Supporting Information

Conversion of Fluoroform to $CHCl_3$ and $AlCl_xF_{3-x}$ via its mechanochemical reaction with $AlCl_3$

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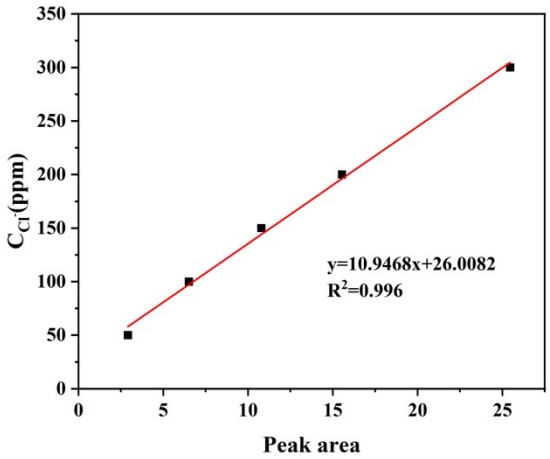

Figure S1. The standard curve and equation between C_{Cl^-} and its peak area.

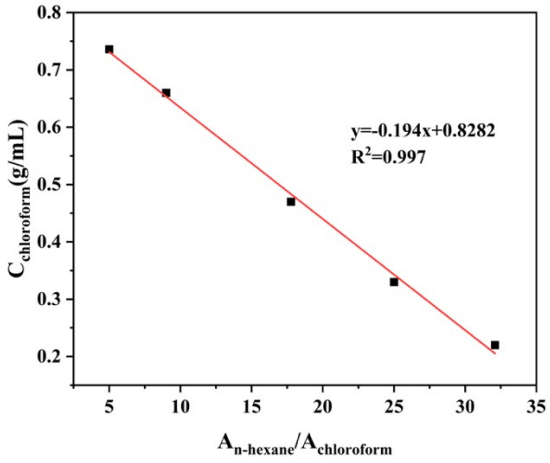

Figure S2. The standard curve and equation between C_{CF} and peak area ratio $A_{n\text{-}hexane}/A_{chloroform}$.

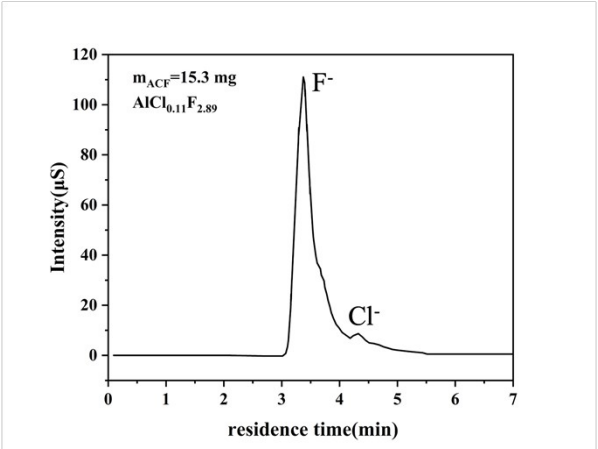

Figure S3. Ion chromatogram for the hydrolyzed solution of ACF produced under BPR=56:1, 450 rpm, 2 h.

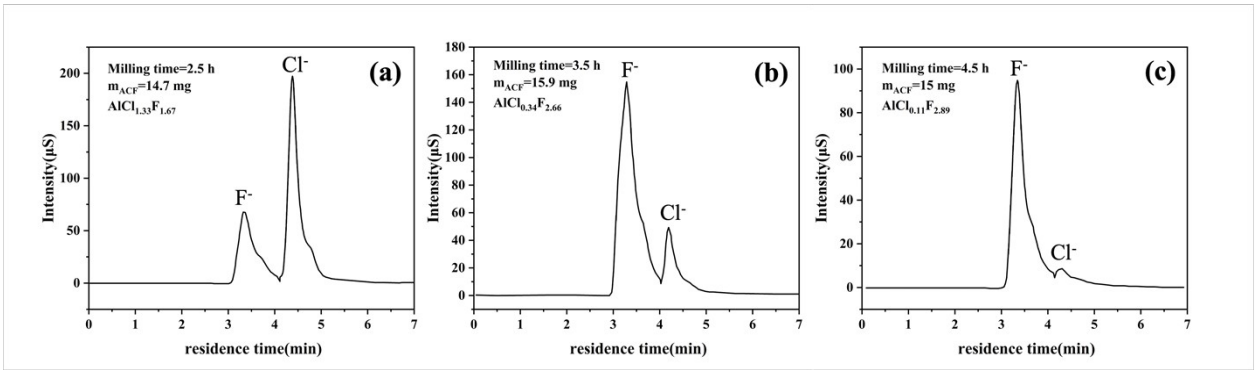

Figure S4. Ion chromatograms for the hydrolyzed solution of ACFs produced under BPR=28:1, 450 rpm.

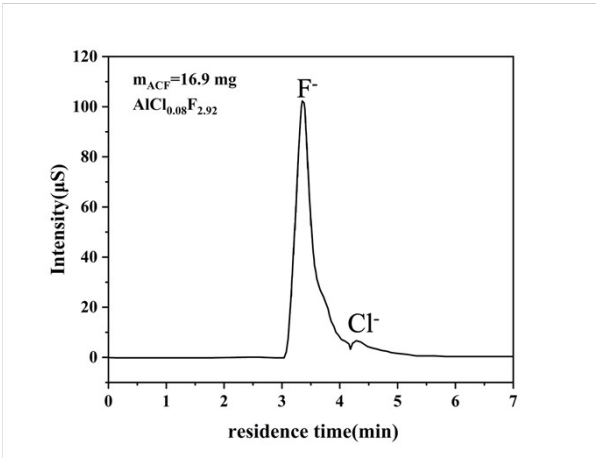

Figure S5. Ion chromatogram for the hydrolyzed solution for ACF produced under BPR=19:1, 450 rpm, 6.5 h.

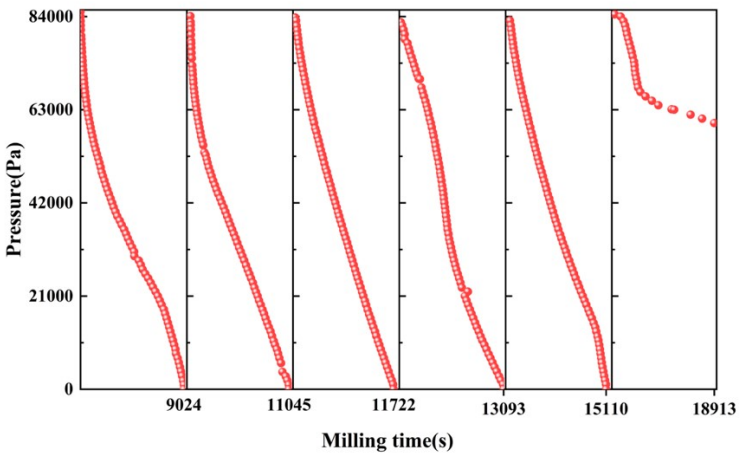

Figure S6. The consecutive pressure dropping of CHF_3 in the milling tank under BPR=56:1 and 350 rpm.

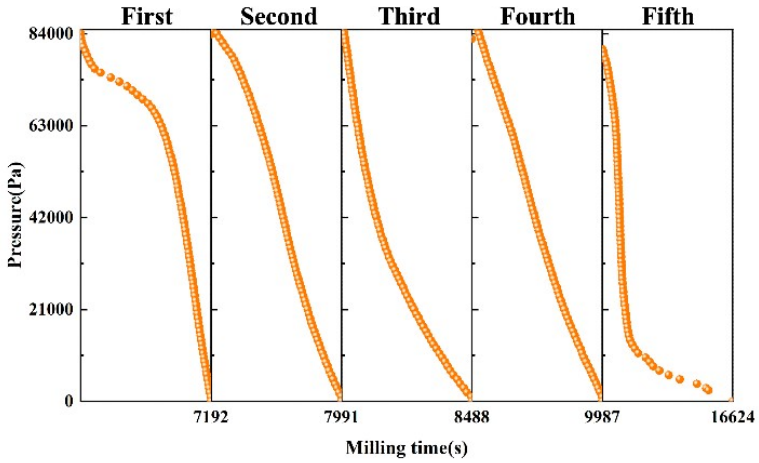

Figure S7. Pressure drop of CHF_3 versus milling time in different rounds of gas charge under BPR=56:1 and 450 rpm.

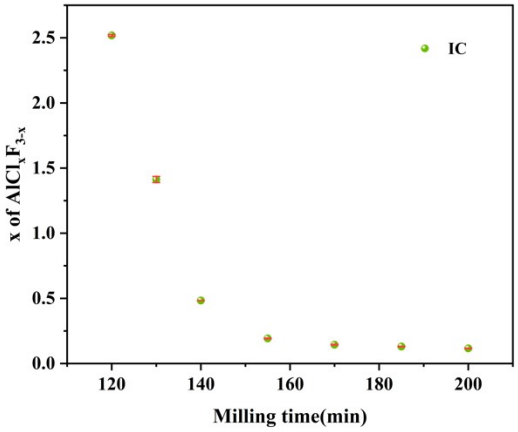

Figure S8. The *x* value of ACFs versus milling time.

Table S1. Experimental chemicals

Reagents	Chemical formula	Specification	Manufacture
Fluoroform	CHF_3	99.99%	Sinochem LantianFluoro Materials Co Ltd
Aluminum chloride	$AlCl_3$	99%	Shanghai Macklin Biochemical Co Ltd
Heptane	C_7H_{16}	AR	Tianjin Fuchen Chem Reagents Factory
Trichloromethane	$CHCl_3$	AR	Beijing Tong Guang Fine Chemicals Company
Sodium carbonate anhydrous	Na_2CO_3	99.8%	Tianjin Fuchen Chem Reagents Factory
Sodium hydrogen carbonate	$NaHCO_3$	99.5%	Tianjin Fuchen Chem Reagents Factory
Deionized water	H_2O	-	Hangzhou Wahaha Group Co Ltd

Table S2. Consumption of CHF_3 and the average *x* values under different reaction conditions in a planetary ball mill

	BPR	Pressure drop of CHF_3/MPa	Milling time/h	Rotation rate/rpm	*x*
Planetary ball mill	56:1	0.4918	2.0	450	0.111
					0.113
					0.108
	28:1	1.1661	4.5		0.112
					0.122
					0.108
	28:1	0.5927	2.5		1.331
					1.284
					1.362
	28:1	0.9511	3.5		0.276
					0.314
					0.339
	19:1	1.6326	6.5		0.088
					0.080
					0.088

Table S3. Raw data for the composition of ACFs in Table 1

BPR	Milling time/h	m_{ACF}/mg	H_2O/g	Peak area of Cl
56:1	2.0	15.3	10.0178	4.0413
		12.9	9.9456	3.1573
		16.6	10.0327	4.3527
28:1	4.5	15.0	9.8958	4.0640
		15.0	10.0860	4.4900
		16.6	10.0327	4.3527
	2.5	14.7	10.0236	57.304
		16.1	10.2085	61.121
		14.3	9.9901	56.8869
	3.5	15.5	10.3534	15.2484
		16.7	10.0600	14.4455
		15.9	10.0114	17.1270
19:1	6.5	18.4	10.1109	3.7335
		19.3	10.0664	3.4333
		16.9	10.0127	3.2749

Table S4. Consumption of CHF_3 and experimental results under different conditions

Gas charge times	BPR	Pressure drop of CHF_3 /kPa	Milling time/s	Rotation rate/rpm	$AlCl_xF_{3-x}$	$CHCl_3$/mol
1	56:1	85.1	9024	350	$AlCl_{0.12}F_{2.88}$	0.14
2		84.1	2021			
3		83.8	677			
4		82.7	1371			
5		83.1	2017			
6		24.5	3803			
1	56:1	86.1	7523	450	$AlCl_{0.11}F_{2.89}$	0.18
2		81.3	1362			
3		84.4	617			
4		85.7	555			
5		87.5	736			
6		31.1	3278			
1	56:1	85.0	5131	550	$AlCl_{0.11}F_{2.89}$	0.19
2		85.8	2512			
3		82.2	669			
4		88.3	451			
5		84.6	477			
6		43.6	5097			
1	112:1	87.5	4628	450	$AlCl_{0.10}F_{2.90}$	0.11
2		83.2	1940			
3		84.0	4546			
1	37.5:1	83.7	9154	450	$AlCl_{0.10}F_{2.90}$	0.25
2		84.8	2780			
3		87.4	1699			
4		84.9	564			
5		83.4	230			
6		85.4	282			
7		82.3	428			
8		41.6	3563			

Conditions: 1.5 kg S.S balls, tank volume 1 L, room temperature, reacted in a stirring ball mill.

Table S5. Cl-content of ACFs ($AlCl_xF_{3-x}$) after different times of gas charge as determined by different analysis methods.

Gas charge times	Pressure drop of CHF_3 /kPa	x_{IC}	X_{XPS}	Theoretical x
First	84.1	-	-	-
Second	84.8	1.656	1.47	2.32
		1.737		
		1.706		
Third	84.6	0.800	0.92	1.47
		0.799		
		0.789		
Fourth	87.5	0.237	0.19	0.73
		0.249		
		0.217		
Fifth	80.5	0.105	0.095	0.45
		0.110		
		0.109		

Conditions: 0.2 mol $AlCl_3$, 450 rpm, BPR=56:1, tank volume 1 L, room temperature, reacted in a stirring ball mill.

Table S6. Specie information of ACFs determined from XPS spectrum.

Gas charge times	Al 2p		Cl 2p		F 1s	
	Peak position (eV)	Species	Peak position (eV)	Species	Peak position (eV)	Species
Second	76.01	$AlCl_xF_{3-x}$	199.57	$AlCl_xF_{3-x}$	686.44	$AlCl_xF_{3-x}$
Third	76.10	$AlCl_xF_{3-x}$	199.64	$AlCl_xF_{3-x}$	686.55	$AlCl_xF_{3-x}$
Fourth	76.81	$AlCl_xF_{3-x}$	200.32	$AlCl_xF_{3-x}$	687.42	$AlCl_xF_{3-x}$
Fifth	76.30	$AlCl_xF_{3-x}$	200.50	$AlCl_xF_{3-x}$	687.10	$AlCl_xF_{3-x}$
	77.30	AlF_3			688.2	AlF_3

Table S7. Detailed Cl-content of ACFs in different milling time

	Milling time/min	x_{IC} of $AlCl_xF_{3-x}$
1	120	2.51
2		2.52
3		2.52
1	130	1.40
2		1.40
3		1.44
1	140	0.48
2		0.48
3		0.48
1	155	0.19
2		0.19
3		0.19
1	170	0.15
2		0.15
3		0.140
1	185	0.13
2		0.13
3		0.13
1	200	0.12
2		0.12
3		0.11

Conditions: 0.2 mol $AlCl_3$, 450 rpm, BPR=56:1, tank volume 1 L, P_{CHF3}=80 kPa, room temperature, reacted in a stirring ball mill.

Text S1 Ion chromatography

This method is based on the facile hydrolysis of the Al-Cl bond to water. ACFs ($AlCl_xF_{3-x}$, $0 \leq x \leq 3$) will be fully hydrolyzed to $Al(OH)_xF_{3-x}$ when it is soaked by water. About 20 mg of ACFs and some water were weighed accurately, added to a glass vial, and sonicated for 30 minutes in a ultrasound bath for its complete hydrolysis. The suspension is filtrated, and the filtrate was diluted by pure water to a constant volume. The Cl^- concentration of the above solution was determined three times by ion chromatography with the standard curve (Figure S1), and the average value was taken

as the reported value. The *x* value of ACFs is calculated by equation (1).

$$\frac{C_{Cl^-} \times V}{M_{ACF}} = \frac{35.5x}{27 + 35.5x + 19(3-x)} \quad (1)$$

where C_{Cl-}, V and M_{ACF} denote the concentration of chloride ions (ppm), the solution volume (L) and the mass of ACF (mg) respectively.

Text S2 Characterization

X-ray diffraction (XRD) pattern was recorded on Ultima IV, Japan, and each XRD pattern was acquired from 5° to 90°at a rate of 10°/s. X-ray photoelectron spectroscopy (XPS, Thermo Scientific K-Alpha, USA) measurements were performed on the surface elemental composition of ACF. NH_3-Temperature programmed desorption (NH_3-TPD): the acidity of ACF was characterized using ammonia thermal programmed temperature desorption on a chemical adsorption analyzer (Quantachrome Autosorb-iQ). A sample of 50-100 mg was treated under He flow rate of 20 mL/min, heated from room temperature to 300℃ at 10 ℃/min and dried, then cooled to 120℃, and finally saturated with 5% NH_3 in He for 60 min. Residual ammonia was flushed at 60 ℃. In the end, the sample was heated in He flow to 700 ℃ at 10 ℃/min, and the desorbing ammonia from the sample was detected by a thermal conductivity detector (TCD).

The gas composition was determined with gas chromatograph (GC, SHIMADZU GC2010) equipped with a hydrogen flame ionization detector (FID) and packed columns of Agilent PoraplotQ (25 m × 0.32 mm × 10 μm). N_2 was used as the carrier gas at a flow rate of 30 mL min^{-1}. The temperature of injection and detector were 250℃, while the temperature program of the column was 100℃ for 3 min and 10 ℃ min^{-1} to 150℃ for 8 min.

Qualitative analysis of the liquid product was performed on an Agilent 7890B GC−MS equipped with an HP-5MS capillary column (30 m × 0.25 mm × 0.25 μm) and a quadrupole analyzer system (5977A) with a high efficiency ion source operated at 230℃. Helium was used as the carrier gas at a flow rate of 1.0 mL min^{-1}, the sample size was 1.0 μL, and the split ratio was 10:1.

Quantitative analysis of the liquid product was performed on a SHIMADZU GC2010 gas chromatograph (GC) equipped with an FFAP capillary column (30 m × 0.53 mm × 1 μm) and an FID detector. n-Heptane was used as the internal standard. N_2 was the carrier gas at a flow rate of 30 mL min^{-1}. The temperature of injection and detector were 200℃, while the temperature program of the column was 40℃ for 3 min, 15 ℃ min^{-1} to 60℃ for 1 min, 15 ℃ min^{-1} to 90℃ for 1 min, and 20 ℃ min^{-1} to 150℃ for 0.5 min.

Text S3 Cartesian coordinates and energy information of optimized structure

(1) Pure component

$AlCl_3$

Al	-1.10619470	0.48672566	0.00000000
Cl	1.13380530	0.48672566	0.00000000
Cl	-2.22619470	-1.45317125	0.00000000
Cl	-2.22619470	2.42662256	0.00000000

$AlCl_2F$

Al	4.17369316	1.03709948	0.00000000
F	6.00369316	1.03709948	0.00000000
Cl	3.05369315	-0.90279742	0.00000000
Cl	3.05369315	2.97699638	0.00000000

$AlClF_2$

Al	0.00000000	0.00000000	0.36261100
F	0.00000000	0.00000000	2.00504600
Cl	0.00000000	-1.83774600	-0.66939300
F	0.00000000	1.59562397	-0.53342704

AlF_3

Al	0.00000000	0.43377600	0.00000000
F	-1.41406800	1.26266900	0.00000000
F	1.41316900	1.26435400	0.00000000
F	0.00041414	-1.39622395	0.00000000

CHF_3

C	-3.05309736	-0.15042958	-0.00196923
H	-4.12309736	-0.15041640	-0.00196923
F	-2.60308957	0.48596066	-1.10423982
F	-2.60308957	0.48596066	1.10030136

F	-2.60311281	-1.42322725	-0.00196923

CHF_2Cl

Cl	0.96247400	-0.69914100	-0.94771200
C	2.23934800	-0.13314800	0.30022300
H	1.82859300	-0.39783200	1.27330900
F	3.36810000	-0.75925400	0.00602400
F	2.38248700	1.17508500	0.15092700

$CHFCl_2$

Cl	1.29170200	-0.00008900	-0.05015600
C	-0.45610900	0.00003400	0.36636200
H	-0.55011500	0.00027900	1.45356800
F	-1.03750900	-1.09041500	-0.15548500
Cl	-1.21854090	1.43089856	-0.31841841

$CHCl_3$

Cl	-1.48073000	-0.50392800	-0.06376600
C	-0.00005100	0.38539300	0.40282600
H	-0.00014600	0.49545800	1.48577300
Cl	1.48099800	-0.50356900	-0.06377300
Cl	-0.00058237	1.96337884	-0.37663561

(2) Cartesian coordinates for the reaction

(a) $CHF_3 + AlCl_3 \rightarrow CHF_2Cl + AlCl_2F$

Reactant

Thermal Correction to Free Energy = -5.52397053 Hartree

Electronic Energy (EE) = -1231004.124 Hartree

Al	-0.83996800	0.03592800	0.21026100
Cl	0.47651000	0.16698400	1.89721000
Cl	-1.92038100	1.78182900	-0.40789100
Cl	-1.82949900	-1.83397300	-0.13928000
C	2.16307800	-0.05979400	-1.06763700
H	2.52664900	-0.00868200	-2.09276200
F	2.56970300	0.94624000	-0.32736700
F	0.73258300	0.04229400	-1.18331900
F	2.41536600	-1.21270800	-0.48746700

TS

Thermal Correction to Free Energy = -6.73820238 Hartree

Electronic Energy (EE) = -1230972.20 Hartree

Al	0.80069222	0.15900823	0.08876088

Cl	1.41287351	2.20688006	-0.37992918
Cl	0.55253436	-0.28240033	2.27077283
Cl	2.12676711	-1.44291532	-0.74368512
C	-0.56948348	2.83525001	-1.59344595
H	-1.49746624	2.96664777	-2.10966550
F	-0.89128444	3.85022585	-0.76352535
F	-0.49775281	1.44940037	-0.81231724
F	0.11628188	3.07401242	-2.73152257

Product

Thermal Correction to Free Energy = -6.02472351 Hartree

Electronic Energy (EE) = -1231005.694 Hartree

Al	-1.08847200	-0.03436400	-0.40398700
Cl	0.91280900	0.16879300	1.22930100
Cl	-2.09263400	1.83527200	-0.15591500
Cl	-2.01212000	-1.87652200	0.14396100
C	2.25969400	0.12913800	-0.10232700
H	1.77197600	0.46978100	-1.01057100
F	3.23463600	0.92043900	0.30931100
F	-0.01012400	-0.09058600	-1.66910600
F	2.67520100	-1.12229400	-0.18889500

(b) $CHF_3 + AlCl_2F \rightarrow CHF_2Cl + AlClF_2$

Reactant

Thermal Correction to Free Energy = -4.24698768 Hartree

Electronic Energy (EE) = -1004883.071 Hartree

Al	0.93564900	-0.27392800	-0.28239900
Cl	-0.25468000	0.76743300	-1.72621600
Cl	2.50235400	0.81907600	0.68551700
C	-1.99884600	-0.24477800	1.04748100
H	-2.36549900	-0.50561200	2.03918600
F	-2.27998600	0.99131400	0.70346700
F	-0.56952500	-0.34307700	1.14688500
F	-2.37567300	-1.09686300	0.11843400
F	1.14727800	-1.90107100	-0.42198800

TS

Thermal Correction to Free Energy = -5.33320749 Hartree

Electronic Energy (EE) = -1004850.798 Hartree

Al	0.80069222	0.15900823	0.08876088
Cl	1.41287351	2.20688006	-0.37992918

Cl	0.55253436	-0.28240033	2.27077283
C	-0.56948348	2.83525001	-1.59344595
H	-1.49746624	2.96664777	-2.10966550
F	-0.89128444	3.85022585	-0.76352535
F	-0.49775281	1.44940037	-0.81231724
F	0.11628188	3.07401242	-2.73152257
F	1.88404804	-1.14970610	-0.59131777

Product

Thermal Correction to Free Energy = -4.58521557 Hartree

Electronic Energy (EE) = -1004884.279 Hartree

Al	1.18780800	-0.58267600	0.19635800
Cl	-0.71029500	0.63498500	-1.06548300
Cl	2.67877800	0.91990100	0.44522300
C	-2.04938000	0.29789000	0.21390900
H	-1.53383200	0.27462400	1.16965700
F	-2.93700500	1.27380500	0.11024500
F	0.16511100	-0.80985100	1.48503200
F	-2.59851400	-0.86583600	-0.09266600
F	1.43607200	-1.83528200	-0.83697500

(c) $CHF_3 + AlClF_2 \rightarrow CHF_2Cl + AlF_3$

Reactant

Thermal Correction to Free Energy = -2.50564743 Hartree

Electronic Energy (EE) = -778764.9288 Hartree

Al	1.13646900	-0.05217300	0.24051300
Cl	1.03709300	-2.13424100	-0.22448500
C	-1.69521600	0.89548600	0.04207600
H	-1.38715800	1.35166400	0.97575900
F	-2.42390600	1.67525000	-0.72658000
F	-0.48883800	0.64388200	-0.71158400
F	-2.26565800	-0.28009600	0.19900200
F	0.50693600	0.44064300	1.69091600
F	2.29289500	0.88542500	-0.45847700

TS

Thermal Correction to Free Energy = -3.16139538 Hartree

Electronic Energy (EE) = -778733.2182 Hartree

Al	0.80069222	0.15900823	0.08876088
Cl	1.41287351	2.20688006	-0.37992918

C	-0.56948348	2.83525001	-1.59344595
H	-1.49746624	2.96664777	-2.10966550
F	-0.89128444	3.85022585	-0.76352535
F	-0.49775281	1.44940037	-0.81231724
F	0.11628188	3.07401242	-2.73152257
F	1.88404804	-1.14970610	-0.59131777
F	0.59795611	-0.20160680	1.87138672

Product

Thermal Correction to Free Energy = -3.3571785 Hartree

Electronic Energy (EE) = -778762.9064 Hartree

Al	1.35439900	0.70957000	0.04011300
Cl	-0.19063100	-1.30346300	-0.34072500
C	-1.70071100	-0.45064300	0.36572900
H	-1.36133800	-0.01019200	1.29693300
F	-2.09029200	0.45562500	-0.52134400
F	0.90592500	1.67264600	-1.21952500
F	-2.63633100	-1.37356900	0.52311200
F	0.59393400	0.97909700	1.48799000
F	2.80056500	-0.05716800	0.00013800

(d) $AlCl_3 + CHF_2Cl \rightarrow AlCl_2F + CHFCl_2$

Reactant

Thermal Correction to Free Energy = -7.59349851 Hartree

Electronic Energy (EE) = -1457123.71 Hartree

Al	1.03281500	0.01122000	0.23693700
Cl	0.14166800	-1.34673500	1.63957500
Cl	2.87080700	-0.60105800	-0.67946800
Cl	0.77527900	2.13326000	0.42662700
C	-1.87561300	-0.36098900	-1.12658200
H	-2.19979600	-0.25605100	-2.16007100
F	-2.15935800	-1.54927800	-0.62803900
F	-0.43344700	-0.28698400	-1.21849000
Cl	-2.46896300	0.93476600	-0.11748600

TS

Thermal Correction to Free Energy = -7.89093825 Hartree

Electronic Energy (EE) = -1457099.914 Hartree

Al	0.80069222	0.15900823	0.08876088
Cl	1.41287351	2.20688006	-0.37992918
Cl	0.55253436	-0.28240033	2.27077283

Cl	2.12676711	-1.44291532	-0.74368512
C	-0.59669474	2.87018657	-1.54845857
H	-1.52114960	3.02141031	-2.06558001
F	-0.80006947	4.01218976	-0.85783028
F	-0.47753915	1.38354498	-0.77287699
Cl	0.28423100	2.89486244	-3.07192860

Product

Thermal Correction to Free Energy = -7.68950754 Hartree

Electronic Energy (EE) = -1457127.306 Hartree

Al	1.27958100	0.33324100	-0.46797600
Cl	-0.41778900	-1.05165200	0.93530300
Cl	3.03847200	-0.81475200	-0.10643200
Cl	1.07237500	2.26926400	0.40624000
C	-1.89684000	-0.83050000	-0.17842900
H	-1.47439200	-0.78661400	-1.18146800
F	-2.67954900	-1.89129900	0.00856900
F	0.38273600	0.02240800	-1.83194500
Cl	-2.73910200	0.66304200	0.21188500

(e) $AlCl_3 + CHFCl_2 \rightarrow AlCl_2F + CHCl_3$

Reactant

Thermal Correction to Free Energy = -8.90624943 Hartree

Electronic Energy (EE) = -1683246.101 Hartree

Al	1.22897200	-0.01888900	0.31336300
Cl	0.30894700	-1.18768200	1.85750800
Cl	2.66875800	-0.96276100	-0.97196400
Cl	1.42028900	2.09090000	0.65142600
C	-1.70949300	0.11658200	-1.11425700
H	-1.91364900	0.34472800	-2.15636700
F	-0.26865000	-0.02854500	-1.08759800
Cl	-2.14687400	1.45687200	-0.08285100
Cl	-2.41163600	-1.41718900	-0.66050000

TS

Thermal Correction to Free Energy = -9.70381464 Hartree

Electronic Energy (EE) = -1683228.977 Hartree

Al	1.08706800	-0.01851200	-0.09261300
Cl	0.03142300	-1.28833600	1.36360900
Cl	3.13106700	-0.52894300	-0.44789400
Cl	0.69705300	2.05816400	0.45998800

C	-2.21414100	-0.48752100	-0.77001000
H	-1.75825200	-0.56220400	-1.75264800
F	0.08274600	-0.29498700	-1.46949900
Cl	-2.44111100	0.95266900	-0.03325400
Cl	-2.83247844	-1.95197366	-0.01460467

Product

Thermal Correction to Free Energy = -9.36558675 Hartree

Electronic Energy (EE) = -1683251.224 Hartree

Al	1.54056300	0.28002000	-0.46864400
Cl	-0.32232600	-0.93684700	0.87484700
Cl	3.14186900	-1.09267500	-0.15227500
Cl	1.59050500	2.18779100	0.49075200
C	-1.75841700	-0.39837700	-0.17358100
H	-1.35943000	-0.42405100	-1.18607600
F	0.61677200	0.13947100	-1.83961100
Cl	-2.21867300	1.25478200	0.22826400
Cl	-3.07254000	-1.55595500	0.01321300

(f) $AlCl_2F + CHF_2Cl \rightarrow AlClF_2 + CHFCl_2$

Reactant

Thermal Correction to Free Energy = -6.05798154 Hartree

Electronic Energy (EE) = -1231002.625 Hartree

Al	-1.07203100	0.15823200	0.44138000
Cl	-0.23538700	-1.58427600	1.35889800
Cl	-2.76656100	-0.08506700	-0.84186600
C	1.69672000	0.21806700	-1.17600200
H	1.97993900	0.71039900	-2.10377000
F	0.28639700	0.45791200	-1.06807300
F	1.85045500	-1.09195700	-1.23505500
Cl	2.49095200	0.92149100	0.21320400
F	-0.85053800	1.61041300	1.18659200

TS

Thermal Correction to Free Energy = -6.85366422 Hartree

Electronic Energy (EE) = -1230977.797 Hartree

Al	-0.90675200	0.00275600	-0.07102400
Cl	0.58885500	0.17400600	1.56919000
Cl	-1.98051000	-1.85085300	0.01350900
C	2.45930600	0.05862100	-0.70111100

H	2.07544900	0.34533500	-1.67128600
F	0.29190400	-0.06836700	-1.33088200
F	2.62914200	-1.15094800	-0.40147400
Cl	3.26741784	1.24246836	0.32019242
F	-1.89073482	1.53517673	-0.25092543

Product

Thermal Correction to Free Energy = -6.53739918 Hartree

Electronic Energy (EE) = -1231005.723 Hartree

Al	-1.30778400	0.68368000	-0.19760800
Cl	0.30103100	-1.17276600	0.61856800
Cl	-3.14418600	-0.38492000	-0.15215800
C	1.78714600	-0.60428300	-0.35346500
H	1.37458000	-0.26654400	-1.30164300
F	-0.45242600	0.77332600	-1.61714300
F	2.59059400	-1.65802900	-0.47981600
Cl	2.59300300	0.71750100	0.48395700
F	-1.02215400	1.85602700	0.92064600

$AlClF_2 + CHFCl_2 \rightarrow AlF_3 + CHCl_3$

Reactant

Thermal Correction to Free Energy = -6.13328274 Hartree

Electronic Energy (EE) = -1231003.952 Hartree

Al	1.58654854	0.07082412	-0.04559208
Cl	0.69502098	-1.42809545	-1.28515480
C	-1.42485289	0.40230707	0.87901271
H	-1.79199764	0.85748824	1.79368891
F	-0.03810077	0.09950473	1.21040842
Cl	-1.47329808	1.53525401	-0.44525581
F	1.45459751	1.66505182	-0.43571649
F	2.92761308	-0.34699189	0.81313335
Cl	-2.26541497	-1.09473148	0.54959185

TS

Thermal Correction to Free Energy = -7.43473848 Hartree

Electronic Energy (EE) = -1230985.209 Hartree

Al	-1.09921500	0.24174600	0.03819600
Cl	-0.10317500	-1.51869100	0.92310800
C	2.09333100	-0.06666500	-0.81073800
H	1.63202300	0.25155200	-1.74088000
F	-0.17130500	0.34020100	-1.42016500

Cl	2.36996000	0.98066800	0.41817200
F	-0.61656300	1.58380500	0.91509500
F	-2.89054908	0.03981561	-0.27683786
Cl	2.71671624	-1.70849153	-0.69499480

Product

Thermal Correction to Free Energy = -7.09462806 Hartree

Electronic Energy (EE) = -1231008.039 Hartree

Al	1.80324788	0.20798941	0.33774269
Cl	0.28583068	-1.14722782	-0.95219865
C	-1.33510186	-0.05717578	0.14996200
H	-0.69495444	-0.00448202	1.03089316
F	0.91150563	0.03133477	1.74944939
Cl	-1.64139710	1.44191549	-0.60825368
F	1.47871562	1.62459595	-0.44564743
F	3.33007808	-0.39806305	0.37891759
Cl	-2.66542183	-1.11881324	0.30446870