.37292000	1.85004700	-1.67905700
O	1.13277000	2.59266000	2.19836300
O	1.20890100	2.19281900	-0.70166900
Al	2.32187300	0.90491800	-0.57141900
Al	1.33811600	0.84441500	2.33853700
O	0.62902600	-2.16524900	-2.45783800
O	0.57121300	-1.72078200	0.42080700
Al	0.42785300	-0.42272700	-2.60212300
Al	2.14780800	-1.43731600	1.41303100
O	-0.81365900	0.06574200	-1.26427700
O	-1.16483800	2.81282700	-0.42506500

C	-4.19912500	1.15063000	0.03734200
H	-4.70209200	1.19420600	1.00371200
H	-4.83024100	1.67830100	-0.68868800
H	-3.24673100	1.68513600	0.08126300
C	-4.05734700	-0.24859500	-0.46594500
H	-3.46231700	-0.34602700	-1.36896700
H	-4.98211500	-0.81440900	-0.52808100
Br	-2.98934500	-1.43256400	0.86285000

Al_8O_{12}---C_2H_5Br TS1 geometry:
v1=-336.30 cm^{-1}

0 1

O	0.49872900	1.37658700	0.41861100
O	-1.56128900	2.99164000	-0.85232100
Al	0.62225100	0.18665600	-0.85688200
Al	0.46400400	0.99706400	2.20927800
O	-2.28438800	-1.57258100	0.20667300
O	-0.17248900	-3.14684700	1.45128600
Al	-2.18377900	-1.10231600	-1.65752600
O	-2.41332600	1.25967400	0.68962600
O	-3.35890900	0.19081700	-1.87292300
Al	0.56712600	-1.59002900	1.77201800
O	-0.40957900	2.50429500	2.40865400
O	-0.76811500	-0.41605800	2.37447600
Al	-2.11700900	-0.29270000	1.31138700
Al	-0.97761300	2.49543000	0.72713900
O	-1.32042100	-2.63112900	-1.80592000
O	-0.90057600	0.26416000	-1.69311400
Al	-0.75614900	-2.63268400	-0.14375400
Al	-2.29279800	1.43376800	-1.22539500
O	0.63187900	-1.36714000	-0.04847100
O	1.69574100	-0.31597000	2.37665900
C	4.16608100	-0.11325500	1.24363800
H	4.54635300	0.78778400	1.72140000
H	4.47090200	-1.03230200	1.75955200
H	3.01952000	-0.18220300	1.59565900
C	4.48095600	-0.21550500	-0.13358500
H	4.49035800	-1.18465700	-0.61713000
H	5.04648500	0.55974800	-0.63273300
Br	2.74879100	0.47106200	-1.92812600

Al_8O_{12}---C_2H_5Br product-1 geometry:
v1=18.63 cm^{-1}

0 1

O	-0.59684900	0.07902200	1.36966300
O	1.64669300	-1.13906600	2.84947400
Al	-0.52670200	-1.06691000	-0.00035100
Al	-0.78251200	1.86243500	1.35662100
O	2.23023600	0.82242200	-1.45156900
O	-0.00693500	1.93736800	-2.90236800
Al	2.44581800	-1.10112800	-1.28358900
O	2.23137200	0.82065600	1.45120500
O	3.63087500	-1.32626500	-0.00212100
Al	-0.78361800	1.86433200	-1.35348300
O	-0.00463900	1.93369000	2.90502000
O	0.33241000	2.46438400	0.00155700
Al	1.85485400	1.61113700	0.00045600
Al	0.80884900	0.37276400	2.61389200
O	1.64426200	-1.13549000	-2.85182200
O	1.17031700	-1.51416800	-0.00118300
Al	0.80678400	0.37610400	-2.61378600
Al	2.44695500	-1.10285200	1.28067400
O	-0.59793000	0.08092400	-1.36865500
O	-2.05048300	2.19179500	0.00233900
C	-4.88054900	0.77167400	-0.66477100
H	-5.34073600	1.57240200	-1.23579500
H	-4.45458800	-0.05452000	-1.22567600
H	-2.94916300	1.80608600	0.00230600
C	-4.88082500	0.77181000	0.66564400
H	-4.45526200	-0.05433500	1.22692300
H	-5.34136300	1.57259200	1.23631100
Br	-2.21259500	-2.64090800	-0.00077900

Al_8O_{12}---C_2H_5I reactant geometry:
v1=26.73 cm^{-1}

0 1

O	-0.42753900	0.77473400	1.14331900
O	0.73811700	-1.01930900	3.11906400
Al	-0.54748400	-0.44228200	-0.08764300
Al	0.30621300	2.47448900	0.80943700
O	2.81083200	-0.43400200	-1.09773400
O	1.59808100	1.36554100	-3.05609600
Al	2.03841200	-2.14063200	-0.73551800
O	2.41115900	0.09295700	1.69138900

O	2.74543800	-2.66835000	0.79049300
Al	0.64775200	1.99676300	-1.71458300
O	0.81979700	2.41062700	2.49298400
O	1.84206400	2.13550700	-0.23970500
Al	2.72776300	0.72737800	0.14299800
Al	0.81766900	0.64636200	2.55573100
O	1.51343000	-2.06401200	-2.41551400
O	0.51741200	-1.74422600	0.30278700
Al	1.52127800	-0.30444800	-2.48816600
Al	1.68231800	-1.66892700	1.77854700
O	-0.02963900	0.25716500	-1.58293600
O	-0.42465500	2.99012400	-0.71529900
C	-3.77667800	1.95324700	-0.37297000
H	-2.75072300	2.19131800	-0.66395800
H	-4.19137400	2.85092000	0.10215500
H	-4.37529800	1.74521500	-1.26036400
C	-3.85561200	0.85272100	0.64130900
I	-3.15596200	-1.10820600	-0.17159800
H	-4.86302700	0.59901000	0.95965600
H	-3.19676400	0.98546300	1.49471800

Al_8O_{12}---C_2H_5I TS1 geometry:
v1=-362.58 cm^{-1}

0 1

O	-0.26769900	0.34871300	1.40346600
O	1.44753700	-1.53112200	2.82129500
Al	-0.52366600	-0.65880900	-0.00500200
Al	0.10148300	2.14214800	1.35564700
O	2.63348700	0.16429900	-1.44877400
O	0.86081100	2.01757200	-2.83608000
Al	2.18904800	-1.70437600	-1.32835000
O	2.65279300	0.11440300	1.42826400
O	3.22567400	-2.34662600	-0.05859000
Al	0.08684900	2.18786700	-1.27228100
O	0.89682000	1.91669900	2.90167100
O	1.42761000	2.33013800	0.03578900
Al	2.56778700	1.03928300	0.00595000
Al	1.16968200	0.18833900	2.60349300
O	1.41101500	-1.43080200	-2.88509200
O	0.83345300	-1.74973400	-0.03247400
Al	1.13589900	0.27967500	-2.60261200
Al	2.20587200	-1.74884800	1.24622000
O	-0.28794800	0.39712000	-1.38194700
O	-0.99735100	2.75718300	0.05781700

C	-3.65255800	2.25554400	0.06553100
H	-2.44473300	2.30515100	0.05112500
H	-3.86166100	2.74714600	1.01639500
H	-3.81964800	2.90226000	-0.80064200
C	-4.32792600	1.01747700	-0.07761200
I	-3.00568100	-1.41872200	0.00038900
H	-4.64726800	0.68315300	-1.05617700
H	-4.86071400	0.58506900	0.75857500

Al_8O_{12}---C_2H_5I product-1 geometry:
v1=20.90 cm^{-1}

0 1

O	0.33284600	0.37291400	-1.36916100
O	-1.51313900	-1.39174500	-2.85058800
Al	0.56853900	-0.75296300	-0.00000300
Al	0.03973200	2.14223000	-1.35520000
O	-2.59450500	0.34531400	1.45250600
O	-0.72721800	2.00717100	2.90416700
Al	-2.29463500	-1.56771500	1.28235700
O	-2.59461300	0.34502000	-1.45235400
O	-3.37801800	-2.09590300	0.00034700
Al	0.03989200	2.14251000	1.35471700
O	-0.72756100	2.00660000	-2.90453900
O	-1.19575000	2.42621200	-0.00019200
Al	-2.44114700	1.20411400	-0.00001800
Al	-1.10221700	0.28675500	-2.61380400
O	-1.51283500	-1.39116700	2.85094100
O	-0.95472200	-1.62764100	0.00019000
Al	-1.10192100	0.28727900	2.61377400
Al	-2.29472300	-1.56800100	-1.28186500
O	0.33299300	0.37318200	1.36898900
O	1.17079700	2.79932000	-0.00040600
C	4.31152300	2.38682200	-0.66518400
H	2.14358900	2.70213700	-0.00030900
H	4.19397500	1.46588600	-1.22801000
H	4.46991800	3.29720200	-1.23533100
C	4.31110700	2.38663400	0.66516900
I	2.77948000	-1.93372200	0.00003300
H	4.46909700	3.29684700	1.23569700
H	4.19323300	1.46553200	1.22765800

Al_8O_{12}---C_2H_5F TS2 geometry:
v1=-220.16 cm^{-1}

0 1

O	-0.82689300	-1.37887600	0.39586500
O	-2.74620700	0.00021300	-1.20314700
Al	-0.46749400	-0.00001100	1.43992100
Al	0.43488200	-2.59848400	-0.26139100
O	1.74071700	1.43855200	-0.98798600
O	3.58258300	-0.00021800	0.77377500
Al	0.43519600	2.59848300	-0.26124600
O	-0.46262300	0.00011100	-2.18684400
O	-0.73915400	2.86429000	-1.56591300
Al	2.38157100	-1.28777100	0.82082300
O	-0.73947600	-2.86406600	-1.56609400
O	1.74053000	-1.43865900	-0.98805500
Al	1.18992000	-0.00000100	-1.70295200
Al	-1.49923800	-1.30192700	-1.32333200
O	1.59671500	2.85116200	1.03155800
O	-0.82668900	1.37894500	0.39592600
Al	2.38172400	1.28747500	0.82089300
Al	-1.49909500	1.30222500	-1.32323700
O	1.26130700	-0.00011000	1.59945900
O	1.59636900	-2.85137400	1.03139800
C	-4.71364200	0.00007000	1.75803500
H	-4.96583700	-0.90732000	2.30574100
H	-5.33097400	0.00085800	0.83902600
H	-4.96502300	0.90723700	2.30653200
C	-3.36689200	-0.00015600	1.23345700
H	-2.87450600	0.92519400	0.98894600
H	-2.87458100	-0.92562600	0.98910000
F	-1.73003600	0.00006200	2.67321600

Al_8O_{12}---C_2H_5F product-2 geometry:
v1=38.25 cm^{-1}

0 1

O	0.93462900	1.17639100	0.68772400
O	2.89455100	-0.67944300	-0.39540800
Al	0.05098700	-0.00526000	1.69840100
Al	0.11366500	2.57342900	-0.30099900
O	-1.72080400	-1.23902200	-1.23739800
O	-3.64386300	0.68692600	-0.10176200
Al	-0.94224700	-2.54057100	-0.10436600
O	0.97748300	-0.33108000	-1.79388800

O	0.42981300	-3.16040600	-1.06334600
Al	-2.26089800	1.72496600	0.23014400
O	1.60509900	2.52734600	-1.28036000
O	-1.13300000	1.60672700	-1.34667800
Al	-0.73145600	0.02132900	-1.78754900
Al	1.92759000	0.89794000	-0.77847500
O	-2.42320900	-2.44108500	0.81269300
O	0.37873000	-1.50755000	0.78566300
Al	-2.77761200	-0.78440300	0.32802000
Al	1.37519900	-1.75744100	-0.68178100
O	-1.61298000	0.32163000	1.24960200
O	-1.27257200	3.13736000	0.59639700
C	4.65574900	0.49651300	0.78127500
H	5.16233400	0.75551800	-0.15176100
H	5.41504500	0.40980600	1.56111900
H	3.99305500	1.31702100	1.07910600
C	3.89311700	-0.79860700	0.65054400
H	3.38807800	-1.05086900	1.58676800
H	4.55600800	-1.62076700	0.37401500
F	0.56259200	-0.05226300	3.31219700

Al_8O_{12}-C_2H_5Cl TS2 geometry:
v1=-220.07 cm^{-1}

0 1

O	-0.78076600	-1.37689400	0.22423700
O	-2.51791200	-0.00071200	-1.58666600
Al	-0.50064400	-0.00007400	1.28651900
Al	0.55215700	-2.59570100	-0.30533000
O	1.92534100	1.43910000	-0.90570700
O	3.59143800	0.00079200	1.02357000
Al	0.55103900	2.59575400	-0.30577000
O	-0.14437500	-0.00029300	-2.31269300
O	-0.48543400	2.86141000	-1.72032300
Al	2.39292400	-1.28780400	0.95461600
O	-0.48422200	-2.86201900	-1.71983500
O	1.92596800	-1.43854500	-0.90545000
Al	1.45594200	0.00010900	-1.67717500
Al	-1.26587800	-1.30185000	-1.56180500
O	1.58193200	2.84729300	1.09203200
O	-0.78140600	1.37645000	0.22399100
Al	2.39237100	1.28886400	0.95439500
Al	-1.26638500	1.30091400	-1.56207600
O	1.20043500	0.00033700	1.61576600
O	1.58316300	-2.84655900	1.09252100

C	-4.92586900	0.00022200	0.80968000
H	-5.30511800	-0.90258500	1.28714500
H	-5.30172800	0.00062100	-0.22802200
H	-5.30422600	0.90325700	1.28749600
C	-3.47939800	-0.00044300	0.65547200
H	-2.94207200	0.92324300	0.53625300
H	-2.94286600	-0.92467900	0.53663100
Cl	-2.16091300	-0.00024600	2.80200900

Al_8O_{12}---C_2H_5Cl product-2 geometry:
v1=41.56 cm^{-1}

0 1

O	-0.39170000	1.51254300	0.59572500
O	2.40149600	2.45627000	0.77518200
Al	-0.11632700	0.02624400	1.54993300
Al	-1.30004700	1.73801300	-0.93274200
O	1.25253200	-1.62642000	-1.39732400
O	-1.48359700	-2.55517300	-1.47859700
Al	2.28335000	-1.71917400	0.24706100
O	1.82497800	1.22013400	-1.29328100
O	3.68035300	-0.68121600	-0.01599300
Al	-1.83998800	-0.91990600	-1.02079800
O	-0.33604700	3.13756600	-1.27751200
O	-0.83302100	0.29639300	-1.99671800
Al	0.87384800	-0.04984400	-1.88770200
Al	0.97866900	2.53783800	-0.23062400
O	1.27936200	-3.12997400	0.57168400
O	1.57273400	-0.30320000	1.20970600
Al	-0.05117700	-2.58395900	-0.41559800
Al	2.78763000	0.79352500	0.33908200
O	-0.93124100	-1.17315100	0.50456800
O	-2.82930500	0.65944300	-0.71758300
C	-4.63247700	-0.51080600	0.40329500
H	-5.07974300	-0.81870600	-0.54524100
H	-5.43727300	-0.40969800	1.13427200
H	-3.97168600	-1.30280300	0.77322300
C	-3.89127700	0.79558600	0.26319800
H	-3.44818100	1.09607700	1.21639200
H	-4.55361900	1.59025900	-0.08549500
Cl	-0.88392900	0.11381700	3.54335800

Al_8O_{12}---C_2H_5Br TS2 geometry:
v1=-228.74 cm^{-1}

0 1

O	0.59940500	1.37674700	0.04479600
O	-1.45604000	2.75457100	-1.50011000
Al	0.59511200	-0.07241500	-0.95804200
Al	0.60912800	1.43238300	1.89669700
O	-2.32070100	-1.38743600	0.64017500
O	-0.20537700	-2.72165100	2.13821300
Al	-2.29785300	-1.37138400	-1.28335700
O	-2.30453400	1.48279400	0.43789800
O	-3.43151400	-0.10563700	-1.74599000
Al	0.59728300	-1.16574900	2.07796000
O	-0.17672400	2.98968300	1.73903800
O	-0.67243000	0.17023300	2.42562300
Al	-2.05533300	0.10696400	1.40167400
Al	-0.81770300	2.61314500	0.12850300
O	-1.48733700	-2.92506100	-1.10161800
O	-0.96897600	-0.11700800	-1.70588000
Al	-0.84509500	-2.56498300	0.49132100
Al	-2.28276300	1.19901900	-1.46488800
O	0.58492300	-1.36620400	0.23758300
O	1.80660200	0.15221000	2.33599000
C	4.74188400	0.07419600	0.82592000
H	5.23937500	0.95606500	0.42315900
H	5.27128200	-0.84023000	0.56003900
H	4.76811800	0.15863000	1.92453100
C	3.32079300	0.02671400	0.49777800
H	2.79138300	-0.90849200	0.49333500
H	2.76577300	0.93566600	0.35703000
Br	2.72895900	-0.16096500	-2.08669400

Al_8O_{12}---C_2H_5Br product-2 geometry:
v1=40.33 cm^{-1}

0 1

O	-0.88060900	-0.09815600	-1.18302400
O	1.27257200	0.27899300	-3.17286700
Al	-0.34008400	1.22957500	-0.11349000
Al	-1.40830700	-1.76106400	-0.76268900
O	2.19952300	-0.94782900	1.33730600
O	0.07719200	-1.23590200	3.27519600
Al	2.75993100	0.81110000	0.72966500
O	1.68902600	-1.47428300	-1.47289200

O	3.72322700	0.52092000	-0.71463700
Al	-0.92768600	-1.27201100	1.86235800
O	-0.94129100	-2.28688900	-2.34863300
O	-0.21260600	-2.34607900	0.53184300
Al	1.42365400	-1.87521400	0.15109200
Al	0.20295900	-0.92769100	-2.50725800
O	2.26818300	1.31501700	2.34448900
O	1.38618800	1.25934300	-0.43299400
Al	1.11809900	0.01986600	2.55159700
Al	2.31256500	0.34397300	-1.75224200
O	-0.39771200	0.39516400	1.46803800
O	-2.45440600	-1.53478600	0.79206300
C	-4.47204900	-1.04308000	-0.45490800
H	-3.91993300	-0.63797700	-1.31070400
H	-5.42930300	-0.51868300	-0.42625700
H	-4.67626900	-2.10398700	-0.61968100
C	-3.71894600	-0.82270200	0.83354000
H	-4.27888300	-1.20609200	1.68864800
H	-3.51484400	0.23992100	0.99008400
Br	-1.64868000	3.12189900	-0.23007000

Al_8O_{12}---C_2H_5I TS2 geometry:
v1=-248.11 cm^{-1}

0 1

O	0.30860900	0.36791400	1.37335400
O	1.02099700	2.78215500	-0.00134500
Al	0.54535000	-0.71122000	0.00006500
Al	-1.11936100	0.22911400	2.59409800
O	-2.61911900	0.13830600	-1.43898200
O	-3.22631900	-2.33590700	0.00141900
Al	-1.12055000	0.22714000	-2.59412200
O	-1.41706800	2.33363600	-0.00073600
O	-0.84342100	1.95824300	-2.86365400
Al	-2.18969100	-1.72937100	1.28932000
O	-0.84227500	1.96043000	2.86225800
O	-2.61843000	0.13939600	1.43964300
Al	-2.55190700	1.03786000	-0.00002700
Al	-0.07729700	2.17783300	1.30196900
O	-1.40360700	-1.48633300	-2.84506900
O	0.30778200	0.36672400	-1.37402200
Al	-2.19021200	-1.73036200	-1.28735200
Al	-0.07779100	2.17676600	-1.30382300
O	-0.82870600	-1.77256900	0.00075700
O	-1.40237700	-1.48414400	2.84650800

C	4.15838400	2.12174900	-0.00012800
H	4.74860200	1.94582100	0.89873900
H	3.87180000	3.18467100	-0.00044000
H	4.74890700	1.94553300	-0.89868400
C	2.89170600	1.38828500	-0.00032400
I	3.06043500	-1.43387600	0.00002400
H	2.39912100	1.15259700	-0.92521700
H	2.39840600	1.15293600	0.92431100

Al_8O_{12}---C_2H_5I product-2 geometry:
v1=38.82 cm^{-1}

0 1

O	0.49020400	0.62116700	1.17658200
O	1.03686900	2.76050400	-0.71579400
Al	0.69509900	-0.74484400	0.03932800
Al	-0.81886800	0.70692900	2.55241600
O	-2.64849500	-0.13696600	-1.27726600
O	-3.12684400	-2.27621000	0.69066000
Al	-1.26323100	-0.34461100	-2.54881700
O	-1.28963200	2.27062000	-0.40426200
O	-1.04763300	1.30091400	-3.20360200
Al	-1.97943000	-1.44144500	1.73205400
O	-0.54672400	2.46787300	2.46698700
O	-2.40449600	0.44859500	1.55624300
Al	-2.43415500	1.00381300	-0.04378300
Al	0.07404200	2.33561300	0.85201700
O	-1.56994200	-2.05642000	-2.41270300
O	0.26261700	0.06938000	-1.49477200
Al	-2.19894400	-1.95763400	-0.77033800
Al	-0.16215100	1.78712600	-1.79399500
O	-0.75400100	-1.68487200	0.36049900
O	-1.08194700	-0.91008900	3.15156900
C	3.05695000	3.36262200	0.47877200
H	2.68036500	4.36434200	0.69981100
H	4.14513600	3.42105100	0.41068600
H	2.83188600	2.69255800	1.31633700
C	2.48362400	2.83211600	-0.81153900
I	2.98282900	-1.76319700	0.05373200
H	2.86861100	1.83192100	-1.02723100
H	2.72010200	3.49084800	-1.64938500

Al_6O_9---C_2H_5F reactant geometry:
v1=21.44 cm^{-1}

0 1

O	-1.59991200	-2.60104800	-0.84055000
O	0.12925200	-1.69420800	1.42009800
O	-1.81123400	2.43979500	-0.27707700
O	0.87905600	1.45483500	-1.95292000
O	-1.06568900	-0.09892000	-0.44263000
O	0.92271700	1.00162600	0.57420400
Al	-2.49710700	-1.17315900	-0.60837400
Al	-2.54467500	1.14283300	0.62971000
Al	-0.02464400	-1.96638000	-0.30394700
Al	-0.34021100	1.67491600	-0.74710500
O	-1.67063800	0.76105300	2.08548600
O	1.40765900	-1.46204800	-1.13697000
Al	1.64661600	0.23344100	-0.97920900
O	-3.66146700	-0.07626700	-0.01801000
Al	-0.25351600	-0.02080100	1.48765100
C	4.29715100	-0.71414600	1.26158100
H	3.32060200	-1.16547500	1.44258700
H	4.80529000	-0.60640300	2.22522800
H	4.89365100	-1.37553600	0.63332100
C	4.17648800	0.64675300	0.66824800
H	5.11724700	1.11382000	0.39132300
H	3.52448600	1.32596200	1.21253100
F	3.49276800	0.52582000	-0.66671700

Al_6O_9---C_2H_5F TS1 geometry:
v1=-397.38 cm^{-1}

0 1

O	0.98602100	2.50706500	-1.35191000
O	-0.70248800	1.59655500	1.02344300
O	2.24818000	-2.13695200	0.14300800
O	-0.61265500	-2.17017900	-1.54484300
O	0.99237000	0.11724600	-0.46605700
O	-0.66876300	-1.24841000	0.83133600
Al	2.19650700	1.39684900	-0.90038400
Al	2.69674200	-0.57277100	0.74975900
Al	-0.38015900	1.52534000	-0.75932700
Al	0.62752400	-1.86722000	-0.39281500
O	1.77014700	-0.04075800	2.13110000
O	-1.67838400	0.61464900	-1.40020200
Al	-1.70012100	-1.02579700	-0.77583600

O	3.55403300	0.68719600	-0.16312700
Al	0.19990400	0.15845600	1.45623300
C	-3.41473900	1.33102800	1.35514100
H	-2.22218600	1.32378100	1.14128300
H	-3.54206100	1.18159900	2.42478100
H	-3.50085600	2.37945900	1.04346800
C	-4.20968600	0.51779500	0.52905400
H	-4.36002900	0.79145400	-0.50731600
H	-4.88128200	-0.22539000	0.93572800
F	-3.35332000	-1.21647600	-0.20825400

Al_6O_9---C_2H_5Cl reactant geometry:
v1=15.23 cm^{-1}

0 1

O	1.27968700	2.75560800	-0.78299200
O	0.40238500	1.48128600	1.77297200
O	2.35314500	-2.19777600	-0.72418600
O	-0.81494500	-1.59842800	-1.52681600
O	1.21989500	0.19443400	-0.49279800
O	-0.21469100	-1.26611200	0.93996000
Al	2.40153200	1.48005800	-0.91509100
Al	3.11140900	-0.84897400	0.07687900
Al	0.03917100	1.82544900	0.09699900
Al	0.71591500	-1.66208600	-0.72268500
O	2.61752800	-0.68322500	1.73493000
O	-1.50914800	1.15671300	-0.34499100
Al	-1.44228400	-0.57291400	-0.26714200
O	3.82477200	0.56076600	-0.72945200
Al	0.99086200	-0.12378100	1.63319500
C	-5.54464900	0.78067100	-0.68828200
H	-5.12242400	0.66913500	-1.68680100
H	-5.98733900	1.78082600	-0.62152100
H	-6.34152200	0.05065800	-0.54461100
C	-4.49565100	0.69705900	0.37018300
H	-4.86687400	0.74027400	1.38913800
H	-3.62385900	1.33059800	0.21396700
Cl	-3.68829900	-1.05498700	0.33278800

Al_6O_9---C_2H_5Cl TS1 geometry:
v1=-349.57 cm^{-1}

0 1

O	1.27130200	2.40441600	-1.49172500
O	-0.41150300	1.71633000	0.94675400
O	2.35114700	-2.19414800	0.25040300
O	-0.50317400	-2.19280600	-1.44572800
O	1.18145200	0.06974100	-0.48048800
O	-0.53316000	-1.15268200	0.88424900
Al	2.43801200	1.27455600	-0.97604400
Al	2.86202300	-0.62296200	0.78381100
Al	-0.12603500	1.51329700	-0.83041700
Al	0.74526600	-1.88161500	-0.30495700
O	1.95336900	0.00819600	2.13334600
O	-1.48655400	0.63738900	-1.39785800
Al	-1.55450200	-0.98235500	-0.73087300
O	3.76389200	0.55538200	-0.19217700
Al	0.39112100	0.24463500	1.45253900
C	-3.12880300	1.95495800	1.26811900
H	-3.32192800	1.96747200	2.33782100
H	-2.99240200	2.95867000	0.84033000
H	-1.96745700	1.69510600	1.09601900
C	-4.05792300	1.24708600	0.48476600
H	-4.06145700	1.37436200	-0.59116200
H	-4.92034800	0.76103800	0.92036500
Cl	-3.65510200	-1.22798200	-0.05280300

Al_6O_9---C_2H_5Br reactant geometry:
v1=20.58 cm^{-1}

0 1

O	-2.26330600	-2.34781400	-1.30945400
O	-0.56134200	-1.95351300	1.11372200
O	-2.20809900	2.51981600	0.12261000
O	0.47373100	1.67797200	-1.64257600
O	-1.60118900	0.00665100	-0.46908700
O	0.41246100	0.79288200	0.77006500
Al	-3.08741700	-0.93124200	-0.84854800
Al	-3.04414500	1.13536400	0.77442300
Al	-0.67435600	-1.90738800	-0.63577000
Al	-0.76833900	1.76116600	-0.44345700
O	-2.23925700	0.45400900	2.15869600
O	0.81760300	-1.35869900	-1.32722500
Al	1.14879500	0.26832400	-0.87276700

O	-4.20499200	0.11612800	-0.09913400
Al	-0.85026600	-0.29629000	1.46431200
C	3.30353900	-1.63424400	1.61869600
H	2.31390800	-1.89127500	1.23848700
H	3.32946600	-1.90283300	2.68125900
H	4.05581100	-2.23182700	1.10364000
C	3.58844300	-0.16812600	1.52987700
H	4.57826300	0.12494100	1.86693300
H	2.81737200	0.46807900	1.95474400
Br	3.63236800	0.47424500	-0.42782700

Al_6O_9---C_2H_5Br TS1 geometry:
v1=-406.25 cm^{-1}

0 1

O	1.88076000	2.29343800	-1.55603400
O	0.11234700	1.84681000	0.87434600
O	2.48012300	-2.33632200	0.32818200
O	-0.34170600	-2.10762500	-1.40636100
O	1.54793500	0.01034100	-0.47865600
O	-0.29586900	-0.99764100	0.89047400
Al	2.92320800	1.07108300	-0.98815000
Al	3.13835500	-0.80943900	0.82776100
Al	0.39242100	1.56474900	-0.89540100
Al	0.91896200	-1.88389600	-0.25798200
O	2.27888700	-0.05287300	2.14505000
O	-1.03624800	0.80548600	-1.45822700
Al	-1.27620700	-0.77502900	-0.74644200
O	4.16230800	0.24752500	-0.16609400
Al	0.75755800	0.31538700	1.43151800
C	-2.51112400	2.44614700	1.24661200
H	-1.39032400	2.02484400	1.03739900
H	-2.60822600	2.52431800	2.32728700
H	-2.27663200	3.40169300	0.75965300
C	-3.59045600	1.82947400	0.58776400
H	-3.72116500	1.96051800	-0.47932300
H	-4.44417100	1.45164800	1.13365600
Br	-3.55326200	-0.79905600	-0.02838100

Al_6O_9---C_2H_5I reactant geometry:
v1=16.56 cm^{-1}

0 1

O	2.28786700	2.48733500	-1.30106200
O	0.96629800	1.86155900	1.30766400
O	2.86956400	-2.39182300	-0.06214900
O	-0.10223700	-1.78971600	-1.41649100
O	1.95294200	0.06307300	-0.49419600
O	0.21448200	-0.95695000	0.98253300
Al	3.29413400	1.14508200	-1.00488500
Al	3.64555600	-0.95228000	0.53898100
Al	0.86254800	1.84826700	-0.44026100
Al	1.30152600	-1.76446900	-0.40437200
O	2.96600900	-0.39329900	2.03850600
O	-0.66936000	1.20023300	-0.95578800
Al	-0.79350400	-0.46960400	-0.51068200
O	4.58829900	0.19568100	-0.43155500
Al	1.42465000	0.23105100	1.58560600
C	-3.78912600	2.15525800	1.20099400
H	-4.60395900	1.77059600	1.81520500
H	-3.95096100	3.23137500	1.06856500
H	-2.84568200	2.02995600	1.73252600
C	-3.74926200	1.53910500	-0.16582400
I	-3.45196600	-0.66712600	-0.06835100
H	-2.88322100	1.83375100	-0.75568000
H	-4.67639600	1.62244200	-0.72576600

Al_6O_9---C_2H_5I TS1 geometry:
v1=-503.70 cm^{-1}

0 1

O	2.33920600	2.21489000	-1.58773400
O	0.52627700	1.89222900	0.82601600
O	2.69769300	-2.40520900	0.37653500
O	-0.08844300	-2.07466900	-1.39883600
O	1.88529600	-0.02935700	-0.47644100
O	-0.01908800	-0.93266800	0.88176700
Al	3.31642000	0.95668900	-0.98336900
Al	3.42095000	-0.90410900	0.86362200
Al	0.80971700	1.56543800	-0.93829500
Al	1.16639100	-1.89125900	-0.23704900
O	2.58019600	-0.08707500	2.15655900
O	-0.64682400	0.86651600	-1.50470700
Al	-0.97089900	-0.68958600	-0.77293100

O	4.50462600	0.08833400	-0.13272200
Al	1.08685800	0.33826600	1.41625900
C	-1.99346800	2.76806000	1.18633400
H	-2.02599800	2.91702200	2.26407600
H	-1.68403400	3.66065900	0.62955900
H	-0.91152500	2.21956600	0.98742700
C	-3.16062700	2.21977400	0.62486800
I	-3.43595400	-0.58750300	-0.00396100
H	-3.36272100	2.33642000	-0.43243900
H	-3.99977300	1.93233700	1.24352200

$Al_{12}O_{18}$---C_2H_5F reactant geometry:
v1=18.56 cm^{-1}

0 1

O	-3.56192600	1.71228600	-0.04377100
O	-0.19571900	-0.86247400	3.08119000
O	-0.48455900	-1.13601300	0.50228400
O	-3.37678400	-1.08269800	-0.70333500
Al	-1.39403900	-0.13781400	2.05107400
Al	-3.85725100	0.06675400	0.51026500
Al	0.56676100	-2.17932100	-0.68771300
O	1.61554700	1.22169600	-0.41942000
O	4.67383800	-1.63677300	0.11059900
Al	0.54165200	2.26739000	0.77440900
Al	4.85620500	0.01032100	-0.40235400
O	1.30928000	0.95907500	-2.99810900
O	-1.26024000	0.64174700	-1.47721600
O	-0.39220600	2.87428300	-0.70200200
Al	0.27845300	1.51097700	-1.75649900
O	4.20412800	0.36765700	-1.94333700
Al	2.98713800	-1.81144100	0.34023700
O	4.49326800	1.18723200	0.78483900
O	-0.71481400	-2.32959700	-1.80011500
O	2.09471500	-1.39676600	-1.22226500
Al	2.49179400	0.22653300	-1.96297500
Al	-1.71756500	-1.08625900	-1.10801000
O	-3.09115100	-0.28179600	2.01595100
O	1.82398900	2.41833700	1.88865800
O	-0.97310400	1.47754000	1.31044300
Al	2.82736500	1.17814600	1.20968300
Al	-1.88214500	1.86858600	-0.24680200
O	2.38873800	-0.56130000	1.55864100
O	1.50467300	-2.79465000	0.79171000
Al	0.83174700	-1.41541800	1.84124600

C	-6.69537800	-1.35670700	-1.29506000
H	-5.70414800	-1.73163200	-1.55312200
H	-7.29045100	-1.27959600	-2.21052000
H	-7.19437600	-2.05325700	-0.62095600
C	-6.60215400	0.00628300	-0.70211200
H	-7.53164600	0.40860100	-0.30892700
H	-6.07792800	0.73626700	-1.31577600
F	-5.75212400	-0.07555500	0.53345000

$Al_{12}O_{18}$---C_2H_5F TS1 geometry:
v1=-452.07 cm^{-1}

0 1

O	-3.47546100	1.96155600	-0.41220000
O	-0.30678400	-0.25211100	3.15206400
O	-0.57912700	-0.94175500	0.64863500
O	-3.44899700	-0.92154000	-0.59856700
Al	-1.45186000	0.36628400	1.99888000
Al	-3.96544800	0.48254900	0.40157100
Al	0.42662200	-2.23879600	-0.32271600
O	1.66565100	1.10491100	-0.60329200
O	4.54494700	-1.79375400	0.45402400
Al	0.64674300	2.40278700	0.38036600
Al	4.83001300	-0.26835400	-0.32228000
O	1.35699600	0.42622400	-3.10131200
O	-1.23643000	0.52868300	-1.59465500
O	-0.23698000	2.80265600	-1.19237400
Al	0.35493900	1.24783900	-1.99170800
O	4.20826700	-0.13562700	-1.91075900
Al	2.84942900	-1.82812900	0.68010000
O	4.52521500	1.10666900	0.64826100
O	-0.86530400	-2.49377600	-1.40780700
O	1.99731600	-1.63663900	-0.94777100
Al	2.49046700	-0.17845100	-1.93661700
Al	-1.76410600	-1.07688200	-0.93972100
O	-3.14250800	0.28736700	1.91626000
O	1.92695100	2.66028000	1.47709100
O	-0.91293100	1.80136800	1.01410400
Al	2.85807300	1.26776500	1.03482700
Al	-1.79483300	1.98196400	-0.59567000
O	2.31221300	-0.36247500	1.65958600
O	1.30390200	-2.63787900	1.25987500
Al	0.70117600	-1.06151300	2.04553200
C	-5.82212000	-2.06804500	-1.08372700
H	-4.70779800	-1.61882100	-0.90328300

H	-5.90776300	-2.05671800	-2.16930500
H	-5.75081300	-3.06370300	-0.64879600
C	-6.70511200	-1.19352100	-0.41486300
H	-7.10721800	-1.44675400	0.55748200
H	-7.25763000	-0.43926900	-0.96008000
F	-5.72851500	0.21106400	0.42254300

$Al_{12}O_{18}$---C_2H_5Cl reactant geometry:
v1=15.43 cm^{-1}

0 1

O	-3.20355000	2.17586900	-0.18759300
O	-0.30505100	-0.87874600	2.95427300
O	-0.46286300	-0.99778300	0.35252800
O	-3.25742900	-0.61327500	-0.99707700
Al	-1.36202000	0.01564200	1.90268700
Al	-3.69864900	0.54780500	0.22778800
Al	0.55263100	-2.08501500	-0.83157900
O	1.91442400	1.17405300	-0.32105200
O	4.63667100	-2.00135600	0.21889600
Al	0.87999500	2.26515700	0.86948900
Al	5.01094100	-0.35846800	-0.19376300
O	1.72779400	1.06264200	-2.92157200
O	-0.94429900	0.94499800	-1.55684600
O	0.09983600	3.03466800	-0.61973400
Al	0.68899100	1.66168400	-1.70888200
O	4.48920200	0.13755500	-1.74549000
Al	2.93057800	-2.01458500	0.34706700
O	4.69776300	0.78939100	1.03502500
O	-0.67205200	-2.05301200	-2.01588000
O	2.17861600	-1.44066700	-1.24045600
Al	2.77497300	0.17011200	-1.86709200
Al	-1.58084500	-0.74515900	-1.31162900
O	-3.05863800	0.03432300	1.75105100
O	2.10265400	2.23106600	2.05729400
O	-0.73494500	1.61285000	1.28326200
Al	3.01724200	0.93059000	1.36677200
Al	-1.50900800	2.17340900	-0.29746900
O	2.38633500	-0.77010500	1.59601500
O	1.33209900	-2.86121000	0.66346500
Al	0.73745100	-1.47011700	1.74488100
C	-6.62810000	-2.41167800	-0.03431600
H	-5.83860400	-2.62577500	0.68584100
H	-6.73860000	-3.28904800	-0.68143400
H	-7.57094100	-2.25934200	0.49137600

C	-6.27318000	-1.25960700	-0.91547100
H	-7.05040400	-0.95637400	-1.60968500
H	-5.29230100	-1.32717700	-1.38244100
Cl	-6.07433100	0.33244900	0.14815700

$Al_{12}O_{18}$---C_2H_5Cl TS1 geometry:
v1=-319.59 cm^{-1}

0 1

O	3.27811100	-2.00640000	-0.59142900
O	0.18461000	0.00686900	3.14879300
O	0.44590200	0.86130200	0.69497700
O	3.30583900	0.88111100	-0.57572500
Al	1.30730600	-0.55465600	1.94642000
Al	3.80034900	-0.59321400	0.31123500
Al	-0.54135900	2.24400400	-0.17314600
O	-1.84744300	-1.05313300	-0.66792100
O	-4.65977000	1.82190900	0.61258600
Al	-0.84455800	-2.43507100	0.21483700
Al	-4.98099300	0.35964800	-0.26462800
O	-1.54747700	-0.20917400	-3.11771300
O	1.05292900	-0.46283400	-1.64540400
O	0.01706400	-2.74142700	-1.39105000
Al	-0.55445000	-1.12539600	-2.07606900
O	-4.37649700	0.32655400	-1.86483000
Al	-2.96227800	1.80881300	0.82325500
O	-4.69524300	-1.08518300	0.60452900
O	0.74984000	2.54779900	-1.24702900
O	-2.12805100	1.71629000	-0.82443700
Al	-2.65878400	0.33910500	-1.90554600
Al	1.61742500	1.08014600	-0.88499900
O	2.99819900	-0.49339300	1.84645600
O	-2.12121000	-2.74129400	1.30282800
O	0.73329700	-1.90901800	0.87270100
Al	-3.02839300	-1.30464900	0.96204900
Al	1.59491000	-1.99193800	-0.75733900
O	-2.44404500	0.26779700	1.69072900
O	-1.39656400	2.54730000	1.44195900
Al	-0.81769700	0.90844700	2.11026500
C	5.46240900	2.45368700	-1.01178700
H	4.48496600	1.79295700	-0.83643500
H	5.48605400	2.57319400	-2.09462900
H	5.21896000	3.36811600	-0.47029800
C	6.58385600	1.76356100	-0.48521100
H	6.97464500	2.01227900	0.49291300

H	7.27388500	1.24680100	-1.13946800
Cl	6.04581000	-0.35620900	0.39572800

$Al_{12}O_{18}$---C_2H_5Br reactant geometry:
v1=19.96 cm^{-1}

0 1

O	2.89389600	-2.14462700	-0.23324100
O	-0.01126700	0.85253300	2.95789900
O	0.13312100	1.00350400	0.35810100
O	2.92624100	0.65621400	-1.01119900
Al	1.04603500	-0.01988800	1.88747600
Al	3.38246800	-0.51680300	0.19742900
Al	-0.89438800	2.09699400	-0.80793800
O	-2.23171900	-1.17624900	-0.33277700
O	-4.97349000	1.97368900	0.25797500
Al	-1.18433500	-2.27445700	0.83984900
Al	-5.33823900	0.33328200	-0.17275400
O	-2.05727800	-1.03161800	-2.93203400
O	0.62042500	-0.91170000	-1.57746400
O	-0.40535300	-3.02002000	-0.66203700
Al	-1.00836400	-1.63797300	-1.73180300
O	-4.81989100	-0.14075000	-1.73243400
Al	-3.26702700	1.99723900	0.37899100
O	-5.01182200	-0.82746600	1.04042900
O	0.32469700	2.08942000	-1.99844000
O	-2.51797900	1.44741000	-1.21848500
Al	-3.10591700	-0.16024900	-1.86126800
Al	1.24741600	0.77957800	-1.31678200
O	2.74215200	-0.02631500	1.72932300
O	-2.40247800	-2.26429900	2.03272700
O	0.42748600	-1.61600100	1.25536800
Al	-3.32875500	-0.96147800	1.36247400
Al	1.19888700	-2.15156300	-0.33527500
O	-2.70891300	0.74076800	1.61027600
O	-1.67315700	2.85063500	0.69935100
Al	-1.06489500	1.45106600	1.76203000
C	6.20316900	2.63617700	-0.04196500
H	5.42015100	2.75146600	0.70753700
H	6.20685700	3.54021300	-0.66175500
H	7.17170400	2.56631900	0.45411700
C	5.93613900	1.47855200	-0.95133300
H	6.71579700	1.28381000	-1.68156700
H	4.94069700	1.47273400	-1.39231400
Br	5.90840100	-0.28881900	0.11301300

$Al_{12}O_{18}$---C_2H_5Br TS1 geometry:
v1=-357.32 cm^{-1}

0 1

O	2.96600000	-1.94678800	-0.72072700
O	-0.09743000	-0.10337300	3.13044900
O	0.12580500	0.84641000	0.70729800
O	2.96945800	0.93885600	-0.59740700
Al	1.01521100	-0.61207500	1.89636800
Al	3.49457300	-0.56551100	0.22786600
Al	-0.88301200	2.25467400	-0.09392800
O	-2.16763500	-1.03689600	-0.69760100
O	-4.98709200	1.76542400	0.72298000
Al	-1.14373300	-2.44305800	0.12098900
Al	-5.30669700	0.33572200	-0.20689700
O	-1.90255200	-0.09781600	-3.11730300
O	0.71479800	-0.38620100	-1.68468200
O	-0.29882800	-2.68137000	-1.50548900
Al	-0.89235500	-1.04612800	-2.12200400
O	-4.72097800	0.36932300	-1.81392200
Al	-3.28743500	1.75881200	0.91371500
O	-4.99992900	-1.13908200	0.60239600
O	0.39437000	2.60711500	-1.16991900
O	-2.47203400	1.73702800	-0.74678400
Al	-3.00416300	0.39799700	-1.87437600
Al	1.27122500	1.13036600	-0.87190900
O	2.70324500	-0.52798300	1.77232200
O	-2.40582900	-2.79966500	1.21031800
O	0.43832400	-1.92962300	0.77984300
Al	-3.32752100	-1.35843200	0.93228200
Al	1.28055300	-1.94371800	-0.86281900
O	-2.74593300	0.18947800	1.71412300
O	-1.72036400	2.48612800	1.54181700
Al	-1.12013900	0.82746300	2.13875800
C	4.97568500	2.66282200	-1.02409400
H	4.05607400	1.90177400	-0.83674300
H	4.91445400	2.82939100	-2.09942500
H	4.67557800	3.51994500	-0.42119600
C	6.18039200	2.05475900	-0.60115000
H	6.61395100	2.29799900	0.36012100
H	6.86201300	1.61908900	-1.32007000
Br	5.89542100	-0.29631100	0.29921400

$Al_{12}O_{18}$---C_2H_5I reactant geometry:
v1=5.92 cm^{-1}

0 1

O	-2.58863800	-2.14362700	-0.23797100
O	-0.00338600	2.07566900	-2.02010500
O	0.17609600	1.00523800	0.34481000
O	-2.44116100	-0.01038300	1.70930700
Al	-0.93272100	0.77217500	-1.33515700
Al	-3.07932300	-0.51054300	0.17754900
Al	1.36860600	1.45943100	1.75068400
O	2.53974800	-1.18364700	-0.32153000
O	5.28447600	1.96549900	0.25997300
Al	1.32159200	-1.65180000	-1.72258300
Al	5.64805900	0.32149600	-0.15773000
O	2.69796400	-2.25652600	2.05151700
O	-0.12761300	-1.60803100	1.25798000
O	0.71122700	-3.02593800	-0.64646700
Al	1.48447400	-2.27204500	0.85386000
O	5.31439600	-0.83044200	1.06185000
Al	3.57747100	1.99274900	0.37350300
O	5.13564900	-0.16212900	-1.71644500
O	0.30806200	0.87123300	2.94566400
O	3.01197700	0.74537600	1.61049400
Al	3.62943200	-0.95995600	1.37631100
Al	-0.74578000	-0.00575600	1.87498600
O	-2.61241200	0.65493300	-1.03506900
O	2.37670000	-1.05558700	-2.92253700
O	-0.30648300	-0.92186400	-1.58006000
Al	3.42224600	-0.17862000	-1.85335700
Al	-0.89307200	-2.15204400	-0.33255000
O	2.83433200	1.43398800	-1.22352400
O	1.98395600	2.85123400	0.68141000
Al	1.21008200	2.08862600	-0.82401500
C	-5.67838200	2.85636600	0.02488100
H	-6.62997200	2.89943200	0.55596200
H	-5.57052400	3.78574600	-0.54628900
H	-4.86570000	2.81886500	0.75045300
C	-5.60855500	1.71890200	-0.95105400
I	-5.78583400	-0.24991400	0.07135400
H	-4.63866400	1.61344800	-1.43422000
H	-6.42727600	1.68808600	-1.66449000

$Al_{12}O_{18}$---C_2H_5I TS1 geometry:
v1=-480.97 cm^{-1}

0 1

O	-2.66199000	-1.88935000	0.83720800
O	0.38891100	-0.25042200	-3.11626500
O	0.18638000	0.81565000	-0.73944800
O	-2.65186000	0.98825600	0.57885100
Al	-0.71841800	-0.69485600	-1.85337100
Al	-3.19703100	-0.55392100	-0.17374300
Al	1.20569900	2.25748000	-0.01489800
O	2.47514800	-1.00835800	0.74121400
O	5.30187500	1.70652800	-0.82752200
Al	1.44199600	-2.44749200	-0.00264700
Al	5.61910300	0.32228100	0.16946700
O	2.22794000	0.04634800	3.11438900
O	-0.39855400	-0.29808100	1.71106900
O	0.60385400	-2.60383400	1.63702400
Al	1.20814800	-0.94413300	2.17167500
O	5.04166600	0.43590600	1.77563700
Al	3.60148000	1.69959000	-1.01004400
O	5.30132300	-1.18832700	-0.56616800
O	-0.06585400	2.66666900	1.04833800
O	2.79466000	1.76179900	0.65364800
Al	3.32530600	0.47637700	1.84323700
Al	-0.94609900	1.17871500	0.82609700
O	-2.40401500	-0.58969800	-1.71827800
O	2.69636000	-2.86323400	-1.07957800
O	-0.14165500	-1.95947400	-0.67782200
Al	3.62654300	-1.41493900	-0.87727700
Al	-0.97578700	-1.89132500	0.96726100
O	3.04804300	0.09564000	-1.73180500
O	2.03434000	2.40360800	-1.66417300
Al	1.42296500	0.72099700	-2.17695700
C	-4.51198400	2.82826500	1.03532900
H	-4.36192400	3.00393800	2.10054100
H	-4.16389800	3.63592400	0.39152900
H	-3.65380600	1.97659700	0.81861900
C	-5.78542600	2.32356500	0.70140800
I	-5.78339000	-0.25359500	-0.24657100
H	-6.25609100	2.58651800	-0.23694500
H	-6.45346600	1.95550200	1.46916500

Al_{20}---C_2H_5I reactant geometry:
v1=13.25 cm^{-1}

0 1

Al	1.28970600	1.52816200	-1.61687800
Al	1.27050400	1.80628600	1.34098000
Al	0.98722400	-0.83809100	2.42761600
Al	0.84933400	-2.69282200	0.26853300
Al	1.00497000	-1.28973200	-2.20125600
Al	2.34420200	-0.38023100	0.05584400
Al	-0.13743700	-0.13519500	0.01756300
Al	-1.14261400	0.42360300	-2.42872100
Al	-0.91506200	2.43437700	-0.21880400
Al	-1.17673100	0.86572800	2.30560400
Al	-1.42366600	-1.91069100	1.61009800
Al	-1.42044000	-2.17938300	-1.21159100
Al	-3.91003900	-1.32199100	-2.13630300
Al	-3.76681300	1.25679800	-2.40347600
Al	-3.62422100	2.79984900	-0.31837400
Al	-3.77639300	1.75722000	2.05687000
Al	-3.88783900	-0.81760400	2.36980500
Al	-3.96152600	-2.37350700	0.25970400
Al	-2.64752700	0.15622000	-0.02436800
Al	-5.16642500	0.26804100	-0.02988600
C	5.57568800	1.55380000	-0.70527100
C	5.80258000	2.51570100	0.42646000
H	4.64828700	1.73284000	-1.24680600
H	5.91307700	3.51949200	0.00150700
H	4.95640000	2.53849900	1.11425500
H	6.70887200	2.28648900	0.98821500
H	6.40983900	1.47753400	-1.39728500
I	5.33649500	-0.52100600	0.01159500

Al_{20}---C_2H_5I TS1 geometry:
v1=-148.14 cm^{-1}

0 1

Al	-1.24174300	0.25771800	-2.36620000
Al	-0.88164500	-2.39981500	-1.41559900
Al	-0.88152900	-2.40020800	1.41510600
Al	-1.24159600	0.25708800	2.36644000
Al	-1.43492400	1.95813200	0.00034400
Al	-2.44637400	-0.57603700	0.00006200
Al	0.05467500	-0.24617200	0.00002000

Al	0.84583500	1.85005000	-1.52695500
Al	1.26154000	-0.90371600	-2.31721200
Al	1.47089800	-2.55231300	-0.00039200
Al	1.26170700	-0.90438400	2.31698100
Al	0.84588500	1.84967700	1.52749000
Al	3.48543500	2.53470000	1.29664300
Al	3.48532700	2.53529100	-1.29559900
Al	3.76114000	0.32058900	-2.61021100
Al	3.88502400	-1.92637200	-1.33428700
Al	3.88517400	-1.92698600	1.33320400
Al	3.76149400	0.31937600	2.61016400
Al	2.57679100	0.19814700	0.00003500
Al	5.12931000	0.39153100	-0.00008900
C	-5.79459500	2.14199900	-0.00007100
C	-4.68992700	3.06301000	0.00012800
H	-6.33153600	1.93846500	0.91619200
H	-4.64298800	3.67305300	-0.90199400
H	-4.64305800	3.67283600	0.90239300
H	-3.65643100	2.53722700	0.00003600
H	-6.33119100	1.93851400	-0.91655200
I	-5.09545600	-0.51437700	0.00000500

Al_{20}---C_2H_5I product-1 geometry:
v1=4.96 cm^{-1}

0 1

Al	1.03707600	-0.24953100	2.44288500
Al	0.47218200	-2.65536700	1.07189300
Al	0.57382400	-2.18040800	-1.75750200
Al	1.20862100	0.53358300	-2.22100100
Al	1.42573600	1.74973500	0.39784500
Al	2.30922700	-0.85247700	-0.01397300
Al	-0.19811300	-0.23695600	-0.00238900
Al	-0.95607000	1.61564200	1.84401000
Al	-1.52983800	-1.15281600	2.15572800
Al	-1.85923100	-2.31843400	-0.41054500
Al	-1.36472000	-0.38405600	-2.42879500
Al	-0.84008600	2.12465700	-1.19351500
Al	-3.45539700	2.97853500	-0.90447400
Al	-3.55610500	2.55169600	1.65297800
Al	-3.94379400	0.20857200	2.62943300
Al	-4.15471400	-1.75453400	0.98442100
Al	-4.05916700	-1.31164000	-1.70081700
Al	-3.76175200	1.07599700	-2.60327100
Al	-2.69663500	0.43354400	0.01742700

Al	-5.28766700	0.72331300	-0.02468500
C	8.53454100	3.26651200	0.20291000
C	9.30587000	4.31317800	-0.05273800
H	8.00389200	2.74107700	-0.58437000
H	9.83557500	4.83816000	0.73551600
H	9.44103200	4.69003100	-1.06128000
H	2.39618700	2.97906700	0.63527200
H	8.39911400	2.88936700	1.21138300
I	4.77656300	-1.42082200	-0.01888800

Al_{20}---C_2H_5I TS2 geometry:
v1=-214.91 cm^{-1}

0 1

Al	1.25848500	0.27661200	2.34849200
Al	0.86263100	-2.39521700	1.43090400
Al	0.86242100	-2.39631200	-1.42954700
Al	1.25800300	0.27480000	-2.34932900
Al	1.44671100	2.01011800	-0.00130100
Al	2.44737800	-0.65894700	-0.00016400
Al	-0.04024600	-0.22546000	-0.00008000
Al	-0.85600500	1.86529300	1.51969000
Al	-1.25044400	-0.88597900	2.32567000
Al	-1.48199100	-2.51916700	0.00095200
Al	-1.25084600	-0.88791800	-2.32508100
Al	-0.85660500	1.86391600	-1.52149600
Al	-3.50592600	2.52383300	-1.29699000
Al	-3.50534500	2.52476300	1.29594500
Al	-3.75049600	0.31286300	2.61372800
Al	-3.88851500	-1.93557200	1.32938500
Al	-3.88875100	-1.93625900	-1.32766100
Al	-3.75065600	0.31127000	-2.61368600
Al	-2.56947400	0.19663800	0.00007400
Al	-5.12578100	0.35890500	0.00014200
C	4.44988900	2.09765200	-0.00052300
C	5.50580400	3.12907800	0.00014600
H	3.95883200	1.83326200	-0.92447500
H	6.12949300	3.07192000	0.89335600
H	6.12873700	3.07409400	-0.89374600
H	5.03398800	4.12149500	0.00164100
H	3.95798200	1.83295400	0.92292500
I	5.16354200	-0.53038600	0.00013500

Al_{20}---C_2H_5I product-2 geometry:
v1=8.97 cm^{-1}

0 1

Al	-1.39167400	0.37729400	-2.36759500
Al	-1.25249100	-2.28528500	-1.43194800
Al	-1.25332700	-2.28704800	1.42838400
Al	-1.39113500	0.37285000	2.36910300
Al	-1.42042200	2.06651500	0.00730700
Al	-2.73365200	-0.39516000	-0.00066700
Al	-0.16485600	-0.22630100	-0.00039100
Al	0.89610400	1.73921100	-1.54267300
Al	0.97611900	-0.99485700	-2.32213800
Al	1.10447700	-2.61199600	-0.00101600
Al	0.97573800	-0.99758400	2.32087100
Al	0.89857600	1.73646100	1.54540700
Al	3.62529700	2.16636900	1.29686200
Al	3.62247100	2.16763900	-1.29810200
Al	3.59079800	-0.01334800	-2.65384000
Al	3.45832300	-2.23233900	-1.36237000
Al	3.45847900	-2.23127400	1.36169600
Al	3.58891200	-0.01293800	2.65441300
Al	2.41692500	-0.01450300	-0.00061600
Al	5.01902400	-0.19668100	0.00034500
C	-2.38425200	3.81446800	-0.00124700
C	-1.49943600	5.05927200	-0.00145500
H	-3.04332600	3.80344800	0.87240800
H	-2.10389000	5.97261700	-0.00680300
H	-0.85555200	5.10120800	0.88071000
H	-0.84829000	5.09565700	-0.87853000
H	-3.03670200	3.79838900	-0.87975000
I	-5.26637800	-0.50311500	-0.00021200

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Hydrated alumina clusters (with one H_2O molecule)-

Al_8O_{12}---C_2H_5F reactant geometry:
v1=35.67 cm^{-1}

0 1

O	-1.23541500	0.95005800	0.06039800
O	0.49991600	3.25348100	0.70729500
Al	-0.57437000	-0.21274400	1.25732200

Al	-1.66303100	0.57195100	-1.72444100
O	2.25997400	-0.91953600	-0.81417000
O	0.42402300	-3.08013100	-1.56939400
Al	2.53374600	-0.38228700	0.97229100
O	1.34593900	1.81384600	-1.12501500
O	3.31863900	1.19132400	0.93203900
Al	-0.86704700	-1.86336100	-1.56851100
O	-1.42107400	2.28986500	-2.01440100
O	-0.11392600	-0.32832900	-2.38131100
Al	1.35897000	0.22390200	-1.72811100
Al	-0.37580800	2.47897200	-0.60829800
O	2.07508400	-2.07296000	1.38020200
O	1.01161100	0.53321100	1.46643000
Al	1.21380900	-2.35191800	-0.17401300
Al	1.77711900	2.04169000	0.70673500
O	-0.42153300	-1.61003800	0.20555000
O	-2.41209300	-1.02664300	-1.76013700
C	-4.27883100	-0.51684600	1.26755200
H	-3.79469900	-0.80408700	0.33023200
H	-5.26300800	-0.10384200	1.02335700
H	-4.42966000	-1.39564400	1.89563500
C	-3.51735500	0.54464700	1.98472000
H	-3.92118600	0.82331000	2.95469800
H	-3.27027900	1.41024100	1.37704000
F	-2.17322000	-0.00336200	2.35967200
O	-0.09483500	-1.46024900	2.77435000
H	0.10231600	-1.08045900	3.63669200
H	0.77810400	-1.83791200	2.40832700

Al_8O_{12}---C_2H_5F TS1 geometry:
v1=-497.70 cm^{-1}

0 1

O	-0.71873800	1.27896000	0.55172900
O	1.69189900	2.63975000	1.53256300
Al	-0.52753100	-0.34695100	1.33441000
Al	-1.40986100	1.65091700	-1.08612600
O	1.77184700	-1.16890900	-1.34919400
O	-0.70851200	-2.35177300	-2.33036700
Al	2.35111300	-1.34401100	0.45032400
O	1.83747600	1.66764200	-0.74926500
O	3.61410500	-0.15033000	0.70402300
Al	-1.47781700	-0.87708800	-1.74169800
O	-0.64554500	3.22389800	-0.97856000
O	-0.39610600	0.55957500	-2.25957600

Al	1.23122900	0.41572300	-1.72082600
Al	0.50968500	2.63611700	0.23325000
O	1.43466400	-2.88583200	0.42001600
O	1.25480900	-0.22822700	1.42146800
Al	0.39418500	-2.37930800	-0.94428700
Al	2.43492600	1.14111100	0.99223300
O	-0.86199300	-1.34102600	-0.09720500
O	-2.69241100	0.40046200	-1.34152600
C	-4.33051300	-0.01393600	0.75269200
H	-3.47632300	0.15902000	-0.11436700
H	-4.90333200	0.90050300	0.58962900
H	-4.81768800	-0.90675500	0.35979400
C	-3.89517500	-0.15634500	2.08811700
H	-3.89245600	-1.12824800	2.56269700
H	-3.92154300	0.68800300	2.76356300
F	-1.99473700	-0.16172500	2.36244100
O	-0.29522700	-2.15982500	2.33176000
H	0.07741000	-2.13767100	3.21852800
H	0.37348100	-2.62718200	1.74175200

Al_8O_{12}---C_2H_5F product-1 geometry:
v1=25.65 cm^{-1}

0 1

O	-0.72369300	1.21721400	0.59354700
O	1.69627400	2.74819700	1.38479800
Al	-0.33985500	-0.36247200	1.49505500
Al	-1.51669900	1.57286300	-0.95650100
O	1.73584300	-1.09786600	-1.45019900
O	-0.69661400	-2.48520100	-2.16739100
Al	2.51659600	-1.20073300	0.29342900
O	1.68123600	1.76407700	-0.89932700
O	3.71111000	0.08168900	0.39455900
Al	-1.47336300	-1.04844900	-1.55813200
O	-0.86675000	3.18141800	-0.93090400
O	-0.61871000	0.47266300	-2.17394400
Al	1.07455000	0.44444200	-1.76744700
Al	0.40565300	2.66096400	0.20986900
O	1.73053300	-2.80882300	0.35656000
O	1.43057200	-0.13993900	1.31593100
Al	0.51230000	-2.39579700	-0.86368100
Al	2.48006600	1.29020700	0.79453800
O	-0.75630400	-1.37703700	0.04540900
O	-2.80882300	0.21979400	-1.19664300
C	-5.25231600	0.23918300	0.91549900

H	-3.50997500	0.06849600	-0.53111300
H	-5.17292400	1.30295100	1.11923400
H	-6.06892400	-0.07137900	0.27073900
C	-4.42290000	-0.63803800	1.47603300
H	-4.53395600	-1.70446400	1.30082600
H	-3.62095500	-0.33694400	2.14524300
F	-1.37762600	-0.11727800	2.84697700
O	0.07161700	-2.20803000	2.37360800
H	0.31325700	-2.19998000	3.30371800
H	0.78288100	-2.64860600	1.83864400

$A_{l8}O_{12}$---C_2H_5Cl reactant geometry:
v1=33.93 cm^{-1}

0 1

O	-0.17957400	-1.64551700	-0.17023900
O	2.16280900	-1.87044300	-1.66915600
Al	-0.56687600	-0.23057700	-1.13031500
Al	-0.37887100	-1.99068500	1.63252900
O	1.48475400	1.85773800	1.07257300
O	-1.17878000	2.09209800	2.30766300
Al	1.66813500	2.18392300	-0.78538000
O	2.55634700	-0.78401300	0.53327800
O	3.22443800	1.46057500	-1.23742600
Al	-1.32216400	0.36990400	1.98321500
O	0.98889300	-3.10107500	1.42284700
O	0.36082900	-0.42638900	2.40364400
Al	1.69821700	0.25572500	1.60039600
Al	1.53920200	-2.27136000	-0.02897200
O	0.32049300	3.29633800	-0.57612600
O	0.92038500	0.64697000	-1.50296400
Al	-0.33014500	2.41073700	0.79682400
Al	2.55510600	-0.16549400	-1.24668400
O	-1.16453800	0.84461600	0.16961500
O	-1.94098000	-1.28005200	2.05357000
C	-4.67754500	-0.47082900	-0.16547900
H	-5.20544700	-1.21973900	-0.75665700
H	-5.41058100	0.02509300	0.48078000
H	-3.94009800	-0.95802700	0.47640000
C	-4.06122900	0.58576900	-1.02516400
H	-3.44540800	1.29954100	-0.48843500
H	-4.74392000	1.07300900	-1.71456300
Cl	-2.80346000	-0.19961900	-2.22340400
O	-0.18436600	-1.36584700	-2.76023600
H	-0.09267700	-0.92653200	-3.61257500
H	0.75005400	-1.69771000	-2.50055400

Al_8O_{12}---C_2H_5Cl TS1 geometry:
v1=-381.45 cm^{-1}

0 1

O	0.58175900	-1.44886100	-0.15742800
O	-1.77835900	-2.69944200	0.74572000
Al	0.50827900	-0.34081000	1.22553700
Al	1.03301900	-1.17234700	-1.89695100
O	-1.86740400	1.77590100	-0.72915700
O	0.71281400	3.03044200	-1.36057100
Al	-2.30379500	1.43904200	1.10216700
O	-2.16413400	-1.08878700	-1.10827500
O	-3.63254300	0.26666600	1.04883000
Al	1.28929400	1.37928500	-1.44648400
O	0.05490600	-2.59391900	-2.26558300
O	0.02911900	0.33288300	-2.39349600
Al	-1.52626300	0.40254400	-1.66539600
Al	-0.86602100	-2.40536900	-0.76568500
O	-1.34558000	2.87444500	1.43619500
O	-1.22530500	-0.01746000	1.50305400
Al	-0.33371400	2.65112900	0.01945000
Al	-2.53537900	-1.07229600	0.75285000
O	0.79079400	1.18958800	0.29620600
O	2.40163200	-0.00151000	-1.78523800
C	4.56279800	-0.22766900	-0.17303200
H	4.94244000	-1.22142400	-0.40313000
H	5.06090100	0.56575000	-0.74116800
H	3.51752900	-0.14790800	-0.77552500
C	4.54482400	0.08619100	1.20549400
H	4.55131500	1.12003700	1.52684100
H	4.86945600	-0.63116500	1.94636700
Cl	2.48299700	-0.14673200	2.41940800
O	0.22861300	-2.04146100	2.35695000
H	0.02399300	-1.95529800	3.29302300
H	-0.56328000	-2.46985300	1.89986300

Al_8O_{12}---C_2H_5Cl product-1 geometry:
v1=23.89 cm^{-1}

0 1

O	0.68797100	-1.38312800	0.01273100
O	-1.76129000	-2.78010100	0.63449900
Al	0.36640600	-0.24818000	1.39720600
Al	1.27346900	-1.19052500	-1.66583000
O	-1.84718300	1.66706800	-1.01264600

O	0.68503000	3.07555200	-1.35312000
Al	-2.51269500	1.33895200	0.77274900
O	-1.91757200	-1.23324100	-1.30746900
O	-3.76026100	0.09852700	0.57148300
Al	1.34359700	1.47213800	-1.29664000
O	0.46187700	-2.67447600	-2.08743000
O	0.36087100	0.27129600	-2.34151000
Al	-1.29550800	0.27811000	-1.80543900
Al	-0.64373600	-2.47445400	-0.70808900
O	-1.69548400	2.84134800	1.17416100
O	-1.41449800	-0.04118400	1.32951100
Al	-0.49750400	2.65444900	-0.08324000
Al	-2.56790500	-1.18634700	0.48926900
O	0.66633500	1.24209500	0.33259100
O	2.62174100	0.10686500	-1.53061900
C	4.96232700	0.50928700	0.65877700
H	5.49867700	1.33145800	0.19401800
H	4.28351900	0.75326100	1.47098200
H	3.40467900	0.01618400	-0.95134200
C	5.15729700	-0.74966300	0.27444700
H	4.65028900	-1.57233400	0.76953600
H	5.85850900	-1.00730600	-0.51352500
Cl	1.79092600	0.26581500	2.98923100
O	0.02842100	-2.00791600	2.44380500
H	-0.12664900	-1.94326200	3.39041100
H	-0.71977700	-2.49010800	1.99594100

Al_8O_{12}---C_2H_5Br reactant geometry:
ν1=31.64 cm^{-1}

0 1

O	-0.02689800	-1.10107500	1.19941600
O	1.97538100	-2.74068300	0.16348200
Al	-0.53564800	-0.80726700	-0.45238800
Al	0.11358300	0.04104000	2.64665200
O	1.98047700	1.83672600	-0.80490400
O	-0.38738400	3.34968700	0.08203100
Al	1.81312900	0.65020300	-2.27479900
O	2.82238900	-0.47394600	0.73580100
O	3.22531000	-0.41959100	-2.17350700
Al	-0.65229400	2.00739000	1.18656100
O	1.37474800	-1.07029000	3.21385400
O	1.04651400	1.50985100	1.89255000
Al	2.23088200	1.14078100	0.72625600
Al	1.66378100	-1.69068900	1.59197700

O	0.57326000	1.76131300	-2.84462400
O	0.88380300	-0.75974800	-1.50704100
Al	0.16671700	2.30184200	-1.22162500
Al	2.50566300	-1.37736800	-0.88634600
O	-0.82716400	0.95524500	-0.36236400
O	-1.30760500	1.08465600	2.53921600
C	-4.44800100	0.70309400	0.87133700
H	-5.19333800	-0.04796500	1.13582800
H	-4.91798400	1.68853300	0.97021000
H	-3.61542100	0.65683600	1.57689100
C	-3.99114800	0.56820100	-0.54936900
H	-3.19004400	1.24625200	-0.82658000
H	-4.78877600	0.56648100	-1.28655600
Br	-3.11803600	-1.25527700	-0.85716500
O	-0.50973100	-2.82084000	-0.71238900
H	-0.52900000	-3.15097300	-1.61757400
H	0.44034800	-2.99977100	-0.36718200

Al_8O_{12}---C_2H_5Br TS1 geometry:
v1=-426.70 cm^{-1}

0 1

O	-0.47643100	-1.41917700	-0.06051800
O	1.51400300	-2.38459700	-1.81130500
Al	-0.54403100	0.08365200	-1.00418000
Al	-0.51973800	-1.70250500	1.73864700
O	2.39052000	1.35420400	0.93209400
O	0.12699500	2.42839100	2.47717600
Al	2.41245300	1.61658800	-0.96344600
O	2.43086000	-1.48431400	0.31846700
O	3.58821200	0.44004700	-1.57807200
Al	-0.60780800	0.86933900	2.16882900
O	0.34803300	-3.20326500	1.41454300
O	0.70454300	-0.47950600	2.43939100
Al	2.08226200	-0.23377400	1.44099900
Al	0.96157600	-2.56848200	-0.11984200
O	1.56727700	3.11632100	-0.61200600
O	1.12305800	0.41220800	-1.55043000
Al	0.84077400	2.48349300	0.85549300
Al	2.43192700	-0.87722800	-1.47921600
O	-0.45537100	1.22684900	0.39238100
O	-1.76068400	-0.51794400	2.30264800
C	-4.23227700	-0.61288600	1.26664400
H	-4.33630500	-1.66755800	1.53795900
H	-4.74638300	0.06107600	1.95074400
H	-3.06570500	-0.50190600	1.61601500

C	-4.53811500	-0.39651700	-0.09605000
H	-5.16761600	0.42936000	-0.39822600
H	-4.47377900	-1.21173300	-0.80517100
Br	-2.85773900	0.83150400	-1.58120400
O	-0.69643700	-1.15936800	-2.64113500
H	-0.67115200	-0.77495000	-3.52303800
H	0.12112200	-1.74337000	-2.53026000

Al_8O_{12}---C_2H_5Br product-1 geometry:
v1=18.43 cm^{-1}

0 1

O	0.46962300	0.82978800	-1.17168800
O	-1.77000500	0.25365200	-2.89896400
Al	0.49666200	-0.91543500	-0.65747300
Al	0.64369000	2.39860900	-0.32949200
O	-2.21091000	0.03977100	1.81902700
O	0.17908900	0.37832700	3.45695900
Al	-2.43794100	-1.58842900	0.80578000
O	-2.37374700	1.38408900	-0.76681200
O	-3.70587200	-1.21744100	-0.37331000
Al	0.82165800	1.07601600	2.00493300
O	-0.25452200	3.15543500	-1.61677200
O	-0.39171600	2.24775200	1.19476300
Al	-1.87406400	1.39676900	0.86683200
Al	-1.00086700	1.59432500	-2.02937500
O	-1.53873600	-2.33517400	2.11702200
O	-1.24842200	-1.32532600	-0.58710900
Al	-0.67177300	-0.86927200	2.50524300
Al	-2.57736500	-0.39570700	-1.43602300
O	0.54945900	-0.45640600	1.14035400
O	1.99457600	2.08876500	0.93203500
C	4.89634100	0.70817800	0.61989200
H	5.38078100	1.08581200	1.51538800
H	4.51128900	-0.30691900	0.65071400
H	2.89702500	1.79676400	0.69304100
C	4.81195500	1.44133600	-0.48716600
H	4.36163000	1.04145800	-1.39059700
H	5.22358800	2.44456500	-0.54315500
Br	2.40934000	-2.32119600	-0.64301600
O	0.40141500	-1.26404800	-2.70152400
H	0.48244500	-2.16774800	-3.02013700
H	-0.43527400	-0.84201400	-3.04341500

$Al_{8}O_{12}$---C_2H_5I reactant geometry:
v1=26.24 cm^{-1}

0 1

O	0.50629800	0.94697800	-0.58529800
O	-0.80630000	0.85029800	-3.23717400
Al	0.38551500	-0.78544100	-0.16064100
Al	0.15337300	2.37932200	0.57850100
O	-3.05621800	-0.46867300	0.77220200
O	-1.70894700	-0.16822200	3.35969800
Al	-2.56458900	-1.76683100	-0.49953200
O	-2.33191600	1.36881400	-1.35415000
O	-3.28729600	-1.30359000	-2.03428800
Al	-0.51874300	0.85200300	2.52831900
O	-0.16443400	3.30991900	-0.87989300
O	-1.53334100	1.93500200	1.34738600
Al	-2.60999500	1.12553000	0.30606900
Al	-0.54619300	1.87848000	-1.83443600
O	-1.98071200	-2.70559700	0.92150500
O	-0.96969100	-1.19145000	-1.22396100
Al	-1.84711800	-1.25914900	1.98539800
Al	-1.97277500	-0.16902000	-2.40200000
O	-0.19473700	-0.64208000	1.48786800
O	0.80724700	1.96084900	2.16235900
C	4.09254400	1.70268600	0.75655900
H	3.22840600	1.71285700	1.42495300
H	4.37215700	2.74285600	0.55228100
H	4.93355800	1.22830900	1.26416800
C	3.78220000	1.04974800	-0.56095200
I	3.20139400	-1.06452000	-0.29800000
H	4.62691500	0.98579200	-1.24149300
H	2.90861200	1.45915000	-1.05973500
O	0.54223100	-2.79713000	0.16899500
H	0.60116500	-3.34560700	-0.62170900
H	-0.40380700	-2.95296800	0.53808500

$Al_{8}O_{12}$---C_2H_5I TS1 geometry:
v1=-530.99 cm^{-1}

0 1

O	0.26795300	-0.35854900	-1.20303400
O	-1.47227700	-2.61206000	-1.95660200
Al	0.42140900	-0.65467600	0.57457000
Al	0.18453400	1.22765600	-2.08709500

O	-2.80665800	0.94139600	0.94317600
O	-1.00618600	3.16252100	1.50794400
Al	-2.55127900	-0.80182300	1.65082500
O	-2.60347100	-0.42904300	-1.60937200
O	-3.57767800	-1.88911500	0.73104500
Al	-0.06318300	2.55726300	0.14739100
O	-0.45567800	0.35256200	-3.46129400
O	-1.25253800	2.12017900	-1.22179300
Al	-2.48730300	1.02347100	-0.74150300
Al	-0.97209600	-1.00074400	-2.44035900
O	-1.72585000	0.05017600	2.99935400
O	-1.14199100	-1.50618700	0.70170300
Al	-1.38798500	1.51560000	2.03176300
Al	-2.38806800	-2.02510900	-0.57674800
O	0.11825100	1.01497900	1.09769300
O	1.19551800	2.39529700	-1.14037500
C	3.77266800	2.23068600	-0.49444000
H	2.56875700	2.16727100	-0.77372300
H	4.19738200	2.45905400	-1.47186900
H	3.70249400	3.09971400	0.16488500
C	4.36932500	1.12315400	0.14597100
I	3.04236700	-1.28693200	0.31068900
H	4.41462300	1.07484000	1.22614900
H	5.09194100	0.50860500	-0.37378300
O	0.65458200	-1.05420200	2.58089500
H	0.76356400	-1.96473200	2.87312400
H	-0.21634500	-0.70530500	2.95982800

Al_8O_{12}---C_2H_5I product-1 geometry:
v1=22.26 cm^{-1}

0 1

O	-0.37234900	0.02238600	1.20216100
O	1.24752800	-2.09155500	2.52712100
Al	-0.49747000	-0.75693400	-0.47773200
Al	-0.23710500	1.70743000	1.76297600
O	2.83205400	0.72809500	-0.99585700
O	1.15923700	2.76946100	-2.17645800
Al	2.57888300	-1.14083000	-1.31738800
O	2.45158000	-0.04399000	1.79309000
O	3.52063700	-2.00146100	-0.11305200
Al	0.15743000	2.49644500	-0.77702100
O	0.27735800	1.15354800	3.32355600
O	1.18714700	2.38357800	0.75610200
Al	2.41470900	1.15959800	0.60434100

Al	0.76984800	-0.41484200	2.62872700
O	1.89425800	-0.59542500	-2.88186900
O	1.10066800	-1.55669900	-0.32025100
Al	1.50165600	1.02782600	-2.28568300
Al	2.24688900	-1.83720300	1.10540500
O	-0.07383400	0.80430700	-1.31023400
O	-1.17567600	2.75894600	0.51251000
C	-4.37320500	2.36476200	0.60682400
H	-2.13482000	2.67325200	0.34069300
H	-4.34036300	1.37624800	1.05498500
H	-4.62145500	3.19771000	1.25759400
C	-4.16121800	2.53367700	-0.69562900
I	-2.88753700	-1.69756900	-0.18010300
H	-4.22957600	3.51140500	-1.16321300
H	-3.95083100	1.68782600	-1.34299100
O	-0.56303800	-1.48993900	-2.42188300
H	-0.85232400	-2.39548200	-2.56913800
H	0.33786100	-1.33981800	-2.82626400

Al_8O_{12}---C_2H_5F TS2 geometry:
v1=-273.39 cm^{-1}

0 1

O	-0.76253400	1.22885500	0.58964900
O	1.62936300	2.70304400	1.47513600
Al	-0.43818500	-0.38151100	1.42327300
Al	-1.51475000	1.57076800	-1.05606900
O	1.76097300	-1.11357600	-1.39100500
O	-0.71313600	-2.39728000	-2.25818100
Al	2.42559700	-1.24971900	0.38141500
O	1.73299800	1.72745900	-0.80583600
O	3.64528200	0.00007800	0.56880900
Al	-1.51509600	-0.94011800	-1.67177500
O	-0.81857000	3.17320300	-0.94987500
O	-0.49286200	0.52089700	-2.24217000
Al	1.15448100	0.44687300	-1.75541400
Al	0.39801400	2.63670400	0.22512300
O	1.56870400	-2.82663400	0.39552700
O	1.33161500	-0.17576900	1.40188300
Al	0.44344200	-2.36652300	-0.91825500
Al	2.42555200	1.24100400	0.90979500
O	-0.81955600	-1.36518000	-0.02753600
O	-2.77332200	0.28955300	-1.26045400
C	-4.73830200	-0.13627600	1.47767100
H	-5.02714500	-1.12256700	1.83900900

H	-5.31293300	0.05573200	0.55521100
H	-4.99845700	0.65254000	2.18326100
C	-3.35410900	-0.06834700	1.04327900
H	-2.83783500	0.87163500	1.01443300
H	-2.85616300	-0.95069400	0.68746400
F	-1.85295800	-0.27109400	2.53349500
O	-0.09840800	-2.19495100	2.35192700
H	0.22397200	-2.21187700	3.25752900
H	0.58755300	-2.63197700	1.75775900

Al_8O_{12}---C_2H_5F product-2 geometry:
v1=38.07 cm^{-1}

0 1

O	-0.34170500	1.34701200	0.85737700
O	2.43746000	2.38826900	1.05562800
Al	-0.04799500	-0.31344700	1.64845900
Al	-1.38598700	1.90011600	-0.46874300
O	1.12145700	-1.28125200	-1.70405700
O	-1.61905100	-2.18825900	-1.82674500
Al	2.25472600	-1.59445700	-0.19489200
O	1.71474900	1.52081500	-1.16010500
O	3.65195400	-0.54697900	-0.37777000
Al	-1.96240100	-0.66431500	-1.05239800
O	-0.46700600	3.36594700	-0.59711600
O	-1.01330000	0.70637700	-1.85531800
Al	0.69557000	0.36491500	-1.85820300
Al	0.91477200	2.58056600	0.22004100
O	1.22729400	-3.03992800	0.05306700
O	1.63938000	-0.40093800	1.04576100
Al	-0.14582900	-2.36596400	-0.84251200
Al	2.78419700	0.84145200	0.29704400
O	-0.96960000	-1.18248200	0.34103300
O	-2.92147700	0.80856300	-0.38240100
C	-4.64403900	-0.55238000	0.64641200
H	-3.99294000	-1.43052000	0.72586500
H	-5.21359600	-0.60296800	-0.28476100
H	-5.35081400	-0.61220100	1.47660700
C	-3.84628000	0.72517700	0.73422900
H	-4.49703900	1.60008500	0.68023000
H	-3.27240100	0.76588900	1.66412000
F	-0.65387000	0.05985600	3.21096400
O	0.21587700	-2.24035100	2.40561500
H	0.65667800	-2.30759500	3.25687800
H	0.69690900	-2.77779800	1.72444100

Al_8O_{12}-C_2H_5Cl TS2 geometry:
v1=-270.16 cm^{-1}

0 1

O	0.70608700	-1.36967700	-0.20652100
O	-1.64388600	-2.80481400	0.48736100
Al	0.47728500	-0.39162900	1.27741900
Al	1.20238900	-0.95364200	-1.92650700
O	-1.89390300	1.74713300	-0.67848900
O	0.64047400	3.15781500	-1.10426000
Al	-2.40274700	1.26702000	1.09849900
O	-2.02603500	-1.09350400	-1.26758200
O	-3.66678600	0.04036900	0.89188000
Al	1.29941800	1.55125200	-1.30617600
O	0.32006800	-2.40055900	-2.40945600
O	0.12931000	0.51854700	-2.36216200
Al	-1.45332200	0.46426300	-1.69597100
Al	-0.67066900	-2.35662400	-0.94614400
O	-1.51881300	2.70847500	1.57916100
O	-1.27661000	-0.16341500	1.45320200
Al	-0.43341300	2.63017300	0.20309300
Al	-2.49176300	-1.22294600	0.56535400
O	0.75623200	1.20588600	0.42487300
O	2.51051500	0.26664700	-1.68863400
C	4.93245500	-0.10375800	0.45181000
H	5.30463000	-1.07759700	0.76781800
H	5.37479500	0.70018500	1.03919700
H	5.24288700	0.04540800	-0.59368400
C	3.47373000	-0.03818000	0.42174000
H	2.96727600	0.90297300	0.50823800
H	2.89597700	-0.92415200	0.23804600
Cl	2.36859800	-0.21619600	2.63360100
O	0.23096300	-2.19943900	2.21356500
H	0.04920100	-2.24439100	3.15671300
H	-0.53227000	-2.62546300	1.70328300

Al_8O_{12}---C_2H_5Cl product-2 geometry:
v1=39.14 cm^{-1}

0 1

O	0.93046100	-1.19344000	0.21425000
O	-1.29912100	-3.02383000	0.24974300
Al	0.13551600	-0.21895700	1.52777400
Al	1.81598600	-0.79246700	-1.28717600

O	-1.83845100	1.44336300	-1.25274600
O	0.40700000	3.28400000	-1.00086500
Al	-2.79078700	0.89052400	0.33686900
O	-1.32323400	-1.40045800	-1.63548000
O	-3.72464400	-0.52854800	-0.16081600
Al	1.31699100	1.81603900	-0.84459500
O	1.38865900	-2.36099300	-1.91900200
O	0.81672800	0.53278500	-2.10673600
Al	-0.88984500	0.22328600	-1.94203900
Al	-0.00015300	-2.44331800	-0.80966600
O	-2.36464000	2.48220100	0.94529600
O	-1.59960100	-0.31464600	1.08016100
Al	-0.91644800	2.58627200	-0.02586100
Al	-2.32928700	-1.58283500	-0.01952300
O	0.37076700	1.37023700	0.59403900
O	2.84045200	0.70942000	-0.80681600
C	4.61151800	-0.60990700	0.19679700
H	3.94057300	-1.44186400	0.43881400
H	5.39579800	-0.61110500	0.95653700
H	5.08357600	-0.78843500	-0.77270300
C	3.87317600	0.70523500	0.21664800
H	4.54443000	1.53801800	-0.00170100
H	3.39942800	0.87228300	1.18791000
Cl	1.13580200	0.41216900	3.37470100
O	-0.09716900	-2.07646200	2.42850600
H	-0.44833000	-2.10919200	3.32274800
H	-0.63557000	-2.64866300	1.81637400

Al_8O_{12}---C_2H_5Br TS2 geometry:
v1=-275.49 cm^{-1}

0 1

O	0.41955100	-0.07310200	-1.45748500
O	-1.65540100	-1.83625800	-2.26709200
Al	0.57107500	-1.04017900	0.04264200
Al	0.43488900	1.73443300	-1.79174600
O	-2.24762600	0.96424400	1.47181700
O	0.06994900	2.52430600	2.35011000
Al	-2.26958900	-0.92196500	1.77214800
O	-2.50235300	0.30712400	-1.34800800
O	-3.53140900	-1.54141200	0.69069100
Al	0.66606600	2.22366600	0.73543600
O	-0.52982200	1.36333400	-3.21840100
O	-0.72976000	2.44857800	-0.50831700

Al	-2.07999200	1.45119400	-0.14364400
Al	-1.09817700	-0.15387000	-2.51190700
O	-1.30049200	-0.55386400	3.19165900
O	-1.07701500	-1.53277400	0.49002400
Al	-0.61517800	0.89539100	2.48002500
Al	-2.47156100	-1.47503800	-0.70781800
O	0.60623200	0.42174300	1.14306400
O	1.74410700	2.34628000	-0.70946900
C	4.64220500	1.08258400	-0.45229300
H	5.13876700	0.51998300	-1.24263800
H	5.21718700	1.04745500	0.47259900
H	4.59608900	2.13327000	-0.77382200
C	3.24878500	0.67368100	-0.26134300
H	2.76402100	0.80584900	0.68555600
H	2.68140200	0.28456500	-1.08552800
Br	2.91810600	-1.76932500	0.61643900
O	0.60096800	-2.65873500	-1.21877500
H	0.66343900	-3.55210800	-0.86798700
H	-0.26392500	-2.56313200	-1.73701200

Al_8O_{12}---C_2H_5Br product-2 geometry:
v1=37.41 cm^{-1}

0 1

O	-0.71381700	-0.69491600	-1.09825000
O	1.50044300	-0.59635500	-2.94341400
Al	-0.41111700	1.04548400	-0.66489900
Al	-1.13356700	-2.17353700	-0.18326300
O	2.20099200	-0.29133100	1.73618800
O	-0.12170200	-0.13268700	3.48802000
Al	2.66527200	1.23336500	0.64050900
O	1.99596100	-1.73669800	-0.78791100
O	3.78755000	0.59657600	-0.57163500
Al	-0.94824300	-0.75604800	2.09659800
O	-0.44608200	-3.12742700	-1.47089400
O	-0.01400800	-2.15892400	1.29020800
Al	1.58007000	-1.60113400	0.86364800
Al	0.54904800	-1.74424900	-1.98217800
O	1.98188400	2.17669400	1.95484300
O	1.38057200	1.13873500	-0.68768000
Al	0.88727500	0.90710200	2.44528300
Al	2.47906100	-0.04812200	-1.54613400
O	-0.45604700	0.67137300	1.15382700
O	-2.34264100	-1.55850300	1.11787800
C	-4.25689500	-1.68374100	-0.36385500

H	-5.23729300	-1.25783000	-0.58666600
H	-4.39092400	-2.75044400	-0.16714600
H	-3.64661500	-1.54933400	-1.26436300
C	-3.64127500	-0.97794400	0.81849500
H	-4.25809500	-1.09246000	1.71188600
H	-3.50566600	0.08709100	0.61061300
Br	-2.07260900	2.73614800	-0.63472100
O	-0.35283900	1.29444300	-2.72551900
H	-0.29359600	2.18449700	-3.08447500
H	0.37900300	0.71835600	-3.08209500

Al_8O_{12}---C_2H_5I TS2 geometry:
v1=-293.07 cm^{-1}

0 1

O	-0.36038700	0.23637900	1.20088200
O	1.18784900	-1.67817400	2.85161500
Al	-0.50074700	-0.78538800	-0.30873700
Al	-0.07095300	2.05072000	1.39531400
O	2.85242400	0.31617700	-1.15294100
O	1.24295600	2.26370600	-2.60892500
Al	2.46142300	-1.53577400	-1.12128100
O	2.51168300	0.09182500	1.72413500
O	3.38755500	-2.23702300	0.19509200
Al	0.25670000	2.34669900	-1.15226600
O	0.44871100	1.71022800	3.02798600
O	1.43039800	2.38141300	0.30758800
Al	2.55695900	1.08493900	0.35034500
Al	0.82325900	0.02362300	2.63646700
O	1.70934400	-1.22535900	-2.72382500
O	0.99341500	-1.70271900	-0.02487300
Al	1.47868300	0.52262800	-2.42074900
Al	2.17785300	-1.76077700	1.40167000
O	-0.07452300	0.55755800	-1.41613100
O	-0.99640800	2.83409900	0.05400900
C	-4.04010500	2.30157500	-0.17640500
H	-4.56484400	2.13783600	-1.11732800
H	-3.72103800	3.35260800	-0.15315400
H	-4.70910800	2.14184200	0.66876100
C	-2.81014100	1.50609700	-0.07452100
I	-3.18258900	-1.26282100	0.02376500
H	-2.42320700	1.21504400	0.88208200
H	-2.26884800	1.22816000	-0.95872500
O	-0.72467300	-1.88429100	-2.02985400

H	-0.96405700	-2.81506500	-1.98711400
H	0.18176100	-1.79419000	-2.47651800

Al_8O_{12}---C_2H_5I product-2 geometry:
v1=34.23 cm^{-1}

0 1

O	-0.54962300	0.38491700	1.01853100
O	0.74333600	-1.29372200	3.10786900
Al	-0.56913000	-0.86725100	-0.35261200
Al	-0.33257400	2.15377400	1.05969400
O	2.90670900	0.21620700	-0.87480800
O	1.55138400	1.87521900	-2.81255200
Al	2.53323700	-1.64519100	-0.65024500
O	2.18665800	0.36534600	1.94681600
O	3.27077700	-2.13892300	0.86281800
Al	0.39119400	2.09873300	-1.53124900
O	-0.02434200	2.08111700	2.76554400
O	1.23936300	2.41472600	0.08004300
Al	2.37029700	1.14455800	0.45626500
Al	0.40204300	0.35352800	2.63874700
O	2.06021000	-1.57625000	-2.37797400
O	0.93086700	-1.65624500	0.23580900
Al	1.74827600	0.16934800	-2.35056000
Al	1.89895900	-1.54156800	1.80889500
O	0.06831200	0.33969300	-1.55658100
O	-1.04896800	2.80234600	-0.56220300
C	-3.28381500	3.00291800	0.35106400
H	-4.34753800	2.99780800	0.10489000
H	-3.04923300	3.96631600	0.81081300
H	-3.13187900	2.19700800	1.07817600
C	-2.46381300	2.77164500	-0.89305100
I	-3.05077100	-1.53639400	-0.08464500
H	-2.69800100	1.79847800	-1.33262500
H	-2.63775100	3.55314900	-1.63531500
O	-0.49787600	-2.15849600	-1.97584300
H	-0.85211700	-3.04773200	-1.88071200
H	0.44879600	-2.18811900	-2.29305500